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Présentée par :
Shuiran Peng

Analyse mathématique et numérique de plusieurs problèmes non linéaires

Directeur(s) de Thèse :
Alain Miranville, Laurence Cherfils

Soutenue le 07 décembre 2018 devant le jury

Jury :

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Membre	**Laurence Cherfils**	Maître de conférences, Université de la Rochelle
Membre	**Madalina Petcu**	Maître de conférences, LMA, Université de Poitiers

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Thèse préparée au sein du Laboratoire de Mathématiques et Applications

Dedicated to my beloved family : my mother Longhuai, my father Junming,
my sister Yan and my nephew Chengzhi.
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Chapitre 1

Introduction générale

1.1 Equations aux dérivées partielles non linéaires

Comparé aux équations aux dérivées partielles linéaires, les équations aux dérivées partielles non linéaires sont plus difficiles à analyser, tant du point de vue théorique que du point de vue numérique. Les modèles de séparation de phase et les systèmes micro-électro-mécaniques (abbr. MEMS) sont deux problèmes non linéaires qui peuvent être singuliers (lorsque l'on considère un potentiel logarithmique dans le modèles de séparation de phase).

1.1.1 Modèles de séparation de phase

Les équations de Allen-Cahn et de Cahn-Hilliard sont les deux principales équations qui modélisent la séparation de phase. L'équation de Allen-Cahn a été introduite par Allen et Cahn dans [4] pour décrire l'ordonnancement des atomes dans les solides cristallins. De plus, Cahn et Hilliard ont proposé l'équation de Cahn-Hilliard dans [20] pour décrire le phénomène de séparation de phase (comme par exemple la décomposition spinodale ou la coalescence) dans les alliages binaires (voir aussi [43], [44] et [108]). Ces deux équations sont fondamentales en sciences des matériaux et sont basées sur l'énergie libre de Ginzburg-Landau, qui s'écrit :

$$\Psi_{\mathrm{GL}} = \int_\Omega (\frac{\alpha}{2}|\nabla u|^2 + F(u))dx, \ \alpha > 0, \tag{1.1}$$

où u représente le paramètre d'ordre, comme par exemple la concentration (relative, généralement considérée entre -1 et 1) de l'un des deux composants de l'alliage, α est un coefficient de tension de surface, F est un potentiel à double puits et Ω est le domaine occupé par le système (on suppose le domaine borné et régulier, de frontière Γ). Ces modèles sont supposés isotropes, et à température constante. L'équation de Allen-Cahn, qui correspond à un flot de gradient en norme L^2 de l'énergie libre, s'écrit :

$$\frac{\partial u}{\partial t} - \alpha\Delta u + f(u) = 0, \tag{1.2}$$

où f est la dérivée du potentiel à deux puits F, alors que l'équation de Cahn-Hilliard, qui correspond à un flot de gradient dans la norme H^{-1}, s'écrit :

$$\frac{\partial u}{\partial t} + \alpha\Delta^2 u - \Delta f(u) = 0. \tag{1.3}$$

Conditions aux limites. Parmi les différents choix de conditions aux limites, les conditions de Dirichlet signifient que la condition sur la frontière est fixée, alors que les conditions au bord de type Neumann impliquent qu'il n'y a pas de perte de masse à travers la frontière, et par conséquent, entraînent une conservation de la masse. On trouve aussi les conditions aux limites mixtes, combinaisons entre les conditions de Dirichlet et de Neumann, ou les condition périodiques. Ces dernières, appliquées à des domaines réguliers de type parallélipède, signifient que les conditions sur deux murs opposés sont les mêmes, et ont des valeurs opposées dans la direction des vecteurs normaux orientés vers l'extérieur du domaine. Plus récemment, des études sont effectuées avec des conditions aux limites dynamiques (cf. [28], [82] and [138]), qui impliquent les dérivées en temps de l'inconnue u.

Terme non linéaire. Les deux puits du potentiel correspondent aux deux phases du matériau. Un potentiel pertinent d'un point de vue thermodynamique, dérivant de modèles à champs moyens (cf., [20] and [36]), est le potentiel logarithmique de la forme

$$F(s) = \frac{\lambda_1}{2}(1 - s^2) + \frac{\lambda_2}{2}[(1 + s)\ln(\frac{1 + s}{2}) + (1 - s)\ln(\frac{1 - s}{2})], \ s \in (-1, 1), \ 0 < \lambda_2 < \lambda_1, \tag{1.4}$$

donc,

$$f(s) = -\lambda_1 s + \frac{\lambda_2}{2} \ln \frac{1 + s}{1 - s}, \tag{1.5}$$

où λ_1 et λ_2 sont respectivement proportionnels à la température critique et à la température absolue, supposées constante pendant le processus. De plus, la condition $\lambda_2 < \lambda_1$ garantit que F possède un double puits et donc que la séparation de phases peut se produire. Un système de champs de phase basé sur la loi de conduction de la chaleur de Maxwell-Cattaneo et avec un potentiel logarithmique a été étudié dans [92], alors que les auteurs dans [26] ont étudié l'équation de Cahn-Hilliard-Bertozzi-Esedoglu-Gilette avec une nonlinéarité logarithmique, pour laquelle ils ont obtenu l'existence de solutions locales (en temps) et ont proposé des applications pour la retouche d'images binaires. Voir [29], [30], [70], [94], [96], [99] et [102] pour plus de détails.

Le potentiel logarithmique, pertinent d'un point de vue thermodynamique, est souvent approché par un potentiel polynomial, qui s'écrit

$$F(s) = \frac{1}{4}(s^2 - 1)^2, \tag{1.6}$$

et

$$f(s) = s^3 - s. \tag{1.7}$$

Anisotropie. Lorque l'on tient compte du caractère anisotrope des interfaces, d'un point de vue physique, une anisotropie importante pourrait entraîner que l'énergie surfacique devienne si large ou singulière selon certaines orientations que ces orientations pourraient disparaître dans la forme d'équilibre pour atteindre une énergie bien définie pour le système. En conséquences, l'interface à l'équilibre peut devenir non lisse, et des facettes ou des coins peuvent apparaître.

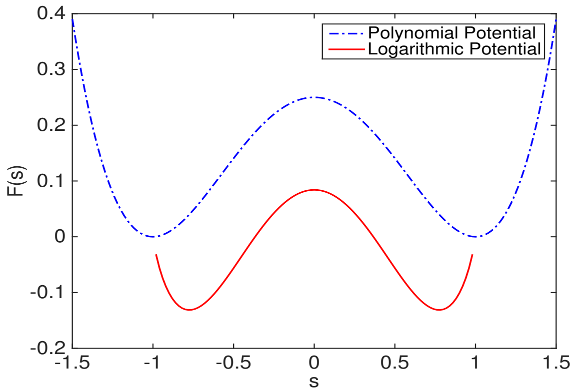

FIGURE 1.1 – Le potentiel logarithmique et le potentiel polynomial.

L'anisotropie jouant un role important dans l'équilibre et la dynamique de l'interface, plusieurs travaux ont porté sur ce point. Dans son article (cf. [80]), R. Kobayashi a étudié la croissance cristalline anisotrope pour deux phases (liquide et solide) pour une énergie libre de type Ginzburg-Landau modifiée. L'anisotropie est prise en compte dans la mobilité de l'interface, fonction de l'orientation. Dans cet article, de nombreuses simulations numériques illustrent les effets de l'anisotropie, notamment la croissance dendritique et de type flocon de neige.

Une autre modification de l'énergie libre de type Ginzburg-Laudau permet de prendre en compte l'anisotropie, la différence avec le modèle précédant étant que la température est omise, (cf. [40], [120], [126] et [133]). L'anisotropie est prise en compte par la fonction énergie interfaciale $\gamma(\mathbf{n})$ qui dépend de l'angle de la tangente à l'interface. Taylor et Cahn (cf. [126]) donnent une idée générale de l'étude du mouvement d'une interface diffuse avec des coins et des faces et le travail de Sekerta (cf. [120]) donne une idée de l'étude des formes à l'équilibre, ainsi que des critères analytiques pour les orientations manquantes des formes à l'équilibre en dimension trois. Wise et al (cf. [133]) et Shen et al. (cf. [40]) ont effectué l'analyse numérique et des simulations pour ces modèles anisotropes en se basant sur une régularisation du problème.

Dans la thèse, on introduit l'anisotropie d'une manière encore différente, en considérant l'énergie libre de type Ginzburg-Landau d'ordre élevé, introduite par G. Caginalp et E. Esenturk dans [23] et qui s'écrit :

$$\Psi_{\text{HOGL}} = \int_\Omega (\frac{1}{2}\sum_{i=1}^{k}\sum_{|\alpha|=i} a_\alpha |\mathcal{D}^\alpha u|^2 + F(u))\, dx,\ k \in \mathbb{N}, \tag{1.8}$$

où $\alpha = (k_1, k_2, k_3) \in (\mathbb{N} \cup \{0\})^3$,

$$|\alpha| = k_1 + k_2 + k_3$$

et, pour $\alpha \neq (0,0,0)$,

$$\mathcal{D}^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{k_1} \partial x_2^{k_2} \partial x_3^{k_3}}$$

(on admet que $\mathcal{D}^{(0,0,0)} v = v$). On remarque que dans (1.8), la température est omise. L'avantage est que ce type d'énergie libre permet de calculer l'anisotropie de manière explicite, en supposant que les tensions de surface sont différentes suivant les différentes orientations. On note alors que l'équation de Cahn-Hilliard d'ordre élevé anisotrope correspond au flot de gradient dans la norme H^{-1} de l'énergie libre (1.8) et s'écrit :

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0.$$

Généralisation. En plus de la séparation de phase, l'équation de Cahn-Hilliard et ses variantes sont aussi utilisées pour modéliser d'autres phénomènes, tels que la dynamique de populations (cf. [31]), la croissance tumorale (cf. [7] et [86]), les films bactériens (cf. [81]), les couches minces (cf. [112] et [129]), la retouche d'image (cf. [8], [9], [21], [27] and [42]) et même les anneaux de Saturne (cf. [130]) et l'agglomérat de moules (cf. [90]).

En particulier, plusieurs de ces phénomèmes peuvent être modélisés par l'équation de Cahn-Hilliard généralisée suivante :

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) + g(x,u) = 0. \tag{1.9}$$

Nous renvoyons le lecteur à [93] et [98] (voir aussi [7], [26], [37], [47]) pour des études détaillées de l'équation (1.9). Etant donné que nous nous intéressons ici aux modèles d'ordre élevé, l'équation suivante sera utilisée :

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) + g(x,u) = 0. \tag{1.10}$$

Cette équation est basée sur l'énergie libre (1.8) mentionnée ci-dessus. Dans (1.10), α représente le multi-indice et le potentiel f est supposé non linéaire mais régulier. En ce qui concerne la fonction g, plusieurs choix sont possibles :
(i) Equation de Cahn-Hilliard-Oono. Dans ce cas,

$$g(x,s) = g(s) = \beta s, \ \beta > 0.$$

Cette fonction a été proposée dans [111] pour prendre en compte les interactions de longue portée (i.e., non locales), mais aussi pour simplifier les simulations numériques. Mentionnons aussi que dans [39], les auteurs ont utilisé une équation similaire à celle de l'équation de Cahn-Hilliard-Oono, pour des applications concernant l'aggrégat de copolymères diblocs, en dessous d'une température critique. Pour plus d'études sur l'équation de Cahn-Hilliard-Oono, voir aussi [15], [38], [95], [131] et [7].
(ii) Terme de prolifération. Dans ce cas,

$$g(x, s) = g(s) = \beta s(s - 1), \ \ \beta > 0.$$

Cette fonction a été introduite dans [86] en vue d'applications à la biologie et, plus précisément, pour modéliser la cicatrisation et la croissance tumorale (en dimension 1 d'espace) et l'agglomérat de cellules cancéreuses dans le cerveau (en dimension deux d'espace) ; voir aussi [7] pour le choix d'un polynôme de degré 4 pour g.
(iii) Terme de fidélité. Dans ce cas,

$$g(x, s) = \lambda_0 \chi_{\Omega\setminus D}(x)(s - \varphi(x)), \ \ \lambda_0 > 0, \ \ D \subset \Omega, \ \ \varphi \in L^2(\Omega),$$

où χ est la fonction indicatrice et λ_0 est un réel positif. Cette fonction a été proposée dans [8] et[9] pour des applications en retouche d'images. Dans ce cas, φ est une image binaire, et D est la zone endommagée (à retoucher), de l'image. Le terme de fidélité $g(x, u)$ est ajouté à l'équation dans le but de garder la solution proche de l'image originale hors de la zone à retoucher. L'idée de la méthode consiste à résoudre l'équation jusqu'à l'état d'équilibre. La solution u obtenue est alors la solution restorée de l'image $\varphi(x)$.

Hyperbolic relaxation. Une relaxation hyperbolique de l'équation de Cahn-Hilliard a été proposée dans [55], dans le but de modéliser la solidification rapide d'un alliage binaire. De plus, S. Gatti et al. ont proposé dans [62] une analyse détaillée du comportement asymptotique des solutions dans le cas de la relaxation hyperbolique de l'équation de Cahn-Hilliard en dimension un.

P. Stefanovic et al. ont proposé dans [123] l'équation appelée "modified phase field crystal equation" (abbr., MPFC), faisant la distinction entre les échelles de temps caractéristiques de la relaxation élastique (rapide) et la diffusion (plus lente), mais sans prendre en compte l'anisotropie. Cette équation s'écrit :

$$\beta\partial_{tt}u + \partial_t u - \Delta[\Delta^2 u + 2\Delta u + f(u)] = 0. \tag{1.11}$$

Dans [75] et [76], M. Grasselli et H. Wu ont établi le caractère bien posé de l'équation MPFC (1.11), ainsi que l'existence d'un attracteur exponentiel, dans le cas de conditions aux limites périodiques. De plus, dans [72], M. Grasselli et M. Pierre ont proposé un schéma de discrétisation en espace, et un schéma de discrétisation en temps et en espace pour le modèle MPFC, et ont notamment établi la convergence de la solution discrétisée vers la solution exacte de l'équation MPFC, ainsi que la convergence de la solution approchée vers une solution stationnaire lorsque le temps tend vers $+\infty$. Nous référons le lecteur à [135], [136] pour plus de schémas numériques appliqués à l'équation MPFC et à [45], [50], [56], [79] pour l'étude théorique et numérique de l'équation de phase-field crystal (sans le terme de relaxation).

Pour tenir compte des effets de l'anisotropie dans l'équation MPFC, l'équation est modifiée et devient, pour $k \in \mathbb{N}$, $k \geq 2$, $x \in \Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$),

$$\beta\partial_{tt}u + \partial_t u - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0. \tag{1.12}$$

On considère également la relaxation hyperbolique des équations de Cahn-Hilliard généralisées, d'ordre élevé et anisotropes, qui s'écrivent :

$$\beta\partial_{tt}u + \partial_t u - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) + \gamma u = 0, \tag{1.13}$$

où $\gamma \geq 0$. Munie du terme γu, l'équation (1.13) tient compte des interactions de longue-portée.

1.1.2 Modélisation mathématique de MSEM

Une autre équation aux dérivées partielles non linéaire apparaît dans la modélisation mathématique de micro-systèmes électro-mécaniques (MSEM en abrégé) tels que, par exemple, les micro-pompes, les micro-interrupteurs, les micro-valves, ..., cf. [114]. Un MSEM idéalisé est présenté dans la Fig. 1.2. Le dispositif contient une membrane déformable élastique mince fixée à ses bords et une plaque électrique rigide parallèle sur le sol. La surface supérieure de la membrane, en principe diélectrique, est recouverte d'un film conducteur métallique d'épaisseur négligeable. Lorsque qu'une tension est appliquée au film conducteur, le membrane élastique se déforme vers la plaque rigide. L'action du système $\mathcal{S}$ consiste en l'énergie cinétique E_k, l'énergie d'amortissement E_d et l'énergie potentielle E_p, à savoir, si $\mathcal{L}$ désigne la Lagrangien,

$$\mathcal{S} = \int_{t_1}^{t_2} \int_{\Omega'} \mathcal{L} dx' dy' dt' := E_k + E_d + E_p, \tag{1.14}$$

où Ω' représente le domaine de la membrane. D'un côté, on applique le principe de Hamilton pour minimiser l'action $\mathcal{S}$, et on obtient un problème élastique. Combinant les effets électrostatiques, une adimensionalisation et certaines hypothèses raisonnables, un problème parabolique non linéaire est obtenu, qui s'écrit :

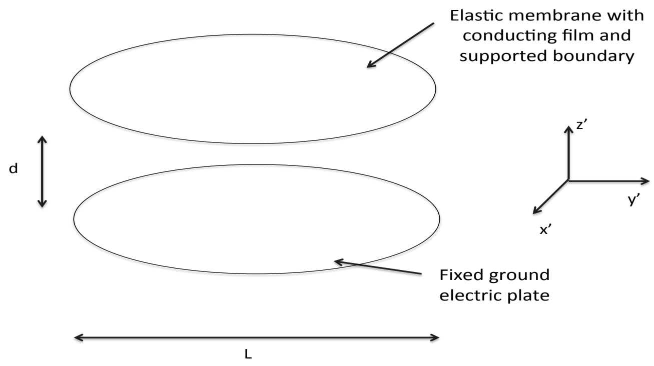

FIGURE 1.2 – MSME idéalisé.

$$
\begin{aligned}
&\frac{\partial w}{\partial t} - \Delta w = \frac{\lambda f(x)}{w^2} \quad \text{in } \Omega, \\
&w(t,x) = 1 \ \text{ on } \partial\Omega; \quad w(0,x) = 1 \quad \text{in } \Omega,
\end{aligned} \tag{1.15}
$$

où w représente la déviation dynamique adimensionalisée, et $f(x)$ décrit la permittivité diélectrique variable de la membrane élastique. Nous renvoyons le lecteur à [46] pour les détails de la dérivation du modèle.

1.2 Problèmes et principaux résultats

On étudie dans cette thèse plusieurs équations aux dérivées partielles non linéaires, telles que les modèles de séparation de phase d'ordre élevé, associés ou non à de l'anisotropie, ainsi qu'une équation aux dérivées partielles singulière issue de la modélisation mathématique de systèmes micro-électromécaniques.

1.2.1 Modèles d'ordre élevé pour la séparation de phase

On considère dans les chapitres 3 et 4 les modèles d'ordre élevé pour la séparation de phase, telles que les équations de Allen-Cahn et de Cahn-Hilliard d'ordre élevé qui s'écrivent :

$$\frac{\partial u}{\partial t} + P(-\Delta)u + f(u) = 0, \tag{1.16}$$

et

$$\frac{\partial u}{\partial t} - \Delta P(-\Delta)u - \Delta f(u) = 0, \tag{1.17}$$

respectivement, avec

$$P(s) = \sum_{i=1}^{k} a_i s^i. \tag{1.18}$$

Les équations (1.16) et (1.17) sont d'ordre élevé en raison du terme $P(-\Delta)$, ce qui les rend difficiles à étudier. Le problème sera encore plus difficile à étudier si la nonlinéarité $f(u)$ est logarithmique. Les conditions aux limites associées à (1.16) et (1.17) sont :

$$u = \Delta u = ... = \Delta^{k-1} u = 0 \text{ on } \Gamma, \tag{1.19}$$

et la condition initiale :

$$u|_{t=0} = u_0. \tag{1.20}$$

Dans le chapitre 3 nous étudions les équations d'ordre élevé de Allen-Cahn (1.16) et de Cahn-Hilliard (1.17) avec un potentiel polynomial et les conditions aux limites (1.19) et donnons pour ces deux problèmes des résultats d'existence et de régularité de solutions. Plus précisément, nous définissons $\dot{H}^m(\Omega) = \{v \in H^m(\Omega), v = \Delta v = \cdots = \Delta^{[\frac{m-1}{2}]} v = 0 \text{ sur } \Gamma\}$, où le symbole $[\cdot]$ représente la partie entière. Pour l'équation de Allen-Cahn d'ordre élevé, nous obtenons :

Théorème 1.2.1. (i) On suppose que $u_0 \in \dot{H}^k(\Omega)$, avec $\int_\Omega F(u_0)dx < +\infty$ lorsque $k = 1$. Alors le problème (1.16), (1.19)-(1.20) possède une unique solution u telle que, $\forall T > 0$, $u \in L^\infty(\mathbb{R}^+; \dot{H}^k(\Omega)) \cap L^2(0, T; \dot{H}^{2k}(\Omega))$, $\frac{\partial u}{\partial t} \in L^2(0, T; L^2(\Omega))$ et

$$\frac{d}{dt}((u, v)) + \sum_{i=1}^{k} a_i(((-\Delta)^{\frac{i}{2}} u, (-\Delta)^{\frac{i}{2}} v)) + ((f(u), v)) = 0, \forall v \in C_c^\infty(\Omega).$$

(ii) Si on suppose de plus que $u_0 \in \dot{H}^{2k}(\Omega)$, alors $u \in L^\infty(\mathbb{R}^+; \dot{H}^{2k}(\Omega))$.

Ensuite on définit le semi-groupe associé et montrons sa dissipativité, ainsi que l'existence de l'attracteur global qui est compact dans $L^2(\Omega)$ et borné dans $\dot{H}^{2k}(\Omega)$. Concernant l'équation de Cahn-Hilliard d'ordre élevé, nous avons le résultat :

Théorème 1.2.2. (i) On suppose que $u_0 \in \dot{H}^k(\Omega)$, avec $\int_\Omega F(u_0)dx < +\infty$ lorsque $k = 1$. Alors le probème (1.17),(1.19)-(1.20) possède une unique solution u, ayant la régularité $u \in L^\infty(\mathbb{R}^+; \dot{H}^k(\Omega)) \cap L^2(0, T; \dot{H}^{2k}(\Omega))$ and $\frac{\partial u}{\partial t} \in L^2(0, T; H^{-1}(\Omega))$;

(ii) Si on suppose que $u_0 \in \dot{H}^{k+1}(\Omega)$, alors $u \in L^\infty(\mathbb{R}^+; \dot{H}^{k+1}(\Omega))$;

(iii) Si de plus on suppose que f est de classe C^{k+1} et $u_0 \in \dot{H}^{2k}(\Omega)$, alors $u \in L^\infty(\mathbb{R}^+; \dot{H}^{2k}(\Omega))$.

Puis nous obtenons la dissipativité du semi-groupe et l'existence de l'attracteur global, qui est de plus compact dans $L^2(\Omega)$ et borné dans $\dot{H}^{2k}(\Omega)$. De plus, nous expliquons comment adapter l'étude pour traiter l'équation de Cahn-Hilliard d'ordre élevé associée aux conditions aux limites de type Neumann homogène.

De plus, nous considérons au Chapitre 4 l'équation de Allen-Cahn d'ordre élevé (1.16) avec le potentiel logarithmique (1.7) et obtenons des solutions variationnelles dans un sens plus faible. Du fait de la singularité du potentiel, nous raisonnons comme dans [104] et construisons une suite de solutions u^N d'approximations régulières du problème singulier. Dans le même temps, nous définissons la solution variationnelle u du problème singulier, et prouvons son existence en montrant que la suite de solutions u^N converge (dans un certain sens) vers u. Plus précisément, nous avons le

Théorème 1.2.3. On suppose que $u_0 \in \dot{H}^k(\Omega)$, avec $-1 < u_0 < 1$ a.e. $x \in \Omega$. Alors, pour f définie par (1.5), le problème (1.16), (1.19) et (1.20) possède une unique solution variationnelle u.

Puis nous définissons le semi-groupe et justifions l'existence de l'attracteur global qui est compact dans $L^2(\Omega)$ et borné dans $H^{k+1}(\Omega)$.

1.2.2 Modèles anisotropes d'ordre élevé

Les problèmes anisotropes correspondant aux équations de Allen-Cahn et Cahn-Hilliard d'ordre élevé, qui sont respectivement les L^2- and H^{-1} flots de gradient de l'énergie libre de Ginzburg-Landau d'ordre élevé (1.8), s'écrivent

$$\frac{\partial u}{\partial t} + \sum_{i=1}^{k}(-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u + f(u) = 0 \tag{1.21}$$

et

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k}(-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0. \tag{1.22}$$

Pour des raisons de simplicité, nous considérons au Chapitre 5 un potentiel polynomial plutôt que le potentiel logarithmique. Les conditions aux limites et la condition initiale sont données par :

$$\mathcal{D}^\alpha u = 0 \text{ on } \Gamma, \ |\alpha| \leq \mathrm{k} - 1, \tag{1.23}$$

$$u|_{t=0} = u_0. \tag{1.24}$$

En résumé, nos résultats pour le problème d'Allen-Cahn anisotrope et d'ordre élevé sont :

Théorème 1.2.4. (i) On suppose que $u_0 \in H_0^k(\Omega)$. Alors, (1.21), (1.23)-(1.24) possède une unique solution faible u telle que, $\forall T > 0$, $u \in L^\infty(\mathbb{R}^+; H_0^k(\Omega)) \cap L^2(0,T; H^{2k}(\Omega) \cap H_0^k(\Omega))$ et $\frac{\partial u}{\partial t} \in L^2(0,T; L^2(\Omega))$.

(ii) Si on suppose de plus que $u_0 \in H^{2k}(\Omega) \cap H_0^k(\Omega)$, alors $u \in L^\infty(\mathbb{R}^+; H^{2k}(\Omega) \cap H_0^k(\Omega))$.

A partir du théorème précédent, on définit le semi-groupe associé au problème (1.21) et on montre que le semi-groupe est dissipatif dans $H^{2k}(\Omega) \cap H_0^k(\Omega)$. On déduit ensuite l'existence de l'attracteur global, compact dans $H_0^k(\Omega)$ et borné dans $H^{2k}(\Omega)$. Nous présentons également des simulations numériques pour le problème de Allen-Cahn anisotrope et d'ordre élevé avec des conditions aux limites périodiques, illustrant l'anisotropie du modèle.

Théorème 1.2.5. (i) On suppose que $u_0 \in H_0^k(\Omega)$. Alors le problème (1.22), (1.23)-(1.24) possède une unique solution faible u telle que, $\forall T > 0$, $u \in L^\infty(\mathbb{R}^+; H_0^k(\Omega)) \cap L^2(0,T; H^{2k}(\Omega) \cap H_0^k(\Omega))$ et $\frac{\partial u}{\partial t} \in L^2(0,T; H^{-1}(\Omega))$.

(ii) Si de plus on suppose que $u_0 \in H^{k+1}(\Omega) \cap H_0^k(\Omega)$, alors, $\forall T > 0$, $u \in L^\infty(\mathbb{R}^+; H^{k+1}(\Omega) \cap H_0^k(\Omega))$ et $\frac{\partial u}{\partial t} \in L^2(0,T; L^2(\Omega))$.

(iii) Si de plus on suppose que f est de classe C^{k+1} et $u_0 \in H^{2k}(\Omega) \cap H_0^k(\Omega)$, alors $u \in L^\infty(\mathbb{R}^+; H^{2k}(\Omega) \cap H_0^k(\Omega))$.

On définit ensuite le semi-groupe associé et on montre qu'il est dissipatif dans $H^{2k}(\Omega) \cap H_0^k(\Omega)$, et on obtient l'existence de l'attracteur global, qui est compact dans $H_0^k(\Omega)$ et borné dans $H^{2k}(\Omega)$.

1.2.3 Equations de Cahn-Hilliard généralisées d'ordre élevé

Dans le Chapitre 6, nous étudions les équations de Cahn-Hilliard généralisées d'ordre élevé introduites dans (1.10) et rappelées ci-dessous :

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) + g(x,u) = 0. \tag{1.25}$$

$$\mathcal{D}^\alpha u = 0 \text{ on } \Gamma,\ |\alpha| \leq \mathrm{k} - 1, \tag{1.26}$$

$$u|_{t=0} = u_0. \tag{1.27}$$

Nous considérons uniquement le cas $k \geq 2$, puisque le cas $k = 1$ peut être traîté comme dans [93]. En ce qui concerne l'étude théorique, nous obtenons des estimations a priori, et la régularité de l'unique solution, à savoir :

Théorème 1.2.6. (i) On suppose que $u_0 \in H_0^k(\Omega)$. Alors, (1.25)-(1.27) possède une unique solution faible u telle que, $\forall T > 0$, $u \in L^\infty(\mathbb{R}^+; H_0^k(\Omega)) \cap L^2(0,T; H^{2k}(\Omega) \cap H_0^k(\Omega))$ et $\frac{\partial u}{\partial t} \in L^2(0,T; H^{-1}(\Omega))$.

(ii) Si on suppose de plus que $u_0 \in H^{k+1}(\Omega) \cap H_0^k(\Omega)$, alors, $\forall T > 0$, $u \in L^\infty(\mathbb{R}^+; H^{k+1}(\Omega) \cap H_0^k(\Omega))$ et $\frac{\partial u}{\partial t} \in L^2(0,T; L^2(\Omega))$.

(iii) En supposant de plus que f est de classe C^{k+1}, que $g(x,s) = g(s)$, avec g de classe C^{k-1} et que $u_0 \in H^{2k}(\Omega) \cap H_0^k(\Omega)$, on obtient $u \in L^\infty(\mathbb{R}^+; H^{2k}(\Omega) \cap H_0^k(\Omega))$.

Nous définissons alors le semi-groupe et montrons qu'il est dissipatif dans $H^{2k}(\Omega) \cap H_0^k(\Omega)$. On en déduit l'existence de l'attracteur global, qui est compact dans $H_0^k(\Omega)$ et borné dans $H^{2k}(\Omega)$. Dans la partie numérique de l'étude, nous choisissons différentes fonctions g, et proposons divers résultats numériques correspondant notamment aux solutions de l'équation de Cahn-Hilliard-Oono, et à celles de l'équation décrivant la croissance tumorale.

1.2.4 L'équation modifiée de Cahn-Hilliard anisotrope d'ordre élevé

On considère au Chapitre 7 une équation modifiée (relaxation hyperbolique) de Cahn-Hilliard anisotrope d'ordre élevé qui s'écrit, pour $k \in \mathbb{N}$, $k \geq 2$, $x \in \Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$,

$$\beta \partial_{tt} u + \partial_t u - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0 \tag{1.28}$$

$$u|_{t=0} = u_0; \ u_t|_{t=0} = v_0. \tag{1.29}$$

On raisonne comme dans l'article de Grasselli et Wu pour l'équation MPFC (cf. [75] et [76]), la difficulté étant d'étendre leurs résultats à l'équation (1.28), comportant de l'anisotropie et des termes d'ordre élevé. Néanmoins, dans le cas de conditions aux limites périodiques, on obtient :

Théorème 1.2.7. (i) Pour toute condition initiale $(u_0, v_0) \in H_0^k(\Omega) \times H^{-1}(\Omega)$, le problème (1.28)-(1.29) possède une unique solution faible (u, u_t) telle que, $\forall\ T > 0$, $u \in L^\infty(\mathbb{R}^+; H_0^k(\Omega))$ et $u_t \in L^2(0,T; H^{-1}(\Omega))$.

(ii) Si on suppose de plus que $(u_0, v_0) \in (H^{k+1}(\Omega) \cap H_0^k(\Omega)) \times L^2(\Omega)$, alors $u \in L^\infty(\mathbb{R}^+; H^{k+1}(\Omega) \cap H_0^k(\Omega))$ et $u_t \in L^2(0,T; L^2(\Omega))$.

(iii) Si on suppose de plus que f est de classe C^{k+1} et que $(u_0, v_0) \in (H^{2k}(\Omega) \cap H_0^k(\Omega)) \times H^{k-1}(\Omega)$, alors $u \in (L^\infty(\mathbb{R}^+; H^{2k}(\Omega) \cap H_0^k(\Omega))$ *et* $u_t \in L^\infty(0,T; H^{k-1}(\Omega))$.

On peut donc définir le semi-groupe associé et montrer que celui-ci est dissipatif dans $H_0^k(\Omega) \cap H^{-1}(\Omega)$. On en déduit l'existence de l'attracteur global, qui est compact dans $H_0^k(\Omega) \cap H^{-1}(\Omega)$. De plus, au Chapitre 8 nous proposons des schémas numériques, basés sur la méthode des éléments finis ou sur une méthode spectrale pour la discrétisation en espace, et sur un schéma d'ordre 2 pour la discrétisation en temps, pour l'équation (1.28) avec un terme additionnel γu, qui s'écrit :

$$\beta\partial_{tt}u + \partial_t u - \Delta\sum_{i=1}^{k}(-1)^i\sum_{|\alpha|=i}a_\alpha\mathcal{D}^{2\alpha}u - \Delta f(u) + \gamma u = 0. \tag{1.30}$$

Nous obtenons des résultats d'existence pour la solution numérique, et des résultats de stabilité basés sur l'énergie pour le schéma semi-discrétisé (en espace) comme pour le schéma entièrement discrétisé. Des simulations numériques illustrent et confirment ces résultats.

1.2.5 Modèles MSEM

Au Chapitre 9, nous étudions le problème parabolique micro-systèmes électro-mécanique (MSEM) suivant :

$$\begin{aligned} &\frac{\partial u}{\partial t} - \Delta u = \frac{\lambda f(x)}{(1-u)^2} \quad \text{in } \Omega,\\ &u(t,x) = 0 \text{ on } \partial\Omega; \quad u(0,x) = 0 \quad \text{in } \Omega, \end{aligned} \tag{1.31}$$

(voir [46] et [114] pour plus de détails). Le problème elliptique associé s'écrit :

$$\begin{aligned} &-\Delta u = \frac{\lambda f(x)}{(1-u)^2} \quad \text{in } \Omega,\\ &u(x) = 0 \text{ on } \partial\Omega; \quad 0 \le u < 1 \quad \text{in } \Omega, \end{aligned} \tag{1.32}$$

avec $u = 1 - w$ (w a été introduit dans (1.15)) et représente la distance adimentionnalisée entre la plaque et la membrane, f décrit le profil diélectrique de la membrane élastique et $\lambda > 0$ représente la tension appliquée. On propose des méthodes numériques stables pour résoudre le problème (1.31) et on discute l'influence de la valeur de λ sur la solution. Plus précisément, on construit un schéma semi-discrétisé (en temps) et semi-implicite : Pour $\tau > 0$ donné, $t_n = n\tau$, $n = 0, 1, \cdots$,

$$\begin{cases} u_{n+1} - \tau\Delta u_{n+1} = u_n + \dfrac{\lambda\tau f(x)}{(1-u_n)^2} \quad \text{in } \Omega,\\ u_{n+1} = 0 \text{ on } \partial\Omega, \end{cases} \tag{1.33}$$

ainsi qu'un schéma semi-discret et implicite :

$$\begin{cases} u_{n+1} - \tau\Delta u_{n+1} = u_n + \dfrac{\lambda\tau f}{(1-u_{n+1})^2} \quad \text{in } \Omega,\\ u_{n+1} = 0 \text{ on } \partial\Omega, \end{cases} \tag{1.34}$$

avec $u_{n+1} \simeq u(t_{n+1}, x)$, $u_n \simeq u(t_n, x)$ et u_0 la condition initiale. On note u_λ l'unique solution minimale du problème (1.32), et λ^* la tension de traction.

En supposant que $\lambda < \lambda^*$, nous avons le résultat suivant pour le schéma (1.33) :

Proposition 1.2.1. *(i) Pour tout $n \in \mathbb{N} \cup \{0\}$, on a $0 \leq u_n(x) \leq u_\lambda(x)$, a.e. $x \in \Omega$; en particulier, pour tout $n \in \mathbb{N} \cup \{0\}$, u_n existe et satisfait $0 \leq u_n(x) < 1$, a.e. $x \in \Omega$.*

(ii) Si on suppose $\frac{1}{1+c_0\tau}\left(1 + \frac{2\lambda\tau}{(1-\overline{u})^3}\right) < 1$, où, $c_0 > 0$ est la constante optimale dans l'inégalité de Poincaré, alors u_n converge vers u_λ dans $L^2(\Omega)$ lorsque $n \to +\infty$.

(iii) Si la condition initiale vérifie $0 \leq u_0 < u_\lambda$, la solution numérique u_n est croissante et bornée par u_λ ; de plus, sous l'hypothèse $\lambda < \lambda^*$, le problème elliptique possède au moins deux solutions notées u_λ, et u_λ^+, avec $u_\lambda < u_\lambda^+$. Si on choisit $u_\lambda \leq u_0 < u_\lambda^+$, alors la solution u_n est décroissante et minorée par u_λ.

Concernant le schéma (1.34), on montre, sous certaines conditions, que u_n converge vers u_λ dans $H_0^1(\Omega)$ lorsque $n \to +\infty$; en particulier, en 1D, u_n converge vers u_λ dans $C(\bar{\Omega})$ lorsque $n \to +\infty$.

Toujours en 1D, on construit ensuite le schéma semi-implicite entièrement discrétisé, qui peut s'écrire :

$$AU^{n+1} = U^n + G(U^n),$$

où A est la matrice des différences finies, U^{n+1} et U^n sont les vecteurs solutions aux $(n+1)$ième et $n$ième pas de temps et G est le vecteur associé au terme non linéaire. On vérifie que, sous des hypothèses raisonnables, la solution numérique U^{n+1} est majorée et croissante, et donc converge. Finalement, des simulations numériques correspondant à différentes conditions initiales et différentes valeurs de λ, sont proposées, pour des domaines Ω de dimensions 1 et 2.

Chapitre 2

General introduction

2.1 Nonlinear partial differential equations

Compared to linear partial differential equations, nonlinear partial differential equations are more complicated to analyze both theoretically and numerically due to their nonlinear nature. Phase separation models and the mathematical models of micro-electro-mechanical systems (abbr. MEMS) are two representatives of nonlinear partial differential equations, which can be (when considering logarithmic potentials in phase separation) singular.

2.1.1 Phase separation models

The Allen-Cahn and Cahn-Hilliard equations are the main equations in phase separation. The classical Allen-Cahn equation was originally introduced by Allen and Cahn in [4] to describe the motion of anti-phase boundaries in crystalline solids. Besides, Cahn and Hilliard established the Cahn-Hilliard equation in [20] to describe the complicated phase separation (for example, spinodal decomposition) phenomena in a solid, especially binary alloy (see also in [43], [44] and [108]) and coarsening. Both of these two equations are central equations in material science and are based on the so-called Ginzburg-Landau free energy, which reads

$$\Psi_{\mathrm{GL}} = \int_\Omega (\frac{\alpha}{2}|\nabla u|^2 + F(u))dx,\ \alpha > 0, \tag{2.1}$$

where u represents the order parameter, say, the concentration of one of the two metallic components (usually being taken between -1 and 1), α is the surface tension, F is a double-well potential and Ω is the domain occupied by the system (we usually set the domain to be bounded and regular, with a boundary of Γ). In this case, isotropy is assumed and also a fixed temperature. The Allen-Cahn equation, which corresponds to an L^2-gradient flow of the Ginzburg-Landau free energy, then reads

$$\frac{\partial u}{\partial t} - \alpha\Delta u + f(u) = 0, \tag{2.2}$$

where f is the derivative of the double-well potential F, while the Cahn-Hilliard equation, which corresponds to an H^{-1}-gradient flow, reads

$$\frac{\partial u}{\partial t} + \alpha\Delta^2 u - \Delta f(u) = 0. \tag{2.3}$$

Boundary conditions. Concerning the boundary condition of these models, the Dirichlet boundary condition indicates that the condition on the boundary is fixed, while the homogenous Neumann boundary condition implies that no mass loss occurs across the boundary walls, which can lead to mass conservation. There is a combination of the Dirichlet and Neumann boundary conditions, which is called mixed boundary condition.

The periodic boundary condition is often considered for a symmetric regular domain, the conditions on two of the symmetric boundary walls are equal in value and opposite in the direction of outer normal vectors. The authors in some references (see [28], [82] and [138]) also study the Cahn-Hilliard equation endowed with dynamic boundary conditions which involves the time derivative of dependent function u.

Nonlinear terms. The double-well potential F possesses two wells which correspond to the phases of the material. A thermodynamically relevant potential F follows from a mean-field model (see, e.g., [20] and [36]) and is a logarithmic function of the form

$$F(s) = \frac{\lambda_1}{2}(1-s^2) + \frac{\lambda_2}{2}[(1+s)\ln(\frac{1+s}{2}) + (1-s)\ln(\frac{1-s}{2})],\ s \in (-1,1),\ 0 < \lambda_2 < \lambda_1, \tag{2.4}$$

therefore,

$$f(s) = -\lambda_1 s + \frac{\lambda_2}{2}\ln\frac{1+s}{1-s}, \tag{2.5}$$

where λ_1 and λ_2 are respectively proportional to a critical temperature and the absolute temperature, which is assumed to be a constant during the process. Moreover, the condition $\lambda_2 < \lambda_1$ ensures that F has a double-well form and the phase separation can occur. A phase-field system based on the Maxwell-Cattaneo heat conduction law with a logarithemic nonlinearity was studied by the author in [92], while the authors in [26] studied the Bertozzi-Esedoglu-Gillette-Cahn-Hilliard equation with logarithmic nonlinear terms in which they obtained the existence of local (in time) solutions and proposed the applications to binary image inpainting. We refer the reader to [29], [30], [70], [94], [96], [99] and [102] for more details.

The thermodynamically relevant potential is generally approximated by a polynomial one, which reads

$$F(s) = \frac{1}{4}(s^2-1)^2, \tag{2.6}$$

and

$$f(s) = s^3 - s. \tag{2.7}$$

We also note the resemblance and difference between the logarithmic potential and the polynomial potential in Fig. 2.1. Both of the potentials have a double-well form ; the wells of the logarithmic potential are at two values of s which are however distinct from ± 1, while the wells of the polynomial potential are located exactly at ± 1. We also notice that the wells of the logarithmic potential would approach to ± 1 when the absolute temperature (or λ_2) is close to the critical temperature (or λ_1). Under this circumstance, the logarithmic potential gets well approximated by the polynomial one.

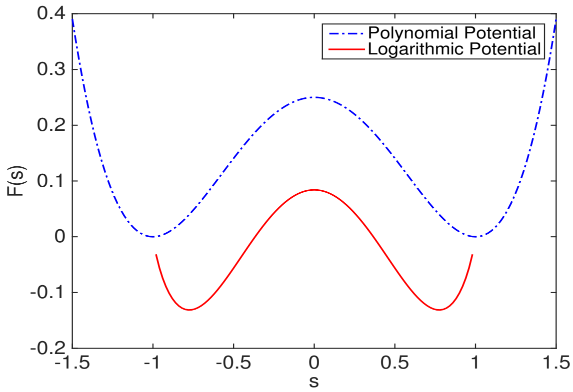

Figure 2.1 – The logarithmic potential and the polynomial potential.

Anisotropy. If we take anisotropy interfaces into account, from a physical point of view, sufficiently strong anisotropy may cause the surface energy function to become so large or singular on certain orientations that these orientations may disappear in the equilibrium shape in order to achieve a well-defined energy for the system. As a result, the interface of equilibrium may become non-smooth curve, moreover facets and corners may appear.

As anisotropy is an important factor in interface equilibria and dynamics, there has been several works on it. In the work of R. Kobayashi (see [80]), the author considered anisotropic crystal growth in two phase field (liquid and solid) based on a modified thermodynamically relevant Ginzburg-Landau type free energy. The anisotropy was introduced by assuming that the mobility of the interface was a function of orientation. In this article, many numerical simulations illustrated anisotropy effects, including dendrite growth and some snowflake-like patterns. Furthermore, one can find more thermodynamically relevant anisotropic phase field models in the works of Wheeler and McFadden et al (see [101], [132] and [134]).

Another approach to take anisotropy into account is to consider another modified Ginzburg-Landau type of free energy, the difference compared to the former one is that temperature has been omitted (see [40], [120], [126] and [133]). The anisotropy was introduced by the interfacial energy function $\gamma(\mathbf{n})$, which depends on the tangent angle on the interface. Taylor and Cahn (see [126]) provided a general outline of an analysis of the motion of diffuse interfaces with sharp corners and facets and the work of Sekerka (see [120]) gave an outline of the study of equilibrium shapes and also analytical criteria for missing orientations on 3D equilibrium shapes. Wise et al (see [133]) and Shen et al. (see [40]) provided some numerical analysis and simulations on these anisotropic models based on the regularization of the problem.

We account for anisotropic phenomenon in a different way (compared to the above) by considering a higher-order Ginzburg-Landau type of free energy, which was proposed by G. Caginalp and E. Esenturk in [23] and reads

$$\Psi_{\text{HOGL}} = \int_\Omega (\frac{1}{2}\sum_{i=1}^{k}\sum_{|\alpha|=i} a_\alpha |\mathcal{D}^\alpha u|^2 + F(u))\, dx,\ k \in \mathbb{N}, \tag{2.8}$$

where, for $\alpha = (k_1, k_2, k_3) \in (\mathbb{N} \cup \{0\})^3$,

$$|\alpha| = k_1 + k_2 + k_3$$

and, for $\alpha \neq (0,0,0)$,

$$\mathcal{D}^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{k_1} \partial x_2^{k_2} \partial x_3^{k_3}}$$

(we agree that $\mathcal{D}^{(0,0,0)} v = v$). We note that, in (2.8), the temperature has been omitted. The advantage is that such a kind of free energy provides an explicit way to compute the anisotropy by supposing that the surface tension being different on different orientations. We then note that the higher-order anisotropic Cahn-Hilliard equation corresponds to the H^{-1}-gradient flow of the free energy (2.8) and reads

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0.$$

Generalization. Despite phase separation, the Cahn-Hilliard equation and some of its variants are also relevant to other phenomenon, such as, population dynamics (see [31]), tumor growth (see [7] and [86]), bacterial films (see [81]), thin films (see [112] and [129]), image processing (see [8], [9], [21], [27] and [42]) and even the rings of Saturn (see [130]) and the clustering of mussels (see [90]).

In particular, several such phenomena can be modeled by the following generalized Cahn-Hilliard equation :

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) + g(x,u) = 0. \tag{2.9}$$

We refer the reader to [93] and [98] (see also [7], [26], [37], [47]) for detailed studies on equation (2.9). Since we focus on the higher-order models in this part, a higher-order generalized Cahn-Hilliard equation will be taken into account, which reads

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) + g(x,u) = 0. \tag{2.10}$$

This equation is actually based on the free energy (2.8) which we mentioned above. In (2.10), α denotes the multi-index and f is considered to be the regular nonlinear term. As far as the function g is concerned, we have several assumptions on it, whereas these assumptions are satisfied in the following cases.
(i) Cahn-Hilliard-Oono equation. In that case,

$$g(x, s) = g(s) = \beta s, \ \beta > 0.$$

This function was proposed in [111] in order to account for long-ranged (i.e., nonlocal) interactions, and also to simplify numerical simulations. We also mention that, in [39], the authors considered a similar form of Cahn-Hilliard-Oono equation which has applications in describing the segregation between the subchains of a diblock copolymer below a critical temperature. We refer the reader to [15], [38], [95], [131] and [7] for more studies on Cahn-Hilliard-Oono equation.
(ii) Proliferation term. In that case,

$$g(x, s) = g(s) = \beta s(s - 1), \ \beta > 0.$$

This function was proposed in [86] in view of biological applications and, more precisely, to model wound healing and tumor growth (in one space dimension) and the clustering of brain tumor cells (in two space dimensions) ; see also [7] for other quadratic functions.
(iii) Fidelity term. In that case,

$$g(x, s) = \lambda_0 \chi_{\Omega \backslash D}(x)(s - \varphi(x)), \ \lambda_0 > 0, \ D \subset \Omega, \ \varphi \in L^2(\Omega),$$

where χ denotes the indicator function and λ_0 is actually a large positive number. This function was proposed in [8] and [9] in view of applications to image inpainting. Here, φ is a given (damaged) image and D is the inpainting (i.e., damaged) region. Furthermore, the fidelity term $g(x, u)$ is added in order to keep the solution close to the image outside the inpainting region. The idea in this model is to solve the equation up to steady state to obtain an inpainted (i.e., restored) version $u(x)$ of $\varphi(x)$.

Hyperbolic relaxation. A hyperbolic relaxation of the Cahn-Hilliard equation has been proposed in [55], in order to model rapid solidification of a binary alloy. Furthermore, S. Gatti et al. provided in [62] a detailed analysis of the longterm properties of the solutions for a hyperbolic relaxation of the one-dimensional Cahn-Hilliard equation in the singular limit when the relaxation parameter goes to zero.

P. Stefanovic et al. proposed in [123] a so-called modified phase field crystal equation (abbr., MPFC) to distinguish between the elastic relaxation and diffusion time scale without consideration of anisotropy, see also in [124], which reads

$$\beta \partial_{tt} u + \partial_t u - \Delta[\Delta^2 u + 2\Delta u + f(u)] = 0. \tag{2.11}$$

The MPFC equation incorporates both fast elastic relaxation and slower mass diffusion. In [75] and [76], M. Grasselli and H. Wu proved the well-posedness and established the existence of an exponential attractor for the MPFC equation (2.11) endowed with periodic boundary conditions. Additionally, in [72], M. Grasselli and M. Pierre proposed a space semi-discrete and a fully discrete finite element scheme for the MPFC model and established their convergence to equilibrium both theoretically and numerically. We refer the readers to [135], [136] for more numerical methods to solve the MPFC model and [45], [50], [56], [79] for the theoretical and numerical study on the phase field crystal model without a relaxation.

As far as the anisotropy is concerned, we take into account the anisotropic effect in the modified phase field crystal equation, then the equation becomes, for $k \in \mathbb{N}$, $k \geq 2$, $x \in \Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$,

$$\beta\partial_{tt}u + \partial_t u - \Delta \sum_{i=1}^{k}(-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0. \tag{2.12}$$

We further consider the numerical approximations for a hyperbolic relaxation of the higher-order anisotropic generalized Cahn-Hilliard models, which read

$$\beta\partial_{tt}u + \partial_t u - \Delta \sum_{i=1}^{k}(-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) + \gamma u = 0, \tag{2.13}$$

where $\gamma \geq 0$ and with the term γu, equation (2.13) can model, e.g., long-ranged interactions.

2.1.2 Mathematical modeling on micro-electromachanical system

Another nonlinear partial differential equation has arisen in the mathematical modeling of micro-electromachanical system (abbr., MEMS), for example, micropumps, microswitches, microvalves, shuffle motor, etc., see [114]. An idealized machinery in MEMS consists of the construction which is shown in Fig. 2.2. The device mainly contains a thin and deformable elastic membrane with fixed boundary and a parallel rigid ground electric plate. The upper surface of the membrane, which is normally dielectric, is coated with a metallic conducting film and the thickness of the film is considered to be negligible. When applying a voltage to the conducting film, the elastic membrane deforms towards the ground plate. The action of the system $\mathcal{S}$ consists of the kinetic energy E_k, damping energy E_d and potential energy E_p, namely, if we denote the Lagrangian by $\mathcal{L}$,

$$\mathcal{S} = \int_{t_1}^{t_2} \int_{\Omega'} \mathcal{L} dx' dy' dt' := E_k + E_d + E_p, \tag{2.14}$$

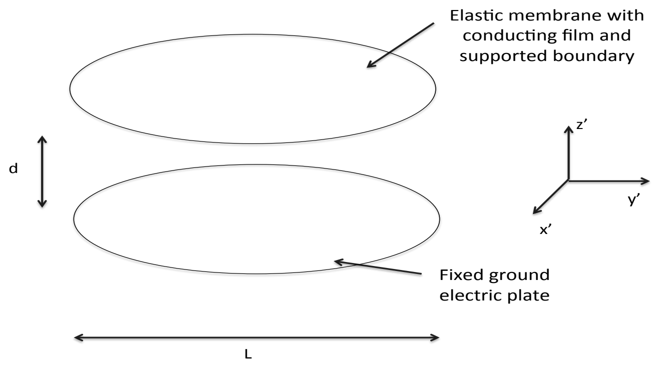

FIGURE 2.2 – An idealized MEMS capacitor.

where Ω' denotes the domain of the membrane. On the one hand, we apply Hamilton's principle to minimize the action $\mathcal{S}$, and obtain an elastic problem. Combining the electrostatic effect, after the dimensionless analysis and under certain reasonable assumptions, a nonlinear parabolic problem can be obtained, which reads

$$\begin{aligned} &\frac{\partial w}{\partial t} - \Delta w = \frac{\lambda f(x)}{w^2} \quad \text{in } \Omega, \\ &w(t,x) = 1 \ \text{ on } \partial\Omega; \quad w(0,x) = 1 \quad \text{in } \Omega, \end{aligned} \tag{2.15}$$

where w denotes the dimensionless dynamic deflection and $f(x)$ describes the varying dielectric permittivity of the elastic membrane. We refer the reader to [46] for the detailed derivation.

2.2 Problems and framework

We study in this thesis several nonlinear partial differential equations, including higher-order models in phase separation endowed or without anisotropy and a typical singular partial differential equation arising in the mathematical modeling of microelectromechanical system.

2.2.1 Higher-order models in phase separation

We consider firstly in Chapter 3 and Chapter 4 the higher-order models in phase separation, namely, the higher-order Allen-Cahn and Cahn-Hilliard equations which read

$$\frac{\partial u}{\partial t} + P(-\Delta)u + f(u) = 0, \tag{2.16}$$

and

$$\frac{\partial u}{\partial t} - \Delta P(-\Delta)u - \Delta f(u) = 0, \tag{2.17}$$

respectively, where

$$P(s) = \sum_{i=1}^{k} a_i s^i. \tag{2.18}$$

Due to $P(s)$, (2.16) and (2.17) may possess higher-order nature, which is the main difficulty to study both of them. Moreover, if the nonlinearity is the logarithmic one, there will be some additional difficulty to deal with the nonlinear term. The boundary condition is set to be

$$u = \Delta u = ... = \Delta^{k-1} u = 0 \text{ on } \Gamma, \tag{2.19}$$

and the initial condition is

$$u|_{t=0} = u_0. \tag{2.20}$$

In Chapter 3 we work on the higher-order Allen-Cahn equation (2.16) and Cahn-Hilliard equation (2.17) with a simplified double-well potential and discuss the regularity results for both of the problems endowed with Dirichlet boundary condition (2.19). More precisely, we set $\dot{H}^m(\Omega) = \{v \in H^m(\Omega), v = \Delta v = \cdots = \Delta^{[\frac{m-1}{2}]} v = 0 \text{ on } \Gamma\}$, where $[\cdot]$ denotes the integer part, and for the higher-order Allen-Cahn equation, we obtain the

Theorem 2.2.1. *(i) We assume that $u_0 \in \dot{H}^k(\Omega)$, with $\int_\Omega F(u_0)dx < +\infty$ when $k = 1$. Then, the problem (2.16), (2.19)-(2.20) possesses a unique solution u such that, $\forall T > 0$, $u \in L^\infty(\mathbb{R}^+; \dot{H}^k(\Omega)) \cap L^2(0, T; \dot{H}^{2k}(\Omega))$, $\frac{\partial u}{\partial t} \in L^2(0, T; L^2(\Omega))$ and*

$$\frac{d}{dt}((u, v)) + \sum_{i=1}^{k} a_i(((-\Delta)^{\frac{i}{2}} u, (-\Delta)^{\frac{i}{2}} v)) + ((f(u), v)) = 0, \forall v \in C_c^\infty(\Omega).$$

(ii) If we further assume that $u_0 \in \dot{H}^{2k}(\Omega)$, then $u \in L^\infty(\mathbb{R}^+; \dot{H}^{2k}(\Omega))$.

Thus, we define the semigroup and deduce the dissipativity of the semigroup, as well as the existence of the global attractor which is compact in $L^2(\Omega)$ and bounded in $\dot{H}^{2k}(\Omega)$. Furthermore, for higher-order Cahn-Hilliard equation, we have the

Theorem 2.2.2. *(i) We assume that $u_0 \in \dot{H}^k(\Omega)$, with $\int_\Omega F(u_0)dx < +\infty$ when $k = 1$. Then, the problem (2.17),(2.19)-(2.20) possesses a unique solution u, $u \in L^\infty(\mathbb{R}^+; \dot{H}^k(\Omega)) \cap L^2(0, T; \dot{H}^{2k}(\Omega))$ and $\frac{\partial u}{\partial t} \in L^2(0, T; H^{-1}(\Omega))$;*

(ii) If we assume that $u_0 \in \dot{H}^{k+1}(\Omega)$, then $u \in L^\infty(\mathbb{R}^+; \dot{H}^{k+1}(\Omega))$;

(iii) If we assume that f is of class C^{k+1} and $u_0 \in \dot{H}^{2k}(\Omega)$, then $u \in L^\infty(\mathbb{R}^+; \dot{H}^{2k}(\Omega))$.

Therefore, we derive the dissipativity of the semigroup and the existence of the global attractor, which is also compact in $L^2(\Omega)$ and bounded in $\dot{H}^{2k}(\Omega)$. In addition, we give some details in order to deal with the higher-order Cahn-Hilliard system associated to the homogenous Neumann boundary condition.

Moreover, we consider the higher-order Allen-Cahn equation (2.16) with the logarithmic nonlinear terms (2.7) in Chapter 4 and also discuss its regularity results in a weaker sense. Due to the singularity of the nonlinearity, we perform as [104] to construct a sequence of solutions u^N under reasonable regular approximations of the singular problem. Meanwhile, we define the variational solution u to the singular problem, verify the existence of u by proving that the sequence of solutions aforementioned are convergent (in some sense) to the variational solution. More precisely, we have the

Theorem 2.2.3. *We assume that $u_0 \in \dot{H}^k(\Omega)$, with $-1 < u_0 < 1$ a.e. $x \in \Omega$. Then, when f is defined in* (2.5)*, problem* (2.16)*,* (2.19) *and* (2.20) *possesses a unique variational solution u.*

Thus, we define the semigroup and claim the existence of the global attractor which is compact in $L^2(\Omega)$ and bounded in $H^{k+1}(\Omega)$.

2.2.2 Higher-order anisotropic models

The corresponding higher-order anisotropic Allen-Cahn and Cahn-Hilliard equations, which are respectively the L^2- and H^{-1}-gradient flow of the higher-order modified Ginzburg-Landau type of free energy (2.8), read

$$\frac{\partial u}{\partial t} + \sum_{i=1}^{k}(-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u + f(u) = 0 \tag{2.21}$$

and

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k}(-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0. \tag{2.22}$$

For the reason of simplicity, we consider in Chapter 5 the polynomial type of potential rather than a thermodynamically relevant potential. The boundary condition and initial condition are set to be

$$\mathcal{D}^\alpha u = 0 \text{ on } \Gamma,\ |\alpha| \leq \mathrm{k} - 1, \tag{2.23}$$

$$u|_{t=0} = u_0. \tag{2.24}$$

In summary, we have the regularity results for the higher-order anisotropic Allen-Cahn problem :

Theorem 2.2.4. *(i) We assume that* $u_0 \in H_0^k(\Omega)$. *Then,* (2.21)*,* (2.23)-(2.24) *possesses a unique weak solution u such that,* $\forall T > 0$, $u \in L^\infty(\mathbb{R}^+; H_0^k(\Omega)) \cap L^2(0, T; H^{2k}(\Omega) \cap H_0^k(\Omega))$ *and* $\frac{\partial u}{\partial t} \in L^2(0, T; L^2(\Omega))$. *(ii) If we further assume that* $u_0 \in H^{2k}(\Omega) \cap H_0^k(\Omega)$*, then* $u \in L^\infty(\mathbb{R}^+; H^{2k}(\Omega) \cap H_0^k(\Omega))$.

Based on this, we define the semigroup and verify that the semigroup is dissipative in $H^{2k}(\Omega) \cap H_0^k(\Omega)$, also the existence of the global attractor, which is compact in $H_0^k(\Omega)$ and bounded in $H^{2k}(\Omega)$. We also display several numerical simulations on the higher-order anisotropic Allen-Cahn problem endowed with periodic boundary condition which illustrate anisotropic effects. For the higher-order anisotropic Cahn-Hilliard problem, we have the

Theorem 2.2.5. *(i) We assume that* $u_0 \in H_0^k(\Omega)$. *Then,* (2.22)*,* (2.23)-(2.24) *possesses a unique weak solution u such that,* $\forall T > 0$, $u \in L^\infty(\mathbb{R}^+; H_0^k(\Omega)) \cap L^2(0, T; H^{2k}(\Omega) \cap H_0^k(\Omega))$ *and* $\frac{\partial u}{\partial t} \in L^2(0, T; H^{-1}(\Omega))$.

(ii) If we further assume that $u_0 \in H^{k+1}(\Omega) \cap H_0^k(\Omega)$*, then,* $\forall T > 0$, $u \in L^\infty(\mathbb{R}^+; H^{k+1}(\Omega) \cap H_0^k(\Omega))$ *and* $\frac{\partial u}{\partial t} \in L^2(0, T; L^2(\Omega))$.

(iii) If we further assume that f *is of class* C^{k+1} *and* $u_0 \in H^{2k}(\Omega) \cap H_0^k(\Omega)$*, then* $u \in L^\infty(\mathbb{R}^+; H^{2k}(\Omega) \cap H_0^k(\Omega))$.

We further define the semigroup and derive that the semigroup is dissipative in $H^{2k}(\Omega) \cap H_0^k(\Omega)$, also the existence of the global attractor, which is compact in $H_0^k(\Omega)$ and bounded in $H^{2k}(\Omega)$.

2.2.3 Higher-order generalized Cahn-Hilliard equations

We then study the higher-order generalized Cahn-Hilliard equation in Chapter 6, which has been shown in (2.10), and is recalled here

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) + g(x, u) = 0. \tag{2.25}$$

$$\mathcal{D}^\alpha u = 0 \text{ on } \Gamma, \ |\alpha| \leq \mathrm{k} - 1, \tag{2.26}$$

$$u|_{t=0} = u_0. \tag{2.27}$$

In this Chapter, we consider only the case $k \geq 2$, since the case $k = 1$ can be treated as in [93]. In the theoretical analysis, we derive the a priori estimates for the problem and the regularity of a unique weak solution, namely,

Theorem 2.2.6. *(i) We assume that* $u_0 \in H_0^k(\Omega)$. *Then,* (2.25)-(2.27) *possesses a unique weak solution u such that,* $\forall T > 0$, $u \in L^\infty(\mathbb{R}^+; H_0^k(\Omega)) \cap L^2(0, T; H^{2k}(\Omega) \cap H_0^k(\Omega))$ *and* $\frac{\partial u}{\partial t} \in L^2(0, T; H^{-1}(\Omega))$.

(ii) If we further assume that $u_0 \in H^{k+1}(\Omega) \cap H_0^k(\Omega)$*, then,* $\forall T > 0$*,* $u \in L^\infty(\mathbb{R}^+; H^{k+1}(\Omega) \cap H_0^k(\Omega))$ *and* $\frac{\partial u}{\partial t} \in L^2(0, T; L^2(\Omega))$*.*

(iii) If we further assume that f *is of class* C^{k+1}*,* $g(x, s) = g(s)$*,* g *is of class* C^{k-1} *and* $u_0 \in H^{2k}(\Omega) \cap H_0^k(\Omega)$*, then* $u \in L^\infty(\mathbb{R}^+; H^{2k}(\Omega) \cap H_0^k(\Omega))$*.*

We then define the semigroup and derive that the semigroup is dissipative in $H^{2k}(\Omega) \cap H_0^k(\Omega)$, also the existence of the global attractor, which is compact in $H_0^k(\Omega)$ and bounded in $H^{2k}(\Omega)$. In the numerical part, we take several different cases into account and demonstrate numerical results to Cahn-Hilliard Oono equation, phase field crystal equation and the equation which describes the tumor growth.

2.2.4 Modified higher-order anisotropic Cahn-Hilliard model

We consider in Chapter 7 the modified higher-order anisotropic Cahn-Hilliard equations which read, for $k \in \mathbb{N}$, $k \geq 2$, $x \in \Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$,

$$\beta \partial_{tt} u + \partial_t u - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0 \tag{2.28}$$

$$u|_{t=0} = u_0; \; u_t|_{t=0} = v_0. \tag{2.29}$$

Based on the work of Grasselli and Wu (see [75] and [76]), the difficulty here to study (2.28) is to extend the regularity analysis to higher-order anisotropy terms. Nevertheless, considering the problem with periodic boundary condition, we have the

Theorem 2.2.7. *(i) For any initial data* $(u_0, v_0) \in H_0^k(\Omega) \times H^{-1}(\Omega)$*, problem* (2.28)-(2.29) *possesses a unique weak solution* (u, u_t)*, such that, for* $\forall\, T > 0$*,* $u \in L^\infty(\mathbb{R}^+; H_0^k(\Omega))$ *and* $u_t \in L^2(0, T; H^{-1}(\Omega))$*.*

(ii) If we assume that $(u_0, v_0) \in (H^{k+1}(\Omega) \cap H_0^k(\Omega)) \times L^2(\Omega)$*, then we have,* $u \in L^\infty(\mathbb{R}^+; H^{k+1}(\Omega) \cap H_0^k(\Omega))$ *and* $u_t \in L^2(0, T; L^2(\Omega))$*.*

(iii) If we further assume that f *is of class* C^{k+1}*, and* $(u_0, v_0) \in (H^{2k}(\Omega) \cap H_0^k(\Omega)) \times H^{k-1}(\Omega)$*, then* $u \in L^\infty(\mathbb{R}^+; H^{2k}(\Omega) \cap H_0^k(\Omega)$ *and* $u_t \in L^\infty(0, T; H^{k-1}(\Omega))$*.*

Therefore, we define the semigroup and claim that the semigroup is dissipative in $H_0^k(\Omega) \cap H^{-1}(\Omega)$, also we have the existence of the global attractor, which is compact in $H_0^k(\Omega) \cap H^{-1}(\Omega)$. Furthermore, in Chapter 8, we develop numerical schemes, which consist of finite element or spectral method in space and a second-order stable scheme in time for equation (2.28) with an additional term γu, which we recall here

$$\beta \partial_{tt} u + \partial_t u - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) + \gamma u = 0. \tag{2.30}$$

We derive the energy stability results and the regularity results for the numerical solution taking both the semi-discrete and fully discrete scheme into account. Numerical simulations illustrate and support the numerical analysis and also the anisotropy effects.

2.2.5 MEMS model

The following idealized parabolic MEMS problem (see [46] and [114] for more detail) will be discussed in Chapter 9,

$$\begin{aligned} &\frac{\partial u}{\partial t} - \Delta u = \frac{\lambda f(x)}{(1-u)^2} \quad \text{in } \Omega, \\ &u(t,x) = 0 \text{ on } \partial\Omega; \quad u(0,x) = 0 \quad \text{in } \Omega, \end{aligned} \tag{2.31}$$

and the corresponding elliptic problem :

$$\begin{aligned} &-\Delta u = \frac{\lambda f(x)}{(1-u)^2} \quad \text{in } \Omega, \\ &u(x) = 0 \text{ on } \partial\Omega; \quad 0 \le u < 1 \quad \text{in } \Omega, \end{aligned} \tag{2.32}$$

where $u = 1 - w$ (w was introduced in (2.15) which represents the dimensionless distance between the membrane and the plate), and f describes the dielectric profile of the elastic membrane and $\lambda > 0$ characterizes the applied voltage. We propose stable and efficient numerical methods to solve problem (2.31) and discuss the influence of the value of λ on the solution. To be exact, we build the semi-implicit semi-discrete scheme : for $\tau > 0$ given, $t_n = n\tau$, $n = 0, 1, \cdots$,

$$\begin{cases} u_{n+1} - \tau\Delta u_{n+1} = u_n + \dfrac{\lambda\tau f(x)}{(1-u_n)^2} \quad \text{in } \Omega, \\ u_{n+1} = 0 \text{ on } \partial\Omega, \end{cases} \tag{2.33}$$

and the implicit semi-discrete scheme :

$$\begin{cases} u_{n+1} - \tau\Delta u_{n+1} = u_n + \dfrac{\lambda\tau f}{(1-u_{n+1})^2} \quad \text{in } \Omega, \\ u_{n+1} = 0 \text{ on } \partial\Omega, \end{cases} \tag{2.34}$$

where $u_{n+1} \simeq u(t_{n+1}, x)$, $u_n \simeq u(t_n, x)$ and u_0 is the initial condition. We also note that the unique minimal solution to problem (2.32) is denoted by u_λ and the so-called pull-in voltage is denoted by λ^*. Then in conclude, assuming that $\lambda < \lambda^*$, we have the following results for scheme (2.33) :

Proposition 2.2.1. *(i) There holds, for all* $n \in \mathbb{N} \cup \{0\}$, $0 \le u_n(x) \le u_\lambda(x)$, *a.e.* $x \in \Omega$; *in particular, for all* $n \in \mathbb{N} \cup \{0\}$, u_n *exists and satisfies* $0 \le u_n(x) < 1$, *a.e.* $x \in \Omega$.

(ii) If we assume $\frac{1}{1+c_0\tau}\left(1+\frac{2\lambda\tau}{(1-\overline{u})^3}\right) < 1$, *where,* $c_0 > 0$ *is the optimal constant in the Poincaré inequality, then,* u_n *converges to* u_λ *in* $L^2(\Omega)$ *as* $n \to +\infty$.

(iii) If we take the initial value $0 \leq u_0 < u_\lambda$, *the numerical solution* u_n *is monotonously increasing and bounded by* u_λ *; we also note that, under the assumption of* $\lambda < \lambda^*$, *the elliptic problem possesses at least two solutions which are denoted by* u_λ, u_λ^+ *and* $u_\lambda < u_\lambda^+$. *If we take* $u_\lambda \leq u_0 < u_\lambda^+$, *it is verified that the numerical solution* u_n *is monotonously decreasing and bounded by* u_λ.

For scheme (2.34), we deduce that, under certain assumption, u_n converges to u_λ in $H_0^1(\Omega)$ as $n \to +\infty$; in particular, in 1D, u_n converges to u_λ in $C(\bar{\Omega})$ as $n \to +\infty$.

We also construct the fully discretized semi-implicit scheme in one dimension, which can be written as

$$AU^{n+1} = U^n + G(U^n),$$

where A is the fully discretized coefficients matrix, U^{n+1} and U^n are the solution vector at $(n+1)$-th and n-th time node and G is the vector associated to the nonlinear term. We verify that, under reasonable assumption, the numerical solution U^{n+1} is bounded and monotone increasing, and converges. Finally, the numerical simulations on the discussion of λ^* and the numerical solution associated to different initial conditions and different λ, both in one dimension and two dimension, are given.

Première partie

Problèmes non linéaires en séparation de phase

Chapitre 3

Higher-order models in phase separation

Modèles d’ordre élevé en séparation de phase

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Higher-order models in phase separation

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Abstract : Our aim in this paper is to study higher-order (in space) Allen-Cahn and Cahn-Hilliard models. In particular, we obtain well-posedness results, as well as the existence of the global attractor.

Key words and phrases : Allen-Cahn model, Cahn-Hilliard model, higher-order models, well-posedness, dissipativity, global attractor.
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3.1 Introduction

The Allen-Cahn (see [4]) and Cahn-Hilliard (see [19] and [20]) equations are central in materials science. They both describe important qualitative features of binary alloys, namely, the ordering of atoms for the Allen-Cahn equation and phase separation processes (spinodal decomposition and coarsening) for the Cahn-Hilliard equation.

These two equations have been much studied from a mathematical point of view ; we refer the readers to the review papers [36] and [108] and the references therein.

Both equations are based on the so-called Ginzburg-Landau free energy,

$$\Psi_{GL} = \int_\Omega (\frac{\alpha}{2}|\nabla u|^2 + F(u))dx,\ \alpha > 0, \tag{3.1}$$

where u is the order parameter, F is a double-well potential and Ω is the domain occupied by the system. The Allen-Cahn equation (which corresponds to an L^2-gradient flow of the Ginzburg-Landau free energy) then reads

$$\frac{\partial u}{\partial t} - \alpha\Delta u + f(u) = 0, \tag{3.2}$$

where $f = F'$, while the Cahn-Hilliard equation (which corresponds to an H^{-1}-gradient flow) reads

$$\frac{\partial u}{\partial t} + \alpha\Delta^2 u - \Delta f(u) = 0. \tag{3.3}$$

In 3.1, the term $|\nabla u|^2$ models short-ranged interactions. It is however interesting to note that such a term is obtained by truncation of higher-order ones (see [20]) ; it can also be seen as a first-order approximation of a nonlocal term accounting for long-ranged interactions (see [65] and [66]). Furthermore, G. Caginalp and E. Esenturk recently proposed in [23] higher-order models in the context of phase-field systems. More precisely, they studied anisotropic higher-order models, which, in the isotropic limit, yield a free energy of the form

$$\begin{aligned}\Psi_{\mathrm{HOGL}} = \int_\Omega \Big(&\sum_{i=1,\dots,k,\ i \text{ even}} a_i |(-\Delta)^{\frac{i}{2}} u|^2 \\ &+ \sum_{i=1,\dots,k,\ i \text{ odd}} a_i |(-\Delta)^{\frac{i-1}{2}} u|^2 + F(u)\Big)dx,\ a_k > 0,\ k \geq 1.\end{aligned} \tag{3.4}$$

The corresponding higher-order Allen-Cahn and Cahn-Hilliard equations then read

$$\frac{\partial u}{\partial t} + P(-\Delta)u + f(u) = 0, \tag{3.5}$$

and

$$\frac{\partial u}{\partial t} - \Delta P(-\Delta)u - \Delta f(u) = 0, \tag{3.6}$$

respectively, where

$$P(s) = \sum_{i=1}^{k} a_i s^i. \tag{3.7}$$

In particular, these models contain sixth-order Cahn-Hilliard models. We can note that there is currently a strong interest in the study of sixth-order Cahn-Hilliard equations. Such equations arise in situations such as strong anisotropy effects being taken into account in phase separation processes (see [128]), atomistic models of crystal growth (see [8], [9] and [56]), the description of growing crystalline surfaces with small slopes which undergo faceting (see [122]), oil-water-surfactant mixtures (see [68] and [69]) and mixtures of polymer molecules (see [50]). We refer the reader to [40], [75], [76],

[79], [84], [85], [95], [96], [97], [99], [115], [116], [117], [118], [135], [136] and [137] for the mathematical and numerical analysis of such models. They also contain the Swift-Hohenberg equation (see [96] and [99]).

Our aim in this paper is to study the well-posedness of (3.5) and (3.6). We also prove the dissipativity of the corresponding solution operators, as well as the existence of the global attractor.

3.1.1 Notation

We denote by $((\cdot,\cdot))$ the usual L^2-scalar product, which associated norm $\|\cdot\|$. We further set $\|\cdot\|_{-1} = \|(-\Delta)^{-\frac{1}{2}}\cdot\|$, where $-\Delta$ denotes the minus Laplace operator associated with (homogeneous) Dirichlet boundary conditions (it is a strictly positive, selfadjoint and unbounded linear operator with compact inverse $(-\Delta)^{-1}$). Note that $\|\cdot\|_{-1}$ is equivalent to the usual H^{-1}-norm on $H^{-1}(\Omega) = H^1_0(\Omega)'$. More generally, $\|\cdot\|_X$ denotes the norm on the Banach space X.

For $m \in \mathbb{N}$, we set $\dot{H}^m(\Omega) = \{v \in H^m(\Omega), v = \Delta v = \cdots = \Delta^{[\frac{m-1}{2}]}v = 0 \text{ on } \Gamma\}$, where $[\cdot]$ denotes the integer part. This space, endowed with the usual H^m-norm, is a closed subspace of $H^m(\Omega)$. Furthermore, $v \mapsto \|(-\Delta)^{\frac{m}{2}}v\|$ is a norm on $\dot{H}^m(\Omega)$ which is equivalent to the usual H^m-norm.

Throughout the paper, the same letters c, c' and c'' denote (generally positive) constants which may vary from line to line. Similarly, the same letter Q denotes (positive) monotone increasing (with respect to each argument) and continuous functions which may vary from line to line.

3.2 The Allen-Cahn theory

3.2.1 Setting of the problem

We consider in this section the following initial and boundary value problem in a bounded and regular domain $\Omega \subset \mathbb{R}^n$, $n = 1,\ 2$ or 3, with boundary Γ :

$$\frac{\partial u}{\partial t} + P(-\Delta)u + f(u) = 0, \tag{3.8}$$

$$u = \Delta u = \cdots = \Delta^{k-1}u = 0,\ \text{on } \Gamma, \tag{3.9}$$

$$u|_{t=0} = u_0. \tag{3.10}$$

We assume that the polynomial P is defined by

$$P(s) = \sum_{i=1}^{k} a_i s^i,\ a_k > 0,\ k \geq 1,\ s \in \mathbb{R}. \tag{3.11}$$

In particular, for $k = 1$, we recover the classical Allen-Cahn equation, while, for $k = 2$, the model contains the Swift-Hohenberg equation.

Furthermore, as far as the nonlinear term f is concerned, we assume that

$$f \in C^1(\mathbb{R}),\ f(0) = 0, \tag{3.12}$$

$$f' \geq -c_0,\ c_0 \geq 0, \tag{3.13}$$

$$f(s)s \geq c_1 F(s) - c_2 \geq -c_3,\ c_1 > 0,\ c_2,\ c_3 \geq 0,\ s \in \mathbb{R}, \tag{3.14}$$

$$F(s) \geq c_3 s^4 - c_4,\ c_3 > 0,\ c_4 \geq 0,\ s \in \mathbb{R}, \tag{3.15}$$

where $F(s) = \int_0^s f(\xi)d\xi$. In particular, the usual cubic nonlinear term $f(s) = s^3 - s$ satisfies these assumption.

We will often use the interpolation inequality

$$\begin{aligned} &\|(-\Delta)^{\frac{1}{2}} v\| \leq c(i)\|(-\Delta)^{\frac{m}{2}} v\|^{\frac{i}{m}} \|v\|^{1-\frac{i}{m}}, \\ &v \in \dot{H}^m(\Omega),\ i \in \{1, \dots, m-1\},\ m \in \mathbb{N},\ m \geq 2. \end{aligned} \tag{3.16}$$

3.2.2 A priori estimates

The estimates derived in this subsection are formal, but they can easily be justified within a Galerkin approximation.

We multiply (3.8) by $\frac{\partial u}{\partial t}$ and have, integrating over Ω and by parts,

$$\frac{d}{dt}(\sum_{i=1}^k a_i \|(-\Delta)^{\frac{i}{2}} u\|^2 + 2\int_\Omega F(u)dx) + 2\|\frac{\partial u}{\partial t}\|^2 = 0, \tag{3.17}$$

meaning that the energy decreases along the trajectories, as expected.

We then multiply (3.8) by u to obtain

$$\frac{1}{2}\frac{d}{dt}\|u\|^2 + \sum_{i=1}^k a_i \|(-\Delta)^{\frac{i}{2}} u\|^2 + ((f(u), u)) = 0, \tag{3.18}$$

We note that it follows from the interpolation inequality (3.16) that, for $i \in \{i, \dots, k-1\}$ and $k \geq 2$,

$$\|(-\Delta)^{\frac{i}{2}} u\|^2 \leq \epsilon \|(-\Delta)^{\frac{k}{2}} u\|^2 + c(i, \epsilon)\|u\|^2, \forall \epsilon > 0. \tag{3.19}$$

It thus follows from (3.14) and (3.18)-(3.19) that

$$\frac{d}{dt}\|u\|^2 + c(\|u\|^2_{H^k(\Omega)} + \int_\Omega F(u)dx) \leq c'(\|u\|^2 + 1),\ c > 0. \tag{3.20}$$

Noting finally that

$$\|u\|^2 \le \epsilon\|u\|^4_{L^4(\Omega)} + c(\epsilon),\ \forall\epsilon > 0, \tag{3.21}$$

we deduce from (3.15) and (3.20) that

$$\frac{d}{dt}\|u\|^2 + c(\|u\|^2_{H^k(\Omega)} + \int_\Omega F(u)dx) \le c',\ c > 0. \tag{3.22}$$

Summing (3.17) and (3.22), we find, noting that $\sum_{i=1}^k a_i\|(-\Delta)^{\frac{i}{2}}u\|^2 \le c\|u\|^2_{H^k(\Omega)}$, a differential inequality of the form

$$\frac{dE_1}{dt} + c(E_1 + \|\frac{\partial u}{\partial t}\|^2) \le c',\ c > 0, \tag{3.23}$$

where

$$E_1 = \sum_{i=1}^k a_i\|(-\Delta)^{\frac{i}{2}}u\|^2 + 2\int_\Omega F(u)dx + \|u\|^2$$

satisfies

$$E_1 \ge c(\|u\|^2_{H^k(\Omega)} + \int_\Omega F(u)dx) - c',\ c > 0. \tag{3.24}$$

Indeed, it follows from the interpolation inequality (3.16) that

$$E_1 \ge c\left(\|u\|^2_{H^k\Omega} + \int_\Omega F(u)dx\right) - c'\|u\|^2 - c''$$

and we conclude by employing (3.15) and (3.21).

We then multiply (3.8) by $-\Delta u$ and have, owing to (3.14),

$$\frac{d}{dt}\|\nabla u\|^2 + 2\sum_{i=1}^k a_i\|(-\Delta)^{\frac{i+1}{2}}u\|^2 \le 2c_0\|\nabla u\|^2. \tag{3.25}$$

Summing (3.23) and δ_1 times (3.25), where $\delta_1 > 0$ is small enough, we obtain, employing once more the interpolation inequality (3.16), a differential inequality of the form

$$\frac{dE_2}{dt} + c(E_2 + \|u\|^2_{H^{k+1}(\Omega)} + \|\frac{\partial u}{\partial t}\|^2) \le c',\ c > 0, \tag{3.26}$$

where

$$E_2 = E_1 + \delta_1\|\nabla u\|^2$$

satisfies

$$E_2 \geq c(\|u\|^2_{H^k(\Omega)} + \int_\Omega F(u)dx) - c',\ c > 0. \tag{3.27}$$

In particular, it follows from (3.26)-(3.27) and Gronwall's lemma that

$$\|u(t)\|^2_{H^k(\Omega)} \leq ce^{-c't}(\|u_0\|^2_{H^k(\Omega)} + \int_\Omega F(u_0)dx) + c'',\ c' > 0,\ t \geq 0, \tag{3.28}$$

and

$$\begin{aligned}&\int_t^{t+r}(\|u\|^2_{H^{k+1}(\Omega)} + \|\frac{\partial u}{\partial t}\|^2)ds \\ &\leq ce^{-c't}(\|u_0\|^2_{H^k(\Omega)} + \int_\Omega F(u_0)dx) + c''(r),\ c' > 0,\ t \geq 0,\end{aligned} \tag{3.29}$$

$r > 0$ given.

Our aim is now to obtain higher-order estimates. To do so, we will distinguish between the cases $k \geq 2$ and $k = 1$.

First case. $k \geq 2$.

We multiply (3.8) by $(-\Delta)^k u$ and find, owing to the interpolation inequality (3.16),

$$\frac{d}{dt}\|(-\Delta)^{\frac{k}{2}}u\|^2 + c\|u\|^2_{H^{2k}(\Omega)} \leq c'\|f(u)\|^2 + c''\|u\|^2,\ c > 0. \tag{3.30}$$

We note that it follows from the continuity of f and the continuous embedding $H^2(\Omega) \subset C(\bar{\Omega})$ that

$$\|f(u)\|^2 \leq Q(\|u\|_{H^2(\Omega)}),$$

hence, owing to (3.28) (recall that $k \geq 2$; also note that it follows from the continuity of F that $|\int_\Omega F(u_0)dx| \leq Q(\|u_0\|_{H^2(\Omega)})$),

$$\|f(u)\|^2 \leq e^{-ct}Q(\|u_0\|_{H^k(\Omega)}) + c',\ c > 0,\ t \geq 0. \tag{3.31}$$

We thus deduce from (3.28) and (3.30)-(3.31) that

$$\frac{d}{dt}\|(-\Delta)^{\frac{k}{2}}u\|^2 + c\|u\|^2_{H^{2k}(\Omega)} \leq e^{-c't}Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0. \tag{3.32}$$

Summing (3.26) and (3.32), we have a differential inequality of the form

$$\frac{dE_3}{dt} + c(E_3 + \|u\|^2_{H^k(\Omega)} + \|\frac{\partial u}{\partial t}\|^2) \leq e^{-c't}Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0, \tag{3.33}$$

where

$$E_3 = E_2 + \|(-\Delta)^{\frac{k}{2}} u\|^2$$

satisfies

$$E_3 \geq c(\|u\|^2_{H^k(\Omega)} + \int_\Omega F(u)dx) - c', \ c > 0. \tag{3.34}$$

We then rewrite (3.8) as an elliptic equation, for $t > 0$ fixed,

$$P(-\Delta)u = -\frac{\partial u}{\partial t} - f(u), \ u = \Delta u = \cdots = \Delta^{k-1} u = 0 \text{ on } \Gamma. \tag{3.35}$$

We multiply (3.35) by $(-\Delta)^k u$ and obtain, employing the interpolation inequality (3.16),

$$\frac{a_k}{2}\|(-\Delta)^k u\|^2 \leq c(\|u\|^2 + \|\frac{\partial u}{\partial t}\|^2 + \|f(u)\|^2),$$

hence, in view of (3.28), (3.31) and standard elliptic regularity results,

$$\|u\|^2_{H^{2k}(\Omega)} \leq c(\|\frac{\partial u}{\partial t}\|^2 + e^{-c't} Q(\|u_0\|_{H^k(\Omega)}) + 1), \ c' > 0. \tag{3.36}$$

We now differentiate (3.8) with respect to time to find

$$\frac{\partial}{\partial t}\frac{\partial u}{\partial t} + P(-\Delta)\frac{\partial u}{\partial t} + f'(u)\frac{\partial u}{\partial t} = 0, \tag{3.37}$$

$$\frac{\partial u}{\partial t} = \Delta\frac{\partial u}{\partial t} = \cdots = \Delta^{k-1}\frac{\partial u}{\partial t} = 0 \text{ on } \Gamma, \tag{3.38}$$

$$\frac{\partial u}{\partial t}(0) = -P(-\Delta)u_0 - f(u_0). \tag{3.39}$$

Note that, if $u_0 \in H^{2k}(\Omega)$, then $\frac{\partial u}{\partial t}(0) \in L^2(\Omega)$ and, owing to the continuous embedding $H^{2k}(\Omega) \subset C(\bar{\Omega})$ and the continuity of f,

$$\|\frac{\partial u}{\partial t}(0)\| \leq Q(\|u_0\|_{H^{2k}(\Omega)}). \tag{3.40}$$

Multiplying (3.37) by $\frac{\partial u}{\partial t}$, we have, owing to (3.13) and the interpolation inequality (3.16),

$$\frac{d}{dt}\|\frac{\partial u}{\partial t}\|^2 \leq c\|\frac{\partial u}{\partial t}\|^2. \tag{3.41}$$

It then follows from (3.29), say, for $r = 1$, and the uniform Gronwall's lemma (see, e.g., [127]) that

$$\|\frac{\partial u}{\partial t}(t)\|^2 \leq e^{-ct}Q(\|u_0\|_{H^k(\Omega)}) + c',\ c > 0,\ t \geq 1. \tag{3.42}$$

Noting that it follows from (3.40)-(3.41) that

$$\|\frac{\partial u}{\partial t}(t)\|^2 \leq e^{ct}Q(\|u_0\|_{H^{2k}(\Omega)}),\ c > 0,\ t \geq 0, \tag{3.43}$$

we finally deduce from (3.42)-(3.43) that

$$\|\frac{\partial u}{\partial t}(t)\|^2 \leq e^{-ct}Q(\|u_0\|_{H^{2k}(\Omega)}) + c',\ c > 0,\ t \geq 0, \tag{3.44}$$

Having this, it follows from (3.36) and (3.44) that

$$\|u(t)\|_{H^{2k}(\Omega)} \leq e^{-ct}Q(\|u_0\|_{H^{2k}(\Omega)}) + c',\ c > 0,\ t \geq 0. \tag{3.45}$$

Remark 3.2.1. *It also follows from the above that*

$$\|u(t)\|_{H^{2k}(\Omega)} \leq e^{-ct}Q(\|u_0\|_{H^k(\Omega)}) + c',\ c > 0,\ t \geq 1. \tag{3.46}$$

Second case. $k = 1$.

We take $a_1 = 1$ for simplicity. We again rewrite (3.8) as an elliptic equation, for $t > 0$ fixed,

$$-\Delta u + f(u) = -\frac{\partial u}{\partial t},\ u = 0 \text{ on } \Gamma. \tag{3.47}$$

We multiply (3.47) by $-\Delta u$ and obtain, employing (3.13) and standard elliptic regularity results,

$$\|u\|^2_{H^2(\Omega)} \leq c(\|\frac{\partial u}{\partial t}\|^2 + \|\nabla u\|^2). \tag{3.48}$$

Next, we differentiate (3.8) with respect to time to find

$$\frac{\partial}{\partial t}\frac{\partial u}{\partial t} - \Delta\frac{\partial u}{\partial t} + f'(u)\frac{\partial u}{\partial t} = 0, \tag{3.49}$$

$$\frac{\partial u}{\partial t} = 0 \text{ on } \Gamma, \tag{3.50}$$

$$\frac{\partial u}{\partial t}(0) = \Delta u_0 - f(u_0). \tag{3.51}$$

Note that, if $u_0 \in H^2(\Omega)$, then $\frac{\partial u}{\partial t}(0) \in L^2(\Omega)$ and

$$\|\frac{\partial u}{\partial t}(0)\| \leq Q(\|u_0\|_{H^2(\Omega)}). \tag{3.52}$$

Proceeding then exactly as above, i.e., multiplying (3.49) by $\frac{\partial u}{\partial t}$, we can prove that

$$\|\frac{\partial u}{\partial t}(t)\| \leq e^{-ct}Q(\|u_0\|_{H^2(\Omega)}) + c',\ c > 0,\ t \geq 0, \tag{3.53}$$

whence, owing to (3.28) for $k = 1$ and (3.48),

$$\|u(t)\|_{H^2(\Omega)} \leq e^{-ct}Q(\|u_0\|_{H^2(\Omega)}) + c',\ c > 0,\ t \geq 0. \tag{3.54}$$

Actually, there also holds, proceeding as above,

$$\|u(t)\|_{H^2(\Omega)} \leq e^{-ct}Q(\|u_0\|^2_{H^1(\Omega)} + \int_\Omega F(u_0)dx) + c',\ c > 0,\ t \geq 1. \tag{3.55}$$

3.2.3 The dissipative semigroup

We have the

Theorem 3.2.1. *(i) We assume that $u_0 \in \dot{H}^k(\Omega)$, with $\int_\Omega F(u_0)dx < +\infty$ when $k = 1$. Then,* (3.8)-(3.10) *possesses a unique solution u such that, $\forall T > 0$, $u(0) = u_0$,*

$$u \in L^\infty(\mathbb{R}^+; \dot{H}^k(\Omega)) \cap L^2(0, T; \dot{H}^{2k}(\Omega)),$$

$$\frac{\partial u}{\partial t} \in L^2(0, T; L^2(\Omega))$$

and

$$\frac{d}{dt}((u, v)) + \sum_{i=1}^{k} a_i(((-\Delta)^{\frac{i}{2}}u, (-\Delta)^{\frac{i}{2}}v)) + ((f(u), v)) = 0, \forall v \in C_c^\infty(\Omega).$$

(ii) If we further assume that $u_0 \in \dot{H}^{2k}(\Omega)$, then

$$u \in L^\infty(\mathbb{R}^+; \dot{H}^{2k}(\Omega)).$$

Proof. **a) Existence :**

The proof of existence is based on the a priori estimates derived in the previous subsection and, e. g., a standard Galerkin scheme.

b) Uniqueness :

Let u_1 and u_2 be two solutions with initial data $u_{0,1}$ and $u_{0,2}$, respectively. We set $u = u_1 - u_2$ and $u_0 = u_{0,1} - u_{0,2}$ and have

$$\frac{\partial u}{\partial t} + P(-\Delta)u + f(u_1) - f(u_2) = 0, \tag{3.56}$$

$$u = \Delta u = \cdots = \Delta^{k-1} u = 0 \text{ on } \Gamma, \tag{3.57}$$

$$u|_{t=0} = u_0. \tag{3.58}$$

We multiply (3.56) by u and have, owing to (3.13) and the interpolation inequality (3.16),

$$\frac{d}{dt}\|u\|^2 + c\|u\|^2_{H^k(\Omega)} \leq c'\|u\|^2, \ c > 0. \tag{3.59}$$

It thus follows from Gronwall's lemma that

$$\|(u_1 - u_2)(t)\| \leq e^{ct}\|u_{0,1} - u_{0,2}\|, \ t \geq 0, \tag{3.60}$$

hence the uniqueness, as well as the continuous dependence with respect to the initial data in the L^2-norm. □

It follows from Theorem 3.2.1 that we can define the semigroup $S(t) : \Phi \to \Phi$, $u_0 \mapsto u(t)$, $t \geq 0$ (i.e., S(0)=I (identity operator) and $S(t+\tau) = S(t) \circ S(\tau)$, $t, \tau \geq 0$), where $\Phi = \dot{H}^{2k}(\Omega)$. Furthermore, $S(t)$ is dissipative in Φ, owing to (3.45) and (3.54), in the sense that it possesses a bounded absorbing set $\mathcal{B}_0$(i.e., $\forall B \subset \Phi$ bounded, $\exists t_0 = t_0(B) \geq 0$ such that $t \geq t_0 \Rightarrow S(t)B \subset \mathcal{B}_0$).

Actually, it follows from (3.60) that we can extend (by continuity and in a unique way) $S(t)$ to $L^2(\Omega)$. Furthermore, it follows from (3.22) that

$$\frac{d}{dt}\|u\|^2 + c\|u\|^2 \leq c', \ c > 0, \tag{3.61}$$

hence, owing to Gronwall's lemma,

$$\|u(t)\| \leq e^{-ct}\|u_0\| + c', \ c > 0, \ t \geq 0, \tag{3.62}$$

i.e., $S(t)$ is dissipative in $L^2(\Omega)$. It then follows from (3.22) and (3.62) that

$$\int_t^{t+r} \|u\|^2_{H^k(\Omega)} ds \leq ce^{-c't}\|u_0\|^2 + c''(r), \ c' > 0, \ t \geq 0, \tag{3.63}$$

$r > 0$ given, so that, applying the uniform Gronwall's lemma to (3.23), we have, for $r = 1$,

$$\|u(t)\|_{H^k(\Omega)} \leq ce^{-c't}\|u_0\| + c'', \ c' > 0, \ t \geq 1. \tag{3.64}$$

This yields the existence of a bounded absorbing set $\mathcal{B}_1$ which is compact in $L^2(\Omega)$ and bounded in $H^k(\Omega)$; actually, it follows from (3.46) and (3.55) that we can take $\mathcal{B}_1$ bounded in $H^{2k}(\Omega)$. We thus deduce (see, e.g., [103] and [127]) the

Theorem 3.2.2. *The semigroup $S(t)$ possesses the global attractor $\mathcal{A}$ which is compact in $L^2(\Omega)$ and bounded in Φ.*

Remark 3.2.2. *(i) We recall that the global attractor $\mathcal{A}$ is the smallest (for the inclusion) compact set of the phase space which is invariant by the flow (i.e., $S(t)\mathcal{A} = \mathcal{A}$, $\forall t \geq 0$) and attracts all bounded sets of initial data as time goes to infinity ; it thus appears as a suitable object in view of the study of the asymptotic behavior of the system. We refer the reader to, e.g., [103] and [127] for more details and discussions on this.*

(ii) We can also prove, based on standard arguments (see, e.g., [103] and [127]) that $\mathcal{A}$ has finite dimension, in the sense of covering dimensions such as the Hausdorff and the fractal dimensions. The finite-dimensionality means, very roughly speaking, that, even though the initial phase space has infinite dimension, the reduced dynamics can be described by a finite number of parameters (we refer the interested reader to, e.g., [103] and [127] for discussions on this subject).

3.3 The Cahn-Hilliard Theory

We now consider the following initial and boundary value problem :

$$(-\Delta)^{-1}\frac{\partial u}{\partial t} + P(-\Delta)u + f(u) = 0, \tag{3.65}$$

$$u = \Delta u = \cdots = \Delta^{k-1}u = 0, \text{ on } \Gamma, \tag{3.66}$$

$$u|_{t=0} = u_0. \tag{3.67}$$

In particular, for $k = 1$, we recover the classical Cahn-Hilliard equation ; the case $k = 2$ corresponds to sixth-order Cahn-Hilliard models.

We make here the same assumptions as in the previous section and we further assume that $f \in C^2(\mathbb{R})$.

3.3.1 A priori estimates

First, repeating the same estimates as those leading to (3.26), we have a differential inequality of the form

$$\frac{dE_4}{dt} + c(E_4 + \|u\|^2_{H^{k+1}(\Omega)} + \|\frac{\partial u}{\partial t}\|^2) \leq c', \ c > 0, \tag{3.68}$$

where

$$E_4 = \sum_{i=1}^{k} a_i\|(-\Delta)^{\frac{i}{2}}u\|^2 + 2\int_\Omega F(u)dx + \|u\|^2_{-1} + \delta_2\|u\|^2,$$

$\delta_2 > 0$ being small enough, satisfies

$$E_4 \geq c(\|u\|^2_{H^k(\Omega)} + \int_\Omega F(u)dx) - c',\ c > 0. \tag{3.69}$$

This yields that

$$\|u(t)\|^2_{H^k(\Omega)} \leq ce^{-c't}(\|u_0\|^2_{H^k(\Omega)} + \int_\Omega F(u_0)dx) + c'',\ c' > 0,\ t \geq 0, \tag{3.70}$$

and

$$\begin{aligned}&\int_t^{t+r}(\|u\|^2_{H^{k+1}(\Omega)} + \|\frac{\partial u}{\partial t}\|^2)ds\\ &\leq ce^{-c't}(\|u_0\|^2_{H^k(\Omega)} + \int_\Omega F(u_0)dx) + c''(r),\ c' > 0,\ t \geq 0,\end{aligned} \tag{3.71}$$

$r > 0$ given.

We now again distinguish between the cases $k \geq 2$ and $k = 1$.

First case. $k \geq 2$.

First, proceeding as in the previous section, we obtain an inequality of the form

$$\frac{dE_5}{dt} + c(E_5 + \|u\|^2_{H^{2k}(\Omega)} + \|\frac{\partial u}{\partial t}\|^2_{-1}) \leq e^{-c't}Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0, \tag{3.72}$$

where

$$E_5 = E_4 + \|u\|^2_{H^{k-1}(\Omega)}$$

satisfies

$$E_5 \geq c(\|u\|^2_{H^k(\Omega)} + \int_\Omega F(u)dx) - c',\ c > 0. \tag{3.73}$$

We then multiply (3.65) by $-\Delta\frac{\partial u}{\partial t}$ and find

$$\frac{d}{dt}(\sum_{i=1}^{k} a_i\|(-\Delta)^{\frac{i+1}{2}}u\|^2) + \|\frac{\partial u}{\partial t}\|^2 \leq \|\Delta f(u)\|^2. \tag{3.74}$$

Since f is of class C^2, it follows from the continuous embedding $H^2(\Omega) \subset C(\bar{\Omega})$ that

$$\|\Delta f(u)\|^2 \leq Q(\|u\|_{H^2(\Omega)}), \tag{3.75}$$

hence, owing to (3.70),

$$\frac{d}{dt}(\sum_{i=1}^{k} a_i\|(-\Delta)^{\frac{i+1}{2}}u\|^2) \leq e^{-ct}Q(\|u_0\|_{H^k(\Omega)}) + c',\ c > 0. \tag{3.76}$$

It finally follows from the interpolation inequality (3.16), (3.71) (for $r = 1$), (3.76) and the uniform Gronwall's lemma that

$$\|u(t)\|_{H^{k+1}(\Omega)} \leq e^{-ct}Q(\|u_0\|_{H^k(\Omega)}) + c',\ c > 0,\ t \geq 1. \tag{3.77}$$

Remark 3.3.1. *Actually, owing again to* (3.76), *there holds*

$$\|u(t)\|_{H^{k+1}(\Omega)} \leq e^{-ct}Q(\|u_0\|_{H^{k+1}(\Omega)}) + c',\ c > 0,\ t \geq 0. \tag{3.78}$$

We now rewrite (3.65) as and elliptic equation, for $t > 0$ fixed,

$$P(-\Delta)u = -(-\Delta)^{-1}\frac{\partial u}{\partial t} - f(u),\ u = \Delta u = \cdots = \Delta^{k-1}u = 0 \text{ on } \Gamma. \tag{3.79}$$

Multiplying (3.79) by $(-\Delta)^k u$, we have, employing the interpolation inequality (3.16),

$$\frac{a_k}{2}\|(-\Delta)^k u\|^2 \leq c(\|u\|^2 + \|f(u)\|^2 + \|\frac{\partial u}{\partial t}\|_{-1}^2),$$

hence, since f and F are continuous and owing to (3.70),

$$\|u\|_{H^{2k}(\Omega)}^2 \leq e^{-ct}Q(\|u_0\|_{H^k(\Omega)}) + c'\|\frac{\partial u}{\partial t}\|_{-1}^2 + c'',\ c > 0,\ t \geq 0. \tag{3.80}$$

Next, we differentiate (3.65) with respect to time to obtain

$$(-\Delta)^{-1}\frac{\partial}{\partial t}\frac{\partial u}{\partial t} + P(-\Delta)\frac{\partial u}{\partial t} + f'(u)\frac{\partial u}{\partial t} = 0, \tag{3.81}$$

$$\frac{\partial u}{\partial t} = \Delta\frac{\partial u}{\partial t} = \cdots = \Delta^{k-1}\frac{\partial u}{\partial t} = 0 \text{ on } \Gamma. \tag{3.82}$$

Multiplying (3.82) by $\frac{\partial u}{\partial t}$, we find, employing (3.13) and the interpolation inequality (3.16),

$$\frac{\partial}{\partial t}\|\frac{\partial u}{\partial t}\|_{-1}^2 + c\|\frac{\partial u}{\partial t}\|_{H^k(\Omega)}^2 \leq c'\|\frac{\partial u}{\partial t}\|^2,$$

which yields, employing the interpolation inequality

$$\|v\|^2 \leq c\|v\|_{-1}\|\nabla v\|,\ v \in H_0^1\Omega, \tag{3.83}$$

the differential inequality

$$\frac{\partial}{\partial t}\|\frac{\partial u}{\partial t}\|_{-1}^2 \leq c\|\frac{\partial u}{\partial t}\|_{-1}^2. \tag{3.84}$$

It then follows from (3.71) (for $r = 1$), (3.84) and the uniform Gronwall's lemma that

$$\|\frac{\partial u}{\partial t}(t)\|_{-1}^2 \leq ce^{-c't}(\|u_0\|_{H^k(\Omega)}^2 + \int_\Omega F(u_0)dx) + c'',\ c' > 0,\ t \geq 1. \tag{3.85}$$

We finally deduce from (3.80) and (3.85) that

$$\|u(t)\|_{H^{2k}(\Omega)} \leq e^{-ct}Q(\|u_0\|_{H^k(\Omega)}) + c',\ c > 0,\ t \geq 1. \tag{3.86}$$

Remark 3.3.2. *We further assume that f is of class C^{k+1}. Multiplying (3.65) by $(-\Delta)^k\frac{\partial u}{\partial t}$, we have*

$$\frac{1}{2}\frac{\partial}{\partial t}(\sum_{i=1}^k a_i\|(-\Delta)^{\frac{i+k}{2}}u\|^2) + \|(-\Delta)^{\frac{k-1}{2}\frac{\partial u}{\partial t}}\|^2 = -(((-\Delta)^{\frac{k+1}{2}}f(u),(-\Delta)^{\frac{k-1}{2}}\frac{\partial u}{\partial t})),$$

which yields, noting that $\|(-\Delta)^{\frac{k+1}{2}}f(u)\|^2 \leq Q(\|u\|_{H^{k+1}(\Omega)})$ and owing to (3.78),

$$\frac{\partial}{\partial t}(\sum_{i=1}^k a_i\|(-\Delta)^{\frac{i+k}{2}}u\|^2) \leq e^{-ct}Q(\|u_0\|_{H^{k+1}(\Omega)}) + c',\ c > 0,\ t \geq 0. \tag{3.87}$$

It follows from the interpolation inequality (3.16) and (3.87) that

$$\|u(t)\|_{H^{2k}(\Omega)} \leq Q(\|u_0\|_{H^{2k}(\Omega)}),\ t \in [0,1],$$

so that, owing to (3.86),

$$\|u(t)\|_{H^{2k}(\Omega)} \leq e^{-ct}Q(\|u_0\|_{H^{2k}(\Omega)}) + c',\ c > 0,\ t \geq 0. \tag{3.88}$$

Second case. k=1.

We now consider the initial and boundary value problem (for simplicity, we take $a_1 = 1$)

$$(-\Delta)^{-1}\frac{\partial u}{\partial t} - \Delta u + f(u) = 0, \tag{3.89}$$

$$u = 0 \text{ on } \Gamma, \tag{3.90}$$

$$u|_{t=0} = u_0. \tag{3.91}$$

Differentiating (3.89) with respect to time, we have

$$(-\Delta)^{-1}\frac{\partial}{\partial t}\frac{\partial u}{\partial t} - \Delta\frac{\partial u}{\partial t} + f'(u)\frac{\partial u}{\partial t} = 0, \tag{3.92}$$

$$\frac{\partial u}{\partial t} = 0, \text{ on } \Gamma. \tag{3.93}$$

Multiplying (3.92) by $\frac{\partial u}{\partial t}$, we obtain, owing to (3.13),

$$\frac{1}{2}\frac{d}{dt}\|\frac{\partial u}{\partial t}\|_{-1}^2 + \|\nabla\frac{\partial u}{\partial t}\|^2 \le c_0\|\frac{\partial u}{\partial t}\|^2,$$

which yields, employing the interpolation inequality (3.83),

$$\frac{d}{dt}\|\frac{\partial u}{\partial t}\|_{-1}^2 \le c\|\frac{\partial u}{\partial t}\|_{-1}^2. \tag{3.94}$$

Let us assume that $u_0 \in H^3(\Omega) \cap H_0^1(\Omega)$. Then, noting that

$$(-\Delta)^{-\frac{1}{2}}\frac{\partial u}{\partial t}(0) = -(-\Delta)^{\frac{3}{2}}u_0 - (-\Delta)^{\frac{1}{2}}f(u_0),$$

we see that $(-\Delta)^{-\frac{1}{2}}\frac{\partial u}{\partial t}(0) \in L^2(\Omega)$ and

$$\|\frac{\partial u}{\partial t}(t)\|_{-1} \le Q(\|u_0\|_{H^3(\Omega)}). \tag{3.95}$$

It thus follows from (3.94)-(3.95) and Gronwall's lemma that

$$\|\frac{\partial u}{\partial t}(t)\|_{-1} \le e^{ct}Q(\|u_0\|_{H^3(\Omega)}),\ t \ge 0. \tag{3.96}$$

Rewriting then (3.89) as an elliptic equation, for $t > 0$ fixed,

$$-\Delta u + f(u) = -(-\Delta)^{-1}\frac{\partial u}{\partial t}(t),\ u = 0 \text{ on } \Gamma, \tag{3.97}$$

we find, multiplying (3.97) by $-\Delta u$ and employing (3.13),

$$\frac{1}{2}\|\Delta u\|^2 \le c_0\|\nabla u\|^2 + c\|\frac{\partial u}{\partial t}\|_{-1}^2. \tag{3.98}$$

We finally deduce from (3.70) (for $k = 1$), (3.96) and (3.98) that

$$\|u(t)\|_{H^2(\Omega)} \le e^{ct}Q(\|u_0\|_{H^3(\Omega)}),\ t \ge 0. \tag{3.99}$$

Actually, (3.99) is not satisfactory , in particular, in view of the study of attractors, and we can do better, namely, we can prove that $u_0 \in H^2(\Omega) \cap H_0^1(\Omega)$ suffices.

Indeed, multiplying (3.89) by $-\Delta\frac{\partial u}{\partial t}$, we have

$$\frac{d}{dt}\|\Delta u\|^2 + \|\frac{\partial u}{\partial t}\|^2 \le \|\Delta f(u)\|^2, \tag{3.100}$$

which yields, proceeding as above,

$$\frac{d}{dt}\|\Delta u\|^2 \le Q(\|\Delta u\|^2). \tag{3.101}$$

We set $y = \|\Delta u\|^2$ and consider the differential inequality

$$y' \le Q(y),\ y(0) = \|\Delta u_0\|^2. \tag{3.102}$$

Let z be a solution to the ODE

$$z' = Q(z),\ z(0) = y(0). \tag{3.103}$$

It follows from the comparison principle that there exists $T_0 = T_0(\|u_0\|_{H^2(\Omega)}) > 0$ (say, belonging to $(0, \frac{1}{2})$) such that

$$y(t) \le z(t),\ t \in [0, T_0], \tag{3.104}$$

hence

$$\|u(t)\|_{H^2(\Omega)} \le Q(\|u_0\|_{H^2(\Omega)}),\ t \in [0, T_0]. \tag{3.105}$$

Next, we multiply (3.92) by $t\frac{\partial u}{\partial t}$ and obtain, proceeding as above,

$$\frac{d}{dt}(t\|\frac{\partial u}{\partial t}\|_{-1}^2) \le ct\|\frac{\partial u}{\partial t}\|_{-1}^2 + \|\frac{\partial u}{\partial t}\|_{-1}^2. \tag{3.106}$$

It follows from (3.68) (for $k = 1$), (3.106) and Gronwall's lemma that

$$\|\frac{\partial u}{\partial t}(T_0)\|_{-1}^2 \le Q(\|u_0\|_{H^2(\Omega)}). \tag{3.107}$$

Then, we deduce from (3.94) and Gronwall's lemma (between T_0 and $t \ge T_0$) that

$$\|\frac{\partial u}{\partial t}(t)\|_{-1}^2 \le e^{c(t-T_0)}\|\frac{\partial u}{\partial t}(T_0)\|_{-1}^2,\ t \ge T_0,$$

so that

$$\|\frac{\partial u}{\partial t}(t)\|_{-1}^2 \le e^{ct}Q(\|u_0\|_{H^2(\Omega)}),\ t \ge T_0. \tag{3.108}$$

Returning to the elliptic problem (3.97) and to (3.98), we now find

$$\|u(t)\|_{H^2(\Omega)}^2 \le e^{ct}Q(\|u_0\|_{H^2(\Omega)}),\ t \ge T_0,$$

hence, owing to (3.105),

$$\|u(t)\|_{H^2(\Omega)} \leq e^{ct} Q(\|u_0\|_{H^2(\Omega)}),\ t \geq 0. \tag{3.109}$$

We can note that the above estimate is not dissipative, as its right-hand side goes to $+\infty$ as t goes to $+\infty$. In order to have a dissipative estimate, we now multiply (3.89) by $-\Delta u$, which gives, owing to (3.13),

$$\frac{1}{2}\frac{d}{dt}\|u\|^2 + \|\Delta u\|^2 \leq c_0\|\nabla u\|^2.$$

This yields, owing to (3.68) (for $k = 1$),

$$\int_0^1 \|\Delta u\|^2 ds \leq c(\|u_0\|^2_{H^1(\Omega)} + \int_\Omega F(u_0)dx) + c'. \tag{3.110}$$

There thus exists $T \in (0, 1)$ such that

$$\|u(T)\|^2_{H^2(\Omega)} \leq c(\|u_0\|^2_{H^1(\Omega)} + \int_\Omega F(u_0)dx) + c'. \tag{3.111}$$

Actually, repeating the above estimates (and employing, in particular, (3.109)), but starting from $t = T$ instead of $t = 0$, we obtain the smoothing property

$$\|u(1)\|^2_{H^2(\Omega)} \leq Q(\|u_0\|^2_{H^1(\Omega)} + \int_\Omega F(u_0)dx). \tag{3.112}$$

Repeating again the above estimates (leading to (3.112)), we find, for $t \geq 1$,

$$\|u(t)\|^2_{H^2(\Omega)} \leq Q(\|u(t-1)\|^2_{H^1(\Omega)} + \int_\Omega F(u(t-1))dx), \tag{3.113}$$

where the function Q does not depend on t (note indeed that (3.103) is an autonomous ODE and that the function Q in (3.113) is thus the same as that in (3.112)). Employing (3.68) (for $k = 1$), we finally deduce that

$$\|u(t)\|_{H^2(\Omega)} \leq e^{-ct} Q(\|u_0\|^2_{H^1(\Omega)} + \int_\Omega F(u_0)dx) + c',\ c > 0,\ t \geq 1, \tag{3.114}$$

hence a dissipative (and also smoothing) estimate.

3.3.2 The dissipative semigroup.

We have the

Theorem 3.3.1. *(i) We assume that* $u_0 \in \dot{H}^k(\Omega)$*, with* $\int_\Omega F(u_0)dx < +\infty$ *when* $k = 1$*. Then,* (3.65)-(3.67) *possesses a unique solution* u *such that,* $\forall T > 0$, $u(0) = u_0$,

$$u \in L^\infty(\mathbb{R}^+; \dot{H}^k(\Omega)) \cap L^2(0, T; \dot{H}^{2k}(\Omega)),$$

$$\frac{\partial u}{\partial t} \in L^2(0, T; H^{-1}(\Omega))$$

and

$$\frac{d}{dt}(((-\Delta)^{-1}u, v)) + \sum_{i=1}^{k} a_i(((-\Delta)^{\frac{i}{2}}u, (-\Delta)^{\frac{i}{2}}v)) + ((f(u), v)) = 0, \ v \in C_c^\infty(\Omega).$$

(ii) If we further assume that $u_0 \in \dot{H}^{k+1}(\Omega)$*, then*

$$u \in L^\infty(\mathbb{R}^+; \dot{H}^{k+1}(\Omega)).$$

(iii) If we further assume that f *is of class* C^{k+1} *and* $u_0 \in \dot{H}^{2k}(\Omega)$*, then*

$$u \in L^\infty(\mathbb{R}^+; \dot{H}^{2k}(\Omega)).$$

The proof of Theorem 3.3.1 is very similar to that of Theorem 3.2.1 ; we just mention that, in order to prove the continuous dependence (with respect to the initial data ; in the H^{-1}−norm here), we need to use the interpolation inequality (3.83).

Proceeding again as in the previous section, we also have the

Theorem 3.3.2. *The corresponding semigroup* $S(t)$ *possesses the global attractor* $\mathcal{A}$ *which is compact in* $L^2(\Omega)$ *and bounded in* Φ*, where* $\Phi = \dot{H}^{2k}(\Omega)$.

Remark 3.3.3. *Actually, the Cahn-Hilliard equation usually is associated with Neumann boundary conditions. In the case of the higher-order Cahn-Hilliard equation* (3.6)*, these read*

$$\frac{\partial u}{\partial \nu} = \frac{\partial \Delta u}{\partial \nu} = \cdots = \frac{\partial \Delta^k u}{\partial \nu} = 0 \text{ on } \Gamma,$$

where ν *denotes the unit outer normal vector. Integrating* (3.6) *over* Ω*, we note that we have the conservation of mass,*

$$\langle u(t) \rangle = \langle u_0 \rangle, \ t \geq 0, \tag{3.115}$$

where, for $v \in L^1(\Omega)$, $\langle v \rangle = \frac{1}{Vol(\Omega)} \int_\Omega v dx$*. We then rewrite* (3.6) *in the equivalent form*

$$(-\Delta)^{-1}\frac{\partial u}{\partial t} + P(-\Delta)u + f(u) - \langle f(u) \rangle = 0, \tag{3.116}$$

where, here, $(-\Delta)^{-1}$ is associated with Neumann boundary conditions and acts on functions with null spatial average. In particular,

$$v \mapsto (\|(-\Delta)^{-\frac{1}{2}}\bar{v}\|^2 + \langle v\rangle^2)^{\frac{1}{2}}$$

is a norm on $H^{-1}(\Omega) = H^1(\Omega)'$ which is equivalent to the usual $H^{-1}-$norm, where $\bar{v} = v - \langle v\rangle$ and being understood that, for $v \in H^{-1}(\Omega)$, $\langle v\rangle = \frac{1}{Vol(\Omega)}\langle v, 1\rangle_{H^{-1}(\Omega),H^1(\Omega)}$. We further consider the spaces

$$\dot{H}^m(\Omega) = \{v \in H^m(\Omega), \frac{\partial u}{\partial \nu} = \frac{\partial \Delta u}{\partial \nu} = \cdots = \frac{\partial \Delta^{[\frac{m-2}{2}]}u}{\partial \nu} = 0 \text{ on } \Gamma\},\ m \in \mathbb{N},\ m \geq 2$$

(we agree that $\dot{H}^1(\Omega) = H^1(\Omega)$), and note that

$$v \mapsto (\|(-\Delta)^{-\frac{m}{2}}\bar{v}\|^2 + \langle v\rangle^2)^{\frac{1}{2}}$$

is a norm on $\dot{H}^m(\Omega)$ which is equivalent to the usual H^m-norm. We can then derive a priori estimates which are similar to those obtained in the previous subsection. To do so, in view of the mass conservation (3.115), we assume that $|\langle u_0\rangle| \leq M$, $M \geq 0$ given. Furthermore, the most delicate step is to multiply (3.116) by $\bar{u} = u - \langle u_0\rangle$ and deal with the nonlinear terms. This is done by replacing (3.14) by

$$f(s)(s-\gamma) \geq c(\gamma)F(s) - c'(\gamma),\ c(\gamma) > 0,\ c'(\gamma) \geq 0,\ s \in \mathbb{R},\ \gamma \in \mathbb{R}, \tag{3.117}$$

where the constants $c(\gamma)$ and $c'(\gamma)$ depend continuously on γ. Note that this assumption is satisfied by the usual cubic nonlinear term $f(s) = s^3 - s$.The other estimates are obtained by proceeding as in the previous subsections. Note however that the constants depend in general on M. Furthermore, in order to have compact attractors, we have to work on subspaces of the phase space on which $|\langle u_0\rangle| \leq M$ (see, e.g., [127] in the case of the classical Cahn-Hilliard equation).

Chapitre 4

Higher-order Allen-Cahn models with logarithmic nonlinear terms

Modèles d'Allen-Cahn d'ordre élevé avec des termes non linéaires logarithmiques

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Higher-order Allen-Cahn models with logarithmic nonlinear terms

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Abstract : Our aim in this paper is to study higher-order (in space) Allen-Cahn models with logarithmic nonlinear terms. In particular, we obtain well-posedness results, as well as the existence of the global attractor.

Key words and phrases : Allen-Cahn equation, higher-order models, logarithmic nonlinear terms, well-posedness, global attractor.
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4.1 Introduction

The Allen-Cahn equation describes the ordering of atoms during the phase separation of a binary alloy (see [4]) and reads

$$\frac{\partial u}{\partial t} - \alpha \Delta u + f(u) = 0, \ \alpha > 0. \tag{4.1}$$

We studied in [32] generalizations of (4.1) of the form

$$\frac{\partial u}{\partial t} + P(-\Delta)u + f(u) = 0, \tag{4.2}$$

where $P(s) = \sum_{i=1}^{k} a_i s^i$, $a_k > 0$, $k \geq 1$; in particular, when $k = 1$, we recover the Allen-Cahn equation (4.1) and, when $k = 2$, the model contains the Swift-Hohenberg equation (see [96] and [99]). Such higher-order (in space) terms were proposed in [23] in the context of phase transition models and in the isotropic limit of more general higher-order terms (also note that a second-order term in phase separation is obtained by truncation of higher-order ones (see [20])).

In [32], we considered regular nonlinear terms (a typical choice is the usual cubic nonlinear term $f(s) = s^3 - s$). It is however important to note that, in phase separation, such a regular nonlinear term actually is an approximation of thermodynamically relevant logarithmic ones of the form $f(s) = -\lambda_1 s + \frac{\lambda_2}{2} \ln \frac{1+s}{1-s}$, $s \in (-1, 1)$, $0 < \lambda_2 < \lambda_1$, which follow from a mean-field model (see [20] and [36] ; in particular, the logarithmic terms correspond to the entropy of mixing).

The study of the classical Allen-Cahn equaiton (4.1) (i.e., $k = 1$ in (4.2)) with logarithmic nonlinear terms is well established (see, e.g., [94]). However, when $k \geq 2$ in (4.2), the situation is much more involved and we are not able to prove the existence of a solution in a classical sense (meaning in a classical weak/variational sense). Nevertheless, we are able to prove the existence of a (weaker) variational solution. This notion of a variational solution was introduced in [104] for the Cahn-Hilliard equation with singular nonlinear terms and dynamic boundary conditions and is based on a variational inequality (see also [70] for a different, though related, approach based on duality techniques). It was also applied with success in other situations in [29], [30], [96] and [99].

Our aim in this paper is to study the well-posedness of (4.2) with a logarithmic nonlinear term in the variational sense mentioned above. We also prove the dissipativity of the corresponding solution operator, as well as the existence of the global attractor.

4.2 Setting of the problem

We consider the following initial and boundary value problem in a bounded and regular domain $\Omega \subset \mathbb{R}^n$, $n = 1,\ 2$ or 3, with boundary Γ :

$$\frac{\partial u}{\partial t} + P(-\Delta)u + f(u) = 0, \tag{4.3}$$

$$u = \Delta u = \cdots = \Delta^{k-1} u = 0, \text{ on } \Gamma, \tag{4.4}$$

$$u|_{t=0} = u_0. \tag{4.5}$$

We assume that the polynomial P is defined by

$$P(s) = \sum_{i=1}^{k} a_i s^i,\ a_k > 0,\ k \geq 1,\ s \in \mathbb{R}. \tag{4.6}$$

As far as the nonlinear term f is concerned, we assume that

$$f(s) = -\lambda_1 s + \frac{\lambda_2}{2}\ln\frac{1+s}{1-s}, \ s\in(-1,1), \ 0<\lambda_2<\lambda_1. \tag{4.7}$$

In particular, it is not difficult to show that it satisfies the following properties :

$$f\in C^\infty(-1,1), \ f(0)=0, \tag{4.8}$$

$$\lim_{s\to\pm1} f = \pm\infty, \ \lim_{s\to\pm1} f' = +\infty, \tag{4.9}$$

$$f' \geq -\lambda_1, \tag{4.10}$$

$$-c_1 \leq F(s) + \frac{1}{2}|f(s)| \leq f(s)s + c_2, \ c_2\geq 0, \ s\in(-1,1), \tag{4.11}$$

where $F(s) = \int_0^s f(\xi)d\xi$. We can also note that F is bounded on $(-1,1)$; indeed, there holds

$$F(s) = -\frac{\lambda_1}{2}s^2 + \frac{\lambda_2}{2}((1+s)\ln(1+s) + (1-s)\ln(1-s)). \tag{4.12}$$

Remark 4.2.1. *We can note that all properties above easily follow from the explicit expression of f. Actually,* (4.10)-(4.11) *follow from* (4.8)-(4.9)*. The only difficulty here is to prove that $F(s) \leq f(s)s + c_2$, $c_2 \geq 0$, $s \in (-1,1)$. To do so, it suffices to study the variations of the function $s \mapsto f(s)s - F(s) + \frac{\lambda_1}{2}s^2$, whose derivative has, owing to* (4.10)*, the sign of s. We can thus consider more general singular nonlinear terms only satisfying* (4.8)-(4.9)*. Indeed, the boundedness of F is not necessary and just allows us to consider more general initial data.*

Setting

$$F(s) = -\frac{\lambda_1}{2}s^2 + F_1(s),$$

we introduce the following approximated functions $F_{1,N}\in C^4(\mathbb{R})$, $N\in\mathbb{N}$:

$$F_{1,N}(s) = \begin{cases} \sum_{i=0}^{4}\frac{1}{i!}F_1^{(i)}(1-\frac{1}{N})(s-1+\frac{1}{N})^i, \ s\geq 1-\frac{1}{N}, \\ F_1(s), \ |s|\leq 1-\frac{1}{N}, \\ \sum_{i=0}^{4}\frac{1}{i!}F_1^{(i)}(-1+\frac{1}{N})(s+1-\frac{1}{N})^i, \ s\leq -1+\frac{1}{N}. \end{cases} \tag{4.13}$$

Setting $F_N(s) = -\frac{\lambda_1}{2}s^2 + F_{1,N}(s)$, $f_{1,N} = F'_{1,N}$ and $f_N = F'_N$, there holds

$$f_N \in C^3(\mathbb{R}),\ f_N(0) = 0, \tag{4.14}$$

$$f'_{1,N} \geq 0,\ f'_N \geq -\lambda_1, \tag{4.15}$$

$$F_N \geq -c_3,\ c_3 \geq 0, \tag{4.16}$$

$$F_N(s) \geq c_4 s^4 - c_5,\ c_4 > 0,\ c_5 \geq 0,\ s \in \mathbb{R}, \tag{4.17}$$

$$f_N(s)s \geq c_6(F_N(s) + |f_N(s)|) - c_7,\ c_6 > 0,\ c_7 \geq 0,\ s \in \mathbb{R}. \tag{4.18}$$

Furthermore, all constants can be chosen independently of N. These properties follow from the fact that we have similar properties for the original singular nonlinear term and from the explicit expression of $F_{1,N}$; we refer the reader to [49], [102] and [104] for more details. We can also note that F_N is bounded, independently of N, in the neighborhood of ± 1.

We then consider the approximated problems

$$\frac{\partial u^N}{\partial t} + P(-\Delta)u^N + f_N(u^N) = 0, \tag{4.19}$$

$$u^N = \Delta u^N = \cdots = \Delta^{k-1} u^N = 0,\ \text{on } \Gamma, \tag{4.20}$$

$$u^N|_{t=0} = u_0. \tag{4.21}$$

The existence, uniqueness and regularity of the solution u^N to (4.19)-(4.21) were proved in [32].

4.2.1 Notations

We denote by $((\cdot,\cdot))$ the usual L^2-scalar product, which associated norm $\|\cdot\|$. More generally, $\|\cdot\|_X$ denotes the norm on the Banach space X.

We then consider the operator $-\Delta$ associated with Dirichlet boundary conditions ; it is a strictly positive, selfadjoint and unbounded linear operator with compact inverse $(-\Delta)^{-1}$, with domain $H^2(\Omega) \cap H^1_0(\Omega)$. In particular, this allows us (see, e.g., [127]) to define the operators $(-\Delta)^m$, $m \in \mathbb{R}$ (being understood that, when $m = 0$, then $(-\Delta)^0$ is the identity operator). For $m \in \mathbb{N}$, $(-\Delta)^m$ has for domain $\{v \in H^{2m}(\Omega),\ v = \Delta v = \cdots = \Delta^{m-1} v = 0 \text{ on } \Gamma\}$. We set, for $m \in \mathbb{N}$,

$$\dot{H}^m(\Omega) = v \in H^m(\Omega), v = \Delta v = \cdots = \Delta^{[\frac{m-1}{2}]} v = 0 \text{ on } \Gamma,$$

where $[\cdot]$ denotes the integer part. This space, endowed with the usual H^m-norm, is a closed subspace of $H^m(\Omega)$. Furthermore, $v \mapsto \|(-\Delta)^{\frac{m}{2}} v\|$ is a norm on $\dot{H}^m(\Omega)$ which is equivalent to the usual H^m-norm.

Throughout the paper, the same letters c, c' and c'' denote (generally positive) constants which may vary from line to line and are independent of N. Similarly, the same letter Q denotes (positive) monotone increasing and continuous functions which may vary from line to line and are independent of N.

4.3 A priori estimates

Our aim in this section is to derive uniform (with respect to N) a priori estimates on u^N which will allow us, in the next section, to pass to the limit $N \to +\infty$ and prove the existence of a solution to the original singular problem, in a suitable setting (i.e., as mentioned in the introduction, based on a proper variational inequality).

Though formal, these a priori estimates can be fully justified in view of the regularity results obtained in [32].

We assume from now on that $-1 < u_0(x) < 1$ a.e. $x \in \Omega$.

Remark 4.3.1. *For a more general singular nonlinear term f, we would need a stronger separation property from the singular values ± 1, namely, $\|u_0\|_{L^\infty(\Omega)} < 1$.*

We multiply (4.19) by $\frac{\partial u^N}{\partial t}$ and have, integrating over Ω and by parts,

$$\frac{d}{dt}\Big(\sum_{i=1}^{k} a_i \|(-\Delta)^{\frac{i}{2}} u^N\|^2 + 2\int_\Omega F_N(u^N)dx\Big) + 2\|\frac{\partial u^N}{\partial t}\|^2 = 0. \tag{4.22}$$

We then multiply (4.19) by u^N to obtain

$$\frac{1}{2}\frac{d}{dt}\|u^N\|^2 + \sum_{i=1}^{k} a_i \|(-\Delta)^{\frac{i}{2}} u^N\|^2 + ((f_N(u^N), u^N)) = 0. \tag{4.23}$$

Employing the interpolation inequality

$$\|(-\Delta)^{\frac{i}{2}} v\| \le c(i)\|(-\Delta)^{\frac{m}{2}} v\|^{\frac{i}{m}} \|v\|^{1-\frac{i}{m}}, \ v \in \dot{H}^m(\Omega), \ i \in \{1, \dots, m-1\}, \ m \in \mathbb{N}, \ m \ge 2, \tag{4.24}$$

from which it follows that, for $i \in \{1, \dots, k-1\}$ and $k \ge 2$,

$$\|(-\Delta)^{\frac{i}{2}} u^N\|^2 \le \epsilon \|(-\Delta)^{\frac{k}{2}} u^N\|^2 + c(i,\epsilon)\|u^N\|^2, \ \forall \epsilon > 0, \tag{4.25}$$

(4.18), (4.23) and (4.25) yield

$$\frac{d}{dt}\|u^N\|^2 + c(\|u^N\|^2_{H^k(\Omega)} + \int_\Omega F_N(u^N)dx + \|f_N(u^N)\|_{L^1(\Omega)}) \le c'(\|u^N\|^2 + 1), \ c > 0. \tag{4.26}$$

Noting finally that

$$\|u^N\|^2 \le \epsilon \|u^N\|^4_{L^4(\Omega)} + c(\epsilon), \ \forall \epsilon > 0, \tag{4.27}$$

we deduce from (4.17) and (4.26)-(4.27) that

$$\frac{d}{dt}\|u^N\|^2 + c(\|u^N\|^2_{H^k(\Omega)} + \int_\Omega F_N(u^N)dx + \|f_N(u^N)\|_{L^1(\Omega)}) \le c',\ c > 0, \tag{4.28}$$

Summing (4.22) and (4.28), we find, noting that $\sum_{i=1}^k a_i\|(-\Delta)^{\frac{i}{2}}u^N\|^2 \le c\|u^N\|^2_{H^k(\Omega)}$, a differential inequality of the form

$$\frac{dE_{1,N}}{dt} + c(E_{1,N} + \|f_N(u^N)\|_{L^1(\Omega)} + \|\frac{\partial u^N}{\partial t}\|^2) \le c',\ c > 0, \tag{4.29}$$

where

$$E_{1,N} = \sum_{i=1}^k a_i\|(-\Delta)^{\frac{i}{2}}u^N\|^2 + 2\int_\Omega F_N(u^N)dx + \|u^N\|^2$$

satisfies

$$E_{1,N} \ge c(\|u^N\|^2_{H^k(\Omega)} + \int_\Omega F_N(u^N)dx) - c',\ c > 0. \tag{4.30}$$

Indeed, it follows from the interpolation inequality (4.24) that

$$E_{1,N} \ge c(\|u^N\|^2_{H^k(\Omega)} + \int_\Omega F_N(u^N)dx) - c'\|u^N\|^2 - c''$$

and we conclude by employing (4.17) and (4.27).

We then multiply (4.19) by $-\Delta u^N$ and have, owing to (4.15),

$$\frac{d}{dt}\|\nabla u^N\|^2 + 2\sum_{i=1}^k a_i\|(-\Delta)^{\frac{i+1}{2}}u^N\|^2 \le 2\lambda_1\|\nabla u^N\|^2. \tag{4.31}$$

Summing (4.29) and δ_1 time (4.31), where $\delta_1 > 0$ is small enough, we obtain, employing once more the interpolation inequality (4.24), a differential inequality of the form

$$\frac{dE_{2,N}}{dt} + c(E_{2,N} + \|u^N\|^2_{H^{k+1}(\Omega)} + \|f_N(u^N)\|_{L^1(\Omega)} + \|\frac{\partial u^N}{\partial t}\|^2) \le c',\ c > 0, \tag{4.32}$$

where

$$E_{2,N} = E_{1,N} + \delta_1\|\nabla u^N\|^2$$

satisfies

$$E_{2,N} \ge c(\|u^N\|^2_{H^k(\Omega)} + \int_\Omega F_N(u^N)dx) - c',\ c > 0. \tag{4.33}$$

In particular, it follows from (4.32)-(4.33) and Gronwall's lemma that

$$\|u^N(t)\|^2_{H^k(\Omega)} \le ce^{-c't}(\|u_0\|^2_{H^k(\Omega)} + \int_\Omega F_N(u_0)dx) + c'',\ c' > 0,\ t \ge 0, \tag{4.34}$$

and

$$\int_t^{t+r} (\|u^N\|^2_{H^{k+1}(\Omega)} + \|\frac{\partial u^N}{\partial t}\|^2)ds \le ce^{-c't}(\|u_0\|^2_{H^k(\Omega)} + \int_\Omega F_N(u_0)dx) + c''(r),\ c' > 0,\ t \ge 0, \tag{4.35}$$

$r > 0$ given. Actually, noting that $F_N(u_0)$ is bounded (independently of N and u_0), there holds

$$\|u^N(t)\|^2_{H^k(\Omega)} \le ce^{-c't}\|u_0\|^2_{H^k(\Omega)} + c'',\ c' > 0,\ t \ge 0, \tag{4.36}$$

and

$$\int_t^{t+r} (\|u^N\|^2_{H^{k+1}(\Omega)} + \|\frac{\partial u^N}{\partial t}\|^2)ds \le ce^{-c't}\|u_0\|^2_{H^k(\Omega)} + c''(r),\ c' > 0,\ t \ge 0,\ r > 0 \text{ given.} \tag{4.37}$$

We now differentiate (4.3) with respect to time to find

$$\frac{\partial}{\partial t}\frac{\partial u^N}{\partial t} + P(-\Delta)\frac{\partial u^N}{\partial t} + f_N'(u^N)\frac{\partial u^N}{\partial t} = 0, \tag{4.38}$$

$$\frac{\partial u^N}{\partial t} = \Delta\frac{\partial u^N}{\partial t} = \cdots = \Delta^{k-1}\frac{\partial u^N}{\partial t} = 0 \text{ on } \Gamma, \tag{4.39}$$

$$\frac{\partial u^N}{\partial t}|_{t=0} = -P(-\Delta)u_0 - f_N(u_0). \tag{4.40}$$

Multiplying (4.38) by $\frac{\partial u^N}{\partial t}$, we have, employing (4.15) and the interpolation inequality (4.24),

$$\frac{d}{dt}\|\frac{\partial u^N}{\partial t}\|^2 \le c\|\frac{\partial u^N}{\partial t}\|^2. \tag{4.41}$$

It then follows from (4.37), say, for $r = 1$, and the uniform Gronwall's lemma (see, e.g., [127]) that

$$\|\frac{\partial u^N}{\partial t}(t)\|^2 \le ce^{-c't}\|u_0\|^2_{H^k(\Omega)} + c'',\ c > 0,\ t \ge 1. \tag{4.42}$$

Remark 4.3.2. *(i) Actually, it follows from the uniform Gronwall's lemma that*

$$\|\frac{\partial u^N}{\partial t}(t+r)\|^2 \leq \frac{c(r)}{r}e^{-c't}\|u_0\|^2_{H^k(\Omega)} + c''(r),\ c'>0,\ t\geq 0,\ r>0 \text{ given}. \tag{4.43}$$

(ii) We assume that $\|u_0\|_{L^\infty(\Omega)} \leq 1$. *We can note that, if* $u_0 \in H^{2k}(\Omega)$*, then* $\frac{\partial u^N}{\partial t}(0) \in L^2(\Omega)$ *and it follows from the continuity of* f *and the continuous embedding* $H^{2k}(\Omega) \subset C(\bar{\Omega})$ *that, for N large enough (note that* $f_{1,N}$ *coincides with* $f_1 = F_1'$ *when* $|s| \leq 1 - \frac{1}{N}$*),*

$$\|\frac{\partial u^N}{\partial t}(0)\| \leq Q(\|u_0\|_{H^{2k}(\Omega)}). \tag{4.44}$$

It then follows from (4.41) *and Gronwall's lemma that*

$$\|\frac{\partial u^N}{\partial t}(t)\| \leq e^{ct}Q(\|u_0\|_{H^{2k}(\Omega)}),\ t\geq 0. \tag{4.45}$$

Collecting (4.42) *and* (4.45) *(for* $t \in [0,1]$*), we finally deduce that*

$$\|\frac{\partial u^N}{\partial t}(t)\| \leq e^{-ct}Q(\|u_0\|_{H^{2k}(\Omega)}) + c',\ c>0,\ t\geq 0. \tag{4.46}$$

We finally rewrite (4.19) as an elliptic equation, for $t > 0$ fixed,

$$P(-\Delta)u^N + f_N(u^N) = -\frac{\partial u^N}{\partial t},\ u^N = \Delta u^N = \cdots = \Delta^{k-1}u^N = 0 \text{ on } \Gamma. \tag{4.47}$$

Multiplying (4.47) by $-\Delta u^N$, we find, owing to (4.15) and employing the interpolation inequality (4.24),

$$\|u^N\|^2_{H^{k+1}(\Omega)} \leq c(\|\frac{\partial u^N}{\partial t}\|^2 + \|u^N\|^2_{H^1(\Omega)}),$$

which yields, owing to (4.36) and (4.42),

$$\|u^N(t)\|^2_{H^{k+1}(\Omega)} \leq ce^{-c't}\|u_0\|^2_{H^k(\Omega)} + c'',\ c'>0,\ t\geq 1. \tag{4.48}$$

Remark 4.3.3. *We assume that* $\|u_0\|_{L^\infty(\Omega)} < 1$. *There also holds, owing to* (4.46) *and for N large enough,*

$$\|u^N(t)\|^2_{H^{k+1}(\Omega)} \leq e^{-ct}Q(\|u_0\|_{H^{2k}(\Omega)}) + c',\ c>0,\ t\geq 0. \tag{4.49}$$

Of course, we have a similar H^{2k}*−estimate on* u^N *(see [32]), but, in that case, the constants and the function* Q *a priori depend on N.*

4.4 The dissipative semigroup

We assume in this section that $k \geq 2$. For $k = 1$, i.e., for the classical Allen-Cahn equation, one can prove the existence (and the uniqueness) of a classical (strong) solution u, owing to the fact that u is strictly separated from the singular values ± 1, meaning that we essentially have to deal with a regular (and even bounded) nonlinear term (see [94]).

Our main aim is to prove the existence (and uniqueness) of solutions to (4.3)-(4.5) in a suitable sense, namely, based on a variational inequality.

To do so, we first derive a variational inequality from (4.3). In this regard, we multiply this equation by $u - v$, where $v = v(x)$ is smooth enough and satisfies $v = \Delta v = \cdots = \Delta^{k-1} v = 0$ on Γ. We then have, recalling that $f(s) = f_1(s) - \lambda_1 s$, $s \in (-1, 1)$,

$$((\frac{\partial u}{\partial t}, u - v)) + \sum_{i=1}^{k} a_i(((-\Delta)^{\frac{i}{2}} u, (-\Delta)^{\frac{i}{2}}(u - v))) + ((f_1(u), u - v)) - \lambda_1((u, u - v)) = 0.$$

Noting that f_1 is monotone increasing, this yields the variational inequality

$$((\frac{\partial u}{\partial t}, u-v)) + \sum_{i=1}^{k} a_i(((-\Delta)^{\frac{i}{2}} u, (-\Delta)^{\frac{i}{2}}(u-v))) + ((f_1(u), u-v)) - \lambda_1((u, u-v)) \leq 0, \quad (4.50)$$

i.e., the nonlinear term now acts on the test functions rather than on the solutions.

Based on this, we give the following definition (see also [104]) :

Definition 4.4.1. We assume that $u_0 \in \dot{H}^k(\Omega)$, with $-1 < u_0(x) < 1$ a.e. $x \in \Omega$. Then $u = u(t, x)$ is a variational solution to (4.3)-(4.5) if, for all $T > 0$,
(i) $-1 < u(t, x) < 1$ a.e. (t, x),
(ii) $u \in C([0, T]; L^2(\Omega)) \cap L^\infty(0, T; \dot{H}^k(\Omega)) \cap L^2(0, T; \dot{H}^{k+1}(\Omega))$,
(iii) $\frac{\partial u}{\partial t} \in L^2(0, T; L^2(\Omega))$,
(iv) $f_1(u) \in L^1((0, T) \times \Omega)$,
(v) $u(0) = u_0$,
(vi) the variational inequality (4.50) is satisfied for every $t > 0$ and every test function $v = v(x)$ such that $v \in \dot{H}^k(\Omega)$, with $f_1(v) \in L^1(\Omega)$.

We first prove the uniqueness of variational solutions. To do so, we need to define as admissible test functions the solutions temselves, i.e., we need to define admissible time-dependent test functions. More precisely, we can admissible any function $v = v(t, x)$ such that $v \in C([0, T]; L^2(\Omega)) \cap L^\infty(0, T; \dot{H}^k(\Omega)) \cap L^2(0, T; \dot{H}^{k+1}(\Omega))$, $f_1(v) \in L^1((0, T) \times \Omega)$ and $\frac{\partial u}{\partial t} \in L^2(0, T; L^2(\Omega))$, $\forall T > 0$.

Next, we write (4.50) for $v = v(t, \cdot)$, for almost every $t > 0$. Noting that, owing to the regularity assumptions on u and v, all terms are L^1 with respect to time, we can integrate with respect to time to obtain

$$\int_s^t [((\frac{\partial u}{\partial t}, u-v)) + \sum_{i=1}^{k} a_i(((-\Delta)^{\frac{i}{2}} u, (-\Delta)^{\frac{i}{2}}(u-v))) + ((f_1(v), u-v)) - \lambda_1((u, u-v))]d\xi \leq 0, \tag{4.51}$$

for all $0 < s < t$ and for every admissible test function $v = v(t, x)$. In particular, since $H^k(\Omega) \subset C(\bar{\Omega})$, $k \geq 2$, then it follows from the above regularity that $((f_1(u), u - v)) \in L^1(\Omega)$, $\forall T > 0$.

Remark 4.4.1. *We can replace (4.50) by (4.51) in Definition 4.4.1, (vi).*

We will actually need a second variational inequality. To do so, let $w = w(t, x)$ be an admissible test function and set

$$v_\eta = (1 - \eta)u + \eta w, \ \eta \in (0, 1].$$

Noting that

$$f_1''(s)\text{sgn}(s) \geq 0, \ s \in (-1, 1), \tag{4.52}$$

it follows that $|f_1|$ is convex, so that

$$|f_1(v_\eta)| \leq |f_1(u)| + |f_1(w)|. \tag{4.53}$$

This yields that $f_1(v_\eta) \in L^1((0, T) \times \Omega)$ and v_η is an admissible test function. Taking $v = v_\eta$ in (4.51) and dividing by η, we find

$$\int_s^t [((\frac{\partial u}{\partial t}, u-w)) + \sum_{i=1}^{k} a_i(((-\Delta)^{\frac{i}{2}} u, (-\Delta)^{\frac{i}{2}}(u-w))) + ((f_1(v_\eta), u-w)) - \lambda_1((u, u-w))]d\xi \leq 0.$$

Passing finally to the limit $\eta \to 0$ and employing Lebesgue's dominated convergence theorem (see (4.53)), we have

$$\int_s^t [((\frac{\partial u}{\partial t}, u-w)) + \sum_{i=1}^{k} a_i(((-\Delta)^{\frac{i}{2}} u, (-\Delta)^{\frac{i}{2}}(u-w))) + ((f_1(u), u-w)) - \lambda_1((u, u-w))]d\xi \leq 0, \tag{4.54}$$

for all $0 < s < t$ and for every test function $w = w(t, x)$.

Let now u_1 and u_2 be two variational solutions with initial data $u_{1,0}$ and $u_{2,0}$, respectively. We take $u = u_1$ and $v = u_2$ in (4.51) and $u = u_2$ and $w = u_1$ in (4.54) and sum the two resulting inequalities. We obtain, after simplifications (recall that f_1 is monotone increasing) and noting that all terms are absolutely continuous from $[0,T]$ onto $L^2(\Omega)$,

$$\frac{1}{2}\|u_1(t)-u_2(t)\|^2-\frac{1}{2}\|u_1(s)-u_2(s)\|^2+\int_s^t(\sum_{i=1}^k\|(-\Delta)^{\frac{i}{2}}(u_1-u_2)\|^2-\lambda_1\|u_1-u_2\|^2)d\xi\leq 0. \tag{4.55}$$

Employing the interpolation inequality (4.24), we deduce that

$$\frac{1}{2}\|u_1(t)-u_2(t)\|^2-\frac{1}{2}\|u_1(s)-u_2(s)\|^2\leq c\int_s^t\|u_1-u_2\|^2d\xi,$$

so that, employing Gronwall's lemma,

$$\|u_1(t)-u_2(t)\|\leq e^{c(t-s)}\|u_1(s)-u_2(s)\|,$$

where the constant c is independent of t, s, u_1 and u_2. Passing finally to the limit $s\to 0$, we find

$$\|u_1(t)-u_2(t)\|\leq e^{ct}\|u_{1,0}-u_{2,0}\|,\ t\geq 0, \tag{4.56}$$

hence the uniqueness, as well as the continuous dependence with respect to the initial data in the L^2-norm.

We now have the

Theorem 4.4.1. *We assume that $u_0\in\dot{H}^k(\Omega)$, with $-1<u_0<1$ a.e. $x\in\Omega$. Then,* (4.3)-(4.5) *possesses a unique variational solution u.*

Proof. There remains to prove the existence of a variational solution. To do so, we consider the solution u_N to the approximated problem (4.19)-(4.21) (as already mentioned, the existence, uniqueness and regularity of u^N is known). Furthermore, proceeding as above, it is easy to see that u^N satisfies a variational inequality which is analogous to (4.51), namely,

$$\begin{aligned}\int_s^t[((\frac{\partial u^N}{\partial t},u^N-v))+\sum_{i=1}^k a_i(((-\Delta)^{\frac{i}{2}}u^N,(-\Delta)^{\frac{i}{2}}(u^N-v)))\\ +((f_{1,N}(v),u^N-v))-\lambda_1((u^N,u^N-v))]d\xi\leq 0,\end{aligned} \tag{4.57}$$

for all $0<s<t$ and for every admissible test function $v=v(t,x)$.

It then follows from the uniform (with respect to N) a priori estimates derived in the previous section (which are fully justified at this stage) that, up to a subsequence, u^N converges to a limit function u such that, $\forall T>0$,

$$u^N \to u \text{ in } \mathrm{L}^\infty(0,\mathrm{T};\mathrm{H}^\mathrm{k}(\Omega)) \text{ weak} - \star \text{ and in } \mathrm{L}^2(0,\mathrm{T};\mathrm{H}^{\mathrm{k}+1}(\Omega)) \text{ weak},$$

$$\frac{\partial u^N}{\partial t} \to \frac{\partial u}{\partial t} \text{ in } \mathrm{L}^2(0,\mathrm{T};\mathrm{L}^2(\Omega)) \text{ weak},$$

$$u^N \to u \text{ in } C([0,\mathrm{T}];\mathrm{H}^{\mathrm{k}-\epsilon}(\Omega)), \mathrm{L}^2(0,\mathrm{T};\mathrm{H}^{\mathrm{k}+1-\epsilon}(\Omega)) \text{ and a.e. in } (0,\mathrm{T})\times\Omega,\ \epsilon > 0.$$

Our aime is to pass to the limit in (4.57). We can note that the above convergences allow us to pass to the limit in all terms in (4.57), except in the nonlinear term $\int_s^t ((f_{1,N}(v), u^N - v))d\xi$. To pass to the limit in the nonlinear term, we can note that, by construction,

$$|f_{1,N}(v)| \leq |f_1(v)|$$

and we are in a position to use Lebesgue's dominated convergence theorem (recall that, since v is an admissible test function, then $f_1(v) \in L^1((0,T)\times\Omega)$; also note that u and v belong to $L^\infty((0,T)\times\Omega)$).

We now need to prove the separation property (i). To do so, we note that, owing to (4.29)-(4.30), $f_{1,N}(u^N)$ is uniformly (with respect to N) bounded in $L^1((0,T)\times\Omega)$. Then, owing to the explicit expression of $f_{1,N}$, we have

$$\mathrm{meas}\{(\mathrm{t},\mathrm{x}) \in (0,\mathrm{T})\times\Omega, |\mathrm{u}^\mathrm{M}(\mathrm{t},\mathrm{x})| > 1 - \frac{1}{\mathrm{N}}\} \leq \frac{\mathrm{c}}{\mathrm{f}_1(1-\frac{1}{\mathrm{N}})},\ \mathrm{M} \geq \mathrm{N}, \tag{4.58}$$

where the constant c is independent of $M \geq N$ and N (note that f_1 and $f_{1,N}$ are odd functions). Indeed, there holds

$$\int_0^T \int_\Omega |f_{1,M}(u^M)|dxdt \geq \int_{E_{N,M}} |f_{1,M}(u^M)|dxdt \geq c'\mathrm{meas}(\mathrm{E}_{\mathrm{N},\mathrm{M}})\mathrm{f}_1(1-\frac{1}{\mathrm{N}}),$$

where

$$E_{N,M} = \{(t,x) \in (0,T)\times\Omega, |u^M(t,x)| > 1 - \frac{1}{N}\},$$

the constant c' being independent of N and M. Passing to the limit $M \to +\infty$ (employing Fatou's Lemma) and then $N \to +\infty$ (noting that $f_1(1-\frac{1}{N}) \to +\infty$ as $N \to +\infty$) in (4.58), it follows that

$$\mathrm{meas}\{(\mathrm{t},\mathrm{x}) \in (0,\mathrm{T})\times\Omega, |\mathrm{u}(\mathrm{t},\mathrm{x})| \geq 1\} = 0, \tag{4.59}$$

hence the separation property.

In order to complete the proof of existence, there remains to prove (iv). To do so, we note that it follows from the almost everywhere convergence of u^N to u, the separation property (i) and the explicit expression of $f_{1,N}$ again that

$$f_{1,N}(u^N) \to f_1(u) \text{ a.e. in } (0,\mathrm{T}) \times \Omega.$$

Then, we deduce from Fatou's lemma that

$$\|f(u)\|_{L^1((0,T)\times\Omega)} \leq \liminf \|f_N(u^N)\|_{L^1((0,T)\times\Omega)} < +\infty,$$

which finishes the proof of existence. □

Remark 4.4.2. *A natural question is whether a solution in the sense of Definition 4.4.1 is a classical variational solution (i.e., it satisfies a variational equality instead of a variational inequality). To prove this, one solution is to obtain a uniform (with respect to N) bound on $f_{1,N}(u^N)$ in $L^p((0,T)\times\Omega)$, for some $p > 1$ (and not just for $p = 1$). Unfortunately, we have not been able to derive such an estimate when $k \geq 2$, so that the question of whether a variational solution is a classical (variational) one is an open problem.*

It follows from Theorem 4.4.1 that we can define the family of operators $S(t) : \Phi \to \Phi, u_0 \mapsto u(t), t \geq 0$, where

$$\Phi = \{v \in \dot{H}^k(\Omega), -1 < v(x) < 1 \text{ a.e. } x \in \Omega\}.$$

This family of operators forms a semigroup (i.e., $S(0) = I$ (identity operator) and $S(t+\tau) = S(t) \circ S(\tau)$, $t, \tau \geq 0$) which is , owing to (4.56), continuous in the L^2-topology. Furthermore, it follows from (4.36) (which also holds in the limit $N \to +\infty$) that this semigroup is dissipative, in the sense that it possesses a bounded absorbing set $\mathcal{B}_0 \subset \Phi$ (i.e., $\forall B \subset \Phi$ bounded, $\exists t_0 = t_0(B) \geq 0$ such that $t \geq t_0 \Longrightarrow S(t)B \subset \mathcal{B}_0$).

It then follows from (4.56) that we can actually extend (in a unique way and by continuity) $S(t)$ to the closure of Φ in the L^2-topology, namely,

$$S(t) : \Phi_1 \to \Phi_1, \ t \geq 0,$$

where

$$\Phi_1 = \{v \in L^\infty, \|v\|_{L^\infty(\Omega) \leq 1}\}.$$

It also follows from the a priori estimates derived in the previous section that $S(t)$ instantaneously regularizes, i.e.,

$$S(t) : \Phi_1 \to \Phi, \ t > 0,$$

and that it possesses a bounded absorbing set $\mathcal{B}_1$ which is compact in $L^2(\Omega)$ and bounded in $H^{k+1}(\Omega)$. We thus deduce from standard results (see, e.g., [103] and [127]) that we have the

Theorem 4.4.2. *The semigroup $S(t)$ possesses the global attractor $\mathcal{A}$ which is compact in $L^2(\Omega)$ and bounded in $H^{k+1}(\Omega)$.*

Remark 4.4.3. *We recall that the global attractor $\mathcal{A}$ is the smallest (for the inclusion) compact set of the phase space which is invariant by the flow (i.e., $S(t)\mathcal{A} = \mathcal{A}$, $\forall t \geq 0$) and attracts all bounded sets of initial data as time goes to infinity ; it thus appears as a suitable object in view of the study of the asymptotic behavior of the system. We refer the reader to, e.g., [103] and [127] for more details and discussions on this.*

Remark 4.4.4. *An important question is whether the global attractor $\mathcal{A}$ has finite dimension, in the sense of covering dimensions such as the Hausdorff and the fractal dimensions. The finite-dimensionality means, very roughly speaking, that, even though the initial phase space has infinite dimension, the reduced dynamics can be described by a finite number of parameters (we refer the interested reader to, e.g., [103] and [127] for discussions on this subject). When $k = 1$, i.e., for the classical Allen-Cahn equation, this can easily be established, owing again to the strict separation from the singular values ± 1 (see, e.g., [94]). However, when $k \geq 2$, the situation is much more involved and one idea could be to proceed as in [104]. This will be addressed elsewhere.*

Remark 4.4.5. *We can adapt the above analysis to the higher-order Cahn-Hilliard model*

$$(-\Delta)^{-1}\frac{\partial u}{\partial t} + P(-\Delta)u + f(u) = 0, \tag{4.60}$$

$$u = \Delta u = \cdots = \Delta^{k-1}u = 0, \text{ on } \Gamma, \tag{4.61}$$

$$u|_{t=0} = u_0. \tag{4.62}$$

where P and f are as above. In particular, for $k = 1$, we recover the classical Cahn-Hilliard equation which describes phase separation processes (spinodal decomposition and coarsening) in binary alloys (see [19], [20] and the review papers [36] and [108] for more details). When $k = 2$, the model contains sixth-order Cahn-Hilliard models. We can note that there is currently a strong interest in the study of sixth-order Cahn-Hilliard equations. Such equations arise in situations such as strong anisotropy effects being taken into account in phase separation processes (see [128]), atomistic models of crystal growth (see, [8], [9] and [56]), the description of growing crystalline surfaces with small slopes which undergo faceting (see [122]), oil-water-surfactant mixtures (see [68] and [69]) and mixtures of polymer molecules (see [50]). We refer the reader to [40], [75], [76], [79], [84], [85], [95], [96], [97], [99], [115], [116], [117], [118], [135], [136] and [137] for the mathematical and numerical analysis of such models.

Chapitre 5

Higher-order anisotropic models in phase separation

Modèles anisotropes d'ordre élevé en séparation de phase

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Higher-order anisotropic models in phase separation

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Abstract : Our aim in this paper is to study higher-order (in space) Allen-Cahn and Cahn-Hilliard models. In particular, we obtain well-posedness results, as well as the existence of the global attractor. We also give, for the Allen-Cahn models, numerical simulations which illustrate the effects of the higher-order terms and the anisotropy.

Key words and phrases : Allen-Cahn model, Cahn-Hilliard model, higher-order models, anisotropy, well-posedness, dissipativity, global attractor, numerical simulations.

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5.1 Introduction

The Allen-Cahn (see [4]) and Cahn-Hilliard (see [19] and [20]) equations are central in materials science. They both describe important qualitative features of binary alloys, namely, the ordering of atoms for the Allen-Cahn equation and phase separation processes (spinodal decomposition and coarsening) for the Cahn-Hilliard equation.

These two equations have been much studied from a mathematical point of view ; we refer the readers to the review papers [36] and [108] and the references therein.

Both equations are based on the so-called Ginzburg-Landau free energy,

$$\Psi_{\rm GL} = \int_\Omega (\frac{\alpha}{2}|\nabla u|^2 + F(u))\, dx,\ \ \alpha > 0, \tag{5.1}$$

where u is the order parameter, F is a double-well potential and Ω is the domain occupied by the system (we assume here that it is a bounded and regular domain of $\mathbb{R}^3$, with boundary Γ ; we can of course also consider bounded and regular domains of $\mathbb{R}$ and $\mathbb{R}^2$). The Allen-Cahn equation (which corresponds to an L^2-gradient flow of the Ginzburg-Landau free energy) then reads

$$\frac{\partial u}{\partial t} - \alpha \Delta u + f(u) = 0, \tag{5.2}$$

where $f = F'$, while the Cahn-Hilliard equation (which corresponds to an H^{-1}-gradient flow) reads

$$\frac{\partial u}{\partial t} + \alpha \Delta^2 u - \Delta f(u) = 0. \tag{5.3}$$

In (5.1), the term $|\nabla u|^2$ models short-ranged interactions. It is however interesting to note that such a term is obtained by truncation of higher-order ones (see [20]) ; it can also be seen as a first-order approximation of a nonlocal term accounting for long-ranged interactions (see [65] and [66]).

G. Caginalp and E. Esenturk recently proposed in [23] (see also [22]) higher-order phase-field models in order to account for anisotropic interfaces (see also [80], [125] and [132] for other approaches which, however, do not provide an explicit way to compute the anisotropy). More precisely, these authors proposed the following modified free energy, in which we omit the temperature :

$$\Psi_{\mathrm{HOGL}} = \int_\Omega \left(\frac{1}{2} \sum_{i=1}^{k} \sum_{|\alpha|=i} a_\alpha |\mathcal{D}^\alpha u|^2 + F(u)\right) dx, \ k \in \mathbb{N}, \tag{5.4}$$

where, for $\alpha = (k_1, k_2, k_3) \in (\mathbb{N} \cup \{0\})^3$,

$$|\alpha| = k_1 + k_2 + k_3$$

and, for $\alpha \neq (0, 0, 0)$,

$$\mathcal{D}^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{k_1} \partial x_2^{k_2} \partial x_3^{k_3}}$$

(we agree that $\mathcal{D}^{(0,0,0)} v = v$).

The corresponding higher-order Allen-Cahn and Cahn-Hilliard equations then read

$$\frac{\partial u}{\partial t} + \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u + f(u) = 0 \tag{5.5}$$

and

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0. \tag{5.6}$$

We studied in [32] (see also [33]) the corresponding higher-order isotropic models, namely,

$$\frac{\partial u}{\partial t} + P(-\Delta)u + f(u) = 0 \tag{5.7}$$

and

$$\frac{\partial u}{\partial t} - \Delta P(-\Delta)u - \Delta f(u) = 0, \tag{5.8}$$

where

$$P(s) = \sum_{i=1}^{k} a_i s^i, \ a_k > 0, \ k \geq 1, \ s \in \mathbb{R}.$$

In particular, these models contain sixth-order Cahn-Hilliard models. We can note that there is currently a strong interest in the study of sixth-order Cahn-Hilliard equations. Such equations arise in situations such as strong anisotropy effects being taken into account in phase separation processes (see [128]), atomistic models of crystal growth (see [8], [9], [45] and [56]), the description of growing crystalline surfaces with small slopes which undergo faceting (see [119]), oil-water-surfactant mixtures (see [68] and [69]) and mixtures of polymer molecules (see [50]). We refer the reader to [40], [75], [76], [79], [84], [85], [95], [96], [97], [99], [115], [116], [117], [118], [135], [136] and [137] for the mathematical and numerical analysis of such models. They also contain the Swift-Hohenberg equation (see [96] and [99]).

Our aim in this paper is to study the well-posedness of (5.5) and (5.6). We also prove the dissipativity of the corresponding solution operators, as well as the existence of the global attractor. We finally give, for the Allen-Cahn models, numerical simulations which show the effects of the higher-order terms and the anisotropy.

5.2 Preliminaries

We assume that $k \in \mathbb{N}$, $k \geq 2$, and

$$a_\alpha > 0, \ |\alpha| = k, \tag{5.9}$$

and we introduce the elliptic operator A_k defined by

$$\langle A_k v, w\rangle_{H^{-k}(\Omega),H_0^k(\Omega)} = \sum_{|\alpha|=k} a_\alpha((\mathcal{D}^\alpha v, \mathcal{D}^\alpha w)), \tag{5.10}$$

where $H^{-k}(\Omega)$ is the topological dual of $H_0^k(\Omega)$. Furthermore, $((\cdot,\cdot))$ denotes the usual L^2-scalar product, with associated norm $\|\cdot\|$. More generally, we denote by $\|\cdot\|_X$ the norm on the Banach space X ; we also set $\|\cdot\|_{-1} = \|(-\Delta)^{-\frac{1}{2}}\cdot\|$, where $(-\Delta)^{-1}$ denotes the inverse minus Laplace operator associated with Dirichlet boundary conditions. We can note that

$$(v,w) \in H_0^k(\Omega)^2 \mapsto \sum_{|\alpha|=k} a_\alpha((\mathcal{D}^\alpha v, \mathcal{D}^\alpha w))$$

is bilinear, symmetric, continuous and coercive, so that

$$A_k : H_0^k(\Omega) \to H^{-k}(\Omega)$$

is indeed well defined. It then follows from elliptic regularity results for linear elliptic operators of order $2k$ (see [1], [2] and [3]) that A_k is a strictly positive, selfadjoint and unbounded linear operator with compact inverse, with domain

$$D(A_k) = H^{2k}(\Omega) \cap H_0^k(\Omega),$$

where, for $v \in D(A_k)$,

$$A_k v = (-1)^k \sum_{|\alpha|=k} a_\alpha \mathcal{D}^{2\alpha} v.$$

We further note that $D(A_k^{\frac{1}{2}}) = H_0^k(\Omega)$ and, for $(v,w) \in D(A_k^{\frac{1}{2}})^2$,

$$((A_k^{\frac{1}{2}} v, A_k^{\frac{1}{2}} w)) = \sum_{|\alpha|=k} a_\alpha((\mathcal{D}^\alpha v, \mathcal{D}^\alpha w)).$$

We finally note that (see, e.g., [127]) $\|A_k\cdot\|$ (resp., $\|A_k^{\frac{1}{2}}\cdot\|$) is equivalent to the usual H^{2k}-norm (resp., H^k-norm) on $D(A_k)$ (resp., $D(A_k^{\frac{1}{2}})$).

Similarly, we can define the linear operator $\overline{A}_k = -\Delta A_k$,

$$\overline{A}_k : H_0^{k+1}(\Omega) \to H^{-k-1}(\Omega)$$

which is a strictly positive, selfadjoint and unbounded linear operator with compact inverse, with domain

$$D(\overline{A}_k) = H^{2k+2}(\Omega) \cap H_0^{k+1}(\Omega),$$

where, for $v \in D(\overline{A}_k)$,

$$\overline{A}_k v = (-1)^{k+1}\Delta \sum_{|\alpha|=k} a_\alpha \mathcal{D}^{2\alpha} v.$$

Furthermore, $D(\overline{A}_k^{\frac{1}{2}}) = H_0^{k+1}(\Omega)$ and, for $(v, w) \in D(\overline{A}_k^{\frac{1}{2}})^2$,

$$((\overline{A}_k^{\frac{1}{2}} v, \overline{A}_k^{\frac{1}{2}} w)) = \sum_{|\alpha|=k} a_\alpha ((\nabla \mathcal{D}^\alpha v, \nabla \mathcal{D}^\alpha w)).$$

Besides, $\|\overline{A}_k \cdot \|$ (resp., $\|\overline{A}_k^{\frac{1}{2}} \cdot \|$) is equivalent to the usual H^{2k+2}-norm (resp., H^{k+1}-norm) on $D(\overline{A}_k)$ (resp., $D(\overline{A}_k^{\frac{1}{2}})$).

We finally consider the operator $\tilde{A}_k = (-\Delta)^{-1} A_k$, where

$$\tilde{A}_k : H_0^{k-1}(\Omega) \to H^{-k+1}(\Omega);$$

note that, as $-\Delta$ and A_k commute, then the same holds for $(-\Delta)^{-1}$ and A_k, so that $\tilde{A}_k = A_k(-\Delta)^{-1}$.

We have the

Lemma 5.2.1. *The operator $\tilde{A}_k$ is a strictly positive, selfadjoint and unbounded linear operator with compact inverse, with domain*

$$D(\tilde{A}_k) = H^{2k-2}(\Omega) \cap H_0^{k-1}(\Omega),$$

where, for $v \in D(\tilde{A}_k)$,

$$\tilde{A}_k v = (-1)^k \sum_{|\alpha|=k} a_\alpha \mathcal{D}^{2\alpha} (-\Delta)^{-1} v.$$

Furthermore, $D(\tilde{A}_k^{\frac{1}{2}}) = H_0^{k-1}(\Omega)$ and, for $(v, w) \in D(\tilde{A}_k^{\frac{1}{2}})^2$,

$$((\tilde{A}_k^{\frac{1}{2}} v, \tilde{A}_k^{\frac{1}{2}} w)) = \sum_{|\alpha|=k} a_\alpha ((\mathcal{D}^\alpha (-\Delta)^{-\frac{1}{2}} v, \mathcal{D}^\alpha (-\Delta)^{-\frac{1}{2}} w)).$$

Besides, $\|\tilde{A}_k \cdot \|$ (resp., $\|\tilde{A}_k^{\frac{1}{2}} \cdot \|$) is equivalent to the usual H^{2k-2}-norm (resp., H^{k-1}-norm) on $D(\tilde{A}_k)$ (resp., $D(\tilde{A}_k^{\frac{1}{2}})$).

Proof. We first note that $\tilde{A}_k$ clearly is linear and unbounded. Then, since $(-\Delta)^{-1}$ and A_k commute, it easily follows that $\tilde{A}_k$ is selfadjoint.

Next, the domain of $\tilde{A}_k$ is defined by

$$D(\tilde{A}_k) = \{v \in H_0^{k-1}(\Omega),\ \tilde{A}_k v \in L^2(\Omega)\}.$$

Noting that $\tilde{A}_k v = f$, $f \in L^2(\Omega)$, $v \in D(\tilde{A}_k)$, is equivalent to $A_k v = -\Delta f$, where $-\Delta f \in H^2(\Omega)'$, it follows from the elliptic regularity results of [1], [2] and [3] that $v \in H^{2k-2}(\Omega)$, so that $D(\tilde{A}_k) = H^{2k-2}(\Omega) \cap H_0^{k-1}(\Omega)$.

Noting then that $\tilde{A}_k^{-1}$ maps $L^2(\Omega)$ onto $H^{2k-2}(\Omega)$ and recalling that $k \geq 2$, we deduce that $\tilde{A}_k$ has compact inverse.

We now note that, considering the spectral properties of $-\Delta$ and A_k (see, e.g., [127]) and recalling that these two operators commute, $-\Delta$ and A_k have a spectral basis formed of common eigenvectors. This yields that, $\forall s_1, s_2 \in \mathbb{R}$, $(-\Delta)^{s_1}$ and $A_k^{s_2}$ commute.

Having this, we see that $\tilde{A}_k^{\frac{1}{2}} = (-\Delta)^{-\frac{1}{2}} A_k^{\frac{1}{2}}$, so that $D(\tilde{A}_k^{\frac{1}{2}}) = H_0^{k-1}(\Omega)$, and, for $(v, w) \in D(\tilde{A}_k^{\frac{1}{2}})^2$,

$$((\tilde{A}_k^{\frac{1}{2}} v, \tilde{A}_k^{\frac{1}{2}} w)) = \sum_{|\alpha|=k} a_\alpha((\mathcal{D}^\alpha (-\Delta)^{-\frac{1}{2}} v, \mathcal{D}^\alpha (-\Delta)^{-\frac{1}{2}} w)).$$

Finally, as far as the equivalences of norms are concerned, we can note that, for instance, the norm $\|\tilde{A}_k^{\frac{1}{2}} \cdot \|$ is equivalent to the norm $\|(-\Delta)^{-\frac{1}{2}} \cdot \|_{H^k(\Omega)}$ and, thus, to the norm $\|(-\Delta)^{\frac{k-1}{2}} \cdot \|$.

□

Throughout the paper, the same letters c, c' and c'' denote (generally positive) constants which may vary from line to line. Similarly, the same letter Q denotes (positive) monotone increasing and continuous functions which may vary from line to line.

5.3 The Allen-Cahn theory

5.3.1 Setting of the problem

We consider in this section the following initial and boundary value problem, for $k \geq 2$ (for $k = 1$, the problem can be treated as in the original Allen-Cahn equation ; see, e.g., [32]) :

$$\frac{\partial u}{\partial t} + \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u + f(u) = 0, \tag{5.11}$$

$$\mathcal{D}^\alpha u = 0 \text{ on } \Gamma, \ |\alpha| \leq k-1, \tag{5.12}$$

$$u|_{t=0} = u_0. \tag{5.13}$$

Remark 5.3.1. *For $k = 1$ (anisotropic Allen-Cahn equation), we have an equation of the form*

$$\frac{\partial u}{\partial t} - \sum_{i=1}^{3} a_i \frac{\partial^2 u}{\partial x_i^2} + f(u) = 0$$

and, for $k = 2$ (fourth-order anisotropic Allen-Cahn equation), we have an equation of the form

$$\frac{\partial u}{\partial t} + \sum_{i,j=1}^{3} a_{ij} \frac{\partial^4 u}{\partial x_i^2 \partial x_j^2} - \sum_{i=1}^{3} b_i \frac{\partial^2 u}{\partial x_i^2} + f(u) = 0.$$

We actually rewrite (5.11) in the equivalent form

$$\frac{\partial u}{\partial t} + A_k u + B_k u + f(u) = 0, \tag{5.14}$$

where

$$B_k v = \sum_{i=1}^{k-1} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} v.$$

As far as the nonlinear term f is concerned, we assume that

$$f \in C^1(\mathbb{R}),\ f(0) = 0, \tag{5.15}$$

$$f' \geq -c_0,\ c_0 \geq 0, \tag{5.16}$$

$$f(s)s \geq c_1 F(s) - c_2 \geq -c_3,\ c_1 > 0,\ c_2,\ c_3 \geq 0,\ s \in \mathbb{R}, \tag{5.17}$$

$$F(s) \geq c_4 s^4 - c_5,\ c_4 > 0,\ c_5 \geq 0,\ s \in \mathbb{R}, \tag{5.18}$$

where $F(s) = \int_0^s f(\xi)\, d\xi$. In particular, the usual cubic nonlinear term $f(s) = s^3 - s$ satisfies these assumptions.

5.3.2 A priori estimates

We multiply (5.14) by $\frac{\partial u}{\partial t}$ and integrate over Ω and by parts. This gives

$$\frac{d}{dt}(\|A_k^{\frac{1}{2}} u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)\, dx) + 2\|\frac{\partial u}{\partial t}\|^2 = 0, \tag{5.19}$$

where

$$B_k^{\frac{1}{2}}[u] = \sum_{i=1}^{k-1} \sum_{|\alpha|=i} a_\alpha \|\mathcal{D}^\alpha u\|^2 \tag{5.20}$$

(note that $B_k^{\frac{1}{2}}[u]$ is not necessarily nonnegative). We can note that, owing to the interpolation inequality

$$\|v\|_{H^i(\Omega)} \le c(i)\|v\|_{H^m(\Omega)}^{\frac{i}{m}} \|v\|^{1-\frac{i}{m}}, \tag{5.21}$$
$$v \in H^m(\Omega),\ i \in \{1, ..., m-1\},\ m \in \mathbb{N},\ m \ge 2,$$

there holds

$$|B_k^{\frac{1}{2}}[u]| \le \frac{1}{2}\|A_k^{\frac{1}{2}} u\|^2 + c\|u\|^2. \tag{5.22}$$

This yields, employing (5.18),

$$\|A_k^{\frac{1}{2}} u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)\,dx \ge \frac{1}{2}\|A_k^{\frac{1}{2}} u\|^2 + \int_\Omega F(u)\,dx + c\|u\|_{L^4(\Omega)}^4 - c'\|u\|^2 - c'',$$

whence

$$\|A_k^{\frac{1}{2}} u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)\,dx \ge c(\|u\|_{H^k(\Omega)}^2 + \int_\Omega F(u)\,dx) - c',\ c > 0, \tag{5.23}$$

noting that, owing to Young's inequality,

$$\|u\|^2 \le \epsilon \|u\|_{L^4(\Omega)}^4 + c(\epsilon),\ \forall \epsilon > 0. \tag{5.24}$$

We then multiply (5.14) by u and have, owing to (5.17) and the interpolation inequality (5.21),

$$\frac{d}{dt}\|u\|^2 + c(\|u\|_{H^k(\Omega)}^2 + \int_\Omega F(u)\,dx) \le c'\|u\|^2 + c'',$$

hence, proceeding as above and employing, in particular, (5.18),

$$\frac{d}{dt}\|u\|^2 + c(\|u\|_{H^k(\Omega)}^2 + \int_\Omega F(u)\,dx) \le c',\ c > 0. \tag{5.25}$$

Summing (5.19) and (5.25), we obtain a differential inequality of the form

$$\frac{dE_1}{dt} + c(E_1 + \|\frac{\partial u}{\partial t}\|^2) \le c',\ c > 0, \tag{5.26}$$

where

$$E_1 = \|A_k^{\frac{1}{2}}u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)\,dx + \|u\|^2$$

satisfies, owing to (5.23),

$$E_1 \geq c(\|u\|^2_{H^k(\Omega)} + \int_\Omega F(u)\,dx) - c',\ c > 0. \tag{5.27}$$

Note indeed that

$$\begin{aligned} E_1 &\leq c\|u\|^2_{H^k(\Omega)} + 2\int_\Omega F(u)\,dx \\ &\leq c(\|u\|^2_{H^k(\Omega)} + \int_\Omega F(u)\,dx) - c',\ c > 0,\ c' \geq 0. \end{aligned}$$

It follows from (5.26)-(5.27) and Gronwall's lemma that

$$\|u(t)\|^2_{H^k(\Omega)} \leq ce^{-c't}(\|u_0\|^2_{H^k(\Omega)} + \int_\Omega F(u_0)\,dx) + c'',\ c' > 0,\ t \geq 0, \tag{5.28}$$

and

$$\int_t^{t+r} \|\frac{\partial u}{\partial t}\|^2\,ds \leq ce^{-c't}(\|u_0\|^2_{H^k(\Omega)} + \int_\Omega F(u_0)\,dx) + c'',\ c' > 0,\ t \geq 0,\ r > 0 \text{ given}. \tag{5.29}$$

Next, we multiply (5.14) by $A_k u$ and find, owing to the interpolation inequality (5.21),

$$\frac{d}{dt}\|A_k^{\frac{1}{2}}u\|^2 + c\|u\|^2_{H^{2k}(\Omega)} \leq c(\|u\|^2 + \|f(u)\|^2). \tag{5.30}$$

It follows from the continuity of f and F, the continuous embedding $H^k(\Omega) \subset C(\overline{\Omega})$ (recall that $k \geq 2$) and (5.28) that

$$\begin{aligned} \|u\|^2 + \|f(u)\|^2 &\leq Q(\|u\|_{H^k(\Omega)}) \\ &\leq e^{-ct}Q(\|u_0\|_{H^k(\Omega)}) + c',\ c > 0,\ t \geq 0, \end{aligned} \tag{5.31}$$

so that

$$\frac{d}{dt}\|A_k^{\frac{1}{2}}u\|^2 + c\|u\|^2_{H^{2k}(\Omega)} \leq e^{-c't}Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0,\ t \geq 0. \tag{5.32}$$

Summing (5.26) and (5.32), we have a differential inequality of the form

$$\frac{dE_2}{dt} + c(E_2 + \|u\|^2_{H^{2k}(\Omega)} + \|\frac{\partial u}{\partial t}\|^2) \leq e^{-c't}Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0,\ t \geq 0, \tag{5.33}$$

where

$$E_2 = E_1 + \|A_k^{\frac{1}{2}} u\|^2$$

satisfies

$$E_2 \geq c(\|u\|^2_{H^k(\Omega)} + \int_\Omega F(u)\,dx) - c',\ c > 0. \tag{5.34}$$

We then rewrite (5.14) as an elliptic equation, for $t > 0$ fixed,

$$A_k u = -\frac{\partial u}{\partial t} - B_k u - f(u),\ \mathcal{D}^\alpha u = 0 \text{ on } \Gamma,\ |\alpha| \leq k - 1. \tag{5.35}$$

Multiplying (5.35) by $A_k u$, we obtain, owing to the interpolation inequality (5.21),

$$\|A_k u\|^2 \leq c(\|u\|^2 + \|f(u)\|^2 + \|\frac{\partial u}{\partial t}\|^2), \tag{5.36}$$

hence, owing to (5.31),

$$\|u\|^2_{H^{2k}(\Omega)} \leq c(e^{-c't} Q(\|u_0\|_{H^k(\Omega)}) + \|\frac{\partial u}{\partial t}\|^2) + c'',\ c' > 0. \tag{5.37}$$

Next, we differentiate (5.14) with respect to time and find

$$\frac{\partial}{\partial t}\frac{\partial u}{\partial t} + A_k \frac{\partial u}{\partial t} + B_k \frac{\partial u}{\partial t} + f'(u)\frac{\partial u}{\partial t} = 0, \tag{5.38}$$

$$\mathcal{D}^\alpha \frac{\partial u}{\partial t} = 0 \text{ on } \Gamma,\ |\alpha| \leq k - 1, \tag{5.39}$$

$$\frac{\partial u}{\partial t}|_{t=0} = -A_k u_0 - B_k u_0 - f(u_0). \tag{5.40}$$

We can note that, if $u_0 \in H^{2k}(\Omega) \cap H^k_0(\Omega)\ (= D(A_k))$, then $\frac{\partial u}{\partial t}(0) \in L^2(\Omega)$ and

$$\|\frac{\partial u}{\partial t}(0)\| \leq Q(\|u_0\|_{H^{2k}(\Omega)}). \tag{5.41}$$

We multiply (5.38) by $\frac{\partial u}{\partial t}$ and have, owing to (5.16) and the interpolation inequality (5.21),

$$\frac{d}{dt}\|\frac{\partial u}{\partial t}\|^2 + c\|\frac{\partial u}{\partial t}\|^2_{H^k(\Omega)} \leq c'\|\frac{\partial u}{\partial t}\|^2,\ c > 0. \tag{5.42}$$

It follows from (5.29) (for $r = 1$), (5.42) and the uniform Gronwall's lemma that

$$\|\frac{\partial u}{\partial t}(t)\|^2 \leq e^{-ct} Q(\|u_0\|_{H^k(\Omega)}) + c',\ c > 0,\ t \geq 1, \tag{5.43}$$

and from (5.41)-(5.42) and Gronwall's lemma that

$$\|\frac{\partial u}{\partial t}(t)\|^2 \le e^{ct}Q(\|u_0\|_{H^{2k}(\Omega)}),\ t \ge 0. \tag{5.44}$$

We finally deduce from (5.37) and (5.43)-(5.44) that

$$\|u(t)\|_{H^{2k}(\Omega)} \le e^{-ct}Q(\|u_0\|_{H^k(\Omega)}) + c',\ c > 0,\ t \ge 1, \tag{5.45}$$

and

$$\|u(t)\|_{H^{2k}(\Omega)} \le e^{-ct}Q(\|u_0\|_{H^{2k}(\Omega)}) + c',\ c > 0,\ t \ge 0. \tag{5.46}$$

5.3.3 The dissipative semigroup

We have the

Theorem 5.3.1. *(i) We assume that $u_0 \in H_0^k(\Omega)$. Then,* (5.11)-(5.13) *possesses a unique weak solution u such that, $\forall T > 0$,*

$$u \in L^\infty(\mathbb{R}^+; H_0^k(\Omega)) \cap L^2(0,T; H^{2k}(\Omega) \cap H_0^k(\Omega))$$

and

$$\frac{\partial u}{\partial t} \in L^2(0,T; L^2(\Omega)).$$

(ii) If we further assume that $u_0 \in H^{2k}(\Omega) \cap H_0^k(\Omega)$, then

$$u \in L^\infty(\mathbb{R}^+; H^{2k}(\Omega) \cap H_0^k(\Omega)).$$

Proof. The proofs of existence and regularity in (i) and (ii) follow from the a priori estimates derived in the previous subsection and, e.g., a standard Galerkin scheme.

Let now u_1 and u_2 be two solutions to (5.11)-(5.12) with initial data $u_{0,1}$ and $u_{0,2}$, respectively. We set $u = u_1 - u_2$ and $u_0 = u_{0,1} - u_{0,2}$ and have

$$\frac{\partial u}{\partial t} + A_k u + B_k u + f(u_1) - f(u_2) = 0, \tag{5.47}$$

$$\mathcal{D}^\alpha u = 0 \text{ on } \Gamma,\ |\alpha| \le k-1, \tag{5.48}$$

$$u|_{t=0} = u_0. \tag{5.49}$$

Multiplying (5.47) by u, we obtain, owing to (5.16) and the interpolation inequality (5.21),

$$\frac{d}{dt}\|u\|^2 + c\|u\|^2_{H^k(\Omega)} \leq c'\|u\|^2, \ c > 0. \tag{5.50}$$

It follows from (5.50) and Gronwall's lemma that

$$\|u(t)\|^2 \leq e^{ct}\|u_0\|^2, \ t \geq 0, \tag{5.51}$$

hence the uniqueness, as well as the continuous dependence with respect to the initial data in the L^2-norm.

□

It follows from Theorem 5.3.1 that we can define the continuous (for the L^2-norm) semigroup $S(t) : \Phi \to \Phi$, $u_0 \mapsto u(t)$, $t \geq 0$ (i.e., $S(0) = I$ (identity operator) and $S(t+\tau) = S(t) \circ S(\tau)$, $t, \tau \geq 0$), where $\Phi = H^k_0(\Omega)$. Furthermore, $S(t)$ is dissipative in Φ, owing to (5.28), in the sense that it possesses a bounded absorbing set $\mathcal{B}_0 \subset \Phi$ (i.e., $\forall B \subset \Phi$ bounded, $\exists t_0 = t_0(B) \geq 0$ such that $t \geq t_0 \implies S(t)B \subset \mathcal{B}_0$).

Remark 5.3.2. *We can also prove the continuous dependence with respect to the initial data in the H^k- and H^{2k}-norms and it then follows from (5.46) that $S(t)$ is defined, continuous and dissipative in $(H^{2k}(\Omega) \cap H^k_0(\Omega))$.*

Actually, it follows from (5.45) that $S(t)$ possesses a bounded absorbing set $\mathcal{B}_1$ such that $\mathcal{B}_1$ is compact in Φ and bounded in $H^{2k}(\Omega)$. It thus follows from classical results (see, e.g., [103] and [127]) that we have the

Theorem 5.3.2. *The semigroup $S(t)$ possesses the global attractor $\mathcal{A}$ which is compact in Φ and bounded in $H^{2k}(\Omega)$.*

Remark 5.3.3. *It follows from (5.51) that we can extend $S(t)$ (by continuity and in a unique way) to $L^2(\Omega)$.*

Remark 5.3.4. *(i) We recall that the global attractor $\mathcal{A}$ is the smallest (for the inclusion) compact set of the phase space which is invariant by the flow (i.e., $S(t)\mathcal{A} = \mathcal{A}$, $\forall t \geq 0$) and attracts all bounded sets of initial data as time goes to infinity ; it thus appears as a suitable object in view of the study of the asymptotic behavior of the system. We refer the reader to, e.g., [103] and [127] for more details and discussions on this.*

(ii) We can also prove, based on standard arguments (see, e.g., [103] and [127]) that $\mathcal{A}$ has finite dimension, in the sense of covering dimensions such as the Hausdorff and the fractal dimensions. The finite-dimensionality means, very roughly speaking, that, even though the initial phase space has infinite dimension, the reduced dynamics can be described by a finite number of parameters (we refer the interested reader to, e.g., [103] and [127] for discussions on this subject).

Remark 5.3.5. *We can also consider periodic boundary conditions, namely,*

$$u \text{ is } \Omega - \text{periodic},$$

in which case $\Omega = \Pi_{i=1}^{3}(0, L_i)$*,* $L_i > 0$*,* $i \in \{1, 2, 3\}$*. In that case, we consider the operator* $\mathbf{A}_k = I + A_k$ *(in order to have a strictly positive operator), where* A_k *is as above, but based on Sobolev spaces with periodic functions (see, e.g., [127]), and rewrite* (5.11) *in the form*

$$\frac{\partial u}{\partial t} + \mathbf{A}_k u + B_k u + g(u) = 0,$$

where $g(s) = f(s) - s$ *(note that* g *satisfies properties which are similar to* (5.15)-(5.18)*).*

5.4 The Cahn-Hilliard theory

5.4.1 Setting of the problem

We consider the following initial and boundary value problem, for $k \in \mathbb{N}$, $k \geq 2$ (the case $k = 1$ can be treated as in the original Cahn-Hilliard equation ; see, e.g., [32]) :

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0, \tag{5.52}$$

$$\mathcal{D}^\alpha u = 0 \text{ on } \Gamma, \ |\alpha| \leq k, \tag{5.53}$$

$$u|_{t=0} = u_0. \tag{5.54}$$

Remark 5.4.1. *For* $k = 1$ *(anisotropic Cahn-Hilliard equation), we have an equation of the form*

$$\frac{\partial u}{\partial t} + \Delta \sum_{i=1}^{3} a_i \frac{\partial^2 u}{\partial x_i^2} - \Delta f(u) = 0$$

and, for $k = 2$ *(fourth-order anisotropic Cahn-Hilliard equation), we have an equation of the form*

$$\frac{\partial u}{\partial t} - \Delta \sum_{i,j=1}^{3} a_{ij} \frac{\partial^4 u}{\partial x_i^2 \partial x_j^2} + \Delta \sum_{i=1}^{3} b_i \frac{\partial^2 u}{\partial x_i^2} - \Delta f(u) = 0.$$

Keeping the same notation as in the previous section, we rewrite (5.52) as

$$\frac{\partial u}{\partial t} - \Delta A_k u - \Delta B_k u - \Delta f(u) = 0. \tag{5.55}$$

As far as the nonlinear term f is concerned, we assume that the assumptions of the previous section hold and that f is of class C^2.

5.4.2 A priori estimates

We multiply (5.55) by $(-\Delta)^{-1}\frac{\partial u}{\partial t}$. This gives

$$\frac{d}{dt}(\|A_k^{\frac{1}{2}}u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)\,dx) + 2\|\frac{\partial u}{\partial t}\|_{-1}^2 = 0. \tag{5.56}$$

We then multiply (5.55) by $(-\Delta)^{-1}u$ and have, owing to (5.17) and the interpolation inequality (5.21) and proceeding as in the previous section,

$$\frac{d}{dt}\|u\|_{-1}^2 + c(\|u\|_{H^k(\Omega)}^2 + \int_\Omega F(u)\,dx) \le c',\ c > 0. \tag{5.57}$$

Summing (5.56) and (5.57), we obtain a differential inequality of the form

$$\frac{dE_3}{dt} + c(E_3 + \|\frac{\partial u}{\partial t}\|_{-1}^2) \le c',\ c > 0, \tag{5.58}$$

where

$$E_3 = \|A_k^{\frac{1}{2}}u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)\,dx + \|u\|_{-1}^2$$

satisfies

$$E_3 \ge c(\|u\|_{H^k(\Omega)}^2 + \int_\Omega F(u)\,dx) - c',\ c > 0. \tag{5.59}$$

It follows from (5.58)-(5.59) and Gronwall's lemma that

$$\|u(t)\|_{H^k(\Omega)}^2 \le ce^{-c't}(\|u_0\|_{H^k(\Omega)}^2 + \int_\Omega F(u_0)\,dx) + c'',\ c' > 0,\ t \ge 0, \tag{5.60}$$

and

$$\int_t^{t+r} \|\frac{\partial u}{\partial t}\|_{-1}^2\,ds \le ce^{-c't}(\|u_0\|_{H^k(\Omega)}^2 + \int_\Omega F(u_0)\,dx) + c'',\ c' > 0,\ t \ge 0,\ r > 0 \text{ given}. \tag{5.61}$$

Multiplying next (5.55) by $\tilde{A}_k u$, we find, owing to the interpolation inequality (5.21) and proceeding as in the previous section,

$$\frac{d}{dt}\|\tilde{A}_k^{\frac{1}{2}}u\|^2 + c\|u\|^2_{H^{2k}(\Omega)} \le e^{-c't}Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0,\ t \ge 0. \tag{5.62}$$

Summing (5.58) and (5.62), we have a differential inequality of the form

$$\frac{dE_4}{dt} + c(E_4 + \|u\|^2_{H^{2k}(\Omega)} + \|\frac{\partial u}{\partial t}\|^2_{-1}) \le e^{-c't}Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0,\ t \ge 0, \tag{5.63}$$

where

$$E_4 = E_3 + \|\tilde{A}_k^{\frac{1}{2}}u\|^2$$

satisfies

$$E_4 \ge c(\|u\|^2_{H^k(\Omega)} + \int_\Omega F(u)\,dx) - c',\ c > 0. \tag{5.64}$$

We also multiply (5.55) by $\frac{\partial u}{\partial t}$ and obtain, noting that f is of class C^2,

$$\frac{d}{dt}(\|\overline{A}_k^{\frac{1}{2}}u\|^2 + \overline{B}_k^{\frac{1}{2}}[u]) + \|\frac{\partial u}{\partial t}\|^2 \le e^{-c't}Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0, \tag{5.65}$$

where

$$\overline{B}_k^{\frac{1}{2}}[u] = \sum_{i=1}^{k-1}\sum_{|\alpha|=i} a_\alpha\|\nabla\mathcal{D}^\alpha u\|^2.$$

Summing finally (5.63) and (5.65), we find a differential inequality of the form

$$\frac{dE_5}{dt} + c(E_5 + \|u\|^2_{H^{2k}(\Omega)} + \|\frac{\partial u}{\partial t}\|^2) \le e^{-c't}Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0,\ t \ge 0, \tag{5.66}$$

where

$$E_5 = E_4 + \|\overline{A}_k^{\frac{1}{2}}u\|^2 + \overline{B}_k^{\frac{1}{2}}[u]$$

satisfies

$$E_5 \ge c(\|u\|^2_{H^{k+1}(\Omega)} + \int_\Omega F(u)\,dx) - c',\ c > 0. \tag{5.67}$$

In particular, it follows from (5.66)-(5.67) that

$$\|u(t)\|_{H^{k+1}(\Omega)} \le e^{-ct}Q(\|u_0\|_{H^{k+1}(\Omega)}) + c',\ c > 0,\ t \ge 0. \tag{5.68}$$

We then differentiate (5.55) with respect to time and have

$$\frac{\partial}{\partial t}\frac{\partial u}{\partial t} - \Delta A_k \frac{\partial u}{\partial t} - \Delta B_k \frac{\partial u}{\partial t} - \Delta(f'(u)\frac{\partial u}{\partial t}) = 0, \tag{5.69}$$

$$\mathcal{D}^\alpha \frac{\partial u}{\partial t} = 0 \text{ on } \Gamma,\ |\alpha| \leq k. \tag{5.70}$$

We multiply (5.69) by $(-\Delta)^{-1}\frac{\partial u}{\partial t}$ and obtain, owing to (5.16) and the interpolation inequality (5.21),

$$\frac{d}{dt}\|\frac{\partial u}{\partial t}\|_{-1}^2 + c\|\frac{\partial u}{\partial t}\|_{H^k(\Omega)}^2 \leq c'\|\frac{\partial u}{\partial t}\|^2,\ c > 0,$$

which yields, employing the interpolation inequality

$$\|v\|^2 \leq c\|v\|_{-1}\|v\|_{H^1(\Omega)},\ v \in H_0^1(\Omega), \tag{5.71}$$

the differential inequality

$$\frac{d}{dt}\|\frac{\partial u}{\partial t}\|_{-1}^2 + c\|\frac{\partial u}{\partial t}\|_{H^k(\Omega)}^2 \leq c'\|\frac{\partial u}{\partial t}\|_{-1}^2,\ c > 0. \tag{5.72}$$

In particular, this yields, owing to (5.61) and employing the uniform Gronwall's lemma,

$$\|\frac{\partial u}{\partial t}(t)\|_{-1} \leq e^{-ct}Q(\|u_0\|_{H^k(\Omega)}) + c',\ c > 0,\ t \geq r,\ r > 0 \text{ given.} \tag{5.73}$$

We finally rewrite (5.55) as an elliptic equation, for $t > 0$ fixed,

$$A_k u = -(-\Delta)^{-1}\frac{\partial u}{\partial t} - B_k u - f(u),\ \mathcal{D}^\alpha u = 0 \text{ on } \Gamma,\ |\alpha| \leq k-1. \tag{5.74}$$

Multiplying (5.74) by $A_k u$, we find, owing to the interpolation inequality (5.21),

$$\|u\|_{H^{2k}(\Omega)}^2 \leq c(e^{-c't}Q(\|u_0\|_{H^k(\Omega)}) + \|\frac{\partial u}{\partial t}\|_{-1}^2) + c'',\ c' > 0. \tag{5.75}$$

In particular, it follows from (5.73) (for $r = 1$) and (5.75) that

$$\|u(t)\|_{H^{2k}(\Omega)} \leq e^{-ct}Q(\|u_0\|_{H^k(\Omega)}) + c',\ c > 0,\ t \geq 1. \tag{5.76}$$

Remark 5.4.2. *If we assume that $u_0 \in H^{2k+1}(\Omega) \cap H_0^k(\Omega)$, we deduce from (5.72), (5.75) and Gronwall's lemma an H^{2k}-estimate on u on $[0,1]$ which, combined with (5.76), gives an H^{2k}-estimate on u, for all times. This is however not satisfactory, in particular, in view of the study of attractors.*

Remark 5.4.3. *We further assume that f is of class C^{k+1}. Multiplying (5.55) by $\tilde{A}_k \frac{\partial u}{\partial t}$, we have*

$$\frac{1}{2}\frac{d}{dt}(\|A_k u\|^2 + ((A_k u, B_k u))) + \|\tilde{A}_k^{\frac{1}{2}}\frac{\partial u}{\partial t}\|^2 = -((\overline{A}_k^{\frac{1}{2}} f(u), \tilde{A}_k^{\frac{1}{2}}\frac{\partial u}{\partial t})),$$

which yields, noting that $\|\overline{A}_k^{\frac{1}{2}} f(u)\|^2 \le Q(\|u\|_{H^{k+1}(\Omega)})$ and owing to (5.68),

$$\frac{d}{dt}(\|A_k u\|^2 + ((A_k u, B_k u))) \le e^{-ct}Q(\|u_0\|_{H^{k+1}(\Omega)}) + c',\ c > 0,\ t \ge 0. \tag{5.77}$$

Combining (5.77) with (5.66), it follows from (5.67) and the interpolation inequality (5.21) that

$$\|u(t)\|_{H^{2k}(\Omega)} \le Q(\|u_0\|_{H^{2k}(\Omega)}),\ t \in [0, 1],$$

so that, owing to (5.76),

$$\|u(t)\|_{H^{2k}(\Omega)} \le e^{-ct}Q(\|u_0\|_{H^{2k}(\Omega)}) + c',\ c > 0,\ t \ge 0. \tag{5.78}$$

5.4.3 The dissipative semigroup

We have the

Theorem 5.4.1. *(i) We assume that $u_0 \in H_0^k(\Omega)$. Then, (5.52)-(5.54) possesses a unique weak solution u such that, $\forall T > 0$,*

$$u \in L^\infty(\mathbb{R}^+; H_0^k(\Omega)) \cap L^2(0, T; H^{2k}(\Omega) \cap H_0^k(\Omega))$$

and

$$\frac{\partial u}{\partial t} \in L^2(0, T; H^{-1}(\Omega)).$$

(ii) If we further assume that $u_0 \in H^{k+1}(\Omega) \cap H_0^k(\Omega)$, then, $\forall T > 0$,

$$u \in L^\infty(\mathbb{R}^+; H^{k+1}(\Omega) \cap H_0^k(\Omega))$$

and

$$\frac{\partial u}{\partial t} \in L^2(0, T; L^2(\Omega)).$$

(iii) If we further assume that f is of class C^{k+1} and $u_0 \in H^{2k}(\Omega) \cap H_0^k(\Omega)$, then

$$u \in L^\infty(\mathbb{R}^+; H^{2k}(\Omega) \cap H_0^k(\Omega)).$$

Proof.

The proofs of existence and regularity in (i), (ii) and (iii) follow from the a priori estimates derived in the previous subsection and, e.g., a standard Galerkin scheme.

Let now u_1 and u_2 be two solutions to (5.52)-(5.53) with initial data $u_{0,1}$ and $u_{0,2}$, respectively. We set $u = u_1 - u_2$ and $u_0 = u_{0,1} - u_{0,2}$ and have

$$\frac{\partial u}{\partial t} - \Delta A_k u - \Delta B_k u - \Delta(f(u_1) - f(u_2)) = 0, \tag{5.79}$$

$$\mathcal{D}^\alpha u = 0 \text{ on } \Gamma, \ |\alpha| \leq k, \tag{5.80}$$

$$u|_{t=0} = u_0. \tag{5.81}$$

Multiplying (5.79) by $(-\Delta)^{-1}u$, we obtain, owing to (5.16) and the interpolation inequalities (5.21) and (5.71),

$$\frac{d}{dt}\|u\|_{-1}^2 + c\|u\|_{H^k(\Omega)}^2 \leq c'\|u\|_{-1}^2, \ c > 0. \tag{5.82}$$

It follows from (5.82) and Gronwall's lemma that

$$\|u(t)\|_{-1}^2 \leq e^{ct}\|u_0\|_{-1}^2, \ t \geq 0, \tag{5.83}$$

hence the uniqueness, as well as the continuous dependence with respect to the initial data in the H^{-1}-norm.

□

It follows from Theorem 5.4.1 that we can define the family of solving operators

$$S(t) : \Phi \to \Phi, \ u_0 \mapsto u(t), \ t \geq 0,$$

where $\Phi = H_0^k(\Omega)$. This family of solving operators forms a semigroup which is continuous with respect to the H^{-1}-topology. Finally, it follows from (5.60) that we have the

Theorem 5.4.2. *The semigroup $S(t)$ is dissipative in Φ.*

Remark 5.4.4. *(i) Actually, it follows from (5.76) that we have a bounded absorbing set $\mathcal{B}_1$ which is compact in Φ and bounded in $H^{2k}(\Omega)$. This yields the existence of the global attractor $\mathcal{A}$ which is compact in Φ and bounded in $H^{2k}(\Omega)$.*

(ii) It follows from (5.78) that, if f is of class C^{k+1}, then $S(t)$ is dissipative in $H^{2k}(\Omega) \cap H_0^k(\Omega)$.

(iii) It follows from (5.83) that we can extend $S(t)$ (by continuity and in a unique way) to $H^{-1}(\Omega)$.

Remark 5.4.5. *The case of periodic boundary conditions is more delicate, since, integrating (formally) (5.52) over Ω, we have the conservation of mass, namely,*

$$\langle u(t)\rangle = \langle u_0\rangle,\ t \geq 0,$$

where $\langle\cdot\rangle = \frac{1}{\mathrm{Vol}(\Omega)}\int_\Omega \cdot\, dx$. As a consequence, we cannot expect to find compact attractors on the whole phase space and have to deal with the nonlocal term $\langle f(u)\rangle$ (see, e.g., [127]).

5.5 Numerical simulations

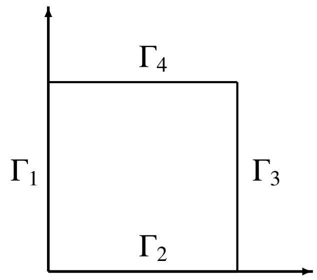


Figure 5.1 – Computational domain : $\Omega = (0,1)\times(0,1)$.

In this section, we give numerical simulations which show the effects of the anisotropy for the generalized Allen-Cahn equations when $k = 1$, 2 and 3 in the domain $\Omega = (0,1)\times(0,1)$ (see Figure 5.1). In particular, this shows how the coefficients of highest orders affect the solutions. Furthermore, we compare the solutions when different k's, time steps or coefficients are taken.

The numerical method applied here is a $P1-$finite element in space and a forward Euler discretization in time. The numerical simulations are performed with the software Freefem++ (see [77]).

For instance, when $k = 2$, the generalized Allen-Cahn equation reads

$$\frac{\partial u}{\partial t} + a_{20}\frac{\partial^4 u}{\partial x^4} + a_{02}\frac{\partial^4 u}{\partial y^4} + a_{11}\frac{\partial^4 u}{\partial x^2\partial y^2} - a_{10}\frac{\partial^2 u}{\partial x^2} - a_{01}\frac{\partial^2 u}{\partial y^2} + f(u) = 0, \tag{5.84}$$

where, here and in all the simulations, $f(s) = s^3 - s$. We further assume that u is $\Omega-$periodic. Finally, we take as initial condition a cross in the center of the computational domain, that is, the initial value in the middle cross is -0.8, while, in the complementary set, it is equal to 0.8, as shown in the following Figure 5.2.

Setting $\frac{\partial^2 u}{\partial x^2} = \omega$ and $\frac{\partial^2 u}{\partial y^2} = p$, then, integrating by parts, the system which needs to be solved reads

$$\begin{cases} (\frac{\partial u}{\partial t}, v) - a_{20}(\frac{\partial \omega}{\partial x}, \frac{\partial v}{\partial x}) - a_{02}(\frac{\partial p}{\partial y}, \frac{\partial v}{\partial y}) - a_{11}(\frac{\partial \omega}{\partial y}, \frac{\partial v}{\partial y}) + a_{10}(\frac{\partial u}{\partial x}, \frac{\partial v}{\partial x}) + a_{01}(\frac{\partial u}{\partial y}, \frac{\partial v}{\partial y}) \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad + (f(u), v) = 0, \\ (\omega, \xi) = -(\frac{\partial u}{\partial x}, \frac{\partial \xi}{\partial x}), \\ (p, \zeta) = -(\frac{\partial u}{\partial y}, \frac{\partial \zeta}{\partial y}), \end{cases} \tag{5.85}$$

where the test functions v, ξ, ζ all belong to $H^1_{per}(\Omega)$.

Next, we introduce the discretization $\mathscr{T}_h$ of $\bar{\Omega}$ and set

$$V_h = \{v_h \in C^0(\bar{\Omega}),\ (v_h)_{|K} \in P_1,\ \forall K \in \mathscr{T}_h,\ v_h \text{ is } \Omega-\text{periodic}\} \subset H^1_{per}(\Omega).$$

As mentioned above, we use a P_1-finite element for the space discretization and a forward Euler scheme for the time discretization. Let $u_h^0 \in V_h$. Then, for $n \geq 0$, we look for $(u_h^{n+1}, \omega_h^{n+1}, p_h^{n+1}) \in V_h \times V_h \times V_h$ such that

$$\begin{cases} \frac{1}{dt}(u_h^{n+1}, v) - a_{20}(\frac{\partial \omega_h^{n+1}}{\partial x}, \frac{\partial v}{\partial x}) - a_{02}(\frac{\partial p_h^{n+1}}{\partial y}, \frac{\partial v}{\partial y}) \\ -a_{11}(\frac{\partial \omega_h^{n+1}}{\partial y}, \frac{\partial v}{\partial y}) + a_{10}(\frac{\partial u_h^{n+1}}{\partial x}, \frac{\partial v}{\partial x}) + a_{01}(\frac{\partial u_h^{n+1}}{\partial y}, \frac{\partial v}{\partial y}) + (f(u_h^n), v) - \frac{1}{dt}(u_h^n, v) = 0, \\ (\omega_h^{n+1}, \xi) = -(\frac{\partial u_h^{n+1}}{\partial x}, \frac{\partial \xi}{\partial x}), \\ (p_h^{n+1}, \zeta) = -(\frac{\partial u_h^{n+1}}{\partial y}, \frac{\partial \zeta}{\partial y}), \end{cases} \tag{5.86}$$

for all v, ξ, $\zeta \in V_h$. We proceed in a similar way for $k = 1$ and 3. In particular, for $k = 3$, we have to deal with a system of 5 second-order equations.

As far as the time step dt is concerned, when $k = 1$, we take $dt = 10^{-7}$ (in Figure 5.3 and Figure 5.7), $dt = 10^{-6}$ (in Figure 5.4) and $dt = 10^{-5}$ (in Figure 5.8). When $k = 2$, we take $dt = 10^{-7}$ and, when $k = 3$, we take $dt = 10^{-10}$ (in Figure 5.6 and Figure 5.12) and $dt = 10^{-8}$ (in Figure 5.10) or $dt = 10^{-7}$ (in Figure 5.3 and Figure 5.7). Here, we use a grid with 150^2 points on the domain Ω.

The next figure (Figure 5.2) shows the initial condition.

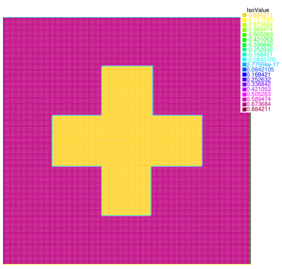
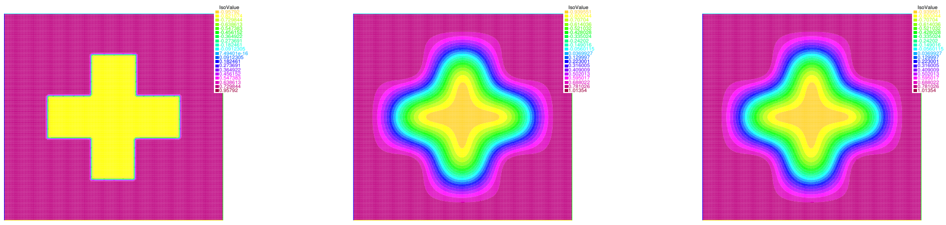


FIGURE 5.2 – Initial condition.

5.5.1 The isotropic case

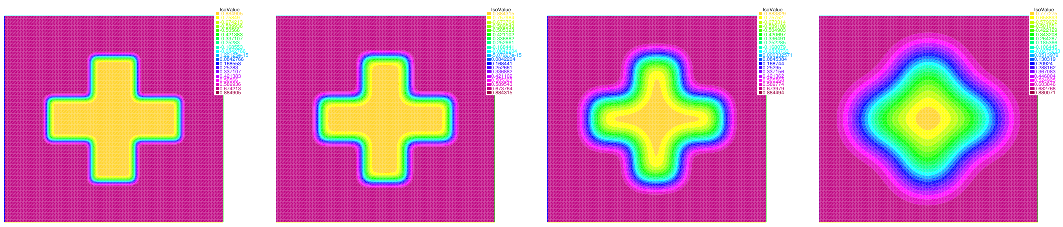
When all the coefficients are set equal to 1, then, as expected, there is no isotropy. The figures below however show the effects of higher-order terms.



(a) $k = 1$, $dt = 10^{-7}$ (b) $k = 2$, $dt = 10^{-7}$ (c) $k = 3$, $dt = 10^{-7}$

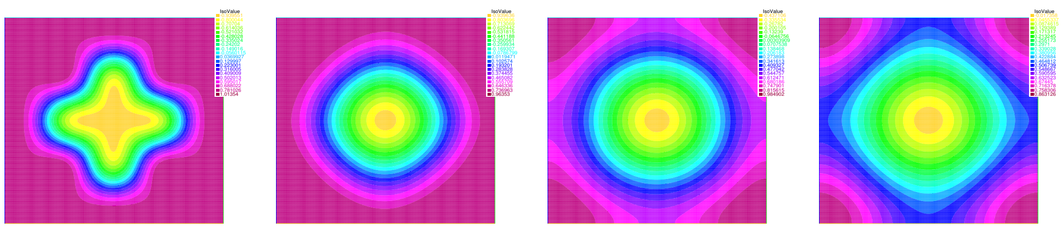
FIGURE 5.3 – Results after 40 iterations with different k's and the same time step size.

In the next figures, we take a different time step. We also note that the higher k is, the smaller the time step has to be taken, since the solution evolves faster in time.



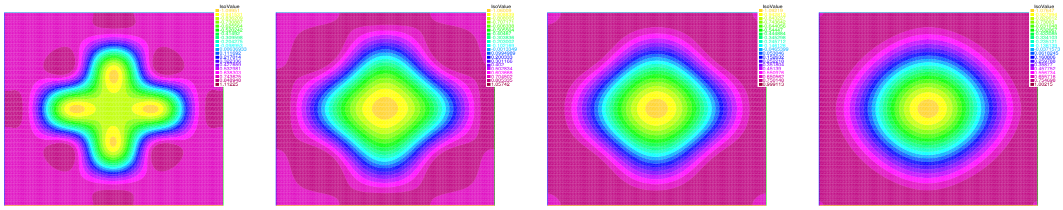
(a) $t = 100 \times dt$ (b) $t = 250 \times dt$ (c) $t = 1000 \times dt$ (d) $t = 4000 \times dt$

FIGURE 5.4 – $k = 1$, $dt = 10^{-6}$.



(a) $t = 40 \times dt$ (b) $t = 400 \times dt$ (c) $t = 2000 \times dt$ (d) $t = 5000 \times dt$

FIGURE 5.5 – $k = 2$, $dt = 10^{-7}$.

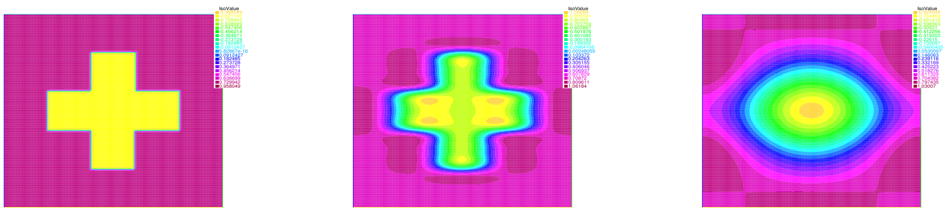


(a) $t = 40 \times dt$ (b) $t = 500 \times dt$ (c) $t = 1000 \times dt$ (d) $t = 2000 \times dt$

FIGURE 5.6 – $k = 3$, $dt = 10^{-10}$.

5.5.2 Anisotropy in the x−direction

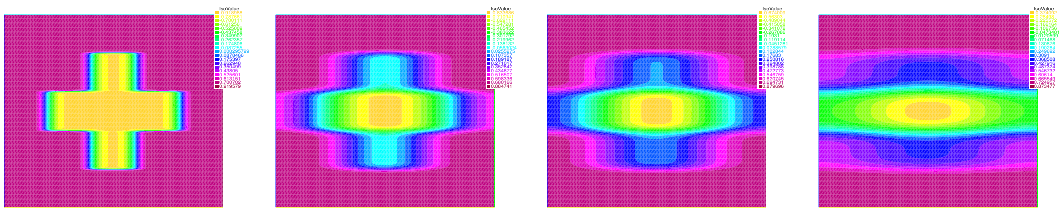
We now illustrate anisotropic situations. We consider the following situations :
(i) $k = 1$, $a_{10} = 1$ and $a_{01} = 0.01$;
(ii) $k = 2$, $a_{20} = 1$ and the other coefficients are set equal to 0.01 ;
(iii) $k = 3$, $a_{30} = 1$ and the other coefficients are set equal to 0.01.
We first investigate the anisotropy in the x−direction after 40 iterations, comparing different k's when the time step is the same.



(a) (b) (c)

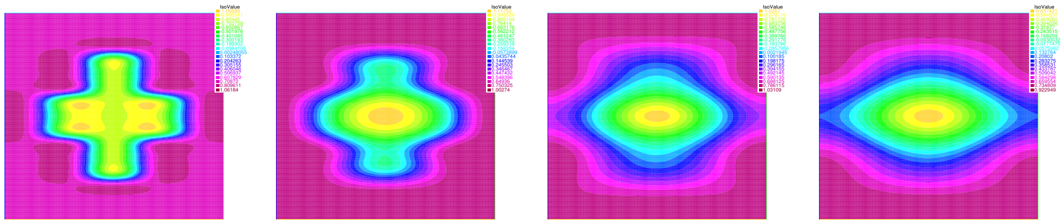
FIGURE 5.7 – (a) $k = 1$, $dt = 10^{-7}$; (b) $k = 2$, $dt = 10^{-7}$; (c) $k = 3$, $dt = 10^{-7}$.

We then illustrate the case when k, as well as the time step, remain unchanged, but the number of iterations increases.



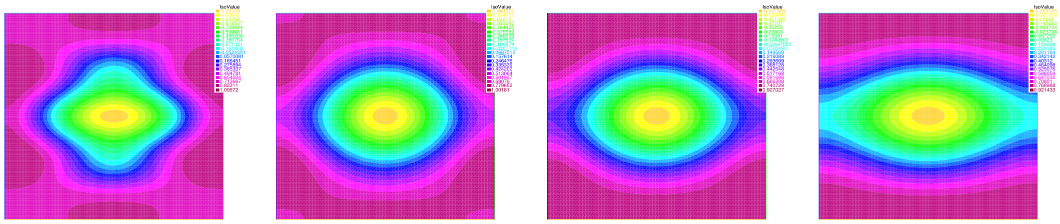
(a) $t = 50 \times dt$ (b) $t = 1000 \times dt$ (c) $t = 2000 \times dt$ (d) $t = 5000 \times dt$

FIGURE 5.8 – $k = 1$, $dt = 10^{-5}$.



(a) $t = 40 \times dt$ (b) $t = 400 \times dt$ (c) $t = 2000 \times dt$ (d) $t = 5000 \times dt$

FIGURE 5.9 – $k = 2$, $dt = 10^{-7}$.



(a) $t = 40 \times dt$ (b) $t = 500 \times dt$ (c) $t = 1000 \times dt$ (d) $t = 2000 \times dt$

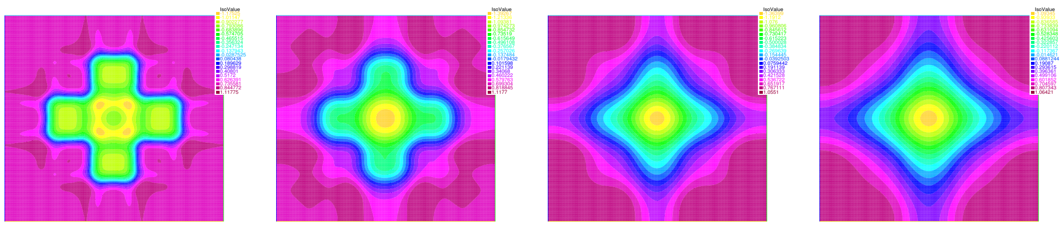
FIGURE 5.10 – $k = 3$, $dt = 10^{-8}$.

We can note that we would have similar results in the $y-$direction.

5.5.3 Influence of the off-diagonal terms

We first note that, when $k = 1$, there is no cross term. We thus consider the following two cases :

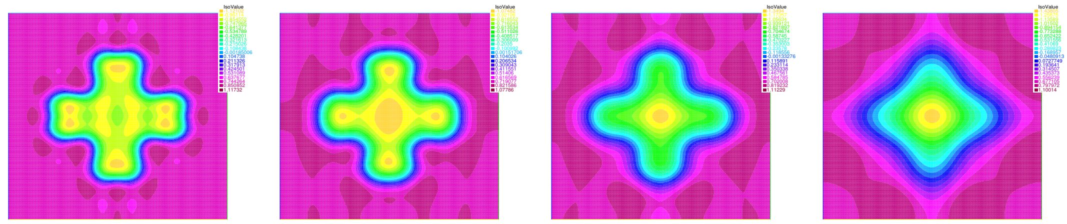
(i) $k = 2$, $a_{11} = 1$ and the other coefficients are set equal to 0.01.



(a) $t = 40 \times dt$ (b) $t = 400 \times dt$ (c) $t = 2000 \times dt$ (d) $t = 5000 \times dt$

FIGURE 5.11 – $k = 2$, $dt = 10^{-7}$.

(ii) $k = 3$, $a_{21} = 1$ and the other coefficients are set equal to 0.01.



(a) $t = 40 \times dt$ (b) $t = 250 \times dt$ (c) $t = 1000 \times dt$ (d) $t = 5000 \times dt$

FIGURE 5.12 – $k = 3$, $dt = 10^{-10}$: (a) after 40 iterations ; (b) after 250 iterations ; (c) after 1000 iterations ; (d) after 5000 iterations.

Chapitre 6

Higher-order generalized Cahn-Hilliard equations

Généralisations d'ordre élevé de l'équation de Cahn-Hilliard

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Higher-order generalized Cahn-Hilliard equations

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Abstract : Our aim in this paper is to study higher-order (in space) anisotropic generalized Cahn-Hilliard models. In particular, we obtain well-posedness results, as well as the existence of the global attractor. Such models can have applications in biology, image processing, etc. We also give numerical simulations which illustrate the effects of the higher-order terms and the anisotropy.

Key words and phrases : Cahn-Hilliard equation, higher-order models, anisotropy, well-posedness, global attractor, numerical simulations.
2010 Mathematics Subject Classification : 35K55, 35J60.

6.1 Introduction

The Cahn-Hilliard equation,

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) = 0, \tag{6.1}$$

plays an essential role in materials science and describes important qualitative features of two-phase systems related with phase separation processes, assuming isotropy and a constant temperature. This can be observed, e.g., when a binary alloy is cooled down sufficiently. One then observes a partial nucleation (i.e., the apparition of nucleides in the material) or a total nucleation, the so-called spinodal decomposition : the material quickly becomes inhomogeneous, forming a fine-grained structure in which each of the two components appears more or less alternatively. In a second stage, which is called coarsening, occurs at a slower time scale and is less understood, these microstructures coarsen. Such phenomena play an essential role in the mechanical properties of the material, e.g., strength. We refer the reader to, e.g., [19], [20], [36], [43], [83], [87], [105], [106], [107] and [108] for more details.

Here, u is the order parameter (e.g., a density of atoms) and f is the derivative of a double-well potential F. A thermodynamically relevant potential F is the following logarithmic function which follows from a mean-field model :

$$F(s) = \frac{\theta_c}{2}(1-s^2) + \frac{\theta}{2}[(1-s)\ln(\frac{1-s}{2}) + (1+s)\ln(\frac{1+s}{2})],\ s \in (-1,1),\ 0 < \theta < \theta_c, \tag{6.2}$$

i.e.,

$$f(s) = -\theta_c s + \frac{\theta}{2}\ln\frac{1+s}{1-s}, \tag{6.3}$$

although such a function is very often approximated by regular ones, typically,

$$F(s) = \frac{1}{4}(s^2-1)^2, \tag{6.4}$$

i.e.,

$$f(s) = s^3 - s. \tag{6.5}$$

Now, it is interesting to note that the Cahn-Hilliard equation and some of its variants are also relevant in other phenomena than phase separation. We can mention, for instance, population dynamics (see [31]), tumor growth (see [7] and [86]), bacterial films (see [81]), thin films (see [112] and [129]), image processing (see [8], [9], [21], [27] and [42]) and even the rings of Saturn (see [130]) and the clustering of mussels (see [90]).

In particular, several such phenomena can be modeled by the following generalized Cahn-Hilliard equation :

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) + g(x,u) = 0. \tag{6.6}$$

We studied in [97] and [99] (see also [7], [27], [37] and [47]) this equation.

The Cahn-Hilliard equation is based on the so-called Ginzburg-Landau free energy,

$$\Psi_{\mathrm{GL}} = \int_\Omega (\frac{1}{2}|\nabla u|^2 + F(u))\,dx, \tag{6.7}$$

where Ω is the domain occupied by the system (we assume here that it is a bounded and regular domain of $\mathbb{R}^n$, $n = 1$, 2 or 3, with boundary Γ). In particular, in (6.7), the term $|\nabla u|^2$ models short-ranged interactions. It is however interesting to note that such a term is obtained by truncation of higher-order ones (see [20]) ; it can also be seen as a first-order approximation of a nonlocal term accounting for long-ranged interactions (see [65] and [66]).

G. Caginalp and E. Esenturk recently proposed in [23] (see also [22]) higher-order phase-field models in order to account for anisotropic interfaces (see also [80], [125] and [132] for other approaches which, however, do not provide an explicit way to compute the anisotropy). More precisely, these authors proposed the following modified free energy, in which we omit the temperature :

$$\Psi_{\mathrm{HOGL}} = \int_\Omega (\frac{1}{2}\sum_{i=1}^{k}\sum_{|\alpha|=i} a_\alpha |\mathcal{D}^\alpha u|^2 + F(u))\,dx,\ k \in \mathbb{N}, \tag{6.8}$$

where, for $\alpha = (k_1, ..., k_n) \in (\mathbb{N} \cup \{0\})^n$,

$$|\alpha| = k_1 + ... + k_n$$

and, for $\alpha \neq (0, ..., 0)$,

$$\mathcal{D}^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{k_1} ... \partial x_n^{k_n}}$$

(we agree that $\mathcal{D}^{(0,...,0)} v = v$). The corresponding higher-order Cahn-Hilliard equation then reads

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0. \tag{6.9}$$

We studied in [32] and [33] the corresponding isotropic model which reads

$$\frac{\partial u}{\partial t} - \Delta P(-\Delta) u - \Delta f(u) = 0, \tag{6.10}$$

where

$$P(s) = \sum_{i=1}^{k} a_i s^i,\ a_k > 0,\ k \in \mathbb{N},\ s \in \mathbb{R}.$$

The anisotropic model (6.9) is treated in [34].

Our aim in this paper is to study the higher-order generalized Cahn-Hillard model

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) + g(x,u) = 0. \tag{6.11}$$

In particular, we study the well-posedness and the regularity of solutions. We also prove the dissipativity of the corresponding solution operators, as well as the existence of the global attractor. We finally give numerical simulations which show the effects of the higher-order terms and the anisotropy.

6.2 Setting of the problem

We consider the following initial and boundary value problem, for $k \in \mathbb{N}$, $k \geq 2$ (the case $k = 1$ can be treated as in [97]) :

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) + g(x,u) = 0, \tag{6.12}$$

$$\mathcal{D}^\alpha u = 0 \text{ on } \Gamma, \ |\alpha| \leq k, \tag{6.13}$$

$$u|_{t=0} = u_0. \tag{6.14}$$

We assume that

$$a_\alpha > 0, \ |\alpha| = k, \tag{6.15}$$

and we introduce the elliptic operator A_k defined by

$$\langle A_k v, w \rangle_{H^{-k}(\Omega), H_0^k(\Omega)} = \sum_{|\alpha|=k} a_\alpha ((\mathcal{D}^\alpha v, \mathcal{D}^\alpha w)), \tag{6.16}$$

where $H^{-k}(\Omega)$ is the topological dual of $H_0^k(\Omega)$. Furthermore, $((\cdot,\cdot))$ denotes the usual L^2-scalar product, with associated norm $\|\cdot\|$. More generally, we denote by $\|\cdot\|_X$ the norm on the Banach space X ; we also set $\|\cdot\|_{-1} = \|(-\Delta)^{-\frac{1}{2}} \cdot\|$, where $(-\Delta)^{-1}$ denotes the inverse minus Laplace operator associated with Dirichlet boundary conditions. We can note that

$$(v,w) \in H_0^k(\Omega)^2 \mapsto \sum_{|\alpha|=k} a_\alpha ((\mathcal{D}^\alpha v, \mathcal{D}^\alpha w))$$

is bilinear, symmetric, continuous and coercive, so that

$$A_k : H_0^k(\Omega) \to H^{-k}(\Omega)$$

is indeed well defined. It then follows from elliptic regularity results for linear elliptic operators of order $2k$ (see [1], [2] and [3]) that A_k is a strictly positive, selfadjoint and unbounded linear operator with compact inverse, with domain

$$D(A_k) = H^{2k}(\Omega) \cap H_0^k(\Omega),$$

where, for $v \in D(A_k)$,

$$A_k v = (-1)^k \sum_{|\alpha|=k} a_\alpha \mathcal{D}^{2\alpha} v.$$

We further note that $D(A_k^{\frac{1}{2}}) = H_0^k(\Omega)$ and, for $(v, w) \in D(A_k^{\frac{1}{2}})^2$,

$$((A_k^{\frac{1}{2}} v, A_k^{\frac{1}{2}} w)) = \sum_{|\alpha|=k} a_\alpha ((\mathcal{D}^\alpha v, \mathcal{D}^\alpha w)).$$

We finally note that (see, e.g., [127]) $\|A_k \cdot\|$ (resp., $\|A_k^{\frac{1}{2}} \cdot\|$) is equivalent to the usual H^{2k}-norm (resp., H^k-norm) on $D(A_k)$ (resp., $D(A_k^{\frac{1}{2}})$).

Similarly, we can define the linear operator $\overline{A}_k = -\Delta A_k$,

$$\overline{A}_k : H_0^{k+1}(\Omega) \to H^{-k-1}(\Omega)$$

which is a strictly positive, selfadjoint and unbounded linear operator with compact inverse, with domain

$$D(\overline{A}_k) = H^{2k+2}(\Omega) \cap H_0^{k+1}(\Omega),$$

where, for $v \in D(\overline{A}_k)$,

$$\overline{A}_k v = (-1)^{k+1} \Delta \sum_{|\alpha|=k} a_\alpha \mathcal{D}^{2\alpha} v.$$

Furthermore, $D(\overline{A}_k^{\frac{1}{2}}) = H_0^{k+1}(\Omega)$ and, for $(v, w) \in D(\overline{A}_k^{\frac{1}{2}})^2$,

$$((\overline{A}_k^{\frac{1}{2}} v, \overline{A}_k^{\frac{1}{2}} w)) = \sum_{|\alpha|=k} a_\alpha ((\nabla \mathcal{D}^\alpha v, \nabla \mathcal{D}^\alpha w)).$$

Besides, $\|\overline{A}_k \cdot\|$ (resp., $\|\overline{A}_k^{\frac{1}{2}} \cdot\|$) is equivalent to the usual H^{2k+2}-norm (resp., H^{k+1}-norm) on $D(\overline{A}_k)$ (resp., $D(\overline{A}_k^{\frac{1}{2}})$).

We finally consider the operator $\tilde{A}_k = (-\Delta)^{-1} A_k$, where

$$\tilde{A}_k : H_0^{k-1}(\Omega) \to H^{-k+1}(\Omega);$$

note that, as $-\Delta$ and A_k commute, then the same holds for $(-\Delta)^{-1}$ and A_k, so that $\tilde{A}_k = A_k(-\Delta)^{-1}$.

We have the

Lemma 6.2.1. *The operator $\tilde{A}_k$ is a strictly positive, selfadjoint and unbounded linear operator with compact inverse, with domain*

$$D(\tilde{A}_k) = H^{2k-2}(\Omega) \cap H_0^{k-1}(\Omega),$$

where, for $v \in D(\tilde{A}_k)$,

$$\tilde{A}_k v = (-1)^k \sum_{|\alpha|=k} a_\alpha \mathcal{D}^{2\alpha}(-\Delta)^{-1} v.$$

Furthermore, $D(\tilde{A}_k^{\frac{1}{2}}) = H_0^{k-1}(\Omega)$ and, for $(v,w) \in D(\tilde{A}_k^{\frac{1}{2}})^2$,

$$((\tilde{A}_k^{\frac{1}{2}} v, \tilde{A}_k^{\frac{1}{2}} w)) = \sum_{|\alpha|=k} a_\alpha ((\mathcal{D}^\alpha (-\Delta)^{-\frac{1}{2}} v, \mathcal{D}^\alpha (-\Delta)^{-\frac{1}{2}} w)).$$

Besides, $\|\tilde{A}_k \cdot \|$ (resp., $\|\tilde{A}_k^{\frac{1}{2}} \cdot \|$) is equivalent to the usual H^{2k-2}-norm (resp., H^{k-1}-norm) on $D(\tilde{A}_k)$ (resp., $D(\tilde{A}_k^{\frac{1}{2}})$).

Proof.

We first note that $\tilde{A}_k$ clearly is linear and unbounded. Then, since $(-\Delta)^{-1}$ and A_k commute, it easily follows that $\tilde{A}_k$ is selfadjoint.

Next, the domain of $\tilde{A}_k$ is defined by

$$D(\tilde{A}_k) = \{v \in H_0^{k-1}(\Omega),\ \tilde{A}_k v \in L^2(\Omega)\}.$$

Noting that $\tilde{A}_k v = f$, $f \in L^2(\Omega)$, $v \in D(\tilde{A}_k)$, is equivalent to $A_k v = -\Delta f$, where $-\Delta f \in H^2(\Omega)'$, it follows from the elliptic regularity results of [1], [2] and [3] that $v \in H^{2k-2}(\Omega)$, so that $D(\tilde{A}_k) = H^{2k-2}(\Omega) \cap H_0^{k-1}(\Omega)$.

Noting then that $\tilde{A}_k^{-1}$ maps $L^2(\Omega)$ onto $H^{2k-2}(\Omega)$ and recalling that $k \geq 2$, we deduce that $\tilde{A}_k$ has compact inverse.

We now note that, considering the spectral properties of $-\Delta$ and A_k (see, e.g., [127]) and recalling that these two operators commute, $-\Delta$ and A_k have a spectral basis formed of common eigenvectors. This yields that, $\forall s_1, s_2 \in \mathbb{R}$, $(-\Delta)^{s_1}$ and $A_k^{s_2}$ commute.

Having this, we see that $\tilde{A}_k^{\frac{1}{2}} = (-\Delta)^{-\frac{1}{2}} A_k^{\frac{1}{2}}$, so that $D(\tilde{A}_k^{\frac{1}{2}}) = H_0^{k-1}(\Omega)$, and, for $(v,w) \in D(\tilde{A}_k^{\frac{1}{2}})^2$,

$$((\tilde{A}_k^{\frac{1}{2}}v, \tilde{A}_k^{\frac{1}{2}}w)) = \sum_{|\alpha|=k} a_\alpha((\mathcal{D}^\alpha(-\Delta)^{-\frac{1}{2}}v, \mathcal{D}^\alpha(-\Delta)^{-\frac{1}{2}}w)).$$

Finally, as far as the equivalences of norms are concerned, we can note that, for instance, the norm $\|\tilde{A}_k^{\frac{1}{2}} \cdot \|$ is equivalent to the norm $\|(-\Delta)^{-\frac{1}{2}} \cdot \|_{H^k(\Omega)}$ and, thus, to the norm $\|(-\Delta)^{\frac{k-1}{2}} \cdot \|$.

□

Having this, we rewrite (6.12) as

$$\frac{\partial u}{\partial t} - \Delta A_k u - \Delta B_k u - \Delta f(u) + g(x,u) = 0, \tag{6.17}$$

where

$$B_k v = \sum_{i=1}^{k-1}(-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} v.$$

As far as the nonlinear term f is concerned, we assume that

$$f \in C^2(\mathbb{R}),\ f(0) = 0, \tag{6.18}$$

$$f' \geq -c_0,\ c_0 \geq 0, \tag{6.19}$$

$$f(s)s \geq c_1 F(s) - c_2 \geq -c_3,\ c_1 > 0,\ c_2,\ c_3 \geq 0,\ s \in \mathbb{R}, \tag{6.20}$$

$$F(s) \geq c_4 s^4 - c_5,\ c_4 > 0,\ c_5 \geq 0,\ s \in \mathbb{R}, \tag{6.21}$$

where $F(s) = \int_0^s f(\xi)\,d\xi$. In particular, the usual cubic nonlinear term $f(s) = s^3 - s$ satisfies these assumptions.

Furthermore, as far as the function g is concerned, we assume that

$$g(\cdot,s) \text{ is measurable, } \forall s \in \mathbb{R},\ g(x,\cdot) \text{ is of class } C^1, \text{ a.e. } x \in \Omega, \tag{6.22}$$
$$\frac{\partial g}{\partial s}(.,s) \text{ is measurable, } \forall s \in \mathbb{R};$$

$$|g(x,s)| \leq h(s), \text{ a.e. } x \in \Omega,\ s \in \mathbb{R}, \tag{6.23}$$

where $h \geq 0$ is continuous and satisfies

$$\|h(v)\|\|v\| \leq \varepsilon \int_\Omega F(v)\,dx + c_\varepsilon,\ \forall \varepsilon > 0, \tag{6.24}$$

$\forall v \in L^2(\Omega)$ such that $\int_\Omega F(v)\,dx < +\infty$, and

$$|h(s)|^2 \leq c_6 F(s) + c_7,\ c_6,\ c_7 \geq 0,\ s \in \mathbb{R}; \tag{6.25}$$

$$|\frac{\partial g}{\partial s}(x,s)| \leq l(s),\ \text{a.e. } x \in \Omega,\ s \in \mathbb{R}, \tag{6.26}$$

where $l \geq 0$ is continuous.

Example 6.2.1. We assume that $f(s) = s^3 - s$. Assumptions (6.22)-(6.26) are satisfied in the following cases.
(i) Cahn-Hilliard-Oono equation (see [95], [111] and [131]). In that case,

$$g(x,s) = g(s) = \beta s,\ \beta > 0.$$

This function was proposed in [111] in order to account for long-ranged (i.e., nonlocal) interactions, but also to simplify numerical simulations.
(ii) Proliferation term. In that case,

$$g(x,s) = g(s) = \beta s(s-1),\ \beta > 0.$$

This function was proposed in [86] in view of biological applications and, more precisely, to model wound healing and tumor growth (in one space dimension) and the clustering of brain tumor cells (in two space dimensions) ; see also [7] for other quadratic functions.
(iii) Fidelity term. In that case,

$$g(x,s) = \lambda_0 \chi_{\Omega\backslash D}(x)(s - \varphi(x)),\ \lambda_0 > 0,\ D \subset \Omega,\ \varphi \in L^2(\Omega),$$

where χ denotes the indicator function. This function was proposed in [8] and [9] in view of applications to image inpainting. Here, φ is a given (damaged) image and D is the inpainting (i.e., damaged) region. Furthermore, the fidelity term $g(x,u)$ is added in order to keep the solution close to the image outside the inpainting region. The idea in this model is to solve the equation up to steady state to obtain an inpainted (i.e., restored) version $u(x)$ of $\varphi(x)$.

Throughout the paper, the same letters c, c' and c'' denote (generally positive) constants which may vary from line to line. Similarly, the same letters Q and Q' denote (positive) monotone increasing and continuous (with respect to each argument) functions which may vary from line to line.

6.3 A priori estimates

We multiply (6.17) by $(-\Delta)^{-1}\frac{\partial u}{\partial t}$ and integrate over Ω and by parts. This gives

$$\frac{d}{dt}(\|A_k^{\frac{1}{2}}u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)\,dx) + 2\|\frac{\partial u}{\partial t}\|_{-1}^2 = -((g(\cdot,u),(-\Delta)^{-1}\frac{\partial u}{\partial t})),$$

where

$$B_k^{\frac{1}{2}}[u] = \sum_{i=1}^{k-1}\sum_{|\alpha|=i} a_\alpha \|\mathcal{D}^\alpha u\|^2$$

(note that $B_k^{\frac{1}{2}}[u]$ is not necessarily nonnegative). This yields, owing to (6.23) and (6.25),

$$\frac{d}{dt}(\|A_k^{\frac{1}{2}}u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)\,dx) + \|\frac{\partial u}{\partial t}\|_{-1}^2 \leq c\int_\Omega F(u)\,dx + c'. \tag{6.27}$$

We can note that, owing to the interpolation inequality

$$\|v\|_{H^i(\Omega)} \leq c(i)\|v\|_{H^m(\Omega)}^{\frac{i}{m}}\|v\|^{1-\frac{i}{m}}, \tag{6.28}$$
$$v \in H^m(\Omega),\ i \in \{1,\dots,m-1\},\ m \in \mathbb{N},\ m \geq 2,$$

there holds

$$|B_k^{\frac{1}{2}}[u]| \leq \frac{1}{2}\|A_k^{\frac{1}{2}}u\|^2 + c\|u\|^2.$$

This yields, employing (6.21),

$$\|A_k^{\frac{1}{2}}u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)\,dx \geq \frac{1}{2}\|A_k^{\frac{1}{2}}u\|^2 + \int_\Omega F(u)\,dx + c\|u\|_{L^4(\Omega)}^4 - c'\|u\|^2 - c'',$$

whence

$$\|A_k^{\frac{1}{2}}u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)\,dx \geq c(\|u\|_{H^k(\Omega)}^2 + \int_\Omega F(u)\,dx) - c',\ c > 0, \tag{6.29}$$

noting that, owing to Young's inequality,

$$\|u\|^2 \leq \varepsilon\|u\|_{L^4(\Omega)}^4 + c_\varepsilon,\ \forall \varepsilon > 0. \tag{6.30}$$

We then multiply (6.17) by $(-\Delta)^{-1}u$ and have, owing to (6.20), (6.23), (6.24) and the interpolation inequality (6.28),

$$\frac{d}{dt}\|u\|_{-1}^2 + c(\|u\|_{H^k(\Omega)}^2 + \int_\Omega F(u)\,dx) \le c'\|u\|^2 + \varepsilon \int_\Omega F(u)\,dx + c''_\varepsilon,\ \forall \varepsilon > 0,$$

hence, proceeding as above and employing, in particular, (6.21),

$$\frac{d}{dt}\|u\|_{-1}^2 + c(\|u\|_{H^k(\Omega)}^2 + \int_\Omega F(u)\,dx) \le c',\ c > 0. \tag{6.31}$$

Summing δ_1 times (6.27) and (6.31), where $\delta_1 > 0$ is small enough, we obtain a differential inequality of the form

$$\frac{dE_1}{dt} + c(E_1 + \|\frac{\partial u}{\partial t}\|_{-1}^2) \le c',\ c > 0, \tag{6.32}$$

where

$$E_1 = \delta_1(\|A_k^{\frac{1}{2}}u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)\,dx) + \|u\|_{-1}^2$$

satisfies, owing to (6.29),

$$E_1 \ge c(\|u\|_{H^k(\Omega)}^2 + \int_\Omega F(u)\,dx) - c',\ c > 0. \tag{6.33}$$

Note indeed that

$$E_1 \le c\|u\|_{H^k(\Omega)}^2 + 2\int_\Omega F(u)\,dx$$

$$\le c(\|u\|_{H^k(\Omega)}^2 + \int_\Omega F(u)\,dx) - c',\ c > 0,\ c' \ge 0.$$

It follows from (6.32)-(6.33) and Gronwall's lemma that

$$\|u(t)\|_{H^k(\Omega)}^2 \le ce^{-c't}(\|u_0\|_{H^k(\Omega)}^2 + \int_\Omega F(u_0)\,dx) + c'',\ c' > 0,\ t \ge 0, \tag{6.34}$$

and

$$\int_t^{t+r} \|\frac{\partial u}{\partial t}\|_{-1}^2\,ds \le ce^{-c't}(\|u_0\|_{H^k(\Omega)}^2 + \int_\Omega F(u_0)\,dx) + c'',\ c' > 0,\ t \ge 0,\ r > 0 \text{ given.} \tag{6.35}$$

Multiplying next (6.17) by $\tilde{A}_k u$, we find, owing to (6.23) and the interpolation inequality (6.28),

$$\frac{d}{dt}\|\tilde{A}_k^{\frac{1}{2}}u\|^2 + c\|u\|_{H^{2k}(\Omega)}^2 \le c(\|u\|^2 + \|f(u)\|^2 + \|h(u)\|^2). \tag{6.36}$$

It follows from the continuity of f, F and h, the continuous embedding $H^k(\Omega) \subset C(\overline{\Omega})$ (recall that $k \geq 2$) and (6.34) that

$$\|u\|^2 + \|f(u)\|^2 + \|h(u)\|^2 \leq Q(\|u\|_{H^k(\Omega)}) \tag{6.37}$$
$$\leq e^{-ct} Q(\|u_0\|_{H^k(\Omega)}) + c',\ c > 0,\ t \geq 0,$$

so that

$$\frac{d}{dt}\|\tilde{A}_k^{\frac{1}{2}} u\|^2 + c\|u\|^2_{H^{2k}(\Omega)} \leq e^{-c't} Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0,\ t \geq 0. \tag{6.38}$$

Summing (6.32) and (6.38), we have a differential inequality of the form

$$\frac{dE_2}{dt} + c(E_2 + \|u\|^2_{H^{2k}(\Omega)} + \|\frac{\partial u}{\partial t}\|^2_{-1}) \leq e^{-c't} Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0,\ t \geq 0, \tag{6.39}$$

where

$$E_2 = E_1 + \|\tilde{A}_k^{\frac{1}{2}} u\|^2$$

satisfies

$$E_2 \geq c(\|u\|^2_{H^k(\Omega)} + \int_\Omega F(u)\, dx) - c',\ c > 0. \tag{6.40}$$

We now multiply (6.17) by $\frac{\partial u}{\partial t}$ and obtain, noting that f is of class C^2, so that

$$\|\Delta f(u)\| \leq Q(\|u\|_{H^k(\Omega)}),$$

and proceeding as above,

$$\frac{d}{dt}(\|\overline{A}_k^{\frac{1}{2}} u\|^2 + \overline{B}_k^{\frac{1}{2}}[u]) + \|\frac{\partial u}{\partial t}\|^2 \leq e^{-c't} Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0, \tag{6.41}$$

where

$$\overline{B}_k^{\frac{1}{2}}[u] = \sum_{i=1}^{k-1} \sum_{|\alpha|=i} a_\alpha \|\nabla \mathcal{D}^\alpha u\|^2.$$

Summing finally (6.39) and (6.41), we find a differential inequality of the form

$$\frac{dE_3}{dt} + c(E_3 + \|u\|^2_{H^{2k}(\Omega)} + \|\frac{\partial u}{\partial t}\|^2) \leq e^{-c't} Q(\|u_0\|_{H^k(\Omega)}) + c'',\ c,\ c' > 0,\ t \geq 0, \tag{6.42}$$

where

$$E_3 = E_2 + \|\overline{A}_k^{\frac{1}{2}} u\|^2 + \overline{B}_k^{\frac{1}{2}}[u]$$

satisfies, proceeding as above,

$$E_3 \geq c(\|u\|^2_{H^{k+1}(\Omega)} + \int_\Omega F(u)\, dx) - c',\ c > 0. \tag{6.43}$$

In particular, it follows from (6.42)-(6.43) that

$$\|u(t)\|_{H^{k+1}(\Omega)} \leq e^{-ct} Q(\|u_0\|_{H^{k+1}(\Omega)}) + c',\ c > 0,\ t \geq 0. \tag{6.44}$$

We then rewrite (6.17) as an elliptic equation, for $t > 0$ fixed,

$$A_k u = -(-\Delta)^{-1} \frac{\partial u}{\partial t} - B_k u - f(u) - (-\Delta)^{-1} g(x,u),\ \mathcal{D}^\alpha u = 0 \text{ on } \Gamma,\ |\alpha| \leq k-1. \tag{6.45}$$

Multiplying (6.45) by $A_k u$, we have, owing to (6.23) and the interpolation inequality (6.28),

$$\|A_k u\|^2 \leq c(\|u\|^2 + \|f(u)\|^2 + \|h(u)\|^2 + \|\frac{\partial u}{\partial t}\|^2_{-1}), \tag{6.46}$$

hence, proceeding as above (employing, in particular, (6.37)),

$$\|u\|^2_{H^{2k}(\Omega)} \leq c(e^{-c't} Q(\|u_0\|_{H^k(\Omega)}) + \|\frac{\partial u}{\partial t}\|^2_{-1}) + c'',\ c' > 0. \tag{6.47}$$

In a next step, we differentiate (6.17) with respect to time and obtain

$$\frac{\partial}{\partial t}\frac{\partial u}{\partial t} - \Delta A_k \frac{\partial u}{\partial t} - \Delta B_k \frac{\partial u}{\partial t} - \Delta(f'(u)\frac{\partial u}{\partial t}) + \frac{\partial g}{\partial s}(x,u)\frac{\partial u}{\partial t} = 0, \tag{6.48}$$

$$\mathcal{D}^\alpha \frac{\partial u}{\partial t} = 0 \text{ on } \Gamma,\ |\alpha| \leq k. \tag{6.49}$$

We multiply (6.48) by $(-\Delta)^{-1}\frac{\partial u}{\partial t}$ and find, owing to (6.19), (6.26), the interpolation inequality (6.28) and the continuous embedding $H^2(\Omega) \subset L^\infty(\Omega)$,

$$\begin{aligned} \frac{d}{dt}\|\frac{\partial u}{\partial t}\|^2_{-1} + c\|\frac{\partial u}{\partial t}\|^2_{H^k(\Omega)} &\leq c'(\|\frac{\partial u}{\partial t}\|^2 + \|l(u)\|\|\frac{\partial u}{\partial t}\|\|(-\Delta)^{-1}\frac{\partial u}{\partial t}\|_{L^\infty(\Omega)}) \\ &\leq c'(\|\frac{\partial u}{\partial t}\|^2 + \|l(u)\|\|\frac{\partial u}{\partial t}\|^2),\ c > 0, \end{aligned}$$

which yields, employing the interpolation inequality

$$\|v\|^2 \leq c\|v\|_{-1}\|v\|_{H^1(\Omega)},\ v \in H^1_0(\Omega), \tag{6.50}$$

and proceeding as above (note that l is continuous), the differential inequality

$$\frac{d}{dt}\|\frac{\partial u}{\partial t}\|_{-1}^2 + c\|\frac{\partial u}{\partial t}\|_{H^k(\Omega)}^2 \le c'(e^{-c''t}Q(\|u_0\|_{H^k(\Omega)}) + 1)\|\frac{\partial u}{\partial t}\|_{-1}^2,\ c,\ c'' > 0. \tag{6.51}$$

In particular, this yields, owing to (6.35) and employing the uniform Gronwall's lemma (see, e.g., [127]),

$$\|\frac{\partial u}{\partial t}(t)\|_{-1} \le \frac{1}{r^{\frac{1}{2}}}Q(e^{-ct}Q'(\|u_0\|_{H^k(\Omega)}) + c'),\ c > 0,\ t \ge r,\ r > 0 \text{ given}, \tag{6.52}$$

where the (continuous and monotone increasing) function Q is of the form $Q(s) = cse^{c's}$.

In particular, it follows from (6.47) and (6.52) (for $r = 1$) that

$$\|u(t)\|_{H^{2k}(\Omega)} \le Q(e^{-ct}Q'(\|u_0\|_{H^k(\Omega)}) + c'),\ c > 0,\ t \ge 1. \tag{6.53}$$

Remark 6.3.1. *If we assume that $u_0 \in H^{2k+1}(\Omega) \cap H_0^k(\Omega)$, we deduce from (6.47), (6.51) and Gronwall's lemma an H^{2k}-estimate on u on $[0, 1]$ which, combined with (6.53), gives an H^{2k}-estimate on u, for all times. This is however not satisfactory, in particular, in view of the study of attractors.*

Remark 6.3.2. *We assume that, for simplicity, $g(x, s) = g(s)$ and we further assume that f is of class C^{k+1} and g is of class C^{k-1}. Multiplying (6.17) by $\tilde{A}_k \frac{\partial u}{\partial t}$, we have*

$$\frac{1}{2}\frac{d}{dt}(\|A_k u\|^2 + ((A_k u, B_k u))) + \|\tilde{A}_k^{\frac{1}{2}}\frac{\partial u}{\partial t}\|^2 = -((\overline{A}_k^{\frac{1}{2}}f(u), \tilde{A}_k^{\frac{1}{2}}\frac{\partial u}{\partial t})) - ((\tilde{A}_k^{\frac{1}{2}}g(u), \tilde{A}_k^{\frac{1}{2}}\frac{\partial u}{\partial t})),$$

which yields, noting that $\|\overline{A}_k^{\frac{1}{2}}f(u)\|^2 + \|\tilde{A}_k^{\frac{1}{2}}g(u)\|^2 \le Q(\|u\|_{H^{k+1}(\Omega)})$ and owing to (6.44),

$$\frac{d}{dt}(\|A_k u\|^2 + ((A_k u, B_k u))) \le e^{-ct}Q(\|u_0\|_{H^{k+1}(\Omega)}) + c',\ c > 0,\ t \ge 0. \tag{6.54}$$

Combining (6.54) with (6.42), it follows from (6.43) and the interpolation inequality (6.28) that

$$\|u(t)\|_{H^{2k}(\Omega)} \le Q(\|u_0\|_{H^{2k}(\Omega)}),\ t \in [0, 1],$$

so that, owing to (6.53),

$$\|u(t)\|_{H^{2k}(\Omega)} \le Q(e^{-ct}Q'(\|u_0\|_{H^{2k}(\Omega)}) + c'),\ c > 0,\ t \ge 0. \tag{6.55}$$

6.4 The dissipative semigroup

We first give the definition of a weak solution to (6.12)-(6.14).

Definition 6.4.1. We assume that $u_0 \in L^2(\Omega)$. A weak solution to (6.12)-(6.14) is a function u such that, for any given $T > 0$,

$$u \in C([0,T]; L^2(\Omega)) \cap L^2(0,T; H_0^k(\Omega)),$$

$$u(0) = u_0 \text{ in } L^2(\Omega)$$

and

$$\frac{d}{dt}(((-\Delta)^{-1}u, v)) + \sum_{i=1}^{k} \sum_{|\alpha|=i} a_i((\mathcal{D}^\alpha u, \mathcal{D}^\alpha v)) + ((f(u), v))$$

$$+(((-\Delta)^{-1}g(x,u), v)) = 0, \ \forall v \in H_0^k(\Omega),$$

in the sense of distributions.

We have the

Theorem 6.4.1. *(i) We assume that $u_0 \in H_0^k(\Omega)$. Then, (6.12)-(6.14) possesses a unique weak solution u such that, $\forall T > 0$,*

$$u \in L^\infty(\mathbb{R}^+; H_0^k(\Omega)) \cap L^2(0,T; H^{2k}(\Omega) \cap H_0^k(\Omega))$$

and

$$\frac{\partial u}{\partial t} \in L^2(0,T; H^{-1}(\Omega)).$$

(ii) If we further assume that $u_0 \in H^{k+1}(\Omega) \cap H_0^k(\Omega)$, then, $\forall T > 0$,

$$u \in L^\infty(\mathbb{R}^+; H^{k+1}(\Omega) \cap H_0^k(\Omega))$$

and

$$\frac{\partial u}{\partial t} \in L^2(0,T; L^2(\Omega)).$$

(iii) If we further assume that f is of class C^{k+1}, $g(x,s) = g(s)$, g is of class C^{k-1} and $u_0 \in H^{2k}(\Omega) \cap H_0^k(\Omega)$, then

$$u \in L^\infty(\mathbb{R}^+; H^{2k}(\Omega) \cap H_0^k(\Omega)).$$

Proof. The proofs of existence and regularity in (i), (ii) and (iii) follow from the a priori estimates derived in the previous section and, e.g., a standard Galerkin scheme. Indeed, we can note that, since the operators $-\Delta$, A_k, $\overline{A}_k$ and $\tilde{A}_k$ are linear, selfadjoint and strictly positive operators with compact inverse which commute, they have a spectral basis formed of common eigenvectors. We then take this spectral basis as Galerkin basis, so that all the a priori estimates derived in the previous section are justified within the Galerkin scheme.

Let now u_1 and u_2 be two solutions to (6.12)-(6.13) with initial data $u_{0,1}$ and $u_{0,2}$, respectively. We set $u = u_1 - u_2$ and $u_0 = u_{0,1} - u_{0,2}$ and have

$$\frac{\partial u}{\partial t} - \Delta A_k u - \Delta B_k u - \Delta(f(u_1) - f(u_2)) + g(x, u_1) - g(x, u_2) = 0, \tag{6.56}$$

$$\mathcal{D}^\alpha u = 0 \text{ on } \Gamma, \ |\alpha| \le k, \tag{6.57}$$

$$u|_{t=0} = u_0. \tag{6.58}$$

Multiplying (6.56) by $(-\Delta)^{-1}u$, we obtain, owing to (6.19), (6.26), (6.34) and the interpolation inequalities (6.28) and (6.50),

$$\frac{d}{dt}\|u\|_{-1}^2 + c\|u\|_{H^k(\Omega)}^2 \le Q\|u\|_{-1}^2, \ c > 0, \tag{6.59}$$

where

$$Q = Q(\|u_{0,1}\|_{H^k(\Omega)}, \|u_{0,2}\|_{H^k(\Omega)}).$$

Here, we have used the fact that, owing to (6.26) and (6.34),

$$\begin{aligned}\|g(x, u_1) - g(x, u_2)\| &\le Q(\|u_1\|_{H^k(\Omega)}, \|u_2\|_{H^k(\Omega)})\|u\| \\ &\le Q(\|u_{0,1}\|_{H^k(\Omega)}, \|u_{0,2}\|_{H^k(\Omega)})\|u\|.\end{aligned}$$

It follows from (6.59) and Gronwall's lemma that

$$\|u(t)\|_{-1}^2 \le e^{Qt}\|u_0\|_{-1}^2, \ t \ge 0, \tag{6.60}$$

hence the uniqueness, as well as the continuous dependence with respect to the initial data in the H^{-1}-norm.

□

It follows from Theorem 6.4.1 that we can define the family of solving operators

$$S(t) : \Phi \to \Phi, \ u_0 \mapsto u(t), \ t \ge 0,$$

where $\Phi = H_0^k(\Omega)$. This family of solving operators forms a semigroup which is continuous with respect to the H^{-1}-topology. Finally, it follows from (6.34) that we have the

Theorem 6.4.2. *The semigroup $S(t)$ is dissipative in Φ, in the sense that it possesses a bounded absorbing set $\mathcal{B}_0 \subset \Phi$ (i.e., $\forall B \subset \Phi$ bounded, $\exists t_0 = t_0(B) \geq 0$ such that $t \geq t_0 \implies S(t)B \subset \mathcal{B}_0$).*

Remark 6.4.1. *(i) Actually, it follows from (6.53) that we have a bounded absorbing set $\mathcal{B}_1$ which is compact in Φ and bounded in $H^{2k}(\Omega)$. This yields the existence of the global attractor $\mathcal{A}$ which is compact in Φ and bounded in $H^{2k}(\Omega)$.*

(ii) We recall that the global attractor $\mathcal{A}$ is the smallest (for the inclusion) compact set of the phase space which is invariant by the flow (i.e., $S(t)\mathcal{A} = \mathcal{A}$, $\forall t \geq 0$) and attracts all bounded sets of initial data as time goes to infinity ; it thus appears as a suitable object in view of the study of the asymptotic behavior of the system. We refer the reader to, e.g., [103] and [127] for more details and discussions on this.

(iii) We can also prove, based on standard arguments (see, e.g., [103] and [127]) that $\mathcal{A}$ has finite dimension, in the sense of covering dimensions such as the Hausdorff and the fractal dimensions. The finite-dimensionality means, very roughly speaking, that, even though the initial phase space has infinite dimension, the reduced dynamics can be described by a finite number of parameters (we refer the interested reader to, e.g., [103] and [127] for discussions on this subject).

Remark 6.4.2. *In the numerical simulations given in the next section below, the equations will be endowed with periodic boundary conditions. From a mathematical point of view, these boundary conditions are much more delicate to handle, since we have to estimate the spatial average of the order parameter $\langle u \rangle = \frac{1}{\mathrm{Vol}(\Omega)} \int_\Omega u\,dx$ (see [27], [36] and [47]). When $g \equiv 0$, this is straightforward, since we have the conservation of mass, namely,*

$$\langle u(t) \rangle = \langle u_0 \rangle, \ \forall t \geq 0.$$

However, when g does not vanish, we are not able to estimate this quantity in general.

6.5 Numerical simulations

We give in this section several numerical simulations in order to illustrate the effects of the higher-order terms on the anisotropy. The computations presented below are performed with the software FreeFem++, for $k = 2$. We also take Ω bi-dimensional and rectangular. Finally, the system is associated with periodic boundary conditions.

The problem can be written as, for $k = 2$,

$$
\begin{cases}
\dfrac{\partial u}{\partial t} + \Delta w + \dfrac{1}{\varepsilon} g(x,u) = 0, \\
w + a_{20}\varepsilon \dfrac{\partial^4 u}{\partial x^4} + a_{02}\varepsilon \dfrac{\partial^4 u}{\partial y^4} + a_{11}\varepsilon \dfrac{\partial^4 u}{\partial x^2 \partial y^2} - a_{10}\varepsilon \dfrac{\partial^2 u}{\partial x^2} - a_{01}\varepsilon \dfrac{\partial^2 u}{\partial y^2} + \dfrac{1}{\varepsilon} f(u) = 0, \\
u,\ w \quad \text{are} \quad \Omega - \text{periodic}, \\
u(0,x,y) = u_0(x,y),
\end{cases}
$$

where $\varepsilon > 0$ is introduced to take into account the diffuse interface thickness. Setting

$$
\frac{\partial^2 u}{\partial x^2} = p, \quad \frac{\partial^2 u}{\partial y^2} = q, \quad \frac{\partial^4 u}{\partial x^2 \partial y^2} = \frac{1}{2}\frac{\partial^2 p}{\partial y^2} + \frac{1}{2}\frac{\partial^2 q}{\partial x^2},
$$

then, integrating by parts, the system which needs to be solved reads

Find $(u, w, p, q) \in H^1_{\text{per}}(\Omega)^4$ such that

$$
\begin{cases}
((\dfrac{\partial u}{\partial t}, v_1)) - ((\nabla w, \nabla v_1)) + \dfrac{1}{\varepsilon}((g(x,u), v_1)) = 0, \\
((w, v_2)) - a_{20}\varepsilon((\dfrac{\partial p}{\partial x}, \dfrac{\partial v_2}{\partial x})) - a_{02}\varepsilon((\dfrac{\partial q}{\partial y}, \dfrac{\partial v_2}{\partial y})) \\
\qquad - \dfrac{a_{11}\varepsilon}{2}((\dfrac{\partial p}{\partial y}, \dfrac{\partial v_2}{\partial y})) - \dfrac{a_{11}\varepsilon}{2}((\dfrac{\partial q}{\partial x}, \dfrac{\partial v_2}{\partial x})) \\
\qquad - a_{10}\varepsilon((p, v_2)) - a_{01}\varepsilon((q, v_2)) + \dfrac{1}{\varepsilon}((f(u), v_2)) = 0, \\
((p, v_3)) + ((\dfrac{\partial u}{\partial x}, \dfrac{\partial v_3}{\partial x})) = 0, \\
((q, v_4)) + ((\dfrac{\partial u}{\partial y}, \dfrac{\partial v_4}{\partial y})) = 0,
\end{cases}
$$

where the test functions v_1, v_2, v_3, v_4 all belong in $H^1_{\text{per}}(\Omega)$.

The mesh is obtained by dividing Ω into 149^2 rectangles, each rectangle being divided along the same diagonal into two triangles. The computations in Fig. 6.2, 6.3, 6.4 are based on a P_1 finite element method for the space discretization, while we used a P_2 finite element method for Fig. 6.5, 6.6, 6.7. The time discretization uses a semi-implicit Euler scheme (implicit for the linear terms and explicit for the nonlinear ones).

We give numerical results concerning a higher-order Cahn-Hilliard-Oono equation (Fig. 6.2), a higher order phase-field crystal equation (Fig. 6.3, 6.4) and a higher-order Cahn-Hilliard equation with a mass source for tumor growth(Fig. 6.5, 6.6, 6.7).

(i) Cahn-Hilliard-Oono equation (See Fig. 6.2)

$$\Omega = [0,1]\times[0,1], \quad \text{coefficients } a_{ij} \text{ in Table 6.1},$$
$$f(u) = u^3 - u, \quad g(x,u) = 0.5u,$$
$$u_0^{(1)} \text{ randomly distributed between -1 and 1}, \quad \varepsilon = 1, \quad \text{step size } \Delta t = 5.10^{-8}.$$

(ii) Phase field crystal equation. (See Fig. 6.3)

$$\text{Coefficients } a_{ij} \text{ in Table 6.2}, \quad \Delta t = 10^{-4},$$
$$f(u) = u^3 + (1-0.025)u, \quad g(x,u) = 2u, \quad \varepsilon = 1,$$
$$u_0^{(2)} \text{ randomly distributed between -0.2 and 0.3}, \quad \Omega = [-10,10]\times[-10,10].$$

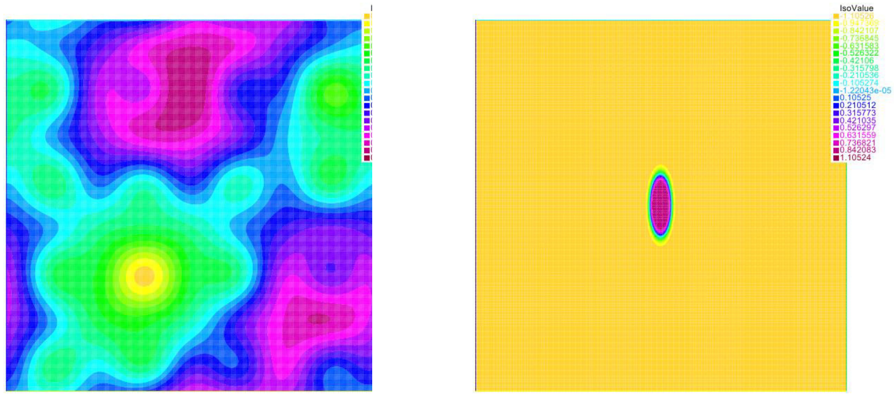
(iii) Phase-field crystal equation. (See Fig. 6.4)

$$\text{Coefficients } a_{ij} \text{ in Table 6.3}, \quad \Delta t = 10^{-3},$$
$$f(u) = u^3 + (1-0.025)u, \quad g(x,u) = 2u, \quad \varepsilon = 1,$$
$$u_0^{(3)} = 0.07 - 0.02\cos\frac{2\pi(x-12)}{32}\sin\frac{2\pi(y-1)}{32} + 0.02\cos^2\frac{\pi(x+10)}{32}\cos^2\frac{\pi(y+3)}{32}$$
$$- 0.01\sin^2\frac{4\pi x}{32}\sin^2\frac{4\pi(y-6)}{32}, \quad \Omega = [0,32]\times[0,32].$$

(iv) Tumor proliferation term. (See Fig. 6.5, 6.6, 6.7)

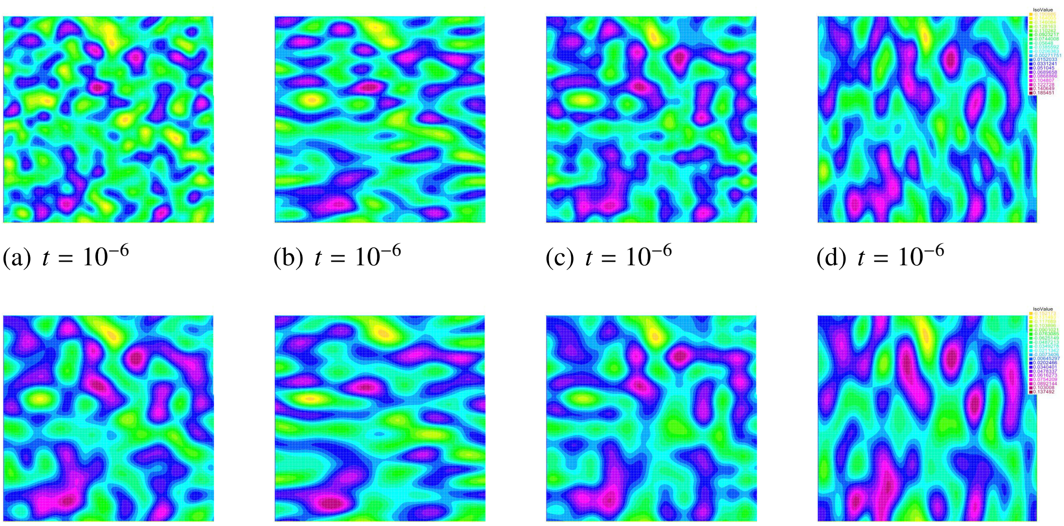
$$\text{Coefficients } a_{ij} \text{ in Table 6.4, 6.5, 6.6}$$
$$f(u) = u^3 - u, \quad \Omega = [-0.7,1,7]\times[-1.7,0.7], \quad \Delta t = 10^{-6}$$
$$g(x,u) = 46(u+1) - 280(u-1)^2(u+1)^2, \varepsilon = 0.0125,$$
$$u_0^{(4)} = -\tanh\left(\frac{1}{\sqrt{2}\varepsilon}\left(\sqrt{2(x-0.5)^2 + 0.25(y+0.5)^2} - 0.1\right)\right) \in [-1,1].$$

The initial conditions $u_0^{(3)}$ and $u_0^{(4)}$ are shown in Fig. 9.9.



(a) Phase-field crystal : $u_0^{(3)}$ (b) Tumor growth : $u_0^{(4)}$

FIGURE 6.1 – Initial conditions $u_0^{(3)}$ and $u_0^{(4)}$.



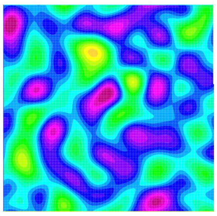
(a) $t = 10^{-6}$ (b) $t = 10^{-6}$ (c) $t = 10^{-6}$ (d) $t = 10^{-6}$

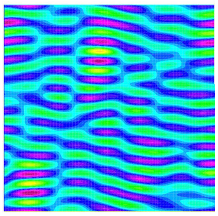
(e) $t = 5 \times 10^{-6}$ (f) $t = 5 \times 10^{-6}$ (g) $t = 5 \times 10^{-6}$ (h) $t = 5 \times 10^{-6}$

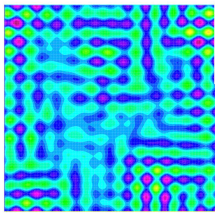
FIGURE 6.2 – Initial condition $u_0^{(1)}$, $f = u^3 - u$, $g = 0.5u$, $\varepsilon = 0.05$, $\Delta t = 5 \times 10^{-8}$.

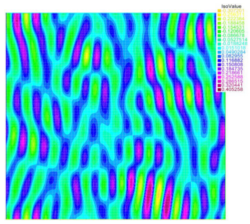
TABLE 6.1 – Coefficients a_{ij} for Fig. 6.2

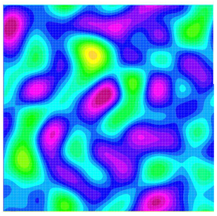
column	a_{20}	a_{11}	a_{02}	a_{10}	a_{01}	Remark
1	0	0	0	1	1	Cahn-Hilliard-Oono
2	1e-2	1e-4	1e-4	1e-4	1e-4	x-direction
3	1e-4	1e-2	1e-4	1e-4	1e-4	cross-direction
4	1e-4	1e-4	1e-2	1e-4	1e-4	y-direction

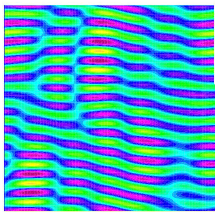

(a) $t = 2.5 \times 10^{-2}$

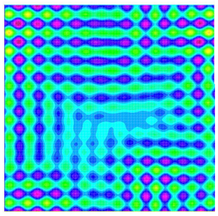

(b) $t = 2.5 \times 10^{-2}$

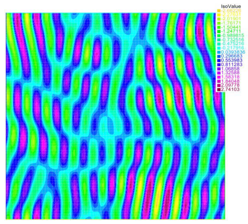

(c) $t = 2.5 \times 10^{-2}$

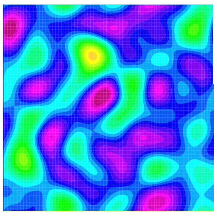

(d) $t = 2.5 \times 10^{-2}$

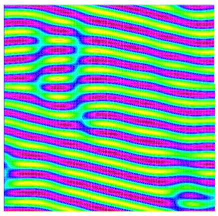

(e) $t = 5 \times 10^{-2}$

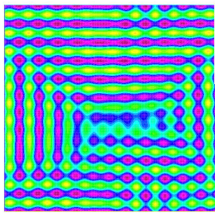

(f) $t = 5 \times 10^{-2}$

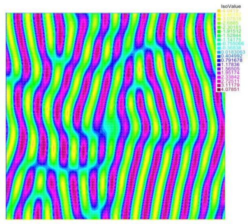

(g) $t = 5 \times 10^{-2}$

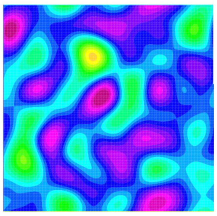

(h) $t = 5 \times 10^{-2}$

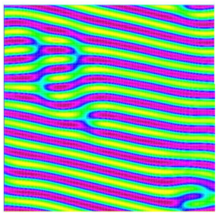

(i) $t = 7.5 \times 10^{-2}$

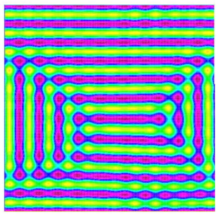

(j) $t = 7.5 \times 10^{-2}$


(k) $t = 7.5 \times 10^{-2}$


(l) $t = 7.5 \times 10^{-2}$


(m) $t = 10^{-1}$


(n) $t = 10^{-1}$


(o) $t = 10^{-1}$

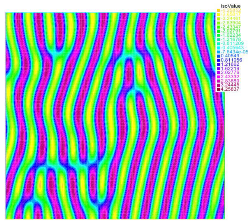
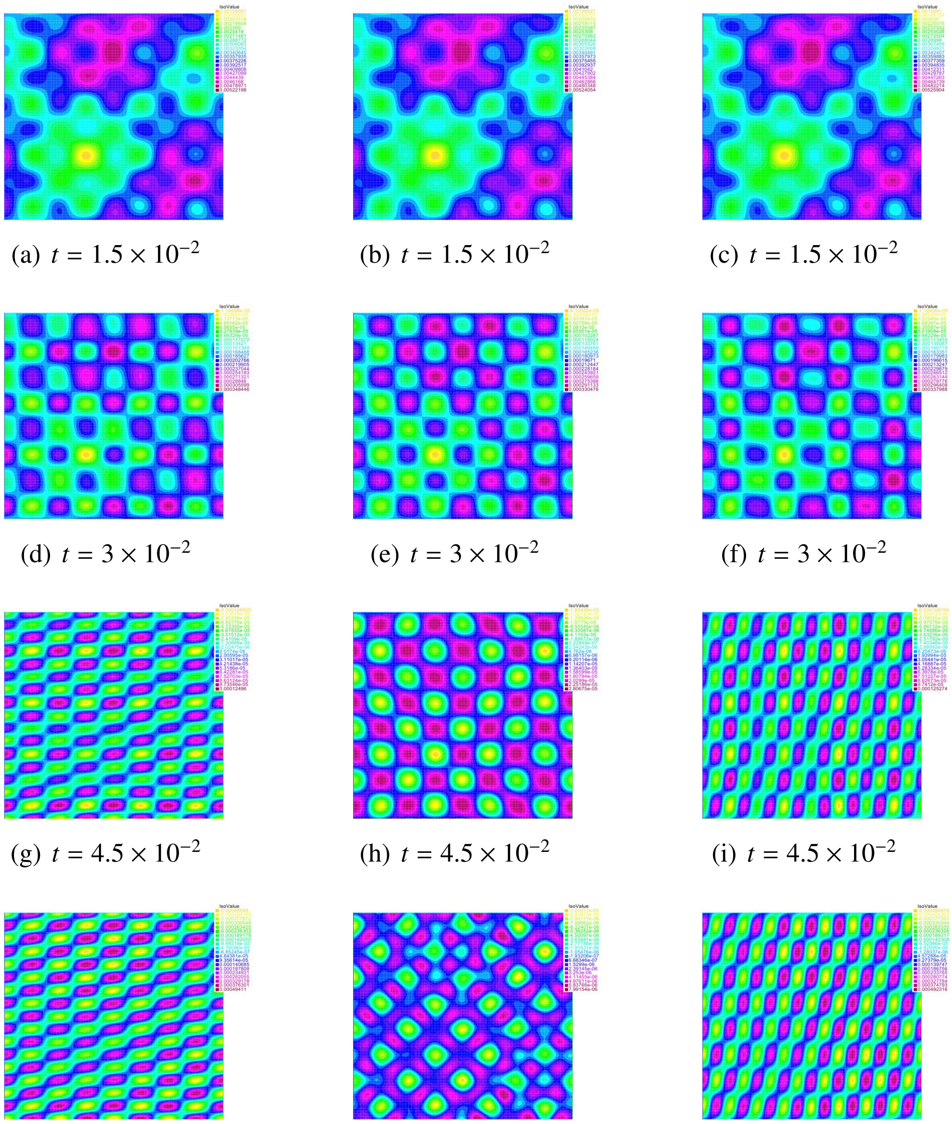

(p) $t = 10^{-1}$

Figure 6.3 – Initial condition $u_0^{(2)}$, $f = u^3 + (1 - 0.025)u, g = 2u$, $\varepsilon = 1$, $\Delta t = 10^{-4}$.

Table 6.2 – Coefficients a_{ij} for Fig. 6.3

Column	a_{20}	a_{11}	a_{02}	a_{10}	a_{01}	Remark
1	1	1	1	-2	-2	Phase-field crystal
2	1	0.1	0.1	-2	-2	x-direction
3	0.1	1	0.1	-2	-2	cross-direction
4	0.1	0.1	1	-2	-2	y-direction



(a) $t = 1.5 \times 10^{-2}$ (b) $t = 1.5 \times 10^{-2}$ (c) $t = 1.5 \times 10^{-2}$

(d) $t = 3 \times 10^{-2}$ (e) $t = 3 \times 10^{-2}$ (f) $t = 3 \times 10^{-2}$

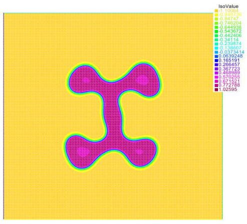
(g) $t = 4.5 \times 10^{-2}$ (h) $t = 4.5 \times 10^{-2}$ (i) $t = 4.5 \times 10^{-2}$

(j) $t = 6 \times 10^{-2}$ (k) $t = 6 \times 10^{-2}$ (l) $t = 6 \times 10^{-2}$

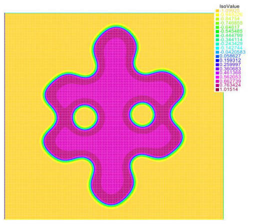
FIGURE 6.4 – Initial condition $u_0^{(3)}$, $f = u^3 + (1 - 0.025)u$, $g = 2u$, $\varepsilon = 1$, $\Delta t = 10^{-3}$.

TABLE 6.3 – Coefficients a_{ij} for Fig.6.4

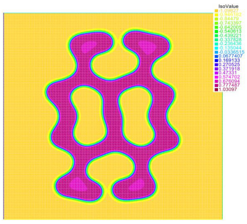
Row	a_{20}	a_{11}	a_{02}	a_{10}	a_{01}	Remark
1	1	0.5	0.5	-2	-2	x-direction
2	0.5	1	0.5	-2	-2	cross-direction
3	0.5	0.5	1	-2	-2	y-direction



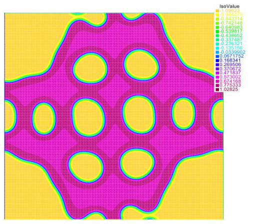
(a) $t = 1.5 \times 10^{-2}$



(b) $t = 1.5 \times 10^{-2}$



(c) $t = 2.5 \times 10^{-2}$

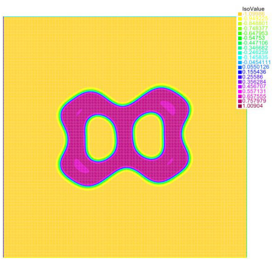


(d) $t = 2.5 \times 10^{-2}$

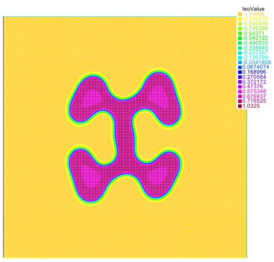
FIGURE 6.5 – Initial condition $u_0^{(4)}$, $f = u^3 - u$, $g = 46(u+1) - 280(u-1)^2(u+1)^2$, $\varepsilon = 0.0125$, $\Delta t = 10^{-6}$.

TABLE 6.4 – Coefficients a_{ij} for Fig. 6.5

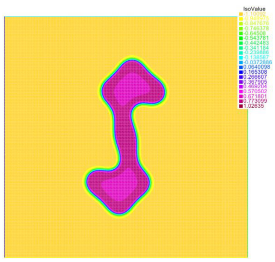
Column	a_{20}	a_{11}	a_{02}	a_{10}	a_{01}	Remark
1	0	0	0	1	1	Cahn-Hilliard
2	5e-5	5e-5	5e-5	1	1	isotropy



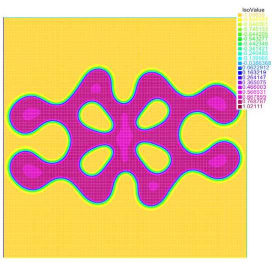
(a) $t = 1.5 \times 10^{-2}$



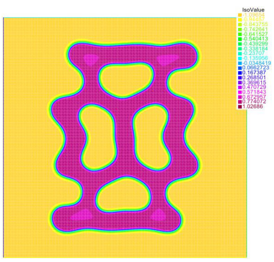
(b) $t = 1.5 \times 10^{-2}$



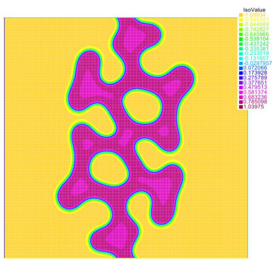
(c) $t = 1.5 \times 10^{-2}$



(d) $t = 2.5 \times 10^{-2}$



(e) $t = 2.5 \times 10^{-2}$

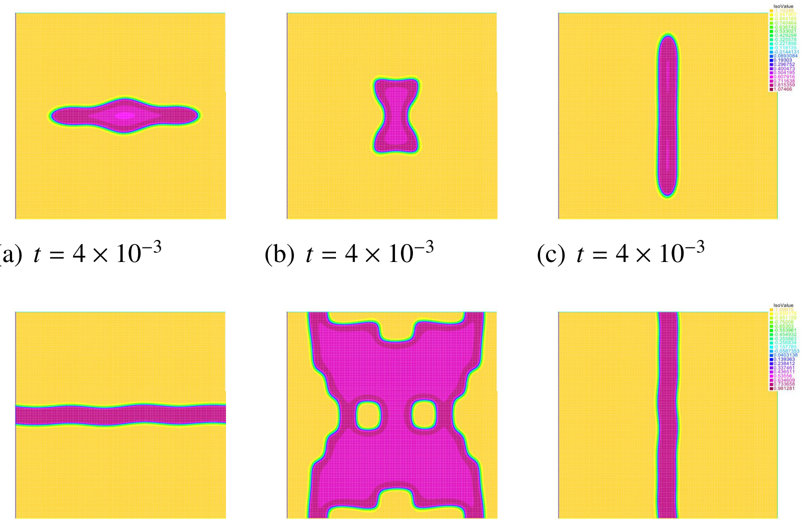


(f) $t = 2.5 \times 10^{-2}$

FIGURE 6.6 – Initial condition $u_0^{(4)}$, $k = 2$, $f = u^3 - u$, $g = 46(u+1) - 280(u-1)^2(u+1)^2$, $\varepsilon = 0.0125$, $\Delta t = 10^{-6}$.

Table 6.5 – Coefficients a_{ij} for Fig. 6.6

Column	a_{20}	a_{11}	a_{02}	a_{10}	a_{01}	Remark
1	1.8e-5	5e-6	5e-6	1	1	x -direction
2	5e-6	1.8e-5	5e-6	1	1	cross-direction
3	5e-6	5e-6	1.8e-5	1	1	y-direction



(a) $t = 4 \times 10^{-3}$ (b) $t = 4 \times 10^{-3}$ (c) $t = 4 \times 10^{-3}$

(d) $t = 2 \times 10^{-2}$ (e) $t = 2 \times 10^{-2}$ (f) $t = 2 \times 10^{-2}$

Figure 6.7 – Initial condition $u_0^{(4)}$, $f = u^3 - u$, $g = 46(u + 1) - 280(u - 1)^2(u + 1)^2$, $\varepsilon = 0.0125$, $\Delta t = 10^{-6}$.

Table 6.6 – Coefficients a_{ij} for Fig. 6.7

Column	a_{20}	a_{11}	a_{02}	a_{10}	a_{01}	Remark
1	5e-4	5e-6	5e-6	1	1	x-direction
2	5e-6	5e-4	5e-6	1	1	cross-direction
3	5e-6	5e-6	5e-4	1	1	y-direction

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The authors wish to thank the Ministère Français des Affaires Etrangères et du Développement International (MAEDI) and the Ministère de l'Education Nationale, de L'Enseignement Supérieur et de la Recherche (MENESR) for their support within the PHC Program Cai Yuanpei 2015 "Modèles fortement anisotropes en séparation de phase".

Chapitre 7

Well-posedness for modified higher-order anisotropic Cahn-Hilliard equations

Caractère bien posé pour des généralisations anisotropes et d'ordre élevé de l'équation de Cahn-Hilliard

Ce chapitre est constitué de l'article **Well-posedness for modified higher-order anisotropic Cahn-Hilliard equations**, *Asymptotic Analysis*, à paraître.
Cet article est écrit en collaboration avec **Hongyi Zhu**.

Asymptotic Analysis, accepted

Well-posedness for modified higher-order anisotropic Cahn-Hilliard equations

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Abstract : Our aim in this paper is to study a modified higher-order (in space) phase field crystal model endowed with anisotropy. In particular, we deduce a priori estimates to obtain the dissipative semigroup which leads to well-posedness results.

Key words and phrases : modified phase field crystal equation, higher-order models, anisotropy, a priori estimates, dissipative semigroup.

7.1 Introduction

We study in this paper the modified higher-order anisotropic Cahn-Hilliard equations which read, for $k \in \mathbb{N}$, $k \geq 2$, $x \in \Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$,

$$\beta\partial_{tt}u + \partial_t u - \Delta \sum_{i=1}^{k}(-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0, \tag{7.1}$$

where Ω is assumed to be a bounded and regular domain occupied by the system with boundary Γ ; u is the order parameter, for instance, the density of atoms ; f is the derivative of a double-well potential F, and $\beta > 0$ is a relaxation time. The Cahn-Hilliard equation ([19, 20]), which describes important features of binary alloys in phase separation processes, such as spinodal decomposition and coarsening,

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) = 0, \tag{7.2}$$

is considered as an H^{-1}-gradient flow of the so-called Ginzburg-Landau (see [68, 69]) free energy,

$$\Psi_{GL} = \int_\Omega \left(\frac{1}{2}|\nabla u|^2 + F(u)\right) dx. \tag{7.3}$$

In (7.3), the term $|\nabla u|^2$ models short-ranged interactions. It is however interesting to note that such a term is obtained by truncation of higher-order ones (see [20]) ; it can also be seen as a first-order approximation of a nonlocal term accounting for long-ranged interactions (see [65] and [66]).

Concerning the inertial term (namely, the hyperbolic term : $\beta\partial_{tt}u$), in fact, a hyperbolic relaxation of the one-dimensional Cahn-Hilliard equation has been proposed in [50], in order to model rapid spinodal decompositions in a binary alloy. Furthermore, S. Gatti et al. provided in [62] a detailed analysis of the longterm properties of the solutions for a hyperbolic relaxation of the one-dimensional Cahn-Hilliard equation in the singular limit when the relaxation parameter goes to zero.

We notice that, when $k = 1$, without consideration of anisotropy, the equation becomes

$$\beta\partial_{tt}u + \partial_t u - \Delta[\Delta^2 u + 2\Delta u + f(u)] = 0, \tag{7.4}$$

which is a so-called modified phase field crystal equation (abbr., MPFC) and was proposed in [123] by P. Stefanovic et al. (see also in [124]). The MPFC equation incorporates both fast elastic relaxation and slower mass diffusion which has achieved to distinguish between the elastic relaxation and diffusion time scales. In [75] and [76], M. Grasselli and H. Wu proved the well-posedness and established the existence of an exponential attractor for the MPFC equation (7.4) endowed with periodic boundary conditions. Additionally, in [72], M. Grasselli and M. Pierre proposed a space semi-discrete and a fully discrete finite element scheme for the MPFC model and established their convergence to equilibrium both theoretically and numerically. We refer the readers to [135, 136] for more numerical methods to solve the MPFC model and [45, 50, 56, 79] for the theoretical and numerical study on the phase field model without a relaxation.

We further studied (7.1) in [140], in which we assumed the well-posedness of solutions, the numerical approximations for a hyperbolic relaxation of the higher-order anisotropic generalized Cahn-Hilliard models which was inspired by the work of M. Grasselli and M. Pierre in [72], employing the finite element and spectral methods. In this article, we will focus on the well-posedness of the hyperbolic equations and their solutions, more precisely, the existence, uniqueness and regularity.

Considering the anisotropic phenomenon, recently, G. Caginalp and E. Esenturk proposed in [23] (see also [22]) higher-order phase-field models in order to account for anisotropic interfaces (see also [40, 80, 119, 125, 128] and [132] for other approaches which, however, do not provide an explicit way to compute the anisotropy). More precisely, these authors proposed the following modified free energy, in which we omit the temperature :

$$\Psi_{\text{HOGL}} = \int_\Omega (\frac{1}{2}\sum_{i=1}^{k}\sum_{|\alpha|=i} a_\alpha |\mathcal{D}^\alpha u|^2 + F(u))\,dx,\ k \in \mathbb{N}, \tag{7.5}$$

where, for $\alpha = (k_1, k_2, k_3) \in (\mathbb{N} \cup \{0\})^3$,

$$|\alpha| = k_1 + k_2 + k_3$$

and, for $\alpha \neq (0, 0, 0)$,

$$\mathcal{D}^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{k_1} \partial x_2^{k_2} \partial x_3^{k_3}}$$

(we agree that $\mathcal{D}^{(0,0,0)} v = v$).

The corresponding higher-order anisotropic Cahn-Hilliard equation (it also corresponds to the case when $\beta = 0$ in equation (7.1)) then reads

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0. \tag{7.6}$$

We studied in [32] the corresponding higher-order isotropic models, namely,

$$\frac{\partial u}{\partial t} - \Delta P(-\Delta) u - \Delta f(u) = 0, \tag{7.7}$$

where

$$P(s) = \sum_{i=1}^{k} a_i s^i,\ a_k > 0,\ k \geq 1,\ s \in \mathbb{R}.$$

We also refer the readers to [84, 85, 95, 96, 97] (see also [117, 118]) the study on higher-order Cahn-Hilliard type equations.The anisotropic model (7.6) was analysed in [34], and the generalized anisotropic model which contains a continuous function $g(x, u)$ was studied in [35], in both of which, numerical simulations were performed to illustrate the anisotropic effects.

Taking the nonlinearity into account, the authors in [33] have considered (7.7) (see also in [30, 36, 41, 70, 96, 99, 104] for other equations) endowed with a thermodynamically relevant potential F which is associated to the mean-field model :

$$F(s) = \frac{\theta_c}{2}(1-s^2) + \frac{\theta}{2}\left((1-s)\ln(\frac{1-s}{2}) + (1+s)\ln(\frac{1+s}{2})\right),$$
$$s \in (-1,1),\ 0 < \theta < \theta_c, \tag{7.8}$$

i.e.,

$$f(s) = -\theta_c s + \frac{\theta}{2}\ln\frac{1+s}{1-s}, \tag{7.9}$$

where θ and θ_c are proportional to the absolute temperature and a critical temperature, respectively. However, in this paper (and also in [72, 75, 76] and [140], etc.), we consider a polynomial type nonlinearity, for example,

$$F(s) = \frac{1}{4}(s^2-1)^2, \tag{7.10}$$

i.e.,

$$f(s) = F'(s) = s^3 - s. \tag{7.11}$$

Our interests in this paper is to study the well-posedness of a hyperbolic relaxation of the higher-order anisotropic Cahn-Hilliard equation. In Section 2, detailed notations on operators, spaces and parameters are provided, then in Section 3, the exact problem is addressed and after which, in Section 4, a priori estimates are derived in detail. In Section 5, the existence and uniqueness of weak solution are given and proved, as well as the dissipativity of semigroup.

7.2 Prelimilaries

For a real Banach space X, we set $\|\cdot\|_X$ as the norm of X and $\langle\cdot,\cdot\rangle$ as the duality product between X and the topological dual of X. Generally, $\|\cdot\|$ denotes the L^2−norm and $\|\cdot\|_{-1} = \|(-\Delta)^{\frac{1}{2}}\cdot\|$, where $(-\Delta)^{-1}$ denotes the inverse minus Laplace operator associated with Dirichlet boundary conditions. Moreover, for $v, w \in H^{-1}(\Omega)$, $((v,w))_{-1} = (((-\Delta)^{-\frac{1}{2}}v, (-\Delta)^{-\frac{1}{2}}w))$, where $((\cdot,\cdot))$ denotes the usual L^2−scalar product.

Assuming that $k \geq 2$ ($k \in \mathbb{N}$), and $a_\alpha > 0$ ($|\alpha| = k$), we define the elliptic operator A_k as

$$\langle A_k v, w\rangle_{H^{-k}(\Omega),H_0^k(\Omega)} = \sum_{|\alpha|=k} a_\alpha((\mathcal{D}^\alpha v, \mathcal{D}^\alpha w)),\ v, w \in H_0^k(\Omega), \tag{7.12}$$

where $H^{-k}(\Omega)$ is the topological dual of $H_0^k(\Omega)$. For arbitrary functions $v, w \in H_0^k(\Omega)$, we note that

$$(v, w) \mapsto \sum_{|\alpha|=k} a_\alpha((\mathcal{D}^\alpha v, \mathcal{D}^\alpha w))$$

is bilinear, symmetric, continuous and coercive, so that

$$A_k : H_0^k(\Omega) \mapsto H^{-k}(\Omega) \tag{7.13}$$

is well defined. It then follows from the elliptic regularity results for linear elliptic operators of order $2k$ (see [1], [2] and [3]) that A_k is a strictly positive, selfadjoint and unbounded linear operator with compact inverse, with domain $D(A_k) = H^{2k}(\Omega) \cap H_0^k(\Omega)$, where, for $v \in D(A_k)$,

$$A_k v = (-1)^k \sum_{|\alpha|=k} a_\alpha \mathcal{D}^{2\alpha} v.$$

We further note that $D(A_k^{\frac{1}{2}}) = H_0^k(\Omega)$ and, for $(v, w) \in D(A_k^{\frac{1}{2}})^2$,

$$((A_k^{\frac{1}{2}} v, A_k^{\frac{1}{2}} w)) = \sum_{|\alpha|=k} a_\alpha((\mathcal{D}^\alpha v, \mathcal{D}^\alpha w)).$$

We then note that (see, e.g., [127]) $\|A_k \cdot\|$ (resp., $\|A_k^{\frac{1}{2}} \cdot\|$) is equivalent to the usual H^{2k}–norm (resp., H^k–norm) on $D(A_k)$ (resp., $D(A_k^{\frac{1}{2}})$).

Similarly, we can define the linear operator $\bar{A}_k = -\Delta A_k$,

$$\bar{A}_k : H_0^{k+1}(\Omega) \mapsto H^{-k-1}(\Omega)$$

which is a strictly positive, selfadjoint and unbounded linear operator with compact inverse, with domain $D(\bar{A}_k) = H^{2k+2}(\Omega) \cap H_0^{k+1}(\Omega)$, where, for $v \in D(\bar{A}_k)$,

$$\bar{A}_k v = (-1)^{k+1} \Delta \sum_{|\alpha|=k} a_\alpha \mathcal{D}^{2\alpha} v.$$

Additionally, $D(\bar{A}_k^{\frac{1}{2}}) = H_0^{k+1}(\Omega)$ and, for $(v, w) \in D(\bar{A}_k^{\frac{1}{2}})^2$,

$$((\bar{A}_k^{\frac{1}{2}} v, \bar{A}_k^{\frac{1}{2}} w)) = \sum_{|\alpha|=k} a_\alpha((\nabla \mathcal{D}^\alpha v, \nabla \mathcal{D}^\alpha w)).$$

Besides, $\|\bar{A}_k \cdot\|$ (resp., $\|\bar{A}_k^{\frac{1}{2}} \cdot\|$) is equivalent to the usual H^{2k+2}–norm (resp., H^{k+1}–norm) on $D(\bar{A}_k)$ (resp., $D(\bar{A}_k^{\frac{1}{2}})$).

We finally define the linear operator $\tilde{A}_k = (-\Delta)^{-1} A_k$,

$$\tilde{A}_k : H_0^{k-1}(\Omega) \mapsto H^{-k+1}(\Omega);$$

as $-\Delta$ and A_k commute, we can note that $(-\Delta)^{-1}$ and A_k commute, so that $\tilde{A}_k = A_k(-\Delta)^{-1}$. Furthermore, according to [34], $\tilde{A}_k$ is strictly positive, selfadjoint and unbounded linear operator with compact inverse, with domain $D(\tilde{A}_k) = H^{2k-2}(\Omega) \cap H^{k-1}(\Omega)$, where, for $v \in D(\tilde{A}_k)$,

$$\tilde{A}_k v = (-1)^k \sum_{|\alpha|=k} a_\alpha \mathcal{D}^{2\alpha}(-\Delta)^{-1} v.$$

Furthermore, $D(\tilde{A}_k^{\frac{1}{2}}) = H_0^{k-1}(\Omega)$ and, for $(v, w) \in D(\tilde{A}_k^{\frac{1}{2}})^2$,

$$((\tilde{A}_k^{\frac{1}{2}} v, \tilde{A}_k^{\frac{1}{2}} w)) = \sum_{|\alpha|=k} a_\alpha((\mathcal{D}^\alpha(-\Delta)^{-\frac{1}{2}} v, \mathcal{D}^\alpha(-\Delta)^{-\frac{1}{2}} w)).$$

Besides, $\|\tilde{A}_k \cdot\|$ (resp., $\|\tilde{A}_k^{\frac{1}{2}} \cdot\|$) is equivalent to the usual H^{2k-2}–norm (resp., H^{k-1}–norm) on $D(\tilde{A}_k)$ (resp., $D(\tilde{A}_k^{\frac{1}{2}})$).

In what follows, the same letters c, c', c'' denote (generally positive) constants which may vary from line to line. Similarly, the same letter Q denotes (positive) monotone increasing and continuous function which may vary from line to line. Furthermore, the boundary conditions are Dirichlet boundary condition for a sufficiently regular boundary.

7.3 Setting of the problem

We consider the following modified higher-order anisotropic phase field crystal equation, for $k \in \mathbb{N}$, $k \geq 2$, $x \in \Omega \subset \mathbb{R}^d$, $t \in (0, +\infty)$,

$$\beta u_{tt} + u_t - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0, \tag{7.14}$$

$$u|_{t=0} = u_0(x), \quad u_t|_{t=0} = v_0(x),\ t \geq 0,\ x \in \Omega, \tag{7.15}$$

where the nonlinearity $f(s)$ is the derivative of a double-well potential F. We consider $F(s)$ in this article as an approximation to the thermodynamically relevant potential F which is a logarithmic function (see [20, 36]). Typically,

$$f(s) = F'(s) = s^3 - s. \tag{7.16}$$

More generally, we assume that

$$f \in C^2(\mathbb{R}),\ f(0) = 0, \tag{7.17}$$

$$f' \geq -c_0,\ c_0 \geq 0, \tag{7.18}$$

$$f(s)s \geq c_1 F(s) - c_2 \geq -c_3,\ c_1 > 0,\ c_2,\ c_3 \geq 0,\ s \in \mathbb{R}, \tag{7.19}$$

$$F(s) \geq c_4 s^4 - c_5,\ c_4 > 0,\ c_5 \geq 0,\ s \in \mathbb{R}, \tag{7.20}$$

It can be verified that f defined by (7.16) satisfies all the assumptions from (7.17) to (7.20).

7.4 A priori dissipative estimates

We rewrite problem (7.14) as

$$\beta u_{tt} + u_t - \Delta(A_k u + B_k u + f(u)) = 0, \tag{7.21}$$

where

$$B_k u := \sum_{i=1}^{k-1} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u. \tag{7.22}$$

Then we have

Lemma 7.4.1. *Suppose (u, u_t) is a regular solution to problem (7.14)-(7.15). Then the following dissipative estimate holds*

$$\|u\|^2_{H^k(\Omega)} + \|u_t\|^2_{-1} + \int_0^t e^{-c'(t-s)} \|u_t(s)\|^2_{-1} ds \leq e^{-c't} Q(\|u_0\|_{H^k(\Omega)}, \|v_0\|_{-1}) + c''; \tag{7.23}$$

Moreover, if we further assume that f is of class C^{k+1}, the following dissipative estimate holds

$$\|u_t\|^2_{H^{k-1}(\Omega)} + \|u\|^2_{H^{2k}(\Omega)} \leq c e^{-c't} Q(\|u_0\|_{H^{2k}(\Omega)}, \|v_0\|_{H^{k-1}(\Omega)}) + c''. \tag{7.24}$$

Proof. Multiplying (7.21) by $(-\Delta)^{-1} u_t$, and integrating over Ω, we obtain

$$\frac{1}{2}\frac{d}{dt}\left(\beta \|u_t\|^2_{-1} + \|A_k^{\frac{1}{2}} u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)dx\right) + \|u_t\|^2_{-1} = 0, \tag{7.25}$$

where

$$B_k^{\frac{1}{2}}[u] := \sum_{i=1}^{k-1} \sum_{|\alpha|=i} a_\alpha \|\mathcal{D}^\alpha u\|^2. \tag{7.26}$$

We can note that, owing to the interpolation inequality

$$\|v\|_{H^i(\Omega)} \leq c(i)\|v\|_{H^m(\Omega)}^{\frac{i}{m}}\|v\|^{1-\frac{i}{m}}, \tag{7.27}$$
$$v \in H^m(\Omega),\ i \in \{1, \cdots, m-1\},\ m \in \mathbb{N},\ m \geq 2,$$

there holds

$$|B_k^{\frac{1}{2}}[u]| \leq \frac{1}{2}\|A_k^{\frac{1}{2}}u\|^2 + c\|u\|^2. \tag{7.28}$$

Multiplying (7.21) by $(-\Delta)^{-1}u$, we obtain

$$\frac{d}{dt}\left(\beta((u_t, u))_{-1} + \frac{1}{2}\|u\|_{-1}^2\right) - \beta\|u_t\|_{-1}^2 + \|A_k^{\frac{1}{2}}u\|^2 + B_k^{\frac{1}{2}}[u] + ((f(u), u)) = 0. \tag{7.29}$$

Multiplying (7.29) by a sufficiently small coefficient η (in fact, normally, we take $\eta \in (0, \frac{1}{2\beta})$), then summing the resulting equation and (7.25), we get the following differential inequality

$$\frac{d}{dt}\mathcal{E}_1(t) + \chi_1(t) = 0, \tag{7.30}$$

where

$$\begin{aligned}
\mathcal{E}_1(t) &= \eta\beta((u_t, u))_{-1} + \frac{1}{2}E_1(u) + \frac{1}{2}\beta\|u_t\|_{-1}^2 + \frac{1}{2}\eta\|u\|_{-1}^2, \\
\chi_1(t) &= (1 - \eta\beta)\|u_t\|_{-1}^2 + \eta\left(\|A_k^{\frac{1}{2}}u\|^2 + B_k^{\frac{1}{2}}[u] + ((f(u), u))\right), \\
E_1(u) &= \|A_k^{\frac{1}{2}}u\|^2 + B_k^{\frac{1}{2}}[u] + 2\int_\Omega F(u)dx,
\end{aligned} \tag{7.31}$$

and E_1 satisfies, owing to (7.20), (7.28) and the Young inequality

$$c\|u\|^2 \leq \frac{c_4}{2}\|u\|_{L^4}^4 + c' \tag{7.32}$$

$$E_1 \geq c\left(\|u\|_{H^k(\Omega)}^2 + \int_\Omega F(u)dx\right) - c',\ c > 0. \tag{7.33}$$

It follows from the Cauchy-Schwarz inequality that

$$\eta\beta|((u_t, u))_{-1}| \leq \frac{\beta}{4}\|u_t\|_{-1}^2 + \eta^2\beta\|u\|_{-1}^2. \tag{7.34}$$

We also note that, according to an embedding theorem,

$$\|u\|_{-1}^2 \leq c\|u\|_{H^k(\Omega)}^2. \tag{7.35}$$

Thus, for $\eta \in (0, \frac{1}{2\beta})$ small enough, we have

$$Q(\|u_t\|_{-1}, E_1(u)) \geq \mathcal{E}_1(t) \geq \frac{1}{2}E_1(t) + \frac{\beta}{4}\|u_t\|_{-1}^2 + (\frac{\eta}{2} - \eta^2\beta)\|u\|_{-1}^2, \tag{7.36}$$

where, $Q(w, z)$ is a positive monotone increasing function with respect to w and z. Furthermore, owing to the assumption (7.19), it is obvious that

$$((f(u), u)) \geq c\int_\Omega F(u)dx - c'|\Omega|, \tag{7.37}$$

with which, according to the definition of $\mathcal{E}_1(t)$ and $\chi_1(t)$, for a sufficient small coefficient $c > 0$, we can obtain

$$\frac{1}{2}\chi_1(t) \geq c\mathcal{E}_1(t) + c'\|u_t\|_{-1}^2 - c''. \tag{7.38}$$

As a result, combining the above inequalities (7.30) - (7.38), we can rewrite (7.30) as

$$\frac{d}{dt}\mathcal{E}_1(t) + c\left(\mathcal{E}_1(t) + \|u_t\|_{-1}^2\right) \leq c', \tag{7.39}$$

where c depends on η and $\mathcal{E}_1$ satisfies

$$\mathcal{E}_1 \geq c\left(\|u\|_{H^k(\Omega)}^2 + \|u_t\|_{-1}^2 + \int_\Omega F(u)dx\right) - c',\ c > 0, \tag{7.40}$$

where c depends on β. We note that, with the continuity of F and the interpolation inequality, we have $|\int_\Omega F(u)dx| \leq Q(\|u\|_{H^k(\Omega)})$. Combining (7.39) and (7.40), and Gronwall's lemma, we obtain, for $c' > 0,\ t \geq 0$,

$$\|u_t\|_{-1}^2 + \|u(t)\|_{H^k(\Omega)}^2 \leq ce^{-c't}Q(\|u_0\|_{H^k(\Omega)}, \|v_0\|_{-1}) + c'', \tag{7.41}$$

and

$$\int_t^{t+r} \|\frac{\partial u}{\partial t}\|_{-1}^2 ds \leq ce^{-c't}Q(\|u_0\|_{H^k(\Omega)}, \|v_0\|_{-1}) + c'',\ r > 0 \text{ given}. \tag{7.42}$$

In addition, applying again Gronwall's lemma on (7.39), we obtain, for $c' > 0,\ t \geq 0$,

$$\mathcal{E}_1(t) + \int_0^t e^{-c'(t-s)}\|u_t(s)\|_{-1}^2 ds \leq \mathcal{E}_1(0)e^{-c't} + c'', \tag{7.43}$$

more precisely, with the definition of $\mathcal{E}_1(t)$, there holds that

$$\|u\|_{H^k(\Omega)}^2 + \|u_t\|_{-1}^2 + \int_0^t e^{-c'(t-s)}\|u_t(s)\|_{-1}^2 ds \leq e^{-c't}Q(\|u_0\|_{H^k(\Omega)}, \|v_0\|_{-1}) + c''.$$

We then multiply (7.21) by u_t and integrate over Ω. It gives :

$$\frac{1}{2}\frac{d}{dt}\left(\beta\|u_t\|^2 + \|\bar{A}_k^{\frac{1}{2}}u\|^2 + \bar{B}_k^{\frac{1}{2}}[u]\right) + \|u_t\|^2 \leq \|\Delta f(u)\|\|u_t\|,$$

with

$$\bar{B}_k^{\frac{1}{2}}[u] = \sum_{i=1}^{k-1}\sum_{|\alpha|=i} a_\alpha\|\nabla D^\alpha u\|^2 \quad \text{and} \quad |\bar{B}_k^{\frac{1}{2}}[u]| \leq c\|u\|_{H^k}^2.$$

Noting that f is of class C^2, so that for $k \geq 2$,

$$\|\Delta f(u)\| \leq Q(\|u\|_{H^k(\Omega)}), \tag{7.44}$$

we get from (7.41) that, for $c' > 0$,

$$\frac{d}{dt}\left(\beta\|u_t\|^2 + \|\bar{A}_k^{\frac{1}{2}}u\|^2 + \bar{B}_k^{\frac{1}{2}}[u]\right) + \|u_t\|^2 \leq e^{-c't}Q(\|u_0\|_{H^k(\Omega)}, \|v_0\|_{-1}) + c''. \tag{7.45}$$

We then test (7.21) by u, and integrate over Ω, owing to (7.41) and (7.44), applying Cauchy-Schwarz inequality, to get

$$\begin{aligned}&\frac{d}{dt}\left(\beta((u_t, u)) + \frac{1}{2}\|u\|^2\right) - \beta\|u_t\|^2 + \|\bar{A}_k^{\frac{1}{2}}u\|^2 + \bar{B}_k^{\frac{1}{2}}[u]\\ &\leq e^{-c't}Q(\|u_0\|_{H^k(\Omega)}, \|v_0\|_{-1}) + c'' + \|u\|^2.\end{aligned} \tag{7.46}$$

Multiplying (7.46) by a sufficient small positive coefficient $\eta' \in (0, \frac{1}{2\beta})$, and summing the resulting inequality with (7.39) and (7.45), it leads to

$$\begin{aligned}\frac{d}{dt}\mathcal{Y}_1(t) + \mathcal{D}_1(t) &\leq e^{-c't}Q(\|u_0\|_{H^k(\Omega)}, \|v_0\|_{-1}) + c'' + \|u\|^2\\ &\leq e^{-c't}Q(\|u_0\|_{H^k(\Omega)}, \|v_0\|_{-1}) + c'',\end{aligned} \tag{7.47}$$

where

$$\begin{aligned}\mathcal{Y}_1(t) &= \mathcal{E}_1 + \frac{\beta}{2}\|u_t\|^2 + \frac{1}{2}\|\bar{A}_k^{\frac{1}{2}}u\|^2 + \frac{1}{2}\bar{B}_k^{\frac{1}{2}}[u] + \eta'\beta((u_t, u)) + \frac{\eta'}{2}\|u\|^2,\\ \mathcal{D}_1(t) &= \eta'\|\bar{A}_k^{\frac{1}{2}}u\|^2 + \eta'\bar{B}_k^{\frac{1}{2}}[u] + (1 - \eta'\beta)\|u_t\|^2 + c\mathcal{E}_1 + c\|u_t\|_{-1}^2.\end{aligned} \tag{7.48}$$

Proceeding as above, according to (7.20), the interpolation and Young inequalities (7.27) and (7.32), it follows that,

$$Q(\|u_t\|, \|u\|_{H^{k+1}(\Omega)}) \geq \mathcal{Y}_1(t) \geq \frac{\beta}{4}\|u_t\|^2 + \frac{1}{4}\|\bar{A}_k^{1/2}u\|^2 - c, \tag{7.49}$$

with which, therefore, we can deduce from the expressions of $\mathcal{Y}_1$ and $\mathcal{D}_1$ that there holds

$$\frac{d}{dt}\mathcal{Y}_1(t) + c_0\mathcal{Y}_1(t) \le ce^{-c't}Q(\|u_0\|_{H^k(\Omega)}, \|v_0\|_{-1}) + c''. \tag{7.50}$$

Owing to Gronwall's lemma and (7.49), we thus obtain

$$\begin{aligned}\mathcal{Y}_1(t) &\le \mathcal{Y}_1(0)e^{-c_0t} + \int_0^t e^{-c_0(t-s)}\left(ce^{-c's}Q(\|u_0\|_{H^k(\Omega)}, \|v_0\|_{-1}) + c''\right)ds \\ &\le e^{-c't}Q(\|u_0\|_{H^{k+1}(\Omega)}, \|v_0\|) + c'',\end{aligned} \tag{7.51}$$

so that

$$\|u_t\|^2 + \|u\|^2_{H^{k+1}(\Omega)} \le e^{-c't}Q(\|u_0\|_{H^{k+1}(\Omega)}, \|v_0\|) + c''. \tag{7.52}$$

Multiplying then (7.21) by $\tilde{A}_k u$, and integrating over Ω, owing to the interpolation inequality (7.27), we have

$$\frac{d}{dt}\left(\beta((\tilde{A}_k^{\frac{1}{2}}u_t, \tilde{A}_k^{\frac{1}{2}}u)) + \frac{1}{2}\|\tilde{A}_k^{\frac{1}{2}}u\|^2\right) - \beta\|\tilde{A}_k^{\frac{1}{2}}u_t\|^2 + \|A_ku\|^2 + ((B_ku, A_ku)) \le |((f(u), A_ku))|.$$

It then follows from the continuity of f and F, and the continuous embedding $H^k \subset C(\overline{\Omega})$ for $k \ge 2$, and (7.41), that

$$\begin{aligned}&\frac{d}{dt}\left(\beta((\tilde{A}_k^{\frac{1}{2}}u_t, \tilde{A}_k^{\frac{1}{2}}u)) + \frac{1}{2}\|\tilde{A}_k^{\frac{1}{2}}u\|^2\right) + c\|A_ku\|^2 - \beta\|\tilde{A}_k^{\frac{1}{2}}u_t\|^2 + ((B_ku, A_ku)) \\ &\le e^{-c't}Q(\|u_0\|_{H^k(\Omega)}, \|v_0\|_{-1}) + c''.\end{aligned} \tag{7.53}$$

Multiplying (7.21) by $\tilde{A}_k u_t$, integrating over Ω and by parts, and noting that the two operators A_k and B_k commute, we obtain

$$\frac{1}{2}\frac{d}{dt}\left(\beta\|\tilde{A}_k^{\frac{1}{2}}u_t\|^2 + \|A_ku\|^2 + ((B_ku, A_ku))\right) + \|\tilde{A}_k^{\frac{1}{2}}u_t\|^2 \le |((\bar{A}_k^{\frac{1}{2}}f(u), \tilde{A}_k^{\frac{1}{2}}u_t))|. \tag{7.54}$$

We further assume that f is of class C^{k+1}, which yields $\|\bar{A}_k^{\frac{1}{2}}f(u)\|^2 \le Q(\|u\|_{H^{k+1}(\Omega)})$. Owing to (7.52) and Cauchy-Schwarz inequality, there holds that

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}\left(\beta\|\tilde{A}_k^{\frac{1}{2}}u_t\|^2 + \|A_ku\|^2 + ((B_ku, A_ku))\right) + \frac{1}{2}\|\tilde{A}_k^{\frac{1}{2}}u_t\|^2 \\ &\le e^{-c't}Q(\|u_0\|_{H^{k+1}(\Omega)}, \|v_0\|) + c''.\end{aligned} \tag{7.55}$$

Multiplying (7.53) by $\eta'' \in (0, \frac{1}{2\beta})$ and summing the resulting inequality with (7.39) and (7.55), we get

$$\frac{d}{dt}\mathcal{Y}_2(t) + \mathcal{D}_2(t) \leq ce^{-c't}Q(\|u_0\|_{H^{k+1}(\Omega)}, \|v_0\|) + c'',\ c,\ c' > 0,\ t > 0, \tag{7.56}$$

where

$$\begin{aligned}\mathcal{Y}_2(t) =& \mathcal{E}_1 + \eta''\beta((\tilde{A}_k^{\frac{1}{2}}u_t, \tilde{A}_k^{\frac{1}{2}}u)) + \frac{\eta''}{2}\|\tilde{A}_k^{\frac{1}{2}}u\|^2 + \frac{\beta}{2}\|\tilde{A}_k^{\frac{1}{2}}u_t\|^2\\ &+ \frac{1}{2}\|A_k u\|^2 + \frac{1}{2}((B_k u, A_k u)),\\ \mathcal{D}_2(t) =& (\frac{1}{2} - \eta''\beta)\|\tilde{A}_k^{\frac{1}{2}}u_t\|^2 + c\eta''\|A_k u\|^2 + \eta''((B_k u, A_k u)).\end{aligned} \tag{7.57}$$

Applying Cauchy-Schwarz, (7.27) and proceeding as above, it follows that,

$$|((B_k u, A_k u))| \leq \frac{1}{4}\|A_k u\|^2 + C\|u\|^2.$$

Then, arguing as previously with (7.20) and (7.32) and for η'' small enough, we have :

$$Q(\|u_t\|_{H^{k-1}(\Omega)}, \|u\|_{H^{2k}(\Omega)}) \geq \mathcal{Y}_2(t) \geq \frac{\beta}{4}\|\tilde{A}_k^{\frac{1}{2}}u_t\|^2 + \frac{1}{4}\|A_k u\|^2 - c, \tag{7.58}$$

with which, we can deduce from the definition of $\mathcal{Y}_2(t)$ and $\mathcal{D}_2(t)$ that there holds

$$\frac{d}{dt}\mathcal{Y}_2(t) + c_0\mathcal{Y}_2(t) \leq ce^{-c't}Q(\|u_0\|_{H^{k+1}(\Omega)}, \|v_0\|) + c'',\ c,\ c' > 0,\ t > 0. \tag{7.59}$$

According to Gronwall's lemma, the interpolation inequality and (7.52), we finally obtain (7.24), then the proof is complete. □

7.5 The dissipative semigroup

Based on the a priori estimates, we have the

Theorem 7.5.1. *(i) For any initial data $(u_0, v_0) \in H_0^k(\Omega)\times H^{-1}(\Omega)$, problem (7.14)-(7.15) possesses a unique weak solution (u, u_t), such that, for $\forall\ T > 0$, u satisfies*

$$u \in L^\infty(\mathbb{R}^+; H_0^k(\Omega)) \text{ and } u_t \in L^2(0, T; H^{-1}(\Omega)).$$

(ii) If we assume that $(u_0, v_0) \in (H^{k+1}(\Omega) \cap H_0^k(\Omega)) \times L^2(\Omega)$, then we have,

$$u \in L^\infty(\mathbb{R}^+; H^{k+1}(\Omega) \cap H_0^k(\Omega)) \text{ and } u_t \in L^2(0, T; L^2(\Omega)).$$

(iii) If we further assume that f is of class C^{k+1}, and $(u_0, v_0) \in (H^{2k}(\Omega) \cap H_0^k(\Omega)) \times H^{k-1}(\Omega)$, then

$$u \in (L^\infty(\mathbb{R}^+; H^{2k}(\Omega) \cap H_0^k(\Omega)) \text{ and } u_t \in L^\infty(0, T; H^{k-1}(\Omega)).$$

Proof. We can prove the existence and the regularities in (i), (ii), (iii) by applying, for instance, a standard Galerkin scheme and the a priori estimates which have been proved in the previous section.

Now we assume that there are at least two pairs of solutions to the problem (7.14)-(7.15), (u_1, v_1) and (u_2, v_2) (where $v_j = \frac{\partial u_j}{\partial t}$, $j = 1, 2$), respectively associated to the initial data $(u_{0,1}, v_{0,1})$ and $(u_{0,2}, v_{0,2})$. Then we set $u = u_1 - u_2$, $v = v_1 - v_2$, $u_0 = u_{0,1} - u_{0,2}$ and $v_0 = v_{0,1} - v_{0,2}$ to have

$$\beta u_{tt} + u_t - \Delta A_k u - \Delta B_k u - \Delta(f(u_1) - f(u_2)) = 0, \tag{7.60}$$

$$\mathcal{D}^\alpha u = 0, \text{ on } \Gamma, \ |\alpha| \le k, \tag{7.61}$$

$$u|_{t=0} = u_0, \ v|_{t=0} = v_0. \tag{7.62}$$

Multiplying (7.60) by $(-\Delta)^{-1} u_t$ and integrating over Ω and by parts, we obtain, adding to both parts of the resulting equation the term $\frac{\gamma}{2}\frac{d}{dt}\|u\|^2$,

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\left(\beta\|u_t\|_{-1}^2 + \|A_k^{1/2}u\|^2 + B_k^{\frac{1}{2}}[u] + \gamma\|u\|^2\right) + \|u_t\|_{-1}^2 \\ \le |((f(u_1) - f(u_2), u_t))| + \gamma|((u, u_t))|. \end{aligned} \tag{7.63}$$

Considering the right-hand side, we note that f is of class C^2, then we have

$$\begin{aligned} \nabla(f(u_1) - f(u_2)) &= f'(u_1)\nabla u_1 - f'(u_2)\nabla u_2 \\ &= (f'(u_1) - f'(u_2))\nabla u_1 + f'(u_2)\nabla u \\ &= f''(\epsilon_{u_1,u_2})u\nabla u_1 + f'(u_2)\nabla u. \end{aligned}$$

Noting that $f''(\epsilon_{u_1,u_2}), f'(u_2) \in L^\infty(\Omega)$ and $u, \nabla u_1 \in L^4(\Omega)$, then

$$\begin{aligned} |((f(u_1) - f(u_2), u_t))| + \gamma|((u, u_t))| &\le \|\nabla(f(u_1) - f(u_2))\|\|u_t\|_{-1} + \|\nabla u\|\|u_t\|_{-1} \\ &\le Q(\|u_{0,1}\|_{H_0^k(\Omega)}, \|u_{0,2}\|_{H_0^k(\Omega)}, \|v_{0,1}\|_{H^{-1}(\Omega)}, \\ &\quad \|v_{0,2}\|_{H^{-1}(\Omega)})(\|u\|_{L^4(\Omega)} + \|u\|_{H^1(\Omega)})\|u_t\|_{-1} \\ &\le c\|u\|_{H^k(\Omega)}\|u_t\|_{-1}. \end{aligned}$$

Using (7.28) and choosing γ large enough, we deduce that

$$\mathcal{E} := \beta\|u_t\|_{-1}^2 + \|A_k^{1/2}u\|^2 + B_k^{\frac{1}{2}}[u] + \gamma\int_\Omega u^2 dx$$
$$\geq \beta\|u_t\|_{-1}^2 + \frac{1}{2}\|A_k^{1/2}u\|^2 \geq \beta\|u_t\|_{-1}^2 + c\|u\|_{H^k}^2.$$

Thus, owing to interpolation inequality and Cauchy-Schwarz inequality, we have

$$\frac{d}{dt}\mathcal{E} + \|u_t\|_{-1}^2 \leq c\|u\|_{H^k(\Omega)}^2 \leq c'\,\mathcal{E}. \tag{7.64}$$

Applying the Gronwall's lemma, we get

$$\|u_t\|_{-1}^2 + \|u\|_{H^k(\Omega)}^2 \leq ce^{c't}(\|u_0\|_{H^1}^2 + \|v_0\|_{-1}^2), \tag{7.65}$$

which yields that the solutions are continuously dependent on the initial condition, as well the uniqueness.

□

Thus, we can define the family of solving operators :

$$S(t) : \Phi \to \Phi,\ (u_0, v_0) \mapsto (u(t), u_t(t)),\ \forall t \geq 0,$$

where $\Phi = H_0^k(\Omega) \times H^{-1}(\Omega)$, and u is the solution given by Theorem 7.5.1. This family of solving operators indeed forms a continuous semigroup for the topology of $H_0^k(\Omega) \times H^{-1}(\Omega)$ ($\forall t \geq 0$). It thus follows from (7.23) and (7.41) (see [103] and [127]) that

Theorem 7.5.2. *The semigroup $S(t)$ is dissipative in Φ, in the sense that $S(t)$ possesses a bounded absorbing set $\mathcal{B}_1$ which is bounded in Φ.*

Remark 7.5.1. *(i) Thus, we can proceed as in [75] and have the existence of the global attractor $\mathcal{A}$ which is compact in Φ.*

(ii) If we further assume that f is of class C^{k+1} and the initial data $(u_0, v_0) \in (H^{2k}(\Omega) \cap H_0^k(\Omega)) \times H^{k-1}(\Omega)$, it follows from (7.24) that the semigroup $S(t)$ is dissipative in $(H^{2k}(\Omega) \cap H_0^k(\Omega)) \times H^{k-1}(\Omega)$.

Chapitre 8

Energy stable finite element/spectral method for modified higher-order generalized Cahn-Hilliard equations

Méthode éléments finis / spectrale stable en énergie pour des généralisations d'ordre élevé de l'équation de Cahn-Hilliard

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Energy stable finite element/spectral method for modified higher-order generalized Cahn-Hilliard equations

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Abstract : Our aim in this paper is to study a fully discrete scheme for modified higher-order (in space) anisotropic generalized Cahn-Hilliard models which have extensive applications in biology, image processing, etc. In particular, the scheme is a combination of finite element or spectral method in space and a second-order stable scheme in time. We obtain energy stability results, as well as the existence and uniqueness of the numerical solution, both for the space semi-discrete and fully discrete cases. We also give several numerical simulations which illustrate the theoretical results and, especially, the effects of the higher-order terms on the anisotropy.

Key words and phrases : modified Cahn-Hilliard equation, higher-order models, energy stability, anisotropy, numerical simulations.

AMS Mathematics Subject Classification : 35K55, 35J60.

8.1 Introduction

The Cahn-Hilliard equation,

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) = 0, \tag{8.1}$$

plays an essential role in materials science and describes important qualitative features of two-phase systems related with phase separation processes, assuming isotropy and a constant temperature (see, e.g., [19], [20], [36], [100] and [108]).

Here, u is the order parameter (e.g., a density of atoms) and f is the derivative of a double-well potential F. A thermodynamically relevant potential F is the following logarithmic function which follows from a mean-field model :

$$F(s) = \frac{\theta_c}{2}(1-s^2) + \frac{\theta}{2}\left((1-s)\ln(\frac{1-s}{2}) + (1+s)\ln(\frac{1+s}{2})\right),\ s \in (-1,1),\ 0 < \theta < \theta_c, \tag{8.2}$$

i.e.,

$$f(s) = -\theta_c s + \frac{\theta}{2}\ln\frac{1+s}{1-s}, \tag{8.3}$$

although such a function is very often approximated by regular ones, typically,

$$F(s) = \frac{1}{4}(s^2-1)^2, \tag{8.4}$$

i.e.,

$$f(s) = s^3 - s. \tag{8.5}$$

Now, it is interesting to note that the Cahn-Hilliard equation and some of its variants are also relevant in other phenomena than phase separation. We can mention, for instance, population dynamics (see [31]), tumor growth (see [7] and [86]), bacterial films (see [81]), thin films (see [112] and [129]), image processing (see [9], [8], [21], [27] and [42]) and even the rings of Saturn (see [130]) and the clustering of mussels (see [90]).

In particular, several such phenomena can be modeled by the following generalized Cahn-Hilliard equation :

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) + g(x,u) = 0. \tag{8.6}$$

We studied in [97] and [99] (see also [7], [27], [37] and [47]) this equation.

The Cahn-Hilliard equation is based on the so-called Ginzburg-Landau free energy,

$$\Psi_{\mathrm{GL}} = \int_\Omega \left(\frac{1}{2}|\nabla u|^2 + F(u)\right) dx, \tag{8.7}$$

where Ω is the domain occupied by the system (we assume here that it is a bounded and regular domain of $\mathbb{R}^d$, $d = 1, 2$ or 3, with boundary Γ). In particular, in (8.7), the term $|\nabla u|^2$ models short-ranged interactions. It is however interesting to note that such a term is obtained by truncation of higher-order ones (see [20]) ; it can also be seen as a first-order approximation of a nonlocal term accounting for long-ranged interactions (see [65] and [66]).

G. Caginalp and E. Esenturk recently proposed in [23] (see also [22]) higher-order phase-field models in order to account for anisotropic interfaces (see also [80], [125] and [132] for other approaches which, however, do not provide an explicit way to compute the anisotropy). More precisely, these authors proposed the following modified free energy, in which we omit the temperature :

$$\Psi_{\mathrm{HOGL}} = \int_\Omega \left(\frac{1}{2}\sum_{i=1}^{k}\sum_{|\alpha|=i} a_\alpha |\mathcal{D}^\alpha u|^2 + F(u)\right) dx, \ k \in \mathbb{N}, \tag{8.8}$$

where, for $\alpha = (\alpha_1, ..., \alpha_d) \in (\mathbb{N} \cup \{0\})^d$,

$$|\alpha| = \alpha_1 + ... + \alpha_d$$

and, for $\alpha \neq (0, ..., 0)$,

$$\mathcal{D}^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} ....\partial x_d^{\alpha_d}}$$

(we agree that $\mathcal{D}^{(0,...,0)}v = v$). The corresponding higher-order Cahn-Hilliard equation then reads

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{k}(-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) = 0. \tag{8.9}$$

We studied in [33] and [32] the corresponding isotropic model which reads

$$\frac{\partial u}{\partial t} - \Delta P(-\Delta)u - \Delta f(u) = 0, \tag{8.10}$$

where

$$P(s) = \sum_{i=1}^{k} a_i s^i, \ a_k > 0, \ k \in \mathbb{N}, \ s \in \mathbb{R}.$$

The anisotropic model (8.9) is treated in [34] and the generalized anisotropic model (8.6) was studied in [35] (there, numerical simulations were also performed to illustrate the effects of the higher-order terms and of the anisotropy). Furthermore, these models contain sixth-order Cahn–Hilliard models, such as the phase-field crystal model (see, e.g., [45], [96] and [97]).

Actually, in this paper, we are interested in the hyperbolic relaxation of the equation, proposed in [57] to model the early stages of spinodal decomposition in certain glasses and in [56] in the context of the phase-field crystal model (in that case, one speaks of the modified phase-field crystal model). In particular, the modified phase-field crystal model was studied in [75].

More precisely, we are interested in the study of numerical approximations for the hyperbolic relaxation of the higher-order anisotropic generalized Cahn-Hilliard models, assuming the existence, uniqueness and regularity of solutions ; these issues will be addressed elsewhere.

A related study, for the modified phase-field crystal model, can be found in [16, 58, 72, 136]. In particular, [58] proposed an unconditionally energy stable (finite element method in space and second-order accurate in time) scheme, but without any theoretical analysis. Furthermore, [72] derived a scheme with a space discretization based on a splitting method and proved its energy stability, as well as its unique solvability. The schemes used in [16, 136] were based on a convex splitting of the pseudo-energy for the time discretization.

The scheme considered in this paper is a combination of finite elements or spectral methods in space and a second-order stable scheme in time. More precisely, the space is discretized by a splitting approach which is inspired by [58, 71, 72] and it turns out that the finite element method, as well as the spectral method, which are contained in an H^1 Galerkin approach, are both applicable. As far as the time discretization is concerned, we apply the modified Crank-Nicolson scheme introduced in [63] which has been successfully applied to the Cahn-Hillard equation, as well as to gradient-like equations.

The structure of the paper is as follows. In section 2, we give some assumptions. In section 3, we discuss the space semi-discrete problem and prove its energy stability and unique solvability. We investigate the fully discrete problem in section 4 and present the main analysis, including consistency, energy stability and unique solvability. In section 5, several numerical simulations are carried out to illustrate the theoretical results and, especially, the effects of the higher-order terms and the anisotropy.

8.2 Setting of the problem and assumptions

In this paper, we consider the following generalized equation which reads, for $k \in \mathbb{N}$, $k \geq 2$, $\mathbf{x} \in \Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$,

$$\beta \frac{\partial^2 u(\mathbf{x},t)}{\partial t^2} + \frac{\partial u(\mathbf{x},t)}{\partial t} - \Delta \sum_{i=1}^{k} (-1)^i \sum_{|\alpha|=i} a_\alpha \mathcal{D}^{2\alpha} u - \Delta f(u) + \gamma u = 0, \tag{8.11}$$

$$u(\mathbf{x},0) = u_0(\mathbf{x}), \qquad \frac{\partial u(\mathbf{x},t)}{\partial t}|_{t=0} = v_0(\mathbf{x}),\ t \geq 0,\ \mathbf{x} \in \Omega, \tag{8.12}$$

with periodic boundary condition for a rectangular (d=2) or cubic (d=3) domain. $\beta > 0$ is a relaxation parameter, $\gamma \geq 0$. The additional term γu can model, e.g., long-ranged interactions (see [111]).

For the sake of simplicity, we assume that $\int_\Omega 1 d\mathbf{x} = |\Omega| = 1$. Besides, we need some assumptions on (8.11). Firstly, we assume that

$$a_\alpha > 0, \quad \text{for } |\alpha| = k. \tag{8.13}$$

Secondly, the nonlinearity f is set to be a polynomial of odd degree with positive leading coefficient and which vanishes at 0, i.e.

$$f(s) = \sum_{i=1}^{2p+1} \kappa_i s^i, \quad s \in \mathbb{R}, \tag{8.14}$$

with $p \in \mathbb{N}^+$ if $d = 2$ and $p \in \{1, 2\}$ if $d = 3$. The restriction on p when $d = 3$ is due to the use of H^1_{per} conforming finite element or spectral spaces (see (8.17)). We denote by F the antiderivative of f which vanishes at 0, i.e.

$$F(s) = \sum_{i=2}^{2p+2} \frac{\kappa_{i-1}}{i} s^i, \quad \forall s \in \mathbb{R}. \tag{8.15}$$

It can be verified that there exist constants $c_1, c_3 > 0, c_2, c_4 \geq 0$, such that

$$\begin{aligned} &(a) \qquad |f(s)| \leq c_1 F(s) + c_2, \quad \forall s \in \mathbb{R}, \\ &(b) \qquad F(s) \geq c_3 s^4 - c_4, \quad \forall s \in \mathbb{R}. \end{aligned} \tag{8.16}$$

In addition, we will make use of the Sobolev embedding $H^1_{per} \subset L^{2p+2}(\Omega)$. In particular, there exists a constant $c_s = c_s(\Omega, p)$ such that

$$||u||_{L^{2p+2}(\Omega)} \leq c_s |u|_1, \quad \forall u \in H^1_{per}, \tag{8.17}$$

where $|\cdot|_1$ is a norm in H^1_{per} defined by $|u|_1^2 = |\langle u \rangle|^2 + ||\nabla u||_0^2$ with $\langle u \rangle = \int_\Omega u dx$, $||\cdot||_0$ is the L^2 norm, and $(\cdot,\cdot)$ is the associated scalar product. The map $v \mapsto f(v)$ is Lipschitz continuous on bounded sets of H^1_{per} with values in $L^{(2p+2)/(2p+1)}(\Omega) \subset H^{-1}_{per}$. We also have $H^2_{per} \subset C^0(\bar{\Omega})$ with continuous injection.

We introduce the pseudo-energy

$$\mathcal{E}(u,v) = \Psi_{\text{HOGL}} + \frac{\beta}{2}\|\dot{v}\|_{-1}^2 + \frac{\gamma}{2}\|\dot{u}\|_{-1}^2,\ \forall (u,v) \in H_{per}^k \times H_{per}^{-1},$$

where $\dot{v} = v - \langle v \rangle$, $\|\cdot\|_{-1} = \|(-\Delta)^{-\frac{1}{2}} \cdot\|$ and $(-\Delta)^{-1}$ denotes the inverse minus Laplace operator associated with periodic boundary conditions with null average ; $\mathcal{E}(u,v)$ is indeed well-defined. Multiplying (8.11) by $(-\Delta)^{-1}\dot{u}_t$ and integrating over Ω, we have

$$\frac{d}{dt}\mathcal{E}(u,u_t) = -\|\dot{u}_t\|_{-1}^2 < 0,$$

which guarantees that the pseudo-energy is nonincreasing in time. As mentioned in the introduction, we will only focus on the numerical approximations in what follows and will address other issues, such as well-posedness and regularity, elsewhere.

8.3 The space semi-discrete problem

8.3.1 The space semi-discrete scheme

For $k = 2$, the original equation (8.11) is equivalent to the following system :

$$\begin{cases} u_t = v, \\ \beta v_t = -v + \Delta w - \gamma u, \\ w = \sum\limits_{|\alpha|=2} a_\alpha D^{2\alpha} u - \sum\limits_{|\alpha|=1} a_\alpha D^{2\alpha} u + f(u). \end{cases} \tag{8.18}$$

For the sake of simplicity, we denote the coefficients a_α by

$$a_\alpha = \begin{cases} a_j, & |\alpha| = 1,\ \alpha_j \neq 0; \\ a_{ij} > 0, & |\alpha| = 2,\ \alpha_i = \alpha_j = 1,\ i = 1, \cdots, j;\ j = 1, \cdots, d. \end{cases} \tag{8.19}$$

Thus, for $d = 2$, the coefficients of $\frac{\partial^4 u}{\partial x_1^4}, \frac{\partial^4 u}{\partial x_1^2 \partial x_2^2}, \frac{\partial^4 u}{\partial x_2^4}$ are a_{11}, a_{12}, a_{22}, respectively, while the coefficients of $\frac{\partial^2 u}{\partial x_1^2}, \frac{\partial^2 u}{\partial x_2^2}$ are a_1, a_2, respectively.

By introducing the variables $p_{ij} = -\frac{\partial^2 u}{\partial x_i \partial x_j}$, $i = 1, \cdots, j,\ j = 1, \cdots, d$, (8.18) can be rewritten as

$$\begin{cases} u_t = v, \\ \beta v_t = -v + \Delta w - \gamma u, \\ p_{ij} = -\dfrac{\partial^2 u}{\partial x_i \partial x_j}, \\ w = -\displaystyle\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}\frac{\partial^2 p_{ij}}{\partial x_i \partial x_j} + \sum_{j=1}^{d} a_j p_{jj} + f(u). \end{cases} \tag{8.20}$$

We now describe the semi-discrete scheme. Let V_h be a finite dimensional subspace of $H^1_{per}(\Omega)$. In practice, V_h could be a space of conforming finite element or a space with spectral basis. Let $\{e_h^k\}_{k=1}^{N_h}$ denote a monic orthonormal basis of V_h for the L^2 scalar product such that $e_h^1 \equiv 1$, where N_h is the dimension of V_h.

We multiply each equation in (8.20) by different test functions in V_h and integrate over Ω and by parts to obtain the space semi-discrete scheme which reads : find u_h, v_h, $p_{ij,h}$, $w_h : \mathbb{R}_+ \to V_h$, such that :

$$\begin{cases} (\partial_t u_h, \phi_h) = (v_h, \phi_h), \\ \beta(\partial_t v_h, \psi_h) = -(v_h, \psi_h) - (\nabla w_h, \nabla \psi_h) - \gamma(u_h, \psi_h), \\ (p_{ij,h}, \zeta_{ij,h}) = \left(\dfrac{\partial u_h}{\partial x_j}, \dfrac{\partial \zeta_{ij,h}}{\partial x_i}\right), \\ (w_h, \xi_h) = \displaystyle\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}\left(\frac{\partial p_{ij,h}}{\partial x_i}, \frac{\partial \xi_h}{\partial x_j}\right) + \sum_{j=1}^{d} a_j (p_{jj,h}, \xi_h) + (f(u_h), \xi_h), \end{cases} \tag{8.21}$$

for all $\phi_h, \psi_h, \zeta_{ij,h}, \xi_h \in V_h$, $i = 1, \cdots, j$, $j = 1 \cdots, d$, with initial conditions :

$$u_h(0) = u_h^0, \quad v_h(0) = v_h^0, \quad u_h^0, v_h^0 \in V_h. \tag{8.22}$$

Then (8.21) can be written in the following equivalent system :

$$\begin{cases} U_t = V, \\ \beta V_t = -V - AW - \gamma U, \\ P_{ij} = A_{ij} U, \\ W = \displaystyle\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij} {A_{ij}}^T P_{ij} + \sum_{j=1}^{d} a_j P_{jj} + \nabla F_h(U), \end{cases} \tag{8.23}$$

where

(a). $A = (\nabla e_h^k, \nabla e_h^l)_{1 \le k,l \le N_h}$, $\quad A_{ij} = (\dfrac{\partial e_h^k}{\partial x_i}, \dfrac{\partial e_h^l}{\partial x_j})_{1 \le k,l \le N_h}$,

$$
\begin{aligned}
&(b).\ u_h(t) = \sum_{i=1}^{N_h} u_i(t) e_h^i \simeq U(t) = (u_1(t), \cdots, u_{N_h}(t))^T,\ v_h \simeq V,\ p_{ij,h} \simeq P_{ij},\ w_h \simeq W, \\
&(c).\ F_h(U) = (F(u_h), 1),\ \ s.t.\ \nabla F_h(U) = ((f(u_h), e_h^1), \cdots, (f(u_h), e_h^{N_h}))^T.
\end{aligned}
\tag{8.24}
$$

We must point out that, for each pair of (i, j), when $i \neq j$, A_{ij} is not symmetric. When there is no risk of confusion, we denote A_{jj} by A_j. Besides, A_j and A have the following relationship :

$$
A = \sum_{j=1}^{d} A_j. \tag{8.25}
$$

Eliminating V, P_{ij}, W, (8.23) is equivalent to

$$
\beta U_{tt} + U_t = -A\left(\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij} {A_{ij}}^T A_{ij} U + \sum_{j=1}^{d} a_j A_j U + \nabla F_h(U)\right) - \gamma U,\ t \geq 0. \tag{8.26}
$$

This corresponds to a space semi-discrete scheme of the original equation. Furthermore, U denotes a solution of (8.26). Notice that the first row and the first column of A are filled with 0, hence the first component of U, i.e. $u_1(t) = (u_h(t), 1)$, satisfies

$$
\beta \partial_{tt} u_1 + \partial_t u_1 + \gamma u_1 = 0, \quad t \geq 0. \tag{8.27}
$$

We consider three cases depending on the sign of the constant $1 - 4\beta\gamma$: (i) $1 - 4\beta\gamma > 0$, (ii) $1 - 4\beta\gamma = 0$, (iii) $1 - 4\beta\gamma < 0$. We solve (8.27) with the initial conditions $u_1(0) = (u_h^0, 1) =: u_1^0$, $\partial_t u_1(0) = (v_h^0, 1) =: v_1^0$ and get

(i)

$$
\begin{aligned}
u_1(t) &= \frac{v_1^0 - \lambda_2 u_1^0}{\lambda_1 - \lambda_2} e^{\lambda_1 t} + \frac{\lambda_1 u_1^0 - v_1^0}{\lambda_1 - \lambda_2} e^{\lambda_2 t}, \\
\partial_t u_1(t) &= \lambda_1 \frac{v_1^0 - \lambda_2 u_1^0}{\lambda_1 - \lambda_2} e^{\lambda_1 t} + \lambda_2 \frac{\lambda_1 u_1^0 - v_1^0}{\lambda_1 - \lambda_2} e^{\lambda_2 t},
\end{aligned}
$$

where

$$
\lambda_1 = \frac{-1 + \sqrt{1 - 4\beta\gamma}}{2\beta} < 0,\ \lambda_2 = \frac{-1 - \sqrt{1 - 4\beta\gamma}}{2\beta} < 0;
$$

(ii)

$$
\begin{aligned}
u_1(t) &= [u_1^0 + (v_1^0 + \frac{1}{2\beta} u_1^0) t] e^{-\frac{1}{2\beta} t}, \\
\partial_t u_1(t) &= [v_1^0 - \frac{1}{2\beta}(v_1^0 + \frac{1}{2\beta} u_1^0) t] e^{-\frac{1}{2\beta} t};
\end{aligned}
$$

(iii)

$$
\begin{aligned}
u_1(t) &= (u_1^0 \cos \lambda t + \frac{u_1^0 + 2\beta v_1^0}{\sqrt{4\beta\gamma - 1}} \sin \lambda t) e^{-\frac{1}{2\beta}t}, \\
\partial_t u_1(t) &= (v_1^0 \cos \lambda t - \frac{v_1^0 + 2\gamma u_1^0}{\sqrt{4\beta\gamma - 1}} \sin \lambda t) e^{-\frac{1}{2\beta}t},
\end{aligned}
\tag{8.28}
$$

where $\lambda = \sqrt{4\beta\gamma - 1}/2\beta$.
Moreover, by a direct calculation, we find

$$
|\partial_t u_1(t)| \leq c(u_1^0, v_1^0, t), \tag{8.29}
$$

where

$$
c(u_1^0, v_1^0, t) = \begin{cases}
|\lambda_1 \dfrac{v_1^0 - \lambda_2 u_1^0}{\lambda_1 - \lambda_2}| e^{\lambda_1 t} + |\lambda_2 \dfrac{\lambda_1 u_1^0 - v_1^0}{\lambda_1 - \lambda_2}| e^{\lambda_2 t}, & 1 - 4\beta\gamma > 0, \\
|v_1^0| e^{-\frac{1}{2\beta}t} + \dfrac{1}{2\beta}|v_1^0 + \dfrac{1}{2\beta} u_1^0| t e^{-\frac{1}{2\beta}t}, & 1 - 4\beta\gamma = 0, \\
(|v_1^0| + \dfrac{1}{\sqrt{4\beta\gamma - 1}}|v_1^0 + 2\gamma u_1^0|) e^{-\frac{1}{2\beta}t}, & 1 - 4\beta\gamma < 0.
\end{cases}
\tag{8.30}
$$

For each vector $R = (r_1, \cdots, r_N)^T \in \mathbb{R}^N$, we set $\dot{R} = (r_2, \cdots, r_N)^T \in \mathbb{R}^{N-1}$. Then $\dot{U} = (U_2(t), \cdots, U_{N_h}(t))^T$ satisfies

$$
\beta \dot{U}_{tt} + \dot{U}_t = -\dot{A} \left(\sum_{j=1}^{d} \sum_{i=1}^{j} a_{ij} \dot{A}_{ij}^T \dot{A}_{ij} \dot{U} + \sum_{j=1}^{d} a_j \dot{A}_j \dot{U} + \dot{\nabla} F_h(U) \right) - \gamma \dot{U}, \tag{8.31}
$$

where $\dot{A} = (a_{kl})_{2 \leq k, l \leq N_h}$, the submatrix of A obtained by deleting the first line and the first column of A, is symmetric and positive definite.

8.3.2 Discrete energy estimate, existence and uniqueness

We start by introducing some norms. Let $|\cdot|$ denote the Euclidean norm in $\mathbb{R}^{N_h}$ or $\mathbb{R}^{N_h - 1}$. Besides, we will also use the quadratic norm $|\cdot|_{-1}$ in $\mathbb{R}^{N_h - 1}$ which is defined by

$$
|\dot{R}|_{-1} = (\dot{R}^T \dot{A}^{-1} \dot{R})^{1/2}, \quad \forall \dot{R} \in \mathbb{R}^{N_h - 1}.
$$

It is easy to show that $|A^s U| = |\dot{A}^s \dot{U}|, \quad \forall s > 0, \ U \in \mathbb{R}^{N_h}$.

Moreover, we define

$$
\begin{aligned}
&(a).\ E_h(U) = \frac{1}{2}\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}|A_{ij}U|^2 + \frac{1}{2}\sum_{j=1}^{d} a_j|A_j^{\frac{1}{2}}U|^2 + F_h(U),\\
&(b).\ \mathcal{E}_h(U,V) = E_h(U) + \frac{\beta}{2}|\dot{V}|_{-1}^2 + \frac{\gamma}{2}|\dot{U}|_{-1}^2.
\end{aligned}
\tag{8.32}
$$

For convenience, we set

$$
\mathcal{E}_h(t) = \mathcal{E}_h(U(t), U_t(t)).
$$

Theorem 8.3.1. *Assume that $U \in C^2([0,T);\mathbb{R}^{N_h})$ is a solution of (8.26). Then it satisfies the energy equality*

$$
\frac{d}{dt}\mathcal{E}_h(t) + |\dot{U}_t|_{-1}^2 = \partial_t u_1(f(u_h),1),
\tag{8.33}
$$

and the energy estimate

$$
\mathcal{E}_h(t) + \int_0^t |\dot{U}_t(s)|_{-1}^2 ds \le (\mathcal{E}_h(0) + c'(\hat{c}|u_1^0| + \check{c}|v_1^0|))e^{2c_1(\hat{c}|u_1^0|+\check{c}|v_1^0|)},
\tag{8.34}
$$

for all $t \in [0,T)$, where c' depends on $f, a_j, a_{jj}, 1 \le j \le d$, $\hat{c}, \check{c}$ given in (8.45).

Proof. Multiplying (8.31) by $\dot{U}_t^T \dot{A}^{-1}$ and using the identity

$$
\dot{U}_t^T \dot{\nabla} F_h(U) = U_t^T \nabla F_h(U) - \partial_t u_1(f(u_h),1) = \frac{d}{dt}F_h(U) - \partial_t u_1(f(u_h),1),
$$

we obtain

$$
\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\left(\beta|\dot{U}_t|_{-1}^2 + \sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}|\dot{A}_{ij}\dot{U}|^2 + \sum_{j=1}^{d} a_j|\dot{A}_j^{\frac{1}{2}}\dot{U}|^2 + \gamma|\dot{U}|_{-1}^2\right) + |\dot{U}_t|_{-1}^2 + \frac{d}{dt}F_h(U)\\
&= \partial_t u_1(f(u_h),1).
\end{aligned}
\tag{8.35}
$$

Note that $|\dot{A}_{ij}\dot{U}|^2 = |A_{ij}U|^2$, $|\dot{A}_j^{\frac{1}{2}}\dot{U}|^2 = |A_j^{\frac{1}{2}}U|^2$. Then reorganising (8.35) yields

$$
\begin{aligned}
&\frac{d}{dt}\left(\frac{1}{2}\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}|A_{ij}U|^2 + \frac{1}{2}\sum_{j=1}^{d} a_j|A_j^{\frac{1}{2}}U|^2 + F_h(U) + \frac{1}{2}\beta|\dot{U}_t|_{-1}^2 + \frac{1}{2}\gamma|\dot{U}|_{-1}^2\right) + |\dot{U}_t|_{-1}^2\\
&= \partial_t u_1(f(u_h),1),
\end{aligned}
\tag{8.36}
$$

which is precisely the energy equality (8.33).

We now prove the energy estimate (8.34). First, by assumption (8.16)(a), (8.33) gives

$$\frac{d}{dt}\mathcal{E}_h(t) + |\dot{U}_t|_{-1}^2 \le |\partial_t u_1|(c_1 F_h(U) + c_2). \tag{8.37}$$

Then by the discrete Hölder's inequality, (8.25), and assumption (8.13), we have

$$|AU|^2 = \Big|\sum_{j=1}^{d} A_j U\Big|^2 \le d\sum_{j=1}^{d}\Big|A_j U\Big|^2 \le \frac{d}{\min\limits_{1\le j\le d}\{a_{jj}\}}\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}|A_{ij}U|^2, \tag{8.38}$$

which, applying Young's inequality, yields

$$\begin{aligned}\Big|\sum_{j=1}^{d} a_j|A_j^{\frac{1}{2}}U|^2\Big| &\le \max_{1\le j\le d}|a_j|\sum_{j=1}^{d}|A_j^{\frac{1}{2}}U|^2 = \max_{1\le j\le d}|a_j|U^T AU\\ &\le \kappa|AU|^2 + \frac{(\max_{1\le j\le d}|a_j|)^2}{4\kappa}|U|^2.\end{aligned} \tag{8.39}$$

Taking $\kappa = \frac{\min_{1\le j\le d}\{a_{jj}\}}{d}$ and applying (8.38) yields

$$\Big|\sum_{j=1}^{d} a_j|A_j^{\frac{1}{2}}U|^2\Big| \le \sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}|A_{ij}U|^2 + \bar{c}|U|^2,\ \text{with}\ \bar{c} = \frac{d(\max_{1\le j\le d}|a_j|)^2}{4\min\limits_{1\le j\le d}\{a_{jj}\}}.$$

As a consequence, we obtain

$$2E_h(U) = \sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}|A_{ij}U|^2 + \sum_{j=1}^{d} a_j|A_j^{\frac{1}{2}}U|^2 + 2F_h(U) \ge 2F_h(U) - \bar{c}|U|^2. \tag{8.40}$$

Note that

$$|U|^2 = \|u_h\|_0^2 \le \|u_h\|_{L^4}^2 \le \frac{c_3}{c}\|u_h\|_{L^4}^4 + \frac{c}{4c_3}, \quad \forall c > 0. \tag{8.41}$$

Then taking $c = \bar{c}$ and by assumption (8.16)(b), we find

$$F_h(U) = (F(u_h), 1) \ge c_3\|u_h\|_{L^4}^4 - c_4 \ge \bar{c}|U|^2 - \grave{c}, \tag{8.42}$$

where $\grave{c} = \dfrac{\bar{c}^2}{4c_3} + c_4$. Hence,

$$2\mathcal{E}_h(t) \ge\ 2E_h(U) \ge F_h(U) - \grave{c}. \tag{8.43}$$

Plugging (8.43) into (8.37), and note (8.29), we deduce

$$\frac{d}{dt}\mathcal{E}_h(t) + |\dot{U}_t|_{-1}^2 \le |\partial_t u_1|(2c_1\mathcal{E}_h(t) + c') \le c(u_1^0, v_1^0, t)(2c_1\mathcal{E}_h(t) + c'),$$

where $c' = c_1\grave{c} + c_2$ depends on $f, a_j, a_{jj}, 1 \le j \le d$. Then applying Gronwall's lemma yields

$$\mathcal{E}_h(t) + \int_0^t |\dot{U}_t(s)|_{-1}^2 e^{\eta(t)-\eta(s)} ds \le \mathcal{E}_h(0)e^{\eta(t)} + \int_0^t c'c(u_1^0, v_1^0, s)e^{\eta(t)-\eta(s)} ds, \tag{8.44}$$

where $\eta(t) = 2c_1 \int_0^t c(u_1^0, v_1^0, s)ds$. According to (8.30), we know that $\eta(t)$ is a monotone increasing function which can be bounded by

$$\eta(t) \le 2c_1(\hat{c}|u_1^0| + \check{c}|v_1^0|),$$

with

$$\begin{array}{llll} (i) & 1-4\beta\gamma > 0, & \hat{c} = \frac{1}{\sqrt{1-4\beta\gamma}}, & \check{c} = \frac{2\beta}{\sqrt{1-4\beta\gamma}}; \\ (ii) & 1-4\beta\gamma = 0, & \hat{c} = 1, & \check{c} = 4\beta; \\ (iii) & 1-4\beta\gamma < 0, & \hat{c} = \frac{4\beta\gamma}{\sqrt{4\beta\gamma-1}}, & \check{c} = \frac{2\beta(1+\sqrt{4\beta\gamma-1})}{\sqrt{4\beta\gamma-1}}. \end{array} \tag{8.45}$$

Thus we derive

$$\mathcal{E}_h(t) + \int_0^t |\dot{U}_t(s)|_{-1}^2 ds \le (\mathcal{E}_h(0) + c'(\hat{c}|u_1^0| + \check{c}|v_1^0|))e^{2c_1(\hat{c}|u_1^0|+\check{c}|v_1^0|)},$$

which finishes the proof. □

Remark 8.3.1. *We can also deduce a lower bound for $\mathcal{E}_h(U,V) : \forall U, V \in \mathbb{R}^{N_h}$,*

$$\mathcal{E}_h(U,V) \ge \frac{\min_{1\le j\le d}\{a_{jj}\}}{4d}|AU|^2 + \frac{1}{2}|U|^2 + \frac{\beta}{2}|\dot{V}|_{-1}^2 + \frac{\gamma}{2}|\dot{U}|_{-1}^2 - c, \tag{8.46}$$

where c depends on $F, a_j, a_{jj}, 1 \le j \le d$.In fact, by (8.38) and taking $\kappa = \frac{\min_{1\le j\le d}\{a_{jj}\}}{2d}$ in (8.39), we get

$$\begin{aligned} E_h(U) &= \frac{1}{2}\sum_{j=1}^d \sum_{i=1}^j a_{ij}|A_{ij}U|^2 + \frac{1}{2}\sum_{j=1}^d a_j|A_j^{\frac{1}{2}}U|^2 + F_h(U) \\ &\ge \frac{\min_{1\le j\le d}\{a_{jj}\}}{4d}|AU|^2 - \bar{c}|U|^2 + F_h(U). \end{aligned}$$

Taking $c = \mu := \bar{c} + \frac{1}{2}$ in (8.41) and plugging it into (8.42), we have

$$E_h(U) \geq \frac{\min_{1\leq j\leq d}\{a_{jj}\}}{4d}|AU|^2 + \frac{1}{2}|U|^2 - (\frac{\mu^2}{4c_3} + c_4),$$

which gives (8.46).

Remark 8.3.2. *If* $\gamma = 0$*, the behavior of* $u_1(t)$ *is straightforward. In fact, in that case, solving* (8.27) *yields*

$$\partial_t u_1(t) = v_1^0 e^{-t/\beta}, \quad u_1(t) = \beta v_1^0 + u_1^0 - \beta v_1^0 e^{-t/\beta},$$

and the energy estimate (8.34) *changes into*

$$\mathcal{E}_h(t) + \int_0^t |\dot{U}_t(s)|_{-1}^2 ds \leq (\mathcal{E}_h(0) + c'\beta|v_1^0|)e^{2c_1\beta|v_1^0|}.$$

Theorem 8.3.2. *For every* U^0*,* V^0 *in* $\mathbb{R}^{N_h}$*,* (8.26) *admits a unique solution* $U \in C^2(\mathbb{R}_+, \mathbb{R}^{N_h})$ *which satisfies* $U(0) = U^0$*,* $U_t(0) = V^0$*.*

Proof. First, by the Cauchy-Lipschitz theorem, we know that (8.26) admits a unique maximal solution $U \in C^2([0, T^+), \mathbb{R}^{N_h})$ for the given initial conditions. Moereover, by the energy estimate (8.34), the definition of $\mathcal{E}_h(t)$ in (8.32), and (8.46), $|\dot{U}_t|_{-1}$ and $|U|$ are uniformly bounded for $t > 0$. Therefore, this and estimate (8.28) on $\partial_t u_1 = \langle \partial_t u \rangle$ imply $T^+ = +\infty$. □

8.4 The fully discrete problem

8.4.1 The fully discrete scheme

We use the scheme proposed by Gomez and Hughes ([63]) to discretize in time which can be regarded as a Crank-Nicolson scheme, together with a second-order stabilization term. For this purpose, we use some decomposition for F and f (such a decomposition is always possible for f satisfying (8.14), see [72]) :

(a) $F = F_+ + F_-$, where F_+ and F_- are polynomials such that

$$F_+^{(4)} \geq 0, F_-^{(4)} \leq 0, \ \deg(\mathrm{F}_-) < \deg(\mathrm{F}).$$

(b) $f = f_+ + f_-$, where $f_+ = F_+'$, $f_- = F_-'$, and there exits two constants $c_5, c_6 > 0$ such that

$$\begin{aligned} &\frac{1}{2}(|f(r)| + |f(s)|) + \frac{1}{12}(s-r)^2(|f_+''(r)| + |f_-''(s)|) \\ &\leq c_5(F(r) + F(s)) + c_6, \ \forall r, s \in \mathbb{R}. \end{aligned} \tag{8.47}$$

Remark 8.4.1. *In particular, for the usual cubic nonlinear term,* $f(s) = s^3 - s$*, then* $f_+ = f$*,* $f_- = 0$*, so that the above assumptions are automatically satisfied.*

Let $\tau > 0$ denote the time step, $(u_h^0, v_h^0) \in V_h \times V_h$ be the initial datum. The fully discrete scheme reads : for $n \geq 0$, find $(u_h^{n+1}, v_h^{n+1}, p_{ij,h}^{n+1/2}, w_h^{n+1/2}) \in (V_h)^{3d}$ such that

$$\begin{cases} (\dfrac{u_h^{n+1} - u_h^n}{\tau}, \phi_h) = (v_h^{n+1/2}, \phi_h), \\ \beta(\dfrac{v_h^{n+1} - v_h^n}{\tau}, \psi_h) = -(v_h^{n+1/2}, \psi_h) - (\nabla w_h^{n+1/2}, \nabla\psi_h) - \gamma(u_h^{n+1/2}, \psi_h), \\ (p_{ij,h}^{n+1/2}, \zeta_{ij,h}) = \left(\dfrac{\partial u_h^{n+1/2}}{\partial x_j}, \dfrac{\partial \zeta_{ij,h}}{\partial x_i}\right), \\ (w_h^{n+1/2}, \xi_h) = \displaystyle\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}\left(\dfrac{\partial p_{ij,h}^{n+1/2}}{\partial x_i}, \dfrac{\partial \xi_h}{\partial x_j}\right) \\ \qquad + \displaystyle\sum_{j=1}^{d} a_j (p_{jj,h}^{n+1/2}, \xi_h) + \left(\dfrac{f(u_h^n) + f(u_h^{n+1})}{2}, \xi_h\right) \\ \qquad - \dfrac{1}{12}((u_h^{n+1} - u_h^n)^2 (f_+''(u_h^n) + f_-''(u_h^{n+1})), \xi_h), \end{cases} \tag{8.48}$$

for all $\phi_h, \psi_h, \zeta_{ij,h}, \xi_h \in V_h, i = 1, \cdots, j,\ j = 1, \cdots, d$. The notation $u_h^{n+1/2} := (u_h^{n+1} + u_h^n)/2$ stands for the appromixation of u_h at time $t_{n+1/2} = (n+1/2)\tau$. The same holds for $p_{ij,h}^{n+1/2}$, $v_h^{n+1/2}$, $w_h^{n+1/2}$.

Following the notation in (8.24), we can rewrite the fully discrete scheme in $\mathbb{R}^{N_h}$: let U^0, V^0 in $\mathbb{R}^{N_h}$. For $n \geq 0$, find $(U^{n+1}, V^{n+1}, P_{ij}^{n+1/2}, W^{n+1/2}) \in (\mathbb{R}^{N_h})^{3d}$ which solves

$$\begin{cases} \dfrac{U^{n+1} - U^n}{\tau} = V^{n+1/2}, \\ \beta\dfrac{V^{n+1} - V^n}{\tau} = -V^{n+1/2} - AW^{n+1/2} - \gamma U^{n+1/2}, \\ P_{ij}^{n+1/2} = A_{ij} U^{n+1/2}, \\ W^{n+1/2} = \displaystyle\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij} A_{ij}{}^T P_{ij}^{n+1/2} + \sum_{j=1}^{d} a_j P_{jj}^{n+1/2} \\ \qquad + \dfrac{\nabla F_h(U^n) + \nabla F_h(U^{n+1})}{2} - G(U^n, U^{n+1}), \end{cases} \tag{8.49}$$

where $G(U^n, U^{n+1}) = \dfrac{1}{12}((u_h^{n+1} - u_h^n)^2 (f_+''(u_h^n) + f_-''(u_h^{n+1})), e_h^i)_{1 \leq i \leq N_h}$.

Eliminating $P_{ij}^{n+1/2}$ and $W^{n+1/2}$, the scheme becomes

$$\begin{cases} \dfrac{U^{n+1}-U^n}{\tau} - V^{n+1/2} = 0, \\ \beta\dfrac{V^{n+1}-V^n}{\tau} + V^{n+1/2} + A(\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}A_{ij}{}^T A_{ij}U^{n+1/2} + \sum_{j=1}^{d} a_j A_j U^{n+1/2} \\ \qquad + \dfrac{\nabla F_h(U^n)+\nabla F_h(U^{n+1})}{2} - G(U^n, U^{n+1})) + \gamma U^{n+1/2} = 0. \end{cases} \tag{8.50}$$

We now check the consistency of the fully discrete problem.

Proposition 8.4.1. (**Consistency**). *The scheme* (8.50) *has a second-order consistency error in time, i.e. any solution of the space semi-discrete problem* (8.23) *satisfies the fully discrete problem* (8.50) *with order* $O(\tau^2)$.

Proof. We need to prove that

$$\frac{U(t_{n+1})-U(t_n)}{\tau} - U_t(t_{n+\frac{1}{2}}) - \left(\frac{V(t_{n+1})+V(t_n)}{2} - V(t_{n+\frac{1}{2}})\right) = O(\tau^2), \tag{8.51}$$

and

$$\begin{aligned} &\beta(\frac{V(t_{n+1})-V(t_n)}{\tau} - V_t(t_{n+\frac{1}{2}})) + \frac{V(t_{n+1})+V(t_n)}{2} - V(t_{n+\frac{1}{2}}) + A[\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}A_{ij}^T A_{ij} \\ &\left(\frac{U(t_{n+1})+U(t_n)}{2} - U(t_{n+\frac{1}{2}})\right) + \sum_{i=1}^{d} a_i A_i\left(\frac{U(t_{n+1})+U(t_n)}{2} - U(t_{n+\frac{1}{2}})\right) \\ &+ \frac{\nabla F_h(U(t_n)) + \nabla F_h(U(t_{n+1}))}{2} - \nabla F_h(U(t_{n+\frac{1}{2}})) - G(U(t_n), U(t_{n+1}))] \\ &+ \gamma\left(\frac{U(t_{n+1})+U(t_n)}{2} - U(t_{n+\frac{1}{2}})\right) = O(\tau^2). \end{aligned} \tag{8.52}$$

Let (U, V) be a solution on a finite time [0, T]. Since f_h is a polynomial, we infer that $(U, V) \in C^\infty([0, T];\ \mathbb{R}^{\mathbb{N}_h} \times \mathbb{R}^{\mathbb{N}_h})$ by a bootstrap argument.Using Taylor's expansion, it is obvious that the midpoint scheme has a local truncation error of order $O(\tau^2)$. Also note that, owing to [72] (see Proposition 4.2, page 16),

$$|G(U(t_n), U(t_{n+1}))|_\infty = O(\tau^2),$$

where $|\cdot|_\infty$ stands for the maximum norm in $\mathbb{R}^{\mathbb{N}_h}$. Hence the proof is complete. □

8.4.2 Existence and discrete energy estimate

Theorem 8.4.1. *(Existence for any τ). For any $(u_h^0, v_h^0) \in V_h \times V_h$, there exists at least one sequence $(u_h^n, v_h^n, p_{ij,h}^{n+1/2}, w_h^{n+1/2})$ in $(V_h)^{3d}$ which complies with (8.48).*

Proof. Let (U^n, V^n) be fixed in $\mathbb{R}^{N_h}$. We eliminate V^{n+1} in (8.50) to obtain

$$\frac{2\beta}{\tau}\left(\frac{U^{n+1}-U^n}{\tau} - V^n\right) + \frac{U^{n+1}-U^n}{\tau} + A\Big[\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}{A_{ij}}^T A_{ij}\frac{U^{n+1}+U^n}{2} \tag{8.53}$$

$$+\sum_{j=1}^{d} a_j A_j \frac{U^{n+1}+U^n}{2} + \frac{\nabla F_h(U^n)+\nabla F_h(U^{n+1})}{2} - \nabla H_h^n(U^{n+1})g\Big] + \gamma\frac{U^{n+1}+U^n}{2} = 0,$$

where $\nabla H_h^n(U^{n+1})$ is defined as follows. First, we introduce a polynomial with two variables

$$g(r,s) = \frac{1}{12}(s-r)^2(f_+''(r) + f_-''(s)), \quad r, s \in \mathbb{R}. \tag{8.54}$$

By assumption (8.47), we know that g is a polynomial of degree at most $2p+1$ and its partial degree with respect to the second variable s is strictly less than $2p+1$. Then g can be written as

$$g(r,s) = \sum_{k,l} b_{k,l} r^k s^l, \tag{8.55}$$

where the coefficients $b_{k,l} \in \mathbb{R}$ and

$$0 \le k \le 2p+1,\ 0 \le l < 2p+1,\ k+l \le 2p+1 \text{ and } \ \text{either } k \le 2 \text{ or } l \le 2.$$

Secondly, let us assume that

$$h(r,s) = \sum_{k,l} b_{k,l} r^k \frac{s^{l+1}}{l+1}, \tag{8.56}$$

so that $\partial_s h(r,s) = g(r,s)$. Then we define $H_h^n(U) = (h(u_h^n, u_h), 1)$ with $u_h \simeq U$, so that

$$\nabla H_h^n(U) = (g(u_h^n, u_h), e_i)_{1\le i\le N_h} = G(U^n, U), \tag{8.57}$$

which explains the presence of $\nabla H_h^n(U)$ in (8.53). Moreover, By (8.56) and Hölder's inequality, we have

$$|H_h^n(U)| \le C_n(\|u_h\|_{L^{2p+2}(\Omega)}^{2p+1} + 1), \quad \forall U \in \mathbb{R}^{N_h}, \tag{8.58}$$

where the constant C_n depends on $\|u_h^n\|_{L^{2p+2}(\Omega)}$.

Then we replace U with $(u_1, \dot{U})$ in (8.53) to get

$$\frac{2\beta}{\tau}\left(\frac{u_1^{n+1}-u_1^n}{\tau}-v_1^n\right)+\frac{u_1^{n+1}-u_1^n}{\tau}+\frac{\gamma}{2}(u_1^{n+1}+u_1^n)=0, \tag{8.59}$$

$$\frac{2\beta}{\tau}\dot{A}^{-1}\left(\frac{\dot{U}^{n+1}-\dot{U}^n}{\tau}-\dot{V}^n\right)+\dot{A}^{-1}\frac{\dot{U}^{n+1}-\dot{U}^n}{\tau}+\sum_{j=1}^{d}\sum_{i=1}^{j}a_{ij}\dot{A}_{ij}^T\dot{A}_{ij}\frac{\dot{U}^{n+1}+\dot{U}^n}{2} \tag{8.60}$$

$$+\sum_{j=1}^{d}a_j\dot{A}_j\frac{\dot{U}^{n+1}+\dot{U}^n}{2}+\frac{\dot{\nabla}F_h(U^n)+\dot{\nabla}F_h(U^{n+1})}{2}-\dot{\nabla}H_h^n(U^{n+1})+\frac{\gamma}{2}\dot{A}^{-1}(\dot{U}^{n+1}+\dot{U}^n)=0.$$

Note that (8.59) determines u_1^{n+1} uniquely. As far as (8.60) is concerned, let us consider the minimization problem for the function

$$\begin{aligned}\mathcal{G}:\dot{U}\in\mathbb{R}^{N_h-1}\mapsto\ &\frac{\beta}{\tau^2}|\dot{U}-\dot{U}^n|_{-1}^2-\frac{2\beta}{\tau}(\dot{V}^n)^T\dot{A}^{-1}\dot{U}+\frac{1}{2\tau}|\dot{U}-\dot{U}^n|_{-1}^2\\ &+\frac{\gamma}{4}|\dot{U}+\dot{U}^n|_{-1}^2+\frac{1}{4}\sum_{j=1}^{d}\sum_{i=1}^{j}a_{ij}|\dot{A}_{ij}(\dot{U}+\dot{U}^n)|^2+\frac{1}{4}\sum_{j=1}^{d}a_j|\dot{A}_j^{\frac{1}{2}}(\dot{U}+\dot{U}^n)|^2\\ &+\frac{(\dot{\nabla}F_h(U^n))^T}{2}\dot{U}+\frac{\tilde{F}_h^n(\dot{U})}{2}-\tilde{H}_h^n(\dot{U}),\end{aligned} \tag{8.61}$$

where $\tilde{F}_h^n(\dot{U}) = F_h(u_1^{n+1},\dot{U})$, $\tilde{H}_h^n(\dot{U}) = H_h^n(u_1^{n+1},\dot{U})$. We show that the minimization problem admits a solution which is precisely a solution of (8.60).

In fact, by (8.14), (8.15) and the Cauchy-Schwartz inequality, we have

$$\begin{aligned}\tilde{F}_h^n(\dot{U}) &= \int_\Omega\sum_{i=2}^{2p+2}\frac{\kappa_{i-1}}{i}(u_1^{n+1}+\sum_{j=2}^{N_h}u_je_h^j)^i dx\\ &\geq\frac{\kappa_{2p+1}}{2p+2}\|u_h\|_{L^{2p+2}}^{2p+2}-c_p'(\|u_h\|_{L^{2p+2}}^{2p+1}+1),\quad\forall\dot{U}\in\mathbb{R}^{N_h-1},\end{aligned} \tag{8.62}$$

where c_p' depends on the coefficients of F. Moreover, by the definition of $\tilde{H}_h^n(\dot{U})$ and Young's inequality, we have

$$|\tilde{H}_h^n(\dot{U})|\leq c_n(\|u_h\|_{L^{2p+2}}^{2p+1}+1),\quad\forall\dot{U}\in\mathbb{R}^{N_h-1}, \tag{8.63}$$

where c_n depends on $\|u_h\|_{L^{2p+2}}$. Notice that

$$|\dot{A}^{-1}\dot{V}|^2 \leq c_{\dagger}|\dot{V}|_{-1}^2, \quad |\dot{A}^{\frac{1}{2}}\dot{V}|^2 \leq c_{\ddagger}|\dot{V}|^2, \quad \forall \dot{V} \in \mathbb{R}^{N_h-1}, \tag{8.64}$$

where the coefficients $c_{\dagger}, c_{\ddagger}$ can be chosen to be

$$c_{\dagger} \geq \frac{1}{\min\limits_{1\leq j\leq N_h-1}\{\lambda_j\}}, \quad c_{\ddagger} \geq \max_{1\leq j\leq N_h-1}\{\lambda_j\},$$

λ_j ($j = 1, \cdots, N_h - 1$) being the eigenvalues of $\dot{A}$. This yields, by the Cauchy-Schwartz inequality, the equivalence of norms in $\mathbb{R}^{N_h-1}$ and (8.64),

$$\begin{aligned}
(a).\ |(\dot{V}^n)^T\dot{A}^{-1}\dot{U}| &\leq \frac{1}{2}|\dot{A}^{-1}\dot{U}|^2 + \frac{1}{2}|\dot{V}^n|^2 \leq \frac{c_{\dagger}}{2}|\dot{U}|_{-1}^2 + \frac{1}{2}|\dot{V}^n|^2 \\
&\leq c|\dot{U}|^2 + \frac{1}{2}|\dot{V}^n|^2 = c\|\dot{u}_h\|_0^2 + \frac{1}{2}|\dot{V}^n|^2, \\
(b).\ |\sum_{j=1}^{d} a_j|\dot{A}_j^{\frac{1}{2}}(\dot{U}+\dot{U}^n)|^2| &\leq \max_{1\leq j\leq d}|a_j|\sum_{j=1}^{d}|\dot{A}_j^{\frac{1}{2}}(\dot{U}+\dot{U}^n)|^2 = \max_{1\leq j\leq d}|a_j||\dot{A}^{\frac{1}{2}}(\dot{U}+\dot{U}^n)|^2 \\
&\leq c_{\ddagger}\max_{1\leq j\leq d}|a_j||\dot{U}+\dot{U}^n|^2 \leq c(\|\dot{u}_h\|_0^2 + \|\dot{u}_h^n\|_0^2).
\end{aligned} \tag{8.65}$$

Combining (8.62) to (8.65), we obtain

$$\mathcal{G}(\dot{U}) \geq \frac{a_{2p+1}}{2(2p+2)}\|u_h\|_{L^{2p+2}}^{2p+2} - (c_n + \frac{c'_p}{2})\|u_h\|_{L^{2p+2}}^{2p+1} - c\|\dot{u}_h\|_0{}^2 - c'',$$

where c, c'' depend on h, F and u_h^n. This implies that $\mathcal{G}(\dot{U})$ tends to $+\infty$ with respect to $|\dot{U}|$. Then the continuous function $\mathcal{G}$ admits a minimizer $\tilde{\dot{U}}$ in $\mathbb{R}^{N_h-1}$, which implies that $\nabla\mathcal{G}(\dot{U})|_{\dot{U}=\tilde{\dot{U}}} = 0$. Therefore, $\tilde{\dot{U}}$ is a solution of (8.60). □

The first component of the numerical solution at each time step u_1^{n+1} can be estimated, due to the special basis $\{e_h^k\}_{k=1}^{N_h}$ chosen in V_h. More precisely, the following estimate holds : for $\gamma > 0$,

$$|v_1^{n+1/2}| \leq \tilde{c}q^n(|u_1^0| + |v_1^0|), \tag{8.66}$$

where $\tilde{c}$ and $q \in (0, 1)$ are given by

$$\begin{aligned}
&(i) \qquad \tilde{c} = \frac{2\gamma + 1 + \sqrt{1-4\beta\gamma}}{\sqrt{1-4\beta\gamma}},\\
&\qquad\quad q = \max\left\{\left|\frac{4\beta + 2\tau\sqrt{1-4\beta\gamma} - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}\right|, \left|\frac{4\beta - 2\tau\sqrt{1-4\beta\gamma} - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}\right|\right\},\\
&(ii) \qquad \tilde{c} = (4\gamma + 2), \quad q = \max\left\{\left|\frac{4\beta + \tau - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}\right|, \left|\frac{4\beta - \tau - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}\right|\right\},\\
&(iii) \qquad \tilde{c} = \frac{2(\gamma + \sqrt{\beta\gamma})}{\sqrt{4\beta\gamma - 1}}, \quad q = \left|\frac{\beta - \gamma\tau^2 + 2\tau i\sqrt{4\beta\gamma - 1}}{4\beta + 2\tau + \gamma\tau^2}\right|,
\end{aligned} \tag{8.67}$$

based on the sign of $1 - 4\beta\gamma$: (i) $1 - 4\beta\gamma > 0$, (ii) $1 - 4\beta\gamma = 0$, (iii) $1 - 4\beta\gamma < 0$. See Appendix for details.

Remark 8.4.2. *When $\gamma = 0$, estimate (8.66) is simpler. Indeed, taking $\psi_h = 1$ in the second equation of (8.48), we find $v_1^{n+1} = qv_1^n$ with $q = \frac{2\beta - \tau}{2\beta + \tau}$. Thus*

$$|v_1^{n+1/2}| \leq |q|^n |v_1^{1/2}| \leq \frac{1 + |q|}{2} |q|^n |v_1^0|. \tag{8.68}$$

It is clear that $|q| < 1$, so that the estimate now only depends on v_1^0.

We now state a Lemma which will be useful in the proof of the energy estimate and was proved in [72].

Lemma 8.4.1. *Let $g \in C^3([0, 1]; \mathbb{R})$. Then the following identities hold*

$$\int_0^1 g(s)ds = \frac{1}{2}(g(0) + g(1)) - \frac{1}{12} g''(0) - \frac{1}{2}\int_0^1 k_2^+(\sigma) g^{(3)}(\sigma) d\sigma, \tag{8.69}$$

$$\int_0^1 g(s)ds = \frac{1}{2}(g(0) + g(1)) - \frac{1}{12} g''(1) + \frac{1}{2}\int_0^1 k_2^-(\sigma) g^{(3)}(\sigma) d\sigma, \tag{8.70}$$

where $k_2^+(\sigma) = (1 - \sigma)^2(2\sigma + 1)/6$, $k_2^-(\sigma) = \sigma^2(3 - 2\sigma)/6$ and $g^{(3)}$ denotes the third derivative of g. In particular, $k_2^+(\sigma) \geq 0$ and $k_2^-(\sigma) \geq 0$ for all $\sigma \in [0, 1]$.

Theorem 8.4.2. (*Energy estimate for any τ*). *If $(U^n, V^n, P_{ij}^{n+\frac{1}{2}}, W^{n+\frac{1}{2}})$ $(n \geq 1)$ is a sequence in $(\mathbb{R}^{N_h})^{3d}$ which complies with (8.49), then for all $n \geq 0$,*

$$\frac{\mathcal{E}_h(U^{n+1}, V^{n+1}) - \mathcal{E}_h(U^n, V^n)}{\tau} + |\dot{V}^{n+1/2}|_{-1}^2 \leq v_1^{n+1/2} w_1^{n+1/2}. \tag{8.71}$$

As a consequence, for all $k \geq 0$, we have

$$\begin{aligned}&\mathcal{E}_h(U^{N_0+k}, V^{N_0+k}) + \sum_{j=0}^{k-1} \tau|\dot{V}^{N_0+j+\frac{1}{2}}|_{-1}^2 \\ &\leq \exp(8c_5\tilde{c}\frac{\tau q^{N_0}}{1-q}(|u_1^0| + |v_1^0|))(\mathcal{E}_h(U^{N_0}, V^{N_0}) + c_7\tilde{c}\frac{\tau q^{N_0}}{1-q}(|u_1^0| + |v_1^0|)),\end{aligned} \tag{8.72}$$

where $N_0 = N_0(\beta, c_5, \tau, |u_1^0|, |v_1^0|) \in \mathbb{N}$ *satisfies*

$$2c_5\tilde{c}\tau q^{N_0}(|u_1^0| + |v_1^0|) \leq \frac{1}{2}, \tag{8.73}$$

with c_7 *depending on* f*,* f_+*,* f_-*,* $\tilde{c}, q$ *and given in* (8.67)*,* $0 < q < 1$.

Proof. Throughout the proof, we will assume that $\gamma > 0$; when $\gamma = 0$, the energy estimate can be proved similarly (in fact, the proof is simpler, see Remark 4.4 below).

Let $\delta u_h^n = u_h^{n+1} - u_h^n$. Since $F'_+ = f_+$ and $F'_- = f_-$, we have

$$F_+(u_h^{n+1}) - F_+(u_h^n) = \delta u_h^n \int_0^1 f_+(u_h^n + s\delta u_h^n)ds, \tag{8.74}$$

$$F_-(u_h^{n+1}) - F_-(u_h^n) = \delta u_h^n \int_0^1 f_-(u_h^n + s\delta u_h^n)ds. \tag{8.75}$$

Setting $g(s) = f_+(u_h^n + s\delta u_h^n)$ in (8.69) and $g(s) = f_-(u_h^n + s\delta u_h^n)$ in (8.70), we get

$$\int_0^1 f_+(u_h^n+s\delta u_h^n)ds = \frac{1}{2}(f_+(u_h^n)+f_+(u_h^{n+1}))-\frac{(\delta u_h^n)^2}{12}f''_+(u_h^n)-\frac{(\delta u_h^n)^3}{2}\int_0^1 k_2^+(\sigma)f'''_+(u_h^n+\sigma\delta u_h^n)d\sigma,$$

$$\int_0^1 f_-(u_h^n+s\delta u_h^n)ds = \frac{1}{2}(f_-(u_h^n)+f_-(u_h^{n+1}))-\frac{(\delta u_h^n)^2}{12}f''_-(u_h^{n+1})+\frac{(\delta u_h^n)^3}{2}\int_0^1 k_2^-(\sigma)f'''_-(u_h^n+\sigma\delta u_h^n)d\sigma.$$

Then combining (8.74) and (8.75) leads to

$$F(u_h^{n+1}) - F(u_h^n) = \delta u_h^n[\frac{1}{2}(f(u_h^n) + f(u_h^{n+1})) - \frac{(\delta u_h^n)^2}{12}(f''_+(u_h^n) + f''_-(u_h^{n+1}))] - \alpha^n, \tag{8.76}$$

where

$$\alpha^n = \frac{(\delta u_h^n)^4}{2}(\int_0^1 k_2^+(\sigma)f'''_+(u_h^n + \sigma\delta u_h^n)d\sigma - \int_0^1 k_2^-(\sigma)f'''_-(u_h^n + \sigma\delta u_h^n)d\sigma) \geq 0,$$

with $k_2^+(\sigma),\ k_2^-(\sigma) \geq 0$ by Lemma 8.4.1 and $f_+''' \geq 0,\ f_-''' \leq 0$ by (8.47)(a).

Choosing $\xi_h = \delta u_h^n$ in the last equation of (8.48) gives

$$\begin{aligned}&(w_h^{n+1/2}, \delta u_h^n) - \sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}(\frac{\partial p_{ij,h}^{n+1/2}}{\partial x_i}, \frac{\partial \delta u_h^n}{\partial x_j}) - \sum_{j=1}^{d} a_j(p_{jj,h}^{n+1/2}, \delta u_h^n)\\ =&(F(u_h^{n+1}), 1) - (F(u_h^n), 1) + (\alpha^n, 1),\end{aligned}$$

which can be rewritten in vector form and simplified by eliminating $P_{ij}^{n+1/2}$,

$$\begin{aligned}&F_h(U^{n+1}) - F_h(U^n) + (\alpha^n, 1) = (W^{n+1/2})^T \delta U^n\\ &-\frac{1}{2}\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}(|A_{ij}U^{n+1}|^2 - |A_{ij}U^n|^2) - \frac{1}{2}\sum_{j=1}^{d} a_j(|A_j^{\frac{1}{2}}U^{n+1}|^2 - |A_j^{\frac{1}{2}}U^n|^2).\end{aligned} \tag{8.77}$$

Notice that the second equation in (8.48) implies that

$$-\dot{W}^{n+\frac{1}{2}} = \dot{A}^{-1}(\beta\frac{\dot{V}^{n+1} - \dot{V}^n}{\tau} + \dot{V}^{n+\frac{1}{2}} + \gamma\dot{U}^{n+\frac{1}{2}}). \tag{8.78}$$

Plugging (8.78) into (8.77) with $\delta U^n = \tau V^{n+\frac{1}{2}}$, we deduce

$$\begin{aligned}E_h(U^{n+1}) - E_h(U^n) + (\alpha^n, 1) + \frac{\beta}{2}(|\dot{V}^{n+1}|_{-1}^2 - |\dot{V}^n|_{-1}^2) + \tau|\dot{V}^{n+\frac{1}{2}}|_{-1}^2&\\ + \frac{\gamma}{2}|\dot{U}^{n+1}|_{-1}^2 - \frac{\gamma}{2}|\dot{U}^n|_{-1}^2 = \tau v_1^{n+\frac{1}{2}} w_1^{n+\frac{1}{2}},&\end{aligned}$$

which yields the energy estimate (8.71). Setting $\xi_h = 1$ in the last equation of (8.48) gives

$$w_1^{n+1/2} = \frac{1}{2}((f(u_h^n) + f(u_h^{n+1})), 1) - \frac{1}{12}((u_h^{n+1} - u_h^n)^2(f_+''(u_h^n) + f_-''(u_h^{n+1})), 1). \tag{8.79}$$

This yields, by (8.71), (8.43), (8.66) and assumption (8.47)(b),

$$\begin{aligned}&\mathcal{E}_h(U^{n+1}, V^{n+1}) - \mathcal{E}_h(U^n, V^n) + \tau|\dot{V}^{n+\frac{1}{2}}|_{-1}^2\\ \leq&\tau|v_1^{n+\frac{1}{2}}||w_1^{n+1/2}|\\ \leq&\tau|v_1^{n+\frac{1}{2}}|\left(c_5(F(u_h^n) + F(u_h^{n+1})) + c_6,\ 1\right)\\ \leq&\tau|v_1^{n+\frac{1}{2}}|(2c_5(E_h(U^{n+1}) + E_h(U^n)) + c_7),\\ \leq&\tau\tilde{c}q^n(|u_1^0| + |v_1^0|)(2c_5(E_h(U^{n+1}) + E_h(U^n)) + c_7),\end{aligned}$$

where $c_7 = c_6 + 2c_5\grave{c}$ depends on f, f_+, f_- and $a_{i,j}$. We set

$$\mathcal{E}_h^n = \mathcal{E}_h(U^n, V^n) = E_h(U^n) + \frac{\beta}{2}|\dot{V}^n|_{-1}^2 + \frac{\gamma}{2}|\dot{U}^n|_{-1}^2, \quad \mathcal{E}_h^{n+1} = \mathcal{E}_h(U^{n+1}, V^{n+1}),$$

and let $N_0 = N_0(\beta, \gamma, c_5, \tau, |u_1^0|, |v_1^0|) \in \mathbb{N}$ satisfy (8.73). Then for $n \geq N_0$,

$$\begin{aligned}&(1 - 2c_5\tilde{c}\tau q^n(|u_1^0| + |v_1^0|))\mathcal{E}_h^{n+1} + \tau|\dot{V}^{n+\frac{1}{2}}|_{-1}^2\\ &\leq (1 + 2c_5\tilde{c}\tau q^n(|u_1^0| + |v_1^0|))\mathcal{E}_h^n + c_7\tilde{c}\tau q^n(|u_1^0| + |v_1^0|).\end{aligned}$$

Dividing this inequality by $(1 - 2c_5\tilde{c}\tau q^n(|u_1^0| + |v_1^0|))$ and noting that

$$1 \leq \frac{1}{1-x}, \quad \frac{1+x}{1-x} \leq 1 + 4x \leq e^{4x}, \quad \forall x \in (0, \frac{1}{2}),$$

we obtain

$$\mathcal{E}_h^{n+1} + \tau|\dot{V}^{n+\frac{1}{2}}|_{-1}^2 \leq e^{8c_5\tilde{c}\tau q^n(|u_1^0|+|v_1^0|)}(\mathcal{E}_h^n + c_7\tilde{c}\tau q^n(|u_1^0| + |v_1^0|)), \quad \forall n \geq N_0.$$

By induction, for all $k \in \mathbb{N}$,

$$\begin{aligned}\mathcal{E}_h^{N_0+k} + \sum_{j=0}^{k-1} \tau|\dot{V}^{N_0+j+\frac{1}{2}}|_{-1}^2 &\leq \exp(8c_5\tilde{c}\tau(|u_1^0| + |v_1^0|) \sum_{j=0}^{k-1} q^{N_0+j})\mathcal{E}_h^{N_0}\\ &+ \sum_{j=0}^{k-1} \exp(8c_5\tilde{c}\tau(|u_1^0| + |v_1^0|) \sum_{i=0}^{k-j-1} q^{N_0+i})c_7\tilde{c}\tau q^{N_0+j}(|u_1^0| + |v_1^0|).\end{aligned}$$

Owing to the fact that $\sum_{j=0}^{k-1} q^{N_0+j} \leq \frac{q^{N_0}}{1-q}$, we deduce (8.72) and the proof is complete. □

Remark 8.4.3. *If the initial conditions satisfy* $(\langle u_h^0 \rangle =)u_1^0 = 0$, $(\langle v_h^0 \rangle =)v_1^0 = 0$, *then estimate* (8.71) *reads :*

$$\mathcal{E}_h(U^{n+1}, V^{n+1}) + \tau|\dot{V}^{n+\frac{1}{2}}|_{-1}^2 \leq \mathcal{E}_h(U^n, V^n), \quad \forall n \geq 0,$$

meaning that the energy decreases. Moreover, the energy estimate (8.72) *reduces to, for any* $k > 0$ *:*

$$\mathcal{E}_h(U^k, V^k) + \sum_{j=0}^{k-1} \tau|\dot{V}^{j+\frac{1}{2}}|_{-1}^2 \leq \mathcal{E}_h(U^0, V^0).$$

Remark 8.4.4. *Since $0 < q < 1$,we infer from the energy estimate (8.72) that, for N_0 large enough,*

$$\sum_{n=N_0}^{\infty} |\dot{V}^{n+\frac{1}{2}}|_{-1}^2 < +\infty.$$

Hence, $\dot{V}^{n+\frac{1}{2}} \to 0$ as n tends to $+\infty$. This, together with the estimate of $v_1^{n+\frac{1}{2}}$ in (8.66), implies that $V^{n+\frac{1}{2}} \to 0$.

Remark 8.4.5. *For the special case $\gamma = 0$, as mentioned in Remark 8.4.2, the estimate for $|v_1^{n+1/2}|$ is much simpler. Furthermore, the energy estimate (8.72) can be simplified to read : for all $k \geq 0$,*

$$\mathcal{E}_h(U^{N_0+k}, V^{N_0+k}) + \sum_{j=0}^{k-1} \tau |\dot{V}^{N_0+j+\frac{1}{2}}|_{-1}^2 \leq \exp(8c_5 \frac{\tau |q|^{N_0}}{1-|q|} |v_1^{\frac{1}{2}}|)(\mathcal{E}_h(U^{N_0}, V^{N_0}) + c_7 \frac{\tau |q|^{N_0}}{1-|q|} |v_1^{\frac{1}{2}}|),$$

where $N_0 = N_0(\beta, c_5, \tau, |v_1^0|) \in \mathbb{N}$ satisfies $2c_5 \tau |q|^{N_0} |v_1^{\frac{1}{2}}| \leq \dfrac{1}{2}$, instead of (8.73). Thus, N_0 does not rely on u_1^0 anymore.

8.4.3 Uniqueness

To prove the uniqueness of the solution of the fully discrete scheme (8.48), we need the following lemma.

Lemma 8.4.2. *For the constant q given in (8.67), the term $\dfrac{\tau}{1-q}$ can be bounded by a constant independent of τ.*

Proof. By (8.67), we know that q has three expressions depending on sign sign of $1 - 4\beta\gamma$. We discuss the three cases separately.

For case (i) $1 - 4\beta\gamma > 0$, if $0 < \tau \leq \sqrt{4\beta/\gamma}$, then

$$\begin{aligned} q &= \max \left\{ \left| \frac{4\beta + 2\tau\sqrt{1-4\beta\gamma} - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2} \right|, \left| \frac{4\beta - 2\tau\sqrt{1-4\beta\gamma} - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2} \right| \right\} \\ &= \frac{4\beta + 2\tau\sqrt{1-4\beta\gamma} - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}, \end{aligned}$$

$$\frac{\tau}{1-q} = \frac{4\beta + 2\tau + \gamma\tau^2}{2(1 - \sqrt{1-4\beta\gamma}) + 2\gamma\tau} \leq \frac{4\beta + 2\tau + \gamma\tau^2}{2(1 - \sqrt{1-4\beta\gamma})} \leq \frac{4\beta + \sqrt{\frac{4\beta}{\gamma}}}{1 - \sqrt{1-4\beta\gamma}};$$

otherwise, if $\sqrt{4\beta/\gamma} < \tau < 1$ (if $\sqrt{4\beta/\gamma} > 1$, it is not necessary to look further, as we always assume that $\tau < 1$),

$$\begin{aligned} q &= \max\left\{\left|\frac{4\beta + 2\tau\sqrt{1-4\beta\gamma} - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}\right|, \left|\frac{4\beta - 2\tau\sqrt{1-4\beta\gamma} - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}\right|\right\} \\ &= \frac{-4\beta + 2\tau\sqrt{1-4\beta\gamma} + \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}, \\ \frac{\tau}{1-q} &= \frac{(4\beta + 2\tau + \gamma\tau^2)\tau}{8\beta + 2\tau(1 - \sqrt{1-4\beta\gamma})} \leq \frac{4\beta + 2\tau + \gamma\tau^2}{2(1 - \sqrt{1-4\beta\gamma})} < \frac{4\beta + 2 + \gamma}{2(1 - \sqrt{1-4\beta\gamma})}. \end{aligned}$$

Similarly, for case (ii) $1 - 4\beta\gamma = 0$, if $0 < \tau \leq \dfrac{1}{\gamma}$, then

$$\begin{aligned} q &= \max\{\left|\frac{4\beta + \tau - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}\right|, \left|\frac{4\beta - \tau - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}\right|\} = \frac{4\beta + \tau - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}, \\ \frac{\tau}{1-q} &= \frac{4\beta + 2\tau + \gamma\tau^2}{1 + 2\gamma\tau} < 4\beta + 2\tau + \gamma\tau^2 \leq \frac{4}{\gamma}; \end{aligned}$$

otherwise, if $\dfrac{1}{\gamma} < \tau < 1$,

$$\begin{aligned} q &= \max\{\left|\frac{4\beta + \tau - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}\right|, \left|\frac{4\beta - \tau - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}\right|\} = \frac{-4\beta + \tau + \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}, \\ \frac{\tau}{1-q} &= \frac{(4\beta + 2\tau + \gamma\tau^2)\tau}{8\beta + \tau} < 4\beta + 2\tau + \gamma\tau^2 < 4\beta + 2 + \gamma. \end{aligned}$$

For case (iii) $1 - 4\beta\gamma < 0$, recall that we always assume $\tau < 1$. Then

$$\begin{aligned} q &= \left|\frac{4\beta - \gamma\tau^2 + 2\tau i\sqrt{4\beta\gamma - 1}}{4\beta + 2\tau + \gamma\tau^2}\right| = \sqrt{\frac{4\beta - 2\tau + \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}}, \\ \frac{\tau}{1-q} &= \frac{\sqrt{4\beta + 2\tau + \gamma\tau^2}(\sqrt{4\beta + 2\tau + \gamma\tau^2} + \sqrt{4\beta - 2\tau + \gamma\tau^2})}{4} \\ &< \frac{4\beta + 2\tau + \gamma\tau^2}{2} < \frac{4\beta + \gamma + 2}{2}. \end{aligned}$$

This completes the proof of the lemma. □

Theorem 8.4.3. **(Uniqueness for small** τ**).** *For any* $(u_h^0, v_h^0) \in V_h \times V_h$, *by choosing* τ *sufficiently small, but depending on h, there is a unique sequence* $(u_h^n, v_h^n, p_{ij,h}^{n+1/2}, w_h^{n+1/2})_{n\geq 1}$ *which complies with* (8.48). *Moreover, the choice of* τ *can be made independent of h if* (u_h^0, v_h^0) *is a family such that*

$$|\langle u_h^0\rangle| + |\langle v_h^0\rangle| + |\mathcal{E}_h(u_h^0, v_h^0)| \leq c^*, \tag{8.80}$$

for some constant c^* independent of h.

Proof. As in Theorem 8.4.2, we only consider the case $\gamma > 0$. Assume that (u_h^n, v_h^n) is uniquely determined for some $n \geq 0$. By (8.59), we know that $u_1^{n+1} = \langle u_h^{n+1}\rangle$ is uniquely determined, so that it is sufficient to show that $\dot{u}_h^{n+1} \simeq \dot{U}^{n+1}$ is uniquely determined by (8.60). Then $v_h^{n+1} \simeq V^{n+1}$ can be recovered by the first equation in (8.50).

Suppose that (8.60) has two solutions $\dot{u}_h^{n+1} \simeq \dot{U}^{n+1}$, $\underline{\dot{u}}_h^{n+1} \simeq \underline{\dot{U}}^{n+1}$. By subtracting the two resulting systems and multiplying by $\delta\dot{U} = \dot{U}^{n+1} - \underline{\dot{U}}^{n+1} \simeq \delta\dot{u}_h = \delta u_h$, we deduce

$$\frac{2\beta}{\tau^2}|\delta\dot{U}|_{-1}^2 + \frac{1}{\tau}|\delta\dot{U}|_{-1}^2 + \frac{1}{2}\sum_{j=1}^{d}\sum_{i=1}^{j} a_{ij}|\dot{A}_{ij}\delta\dot{U}|^2 + \frac{1}{2}\sum_{j=1}^{d} a_j|\dot{A}_j^{\frac{1}{2}}\delta\dot{U}|^2 + \frac{\gamma}{2}|\delta\dot{U}|_{-1}^2 \tag{8.81}$$

$$= -(\delta\dot{U})^T\frac{\dot{\nabla}F_h(U^{n+1}) - \dot{\nabla}F_h(\underline{U}^{n+1})}{2} + (\delta\dot{U})^T(\dot{\nabla}H_h^n(U^{n+1}) - \dot{\nabla}H_h^n(\underline{U}^{n+1})).$$

According to (8.14), f' is a polynomial of even degree with strictly positive leading coefficient, so that there exists a constant $c_f \geq 0$ such that

$$f'(s) \geq -c_f, \quad \forall s \in \mathbb{R}. \tag{8.82}$$

This implies, by the mean value theorem,

$$(\delta\dot{U})^T\frac{\dot{\nabla}F_h(U^{n+1}) - \dot{\nabla}F_h(\underline{U}^{n+1})}{2} = \frac{1}{2}(f(u_h^{n+1}) - f(\underline{u}_h^{n+1}), \delta u_h) \geq -\frac{c_f}{2}|\delta\dot{U}|^2. \tag{8.83}$$

By the definition of $g(r,s)$, (8.17) and Hölder's inequality, we find

$$
\begin{aligned}
&|(\delta\dot{U})^T(\dot{\nabla}H_h^n(U^{n+1})-\dot{\nabla}H_h^n(\underline{U}^{n+1}))| = |(g(u_h^n,u_h^{n+1})-g(u_h^n,\underline{u}_h^{n+1}),\delta u_h)|\\
=&|\sum_{k+l=0}^{2p} b_{k,l}((u_h^n)^k((u_h^{n+1})^l-(\underline{u}_h^{n+1})^l),\delta u_h)| = |\sum_{k+l=0}^{2p} b_{k,l}((u_h^n)^k\delta u_h\sum_{j=0}^{l-1}(u_h^{n+1})^j(\underline{u}_h^{n+1})^{l-j-1},\delta u_h)|\\
\leq&\sum_{k+l=0}^{2p}|b_{k,l}|\cdot|((u_h^n)^k\sum_{j=0}^{l-1}(u_h^{n+1})^j(\underline{u}_h^{n+1})^{l-j-1},(\delta\dot{u}_h)^2)|\\
\leq&\sum_{k+l=0}^{2p}|b_{k,l}|\cdot\|(\delta\dot{u}_h)^2\|_{L^{p+1}}\|(u_h^n)^k\sum_{j=0}^{l-1}(u_h^{n+1})^j(\underline{u}_h^{n+1})^{l-j-1}\|_{L^{\frac{p+1}{p}}}\\
\leq&\|\delta\dot{u}_h\|_{L^{2p+2}}^2\sum_{k+l=0}^{2p}|b_{k,l}|\sum_{j=0}^{l-1}\|(u_h^n)^k(u_h^{n+1})^j(\underline{u}_h^{n+1})^{l-j-1}\|_{L^{\frac{p+1}{p}}}\\
\leq&\|\delta\dot{u}_h\|_{L^{2p+2}}^2\sum_{k+l=0}^{2p}|b_{k,l}|\sum_{j=0}^{l-1}(\|(u_h^n)^{k\frac{p+1}{p}}\|_{L^{\frac{2p}{k}}}\|(u_h^{n+1})^{j\frac{p+1}{p}}(\underline{u}_h^{n+1})^{(l-j-1)\frac{p+1}{p}}\|_{L^{\frac{2p}{2p-k}}})^{\frac{p}{p+1}}\\
=&\|\delta\dot{u}_h\|_{L^{2p+2}}^2\sum_{k+l=0}^{2p}|b_{k,l}|\sum_{j=0}^{l-1}\|u_h^n\|_{L^{2p+2}}^k\|(u_h^{n+1})^j(\underline{u}_h^{n+1})^{l-j-1}\|_{L^{\frac{2p+2}{2p-k}}}\\
\leq&\|\delta\dot{u}_h\|_{L^{2p+2}}^2\sum_{k+l=0}^{2p}|b_{k,l}|\sum_{j=0}^{l-1}\|u_h^n\|_{L^{2p+2}}^k(\|(u_h^{n+1})^{j\frac{2p+2}{2p-k}}\|_{L^{\frac{2p-k}{j}}}\|(\underline{u}_h^{n+1})^{(l-j-1)\frac{2p+2}{2p-k}}\|_{L^{\frac{2p-k}{2p-k-j}}})^{\frac{2p-k}{2p+2}}\\
=&\|\delta\dot{u}_h\|_{L^{2p+2}}^2\sum_{k+l=0}^{2p}|b_{k,l}|\sum_{j=0}^{l-1}\|u_h^n\|_{L^{2p+2}}^k\|u_h^{n+1}\|_{L^{2p+2}}^j\|(\underline{u}_h^{n+1})^{l-j-1}\|_{L^{\frac{2p+2}{2p-k-j}}}\\
\leq&\|\delta\dot{u}_h\|_{L^{2p+2}}^2\sum_{k+l=0}^{2p}|b_{k,l}|\sum_{j=0}^{l-1}\|u_h^n\|_{L^{2p+2}}^k\|u_h^{n+1}\|_{L^{2p+2}}^j\|\underline{u}_h^{n+1}\|_{L^{2p+2}}^{2p-k-j}\\
\triangleq&c_n'\|\delta\dot{u}_h\|_{L^{2p+2}}^2\leq c_n'\|\delta\dot{u}_h\|_{L^{2p+2}}^2\leq c_n'c_s^2|\delta\dot{u}_h|_1^2 = c_n'c_s^2|\dot{A}^{\frac{1}{2}}\delta\dot{U}|^2,
\end{aligned}
\tag{8.84}
$$

where

$$
\begin{aligned}
c_n' =&\sum_{k+l=0}^{2p}|b_{k,l}|\sum_{j=0}^{l-1}\|u_h^n\|_{L^{2p+2}}^k\|u_h^{n+1}\|_{L^{2p+2}}^j\|\underline{u}_h^{n+1}\|_{L^{2p+2}}^{2p-k-j}\\
=&c_n'(\|u_h^n\|_{L^{2p+2}},\|u_h^{n+1}\|_{L^{2p+2}},\|\underline{u}_h^{n+1}\|_{L^{2p+2}})\\
\leq&c_n'(|u_h^n|_1,|u_h^{n+1}|_1,|\underline{u}_h^{n+1}|_1)\\
\leq&c_n'(|AU^n|,|AU^{n+1}|,|A\underline{U}^{n+1}|,|U^n|,|U^{n+1}|,|\underline{U}^{n+1}|),
\end{aligned}
\tag{8.85}
$$

recall (8.17) and the fact that $|v_h|_1^2 = |\langle v_h\rangle|^2+\|\nabla v_h\|_0^2\leq|V|^2+|AV|^2,\ \forall v_h\in V_h$ in the last inequality, and for simplicity, we use the same constant c'_n.

Plugging (8.83) and (8.84) into (8.81), we derive

$$\begin{aligned}&\frac{2\beta}{\tau^2}|\delta\dot{U}|_{-1}^2+\frac{1}{\tau}|\delta\dot{U}|_{-1}^2+\frac{1}{2}\sum_{j=1}^{d}\sum_{i=1}^{j}a_{ij}|\dot{A}_{ij}\delta\dot{U}|^2+\frac{1}{2}\sum_{j=1}^{d}a_j|\dot{A}_j^{\frac{1}{2}}\delta\dot{U}|^2+\frac{\gamma}{2}|\delta\dot{U}|_{-1}^2\\&\le\frac{c_f}{2}|\delta\dot{U}|^2+c'_nc_s^2|\dot{A}^{\frac{1}{2}}\delta\dot{U}|^2.\end{aligned}\tag{8.86}$$

Owing to Young's inequality,

$$|\dot{A}^{\frac{1}{2}}\delta\dot{U}|^2\le\frac{\varepsilon}{2}|\dot{A}\delta\dot{U}|^2+\frac{1}{2\varepsilon}|\delta\dot{U}|^2,\quad\forall\varepsilon>0.$$

Furthermore, owing to the fact that

$$\begin{aligned}&(a).\ \sum_{j=1}^{d}\sum_{i=1}^{j}a_{ij}|\dot{A}_{ij}\delta\dot{U}|^2\ge\frac{\min\limits_{1\le j\le d}\{a_{jj}\}}{d}|\dot{A}\delta\dot{U}|^2,\\&(b).\ |\sum_{j=1}^{d}a_j|\dot{A}_j^{\frac{1}{2}}\delta\dot{U}|^2|\le\max_{1\le j\le d}\{|a_j|\}|\dot{A}^{\frac{1}{2}}\delta\dot{U}|^2,\end{aligned}\tag{8.87}$$

it follows that

$$\frac{2\beta}{\tau^2}|\delta\dot{U}|_{-1}^2+\frac{1}{\tau}|\delta\dot{U}|_{-1}^2+\frac{\gamma}{2}|\delta\dot{U}|_{-1}^2\le(\frac{c_f}{2}+d\frac{(c'_nc_s^2+\frac{1}{2}\max\limits_{1\le j\le d}\{|a_j|\})^2}{2\min\limits_{1\le j\le d}\{a_{jj}\}})|\delta\dot{U}|^2,\tag{8.88}$$

where we set $\epsilon=\min_{1\le j\le d}\{a_{jj}\}/d(c'_nc_s^2+\frac{1}{2}\max_{1\le j\le d}\{|a_j|\})$.

Let (u_h^0,v_h^0) be given initial data. Setting

$$\tau<\frac{1}{4c_5\tilde{c}(|u_1^0|+|v_1^0|)},$$

then (8.73) is satisfied for $N_0=0$. Therefore, by (8.46), the energy estimate (8.72) and (8.85), c'_n in (8.88) is bounded by a constant C which depends on $q,\tau,\mathcal{E}_h(U^0,V^0)$, i.e.

$$c'_n\le C(\frac{\tau}{1-q},\mathcal{E}_h(U^0,V^0)),$$

By Lemma 8.4.2, we know that $\frac{\tau}{1-q}$ is bounded by a constant independent of τ, which means that c'_n is bounded by a constant independent of n and τ, but still depending on h because of $\mathcal{E}_h(U^0,V^0)$. By choosing τ small enough (depending on h) and the equivalence of $|\cdot|$ and $|\cdot|_{-1}$ in $\mathbb{R}^{N_h-1}$, we deduce from (8.88) that $\delta\dot{U}=0$.

Now suppose that (8.80) holds. We estimate (8.86) in a different way. By Young's inequality, we have

$$\begin{aligned}|\dot{A}^{\frac{1}{2}}\delta\dot{U}|^2 \leq& \frac{\varepsilon_1}{2}|\dot{A}\delta\dot{U}|^2 + \frac{1}{2\varepsilon_1}|\delta\dot{U}|^2\\ \leq& \frac{\varepsilon_1}{2}|\dot{A}\delta\dot{U}|^2 + \frac{1}{2\varepsilon_1}(\varepsilon_1|\dot{A}^{\frac{1}{2}}\delta\dot{U}|^2 + \frac{1}{4\varepsilon_1}|\dot{A}^{-\frac{1}{2}}\delta\dot{U}|^2),\end{aligned}$$

i.e.

$$|\dot{A}^{\frac{1}{2}}\delta\dot{U}|^2 \leq \varepsilon_1|\dot{A}\delta\dot{U}|^2 + \frac{1}{4\varepsilon_1^2}|\delta\dot{U}|_{-1}^2, \quad \forall\varepsilon_1 > 0.$$

Owing to this and using Young's inequality again, we find

$$\begin{aligned}|\delta\dot{U}|^2 \leq& |\dot{A}^{\frac{1}{2}}\delta\dot{U}|^2 + \frac{1}{4}|\delta\dot{U}|_{-1}^2\\ \leq& \varepsilon_2|\dot{A}\delta\dot{U}|^2 + (\frac{1}{4\varepsilon_2^2} + \frac{1}{4})|\delta\dot{U}|_{-1}^2, \qquad \forall\varepsilon_2 > 0.\end{aligned}$$

By taking

$$\varepsilon_1 = \frac{\min\limits_{1\leq j\leq d}\{a_{jj}\}}{4d(c_n'c_s^2 + \frac{1}{2}\max\limits_{1\leq j\leq d}\{|a_j|\})}, \quad \varepsilon_2 = \frac{\min\limits_{1\leq j\leq d}\{a_{jj}\}}{2dc_f},$$

and in view of (8.87), we deduce

$$\frac{2\beta}{\tau^2}|\delta\dot{U}|_{-1}^2 + \frac{1}{\tau}|\delta\dot{U}|_{-1}^2 + \frac{\gamma}{2}|\delta\dot{U}|_{-1}^2 \leq \left(\frac{c_f}{2}(\frac{1}{4\varepsilon_2^2} + \frac{1}{4}) + \frac{c_n'c_s^2 + \frac{1}{2}\max\limits_{1\leq j\leq d}\{|a_j|\}}{4\varepsilon_1^2}\right)|\delta\dot{U}|_{-1}^2. \quad (8.89)$$

Thanks to (8.80), let $\tau < \frac{1}{4c_5\tilde{c}c^*}$. Then (8.73) is still satisfied for $N_0 = 0$, and c_n' is bounded by a constant independent of n, τ and h. By taking τ small enough (independent of h), we have $\delta\dot{U} = 0$ and the proof is completed. □

Remark 4.5. For $\gamma = 0$, the uniqueness of the solution also holds, and the condition in (8.80) can be reduced to

$$|\langle v_h^0\rangle| + |\mathcal{E}_h(u_h^0, v_h^0)| \leq c^*,$$

which is independent of $\langle u_h^0\rangle$.

8.5 Numerical simulations

8.5.1 The one-dimensional case

In the one-dimensional case, problem (8.11) reads

$$\beta\partial_{tt}u + \partial_t u - a_2 u^{(6)} + a_1 u^{(4)} - (f(u))'' + \gamma u = 0.$$

We set $\Omega = [0, 2\pi]$, $h = \frac{2\pi}{N}$, $x_i = ih$, $i = 0, \cdots N$. Let V_h be the space of P_1 finite elements, namely $V_h = \{v \in C([0, 2\pi]);\ v|_{[x_i,x_{i+1}]} \in P_1,\ i = 0, \dots N-1;\ \ v_h(0) = v_h(2\pi)\}$, and let $(\varphi_i)_{i=1,\dots,N}$ be the usual corresponding basis. We denote by B and A the matrices $B = (\varphi_i, \varphi_j)_{i,j=1,\dots,N}$ and $A = (\varphi_i', \varphi_j')_{i,j=1,\dots,N}$ and we adapt the schemes of Sections 3 and 4 to this basis. (Indeed, we have to take into account the matrix B since the basis is not orthonormal.)

Mimicking the computations in Section 3, formula (3.14) becomes

$$\beta\dot{B}\dot{U}_{tt} + \dot{B}\dot{U}_t + \dot{A}(a_2\dot{B}^{-1}\dot{A}\dot{B}^{-1}\dot{A}\dot{U} + a_1\dot{B}^{-1}\dot{A}\dot{U} + \dot{B}^{-1}\dot{\nabla}F_h(U)) + \gamma\dot{B}\dot{U} = 0.$$

Hence, multiplying the latter equation by $\dot{U}_t^T\dot{B}\dot{A}^{-1}$, we obtain, instead of (3.15),

$$E_h(U, V) = \frac{a_2}{2}(\dot{U}^T\dot{A}\dot{B}^{-1}\dot{A}\dot{U}) + \frac{a_1}{2}\dot{U}^T\dot{A}\dot{U} + F_h(U),$$

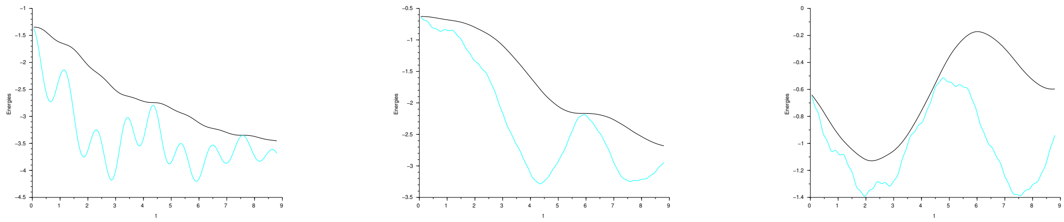
$$\mathcal{E}_h(U, V) = E_h(U, V) + \frac{\beta}{2}\dot{V}^T\dot{B}\dot{A}^{-1}\dot{B}\dot{V} + \frac{\gamma}{2}\dot{U}^T\dot{B}\dot{A}^{-1}\dot{B}\dot{U}.$$

The simulations below were performed with the software MATLAB. we chose $a_1 = -2$, $a_2 = 1, \beta = 5, N = 300, \tau = 0.05, f(u) = u^3 - u$. As far as u_h^0 and v_h^0 are concerned, we use the P_1 projection of 2 kinds of initial conditions :

(i) $u_0(x) = e^{\cos x - 1} - 0.1$ for the case $\langle u_0 \rangle \neq 0$ and $u_0(x) = \cos x + 0.3\cos(3x)$ for the case $\langle u_0 \rangle = 0$;

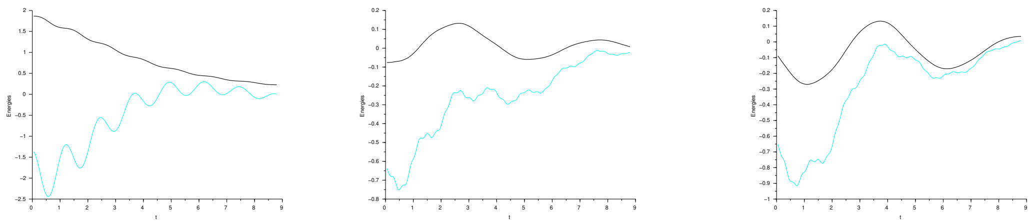
(ii) $v_0 \equiv 0.2$ for the case $\langle v_0 \rangle \neq 0$ and v_0 randomly distributed between -0.05 and 0.05 for the case $\langle v_0 \rangle = 0$.

In Figure 1, 2, 3, we display $E_h(U, V)$ (in blue) and $\mathcal{E}_h(U, V)$ (in black) with respect to t, for different combinations of γ, u_0 and v_0. These simulations are consistent with our theoretical results, namely Theorem 8.4.2 in case $\gamma \neq 0$ and Remark 8.4.5 in case $\gamma = 0$ (see also [72]). Indeed, when $\gamma = 0$, the energy $\mathcal{E}_h$ is decreasing when $\langle v_0 \rangle = 0$, whatever the value of $\langle u_0 \rangle$ is, and, when $\gamma \neq 0$, the energy $\mathcal{E}_h$ is decreasing when $\langle v_0 \rangle = 0$ and $\langle u_0 \rangle = 0$. We recall that in Theorem 8.4.2, $u_1^0 = (u_0, 1)$ and $v_1^0 = (v_0, 1)$ are now written as $|\Omega|\,\langle u_0 \rangle$ and $|\Omega|\,\langle v_0 \rangle$.



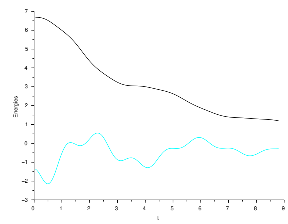
(a) $\gamma = 0$, $\langle v_0 \rangle = 0$, $\langle u_0 \rangle = 0$ (b) $\gamma = 0$, $\langle v_0 \rangle = 0$, $\langle u_0 \rangle \neq 0$ (c) $\gamma = 0$, $\langle v_0 \rangle \neq 0$, $\langle u_0 \rangle \neq 0$

FIGURE 8.1 – E_h (blue) and $\mathcal{E}_h$ (black)



(a) $\gamma = 2$, $\langle v_0 \rangle = 0$, $\langle u_0 \rangle = 0$ (b) $\gamma = 2$, $\langle v_0 \rangle = 0$, $\langle u_0 \rangle \neq 0$ (c) $\gamma = 2$, $\langle v_0 \rangle \neq 0$, $\langle u_0 \rangle \neq 0$

FIGURE 8.2 – E_h (blue) and $\mathcal{E}_h$ (black)



(a) $\gamma = 5$, $\langle v_0 \rangle = 0$, $\langle u_0 \rangle = 0$

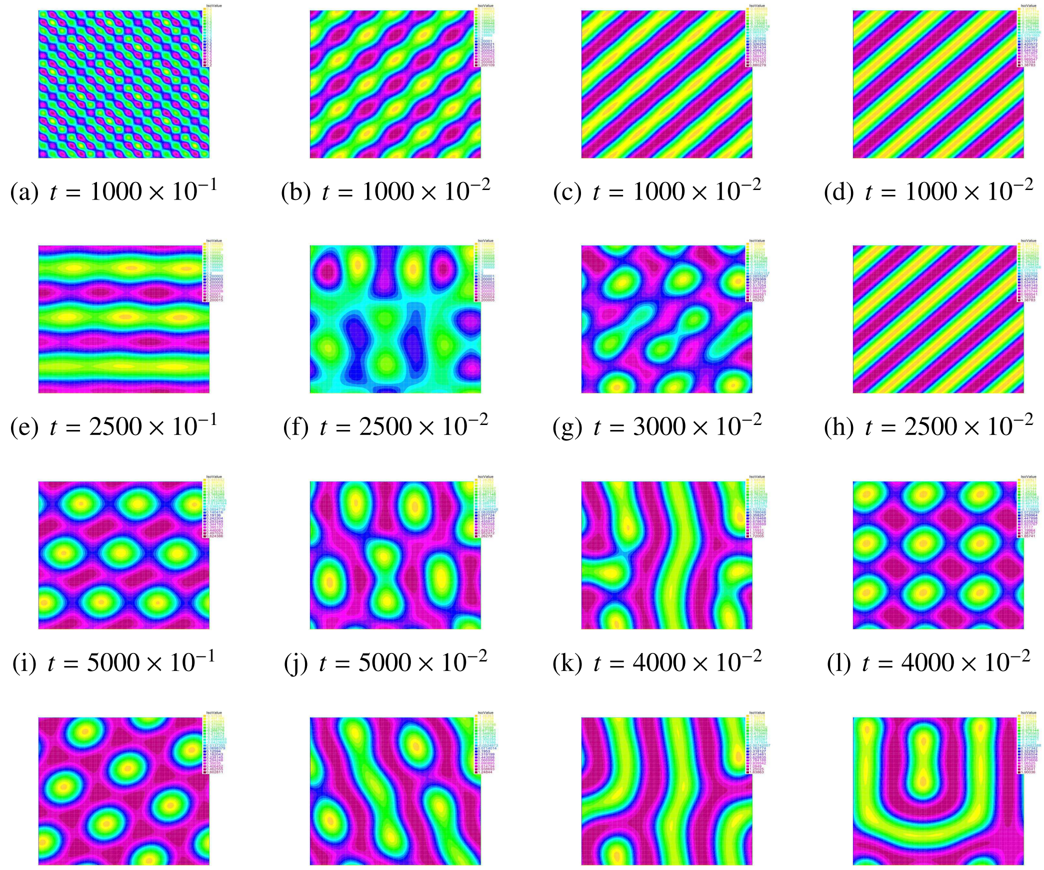
FIGURE 8.3 – E_h (blue) and $\mathcal{E}_h$ (black)

8.5.2 Simulations in two space dimensions

1. Phase-field-crystal simulations ($\gamma = 0$)

This time, the computations were performed with the software FreeFem++ [77], using a slightly different scheme :

Given $(u_h^0, v_h^0) \in V_h \times V_h$, find $(u_h^{n+1}, v_h^{n+1}, p_{i,h}^{n+1/2}, w_h^{n+1/2}) \in (V^h)^5$, $n \geq 0$, $i = 1, 2$, such that :



(a) $t = 1000 \times 10^{-1}$ (b) $t = 1000 \times 10^{-2}$ (c) $t = 1000 \times 10^{-2}$ (d) $t = 1000 \times 10^{-2}$

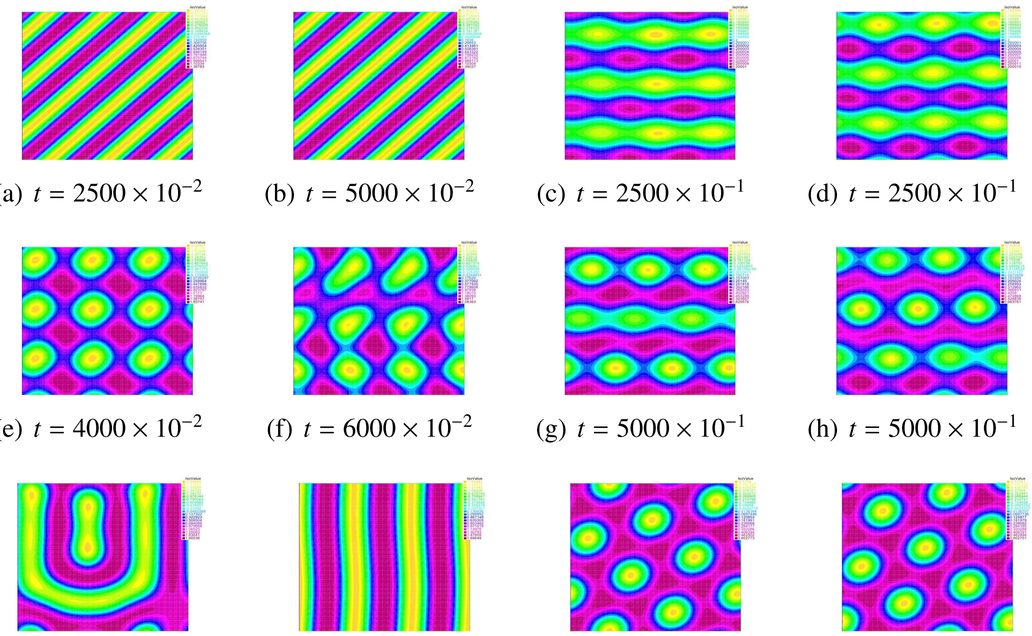
(e) $t = 2500 \times 10^{-1}$ (f) $t = 2500 \times 10^{-2}$ (g) $t = 3000 \times 10^{-2}$ (h) $t = 2500 \times 10^{-2}$

(i) $t = 5000 \times 10^{-1}$ (j) $t = 5000 \times 10^{-2}$ (k) $t = 4000 \times 10^{-2}$ (l) $t = 4000 \times 10^{-2}$

(m) $t = 8000 \times 10^{-1}$ (n) $t = 8000 \times 10^{-2}$ (o) $t = 8000 \times 10^{-2}$ (p) $t = 8000 \times 10^{-2}$

FIGURE 8.4 – $u_0 = u_0^{(1)}$, $\beta = 0.1$, $\varepsilon = 0.2$ (column 1), $\varepsilon = 0.8$ (column 2), $\varepsilon = 1.4$ (column 3), $\varepsilon = 2$ (column 4).

$$\begin{cases} \left(\dfrac{u_h^{n+1} - u_h^n}{\tau}, \phi_h\right) = (v_h^{n+1/2}, \phi_h), \\ \beta\left(\dfrac{v_h^{n+1} - v_h^n}{\tau}, \psi_h\right) = -(v_h^{n+1/2}, \psi_h) - (\nabla w_h^{n+1/2}, \nabla\psi_h) - \gamma(u_h^{n+1/2}, \psi_h), \\ (p_{i,h}^{n+1/2}, \zeta_{i,h}) = -\left(\dfrac{\partial u_h^{n+1/2}}{\partial x_i}, \dfrac{\partial \zeta_{i,h}}{\partial x_i}\right), \ i = 1,2 \\ (w_h^{n+1/2}, \xi_h) + \displaystyle\sum_{i=1}^{2}\left(a_{ii}(\dfrac{\partial p_{i,h}^{n+1/2}}{\partial x_i}, \dfrac{\partial \xi_h}{\partial x_i}) + a_i(p_{h,i}^h, \xi_h)\right) + \dfrac{a_{12}}{2}\left(\dfrac{\partial p_{2,h}^{n+1/2}}{\partial x_1}, \dfrac{\partial \xi_h}{\partial x_1}\right) \\ \qquad + \dfrac{a_{12}}{2}\left(\dfrac{\partial p_{1,h}^{n+1/2}}{\partial x_2}, \dfrac{\partial \xi_h}{\partial x_2}\right) = \left(\dfrac{f(u_h^n) + f(u_h^{n+1})}{2}, \xi_h\right) - \dfrac{1}{12}\left((u_h^{n+1} - u_h^n)^2 (f_+''(u_h^n) + f_-''(u_h^{n+1})), \xi_h\right), \end{cases} \tag{8.90}$$



(a) $t = 2500 \times 10^{-2}$ (b) $t = 5000 \times 10^{-2}$ (c) $t = 2500 \times 10^{-1}$ (d) $t = 2500 \times 10^{-1}$

(e) $t = 4000 \times 10^{-2}$ (f) $t = 6000 \times 10^{-2}$ (g) $t = 5000 \times 10^{-1}$ (h) $t = 5000 \times 10^{-1}$

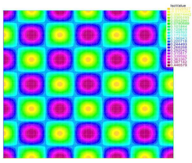
(i) $t = 8000 \times 10^{-2}$ (j) $t = 8000 \times 10^{-2}$ (k) $t = 8000 \times 10^{-1}$ (l) $t = 8000 \times 10^{-1}$

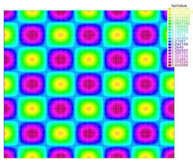
FIGURE 8.5 – $u_0 = u_0^{(1)}$, $\beta = 0.1$, $\varepsilon = 2$ (column 1), $\beta = 1$, $\varepsilon = 2$ (column 2), $\beta = 0.1$, $\varepsilon = 0.2$ (column 3), $\beta = 1$, $\varepsilon = 0.2$ (column 4).

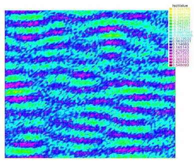
For all $(\phi_h, \psi_h, \zeta_{i,h}, \xi_h) \in (V_h)^5$, $i = 1, 2$.

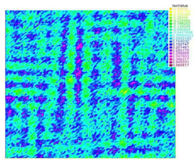
Although our theoretical results claimed in the paper actually don't translate to the latter scheme, it has the advantages of reducing the computation times (5 unknows to compute at each time-step instead of 6 unknows for the scheme (8.48)), and the numerical simulations are consistent with those obtained with (8.48) or in the litterature ([72], [58]). We choose $f(u) = u^3 + (1-\varepsilon)u$, $f_+ = f$, $f_- = 0$, and, in order to deal with a semi-implicit scheme, we use the approximation (also used in [58]) : $u_{n+1}^3 \sim 3u_n^2 u_{n+1} - 2u_n^3$ and $u_{n+1}^2 \sim 2u_n u_{n+1} - u_n^2$. Consequently, the last line of the scheme (8.90) reduces to : $(\dfrac{u_{n+1}(3u_n^2 + 1 - \varepsilon) + (1-\varepsilon)u_n - u_n^3}{2}, \xi_h)$.

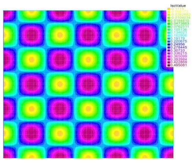
First we test the actual Phase-field crystal equation, corresponding to the coefficients $a_{11} = 1 = a_{22}$, $a_{12} = 2$, $a_1 = -2 = a_2$. The domain Ω is the square $[0, 6\pi] \times [0, 6\pi]$. It is decomposed in 100×100 squares, each square being divided along the same diagonal into two triangles. We choose $u_0^{(1)} = 0.2 + 0.2\cos(x)\cos(y)$ and $v_0 = 0$. The results are displayed in Figures 8.4 and 8.5. In Figure 8.4, we set $\beta = 0.1$ and we compare different solutions u, corresponding to different values of ε. The time stepsize τ is equal to 10^{-1} in the case $\varepsilon = 0.2$ and 10^{-2} in the other cases. In Figure 8.5, we vary ε ($\varepsilon = 0.2$ and $\varepsilon = 2$) and β ($\beta = 0.1$ and $\beta = 1$). In Figure 8.6, we vary the coefficients a_{11}, a_{12}, a_{22}, a_1, a_2 (see Table (8.1)) to illustrate the anisotropy.

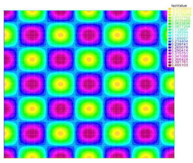

(a) $t = 100 \times 10^{-3}$

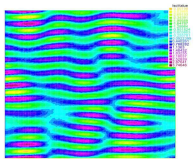

(b) $t = 100 \times 10^{-3}$

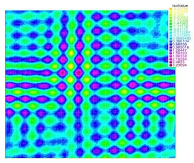

(c) $t = 100 \times 10^{-3}$

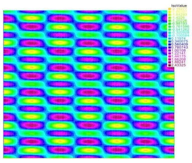

(d) $t = 100 \times 10^{-3}$

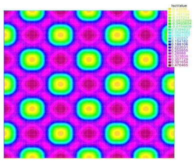

(e) $t = 200 \times 10^{-3}$

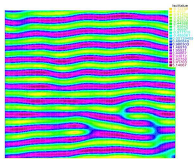

(f) $t = 200 \times 10^{-3}$


(g) $t = 200 \times 10^{-3}$


(h) $t = 200 \times 10^{-3}$


(i) $t = 400 \times 10^{-3}$


(j) $t = 400 \times 10^{-3}$


(k) $t = 400 \times 10^{-3}$

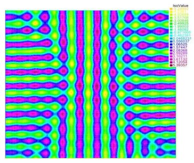

(l) $t = 400 \times 10^{-3}$

FIGURE 8.6 – The anisotropic phenomenon, $u_0 = u_0^{(1)}$ (column 1, 2) , $u_0 = u_0^{(2)}$ (column 3, 4), $\varepsilon = 0.2, \beta = 0.1, \Delta t = 10^{-3}$.

TABLE 8.1 – Coefficients for Figure 8.6 : $\beta = 0.1,\ \varepsilon = 0.2$

Column	a_{11}	a_{12}	a_{22}	a_1	a_2	Initial value	Remark
1	1	0.2	0.1	-2	-2	$u_0^{(1)}$	x-dir
2	0.1	2	0.1	-2	-2		cross-dir
3	1	0.2	0.1	-2	-2	$u_0^{(2)}$	x-dir
4	0.1	2	0.1	-2	-2		cross-dir

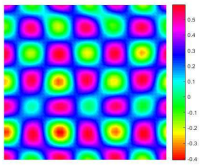
2. Simulations with $\gamma \neq 0$

In this paragraph, the computations have been made with the actual scheme (8.48), the space V_h (now denoted by V_N, $N \in \mathbb{N}$) being a space with Fourier spectral basis. Spectral methods have the advantage of requiring low computation times and the simulations were performed with the software Matlab. More precisely, the domain $\Omega = [0, 6\pi] \times [0, 6\pi]$ is now decomposed in N^2 squares, and the approximate solution (at step $n+1$) $u_N^{n+1} \in V_N$ is searched as :

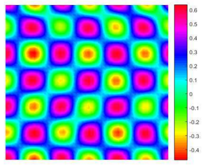
$$u_N^{n+1} = \sum_{k_x=-N/2}^{N/2-1} \sum_{k_y=-N/2}^{N/2-1} \hat{u}_{k_x}^{n+1} \hat{u}_{k_y}^{n+1} e^{ik_x x} e^{ik_y y}.$$

We choose again $f(u) = u^3 + (1-\varepsilon)u$, $f_+ = f$, $f_- = 0$, and the nonlinear system at each step is solved by a Newton algorithm. We take $a_{11} = 1 = a_{22}$, $a_{12} = 2$, $a_1 = -2 =$

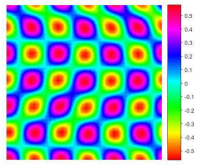
a_2, $u_0^{(1)} = 0.2 + 0.2\cos(x)\cos(y)$ and $v_0 = 0$. The figures 8.7, 8.8, 8.9 and 8.10 display the solution u_N at different times. In Figure 8.7, we take $\varepsilon = 2$, $\beta = 0.5$ and we vary γ. In Figure 8.8, we take $\varepsilon = 2$, $\beta = 5$ and we vary γ. In Figure 8.9, we take $\varepsilon = 0.2$, $\beta = 0.5$ and we vary γ. In Figure 8.10, we take $\varepsilon = 0.2$, $\beta = 5$ and we vary γ.



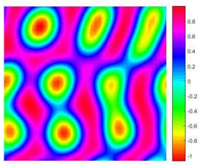
(a) $t = 6000 \times 0.005$



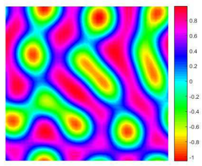
(b) $t = 6000 \times 0.005$



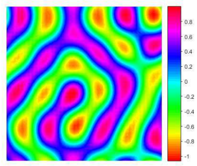
(c) $t = 6000 \times 0.005$



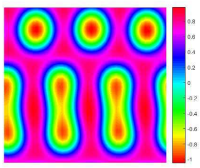
(d) $t = 7000 \times 0.005$



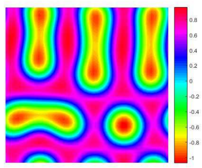
(e) $t = 7000 \times 0.005$



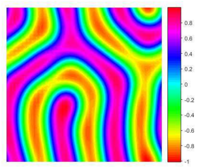
(f) $t = 7000 \times 0.005$



(g) $t = 10^4 \times 0.005$



(h) $t = 10^4 \times 0.005$



(i) $t = 10^4 \times 0.005$

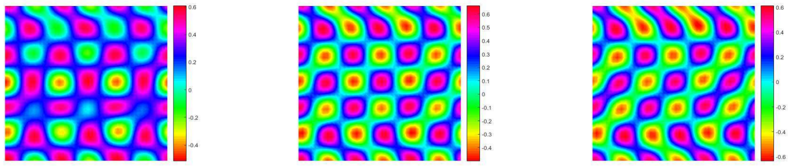
FIGURE 8.7 – $N = 40$, $\tau = 0.005$, $\varepsilon = 2$, $\beta = 0.5$, $\gamma = 0$ (column 1), $\gamma = 0.01$ (column 2), $\gamma = 0.1$ (column 3)

8.6 Appendix

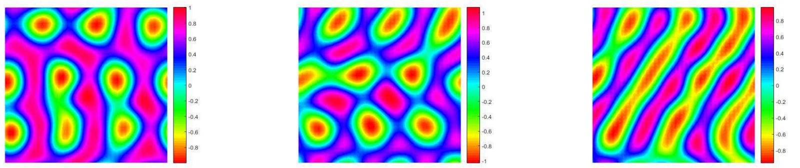
We prove (8.66). By choosing $\phi_h = 1, \psi_h = 1$ in the first and second equations of (8.48), respectively, we have

$$\begin{cases} \dfrac{u_1^{n+1} - u_1^n}{\tau} = \dfrac{v_1^{n+1} + v_1^n}{2}, \\ \beta \dfrac{v_1^{n+1} - v_1^n}{\tau} = -\dfrac{v_1^{n+1} + v_1^n}{2} - \gamma \dfrac{u_1^{n+1} + u_1^n}{2}. \end{cases}$$

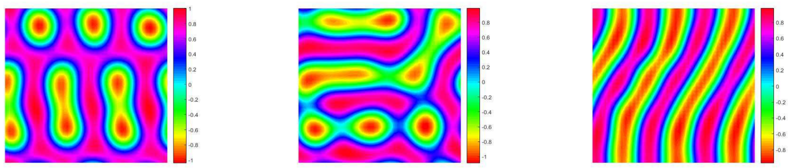
Solving the linear system gives



(a) $t = 13000 \times 0.005$ (b) $t = 13000 \times 0.005$ (c) $t = 13000 \times 0.005$



(d) $t = 15000 \times 0.005$ (e) $t = 15000 \times 0.005$ (f) $t = 15000 \times 0.005$



(g) $t = 17000 \times 0.005$ (h) $t = 17000 \times 0.005$ (i) $t = 17000 \times 0.005$

FIGURE 8.8 – $N = 40$, $\tau = 0.005$, $\varepsilon = 2$, $\beta = 5$, $\gamma = 0$ (column 1), $\gamma = 0.01$ (column 2), $\gamma = 0.1$ (column 3)

$$\begin{pmatrix} u_1^{n+1} \\ v_1^{n+1} \end{pmatrix} = \frac{1}{4\beta + 2\tau + \gamma\tau^2} B \begin{pmatrix} u_1^n \\ v_1^n \end{pmatrix} = \frac{1}{(4\beta + 2\tau + \gamma\tau^2)^{n+1}} B^{n+1} \begin{pmatrix} u_1^0 \\ v_1^0 \end{pmatrix},$$

where

$$B = \begin{pmatrix} 4\beta + 2\tau - \gamma\tau^2 & 4\beta\tau \\ -4\gamma\tau & 4\beta - 2\tau - \gamma\tau^2 \end{pmatrix}.$$

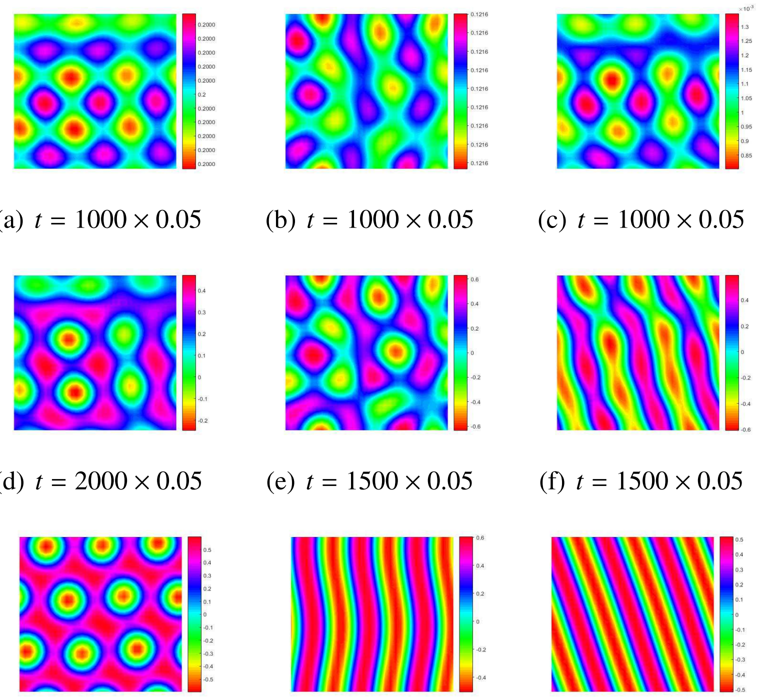
Now we decompose B into $B = B_1 + B_2$, with

$$B_1 = \begin{pmatrix} 4\beta - \gamma\tau^2 & 0 \\ 0 & 4\beta - \gamma\tau^2 \end{pmatrix}, \quad B_2 = \begin{pmatrix} 2\tau & 4\beta\tau \\ -4\gamma\tau & -2\tau \end{pmatrix}.$$

Since B_1 and B_2 commute, then

$$B^{n+1} = \sum_{j=0}^{n+1} \frac{(n+1)!}{j!(n+1-j)!} B_1^{n+1-j} B_2^j.$$

Based on the sign of $1 - 4\beta\gamma$: (i) $1 - 4\beta\gamma > 0$, (ii) $1 - 4\beta\gamma = 0$, (iii) $1 - 4\beta\gamma < 0$,



(a) $t = 1000 \times 0.05$ (b) $t = 1000 \times 0.05$ (c) $t = 1000 \times 0.05$

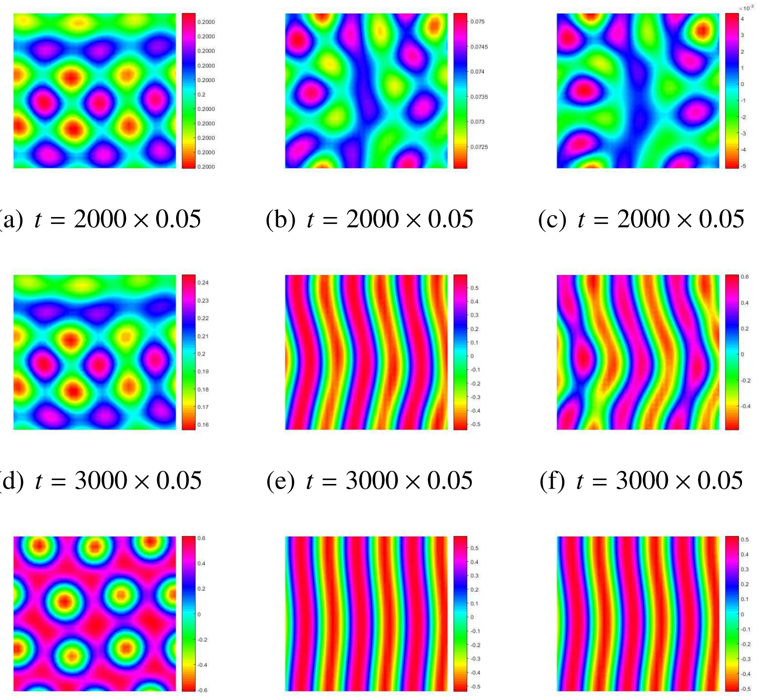
(d) $t = 2000 \times 0.05$ (e) $t = 1500 \times 0.05$ (f) $t = 1500 \times 0.05$

(g) $t = 3000 \times 0.05$ (h) $t = 2500 \times 0.05$ (i) $t = 2000 \times 0.05$

FIGURE 8.9 – $N = 30$, $\tau = 0.05$, $\varepsilon = 0.2$, $\beta = 0.5$, $\gamma = 0$ (column 1), $\gamma = 0.01$ (column 2), $\gamma = 0.1$(column 3)

we diagonalize B_2 to obtain B_2^j :

$$
\begin{aligned}
&(i) \quad B_2^j = C\begin{pmatrix} \rho_1^j & 0 \\ 0 & \rho_2^j \end{pmatrix} C^{-1}, \rho_1 = 2\tau\sqrt{1-4\beta\gamma},\ \rho_2 = -2\tau\sqrt{1-4\beta\gamma},\\
&\qquad C = \frac{1}{2\beta}\begin{pmatrix} 2\beta & 2\beta \\ \sqrt{1-4\beta\gamma}-1 & -\sqrt{1-4\beta\gamma}-1 \end{pmatrix},\\
&\qquad C^{-1} = \frac{1}{2\sqrt{1-4\beta\gamma}}\begin{pmatrix} \sqrt{1-4\beta\gamma}+1 & 2\beta \\ \sqrt{1-4\beta\gamma}-1 & -2\beta \end{pmatrix}.\\
&(ii) \quad B_2^j = 0,\ j \geq 2. \\
&(iii) \quad B_2^j = C\begin{pmatrix} \rho_1^j & 0 \\ 0 & \rho_2^j \end{pmatrix} C^{-1},\ \rho_1 = 2\tau i\sqrt{4\beta\gamma-1},\ \rho_2 = -2\tau i\sqrt{4\beta\gamma-1},\\
&\qquad C = \frac{1}{2\beta}\begin{pmatrix} 2\beta & 2\beta \\ i\sqrt{4\beta\gamma-1}-1 & -i\sqrt{4\beta\gamma-1}-1 \end{pmatrix},\\
&\qquad C^{-1} = \frac{i}{2\sqrt{4\beta\gamma-1}}\begin{pmatrix} -i\sqrt{4\beta\gamma-1}-1 & -2\beta \\ -i\sqrt{4\beta\gamma-1}+1 & 2\beta \end{pmatrix}.
\end{aligned}
\tag{8.91}
$$



(a) $t = 2000 \times 0.05$ (b) $t = 2000 \times 0.05$ (c) $t = 2000 \times 0.05$

(d) $t = 3000 \times 0.05$ (e) $t = 3000 \times 0.05$ (f) $t = 3000 \times 0.05$

(g) $t = 4000 \times 0.05$ (h) $t = 4000 \times 0.05$ (i) $t = 5000 \times 0.05$

FIGURE 8.10 – $N = 30$, $\tau = 0.05$, $\varepsilon = 0.2$, $\beta = 5$, $\gamma = 0$ (column 1), $\gamma = 0.01$ (column 2), $\gamma = 0.1$(column 3)

Therefore,

$$B^{n+1} = \begin{cases} \displaystyle\sum_{j=0}^{n+1} \frac{(n+1)!}{j!(n+1-j)!}(4\beta - \gamma\tau^2)^{n+1-j} B_2^j I, & cases\ (i),\ (iii), \\ B_1^{n+1} + (n+1)(4\beta - \gamma\tau^2)^n B_2, & case\ (ii). \end{cases}$$

Now we derive the expression of $v_1^{n+1/2}$. For cases (i) and (iii), setting $C = (c_{ij})_{1\le i,j\le 2}$, $C^{-1} = (d_{ij})_{1\le i,j\le 2}$, then

$$\begin{aligned} (B^{n+1})_{21} =& \sum_{j=0}^{n+1} \frac{(n+1)!}{j!(n+1-j)!}(4\beta - \gamma\tau^2)^{n+1-j}(c_{21}d_{11}\rho_1^j + c_{22}d_{21}\rho_2^j) \\ =& c_{21}d_{11}[(4\beta - \gamma\tau^2 + \rho_1)^{n+1} - (4\beta - \gamma\tau^2 + \rho_2)^{n+1}], \\ (B^{n+1})_{22} =& \sum_{j=0}^{n+1} \frac{(n+1)!}{j!(n+1-j)!}(4\beta - \gamma\tau^2)^{n+1-j}(c_{21}d_{12}\rho_1^j + c_{22}d_{22}\rho_2^j) \\ =& c_{21}d_{12}(4\beta - \gamma\tau^2 + \rho_1)^{n+1} + c_{22}d_{22}(4\beta - \gamma\tau^2 + \rho_2)^{n+1}. \end{aligned}$$

We thus have

$$\begin{aligned}
v_1^{n+1} =& \frac{1}{(4\beta+\gamma\tau^2+2\tau)^{n+1}}[(B^{n+1})_{21}u_1^0+(B^{n+1})_{22}v_1^0] \\
=& c_{21}d_{11}[(\frac{4\beta-\gamma\tau^2+\rho_1}{4\beta+\gamma\tau^2+2\tau})^{n+1}-(\frac{4\beta-\gamma\tau^2+\rho_2}{4\beta+\gamma\tau^2+2\tau})^{n+1}g]u_1^0 \\
&+[c_{21}d_{12}(\frac{4\beta-\gamma\tau^2+\rho_1}{4\beta+\gamma\tau^2+2\tau})^{n+1}+c_{22}d_{22}(\frac{4\beta-\gamma\tau^2+\rho_2}{4\beta+\gamma\tau^2+2\tau})^{n+1}]v_1^0.
\end{aligned}$$

Furthermore,

$$\begin{aligned}
v_1^{n+1/2} =& \frac{c_{21}d_{11}}{2}\Big[(\frac{4\beta-\gamma\tau^2+\rho_1}{4\beta+\gamma\tau^2+2\tau})^{n+1}-(\frac{4\beta-\gamma\tau^2+\rho_2}{4\beta+\gamma\tau^2+2\tau})^{n+1}+(\frac{4\beta-\gamma\tau^2+\rho_1}{4\beta+\gamma\tau^2+2\tau})^{n} \\
&-(\frac{4\beta-\gamma\tau^2+\rho_2}{4\beta+\gamma\tau^2+2\tau})^{n}\Big]u_1^0+\Big[\frac{c_{21}d_{12}}{2}(\frac{4\beta-\gamma\tau^2+\rho_1}{4\beta+\gamma\tau^2+2\tau})^{n+1}+\frac{c_{21}d_{12}}{2}(\frac{4\beta-\gamma\tau^2+\rho_1}{4\beta+\gamma\tau^2+2\tau})^{n} \\
&+\frac{c_{22}d_{22}}{2}(\frac{4\beta-\gamma\tau^2+\rho_2}{4\beta+\gamma\tau^2+2\tau})^{n+1}+\frac{c_{22}d_{22}}{2}(\frac{4\beta-\gamma\tau^2+\rho_2}{4\beta+\gamma\tau^2+2\tau})^{n}\Big]v_1^0.
\end{aligned}$$

For case (*ii*), since

$$\begin{aligned}
(B^{n+1})_{21} &= (n+1)(4\beta-\gamma\tau^2)^n(B_2)_{21} = -4\gamma(n+1)\tau(4\beta-\gamma\tau^2)^n, \\
(B^{n+1})_{22} &= (4\beta-\gamma\tau^2)^{n+1}+(n+1)(4\beta-\gamma\tau^2)^n(B_2)_{22} \\
&= (4\beta-\gamma\tau^2)^{n+1}-2\tau(n+1)(4\beta-\gamma\tau^2)^n,
\end{aligned}$$

then

$$\begin{aligned}
v_1^{n+1} =& \frac{1}{(4\beta+\gamma\tau^2+2\tau)^{n+1}}[(B^{n+1})_{21}u_1^0+(B^{n+1})_{22}v_1^0] \\
=& \frac{-4\gamma\tau(n+1)(4\beta-\gamma\tau^2)^n}{(4\beta+\gamma\tau^2+2\tau)^{n+1}}u_1^0+\frac{(4\beta-\gamma\tau^2)^{n+1}-2\tau(n+1)(4\beta-\gamma\tau^2)^n}{(4\beta+\gamma\tau^2+2\tau)^{n+1}}v_1^0.
\end{aligned} \tag{8.92}$$

Therefore, we get the expression of $v_1^{n+1/2}$:

$$\begin{aligned}
(i)\ v_1^{n+1/2} =& -\frac{\gamma}{2\sqrt{1-4\beta\gamma}}(q_1^{n+1}-q_2^{n+1}+q_1^n-q_2^n)u_1^0 \\
&+\frac{1}{4\sqrt{1-4\beta\gamma}}[(\sqrt{1-4\beta\gamma}-1)(q_1^{n+1}+q_1^n)+(\sqrt{1-4\beta\gamma}+1)(q_2^{n+1}+q_2^n)]v_1^0, \\
\text{where } \mathrm{q}_1 =& \frac{4\beta+2\tau\sqrt{1-4\beta\gamma}-\gamma\tau^2}{4\beta+2\tau+\gamma\tau^2}, \mathrm{q}_2 = \frac{4\beta-2\tau\sqrt{1-4\beta\gamma}-\gamma\tau^2}{4\beta+2\tau+\gamma\tau^2}.
\end{aligned} \tag{8.93}$$

$$(ii)\ v_1^{n+1/2} = \frac{(4\beta-\gamma\tau^2)^n}{2(4\beta+2\tau+\gamma\tau^2)^{n+1}}[-4\gamma(n+1)\tau u_1^0 + (4\beta - 2\tau(n+1) - \gamma\tau^2)v_1^0]$$
$$+ \frac{(4\beta-\gamma\tau^2)^{n-1}}{2(4\beta+2\tau+\gamma\tau^2)^{n}}[-4\gamma n\tau u_1^0 + (4\beta - 2\tau n - \gamma\tau^2)v_1^0].$$

$$(iii)\ v_1^{n+1/2} = \frac{\gamma i}{2\sqrt{4\beta\gamma-1}}(q_3^{n+1} - q_4^{n+1} + q_3^n - q_4^n)u_1^0$$
$$+ \frac{1}{4\sqrt{4\beta\gamma-1}}[(\sqrt{4\beta\gamma-1}+i)(q_3^{n+1}+q_3^n) + (\sqrt{4\beta\gamma-1}-i)(q_4^{n+1}+q_4^n)]v_1^0,$$

where $q_3 = \dfrac{4\beta-\gamma\tau^2+2\tau i\sqrt{4\beta\gamma-1}}{4\beta+2\tau+\gamma\tau^2}, q_4 = \dfrac{4\beta-\gamma\tau^2-2\tau i\sqrt{4\beta\gamma-1}}{4\beta+2\tau+\gamma\tau^2}.$

We are now ready to estimate $v_1^{n+1/2}$. For case (i), note that $|q_1| < 1,\ |q_2| < 1$. Then by (8.93), we deduce

$$\begin{aligned}
|v_1^{n+1/2}| \le& \frac{\gamma}{\sqrt{1-4\beta\gamma}}(|q_1|^n + |q_2|^n)|u_1^0| + g(\frac{1-\sqrt{1-4\beta\gamma}}{2\sqrt{1-4\beta\gamma}}|q_1|^n + \frac{1+\sqrt{1-4\beta\gamma}}{2\sqrt{1-4\beta\gamma}}|q_2|^n g)|v_1^0| \\
\le& \frac{\gamma}{\sqrt{1-4\beta\gamma}}(|q_1|^n + |q_2|^n)|u_1^0| + \frac{1+\sqrt{1-4\beta\gamma}}{2\sqrt{1-4\beta\gamma}}(|q_1|^n + |q_2|^n)|v_1^0| \\
\le& \frac{2\gamma+1+\sqrt{1-4\beta\gamma}}{\sqrt{1-4\beta\gamma}}q^n(|u_1^0| + |v_1^0|), \quad q = max\{|q_1|, |q_2|\}.
\end{aligned} \tag{8.94}$$

Similarly, the following estimate holds for case (iii) :

$$\begin{aligned}
|v_1^{n+1/2}| \le& \frac{\gamma}{\sqrt{4\beta\gamma-1}}(|q_3|^n + |q_4|^n)|u_1^0| + \frac{\sqrt{\beta\gamma}}{\sqrt{4\beta\gamma-1}}(|q_3|^n + |q_4|^n)|v_1^0| \\
\le& \frac{2(\gamma+\sqrt{\beta\gamma})}{\sqrt{4\beta\gamma-1}}q^n(|u_1^0| + |v_1^0|), \quad q = |q_3| = |q_4|.
\end{aligned} \tag{8.95}$$

We mainly discuss case (ii). Here we will frequently use three inequalities obtained by the mean value theorem :

$$\begin{aligned}
&(a)\quad (4\beta+\tau-\gamma\tau^2)^{n+1} - (4\beta-\gamma\tau^2)^{n+1} > \tau(n+1)(4\beta-\gamma\tau^2)^n, \quad \text{if } \tau \le 4\beta; \\
&(b)\quad (4\beta-\tau-\gamma\tau^2)^{n+1} - (4\beta-\gamma\tau^2)^{n+1} > -\tau(n+1)(4\beta-\gamma\tau^2)^n, \text{ if } \tau > 4\beta, \text{n is odd}; \\
&(c)\quad (4\beta-\gamma\tau^2)^{n+1} - (4\beta-\tau-\gamma\tau^2)^{n+1} > \tau(n+1)(4\beta-\gamma\tau^2)^n, \quad \text{if } \tau > 4\beta, \text{n is even}.
\end{aligned} \tag{8.96}$$

Let

$$q_5 = \frac{4\beta + \tau - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}, \ q_6 = \frac{4\beta - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}, \ q_7 = \frac{4\beta - \tau - \gamma\tau^2}{4\beta + 2\tau + \gamma\tau^2}.$$

Then $-1 < q_7 < q_6 < q_5 < 1$.

If $4\beta - \gamma\tau^2 \geq 0$, i.e. $\tau \leq 4\beta$, $0 \leq q_6 < q_5 < 1$, by (8.92), (8.96)(a), we derive

$$\begin{aligned} |v_1^{n+1}| \leq& 4\gamma(q_5^{n+1} - q_6^{n+1})|u_1^0| + 2q_5^{n+1}|v_1^0| \\ <& 4\gamma q_5^{n+1}|u_1^0| + 2q_5^{n+1}|v_1^0| \\ <& (4\gamma + 2)|q_5|^{n+1}\left(|u_1^0| + |v_1^0|\right). \end{aligned}$$

If $4\beta - \gamma\tau^2 < 0$, i.e. $\tau > 4\beta$, $-1 < q_7 < q_6 < 0$, for n odd, by (8.96)(b),

$$\begin{aligned} |v_1^{n+1}| \leq& 4\gamma(q_7^{n+1} - q_6^{n+1})|u_1^0| + 2q_7^{n+1}|v_1^0| \\ <& 4\gamma q_7^{n+1}|u_1^0| + 2q_7^{n+1}|v_1^0| \\ <& (4\gamma + 2)|q_7|^{n+1}\left(|u_1^0| + |v_1^0|\right). \end{aligned}$$

For n even, by (8.96)(c),

$$\begin{aligned} |v_1^{n+1}| \leq& 4\gamma(q_6^{n+1} - q_7^{n+1})|u_1^0| - 2q_7^{n+1}|v_1^0| \\ <& 4\gamma|q_7|^{n+1}|u_1^0| + 2|q_7|^{n+1}|v_1^0| \\ <& (4\gamma + 2)|q_7|^{n+1}\left(|u_1^0| + |v_1^0|\right). \end{aligned}$$

In short, we have

$$|v_1^{n+1}| < (4\gamma + 2)q^{n+1}\left(|u_1^0| + |v_1^0|\right), \ q = \max\{|q_5|, |q_7|\}.$$

This yields

$$\begin{aligned} |v_1^{n+1/2}| \leq& \frac{1}{2}\left[(4\gamma + 2)(q^{n+1} + q^n)\left(|u_1^0| + |v_1^0|\right)\right] \\ <& (4\gamma + 2)q^n\left(|u_1^0| + |v_1^0|\right). \end{aligned} \tag{8.97}$$

Combining (8.94), (8.95) and (8.97), we deduce (8.66), with the coefficients satisfying (8.67).

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Deuxième partie

Problèmes non linéaires pour des micro-systèmes électro-mécaniques

Chapitre 9

Analysis of discretized parabolic problems modeling electrostatic micro-electromechanical systems

Analyse de problèmes paraboliques discrétisés modélisant un système micro-électromécanique électrostatique

Ce chapitre est constitué de l'article **Analysis of discretized parabolic problems modeling electrostatic micro-electromechanical systems**, *Discrete and Continuous Dynamical Systems Series S*, à paraître.
Cet article est écrit en collaboration avec **Laurence Cherfils**, **Alain Miranville** et **Chuanju Xu**.

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Analysis of discretized parabolic problems modeling electrostatic micro-electromechanical systems

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Abstract : Our aim in this paper is to study discretized parabolic problems modeling electrostatic micro-electromechanical systems (MEMS). In particular, we prove, both for semi-implicit and implicit semi-discrete schemes, that, under proper assumptions, the solutions are monotonically and pointwise convergent to the minimal solution to the corresponding elliptic partial differential equation. We also study the fully discretized semi-implicit scheme in one space dimension. We finally give numerical simulations which illustrate the behavior of the solutions both in one and two space dimensions.

Key words and phrases : Micro-electromechanical systems (MEMS), semi-implicit scheme, implicit scheme, fully discretized scheme, pull-in voltage, minimal solution, numerical simulations.

2010 Mathematics Subject Classification : 35K55, 35J60, 65N06, 65N12

9.1 Introduction

MEMS (micro-electromechanical systems) combine electronics and micro-size mechanical devices in order to decrease the scaling of electromechanical systems to micro-scale ; this is similar to NEMS (nano-electromechanical systems) which go to nano-scale (see [114]). The idea of micro-machineries was presented by Feynman in his famous lecture (see [48]) at the end of the 1950's. Several years later, the earliest micro-machinery, named resonant gate transistor and which served as a tuner for micro-electronic radios (see [109]), was created by Nathanson and his coworkers (see [110]) at Westinghouse research labs. From then on, MEMS devices have been extensively applied to many commercial systems, including inkjet printers, MEMS microphones in portable devices, accelerometers for airbag deployment and electronic stability control in modern cars, biosensors, silicon pressure sensors, such as disposable blood pressure sensors, and so on (see more examples in [17] and [114]).

From a mathematical point of view and with the fundamental works by Pelesko and Bernstein (see [114]), we consider an idealized MEMS device which is described in the following sketch (Fig. 9.1). The device mainly contains a thin and deformable elastic membrane with supported boundary and a parallel rigid ground electric plate.

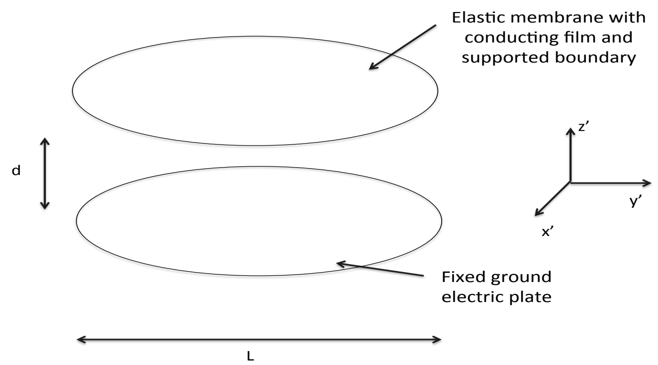


FIGURE 9.1 – An idealized MEMS capacitor.

The upper surface of the membrane, which is normally dielectric, is coated with a metallic conducting film and the thickness of the film is considered to be negligible. When applying a voltage to the conducting film, the elastic membrane deforms towards the ground plate. Considering both the dynamics and electrostatic processes (see [46] and [114] for details) and applying dimensionless analysis, we obtain the following idealized parabolic MEMS problem :

$$\begin{aligned} &\frac{\partial u}{\partial t} - \Delta u = \frac{\lambda f(x)}{(1-u)^2} \quad \text{in } \Omega, \\ &u(t,x) = 0 \text{ on } \partial\Omega; \quad u(0,x) = 0 \quad \text{in } \Omega, \end{aligned} \tag{9.1}$$

and the corresponding elliptic problem :

$$\begin{aligned} &-\Delta u = \frac{\lambda f(x)}{(1-u)^2} \quad \text{in } \Omega, \\ &u(x) = 0 \text{ on } \partial\Omega; \quad 0 \le u < 1 \quad \text{in } \Omega, \end{aligned} \tag{9.2}$$

where $u = 1-d$ and d corresponds to the dimensionless distance between the membrane and the plate. Furthermore, f describes the dielectric profile of the elastic membrane and $\lambda > 0$ characterizes the applied voltage.

There are several central problems in the study of problem (9.1) and its corresponding elliptic problem (9.2). For instance, when the applied voltage λ increases to some threshold, the device cannot remain stable and a touchdown phenomenon appears, which means that u goes to 1 in finite time. The threshold value is called the pull-in voltage, denoted by λ^*, and is defined by

$$\lambda^*(\Omega, f) = \sup\{\lambda > 0 \mid \text{problem (9.2) possesses at least one solution}\}.$$

The questions of the evaluation of λ^* and of how λ, as well as λ^*, influence the solutions to MEMS problems are among the central questions in the mathematical study of MEMS. Moreover, we list below the definitions of quenching time and quenching set (see [51], [52] and [88]) which are also important problems in the study of MEMS parabolic problem.

Definition 9.1.1. We call T the quenching time of problem (9.1) if T satisfies

$$T = \sup\{t > 0 \mid \text{for } s \in [0,t], \sup_{\Omega} u(\cdot, s) < 1\}. \tag{9.3}$$

Definition 9.1.2. We call Σ the quenching set of problem (9.1) if Σ satisfies

$$\Sigma = \{\mathbf{x} \in \overline{\Omega} \mid \exists (\mathbf{x}_n, t_n) \in \Omega \times (0,T), \mathbf{x}_n \to \mathbf{x},\ t_n \to t,\ u(\mathbf{x}_n, t_n) \to 1\}. \tag{9.4}$$

Besides, the diversification of materials for the membrane leads to different dielectric profiles f and corresponding solutions. We refer the readers to [46], [59], [60], [53], [73], [78], [91], [114] and references therein for more details, including the evaluation of λ^*, discussions on the touchdown phenomenon and the existence and properties of the global solutions to both the elliptic and parabolic problems, as well as the study of the equations with varying dielectric properties from a theoretical perspective. Furthermore, we refer the readers to [89] for modified MEMS problems with a non-local term, to [139] for an advection term and to [24] and references therein for fourth-order problems.

We are interested in this paper in the numerical approximation of problem (9.1). In particular, we prove that, both for semi-implicit and implicit semi-discrete schemes, the solutions are monotonically and pointwise convergent to the minimal solution to the corresponding elliptic partial differential equation, under proper assumptions. We also study the fully discretized semi-implicit scheme in one space dimension. We finally give numerical simulations which illustrate the behavior of the solutions, as well as the touchdown phenomenon, with different schemes and different initial conditions.

9.2 Setting of the problem

We consider the following initial and boundary value problem :

$$\begin{aligned} &\frac{\partial u}{\partial t} - \Delta u = \frac{\lambda f(x)}{(1-u)^2} \quad \text{in } \Omega, \\ &u(t,x) = 0 \ \text{ on } \partial\Omega; \quad u(0,x) = u_0(x) \quad \text{in } \Omega, \end{aligned} \tag{9.5}$$

where f describes the permittivity profile of the elastic membrane and $\lambda > 0$ characterizes the applied voltage. We make the following assumptions :

- Ω is a bounded and regular domain of $\mathbb{R}^N$, $N = 1,\ 2$ or 3 ;
- $f \in C^\alpha(\overline{\Omega})$ for some $\alpha \in (0,1]$ and f satisfies the condition $0 \le f \le 1$, but is not reduced to the null function.
- $u_0 \in L^2(\Omega)$ and $0 \le u_0 < 1$ a.e..

In particular, when $u_0 = 0$, there exists $\lambda^* > 0$ such that, if $0 \le \lambda \le \lambda^*$, then (9.5) possesses a unique solution which globally converges as $t \to +\infty$, monotonically and pointwise, to its unique minimal steady state. Furthermore, when $\lambda > \lambda^*$, the unique solution reaches the singular value 1 in finite time. We refer the interested reader to [46] for more details.

9.3 The semi-implicit scheme

We set, for $\tau > 0$ given, $t_n = n\tau$, $n = 0, 1, \cdots$, and consider the semi-implicit semi-discrete scheme :

$$\begin{cases} u_{n+1} - \tau\Delta u_{n+1} = u_n + \dfrac{\lambda\tau f(x)}{(1-u_n)^2} \ \text{ in } \Omega, \\ u_{n+1} = 0 \ \text{ on } \partial\Omega, \end{cases} \tag{9.6}$$

where $u_{n+1} \simeq u(t_{n+1}, x)$, $u_n \simeq u(t_n, x)$ and u_0 is as in (9.5).

We can note that, if $u_n \in H^2(\Omega) \cap H^1_0(\Omega)$, then $u_{n+1} \in H^2(\Omega) \cap H^1_0(\Omega)$ and

$$u_{n+1} = (I - \tau\Delta)^{-1}(u_n + \frac{\lambda\tau f}{(1-u_n)^2}),$$

as long as this makes sense, i.e., u_n does not reach the singular value 1. Actually, it follows from classical elliptic regularity results that, if $f \in H^2(\Omega)$, then $u_{n+1} \in H^4(\Omega)$. Thus, if $u_0 \in H^2(\Omega)$ and $f \in H^{2n}(\Omega)$, then $u_n \in H^{2n+2}(\Omega)$ and, if $u_0, f \in C^\infty(\overline{\Omega})$, then $u_n \in C^\infty(\overline{\Omega})$ (as long as it exists).

We also know that (see [46]), for $0 \leq \lambda < \lambda^*$, where $\lambda^* > 0$ denotes the pull-in voltage and is the same as above, the elliptic problem

$$\begin{aligned} -\Delta u &= \frac{\lambda f(x)}{(1-u)^2} \quad \text{in } \Omega, \\ 0 \leq u < 1 &\text{ in } \Omega \quad \text{and} \quad u = 0 \text{ on } \partial\Omega, \end{aligned} \tag{9.7}$$

possesses at least one solution $u = u_\lambda$. Furthermore, we assume that u_λ is the unique minimal solution (see [46]) to (9.7), i.e., for any other solution v to (9.7), there holds $u_\lambda(x) \leq v(x)$ a.e. in Ω. Actually, there exists $\overline{u} \in (0, 1)$ independent of λ such that

$$\|u_\lambda\|_{L^\infty(\Omega)} \leq \overline{u}, \ \forall \lambda \in [0, \lambda^*). \tag{9.8}$$

We additionally assume that

$$0 \leq u_0(x) \leq u_\lambda(x), \text{ a.e. } x \in \Omega. \tag{9.9}$$

We first establish a number of propositions and corollaries as follows.

Proposition 9.3.1. *There holds, for all $n \in \mathbb{N} \cup \{0\}$,*

$$0 \leq u_n(x) \leq u_\lambda(x), \ a.e. \ x \in \Omega; \tag{9.10}$$

in particular, for all $n \in \mathbb{N} \cup \{0\}$, u_n exists and satisfies

$$0 \leq u_n(x) < 1, \ a.e. \ x \in \Omega.$$

Proof. We already assumed that (9.9) holds for $n = 0$. Let us assume that, for a given $n \in \mathbb{N} \cup \{0\}$, there holds $0 \leq u_n(x) \leq u_\lambda(x)$, $a.e.$ $x \in \Omega$. The function $v_{n+1} = u_{n+1} - u_\lambda$ satisfies

$$v_{n+1} - \tau\Delta v_{n+1} = u_n - u_\lambda + \frac{\lambda\tau f}{(1-u_n)^2} - \frac{\lambda\tau f}{(1-u_\lambda)^2} \leq 0 \tag{9.11}$$

and

$$v_{n+1} = 0 \text{ on } \partial\Omega. \tag{9.12}$$

Multiplying (9.11) by v_{n+1}^+, where $\cdot^+ = \max\{0, \cdot\}$, we obtain, integrating over Ω and by parts and owing to (9.12),

$$\|v_{n+1}^+\|^2 \leq 0,$$

where $\|\cdot\|$ denotes the L^2-norm. This means that $v_{n+1}^+ = 0$ and $u_{n+1} \leq u_\lambda$ a.e. $x \in \Omega$.

Alternatively, we can note that

$$u_\lambda - \tau\Delta u_\lambda = u_\lambda + \frac{\lambda\tau f}{(1-u_\lambda)^2} \geq u_n + \frac{\lambda\tau f}{(1-u_n)^2},$$

so that u_λ is a supersolution to (9.6). Noticing that 0 is a subsolution to (9.6), it follows from the sub and supersolutions theorem (see, e.g., [18]) that

$$0 \leq u_{n+1} \leq u_\lambda, \quad \text{a.e.} \quad x \in \Omega,$$

which completes the proof. □

Proposition 9.3.2. *There holds, for $n \in \mathbb{N} \cup \{0\}$,*

$$\|u_{n+1} - u_\lambda\| \leq \frac{1}{1+c_0\tau}\left(1 + \frac{2\lambda\tau}{(1-\overline{u})^3}\right)\|u_n - u_\lambda\|, \tag{9.13}$$

where $\overline{u}$ was given in (9.8), and $c_0 > 0$ is the optimal constant in the Poincaré inequality

$$\|\nabla v\|^2 \geq c_0\|v\|^2, \quad v \in H_0^1(\Omega). \tag{9.14}$$

Proof. We have, setting $v_n = u_n - u_\lambda$ and $v_{n+1} = u_{n+1} - u_\lambda$,

$$v_{n+1} - \tau\Delta v_{n+1} = v_n + \frac{\lambda\tau f}{(1-u_n)^2} - \frac{\lambda\tau f}{(1-u_\lambda)^2} \quad \text{in} \quad \Omega,$$
$$v_{n+1} = 0 \quad \text{on} \quad \partial\Omega.$$

We thus deduce that

$$\begin{aligned} v_{n+1} - \tau\Delta v_{n+1} &= v_n + \frac{\lambda\tau f v_n(1-u_\lambda+1-u_n)}{(1-u_n)^2(1-u_\lambda)^2} \\ &= v_n + \left[\frac{\lambda\tau f}{(1-u_n)^2(1-u_\lambda)} + \frac{\lambda\tau f}{(1-u_n)(1-u_\lambda)^2}\right]v_n. \end{aligned} \tag{9.15}$$

Multiplying (9.15) by v_{n+1} and integrating over Ω and by parts, we obtain

$$\begin{aligned} \|v_{n+1}\|^2 + \tau\|\nabla v_{n+1}\|^2 &= ((v_n, v_{n+1})) \\ &\quad + ((\left[\frac{\lambda\tau f}{(1-u_n)^2(1-u_\lambda)} + \frac{\lambda\tau f}{(1-u_n)(1-u_\lambda)^2}\right]v_n, v_{n+1})), \end{aligned}$$

which yields, noting that v_n and v_{n+1} are nonnegative and recalling that $u_n \leq u_\lambda$ and the assumptions on f,

$$\begin{aligned}\|v_{n+1}\|^2 + \tau\|\nabla v_{n+1}\|^2 &\leq ((v_n, v_{n+1})) + ((\frac{2\lambda\tau}{(1-\overline{u})^3}v_n, v_{n+1})) \\ &= ((\left(1 + \frac{2\lambda\tau}{(1-\overline{u})^3}\right)v_n, v_{n+1})) \\ &\leq \left(1 + \frac{2\lambda\tau}{(1-\overline{u})^3}\right)\|v_n\|\|v_{n+1}\|.\end{aligned}$$

It thus follows from (9.12) and the Poincaré inequality that

$$(1 + c_0\tau)\|v_{n+1}\|^2 \leq \left(1 + \frac{2\lambda\tau}{(1-\overline{u})^3}\right)\|v_{n+1}\|\|v_n\|.$$

This completes the proof. □

As a consequence of Proposition 9.3.1, we deduce the following corollary.

Corollary 1. We assume that

$$\frac{1}{1 + c_0\tau}\left(1 + \frac{2\lambda\tau}{(1-\overline{u})^3}\right) < 1. \tag{9.16}$$

Then, u_n converges to u_λ in $L^2(\Omega)$ as $n \to +\infty$.

Remark 9.3.1. *We can note that* (9.16) *holds for*

$$\lambda < \frac{1}{2}c_0(1-\overline{u})^3.$$

In particular, this estimate does not depend on the choice of $\tau > 0$.

Remark 9.3.2. *Let us take* $u_0 = 0$. *It is clear that* $u_1 \geq u_0 = 0$. *Let us then assume that, for a given* $n \in \mathbb{N}$, $u_n \geq u_{n-1}$. *We have, setting* $v_{n+1} = u_{n+1} - u_n$,

$$v_{n+1} - \tau\Delta v_{n+1} = u_n - u_{n-1} + \frac{\lambda\tau f}{(1-u_n)^2} - \frac{\lambda\tau f}{(1-u_{n-1})^2} \geq 0 \text{ in } \Omega \tag{9.17}$$

and

$$v_{n+1} = 0 \text{ on } \partial\Omega.$$

Multiplying (9.17) *by* $-v_{n+1}^-$, *where* $\cdot^- = \max\{0, -\cdot\}$, *we deduce that* $\|v_{n+1}^-\| = 0$, *whence* $u_{n+1} \geq u_n$. *Therefore, for every* $x \in \Omega$, *the sequence* $\{u_n(x)\}$ *is monotone increasing and bounded from above by* u_λ. *Hence it converges monotonically as* $n \to +\infty$.

Moreover, it is verified numerically (see [46] for details) that, if $\lambda < \lambda^*$ and is close to λ^*, with given f and N, there may exist another stable solution to the elliptic problem (9.7) which is denoted by u_λ^+ and satisfies $u_\lambda < u_\lambda^+ < 1$. We now assume that the stationary problem possesses at least 2 solutions $u_\lambda < u_\lambda^+ < 1$ and that the initial condition satisfies $u_\lambda \leq u_0 < u_\lambda^+ < 1$. Then, we additionally have the following proposition.

Proposition 9.3.3. *We consider the semi-implicit scheme (9.6), with $0 < \lambda < \lambda^*$ and f satisfying the assumptions mentioned in Section 9.2. Then, if the initial condition satisfies $u_\lambda \leq u_0 < u_\lambda^+ < 1$, there holds, for all $n \in \mathbb{N} \cup \{0\}$, $u_\lambda \leq u_n < u_\lambda^+ < 1$, a.e. $x \in \Omega$.*

Proof. We proceed as above. On the one hand, for $n = 0$, then $u_\lambda \leq u_0 < 1$. We further assume that, for a given $n \in \mathbb{N} \cup \{0\}$, there holds $u_\lambda \leq u_n < 1$, a.e. $x \in \Omega$. Then, the function $v_{n+1} = u_\lambda - u_{n+1}$ satisfies

$$v_{n+1} - \tau \Delta v_{n+1} = v_n + \frac{\lambda \tau f(x)}{(1-u_\lambda)^2} - \frac{\lambda \tau f(x)}{(1-u_n)^2} \leq 0 \tag{9.18}$$

and

$$v_{n+1} = 0 \quad \text{on} \quad \partial\Omega. \tag{9.19}$$

Multiplying (9.18) by v_{n+1}^+ and integrating over Ω and by parts, we obtain, owing to (9.19),

$$\|v_{n+1}^+\|^2 + \tau \|\nabla v_{n+1}^+\|^2 \leq 0, \tag{9.20}$$

which implies $v_{n+1} \leq 0$, i.e., $u_\lambda \leq u_{n+1}$, a.e. $x \in \Omega$. On the other hand, we already assumed that $u_\lambda \leq u_0 < u_\lambda^+ < 1$ and we further assume that, for a given $n \in \mathbb{N} \cup \{0\}$, there holds $u_\lambda \leq u_n < u_\lambda^+ < 1$, a.e. $x \in \Omega$. Then, the function $w_{n+1} = u_{n+1} - u_\lambda^+$ satisfies

$$w_{n+1} - \tau \Delta w_{n+1} = w_n + \frac{\lambda \tau f(x)}{(1-u_n)^2} - \frac{\lambda \tau f(x)}{(1-u_\lambda^+)^2} < 0 \tag{9.21}$$

and

$$w_{n+1} = 0 \quad \text{on} \quad \partial\Omega. \tag{9.22}$$

Multiplying (9.21) by w_{n+1}^+ and integrating over Ω and by parts, we obtain, owing to (9.22),

$$\|w_{n+1}^+\|^2 + \tau \|\nabla w_{n+1}^+\|^2 < 0, \tag{9.23}$$

which implies $w_{n+1} < 0$, i.e., $u_{n+1} < u_\lambda^+$, a.e. $x \in \Omega$. □

Remark 9.3.3. *Let us take u_0 such that $u_\lambda \leq u_0 < u_\lambda^+ < 1$. It was numerically verified that $u_\lambda \leq u_1 \leq u_0 < u_\lambda^+$. Assuming that, for a given $n \in \mathbb{N} \cup \{0\}$, $u_\lambda \leq u_n \leq u_{n-1} < u_\lambda^+$ and setting $v_{n+1} = u_{n+1} - u_n$, we deduce that*

$$v_{n+1} - \tau \Delta v_{n+1} = v_n + \frac{\lambda \tau f(x)}{(1-u_n)^2} - \frac{\lambda \tau f(x)}{(1-u_{n-1})^2} \leq 0 \tag{9.24}$$

and

$$v_{n+1} = 0 \quad \text{on} \quad \partial\Omega. \tag{9.25}$$

Multiplying (9.24) *by* v_{n+1}^+ *and integrating over* Ω *and by parts, we obtain, owing to* (9.25),

$$\|v_{n+1}^+\|^2 + \tau\|\nabla v_{n+1}^+\|^2 \leq 0, \tag{9.26}$$

whence $u_\lambda \leq u_{n+1} \leq u_n < u_\lambda^+$. *Therefore, for* $x \in \Omega$, *the sequence* $\{u_n(x)\}$ *is monotonously decreasing and bounded from below by* u_λ, *i.e., it converges as* $n \to +\infty$.

9.4 The implicit scheme

We consider in this section the implicit semi-discrete scheme : for $n \in \mathbb{N} \cup \{0\}$,

$$\begin{cases} u_{n+1} - \tau\Delta u_{n+1} = u_n + \dfrac{\lambda\tau f}{(1-u_{n+1})^2} \ \text{ in } \ \Omega, \\ u_{n+1} = 0 \ \text{ on } \ \partial\Omega, \end{cases} \tag{9.27}$$

where, again, $u_{n+1} \simeq u(t_{n+1}, x)$, $u_n \simeq u(t_n, x)$. We suppose that the assumptions on Ω, f, and (9.9)-(9.10) still hold.

Proposition 9.4.1. *For* $0 \leq u_n \leq u_\lambda < 1$, *a.e.* $x \in \Omega$, *problem* (9.27) *possesses at least one solution such that*

$$0 \leq u_{n+1} \leq u_\lambda < 1, \ \ a.e. \ \ x \in \Omega, \tag{9.28}$$

where u_λ *is the minimal solution to* (9.7).

Proof. It is obvious that 0 is a subsolution to problem (9.27). Furthermore, we note that

$$\begin{aligned} u_\lambda - \tau\Delta u_\lambda &= u_\lambda + \frac{\lambda\tau f}{(1-u_\lambda)^2} \\ &\geq u_n + \frac{\lambda\tau f}{(1-u_\lambda)^2}, \end{aligned}$$

so that u_λ is a supersolution to (9.27). The proof is completed. □

Proceeding as in the proof of Proposition 9.3.2 and setting $v_n = u_n - u_\lambda$, $v_{n+1} = u_{n+1} - u_\lambda$, we have

$$v_{n+1} - \tau\Delta v_{n+1} = v_n + \left[\frac{\lambda\tau f}{(1-u_\lambda)(1-u_{n+1})^2} + \frac{\lambda\tau f}{(1-u_\lambda)^2(1-u_{n+1})}\right] v_{n+1} \ \text{ in } \ \Omega, \tag{9.29}$$

$$v_{n+1} = 0 \ \text{ on } \ \partial\Omega. \tag{9.30}$$

Multiplying (9.29) by v_{n+1} and applying the Poincaré inequality, we obtain

$$\begin{aligned}\|v_{n+1}\|^2 + c_0\tau\|v_{n+1}\|^2 &\leq ((v_n, v_{n+1})) + \frac{2\lambda\tau}{(1-\overline{u})^3}\|v_{n+1}\|^2 \\ &\leq \|v_n\|\|v_{n+1}\| + \frac{2\lambda\tau}{(1-\overline{u})^3}\|v_{n+1}\|^2,\end{aligned}$$

whence

$$\left(1 + c_0\tau - \frac{2\lambda\tau}{(1-\overline{u})^3}\right)\|v_{n+1}\| \leq \|v_n\|. \tag{9.31}$$

This yields the following result.

Proposition 9.4.2. *We assume that,*

$$\lambda < \frac{1}{2}(1-\overline{u})^3 c_0. \tag{9.32}$$

Then, u_n converges to u_λ in $L^2(\Omega)$ as $n \to +\infty$.

Remark 9.4.1. *We again take $u_0 = 0$. Then, $u_1 \geq u_0$. Let us assume that, for a given $n \in \mathbb{N}$, $u_n \geq u_{n-1}$. Then, the function $v_{n+1} = u_{n+1} - u_n$ satisfies*

$$\begin{aligned}v_{n+1} - \tau\Delta v_{n+1} &= u_n - u_{n-1} + \frac{\lambda\tau f}{(1-u_{n+1})^2} - \frac{\lambda\tau f}{(1-u_n)^2} \\ &\geq \left(\frac{\lambda\tau f}{(1-u_{n+1})(1-u_n)^2} + \frac{\lambda\tau f}{(1-u_n)(1-u_{n+1})^2}\right)v_{n+1} \ \text{ in } \ \Omega\end{aligned} \tag{9.33}$$

and

$$v_{n+1} = 0 \ \text{ on } \ \partial\Omega.$$

Multiplying (9.33) by $-v_{n+1}^-$ and integrating over Ω and by parts, we find

$$\begin{aligned}\|v_{n+1}^-\|^2 + \tau\|\nabla v_{n+1}^-\|^2 &\leq \left(\frac{\lambda\tau f}{(1-u_{n+1})(1-u_n)^2} + \frac{\lambda\tau f}{(1-u_n)(1-u_{n+1})^2}\right)\|v_{n+1}^-\|^2 \\ &\leq \frac{2\lambda\tau}{(1-\overline{u})^3}\|v_{n+1}^-\|^2,\end{aligned}$$

whence

$$\left(1 + c_0\tau - \frac{2\lambda\tau}{(1-\overline{u})^3}\right)\|v_{n+1}^-\|^2 \leq 0. \tag{9.34}$$

Therefore, for a given λ, if $\tau \leq \tau_0$, where τ_0 is small enough so that

$$1 + c_0\tau_0 - \frac{2\lambda\tau_0}{(1-\overline{u})^3} > 0, \tag{9.35}$$

then $v_{n+1}^- = 0$ and thus $u_{n+1} \geq u_n$. It thus follows from Propersition 9.4.1 that u_n converges monotonically and pointwise.

Remark 9.4.2. *Multiplying (9.29) by $-\Delta v_{n+1}$ and integrating over Ω and by parts, we have*

$$\|\nabla v_{n+1}\|^2 + \tau\|\Delta v_{n+1}\|^2 \le \|\nabla v_n\|\|\nabla v_{n+1}\| + \frac{2\lambda\tau}{(1-\overline{u})^3}\|v_{n+1}\|\|\Delta v_{n+1}\|. \tag{9.36}$$

Then, since

$$\|\Delta v\|^2 \ge c_0\|\nabla v\|^2, \quad v \in H^2(\Omega)\cap H_0^1(\Omega),$$

applying the Cauchy-Schwarz inequality, we obtain

$$\|\nabla v_{n+1}\|^2 + c_0^{1/2}\tau\|\nabla v_{n+1}\|\|\Delta v_{n+1}\| \tag{9.37}$$

$$\le \|\nabla v_n\|\|\nabla v_{n+1}\| + \frac{2\lambda\tau}{c_0^{1/2}(1-\overline{u})^3}\|\nabla v_{n+1}\|\|\Delta v_{n+1}\|,$$

whence

$$\|\nabla v_{n+1}\| + \left(c_0^{1/2}\tau - \frac{2\lambda\tau}{c_0^{1/2}(1-\overline{u})^3}\right)\|\Delta v_{n+1}\| \le \|\nabla v_n\|.$$

Therefore,

$$(1 + c_0\tau - \frac{2\lambda\tau}{(1-\overline{u})^3})\|\nabla v_{n+1}\| \le \|\nabla v_n\|. \tag{9.38}$$

Finally, if

$$\lambda < \frac{1}{2}(1-\overline{u})^3 c_0,$$

or equivalently

$$\left(1 + c_0\tau - \frac{2\lambda\tau}{(1-\overline{u})^3}\right)^{-1} < 1,$$

then u_n converges to u_λ in $H_0^1(\Omega)$ as $n \to +\infty$. In particular, in one space dimension, u_n converges to u_λ in $C(\overline{\Omega})$ as $n \to +\infty$.

9.5 The fully discretized semi-implicit scheme

We only consider the one-dimensional problem in this section. We believe that similar results hold in two-dimensional space and will address this elsewhere.

Let $M > 0$ be an integer, $h = (b-a)/(M+1)$ denote the spatial mesh size, and $x_i = a + ih$, $i = 0, \cdots, M+1$. We consider the fully discretized semi-implicit scheme as follows : for $n \in \mathbb{N}\cup\{0\}$,

$$\begin{cases} \dfrac{u_i^{n+1} - u_i^n}{\tau} - \dfrac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{h^2} = \dfrac{\lambda f(x_i)}{(1-u_i^n)^2}, \ i = 1, \cdots, M; \\ u_0^{n+1} = u_{M+1}^{n+1} = 0, \end{cases} \tag{9.39}$$

where $u_i^n \approx u(t^n, x_i)$. Problem (9.39) can be rewritten equivalently as

$$(1 + 2\frac{\tau}{h^2})u_i^{n+1} - \frac{\tau}{h^2}u_{i+1}^{n+1} - \frac{\tau}{h^2}u_{i-1}^{n+1} = u_i^n + \frac{\lambda\tau f(x_i)}{(1-u_i^n)^2}. \tag{9.40}$$

We then rewrite (9.40) in vector form as

$$AU^{n+1} = F(U^n), \quad U^0 = 0, \tag{9.41}$$

where $U^n = \left(u_1^n, u_2^n, \cdots, u_M^n\right)^t$ and

$$A = \begin{pmatrix} 1+2\frac{\tau}{h^2} & -\frac{\tau}{h^2} & & & \\ -\frac{\tau}{h^2} & 1+2\frac{\tau}{h^2} & -\frac{\tau}{h^2} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{\tau}{h^2} & 1+2\frac{\tau}{h^2} & -\frac{\tau}{h^2} \\ & & & -\frac{\tau}{h^2} & 1+2\frac{\tau}{h^2} \end{pmatrix}, \quad F(U^n) = \begin{pmatrix} u_1^n + \frac{\lambda\tau f(x_1)}{(1-u_1^n)^2} \\ u_2^n + \frac{\lambda\tau f(x_2)}{(1-u_2^n)^2} \\ \vdots \\ u_M^n + \frac{\lambda\tau f(x_M)}{(1-u_M^n)^2} \end{pmatrix}.$$

We can rewrite (9.41) equivalently as

$$AU^{n+1} = U^n + G(U^n), \tag{9.42}$$

where

$$G(U^n) = \lambda\tau \begin{pmatrix} \frac{f(x_1)}{(1-u_1^n)^2} \\ \frac{f(x_2)}{(1-u_2^n)^2} \\ \vdots \\ \frac{f(x_M)}{(1-u_M^n)^2} \end{pmatrix}.$$

We note that

$$A = I + \frac{\tau}{h^2}B,$$

where

$$B = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}.$$

It is well known that A is positive definite, and thus invertible. Furthermore,

$$A = \left(1 + \frac{2\tau}{h^2}\right)\left(I - \frac{\tau/h^2}{1+2\tau/h^2}C\right),$$

where

$$C = \begin{pmatrix} 0 & 1 & & & \\ 1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & 1 \\ & & & 1 & 0 \end{pmatrix},$$

so that

$$\begin{aligned} A^{-1} &= \left(1 + \frac{2\tau}{h^2}\right)^{-1} \left(I - \frac{\tau/h^2}{1 + 2\tau/h^2} C\right)^{-1} \\ &= \left(1 + \frac{2\tau}{h^2}\right)^{-1} \sum_{j=0}^{+\infty} \left(\frac{\tau/h^2}{1 + 2\tau/h^2}\right)^j C^j. \end{aligned} \tag{9.43}$$

This yields that $A^{-1} \geq 0$.

We now consider the equation

$$AU^* = U^* + G(U^*), \tag{9.44}$$

which is the centered difference scheme of the steady state problem (9.7).

Equation (9.44) can be rewritten as

$$BU^* = \lambda h^2 \begin{pmatrix} \frac{f(x_1)}{(1-u_1^*)^2} \\ \frac{f(x_2)}{(1-u_2^*)^2} \\ \vdots \\ \frac{f(x_M)}{(1-u_M^*)^2} \end{pmatrix}. \tag{9.45}$$

The solvability of the above problem is given in the following theorem.

Theorem 9.5.1. *We assume that* $0 \leq \lambda \leq \dfrac{8(1-\delta)\delta^2}{(b-a)^2}$, *for some* $\delta \in (0, 1)$. *Then* (9.45) *possesses a solution* U^* *such that* $0 \leq U^* < E$, *where* $E = (1, 1, \cdots, 1)^t_{1\times M}$.

Proof. First note that B is invertible and (as above) $B^{-1} \geq 0$. We rewrite (9.45) in the form

$$U^* = \mathcal{H}(U^*), \tag{9.46}$$

where

$$\mathcal{H}(U^*) = \lambda h^2 B^{-1} \begin{pmatrix} \frac{f(x_1)}{(1-u_1^*)^2} \\ \frac{f(x_2)}{(1-u_2^*)^2} \\ \vdots \\ \frac{f(x_M)}{(1-u_M^*)^2} \end{pmatrix}.$$

We then consider the sequence

$$W^{k+1} = \mathcal{H}(W^k), \quad W^0 = 0. \tag{9.47}$$

Note that W^1 exists and, since $B^{-1} \geq 0$, $W^1 \geq 0$. Actually, as long as it exists,

$$W^k \geq 0.$$

Furthermore,

$$W^{k+2} - W^{k+1} = \lambda h^2 B^{-1} \begin{pmatrix} \frac{f(x_1)}{(1-w_1^{k+1})^2} - \frac{f(x_1)}{(1-w_1^k)^2} \\ \frac{f(x_2)}{(1-w_2^{k+1})^2} - \frac{f(x_2)}{(1-w_2^k)^2} \\ \vdots \\ \frac{f(x_M)}{(1-w_M^{k+1})^2} - \frac{f(x_M)}{(1-w_M^k)^2} \end{pmatrix}.$$

Therefore, since $W^1 \geq W^0$, we deduce that

$$W^{k+1} \geq W^k, \tag{9.48}$$

as long as this makes sense.

Now, recalling the assumptions on f, we have

$$\|\mathcal{H}(\chi)\|_\infty \leq \lambda h^2 \|B^{-1}\|_\infty \max_j \left(\frac{1}{(1-\chi_j)^2} \right). \tag{9.49}$$

We denote by D_M the determinant of B. It is easy to see that

$$D_M = 2D_{M-1} - D_{M-2}.$$

Therefore, since $D_2 = 3$ and $D_3 = 4$, it follows that $D_M = M + 1$. It thus follows from [12] (see also [74]) that B^{-1} is the factorizable matrix $\{M_{ij}\}$, $M_{ij} = a_i b_j$, $i \leq j$, $M_{ij} = M_{ji}$, where

$$a_i = i, \quad b_j = 1 - \frac{j}{M+1}.$$

We deduce from the structure of B^{-1} that

$$\|B^{-1}\|_\infty = \max \left(\sum_{j=1}^{M} b_j, (\sum_{i=1}^{M} a_i) b_M, \max_{i=2,\cdots,M-1} \left(b_i \sum_{j=1}^{i-1} a_j + a_i \sum_{j=i}^{M} b_j \right) \right),$$

that is to say

$$\|B^{-1}\|_\infty = \max \left(\frac{M}{2}, \max_{i=2,\cdots,M-1} \left(i \frac{M+1-i}{2} \right) \right).$$

Studying the variations of the function $x \mapsto x\dfrac{M+1-x}{2}$, it is easy to see that

$$\max_{i=2,\cdots,M-1}\left(i\frac{M+1-i}{2}\right) \leq \frac{(M+1)^2}{8},$$

so that (taking M large enough)

$$\|B^{-1}\|_\infty \leq \frac{(M+1)^2}{8} = \frac{(b-a)^2}{8h^2},$$

whence

$$\|\mathcal{H}(\chi)\|_\infty \leq \frac{(b-a)^2}{8}\lambda \max_i\left(\frac{1}{(1-\chi_i)^2}\right). \tag{9.50}$$

Let us now assume that

$$0 \leq \chi_i \leq 1-\delta,\ i = 1, \cdots, M,\ \delta \in (0,1).$$

Then, we have

$$\|\mathcal{H}(\chi)\|_\infty \leq \frac{(b-a)^2}{8\delta^2}\lambda.$$

Therefore, if

$$\lambda \leq \frac{8(1-\delta)\delta^2}{(b-a)^2},$$

then

$$\|\mathcal{H}(\chi)\|_\infty \leq 1-\delta.$$

This yields that $\{W^k\}$ exists for all $k \in \mathbb{N} \cup \{0\}$ and

$$0 \leq W^k \leq \begin{pmatrix} 1-\delta \\ 1-\delta \\ \vdots \\ 1-\delta \end{pmatrix}. \tag{9.51}$$

Hence, each component of $\{W^k\}$ is bounded and monotone increasing, and thus converges. This finishes the proof. □

Remark 9.5.1. *Note that, when δ goes to 0, i.e., the χ_i's approach 1, then λ goes to 0.*

We assume from now on that the assumptions of Theorem 9.5.1 hold, so that $0 \leq U^1 \leq U^*$. Let us assume that $0 \leq U^n \leq U^*$. Then, setting $V^n = U^n - U^*$, there holds

$$V^{n+1} = A^{-1}\left(V^n + G(U^n) - G(U^*)\right),$$

so that (since $A^{-1} \geq 0$)

$$U^{n+1} \leq U^*.$$

Furtheremore, since $A^{-1} \geq 0$, $U^{n+1} \geq 0$. It thus follows that $\{U^n\}$ is well-defined and

$$0 \leq U^n \leq U^*, \quad n \in \mathbb{N} \cup \{0\}.$$

We can also prove, proceeding as above, that

$$0 \leq U^n \leq U^{n+1}, \quad n \in \mathbb{N} \cup \{0\},$$

whence $\{U^n\}$ converges.

Remark 9.5.2. *We have, for all* $\{V^{n+1}\}$ *with* $v_0^{n+1} = 0$,

$$\begin{aligned}((AV^{n+1}, V^{n+1})) \quad &= (1 + \frac{2\tau}{h^2}) \sum_{j=1}^{M} (v_j^{n+1})^2 - \frac{2\tau}{h^2} \sum_{j=1}^{M-1} v_j^{n+1} v_{j+1}^{n+1} \\ &= (1 + \frac{\tau}{h^2}) \left((v_1^{n+1})^2 + (v_M^{n+1})^2\right) + \sum_{j=2}^{M-1} (v_j^{n+1}) + \frac{\tau}{h^2} \sum_{j=1}^{M-1} |v_j^{n+1} - v_{j+1}^{n+1}|^2 \\ &\geq \sum_{j=1}^{M} (v_j^{n+1})^2 + \frac{\tau}{h^2} \sum_{j=0}^{M-1} |v_j^{n+1} - v_{j+1}^{n+1}|^2,\end{aligned}$$

where $((\cdot,\cdot))$ *denotes the usual Euclidean scalar product, with associated norm* $\|\cdot\|$. *It follows from the discrete Poincaré inequality that*

$$\sum_{j=0}^{M-1} |v_j^{n+1} - v_{j+1}^{n+1}|^2 \geq \frac{2h^2}{(b-a)^2} \sum_{j=1}^{M} |v_j^{n+1}|^2,$$

which yields

$$((AV^{n+1}, V^{n+1})) \geq \left(1 + \frac{2\tau}{(b-a)^2}\right) \|V^{n+1}\|^2. \tag{9.52}$$

We now have

$$AV^{n+1} = V^n + G(U^n) - G(U^*),$$

so that, taking the scalar product with V^{n+1},

$$\left(1 + \frac{2\tau}{(b-a)^2}\right)\|V^{n+1}\|^2 \le \|V^n + G(U^n) - G(U^*)\|\|V^{n+1}\|.$$

Therefore,

$$\begin{aligned}
\|V^{n+1}\| &\le \left(1 + \frac{2\tau}{(b-a)^2}\right)^{-1} (\|V^n\| + \|G(U^n) - G(U^*)\|) \\
&\le \left(1 + \frac{2\tau}{(b-a)^2}\right)^{-1} \left(\|V^n\| + \lambda\tau \left(\sum_{j=1}^{M} \left(\frac{V_j^n(2 - u_j^n - u_j^*)}{(1-u_j^n)^2(1-u_j^*)^2}\right)^2\right)^{\frac{1}{2}}\right) \\
&\le \left(1 + \frac{2\tau}{(b-a)^2}\right)^{-1} \left(\|V^n\| + 2\lambda\tau \frac{1}{(1-\|U^*\|_\infty)^3}\|V^n\|\right) \\
&\le \left(1 + \frac{2\tau}{(b-a)^2}\right)^{-1} \left(1 + 2\lambda\tau \frac{1}{(1-\|U^*\|_\infty)^3}\right)\|V^n\|.
\end{aligned}$$

Therefore, if

$$\left(1 + \frac{2\tau}{(b-a)^2}\right)^{-1} \left(1 + 2\lambda\tau \frac{1}{(1-\|U^*\|_\infty)^3}\right) < 1,$$

i.e. $\lambda < (1 - \|U^\star\|_\infty)^3/(b-a)^2$, then $\{U^n\}$ converges to U^*.

Remark 9.5.3. *The above results, as well as those in the previous sections, can be improved by taking an assumption on f of the form*

$$0 \le f \le \overline{f},\ 0 \le \overline{f} \le 1.$$

In particular, in Theorem 9.5.1, we then have the more general assumption

$$0 \le \lambda \bar{f} \le \frac{8(1-\delta)\delta^2}{(b-a)^2},$$

which allows for a larger λ when $\bar{f}$ is small.

9.6 Numerical simulations

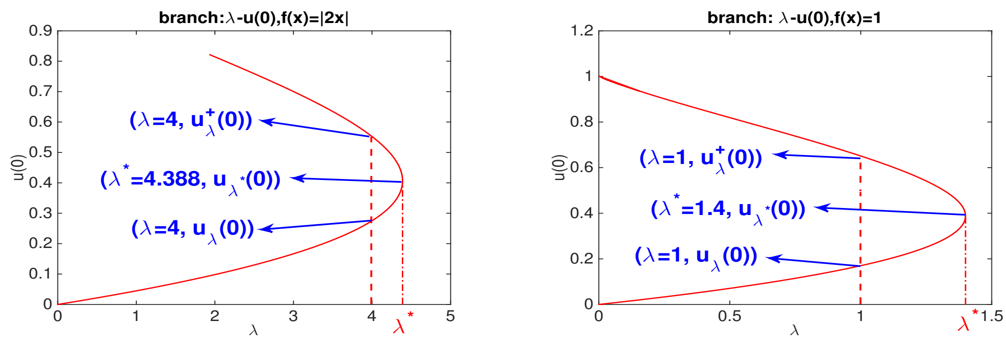
In this section, we give several numerical simulations which show the behavior of the solutions u corresponding to different schemes, different λ's and different initial conditions (see Proposition 9.3.3 and Remark 9.3.3). In particular, it is verified that, when $0 < \lambda \le \lambda^*$, the solutions to problem (9.5) tend to a stable solution u_λ as time grows. Furthermore, if $\lambda > \lambda^*$, one can observe the so-called touchdown phenomenon. The numerical simulations are performed with MATLAB.

9.6.1 The elliptic problem

In this subsection, we study the elliptic problem (9.7). Theoretically, it has been shown (see, e.g., [46]) that there exists λ^* depending on the domain Ω as well as the permittivity profile f such that when $\lambda \leq \lambda^*$, problem (9.7) possesses a unique minimal solution.

The 1D elliptic problem

Employing the continuation method described in Appendix A and considering the one-dimensional elliptic problem, we draw the branch of solutions $u(0)$ as a function of λ. Setting $\Omega = (-0.5, 0.5)$, $M = 199$ and $f(x) = |2x|$ or $f(x) \equiv 1$, we obtain Fig. 9.2



(a) (b)

FIGURE 9.2 – The branch of solutions $u(0)$ as a function of λ : (a) $f(x) = |2x|$; (b) $f(x) \equiv 1$.

in which we observe the existence of λ^* (when $f(x) = |2x|$, $\lambda^* \approx 4.388$, see Fig. 9.2(a), and, when $f \equiv 1$, $\lambda^* \approx 1.4$, see Fig. 9.2(b)) and that, when $\lambda < \lambda^*$ but is close to λ^*, the branches display two solutions $u_\lambda(0)$ and $u_\lambda^+(0)$. The results are consistent with [46].

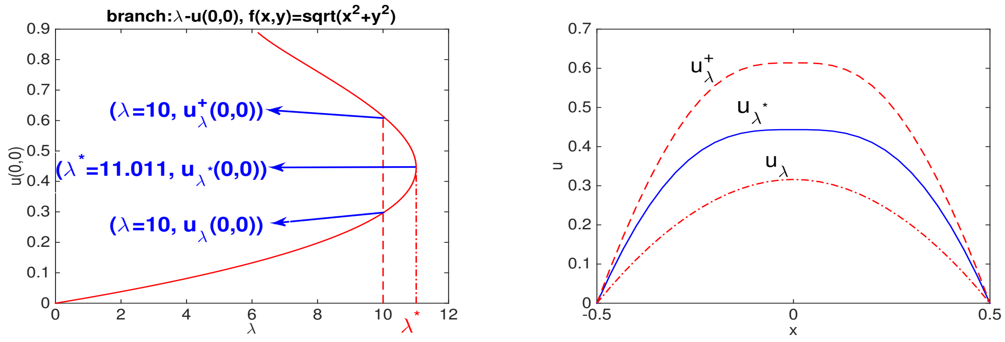
The 2D elliptic problem

As far as the 2D elliptic problem is concerned, applying the 5-point centered difference to approximate the Laplace operator, we have the discrete scheme :

$$\begin{cases} -4u_{i,j} + u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} + \dfrac{\lambda h^2 f(x_i, y_j)}{(1-u_{i,j})^2} = 0, \; i, \; j = 1, \cdots, M, \\ u_{0,j} = u_{M+1,j} = u_{i,0} = u_{i,M+1} = 0, \; i, \; j = 0, \cdots, M+1, \end{cases} \tag{9.53}$$

where $h = 1/(M+1)$ denotes the spatial mesh size of the computational domain $\Omega = (-0.5, 0.5) \times (-0.5, 0.5)$ and $u_{i,j} \simeq u(x_i, y_j)$, with $(x_i, y_j) = (-0.5 + ih, -0.5 + jh)$, $i, j =$

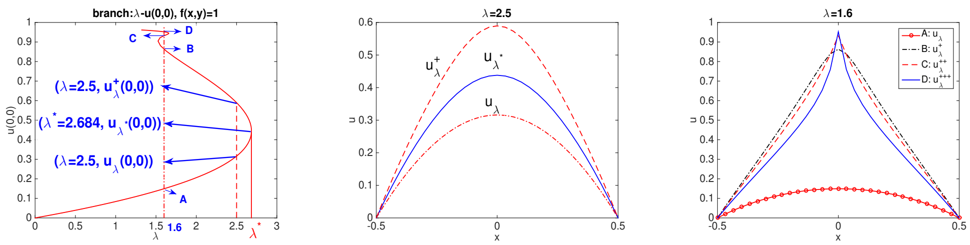
$0, \cdots, M+1$. Similarly, we display the branch of solutions $u(0,0)$ as a function of λ in Fig. 9.3(a) for $f(x,y) = \sqrt{x^2+y^2}$ and in Fig. 9.4(a) for $f(x,y) \equiv 1$; here $M = 29$. We



(a) (b)

FIGURE 9.3 – The branch of solutions $u(0,0)$ as a function of λ : (a) $f(x,y) = \sqrt{x^2+y^2}$; (b) $\lambda = 10$, u_λ, u_{λ^*}, and u_λ^+.

observe in Fig. 9.3(a) and Fig. 9.4(a) that there exists a maximal value of λ, namely, $\lambda^* \approx 11.011$ when $f(x,y) = \sqrt{x^2+y^2}$ and $\lambda^* \approx 2.684$ when $f(x,y) \equiv 1$, such that, if $0 < \lambda \leq \lambda^*$, problem (9.7) possesses at least one solution, and, if $\lambda > \lambda^*$, there does not exist a solution to the elliptic problem. Simultaneously, we observe that, when λ is less than but is close to λ^*, there are two values of $u(0,0)$ which are denoted by $u_\lambda(0,0)$ and $u_\lambda^+(0,0)$, as illustrated in Fig. 9.3(a) for $\lambda = 10$ and in Fig. 9.4(a) for $\lambda = 2.5$. In Fig. 9.3(b) (resp. Fig. 9.4(b)), we display the two corresponding solutions u_λ, u_λ^+ with $\lambda = 10$ (resp. $\lambda = 2.5$) and u_{λ^*}. Furthermore, Fig. 9.4(c) shows four solutions to problem (9.7) with $\lambda = 1.6$ which become sharper and sharper as the computation goes on. In the two dimensional simulations, here and below, otherwise specified, the solutions correspond to the section $y = 0$.



(a) (b) (c)

FIGURE 9.4 – The branch of solutions $u(0,0)$ as a function of λ : (a) $f(x,y) \equiv 1$; (b) $\lambda = 2.5$, u_λ, u_{λ^*} and u_λ^+ ; (c) $\lambda = 1.6$, four corresponding solutions.

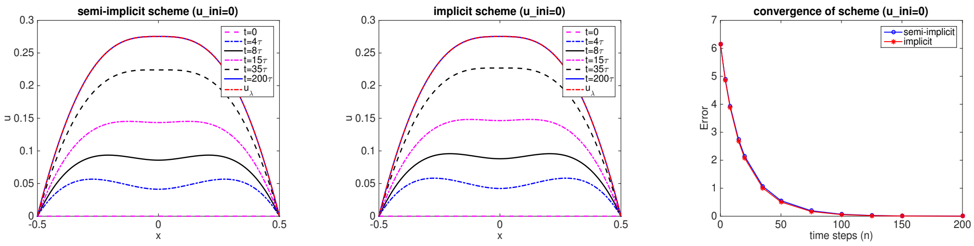
The branches and solutions for the one- and two-dimensional elliptic problems are helpful in view of the study of the parabolic problems.

9.6.2 The parabolic problem

We set $t^n = n\tau$, $n = 0, \cdots, K$, and write the time steps as superscripts and the spatial nodes as subscripts.

The 1D problem

Setting $\Omega = (-0.5, 0.5)$, we display in Fig. 9.5 the one-dimensional results for problem (9.5) applying both the semi-implicit and implicit schemes when $\lambda = 4.0$, $f(x) = |2x|$, $M = 199$ and $u\_ini = 0$; these are consistent with the theoretical results.



(a) (b) (c)

FIGURE 9.5 – 1D, τ=0.01. (a) Semi-implicit scheme ; (b) Implicit scheme ; (c) Convergence : $error = \|u^n - u_\lambda\|$.

Moreover, the results for the semi-implicit scheme for the initial condition

$$\text{pointwise\_ini :} \quad u\_ini\_pw = \frac{9}{10}u_\lambda^+ + \frac{1}{10}u_\lambda \tag{9.54}$$

which is larger than u_λ and less than but close to u_λ^+ show that the solution decreases and converges to u_λ (see Fig. 9.6(a)). In Fig. 9.6(b), the solution for the nonsymmetric initial condition

$$u\_ini\_nonsym = 4(x + 0.33)^2(x + 0.5)^2|x - 0.5|, \quad x \in [-0.5, 0.5], \tag{9.55}$$

also converges to u_λ. However, for $\lambda = 4.45 > \lambda^*$ and a smaller time step $\tau = 0.001$, we observe in Fig. 9.6(c) that, after 2654 steps, there does not exist a stable solution to the parabolic problem. We have similar results when applying the implicit scheme ; these are not displayed here.

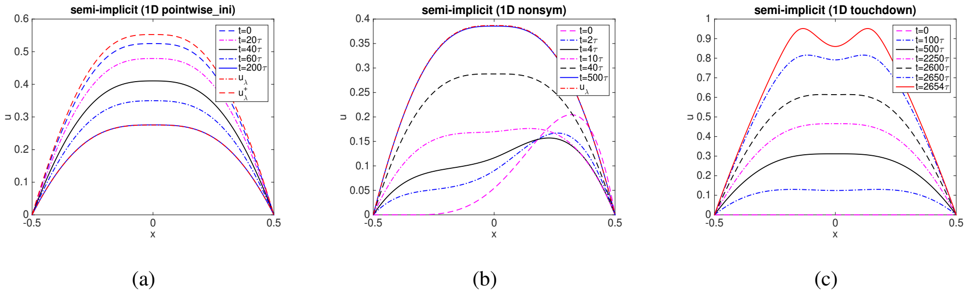


FIGURE 9.6 – 1D, $M = 199$, $f(x) = |2x|$. (a) $\tau = 0.01$, $\lambda = 4.0$, u_ini =pointwise_ini ; (b) $\tau = 0.01$, $\lambda = 4.0$, u_ini is nonsymmetric ; (c) touchdown phenomenon : λ=4.45, τ=0.001.

The 2D problem

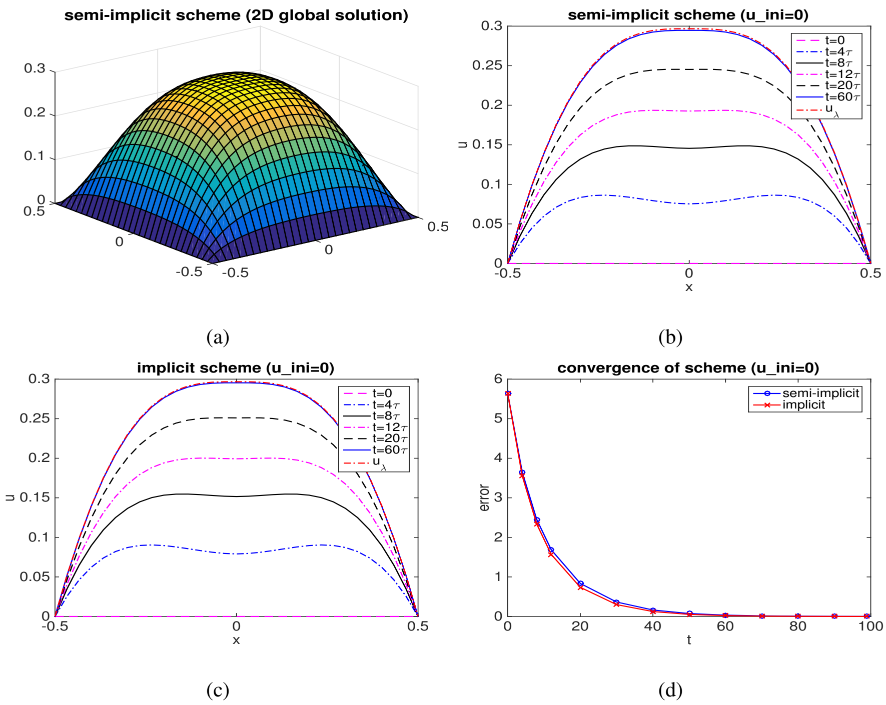


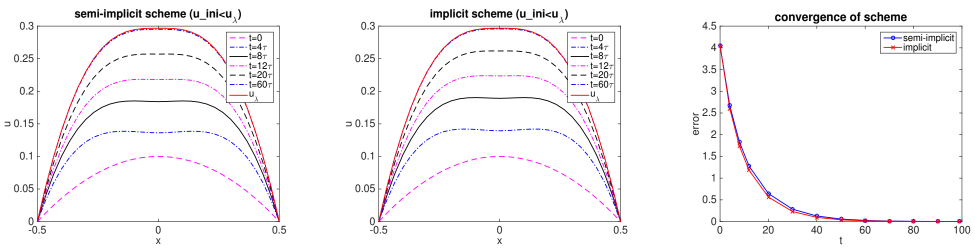
FIGURE 9.7 – 2D, λ=10.0, $f(x, y) = \sqrt{x^2 + y^2}$, τ=0.01, $M = 29$. (a) The global solution when $t = 100\tau$; (b) Semi-implicit scheme ; (c) Implicit scheme ; (d) Convergence.

Applying the centered scheme for the spatial discretization, we have the fully discrete semi-implicit scheme

$$(h^2 - 4\tau)u_{i,j}^{n+1} - \tau u_{i-1,j}^{n+1} - \tau u_{i+1,j}^{n+1} - \tau u_{i,j-1}^{n+1} - \tau u_{i,j+1}^{n+1} = h^2 u_{i,j}^n + \frac{\lambda\tau h^2 f(x_i, y_j)}{(1 - u_{i,j}^n)^2}, \qquad (9.56)$$

with i, $j = 1, \cdots, M$, $u^n_{0,j} = u^n_{M+1,j} = u^n_{i,0} = u^n_{i,M+1} = 0$ (i, $j = 0, \cdots, M+1$), and $n = 0$, $\cdots$, K. Then, one can easily get the two-dimensional fully-discrete implicit scheme, keeping the same notation and boundary conditions. Here, again, $\Omega = (-0.5, 0.5) \times (-0.5, 0.5)$.

In Fig. 9.7, we illustrate the two-dimensional results for $\lambda = 10.0$, $f(x, y) = \sqrt{x^2 + y^2}$ and $u\_ini = 0$, using both the semi-implicit and implicit schemes, as well as the corresponding convergence. We observe that, with each scheme, the solution increases and pointwise converges to u_λ.



(a) (b) (c)

FIGURE 9.8 – 2D, λ=10.0, $f(x, y) = \sqrt{x^2 + y^2}$, τ=0.01, $M = 29$. (a) Semi-implicit scheme ; (b) Implicit scheme ; (c) Convergence.

As shown in Fig. 9.8, when the initial value u_ini is less than u_λ (more precisely, we apply the cubic Lagrange polynomial on five points, (-0.5, -0.5, 0), (-0.5, 0.5, 0), (0, 0, 0.1), (0.5, -0.5, 0) and (0.5, 0.5, 0), to interpolate the initial value u_ini), the solutions corresponding to the semi-implicit and implicit schemes both increase and converge to u_λ.

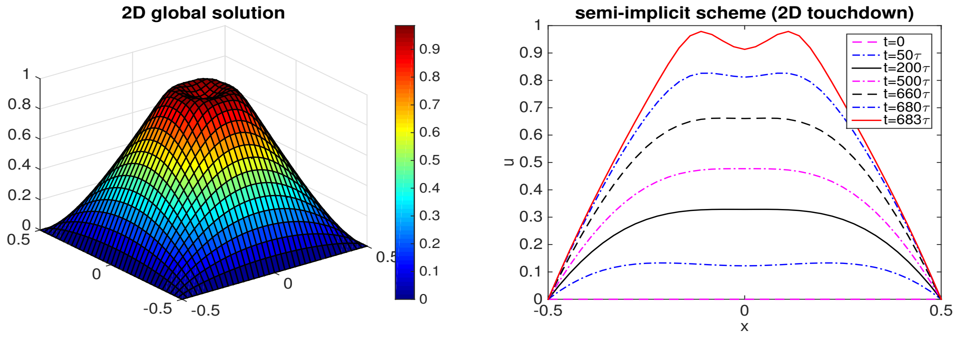
Finally, setting $\tau = 0.001$, $\lambda = 11.5$ (which is larger than λ^*) and $M = 35$, the touchdown phenomenon can be observed (see Fig. 9.9).

9.7 The continuation method

In this appendix, we explain how to compute the upper bound on λ (namely, the pull-in voltage λ^*) by applying a continuation method (see [5]) which we describe for the two-dimensional problem. The elliptic system (9.53) can be rewritten as

$$H(w) = 0, \tag{9.57}$$

where $w = (\mathbf{U}\ \lambda)^t$ and $\mathbf{U} = (u_{1,1}, \cdots, u_{M,1}, \cdots, u_{1,M}, \cdots, u_{M,M})$ is the reordered row vector of the solution to the elliptic problem (9.53). Let $H'(u)$ denote the Jacobian of $H(u)$ and $t(A)$ denote the tangent vector induced by A, which is defined by



(a) (b)

FIGURE 9.9 – 2D, $f(x, y) = \sqrt{x^2 + y^2}$, touchdown phenomenon. (a) Global solution when $t = 683\tau$; (b) Section $y = 0$.

Definition 9.7.1. Let A be an $\overline{M} \times (\overline{M} + 1)$ matrix with maximal rank. The unique vector $t(A) \in \mathbb{R}^{\overline{M}+1}$ satisfying the conditions

$$At = 0, \ \|t\| = 1, \ det\begin{pmatrix} A \\ t^* \end{pmatrix} > 0, \tag{9.58}$$

is called the tangent vector induced by A, where $(\cdot)^*$ denotes the Hermitian transpose.

Here and below, $\overline{M} = M^2$.

We then use an approximate Euler predictor and Newton-type iterations as corrector steps, described in the following algorithm, see [5].

Algorithm 1 Continuation Method

Input $Npas$, ϵ and w such that $H(w) = 0$
for $n = 1, Npas$ **do**
  Estimate $A = H'(w)$
  Compute A^+ and the tangent vector $t(A)$
  $w := w + \epsilon t(A)$ % prediction
  while error larger than tolerance and Newton's iteration step is bounded **do**
    $w := w - A^+ H(w)$ % corrections
  end while
end for

In this algorithm, A^+ denotes the Moore–Penrose inverse of A and ϵ stands for the current step size. We refer the readers to [14] and [113] for Newton's method based on the Moore–Penrose inverse and [6] for a convergence result which ensures that the above algorithm is applicable and effective under reasonable assumptions. To compute

A^+ and $t(A)$, we use a QR factorization (see [5] for details), that is to say, A being a maximal rank $\overline{M} \times (\overline{M} + 1)$ matrix and A^* representing its conjugate transpose, we have

$$A^+ = A^*(AA^*)^{-1} = Q \begin{pmatrix} (R^*)^{-1} \\ 0^* \end{pmatrix}, \qquad (9.59)$$

with the QR factorization, $A^* = Q \begin{pmatrix} R \\ 0^* \end{pmatrix}$, where Q is an $(\overline{M}+1)\times(\overline{M}+1)$ orthogonal matrix and R is a nonsingular $\overline{M} \times \overline{M}$ upper triangular matrix. Then, we compute $t(A) = \sigma q$, where q denotes the last column of Q and, in order to satisfy the orientation which has been defined in [5](2.5), we can choose $\sigma = \text{sign}(\det Q \det R)$.

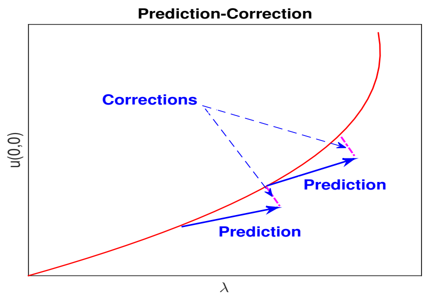


FIGURE 9.10 – The main idea of the continuation method.

The main idea of the continuation method is displayed in Fig. 9.10, using a rough prediction and several steps of corrections.

Chapitre 10

Conclusion générale et perspectives

We introduced and studied several nonlinear partial differential equations associated to mathematical modeling of phase separation and micro-electromechanical system (MEMS). For the phase separation, we introduced several models : the higher-order models with regular potential, the higher-order Allen-Cahn model with logarithmic potential, the higher-order anisotropic models, the higher-order generalized Cahn-Hilliard equation and the higher-order anisotropic model endowed with an inertial term, namely, the hyperbolic relaxation. In particular, we obtained the well-posedness results for each model and the existence of global attractors, which are essential in the analysis of asymptotic behavior. For the micro-electromechanical system, we studied a model which describes an idealized MEMS capacitor and contains singularity. We conclude our achievement below :

- In the study of the higher-order models with regular potential, we mainly considered the higher-order Allen-Cahn and Cahn-Hilliard equations endowed with Dirichlet boundary condition. In particular, for both of the equations, regularity results have been established, moreover dissipative semigroups and the existence of global attractors. We also gave the main idea to study the higher-order Cahn-Hilliard equation endowed with Neumann boundary condition which leads to the conservation of mass.

- We studied the well-posedness results for the higher-order Allen-Cahn models with logarithmic potential, however not in a classical way, but in a variational sense which was introduced in [104]. By deriving uniform (with respect to N) a priori estimates on the solution u^N to the approximated problems and passing to the limit $N \to \infty$, we proved the existence and uniqueness of the variational solution, as well as the dissipative semigroup and the existence of global attractor.

- We then built the higher-order anisotropic models in phase separation to describe explicitly the anisotropic phenomenon based on the work of G. Caginalp and E. Esenturk in [23]. Both for the higher-order anisotropic Allen-Cahn and Cahn-Hilliard equations with regular potential and Dirichlet/periodic boundary condition, we derived the a priori estimates and constructed dissipative semigroups, moreover obtained the existence of global attractors. Furthermore, we also gave numerical simulations to show the anisotropic effects intuitively.

- We considered other phenomenon than phase separation by studying the higher-order generalized Cahn-Hilliard equations, which have applications in biology, image processing, etc. The a priori estimates have been derived, as well as the regularity results. We further obtained the dissipative semigroup and the existence of the global attractor with finite dimension. Moreover, numerical simulations in 2D for the Cahn-Hilliard-Oono equation, phase field crystal equation and the equation which is modeling tumor proliferation growth, have illustrated the anisotropy effects.

- An inertial term, i.e., the second order derivative of u with respect to time t, has been added to the higher-order Cahn-Hilliard equation for the purpose of incorporating both fast elastic relaxation and slower mass diffusion. We studied the well-posedness of such a model, in particular, the regularity results, the dissipative semigroup and the existence of global attractor. In addition, numerical scheme, based on the finite element/spectral method in space and second order stable scheme in time, for solving the modified higher-order generalized (in the sense that an additional term γu has been added to the equation) Cahn-Hilliard equation has been developed. Furthermore,the energy stability results for the numerical scheme have been derived, as well as the existence and uniqueness of the numerical solution, both for semi-discrete and fully discrete scheme. Moreover, the numerical simulations have been illustrated to support the numerical analysis and show anisotropic effects.

- The last model describes the elastic and electrostatic effects in an idealized MEMS capacitor. Both for semi-implicit and implicit semi-discrete schemes, we proved that, under proper assumptions, the solutions are monotonically and pointwise convergent to the steady state, which is actually the minimal solution to the corresponding elliptic partial differential equation. Moreover, the fully discretized semi-implicit scheme was studied in 1D and numerical simulations were illustrated to show the behavior of the solutions which support the theoretical analysis both in 1D and 2D.

Based on what we have done, we provide here some perspectives on these models.

- For the phase separation models, considering the consistence between the mathematical modeling and the physical phenomena, one can further take long-ranged interactions into account. In this situation, the governing equation may turn out to be nonlocal and the study of nonlocal partial differential equations may be involved in. We refer the reader to [25, 61, 64, 65, 66] several literatures on nonlocal phase separation models, which may help to build nonlocal anisotropic models in phase separation.

- For the higher-order models in phase separation, one can further construct the exponential attractors which are more robust, i.e., not sensitive to perturbation, and can attract the trajectory much more faster.

- We note that for the higher-order models with logarithmic nonlinear term in Chapter 4, the results are associated to Allen-Cahn equation, so one can consider the well-posedness properties for higher-order Cahn-Hilliard equation with logarithmic nonlinear term. As what mentioned in Chapter 4, when $k \geq 2$, the question that whether a variational solution is a classical (variational) solution or not is an open issue.

- And for the higher-order models (when $k \geq 2$), both Allen-Cahn and Cahn-Hilliard, one can try to analysis whether the global attractors have finite dimension or not. Moreover, one can further develop more efficient and higher-performance numerical methods to simulate the higher-order models.

- Finally, as the MEMS machineries are essential components in many commercial devices, it is necessary to study more realistic models, which may contain fourth order derivatives, or non-local terms. And since the pull-in voltage is an important factor, not only in mathematical analysis, but also in the real MEMS machineries, it is also worth spending efforts on estimating and calculating the pull-in voltage, as well as the quenching time and quenching set.

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Résumé : Cette thèse est consacré à l'étude théorique et numérique de plusieurs équations aux dérivées partielles non linéaires qui apparaissent dans la modélisation de la séparation de phase et des micro-systèmes électro-mécaniques (MSEM). Dans la première partie, nous étudions des modèles d'ordre élevé en séparation de phase pour lesquels nous obtenons le caractère bien posé et la dissipativité, ainsi que l'existence de l'attracteur global et, dans certains cas, des simulations numériques. De manière plus précise, nous considérons dans cette première partie des modèles de type Allen-Cahn et Cahn-Hilliard d'ordre élevé avec un potentiel régulier et des modèles de type Allen-Cahn d'ordre élevé avec un potentiel logarithmique. En outre, nous étudions des modèles anisotropes d'ordre élevé et des généralisations d'ordre élevé de l'équation de Cahn-Hilliard avec des applications en biologie, traitement d'images, etc. Nous étudions également la relaxation hyperbolique d'équations de Cahn-Hilliard anisotropes d'ordre élevé. Dans la seconde partie, nous proposons des schémas semi-discrets semi-implicites et implicites et totalement discrétisés afin de résoudre l'équation aux dérivées partielles non linéaire décrivant à la fois les effets élastiques et électrostatiques de condensateurs MSEM. Nous faisons une analyse théorique de ces schémas et de la convergence sous certaines conditions. De plus, plusieurs simulations numériques illustrent et appuient les résultats théoriques.

Mots clés : séparation de phase, équations d'Allen-Cahn et Cahn-Hilliard, anisotropie, modèles d'ordre élevé, caractère bien posé, attracteur global, micro-systèmes électro-mécaniques (MSEM), schémas semi-implicites et implicites, simulations numériques

Abstract : This thesis is devoted to the theoretical and numerical study of several nonlinear partial differential equations, which occur in the mathematical modeling of phase separation and micro-electromechanical system (MEMS). In the first part, we study higher-order phase separation models for which we obtain well-posedness and dissipativity results, together with the existence of global attractors and, in certain cases, numerical simulations. More precisely, we consider in this first part higher-order Allen-Cahn and Cahn-Hilliard equations with a regular potential and higher-order Allen-Cahn equation with a logarithmic potential. Moreover, we study higher-order anisotropic models and higher-order generalized Cahn-Hilliard equations, which have applications in biology, image processing, etc. We also consider the hyperbolic relaxation of higher-order anisotropic Cahn-Hilliard equations. In the second part, we develop semi-implicit and implicit semi-discrete, as well as fully discrete, schemes for solving the nonlinear partial differential equation, which describes both the elastic and electrostatic effects in an idealized MEMS capacitor. We analyze theoretically the stability of these schemes and the convergence under certain assumptions. Furthermore, several numerical simulations illustrate and support the theoretical results.

Keywords : phase separation, Allen-Cahn and Cahn-Hilliard equations, higher-order models, anisotropy, well-posedness, global attractor, micro-electromechanical system (MEMS), semi-implicit and implicit schemes, numerical simulations