Numerical aspects for stochastic PDEs of Fluctuating Hydrodynamics.*

Stochastic equations and particle systems, 7-9 April 2025

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UNIVERSITY OF BATH

*based on joint works with J. Fischer (IST Austria), J. Ingmanns (IST Austria), C. Raithel (TU Wien)

Particle systems are often (exact) solutions to (singular) SPDEs

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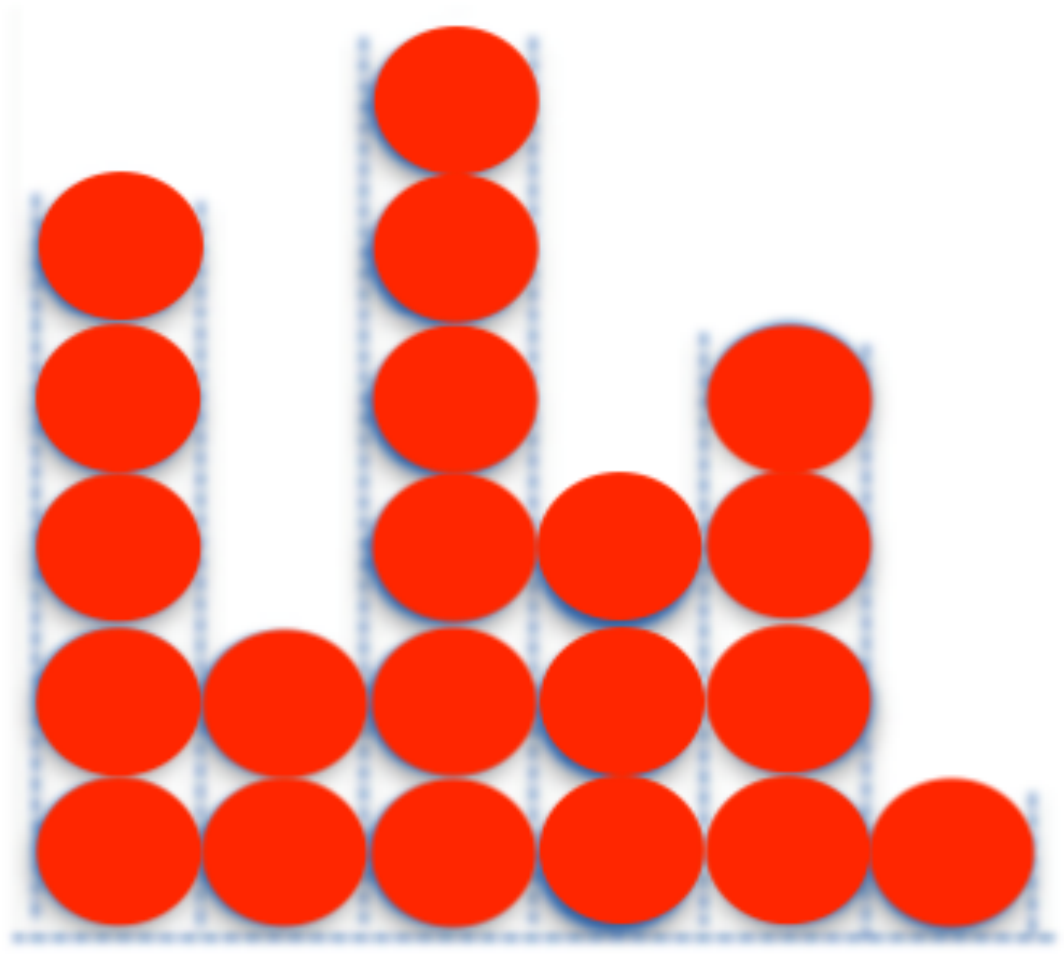

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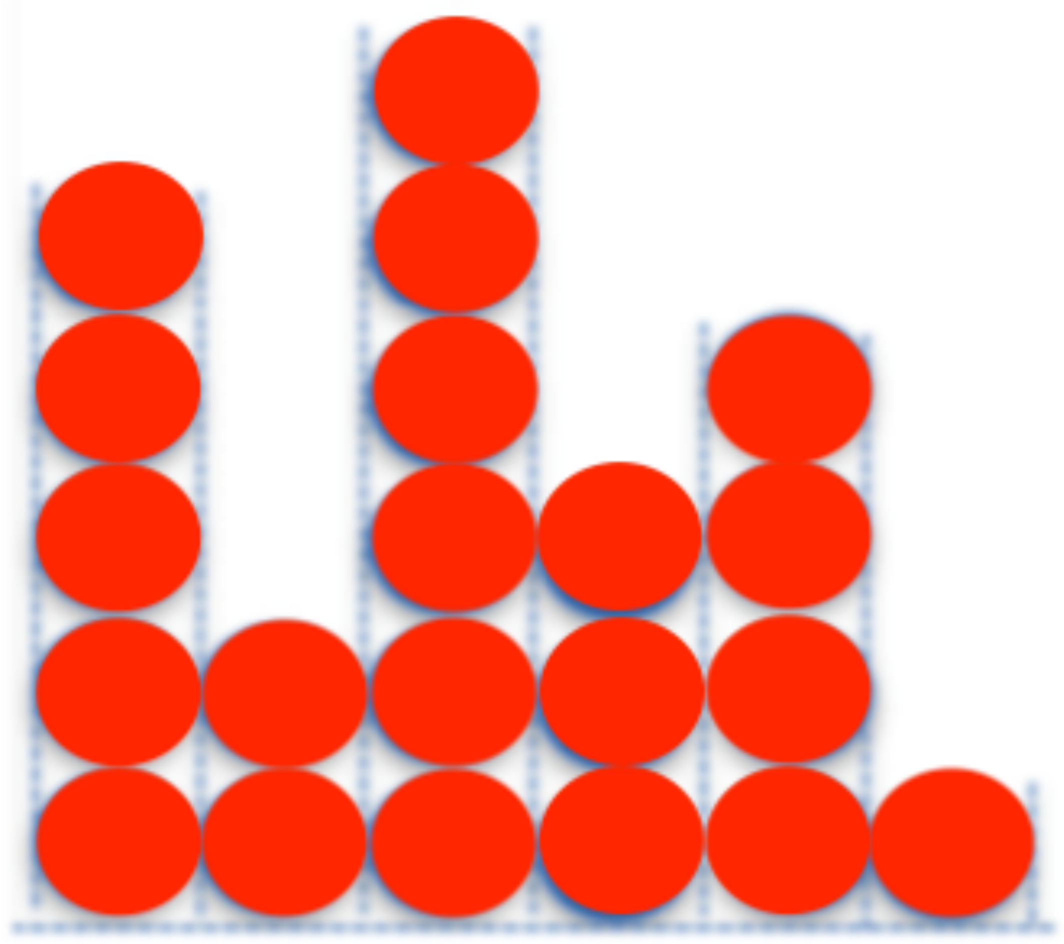

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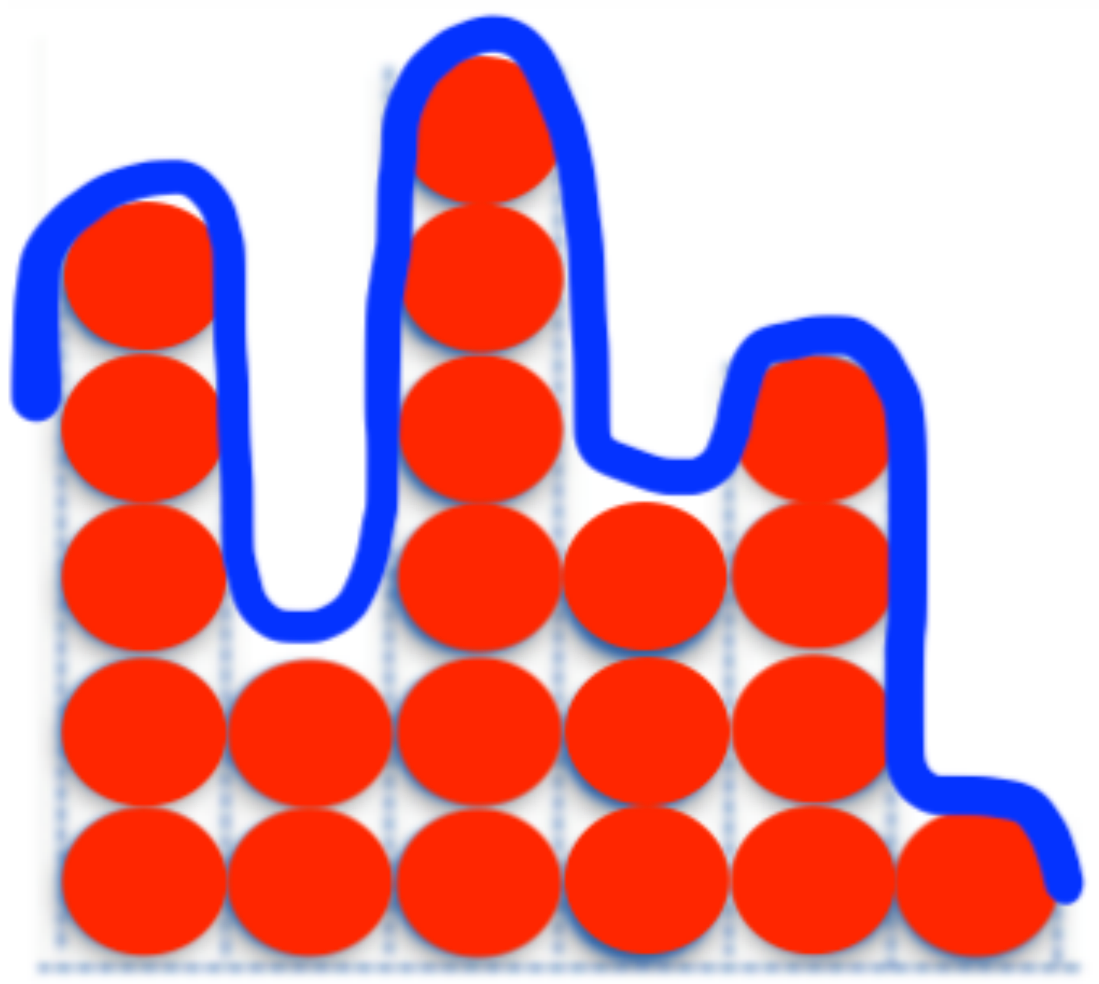
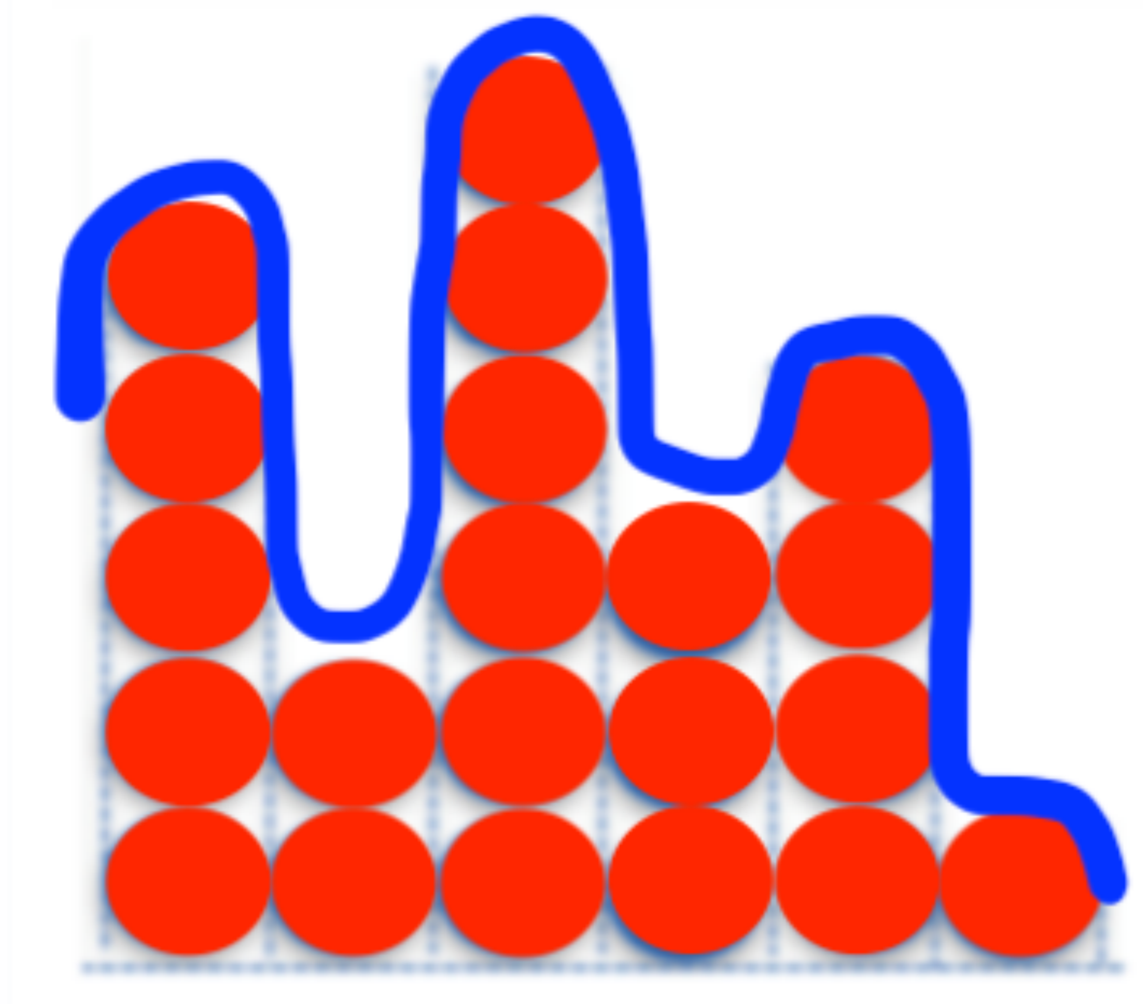


Particle systems are often (exact) solutions to (singular) SPDEs

Particle empirical density

μ



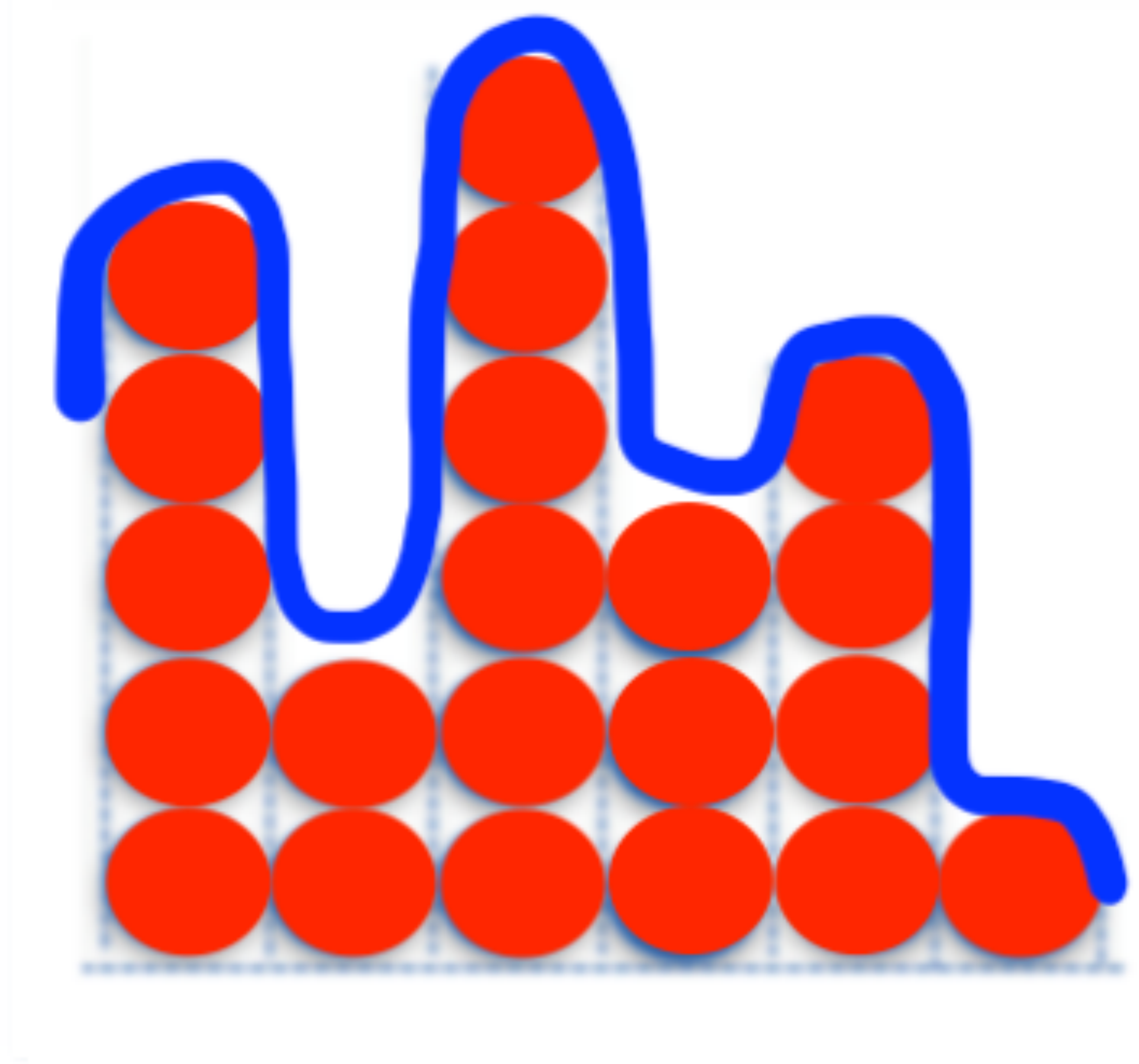
Continuous density

ρ

Particle systems are often (exact) solutions to (singular) SPDEs

Particle **fluctuations**

$\mu - \overline{\mu}$



Continuous **fluctuations**

$\rho - \overline{\rho}$

Particle systems are often (exact) solutions to (singular) SPDEs

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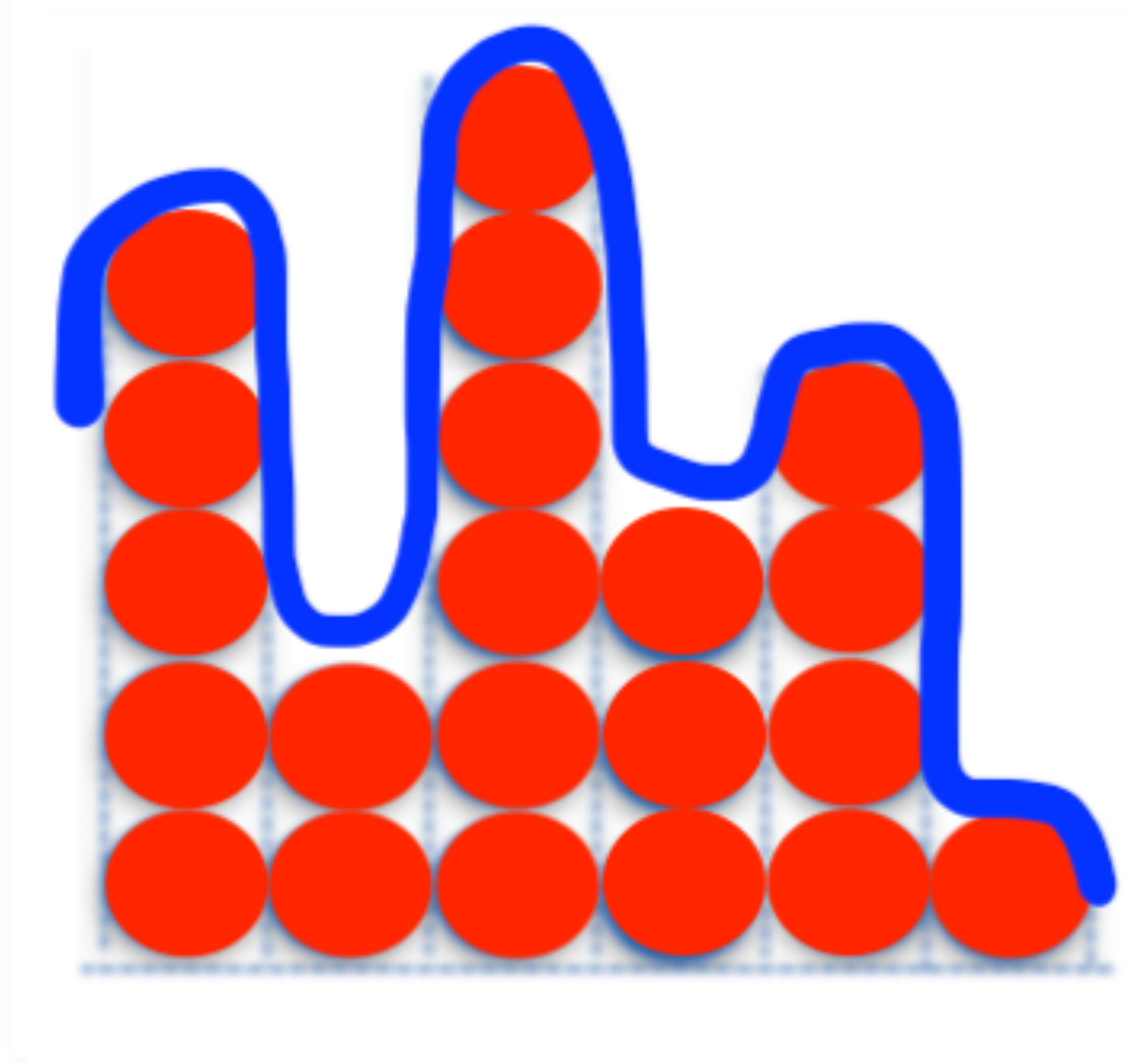

Continuous **fluctuations**

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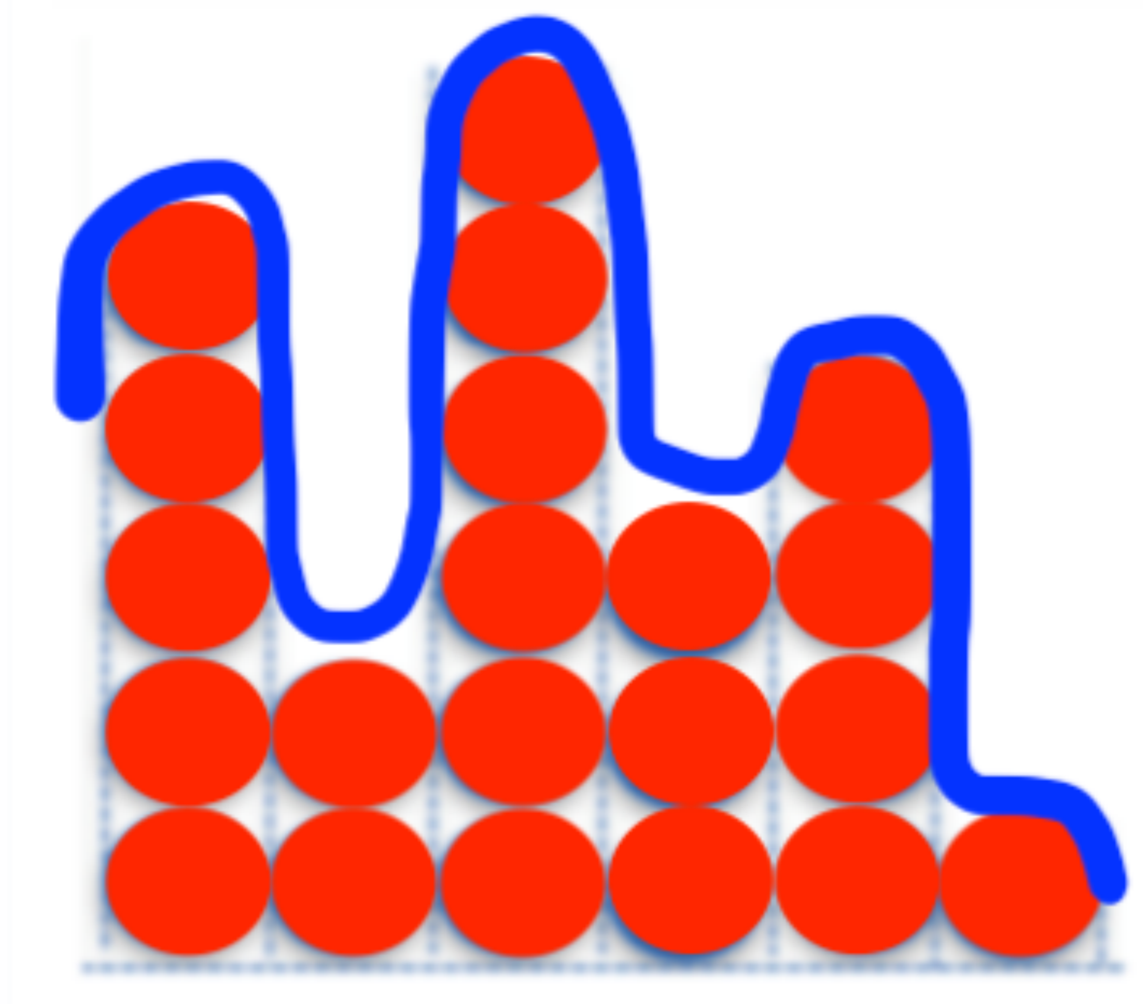
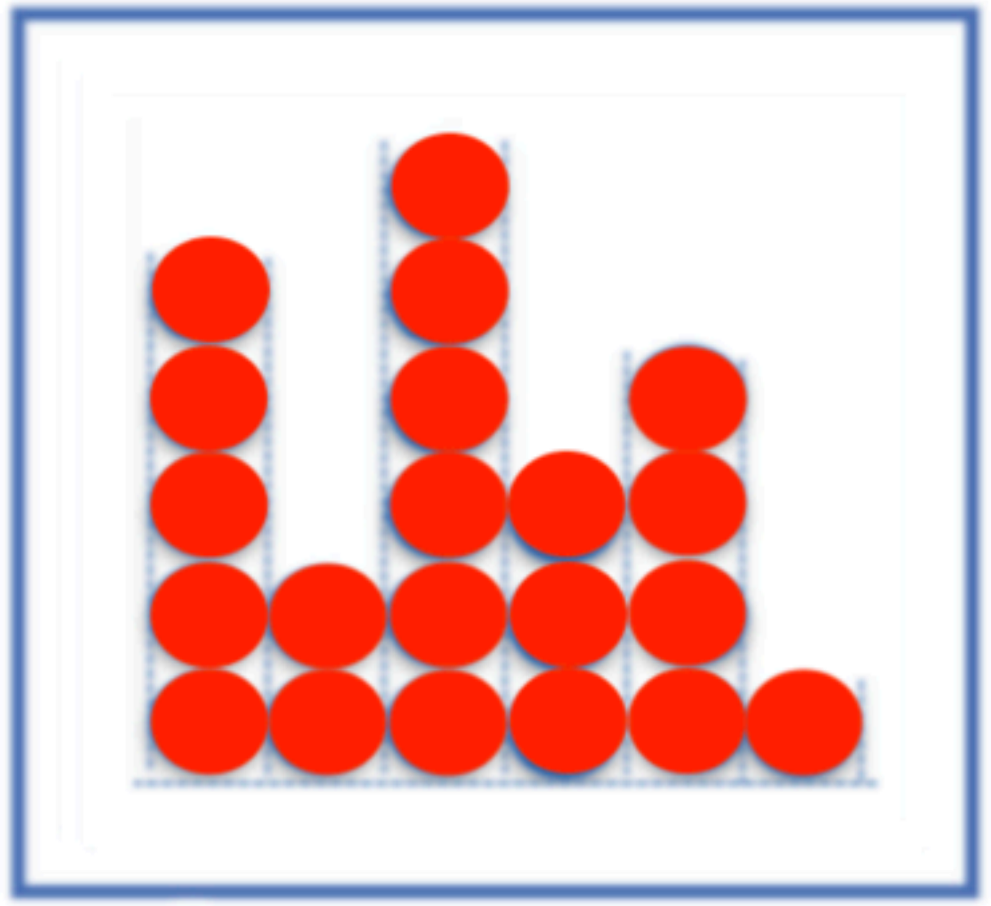


Continuous **fluctuations**

$\rho - \overline{\rho}$

Theory of **Fluctuating Hydrodynamics**

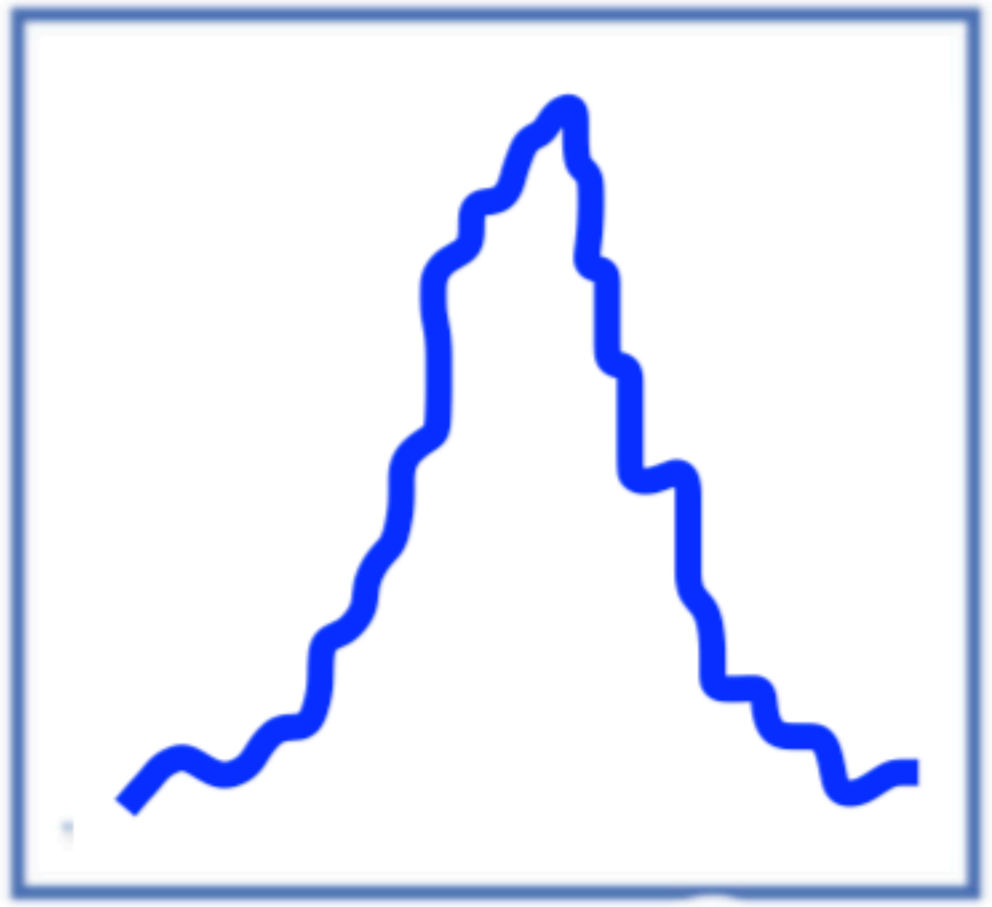
N particles



μ

Particle fluctuations $\mu - \overline{\mu}$

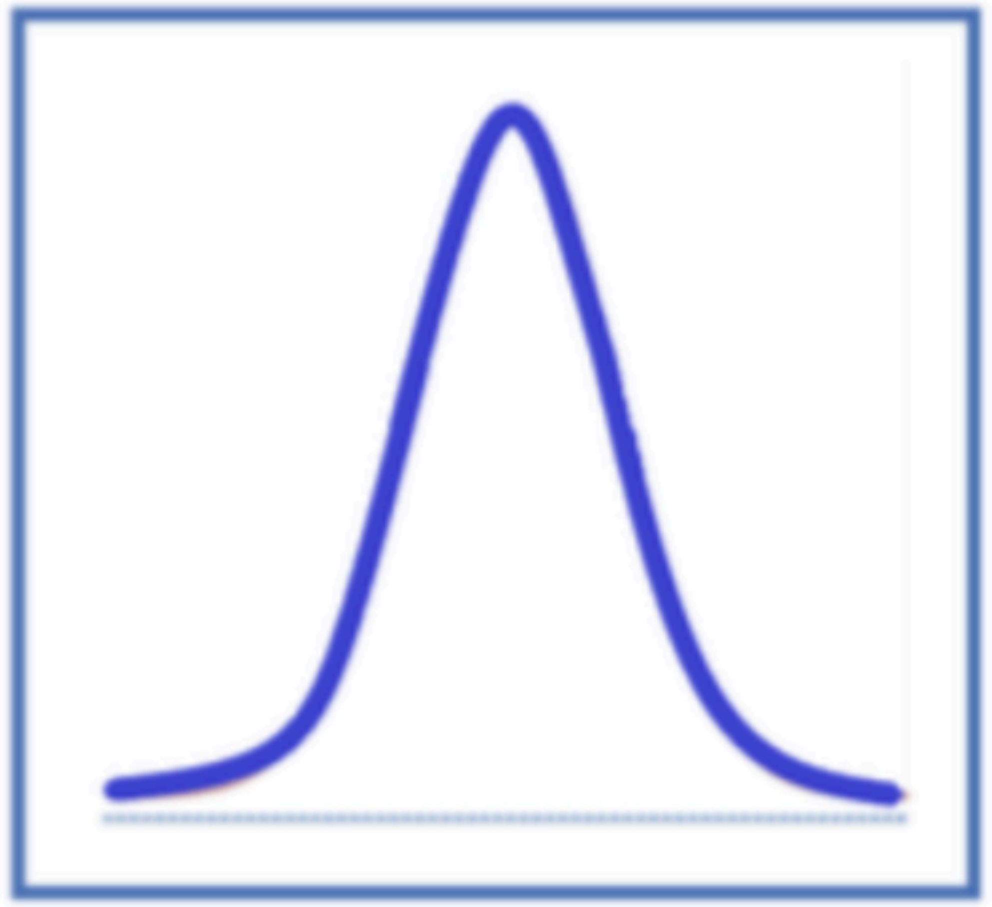
SPDE



ρ

Continuous fluctuations $\rho - \overline{\rho}$

Mean-field limit PDE ($N \to \infty$)



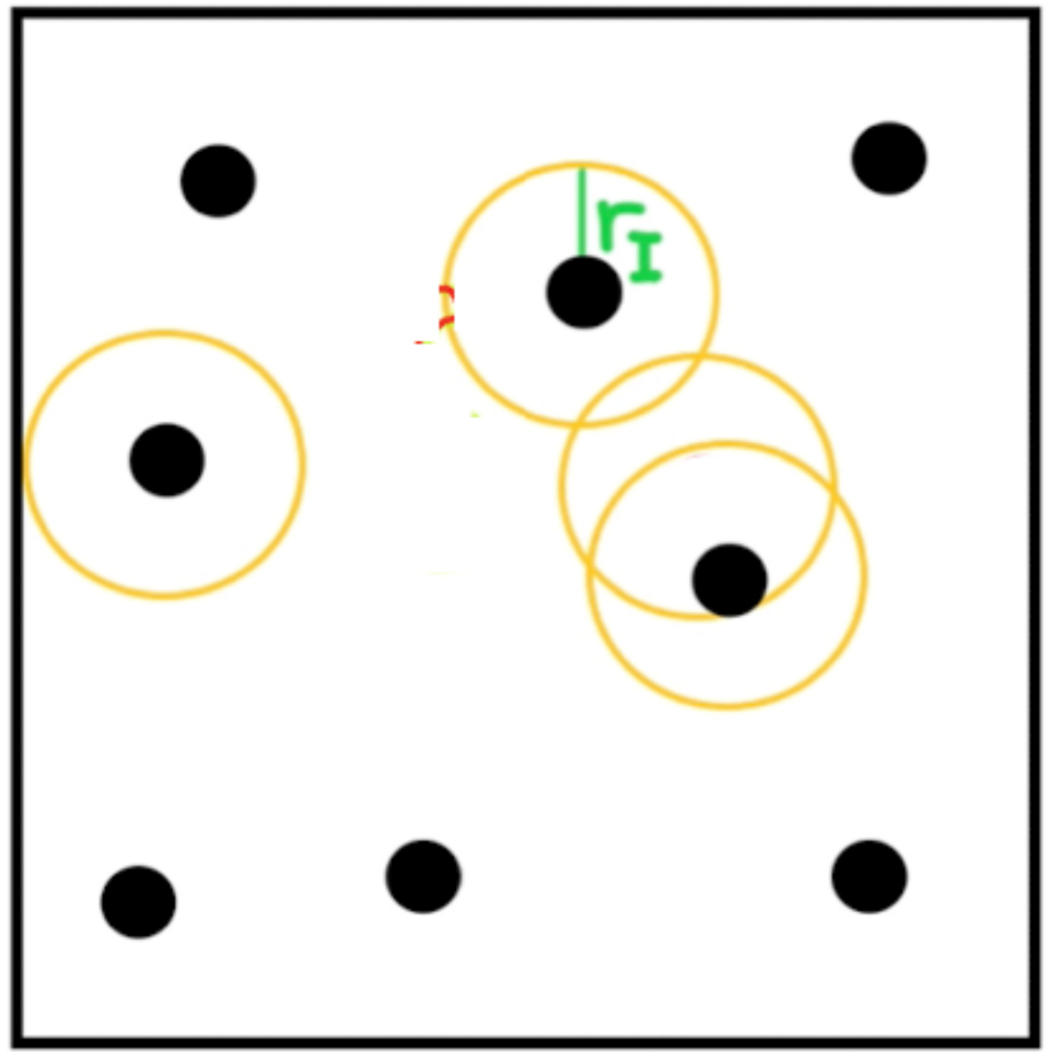
$\overline{\rho}$

Why moving from particles to **SPDEs**?

Computational efficiency for large particle systems ($N \gg 1$).

In this talk:

Part A: a specific setting
Part B: aspects of interest



For **Part A** of talk: consider **one** self-interacting species

$$dX_i = -N^{-1}\sum_{j=1}^{N}\nabla V(X_i - X_j)dt + dW_i$$

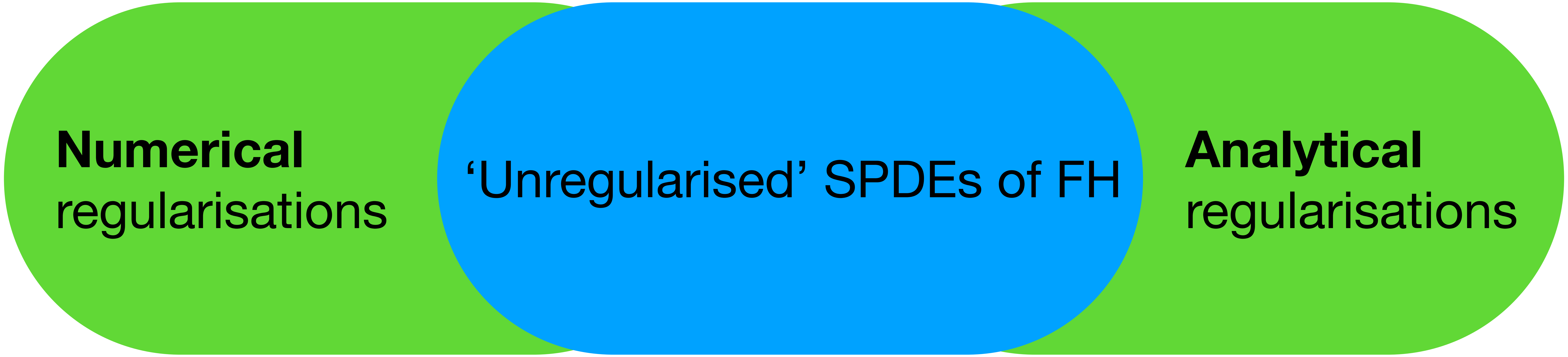
$$\partial_t \rho = \frac{1}{2}\Delta\rho + \nabla\cdot\left(\rho\nabla V * \rho\right) + N^{-1/2}\nabla\cdot(\sqrt{\rho}\xi)$$

Goal: study empirical density $\mu(t) := N^{-1}\sum_{i=1}^{N}\delta_{X_i(t)}$ of N weakly interacting particles in $\mathbb{T}^d$

$$dX_i = -N^{-1}\sum_{j=1}^{N}\nabla V(X_i - X_j)dt + dW_i$$

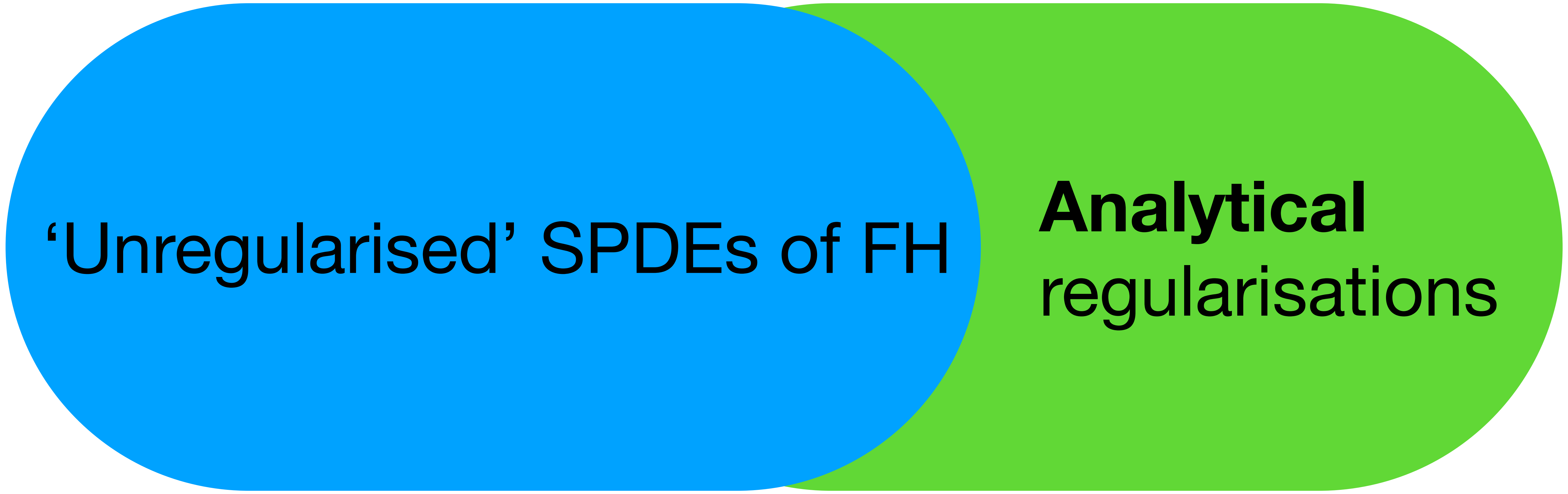
$\mu(t) = N^{-1} \sum_{i=1}^{N} \delta_{X_i(t)}$ is precisely the **only** solution to (DK) eqn. ($\mu \equiv \rho$)

[T. Lehmann, V. Konarovskyi, M.-K. von Renesse, '19]

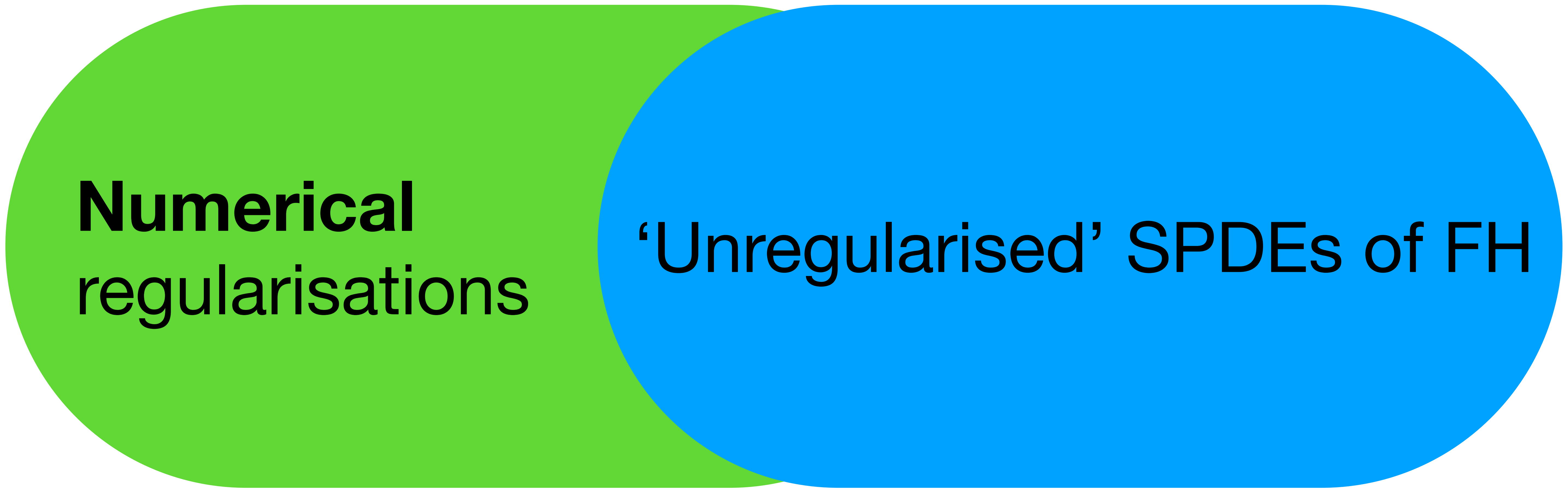

Numerical regularisations
‘Unregularised’ SPDEs of FH
Analytical regularisations

‘Unregularised’ SPDEs of FH

- *[Konarovskyi, Lehmann, von Renesse]*
- *[Dirr, Zimmer, Stamatakis]*
- *[Fehrman, Gess]*
- *[von Renesse, Sturm]*
- *[Marx]*
- *[Ayala, Zimmer]*
- *[Dello Schiavo]*
- …………………..



- *[Fehrman, Gess]*
- *[Gess, Gvalani, Konarovskyi]*
- *[Fehrman, Gess, Gvalani]*
- *[Djurdjevac, Kremp, Perkowski]*
- *[C., Shardlow, Zimmer]*
- *[Fehrman, Clini]*
- *[Martini, Mayorcas]*
- *[Grün]*
- *[Popat]*
- *[Gess, Zhang, Wu]*
- *……………..*



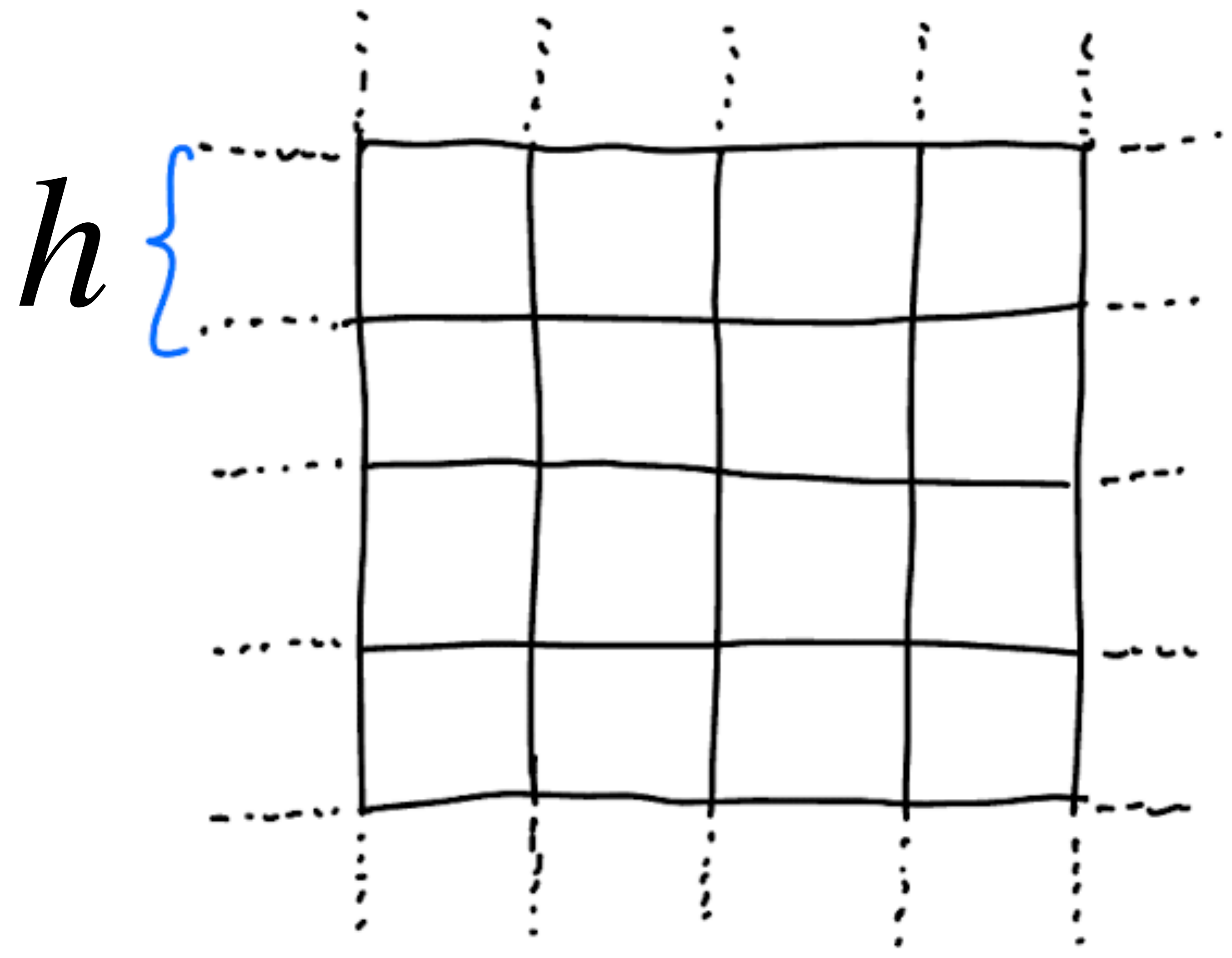
- *[Baňas, Gess, Vieth]*: **finite elements** (for weak formulation of regularised DK equation)
- [*L. Helfmann et al.*], [*C. Kim et al.*]: **finite elements** for reaction/diffusion equations
- [*A. Russo et al.*] [*A. Donev, E. Vanden-Eijnden, A. Garcia, and J. Bell.*] **Finite volume** schemes for stochastic gradient flow equations
- *[X. Li, N. Dirr, P. Embacher, J. Zimmer, C. Reina]:* full reconstruction of dissipative operators
- *[C., Shardlow]* **discontinuous Galerkin** + modelling for inertial DK systems
- *[N. Gerber, A. Schlichting, R. Gvalani, G. Pavliotis, A. Shalova]* Phase transitions, metastability, and coarsening .
- *[C. and J. Fischer] [C., Fischer, Ingmanns, C. Raithel]* High-order approximation for density fluctuation (**finite differences**) in diffusive / weakly interacting particle systems
- *[C., Fischer]:* **multilevel Monte Carlo** methods
- *[Djdurdjevac, Almgren, Bell], [Djdurdjevac, Le Bris, Süli]* **Hybrid models** (SPDE / particles), positivity-preserving schemes
- …………..

$$\partial_t \rho = \frac{1}{2}\Delta\rho + \nabla\cdot\left(\rho\nabla V * \rho\right) + N^{-1/2}\nabla\cdot(\sqrt{\rho}\,\xi)$$

<u>Goal</u>: study empirical density $\mu(t) := N^{-1}\sum_{i=1}^{N}\delta_{X_i(t)}$ of N weakly interacting particles in $\mathbb{T}^d$

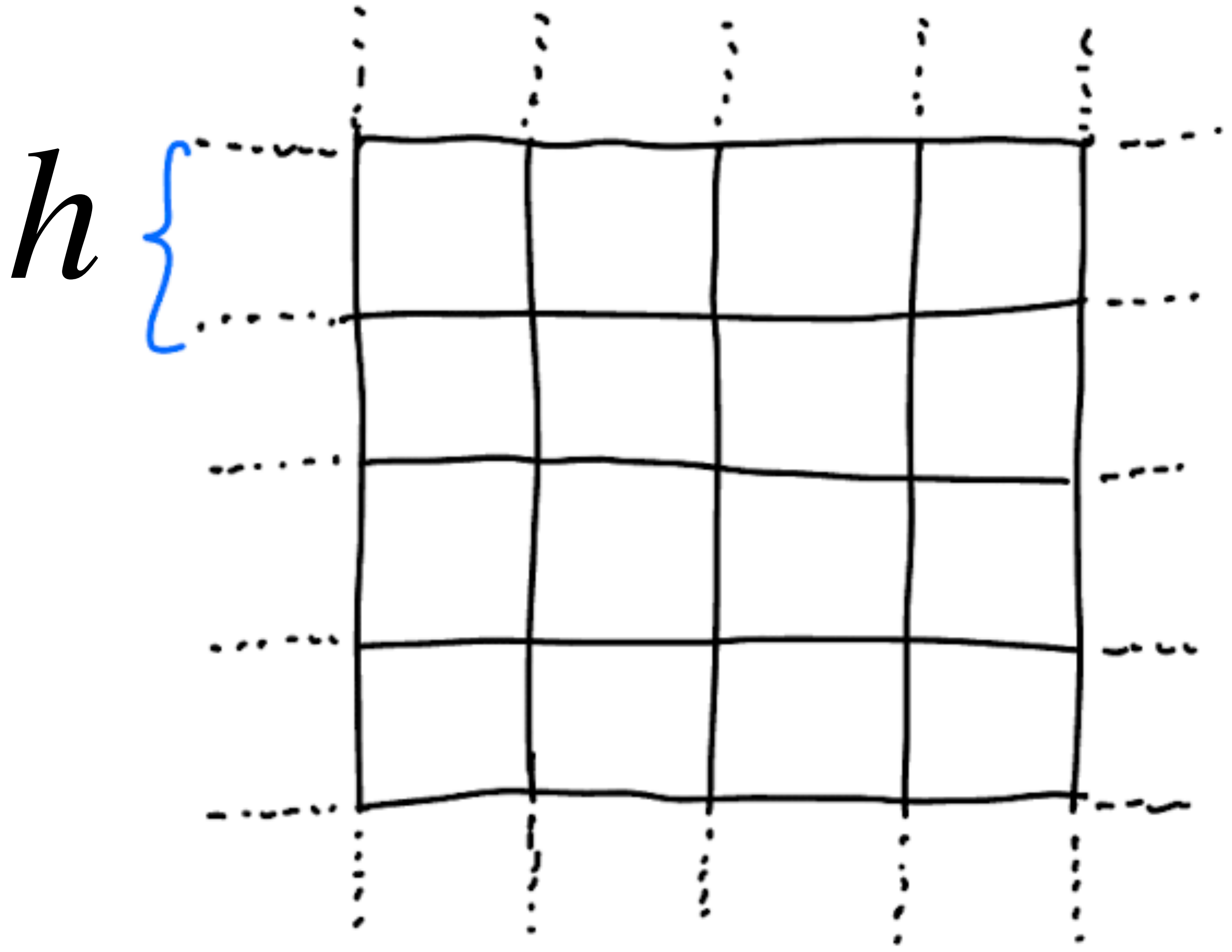
$$dX_i = -N^{-1}\sum_{j=1}^{N}\nabla V(X_i - X_j)dt + dW_i$$

Q: how to describe microscopic fluctuation $\mu - \overline{\mu}$ of N particles in $\mathbb{T}^d$ in terms of fluctuations $\rho_h - \overline{\rho}_h$ for a **discretised** version of DK?



$$\partial_t \rho_h = \frac{1}{2}\Delta_h \rho_h + \nabla_h \cdot \left(\rho_h \nabla_h V_h * \rho_h\right)_h + N^{-1/2} \nabla_h \cdot \left(\sqrt{\rho_h^+}\,\xi_h\right)$$

with Δ_h, ∇_h finite-difference operators

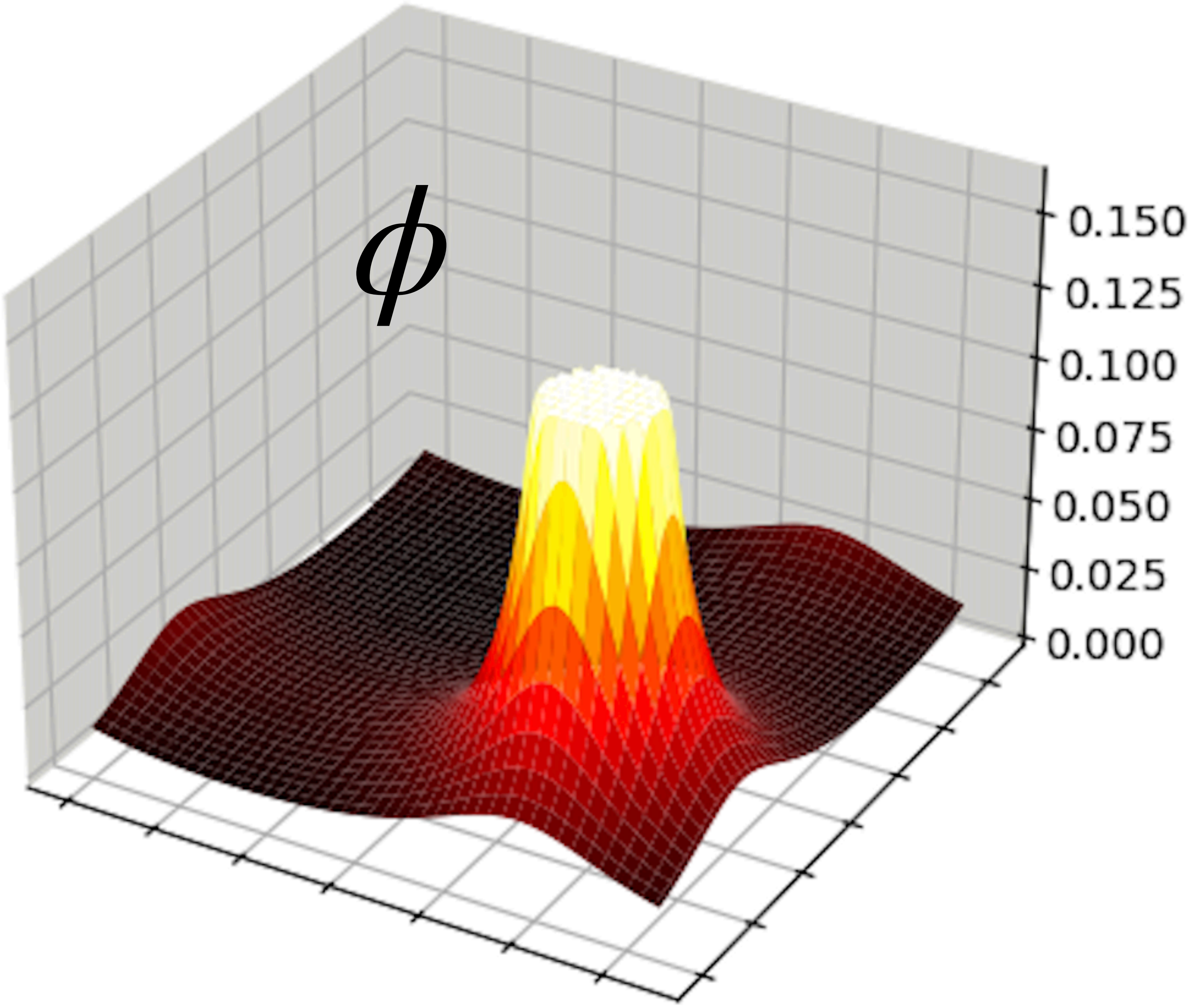


G_h

$$\xi_h(x,t) = \sum_{y \in G_h} e_y(x)\beta_y(t)$$

Expressing **fluctuations** in particle system:

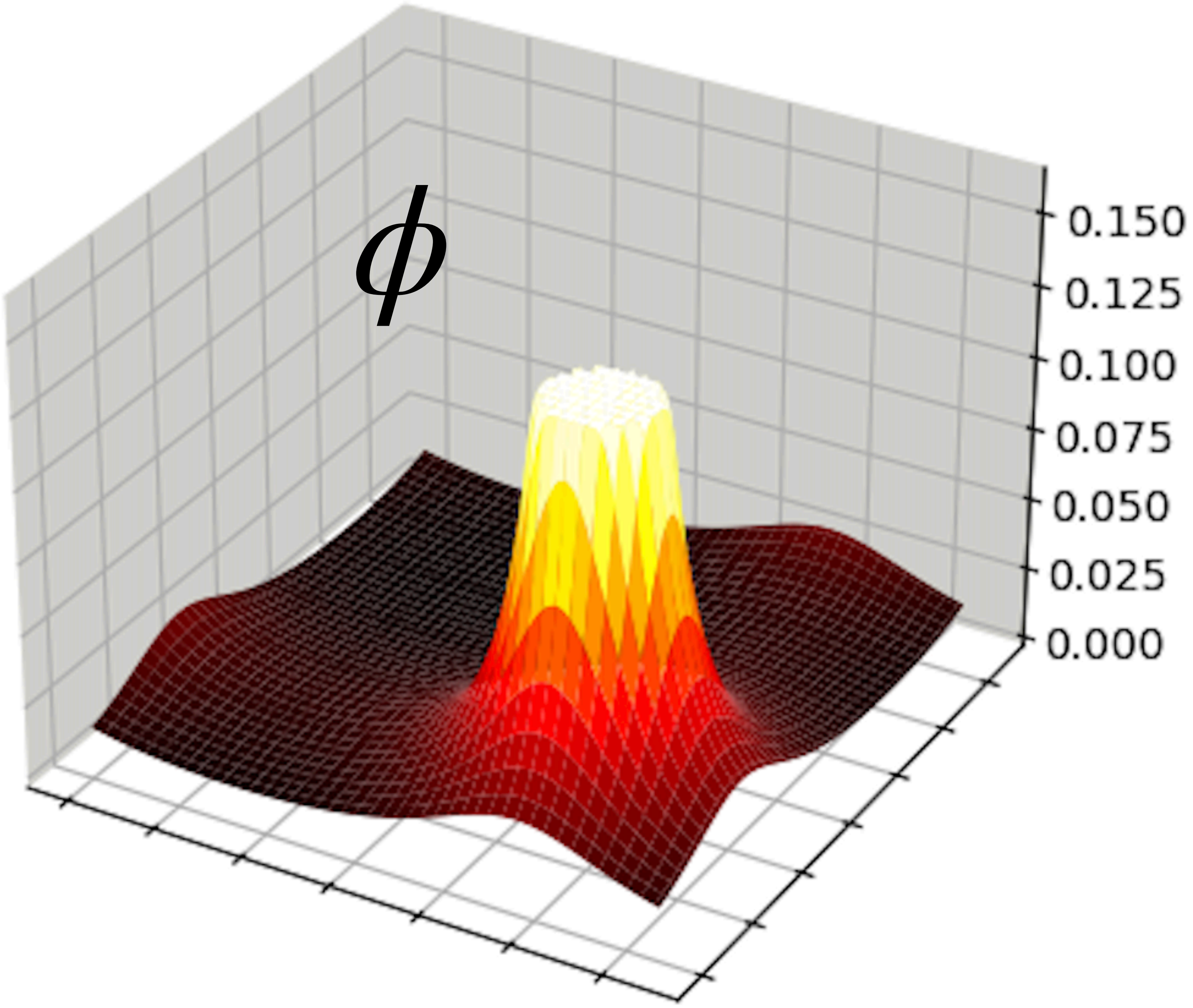
$$\mathbb{E}[\psi(N^{1/2}(\mu - \bar{\mu}, \phi))]$$



- ϕ? identify regions of interest.
- ψ? statistical properties of fluctuations (e.g., moments)
- $N^{1/2}$? scales fluctuations to $O(1)$

Computing **fluctuations** in particle system using DK model:

$$\mathbb{E}[\psi(N^{1/2}(\mu - \overline{\mu}, \phi))] \approx \mathbb{E}[\psi(N^{1/2}(\rho_h - \overline{\rho}_h, \phi_h)_h)]$$



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Natural (negative Sobolev-type) metric:

$$d_{-j}(\mu - \bar{\mu}, \rho_h - \bar{\rho}_h)$$
$$:= \sup_{\phi, \psi \in H^j_w} \left| \mathbb{E}[\psi(N^{1/2}(\mu - \bar{\mu}, \phi))] - \mathbb{E}[\psi(N^{1/2}(\rho_h - \bar{\rho}_h, \phi_h)_h)] \right|$$

Computing **fluctuations** in particle system using DK model:

$$\underbrace{\mathbb{E}[\psi(N^{1/2}(\mu - \overline{\mu}, \phi))]}_{=:P} \approx \underbrace{\mathbb{E}[\psi(N^{1/2}(\rho_h - \overline{\rho}_h, \phi_h)_h)]}_{=:P_h}$$

We want $MSE := \mathbb{E}[\,|\,P_h - \mathbb{E}[P]\,|^2\,] \lesssim \varepsilon^2$,

A. $|\,\mathbb{E}[P_h - E[P]]\,|^2 \lesssim \varepsilon^2$ (i.e., **small bias**)

B. $Var[P_h] \lesssim \varepsilon^2$ (i.e., **small variance**)

Small bias?

Theorem [F.C., J. Fischer, J. Ingmanns, C. Raithel, AoP 2025+] For $h > 0$ and $p \in \mathbb{N}$, there exists a finite-difference discretisation of (DK) on $[0,T]$ such that:

A. Solution ρ_h is **non-negative** up to stopping time τ, with

$$\mathbb{P}(\tau < T) \lesssim exp\{-N^\delta\}, \quad \text{for some } \delta > 0, \quad \text{subject to } \boxed{Nh^d \gg 1}$$

B. For test functions being differentiable j times, up to stopping time τ, fluctuations bounded by

$$d_{-j}(\mu - \bar{\mu}, \rho_h - \bar{\rho}_h) \lesssim \underbrace{h^{p+1}}_{Err_{num}} + \underbrace{N^{-j/2}}_{Err_{fluct}}$$

Main idea

Goal: estimate

$$M(\psi, \phi) := \mathbb{E}[\psi(N^{1/2}(\mu - \overline{\mu}, \phi))] - \mathbb{E}[\psi(N^{1/2}(\rho_h - \overline{\rho}_h, \phi_h)_h)]$$

Main idea

Goal: estimate

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Method: Itô calculus for $M(\psi, \phi)$ leads to:

Main idea

Goal: estimate

$$M(\psi, \phi) := \mathbb{E}[\psi(N^{1/2}(\mu - \bar{\mu}, \phi))] - \mathbb{E}[\psi(N^{1/2}(\rho_h - \bar{\rho}_h, \phi_h)_h)]$$

Method: Itô calculus for $M(\psi, \phi)$ leads to:

A. More terms of same kind $N^{-1/2}M(\tilde{\psi}, \tilde{\phi})$ (**iteration!!!**)
B. Residuals, including numerical error (**NO iteration!!!**)

Ito formula for $M(\psi, \phi)$

$$d(\mathbb{E}[\psi(N^{1/2}(\mu - \bar{\mu}, \phi))] - \mathbb{E}[\psi(N^{1/2}(\rho_h - \bar{\rho}_h, \phi_h)_h)])$$

$$\propto N^{-1/2} \cdot \{\mathbb{E}[\tilde{\psi}(N^{1/2}(\rho_h - \bar{\rho}_h, \phi_h)_h) N^{1/2}(\rho_h - \bar{\rho}_h, |\nabla_h \phi_h|^2)_h]$$

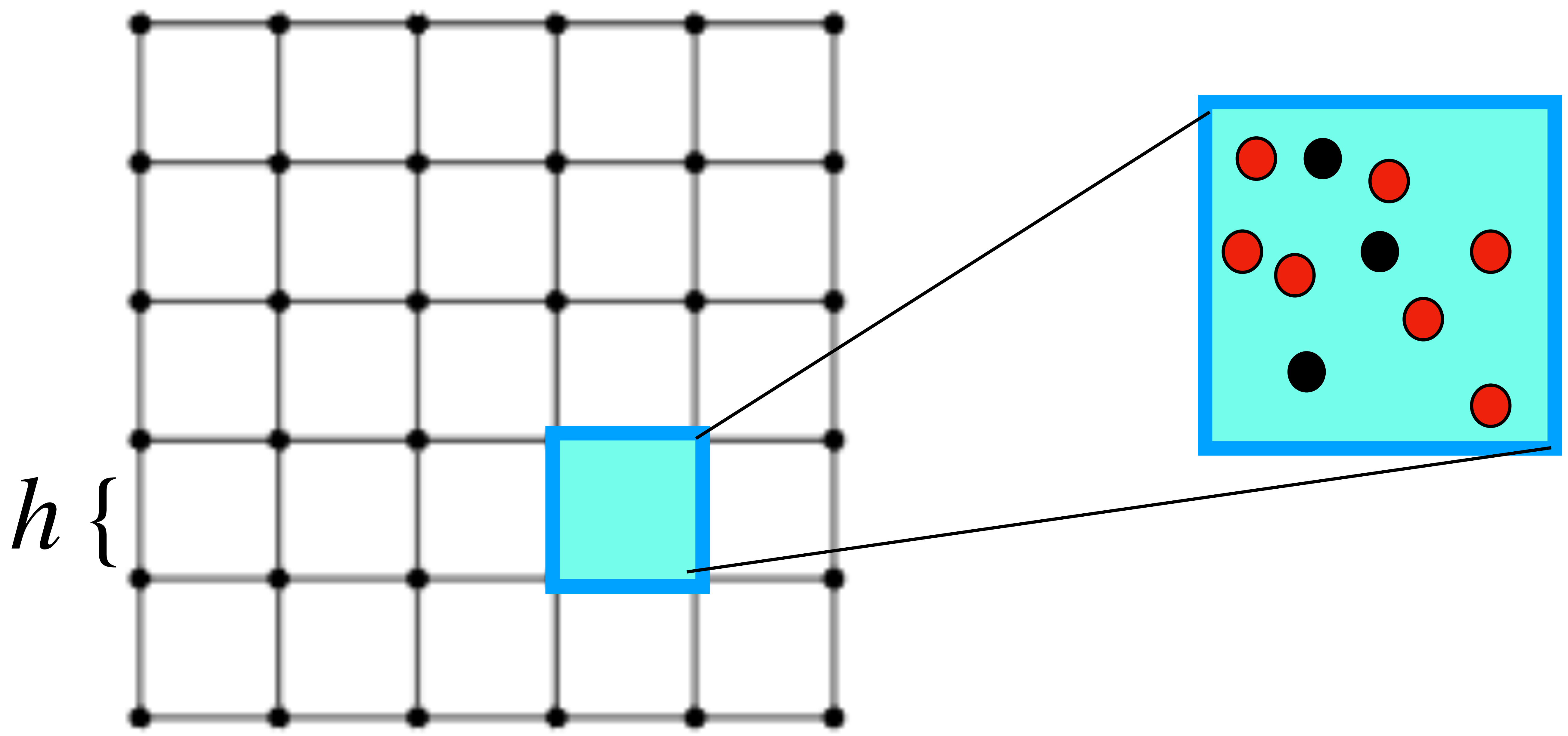
$$-\mathbb{E}[\tilde{\psi}(N^{1/2}(\mu - \bar{\mu}, \phi)) N^{1/2}(\mu - \bar{\mu}, |\nabla \phi_1|^2)]\} dt$$

$+[$**nonlinear convolution terms**$]dt$

$+[$**residuals**$]dt$

Cross-variation of DK noise is linear in the density!

We have $\rho_h \geq 0$ up to τ, with $\mathbb{P}(\tau < T) \approx exp\{-N^\delta\}$, if $\boxed{Nh^d \gg 1}$



$\boxed{Nh^d \gg 1}$: SPDE **cheaper** when # particles $N \gg$ # grid points h^{-d}

Linearising convolutional terms

Idea: linearise using Fourier expansion (separation of variables)

$$
\begin{aligned}
&(\rho_h - \bar{\rho}_h)\, \nabla_h V * (\rho_h - \bar{\rho}_h) \\
&\quad = \{\, \nabla_h V(x - y) = \sum_{m,n} F_{m,n} e^{im\cdot x} e^{in\cdot y} \} \\
&\quad = \sum_{m,n} F_{m,n} \underbrace{(\rho_h(x) - \bar{\rho}_h(x), e^{im\cdot x})_h}\, \cdot\, \underbrace{(\rho_h(y) - \bar{\rho}_h(y), e^{in\cdot y})_h}
\end{aligned}
$$

$$M(\psi,\phi) \propto N^{-1/2}\cdot M(\tilde{\psi},\tilde{\phi}) + \underbrace{h^{p+1}}_{Err_{num}} + \underbrace{\exp(-N^{\delta})}_{Err_{negativity}}$$

Iterate!

Fluctuations error "scaling gain" for each iteration step

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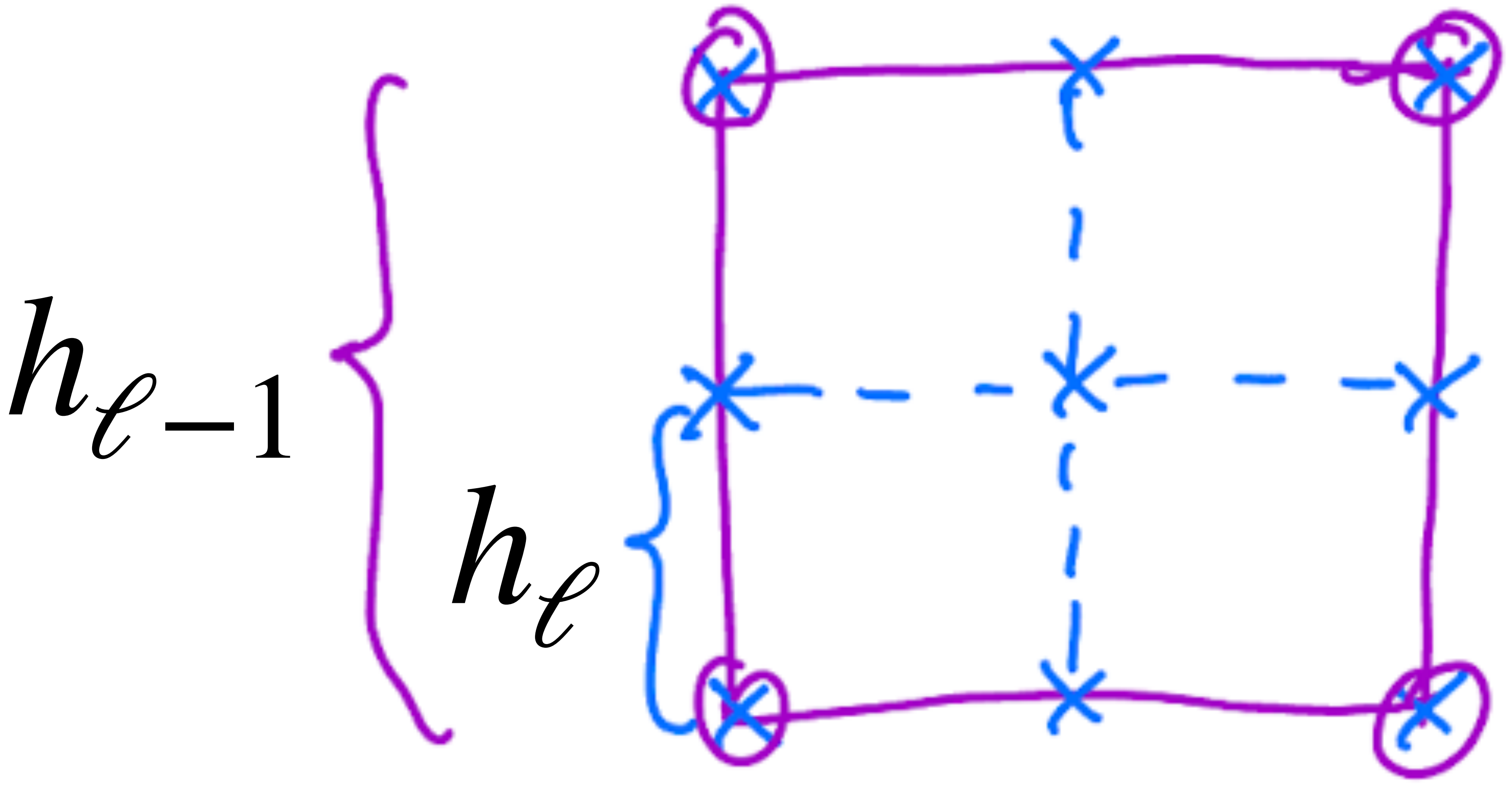
Small variance?



Need to produce coupled SPDE estimators $P_\ell, P_{\ell-1}$

Theorem [FC, J. Fischer, SIAM J. Numer. Anal., 25+] For fixed $\varepsilon > 0$, and in the particle <u>high-density regime</u>, we can set up **Multilevel** MC method reducing cost of standard MC method by

$$F_{cost\ red} \propto \begin{cases} \epsilon^{-2}, & \text{for noise coupling on Fourier modes,} \\ \epsilon^{-1}, & \text{for noise coupling on neighbouring points,} \end{cases}$$

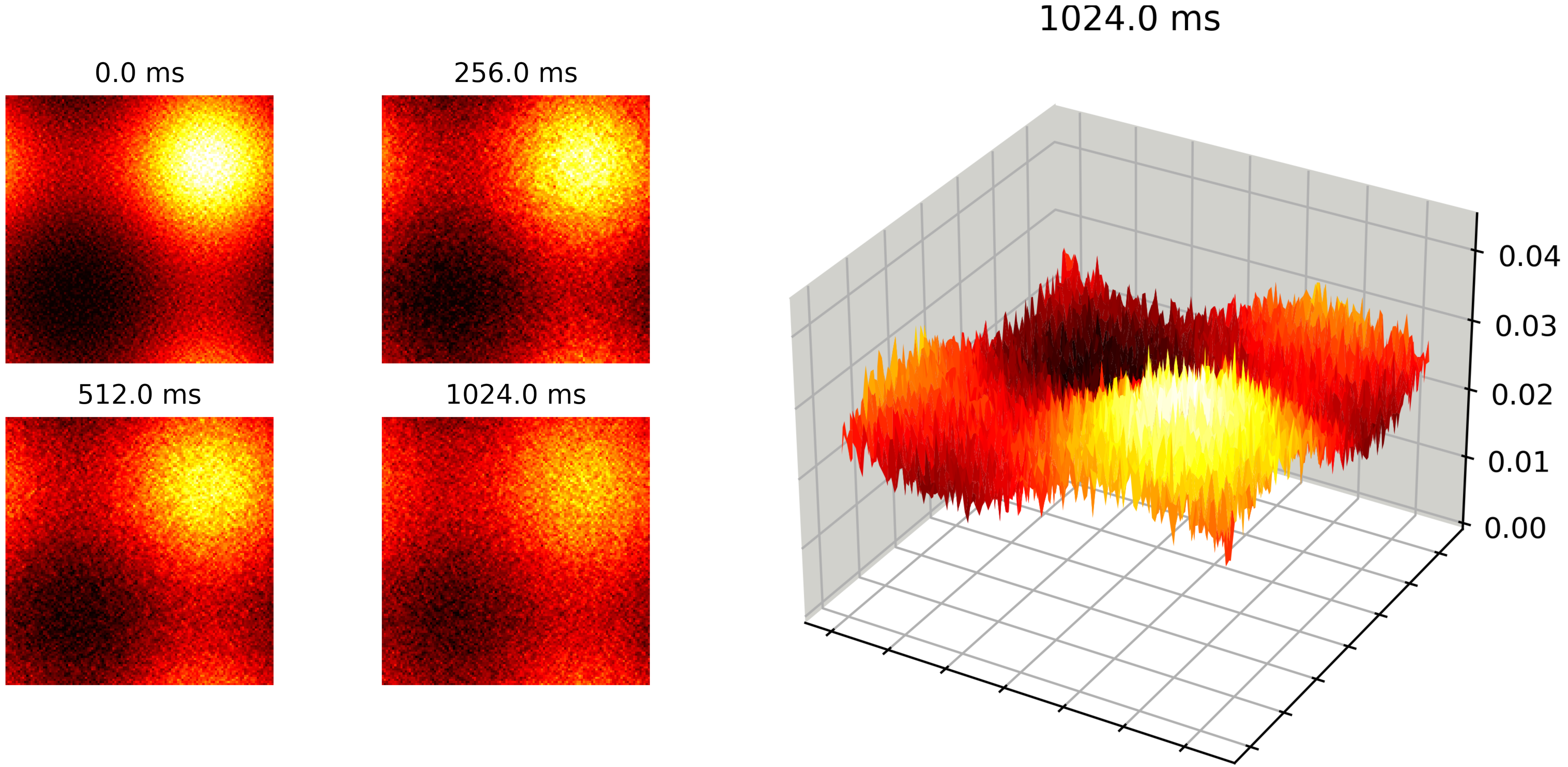
Key ingredient for variance reduction

$$Var[P_\ell - P_{\ell-1}] \lesssim (Nh_\ell^d)^{-1} + h_\ell^2$$

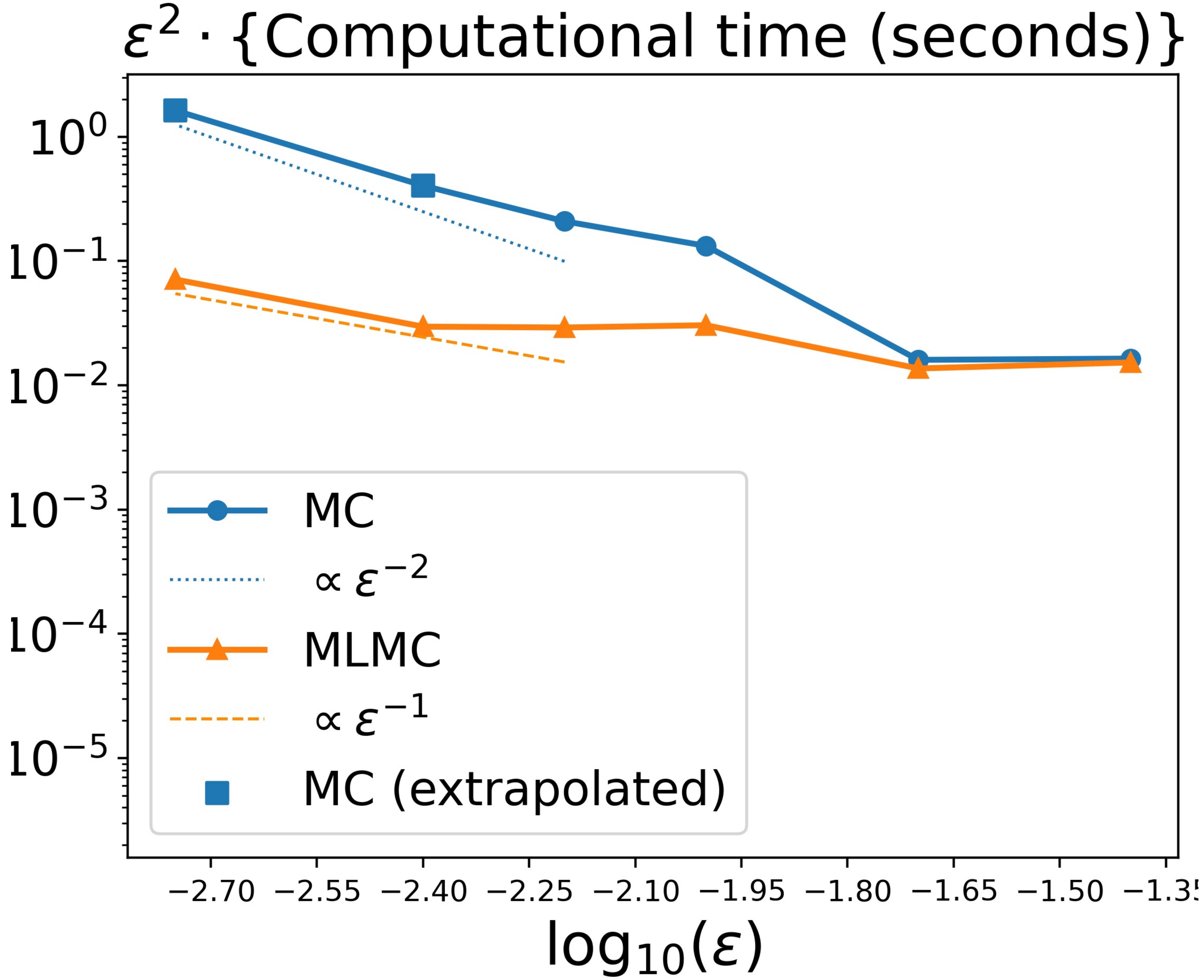
(inverse of) average particle density
= **“size of SPDE noise”**

Numerical
error

ρ_h for 'small' h

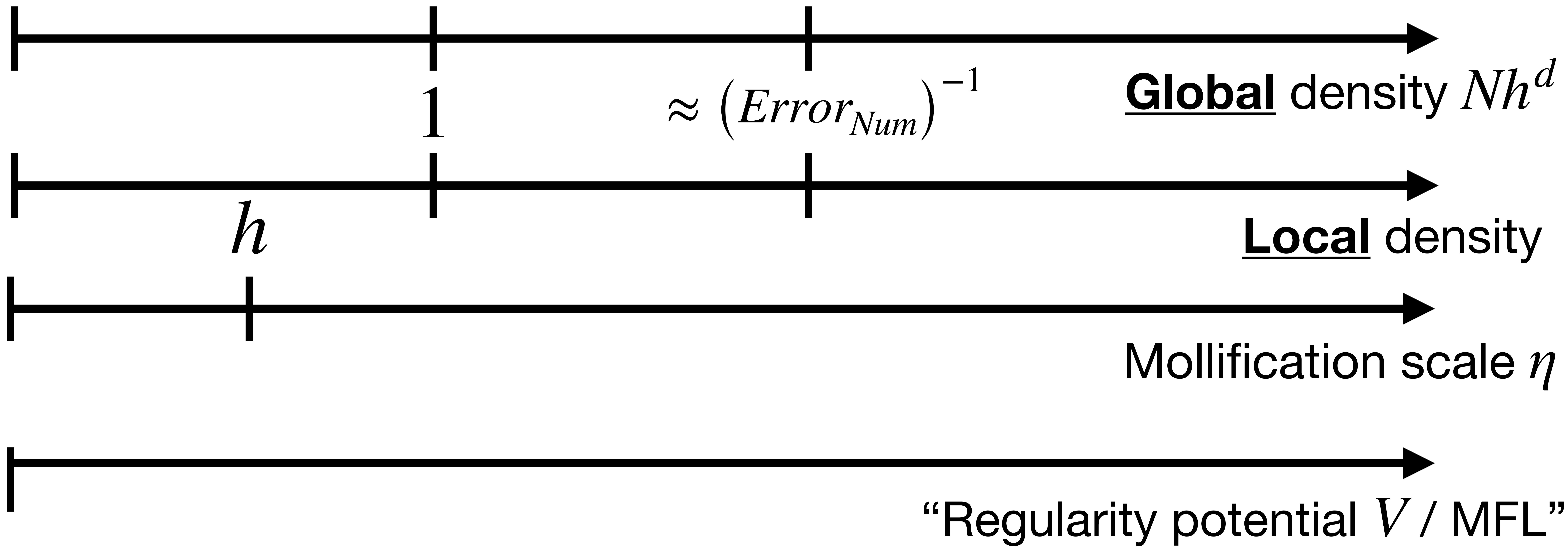


High-density: $Nh_{min}^2 \gtrsim h_{min}^{-2}$

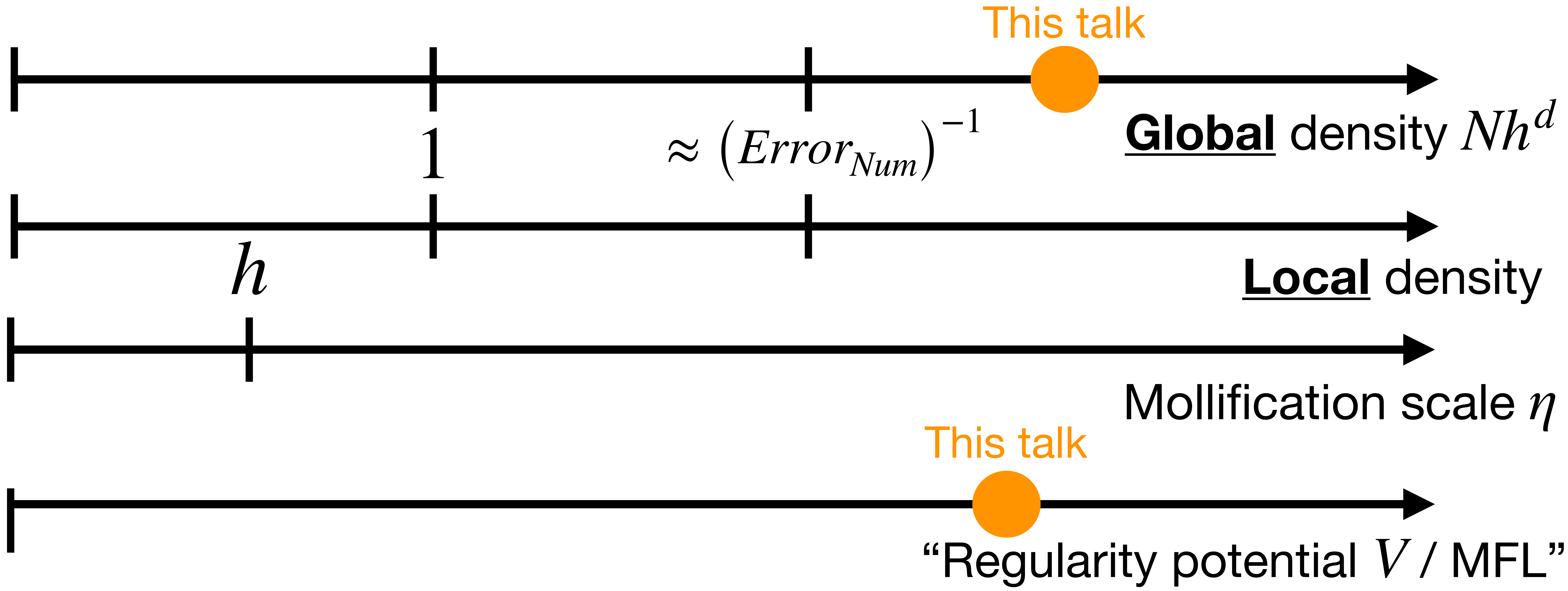


Although DK SPDE is singular, numerical discretisations work well in high-density regime $Nh^d \gg 1$

Part B: aspects of interest



1
$\approx \left(Error_{Num}\right)^{-1}$
Global density Nh^d
h
Local density
Mollification scale η
"Regularity potential V / MFL"


This talk
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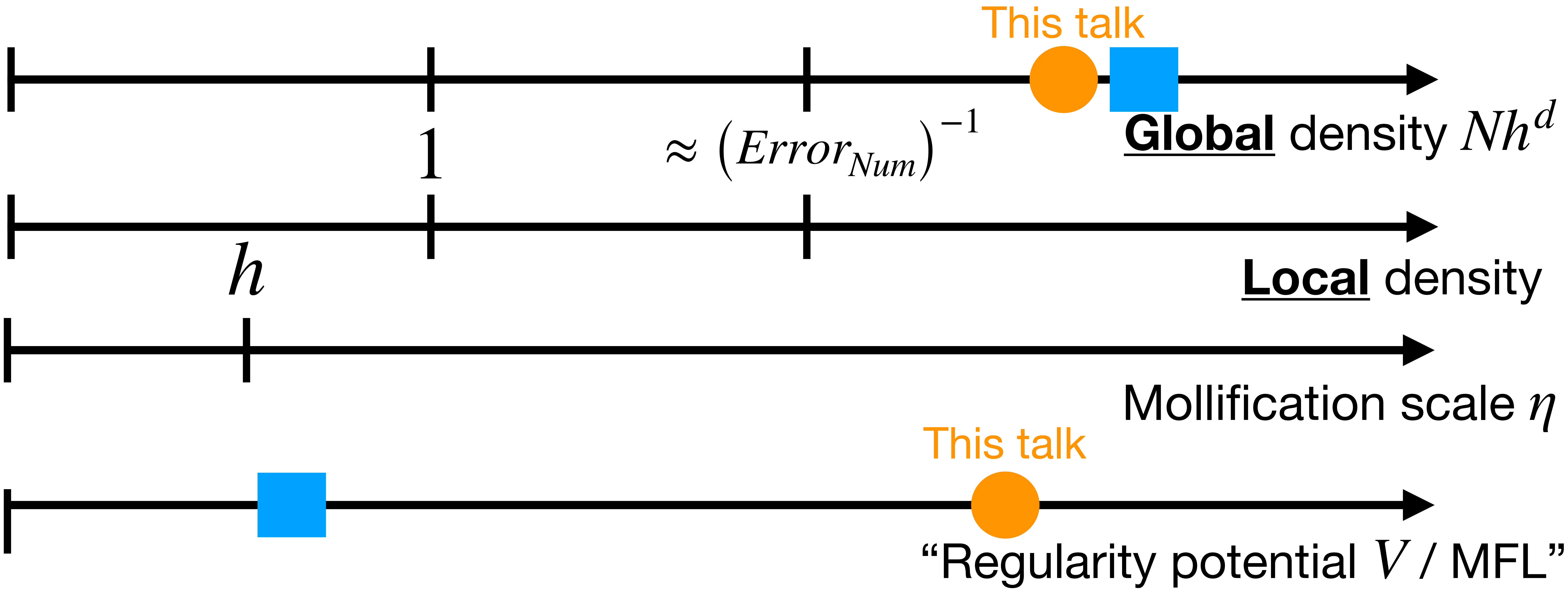
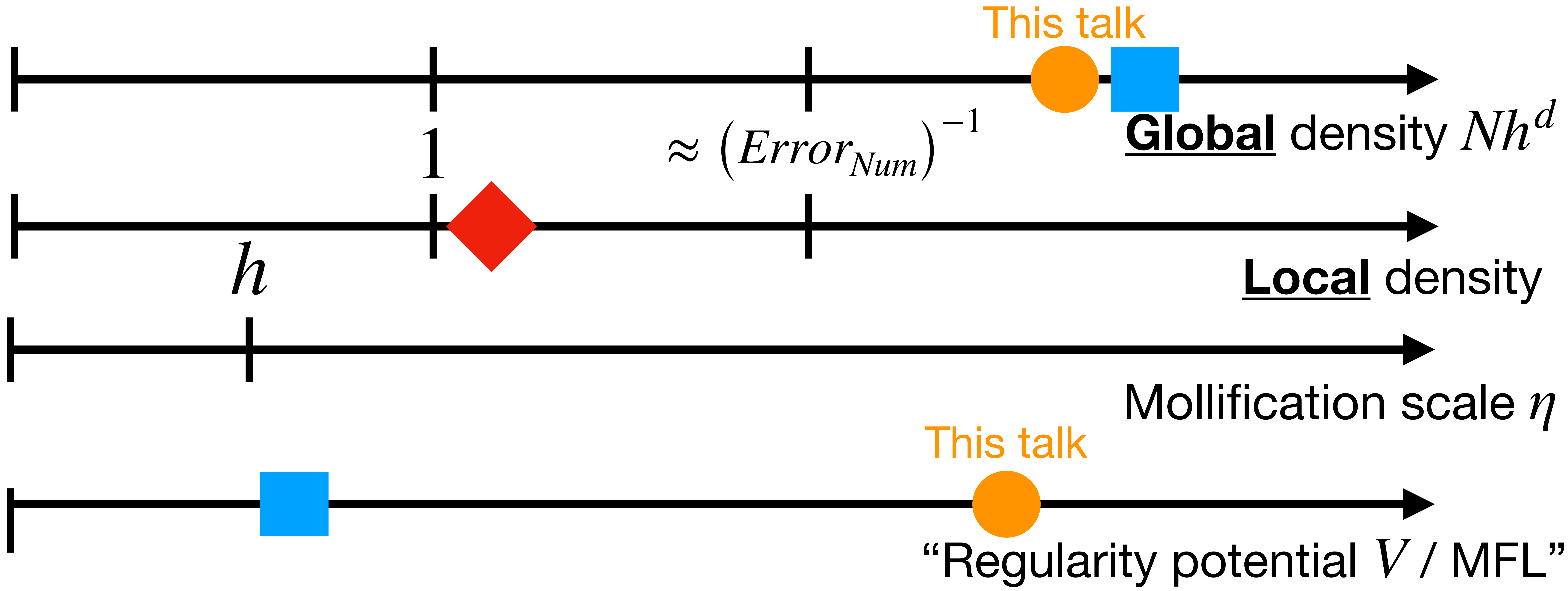


- A1: low-regularity of V (work in progress on cross-diffusion with J. Ingmanns / C. Raithel)



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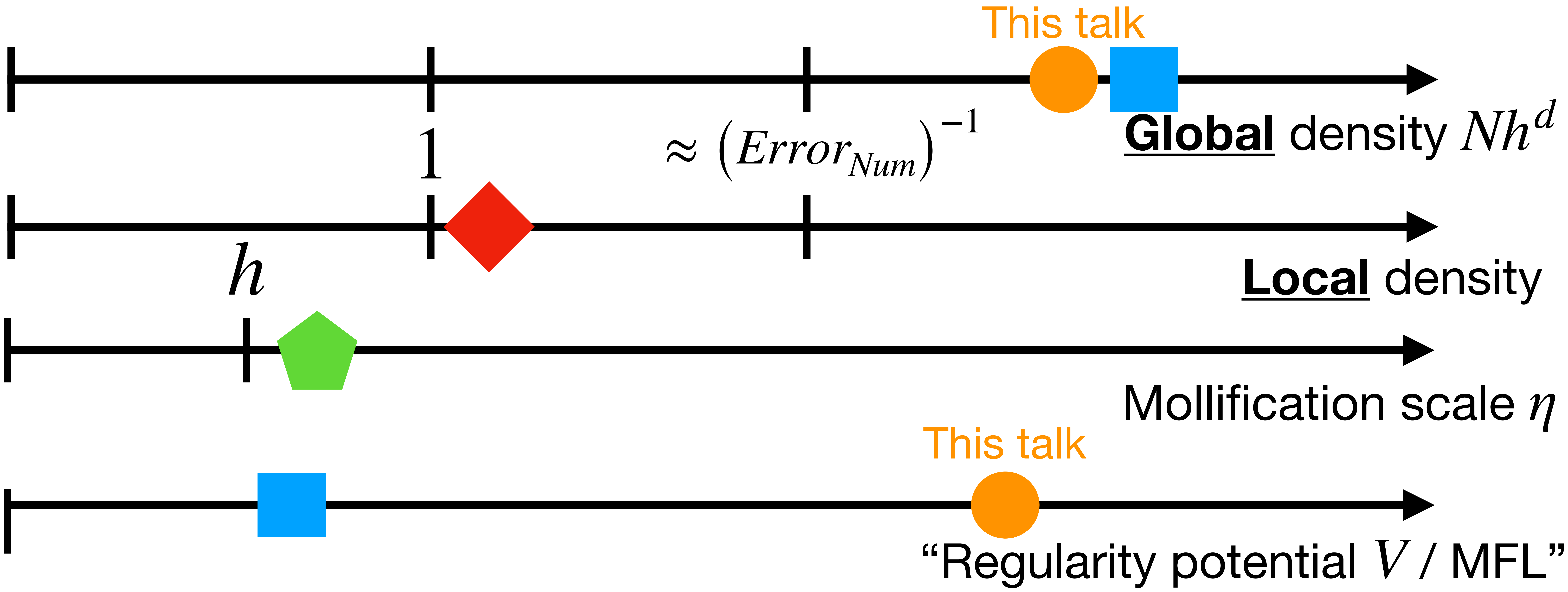
- A2: Hybrid particles/SPDE models (A. Djurdjevac, A. Almgren, J. Bell)



- A1: low-regularity of V (work in progress on cross-diffusion with J. Ingmanns / C. Raithel)
- A2: Hybrid particles/SPDE models (A. Djurdjevac, A. Almgren, J. Bell)
- A3: h (numerical scale) vs. η (analytical scale): approximating radial distribution function / coarse graining

[1] FC and J. Fischer, *The Dean-Kawasaki equation and the structure of density fluctuations in systems of diffusing particles*,
Arch. Rational Mech. Anal. (2023)

[2] FC, J. Fischer, J. Ingmanns, C. Raithel, *Density fluctuations in weakly interacting particle systems via the Dean-Kawasaki equation,*
Ann. Probab. (to appear, 2025)

[3] FC and J. Fischer, *Multilevel Monte Carlo methods for the Dean-Kawasaki equation from Fluctuating Hydrodynamics*,
SIAM J. Numer. Anal. (2025)

[4] FC, J. Ingmanns, C. Raithel, *Quantitative fluctuation bounds in models of cross-diffusion (in preparation)*

Thanks for listening!