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Following Top-Down (↓) and Bottom-Up (↑) Approaches to Discretize Non-Linear Stochastic Diffusion Equations

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A Non-Linear Diffusion Equation

- Diffusion processes in softmatter are generally described by Non-Linear PDEs

$$\frac{\partial c}{\partial t}(\mathbf{r}, t) = \boldsymbol{\nabla} \cdot \left[\Gamma(c(\mathbf{r}, t)) \boldsymbol{\nabla} \frac{\delta \mathcal{F}}{\delta c(\mathbf{r}, t)} [c(\mathbf{r}, t)] \right] .$$

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- Fluctuations are relevant when Brownian motion, critical phenomena, transition events, etc., are of interest.
- Landau and Lifshitz added thermal fluctuations through the divergence of a stochastic flux

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with

$$\tilde{\mathbf{J}}(\mathbf{r},t) = \sqrt{2 k_B T \Gamma[c(\mathbf{r},t)]} \zeta(\mathbf{r},t) .$$

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- Here, δ_μ is a generic smoothing kernel with support μ that converges to a delta "function" when $\mu \to 0$.
- In the limit $\mu \to 0$ (NO CG), for a dilute solution, the SPDE for $c(\mathbf{r}, t)$ turns into

$$\frac{\partial c}{\partial t}(\mathbf{r}, t) = D\nabla^2 c + \boldsymbol{\nabla} \cdot \sqrt{2Dc}\zeta(\mathbf{r}, t).$$

Microscopic Description

- In a microscopic level of description, the evolution equation for the microscopic variables $\mathbf{z} \equiv \{\mathbf{q}_i, \mathbf{p}_i, \mathbf{Q}_j, \mathbf{P}_j\}$ is given by Hamilton's equations

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- We define as CG variable the discrete concentration field $\hat{\mathbf{c}}(\mathbf{z})$

$$\hat{c}_\mu(\mathbf{z}) = \sum_{i=1}^{N} \delta_\mu(\mathbf{r}_i)$$

Mesoscopic Description

- The mesoscopic probability of finding the mesoscopic variables $\hat{\mathbf{c}}(\mathbf{z})$ at a given configuration $\mathbf{c}$ at a time t is given by

$$P(\mathbf{c}, t) = \int d\mathbf{z}\, \rho(\mathbf{z}, t)\delta(\hat{\mathbf{c}}(\mathbf{z}) - \mathbf{c})$$

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$$\frac{\partial P}{\partial t}(\mathbf{c}, t) = \frac{\partial}{\partial c_\mu}\left[-\hat{v}_\mu(\mathbf{c}) + \hat{D}_{\mu\nu}(\mathbf{c})\frac{\partial \hat{F}}{\partial c_\nu}(\mathbf{c})\right] P(\mathbf{c}, t) + k_{\mathrm{B}} T \frac{\partial}{\partial c_\mu}\hat{D}_{\mu\nu}(\mathbf{c})\frac{\partial P}{\partial c_\nu}(\mathbf{c}, t)$$

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- or its mathematically equivalent Ito SDE for the CG variable

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- All the quantities involved in the SDE are defined microscopically.

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- The dissipative matrix $\hat{\mathbf{D}}(\mathbf{c})$, for a **infinitely diluted suspension** with a **separation of scales between positions and velocities**, is given by

$$\hat{D}_{\mu\nu} = \frac{D}{k_{\mathrm{B}} T} \int d\mathbf{r} \, \nabla \delta_{\nu}(\mathbf{r}) \nabla \delta_{\mu}(\mathbf{r}) \, \langle \hat{c}_{\mathbf{r}} \rangle^{\mathbf{c}}$$

where

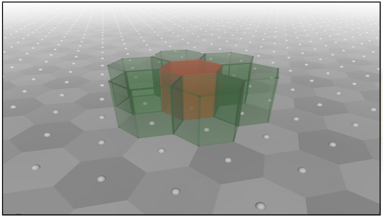
$$D = \int_0^{\infty} dt \, \langle \mathbf{v}_i \mathbf{v}_i(t) \rangle^{\mathbf{c}} \quad \text{and} \quad \langle \hat{c}_{\mathbf{r}} \rangle^{\mathbf{c}} = \left\langle \sum_i \delta(\mathbf{r} - \mathbf{r}_i) \right\rangle^{\mathbf{c}}$$

Finite Elements

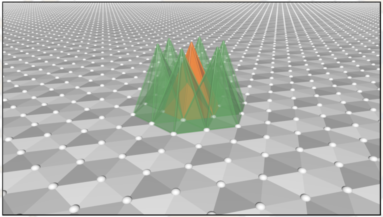
- The dissipative matrix $\hat{\mathbf{D}}(\mathbf{c})$ shows that choosing a good definition for the finite element $\delta_\mu(\mathbf{r})$ is a sensitive issue [P. Español & I. Zúñiga, JCP 131(16), 2009].

$$\hat{D}_{\mu\nu} = \frac{D}{k_{\mathrm{B}} T} \int d\mathbf{r}\, \nabla\delta_\nu(\mathbf{r}) \nabla\delta_\mu(\mathbf{r}) \left\langle \hat{c}_{\mathbf{r}} \right\rangle^{\mathbf{c}}$$

- A finite element based on the Voronoi construction assigns a particle to the nearest node.



- A finite element based on the Delaunay triangulation assigns a particle to a node following a linear piece-wise function.

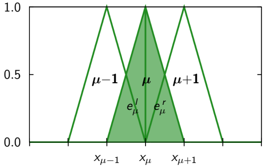


Finite Elements

- A finite element based on the Delaunay triangulation (which is well behaved) define the discrete concentration field as

$$\hat{c}_\mu(\mathbf{r}) = \sum_{i=1}^{N} \delta_\mu(\mathbf{r}_i) \quad \left(\delta_\mu(\mathbf{r}) \to \frac{\psi_\mu(\mathbf{r})}{V_\mu}\right)$$

$$\psi_\mu(\mathbf{r}) = \sum_{e\in\mu} (a_{e_\mu} + \mathbf{b}_{e\to\mu} \cdot \mathbf{r})\theta_{e_\mu}$$



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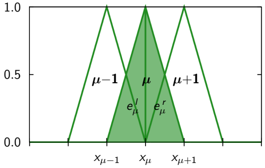

- By using the finite element with support on the Delaunay triangulation, the SDE is explicitly written as [J. A. de la Torre & P. Español, JCP 135(11), 2011].

$$dc_\mu(t) = -\frac{D}{k_\mathrm{B}T} \sum_{\nu} \sum_{e\in\mu\nu} \mathbf{b}_{e\to\mu} \cdot \mathbf{b}_{e\to\nu} \frac{V_e}{V_\mu V_\nu} c_e \frac{\partial \hat{F}}{\partial c_\nu} dt$$

$$+ D \sum_{\nu} \sum_{e\in\mu\nu} \mathbf{b}_{e\to\mu} \cdot \mathbf{b}_{e\to\nu} \frac{V_e}{V_\mu V_\nu} \frac{\partial c_e}{\partial c_\nu} dt$$

$$+ \sum_{e\in\mu} \sqrt{2Dc_e V_e} \frac{1}{V_\mu} \mathbf{b}_{e\to\mu} \cdot d\mathcal{W}_e$$

Thermodynamic Limit

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- If we define a discrete concentration field, and an interpolated concentration field (namely, a (Petrov) Galerkin discretization method)

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- The discrete evolution equations (without fluctuations)

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obtained from microscopic principles by using the ToCG, can be understood as a discrete version of the continuum equation

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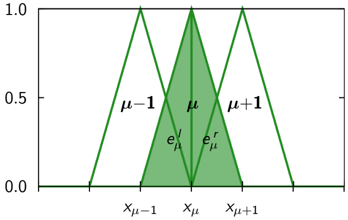
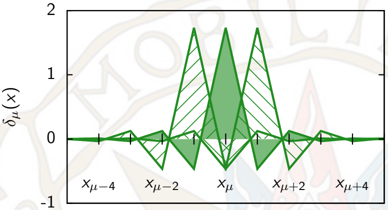
- Reciprocically, the continuum PDE can be obtained from Hamilton's equations, by using the ToCG. This is the Bottom-Up (↑) Approach [P. Español & H. Löwen, JCP 131(24), 2009].

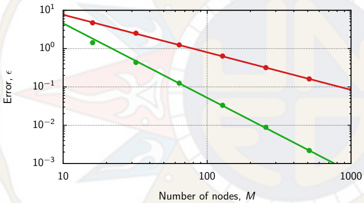
Conjugate Finite Elements

- Consider now $\delta_\mu(\mathbf{r}) \to \sum_\nu M^\delta_{\mu\nu}\psi_\nu(\mathbf{r})$, which is different from the previous definition $\delta_\mu(\mathbf{r}) \to \psi_\mu(\mathbf{r})/V_\mu$. [J. A. de la Torre, P. Español, & A. Donev, JCP 142(9), 2015].





- The discretization method gives a **discrete** Laplacian $\Delta = \mathbf{M}^\delta \mathbf{L}^\psi$, where $\mathbf{M}^\delta = (\boldsymbol{\delta}, \boldsymbol{\delta}) = \left(\mathbf{M}^\psi\right)^{-1}$ and $\mathbf{L}^\psi = (\nabla\boldsymbol{\psi}, \nabla\boldsymbol{\psi})$.
- This discrete Laplacian gives a **second order accuracy scheme** for linearly consistent basis functions.



Conjugate Finite Elements

- Define a **new** (conjugate) CG variable

$$\hat{c}_\mu(\mathbf{z}) = \sum_{i=1}^{N} \delta_\mu(\mathbf{r}_i) \qquad \left(\delta_\mu(\mathbf{r}) \rightarrow M^{\delta}_{\mu\nu}\psi_\nu(\mathbf{r})\right)$$

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with $\hat{D}_{\mu\nu}(\mathbf{c}) = \sum_{e\in\mu\nu} \mathbf{b}_{e\to\mu}\cdot\mathbf{b}_{e\to\nu}\frac{V_e}{V_\mu V_\nu}\Gamma_e(\mathbf{c})$.

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- The dissipative matrix coincides with the one obtained in the Top-Down (↓) Approach.

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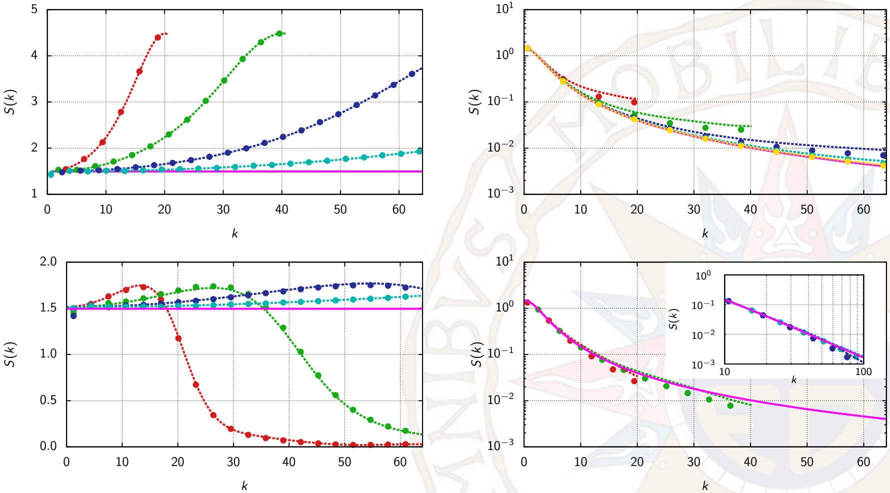
- The dissipative matrix takes the form, by assuming a constant mobility $\Gamma(\mathbf{c})$

$$\mathbf{D} = \frac{Dc_0}{k_{\mathrm{B}} T} \mathbf{L}^{\delta}$$

where $L^{\delta}_{\mu\nu} = (\nabla \delta_\mu, \nabla \delta_\nu)$.

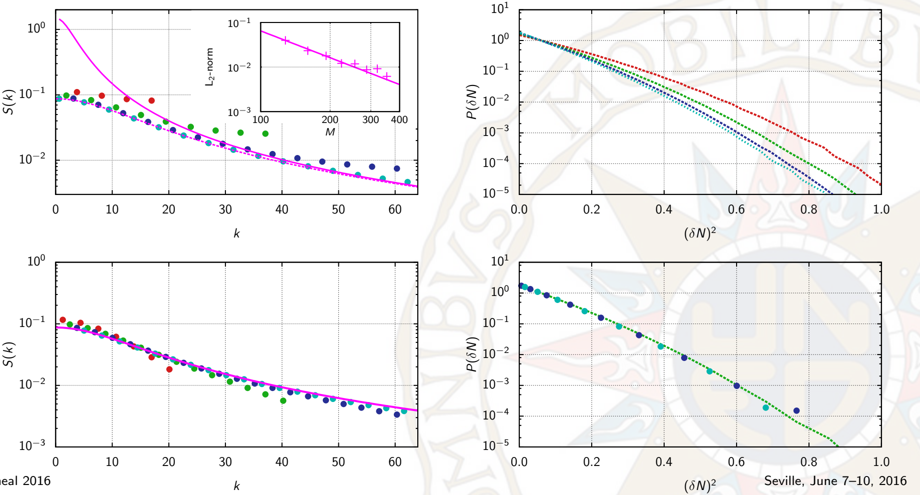
Results – 1D

- Structure factors (discrete Fourier Transform of the matrix of covariances) in Gaussian models for **regular** (top) and **irregular** (bottom) grids



Results – 1D

- Structure factors and probability of finding a given number of particle in a finite region, in Ginzburg-Landau models for **regular** (top) and **irregular** (bottom) grids



Conclusions

- In 1D, Gaussian models have a continuum limit.
- In 1D, Ginzburg-Landau model also has a continuum limit.
- For $D > 1$, Gaussian fields are extremely rough, and should be understood as distributions (*à la* Schwartz).

$$\langle \delta c(\mathbf{r}) \delta c(\mathbf{r}') \rangle = \begin{cases} 1D & \rightarrow \quad \frac{c_0^2 k_0}{2 r_0} e^{-k_0 |r - r'|} \\ 2D & \rightarrow \quad \frac{c_0^2 k_0^2}{4\pi r_0} K_0(k_0 |\mathbf{r} - \mathbf{r}'|) \\ 3D & \rightarrow \quad \frac{c_0^2 k_0^2}{4\pi r_0} \frac{e^{-k_0 |r - r'|}}{|\mathbf{r} - \mathbf{r}'|} \end{cases}$$

- Non-linear equations are not well defined.
- SPDEs can be constructed, but they do not have a physical meaning.
- In the GL model, an observable like the fluctuations of the number of particles in a finite region depends on the resolution of the grid.

References

- J. A. de la Torre, P. Español, and A. Donev, JCP **142**(9), 2015
- S. Delong, Y. Sun, B. E. Griffith, E. Vanden-Eijnden, and A. Donev, PRE **90**(6), 2014
- S. Delong, B. E. Griffith, E. Vanden-Eijnden, and A. Donev, PRE **87**(3), 2013
- J. A. de la Torre, and P. Español, JCP **135**(11), 2011
- P. Español, and I. Zúñiga, JCP **131**(16), 2009
- P. Español, and H. Löwen, JCP **131**(24), 2009
- R. Zwanzig, PR **124**(4), 1961

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Following Top-Down (↓) and Bottom-Up (↑) Approaches to Discretize Non-Linear Stochastic Diffusion Equations

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