### The role of randomness in stochastic phase-field modelling

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#### Mixtures: Modeling, analysis and computing EMS Topical Activity Group conference

5-7 February 2025, Charles University, Prague





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3 An example: the stochastic Allen-Cahn equation

Open problems and ongoing work

# Phase field modelling

Phase-field approach to phase-separation:

- evolution of a material with 2 different features, mixtures, ...
- $\bullet$  phase variable  $\varphi \in [-1,1]:$  pure phases are  $\{\varphi = 1\}$  and  $\{\varphi = -1\}$
- intermediate values  $\varphi \in (-1,1)$  are allowed: diffuse (narrow) interface

Advantages with respect to sharp interface models:

- no need of boundary conditions at the interface
- no need to track the interface at all times
- no difficulties in case of topological changes

Applications:

- physics and engineering: phase separation, alloys, fluid mixtures, ...
- biology: tumour growth dynamics, RNA-protein formation, ...

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$$\mathcal{E}(\varphi) := rac{1}{2} \int_{\mathcal{O}} |\nabla \varphi|^2 + \int_{\mathcal{O}} F(\varphi) \,,$$

along with its variational derivative (chemical potential)

$$\mu = -\Delta \varphi + F'(\varphi).$$

Deterministic approach:

neglect other possible energy contributions (temperature, magnetic, vibrational effects)

Allen-Cahn model:

- $\partial_t \varphi + \mu = 0$
- no-flux boundary conditions for  $\varphi$
- no mass-conservation

Cahn-Hilliard model:

- $\partial_t \varphi \Delta \mu = 0$
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### Classical Allen-Cahn and Cahn-Hilliard equations

Typical form of the AC equation:

$$\begin{cases} \partial_t \varphi - \Delta \varphi + F'(\varphi) = 0 & \text{in } (0, T) \times \mathcal{O}, \\ \partial_n \varphi = 0 & \text{in } (0, T) \times \partial \mathcal{O}, \\ \varphi(0) = \varphi_0 & \text{in } \mathcal{O}. \end{cases}$$

Typical form of the CH equation:

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Physically-relevant choice of double-well potential:

$$F_{log}(r) := \frac{\theta}{2} \left[ (1+r) \ln(1+r) + (1-r) \ln(1-r) \right] - \frac{\theta_0}{2} r^2 \,, \quad r \in [-1,1] \,, \qquad 0 < \theta < \theta_0 \,.$$

Initial datum with finite energy:

 $\varphi_0 \in H^1(\mathcal{O})\,, \qquad |\varphi_0| \le 1 \text{ a.e. in } \mathcal{O}\,.$ 

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3 An example: the stochastic Allen-Cahn equation

Open problems and ongoing work

Phase separation may be affected by:

- unpredictable temperature oscillations, microscopic movements, magnetic effects, ...
- measurement uncertainty, environmental disturbance, ...

#### Possible solutions (Cook, 1970):

- deterministic model is too "simple" to capture such background noise
- addition of a suitable stochastic forcing in the equation: gaussian noise

General form of the stochastic Allen-Cahn ( $\alpha = 0$ ) and Cahn-Hilliard ( $\alpha = 1$ ) equations:

$$\begin{cases} d\varphi + (1 - \alpha)\mu \, dt - \alpha \Delta \mu \, dt = G(\varphi) \, dW & \text{in } (0, T) \times \mathcal{O} \,, \\ \mu = -\Delta \varphi + F'(\varphi) & \text{in } (0, T) \times \mathcal{O} \,, \\ \partial_{n}\varphi = \alpha \partial_{n}\mu = 0 & \text{in } (0, T) \times \partial \mathcal{O} \,, \\ \varphi(0) = \varphi_{0} & \text{in } \mathcal{O} \,. \end{cases}$$

Stochastic forcing:

- $(\Omega, \mathscr{F}, (\mathscr{F}_t)_{t \ge 0}, \mathbb{P})$ : filtered probability space
- W: cylindrical Wiener process on a abstract Hilbert space U i.e.

$$W = \sum_{k=0}^{\infty} eta_k e_k$$
,  $(e_k)_k$  c.o.s. of  $U$ ,  $(eta_k)_k$  independent Brownian motions.

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Noise coefficient: Hilbert-Schmidt from a abstract space U to the reference space  $L^2(\mathcal{O})$ , i.e.  $G(\varphi) \in \mathscr{L}^2(U, L^2(\mathcal{O})) \quad \forall \varphi \in L^2(\mathcal{O}).$ 

Possible choice of the noise:

•  $G: L^2(\mathcal{O}) \to \mathscr{L}^2(U, L^2(\mathcal{O}))$  given by

 $G(\varphi)[e_k] = g_k(\varphi)$ , with  $(g_k)_k \subset C^{0,1}([-1,1])$ 

• structure:

$$g_k(\pm 1)=0\,,\quad {F''g_k^2}\in L^\infty(-1,1)\qquad ext{for all }k\in\mathbb{N}$$

• Hilbert-Schmidt condition:

$$\sum_{k\in\mathbb{N}} \left( \|g_k\|_{C^{0,1}([-1,1])}^2 + \|F''g_k^2\|_{L^{\infty}(-1,1)} \right) < +\infty$$

- interpretation: G(arphi) behaves as a degenerate mobility-type function
- advantage: G is of "local" type (superposition operator)
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### Stochastic Allen-Cahn equation

#### Theorem (Bertacco, Orrieri, S. (2020-2023))

In this setting, for every  $\varphi_0 \in H^1(\mathcal{O})$  with  $\|\varphi_0\|_{L^{\infty}(\mathcal{O})} \leq 1$ , there exists a unique process

$$\begin{split} \varphi \in L^2(\Omega; C^0([0,T]; L^2(\mathcal{O})) \cap L^\infty(0,T; H^1(\mathcal{O})) \cap L^2(0,T; H^2_n(\mathcal{O}))) \,, \\ |\varphi| < 1 \quad \text{a.e. in } \Omega \times (0,T) \times \mathcal{O} \,, \end{split}$$

such that for every  $t \in [0, T]$ ,  $\mathbb{P}$ -almost surely,

$$\varphi(t) - \int_0^t \Delta \varphi(s) \, ds + \int_0^t F'_{log}(\varphi(s)) v \, ds = \varphi_0 + \int_0^t G(\varphi(s)) \, dW(s) \quad \text{in } L^2(\mathcal{O}) \, .$$

Moreover, the solution map  $\varphi_0 \mapsto \varphi$  is Lipschitz-continuous as a map

 $L^{2}(\mathcal{O}) \rightarrow L^{2}(\Omega; C^{0}([0, T]; L^{2}(\mathcal{O})) \cap L^{2}(0, T; H^{1}(\mathcal{O}))).$ 

If also  $\varphi_0 \in H^2_n(\mathcal{O})$  satisfies  $\|\varphi_0\|_{L^{\infty}(\mathcal{O})} < 1$ , then a random separation property holds:

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### Formal energy balance

Itô formula yields the formal energy balance:

$$\begin{split} &\frac{1}{2} \int_{\mathcal{O}} |\nabla \varphi(t)|^2 + \int_{\mathcal{O}} F(\varphi(t)) + \int_0^t \int_{\mathcal{O}} |\mu(s)|^2 \, ds \\ &= \frac{1}{2} \int_{\mathcal{O}} |\nabla \varphi_0|^2 + \int_{\mathcal{O}} F(\varphi_0) + \int_0^t (\mu(s), G(\varphi(s)) \, dW(s)) \\ &\quad + \frac{1}{2} \int_0^t \sum_{k=0}^\infty \int_{\mathcal{O}} |g_k'(\varphi(s)) \nabla \varphi(s)|^2 \, ds + \frac{1}{2} \int_0^t \sum_{k=0}^\infty \int_{\mathcal{O}} F''(\varphi(s)) |g_k(\varphi(s))|^2 \, ds \, . \end{split}$$

Extra terms:

dW(s) : first order martingale term,

 $\frac{1}{2}\int_0^t\sum_{k=0}^\infty\int_{\mathcal{O}}|g_k'(\varphi(s))\nabla\varphi(s)|^2\,ds$ 

second order proliferation term (gradient o

$$\frac{1}{2}\int_0^t\sum_{k=0}^\infty\int_{\mathcal{O}}F''(\varphi(s))|g_k(\varphi(s))|^2\,ds$$

second order proliferation term (potential contribution).

### Formal energy balance

Itô formula yields the formal energy balance:

$$\begin{split} &\frac{1}{2} \int_{\mathcal{O}} |\nabla \varphi(t)|^2 + \int_{\mathcal{O}} F(\varphi(t)) + \int_0^t \int_{\mathcal{O}} |\mu(s)|^2 \, ds \\ &= \frac{1}{2} \int_{\mathcal{O}} |\nabla \varphi_0|^2 + \int_{\mathcal{O}} F(\varphi_0) + \int_0^t (\mu(s), G(\varphi(s)) \, dW(s)) \\ &\quad + \frac{1}{2} \int_0^t \sum_{k=0}^\infty \int_{\mathcal{O}} |g_k'(\varphi(s)) \nabla \varphi(s)|^2 \, ds + \frac{1}{2} \int_0^t \sum_{k=0}^\infty \int_{\mathcal{O}} F''(\varphi(s)) |g_k(\varphi(s))|^2 \, ds \, . \end{split}$$

Extra terms:

$$\begin{split} & \int_0^t \left(\mu(s), G(\varphi(s)) \, dW(s)\right): & \text{first order martingale term,} \\ & \frac{1}{2} \int_0^t \sum_{k=0}^\infty \int_{\mathcal{O}} |g_k'(\varphi(s)) \nabla \varphi(s)|^2 \, ds & \text{second order proliferation term (gradient contribution),} \\ & \frac{1}{2} \int_0^t \sum_{k=0}^\infty \int_{\mathcal{O}} F''(\varphi(s)) |g_k(\varphi(s))|^2 \, ds & \text{second order proliferation term (potential contribution).} \end{split}$$

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ISSUE: blow-up of F'' should be compensated by degeneracy of G!

2 Stochastic approach to phase-field models

3 An example: the stochastic Allen-Cahn equation

Open problems and ongoing work

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#### 1) Stochastic conservative Allen-Cahn equation with conservative noise

Divergence-form noise:  

$$\begin{cases}
d\varphi + (\mu - \overline{\mu}) dt = -\operatorname{div} \mathbf{G}(\varphi) dW & \text{in } (0, T) \times \mathbb{T}, \\
\mu = -\Delta\varphi + F'(\varphi) & \text{in } (0, T) \times \mathbb{T}, \\
\varphi(0) = \varphi_0 & \text{in } \mathbb{T},
\end{cases}$$

$$Zero-order \text{ noise:}$$

$$\begin{cases}
d\varphi + (\mu - \overline{\mu}) dt = (G(\varphi) - \overline{G(\varphi)}) dW & \text{in } (0, T) \times \mathbb{T}, \\
\mu = -\Delta\varphi + F'(\varphi) & \text{in } (0, T) \times \mathbb{T}, \\
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\end{cases}$$
(4.2)

- more coherent with the model derivation
- (4.1): treated in collaboration with Andrea Di Primio and Maurizio Grasselli
- (4.2): energy proliferation reads as

$$\frac{1}{2} \mathbb{E} \int_0^t \sum_{k=0}^\infty \int_{\mathbb{T}} |F''(\varphi(s))| |g_k(\varphi(s)) - \overline{g_k(\varphi(s))}|^2 \, ds$$

ullet problem: nonlocal term prevents to control the blow-up of F'' locally at  $\pm 1$ 

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- 2) Long-time behaviour for stochastic Allen-Cahn-type equations
  - behaviour of the law of the random variable  $arphi(t):\Omega
    ightarrow L^2(\mathcal{O}),$  as  $t
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  - existence uniqueness of an invariant measure  $\nu$
  - convergence of the laws towards u
  - asymptotic stability in Wasserstein distances
  - elliptic Kolmogorov equation in  $L^2(H, \nu)$ , where  $H = L^2(\mathcal{O})$
  - stochastic Allen-Cahn equation: treated in collaboration with Margherita Zanella
- 3) Coupled stochastic Allen-Cahn-Navier-Stokes systems

 $\begin{cases} d\mathbf{u} - \Delta \mathbf{u} \, dt + (\mathbf{u} \cdot \nabla) \mathbf{u} \, dt = \mu \nabla \varphi \, dt + G_1(\mathbf{u}) \, dW & \text{in } (0, T) \times \mathcal{O}, \\ d\varphi + \mu \, dt + \mathbf{u} \cdot \nabla \varphi \, dt = G_2(\varphi) \, dW & \text{in } (0, T) \times \mathcal{O}, \\ \mu = -\Delta \varphi + F'(\varphi) & \text{in } (0, T) \times \mathcal{O}, \\ \mathbf{u}(0) = \mathbf{u}_0, \quad \varphi(0) = \varphi_0 & \text{in } \mathcal{O}, \end{cases}$ (4.3)

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	$\int d\mathbf{u} - \Delta \mathbf{u}  dt + (\mathbf{u} \cdot \nabla) \mathbf{u}  dt = \mu \nabla \varphi  dt + G_1(\mathbf{u})  dW$	in $(0, T) \times \mathcal{O}$ ,	
	$d arphi + \mu  dt + \mathbf{u} \cdot  abla arphi  dt = G_2(arphi)  dW$	in $(0, T) \times \mathcal{O}$ ,	(12)
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#### 4) Stochastic Cahn-Hilliard equation

$$\begin{cases} d\varphi - \operatorname{div}[m(\varphi)\nabla\mu] \, dt = G(\varphi) \, dW & \text{in } (0, T) \times \mathcal{O}, \\ \mu = -\Delta\varphi + F'(\varphi) & \text{in } (0, T) \times \mathcal{O}, \\ \partial_{n}\varphi = m(\varphi)\partial_{n}\mu = 0 & \text{in } (0, T) \times \partial\mathcal{O}, \\ \varphi(0) = \varphi_{0} & \text{in } \mathcal{O}. \end{cases}$$

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- (4.4) with degenerate mobility and singular potential treated by **S**. (2021) with non-conservative noise
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#### 5) Uniqueness by noise for phase-field models

III-posed deterministic evolution equation:  $\partial_t u + Au + B(u) = 0.$   $\Downarrow$ Well-posed stochastic evolution equation: du + Au dt + B(u) dt = G dV

- uniqueness by noise: well-known in finite dimensions
- infinite dimensions with perturbation *B* of order zero: Da Prato, Flandoli, Priola, Röckner (2013)
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#### 6) Joint hydrodynamic and nonlocal-to-local convergence for Cahn-Hilliard

Microscopic derivation of the nonlocal Cahn-Hilliard equation:

- Giacomin, Lebowitz (1997): probabilistic limit
- from lattice gas model to nonlocal Cahn-Hilliard equation  $(n 
  ightarrow \infty)$

Convergence of the nonlocal Cahn-Hilliard equation to the local one:

- Davoli, S., Trussardi (2020-2021): constant mobility and singular potential
- Abels, Terasawa (2022): coupled Cahn-Hilliard-Navier-Stokes
- Elbar, Skrzeczkowski (2023): degenerate mobility
- ullet interaction kernels suitably scaled around a Dirac delta (arepsilon 
  ightarrow 0)

Possible idea for microscopic derivation of the local Cahn-Hilliard equation:

- lattice gas (*n* particles) with scaled interaction potential ( $\varepsilon$ )
- joint limiting procedure as  $n \to \infty$  and  $\varepsilon \to 0$ .

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#### Thank you

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# THANK YOU FOR YOUR ATTENTION!