Finite Element Methods for a class of Stochastic PDEs from phase transitions

Dimitra Antonopoulou

University of Athens, Greece

HELLENIC REPUBLIC
National and Kapodistrian University of Athens
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Phase separation

- In a vessel $\mathcal{D}$ a two-phases mixture is forced to homogenization,

$\hookrightarrow$ reducing the temperature the binary alloy starts to separate rapidly,

$\hookrightarrow$ thin transition layers of width an order of ε are formed and the evolution slows down (ε small enough).

$\hookrightarrow$ ε-dependent spdes for the concentration.

$\hookrightarrow$ sharp interface limit as $\varepsilon \to 0$.

Some essentials for the numerical approximation:

- underlying existence-regularity theory,
- noise definition and its numerical implementation,
- sufficient theory (at least numerical convergence) so that the applied scheme will lead somewhere we provisionally trust.

A class of ε-dependent spdes

$$
\begin{aligned}
& u_t = -\delta(\varepsilon)\,\Delta\big(\varepsilon^2\Delta u - f(u)\big) + \mu(\varepsilon)(\varepsilon^2\Delta u - f(u)) + \mathcal{F}(u, x, t; \varepsilon), \\
& \qquad x \in \mathcal{D}, \quad t > 0, \\
& u(x, 0) = u_0(x; \varepsilon), \; x \in \mathcal{D} \; \text{ (possibly layered)}, \\
& \text{and b.c. on } \; \partial\mathcal{D},
\end{aligned}
\tag{1}
$$

for u the concentration of one of the components of the binary alloy, and

$$0 < \varepsilon \ll 1.$$

$f(u) = F'(u)$, is the derivative of a double equal-well potential, typical example

$$f(u) = u^3 - u, \quad F(u) := \frac{1}{4}(u^2 - 1)^2,$$

and the ε-dependent weights satisfy

$$\delta(\varepsilon) \geq 0, \quad \mu(\varepsilon) \geq 0.$$

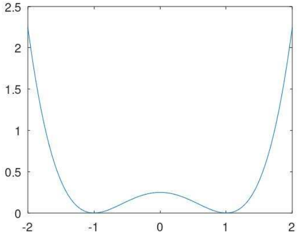

Figure: The potential F

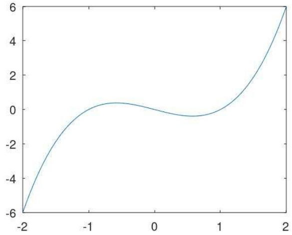

Figure: The nonlinearity $f = F'$

Main cases

- $\delta(\varepsilon) > 0, \quad \mu(\varepsilon) = 0$ Cahn-Hilliard equation (Model B).
- $\delta(\varepsilon) = 0, \quad \mu(\varepsilon) > 0$ Allen-Cahn equation (Model A).
- $\delta(\varepsilon) > 0, \quad \mu(\varepsilon) > 0$ 'competition' of Cahn-Hilliard and Allen-Cahn operators (Model B/A).

$$\mathcal{F} \equiv 0 \text{ the homogeneous problem,}$$

$$\mathcal{F} \neq 0 = \begin{cases} \text{smooth stochastic perturbation,} \\ \text{non smooth stochastic perturbation.} \end{cases}$$

Questions: Existence, regularity, transitions profile, sharp interface limit as $\varepsilon \to 0$, numerical approximation.

Numerical Difficulty: $\varepsilon \ll 1$ in physical scale

$\hookrightarrow$ severe rounding errors.

1. The stochastic Cahn-Hilliard equation

$$
\begin{aligned}
&u_t = \Delta(-\varepsilon\Delta u + \varepsilon^{-1} f(u)) + \varepsilon^{\gamma}\dot{W}(x,t), \quad x \text{ in } \mathcal{D}, \\
&\frac{\partial u}{\partial \nu} = \frac{\partial \Delta u}{\partial \nu} = 0 \text{ on } \partial\mathcal{D} \quad \text{(Neumann b.c.)}
\end{aligned} \tag{2}
$$

Here

$$\delta(\varepsilon) := \varepsilon^{-1}, \quad \text{and} \quad \mu(\varepsilon) \equiv 0,$$

with

$$\mathcal{F}(u,x,t;\varepsilon) := \mathcal{F}(x,t;\varepsilon) = \varepsilon^{\gamma}\dot{W} = \varepsilon^{\gamma}\sum_{i=1}^{\infty} a_i\dot{\beta}_i(t)e_i(x),$$

for β_i stochastically independent brownian motions.

Let the chemical potential $v = v(\varepsilon)$ and derive the stochastic system:

$$
\begin{aligned}
&u_t = -\Delta v + \varepsilon^{\gamma}\dot{W} \\
&v = -\varepsilon^{-1} f(u) + \varepsilon\Delta u.
\end{aligned} \tag{3}
$$

In $d = 2, 3$, by applying a boot-strap stochastic argument, in A, Blömker, Karali, A.I.H.P. Prob.-Stat, 2018, we proved the next theorem for the Stochastic sharp interface limit.

Theorem: Let $\gamma > \gamma_0 > 1$. The limit of v as $\varepsilon \to 0^+$ solves on $[0, T]$ the deterministic Hele-Shaw problem

$$\Delta v = 0 \ \text{ in } \mathcal{D}\backslash\Gamma(t), \quad t > 0$$
$$\partial_n v = 0 \ \text{ on } \partial\mathcal{D}$$
$$v = \lambda H \ \text{ on } \Gamma(t)$$
$$V = \frac{1}{2}(\partial_n v^+ - \partial_n v^-) \ \text{ on } \Gamma(t)$$
$$\Gamma(0) = \Gamma_0,$$

where H is the mean curvature, and V the velocity of the surface $\Gamma(t)$.

Remarks:

- The above was derived when

$$\int_{\mathcal{D}} W(x,t)dx = 0 \ \text{ (mass conservation).}$$

- This problem coincides to the limit problem of deterministic C-H of Alikakos, Bates, Chen, ARMA 1994.

- When γ smaller formal asymptotics indicated convergence but with

$$v = \lambda H + W \ \text{ on } \Gamma(t).$$

Numerical approximation

In (2), we consider one mode in the noise series, i.e.,

$$\mathcal{F}(u,x,t;\varepsilon) := \mathcal{F}(x,t;\varepsilon) = \varepsilon^\gamma \dot{W} = \varepsilon^\gamma \sigma(x)\dot{\beta}(t).$$

The non-smooth in time noise is approximated, by using the increments of the brownian motion $\beta(t) \equiv N(0,t)$, as follows

$$\dot{\beta}(t) \cong \text{rate of change} = \frac{\beta(t^i) - \beta(t^{i-1})}{t^i - t^{i-1}} \sim k^{-1/2} N(0,1) = N(0,k^{-1}).$$

In A, Banas, Nürnberg, Prohl, Numer. Math. 2021, we defined the next semi-discretization in time:

Let $0 = t^0 < t^1 < \cdots < t^J = T$ a uniform partition, with step-size $k = \frac{T}{J}$. For $1 \le j \le J$, let

$$\Delta_j \beta := \beta(t^j) - \beta(t^{j-1}) \sim N(0,k),$$

the corresponding brownian increments.

We seek in $H^1(\mathcal{D})$ approximations of the solution u and of the chemical potential v

$$U^j(x) \simeq u(x, t^j), \quad V^j(x) \simeq v(x, t^j)$$

satisfying the discrete weak formulation of the system (3)

$$(U^j - U^{j-1}, \varphi) + k(\nabla W^j, \nabla\varphi) = \varepsilon^\gamma (\sigma, \varphi) \Delta_j \beta \quad \forall\, \varphi \in H^1(\mathcal{D}),$$

$$\varepsilon(\nabla U^j, \nabla\psi) + \frac{1}{\varepsilon}(f(U^j), \psi) = (V^j, \psi) \quad \forall\, \psi \in H^1(\mathcal{D}),$$

$$U^0(x) = u_0(x;\varepsilon) \in H^1(\mathcal{D}).$$

Remark: The scheme without noise was introduced and analyzed in Feng, Prohl Numer. Math. 2004.

In dimensions $d = 2$,
- by a discrete boot-strap argument, we estimated the error in expectation in H^{-1} for $k < \varepsilon^\ell$ for some $\ell > 0$ sufficiently large,

- the convergence to the Hele-Shaw was experimentally investigated for a fully discrete space-time scheme.

Remark: This result was derived by energy estimates, i.e., up to $H^1(\mathcal{D})$ regularity used for the stochastic C-H.

But how smooth the solution can really be?

Let us consider the more general case of multiplicative noise, where

$$\mathcal{F}(u,x,t;\varepsilon) := \sigma(u)\varepsilon^{\gamma}\dot{W} = \sigma(u)\varepsilon^{\gamma}\sum_{i=1}^{\infty} a_i\dot{\beta}_i(t)e_i(x).$$

In A Nonlinearity, 2023, the next result was derived.

Theorem: Let $\|u_0\|_{H^2(\mathcal{D})}$ have bounded p-moments, $d = 1, 2, 3$, and

$$|\sigma(x)| + |\sigma'(x)| + |\sigma''(x)| \leq c, \ \ \forall\, x \in \mathbb{R}, \ \text{ and } \ \sum_{i=1}^{\infty} a_i^2 \|e_i\|^2_{H^4(\mathcal{D})} < \infty.$$

Then for any $T > 0$, and some $k = k(p) > 0$, and for any $p \geq 1$

$$\mathbb{E}\Big(\sup_{0\leq t\leq T} \|u\|^{2p}_{L^\infty(\mathcal{D})}\Big) \leq c\mathbb{E}\Big(\sup_{0\leq t\leq T} \|u\|^{2p}_{H^2(\mathcal{D})}\Big) \leq c\varepsilon^{-k(p)}.$$

Moreover, if $\partial\mathcal{D}$ is C^1, for

$$\|u(\cdot,t)\|_{C^{0,\theta}(\overline{\mathcal{D}})} := \sup_{x\neq y\in\overline{\mathcal{D}}} \frac{|u(x,t)-u(y,t)|}{|x-y|^\theta},$$

it follows for any $0<\theta<1$ for $d=2$, and for $\theta=\frac{1}{2}$ when $d=3$

$$\mathbb{E}\Big(\sup_{0\leq t\leq T}\|u(\cdot,t)\|^{2p}_{C^{0,\theta}(\overline{\mathcal{D}})}\Big) \leq c\mathbb{E}\Big(\sup_{0\leq t\leq T}\|u(\cdot,t)\|^{2p}_{H^2(\mathcal{D})}\Big) \leq c\varepsilon^{-k(p)}.$$

Additionally, if the initial data are layered, then $u\to\pm1$ a.s. In particular, for any $\gamma>0$ (of noise), and any $0<\alpha<\min\{\gamma,1/2\}$

$$\lim_{\varepsilon\to0^+} P(\||u|-1\|_{L^2(\mathcal{D})}\geq\varepsilon^\alpha)=0.$$

Remark: The $H^2(\mathcal{D})$ estimate, establishes a.s. convergence in $L^2(\mathcal{D})$ to the step function through a.s. continuous paths.

The H^2 regularity was derived by applying a proper version of BDG inequality (see for example in Marinelli, Röckner, Exp. Math. 2016), for the a priori estimates in expectation up to H^2 (inspired by Elliott, Songmu, ARMA, 1986, made for the determ. CH.)

2. The stochastic Allen-Cahn equation with mild noise

$$
\begin{aligned}
& w_t = \Delta w + \frac{f(w)}{\varepsilon^2} + \frac{\dot{W}(x,t;\varepsilon)}{\varepsilon}, \quad x \in \Omega, \quad 0 < t \leq T, \\
& w(x,0) = w_0(x), \quad x \in \Omega, \\
& \frac{\partial w}{\partial \eta} = 0, \quad x \in \partial\Omega, \quad 0 < t \leq T \quad \text{(Neumann b.c.)}
\end{aligned} \tag{4}
$$

Here

$$\delta(\varepsilon) \equiv 0, \quad \text{and} \quad \mu(\varepsilon) = \varepsilon^{-2}.$$

with

$$\mathcal{F}(u,x,t;\varepsilon) := \mathcal{F}(x,t;\varepsilon) = \frac{\dot{W}(x,t;\varepsilon)}{\varepsilon},$$

for

$\dot{W}(x,t;\varepsilon)$ a mild noise tending to rough as $\varepsilon \to 0$.)

- In A IMA NA 2020, a DG nonlinear method was introduced

$\hookrightarrow$ existence and uniqueness of the numerical solution were proved

$\hookrightarrow$ optimal error estimates were derived.

- In A, Egwu, Yan IMA NA 2023, the mild noise was numerically approximated

$\hookrightarrow$ and we applied an a posteriori error analysis on the scheme.

Smooth time-noise definition (H. Weber AIHP P.Stat., 2010)

Let $\rho : \mathbb{R} \to \mathbb{R}^+$
- compactly supported in $[-1, 1]$,
- symmetric around zero,
- it satisfies

$$\int_{-\infty}^{\infty} \rho(s) ds = 1.$$

Define for $0 < \gamma < \frac{2}{3}$

$$\rho^{\varepsilon}(s) := \varepsilon^{-\gamma} \rho\Big(\frac{s}{\varepsilon^{\gamma}}\Big).$$

Let $\beta(t), \widetilde{\beta}(t) \sim N(0, t)$, $t \geq 0$ two **stochastically independent** Brownian Motions.

The smooth approximation of a brownian $\beta(t)$ is given by,

$$\beta_{\varepsilon}(t) := \int_{-\infty}^{0} \rho^{\varepsilon}(t-s)\widetilde{\beta}(-s)ds + \int_{0}^{\infty} \rho^{\varepsilon}(t-s)\beta(s)ds,$$

and the smooth approximation of its formal derivative by

$$\dot{\beta}_\varepsilon(t) := \int_{-\infty}^{0} \partial_t(\rho^\varepsilon(t-s))\widetilde{\beta}(-s)ds + \int_{0}^{\infty} \partial_t(\rho^\varepsilon(t-s))\beta(s)ds,$$

which is the smooth approximation of $\dot{\beta}$.

Numerical implementation of smooth noise

How we insert x-dependence in the mild noise?

An answer: In A IMA NA 2020, the smooth space-time noise was defined by the convolution

$$\dot{W}(x,t;\varepsilon) := G(x)\dot{\beta}_\varepsilon(t),$$

for $G \in C^\infty$.

How we select ρ?

How we construct the convolution integral numerically?

In A, Egwu, Yan IMA NA 2023, the bump function was selected and the composite trapezoidal rule on the convolution was used.

Let the compactly supported bump function $r : \mathbb{R} \to \mathbb{R}^+$, with

$$r(s) := \begin{cases} e^{-\frac{1}{1-s^2}} & s \in (-1,1) \\ 0 & \text{otherwise} \end{cases}, \text{ and define}$$

$$\rho(s) := r(s)\left[\int_{-1}^{1} r(s)ds\right]^{-1} = \begin{cases} e^{-\frac{1}{1-s^2}}\left[\int_{-1}^{1} e^{-\frac{1}{1-s^2}} ds\right]^{-1} & s \in (-1,1), \\ 0 & \text{otherwise.} \end{cases}$$

Then ρ satisfies all the properties required in the convolution definitions.

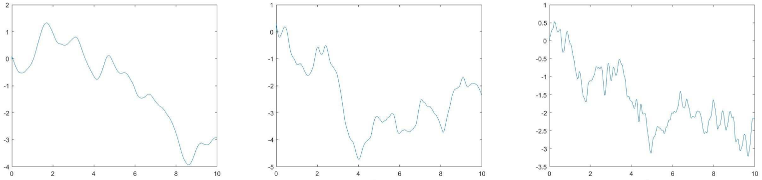

Figure: The smooth approximation $\beta_\varepsilon(t)$ of the brownian for $\gamma = \frac{1}{8} < \frac{2}{3}$ and $T = 10$, for $\varepsilon = 10^{-3},\ 10^{-6},\ 10^{-9}$ (from the left to the right).

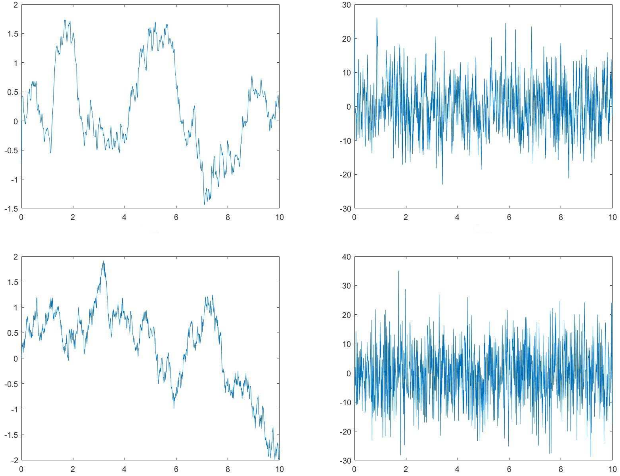

Figure: First row: The smooth approximation $\beta_\varepsilon(t)$ of the brownian and $\dot{\beta}_\varepsilon(t)$ the smooth approximation of the formal derivative of the brownian, for $\gamma = \frac{1}{8} < \frac{2}{3}$, $T = 10$, and $\varepsilon = 10^{-14}$. Second row: A brownian path (with D. Higham's algorithm, SIAM Rev. 2001), and its formal derivative.

The DG scheme for the mild stochastic AC, motivated by Jamet SINUM 1978.

We apply the exponential transformation

$$w = e^{b(\varepsilon)t}u, \quad \text{with} \quad \inf_{\varepsilon\in(0,1)}\big(b(\varepsilon) - \varepsilon^{-2}\big) \geq \hat{c}_0 > 0,$$

which is analogous to these of A, Plexousakis Numer.Math. 2010, A, Plexousakis ESAIM M2AN 2019, and obtain

$$\begin{aligned} u_t &= \Delta u - b(\varepsilon)u + \frac{g(u,\varepsilon,t)}{\varepsilon^2} \\ &+ m(\varepsilon,t)\frac{\dot{W}(x,t;\varepsilon)}{\varepsilon}, \quad x \in \mathcal{D}, \quad 0 < t \leq T, \end{aligned}$$

for

$$g(u,\varepsilon,t) := u - e^{2b(\varepsilon)t}u^3, \quad m(\varepsilon,t) := e^{-b(\varepsilon)t}.$$

The exponential transformation resulted to numerical stability on:

- linear parabolic equations (linear Schrödinger, Heat)
- stochastic Allen-Cahn.

Let $0 = t^0 < t^1 < \cdots < t^N = T$, a partition of $[0, T]$, and set

$$G^n := \mathcal{D} \times (t^n, t^{n+1}).$$

For each $0 \le n \le N - 1$

let a family $\{V_h^n\}$ of finite dimensional subspaces of $H^1(G^n)$, and define V_h such that

$$V_h|_{(t^n, t^{n+1})} := V_h^n.$$

Remark: The functions of V_h are in general discontinuous at the temporal nodes t^n.

$\hookrightarrow$ We seek $u_h \in V_h$ such that:

$$
\begin{aligned}
&-((u_h, \partial_t v_h))_{G^n} + ((\nabla u_h, \nabla v_h))_{G^n} + b(\varepsilon)((u_h, v_h))_{G^n} \\
&-\varepsilon^{-2}((u_h, v_h))_{G^n} + \varepsilon^{-2}((e^{2b(\varepsilon)t}(u_h)^3, v_h))_{G^n} \\
&+(u_h^{n+1}, v_h^{n+1})_{\mathcal{D}} - (u_h^n, v_h^{n+0})_{\mathcal{D}} = \varepsilon^{-1}((e^{-b(\varepsilon)t}\xi_t^\varepsilon, v_h))_{G^n}, \\
&\quad \forall v_h \in V_h^n, \; n = 0, \dots, N-1, \quad u_h^0 = u_0,
\end{aligned}
$$

for $\xi_t^\varepsilon := \dot{W}(x, t; \varepsilon)$ the mild noise.

Here, $((\cdot,\cdot))_{G^n}$, $(\cdot,\cdot)_{\mathcal{D}}$ denote the $L^2(G^n)$ and the $L^2(\mathcal{D})$ inner products respectively, while $|\cdot|_{\mathcal{D}} := \|\cdot\|_{L^2(\mathcal{D})}$.

Remarks: The DG scheme is nonlinear, time discontinuous, adaptive in t, while u_h^0 coincides with the continuous problem initial data.

The weak formulation and the inner product is defined by L^2 double integration in space-time.

3. Coexistence of both Cahn-Hilliard and Allen-Cahn operators

Let us recall the CH/AC equation

$$u_t = -\delta(\varepsilon)\Delta\big(\varepsilon^2\Delta u - f(u)\big) + \mu(\varepsilon)(\varepsilon^2\Delta u - f(u)) + \mathcal{F}, \quad x \in \mathcal{D}, \quad t > 0,$$

where

$$\delta(\varepsilon) > 0, \quad \mu(\varepsilon) \geq 0.$$

For the homogeneous problem ($\mathcal{F} \equiv 0$ and so deterministic) in $d = 1$, A, Karali, Tzirakis, in Cal.Var. 2021

↪ we estimated the spectrum of the linearized CH/AC operator,

↪ determined families of weights $\delta(\varepsilon)$, $\mu(\varepsilon)$, for which the dynamics of N layers are stable and rest exponentially small in ε,

↪ derived a system of ODEs for the layers motion.

For the same problem, in A, Karali, D. Li, J.Sc.Comput. 2025,

$\hookrightarrow$ we applied a **SAV**-linearized RK method in $d = 1, 2, 3$

- we proved optimal error estimates,

- we had the first simulations for the mixed problem (deterministic) by further discretizing in space by FEM.

In progress: The SAV method for stochastic equations.

Thank you!

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