Fluctuations in Hybrids

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Multi-algorithm Methods for Multiscale Simulations
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Outline

Problem Statement

Fluctuations

Hybrids

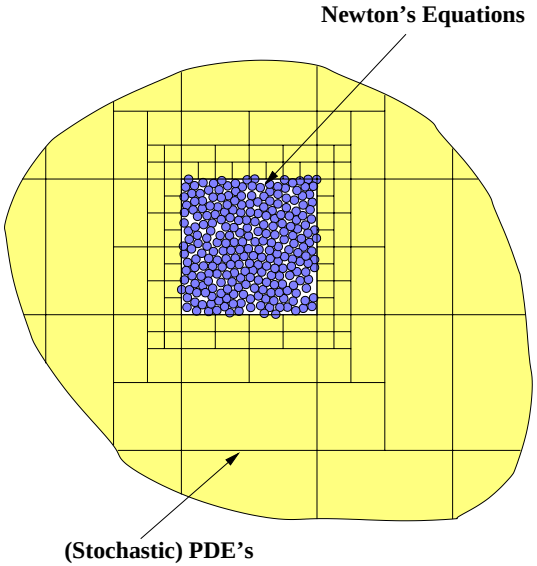
- Linear Diffusion
- Transport with Correlations
- Phase Ordering Dynamics

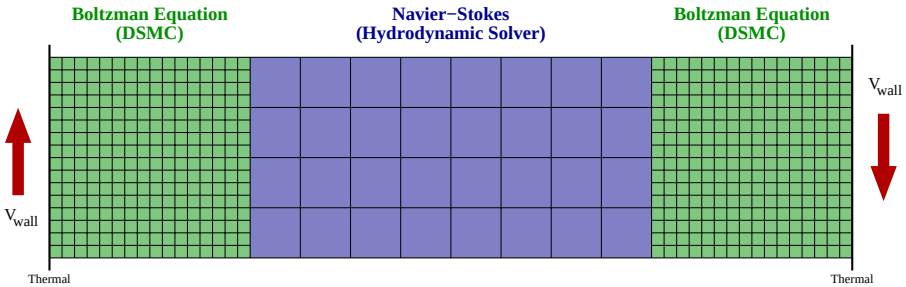
Conclusions

Goal (Motherhood and Apple Pie)

The accurate and efficient simulation of multiscale phenomena

- Different spatial regions require different physics/resolutions
- Use computationally cheapest, ***valid***, method in each region
- Dynamically couple methods
- Computational Gain $=V_{macro}/V_{micro}$
- Analogous to improvements on Landau theory of phase transitions in the 1960's





Why look at fluctuations?

- Fluctuations drive some physical phenomena
- Fluctuations are largely ignored in other work
- Fluctuations set time-scales: e.g.,

  Fluid Instabilities (e.g., Rayleigh-Benard)

  Nucleation (metals under extreme conditions)

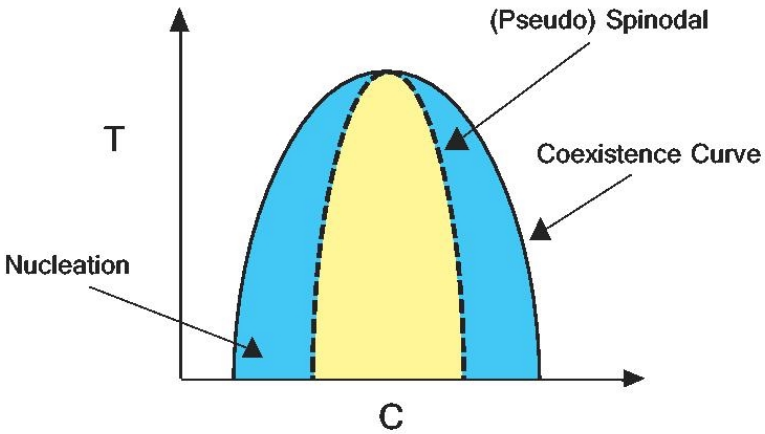
  Source of energy (Brownian Motors)

  Rare events (Failures)
- If fluctuations drive the physics, then the hybrid must not alter the fluctuations (neither enhance or reduce).

Fluctuations: Nucleation

- Temperature Dependent Nucleation Rate
- $\Gamma = \exp(-\Delta F/k_B T)$

$\Delta F = (16\pi\sigma^3)/(3(\Delta\varphi)^2 H^2)$



Fluctuations: Particle Filters/State Estimation:

State Variable

$$\frac{d\mathbf{x}}{dt} = f(\mathbf{x},t) + \mathbf{D}^{1/2}(\mathbf{x},t)\mathbf{q}(\mathbf{x},t)$$

Stochastic Nonlinear Dynamics
PDE, ODE, etc.

Noise Covariance
Possible Time Dependence

Noise :Additive, Multiplicative
Gaussian, Non-Gaussian etc

Function of state variable

Observations

$$\mathbf{r}_m = \mathbf{Z}(\mathbf{x}(t_m),t_m) + \boldsymbol{\rho}_m$$

Measurement Error

$$i = 1,\ldots,M$$

Index of Measurements

Fluctuations: Particle Filters/ State Estimation:

- Determine best estimate of the state at various times
- Determine uncertainty in these measurements
- Three Classes of problems:

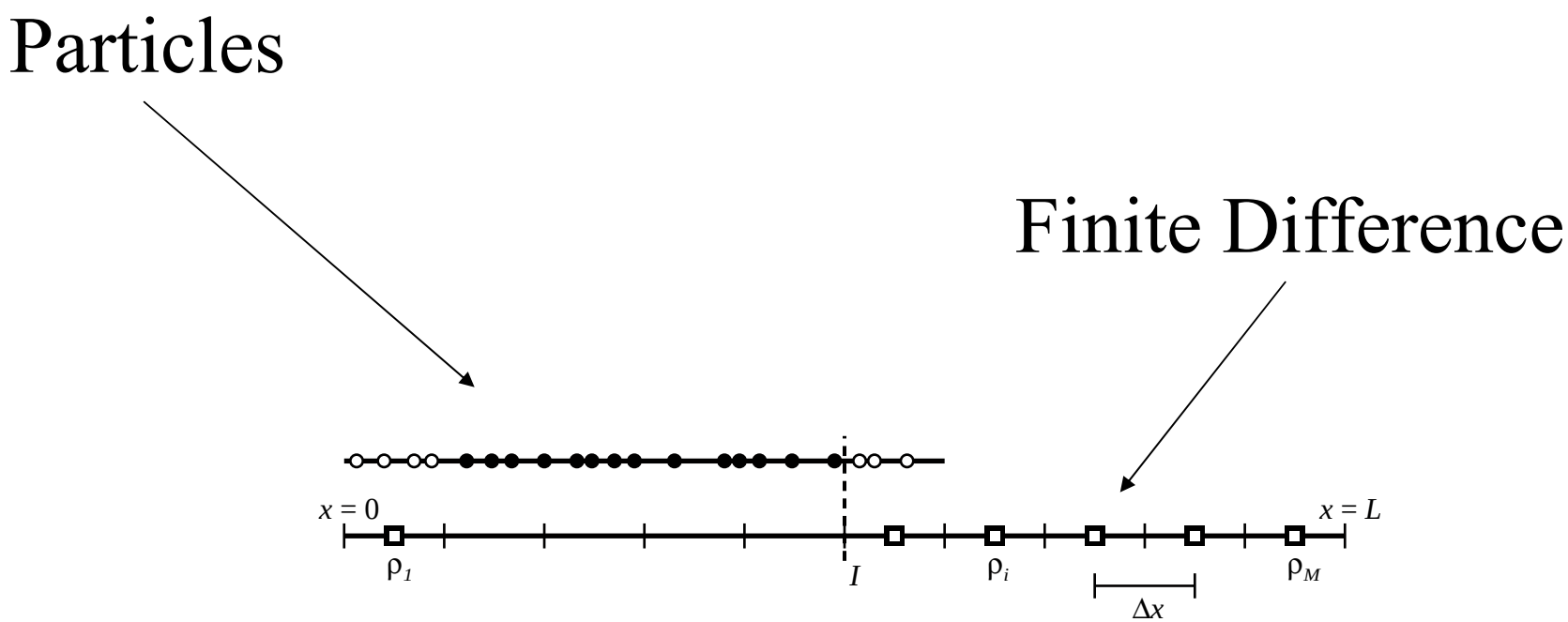
$$\mathbf{x}_B(t) = E[\mathbf{x}(t) \mid \mathbf{r}_1, \ldots, \mathbf{r}_k]$$

$$\mathbf{C}_B(t) = E[(\mathbf{x}(t) - \mathbf{x}_B(t))(\mathbf{x}(t) - \mathbf{x}_B(t))^T \mid \mathbf{r}_1, \ldots, \mathbf{r}_M]$$

1. Smoothing: $\rightarrow$ $k = M, t < t_M$
2. Filtering: $\rightarrow$ $t_{k+1} > t \geq t_k$
3. Prediction: $\rightarrow$ $t > t_M$

Linear Diffusion

- Simplest example
- Coarse-grained / Rescaled Independent Random Walkers converges to solution of Linear Diffusion Equation



Linear Diffusion

$$X_k(t+\Delta t) - X_k(t) = \sqrt{2D\Delta t}\,\Re_k \qquad (1$$

$$\frac{\rho_{i;n+1} - \rho_{i;n}}{\Delta t} = -\left(\frac{F^{+}_{i;n} - F^{-}_{i;n}}{\Delta x}\right) \qquad (2$$

$$F^{\pm}_{i;n} = \mp D\left(\frac{\rho_{i\pm1;n} - \rho_{i;n}}{\Delta x}\right) + f^{\pm}_{i;n} \qquad (3$$

Linear Diffusion

$$\langle f^+_{i;n} f^+_{j;m} \rangle = \frac{(A_{i;n} + A_{i+1;n})\delta_{i,j}\delta_{n,m}}{2\Delta x \Delta t} \quad (4$$

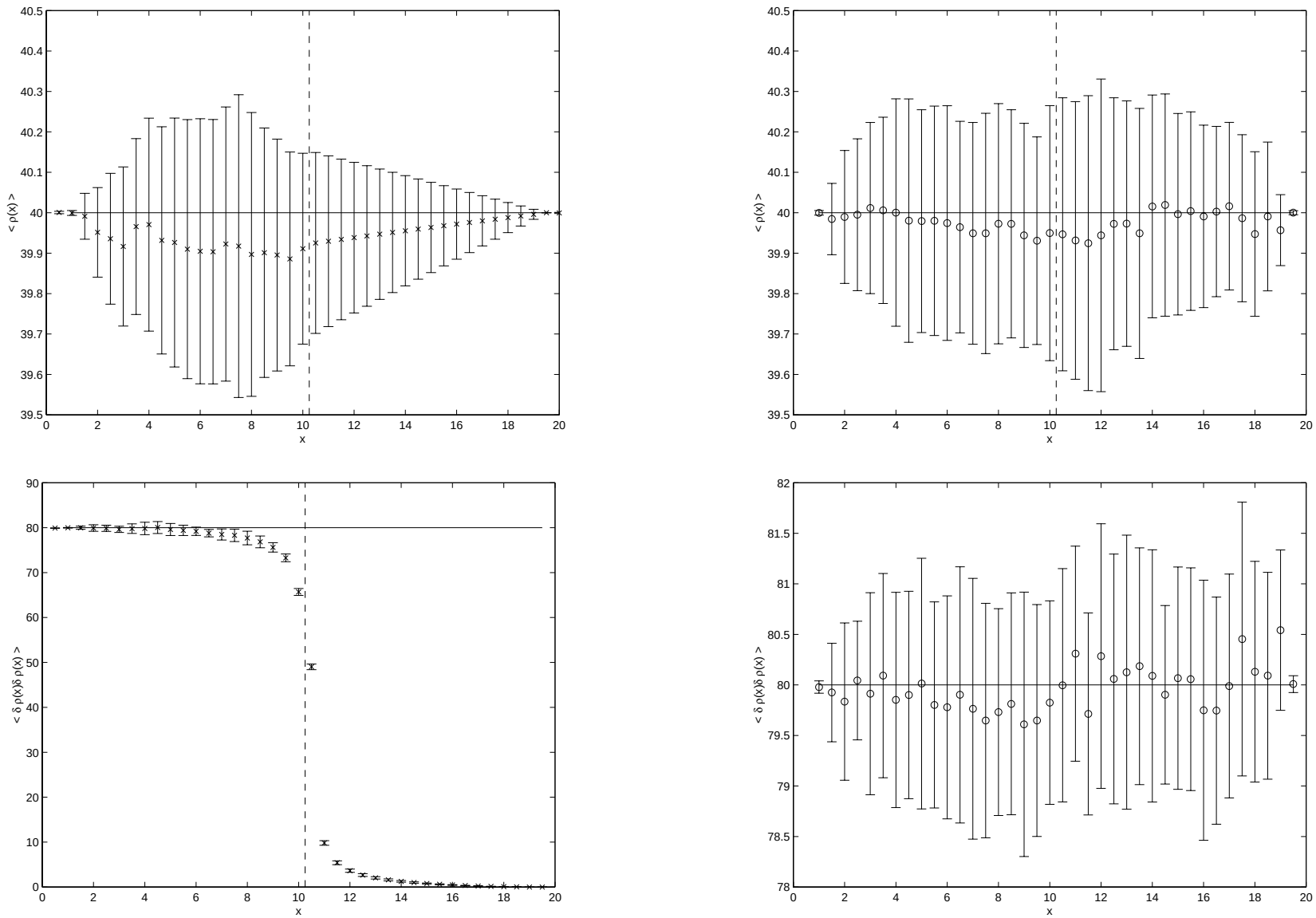
$$\langle f^-_{i;n} f^-_{j;m} \rangle = \frac{(A_{i;n} + A_{i-1;n})\delta_{i,j}\delta_{n,m}}{2\Delta x \Delta t} \quad (5$$

$$f^+_{i;n} = f^-_{i+1;n} = \sqrt{\frac{(A_{i;n} + A_{i+1;n})}{2\Delta x \Delta t}}\Re_{i;n} \quad (6$$

$$A = 2D\bar{\rho}(x,t) \quad (7$$

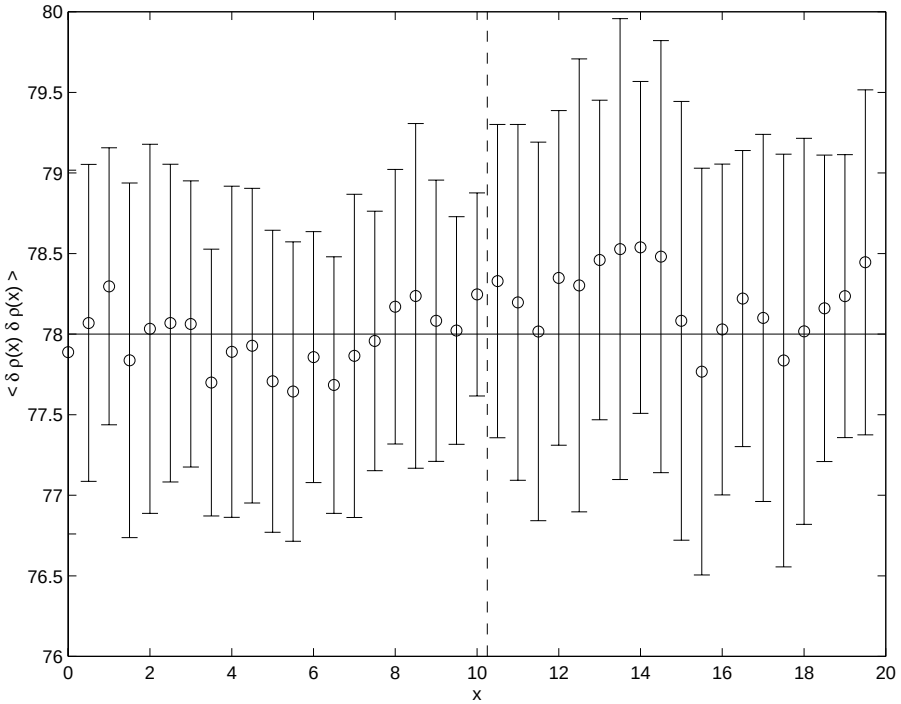
$$
\begin{aligned}
\rho_{i;n+1} &= \rho_{i;n} + \frac{D\Delta t}{\Delta x^2}\left(\rho_{i+1;n} + \rho_{i-1;n} - 2\rho_{i;n}\right) \\
&- \sqrt{\frac{D\Delta t}{\Delta x^3}}\left(\sqrt{\bar{\rho}_{i;n} + \bar{\rho}_{i+1;n}}\,\Re_{i;n} - \sqrt{\bar{\rho}_{i;n} + \bar{\rho}_{i-1;n}}\,\Re_{i-1;n}\right)
\end{aligned}
\qquad (8
$$

Linear Diffusion Open Equilibrium System

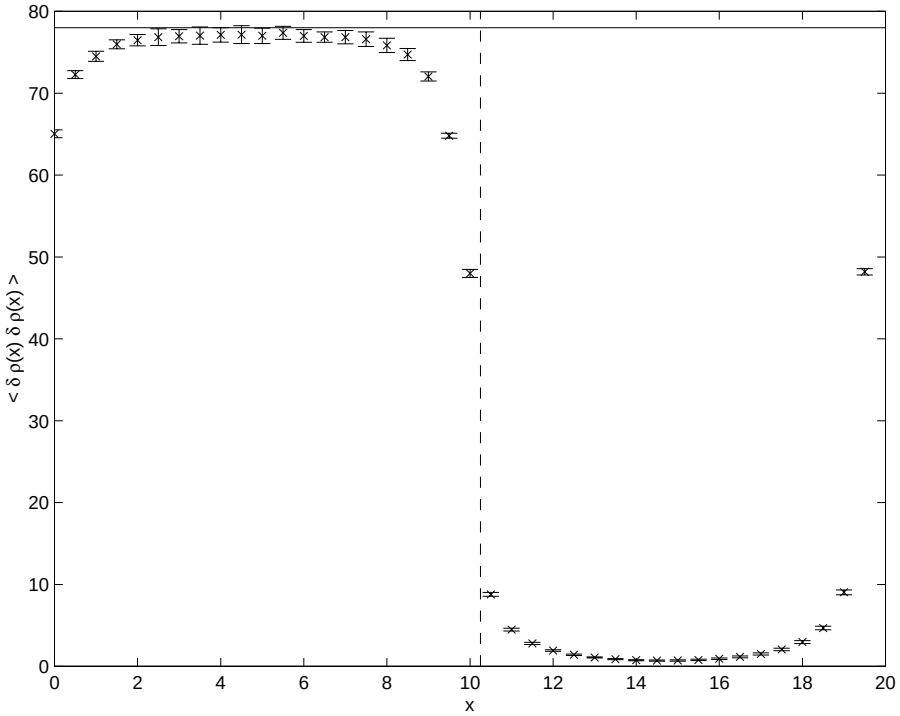


Linear Diffusion: Closed Equilibrium System

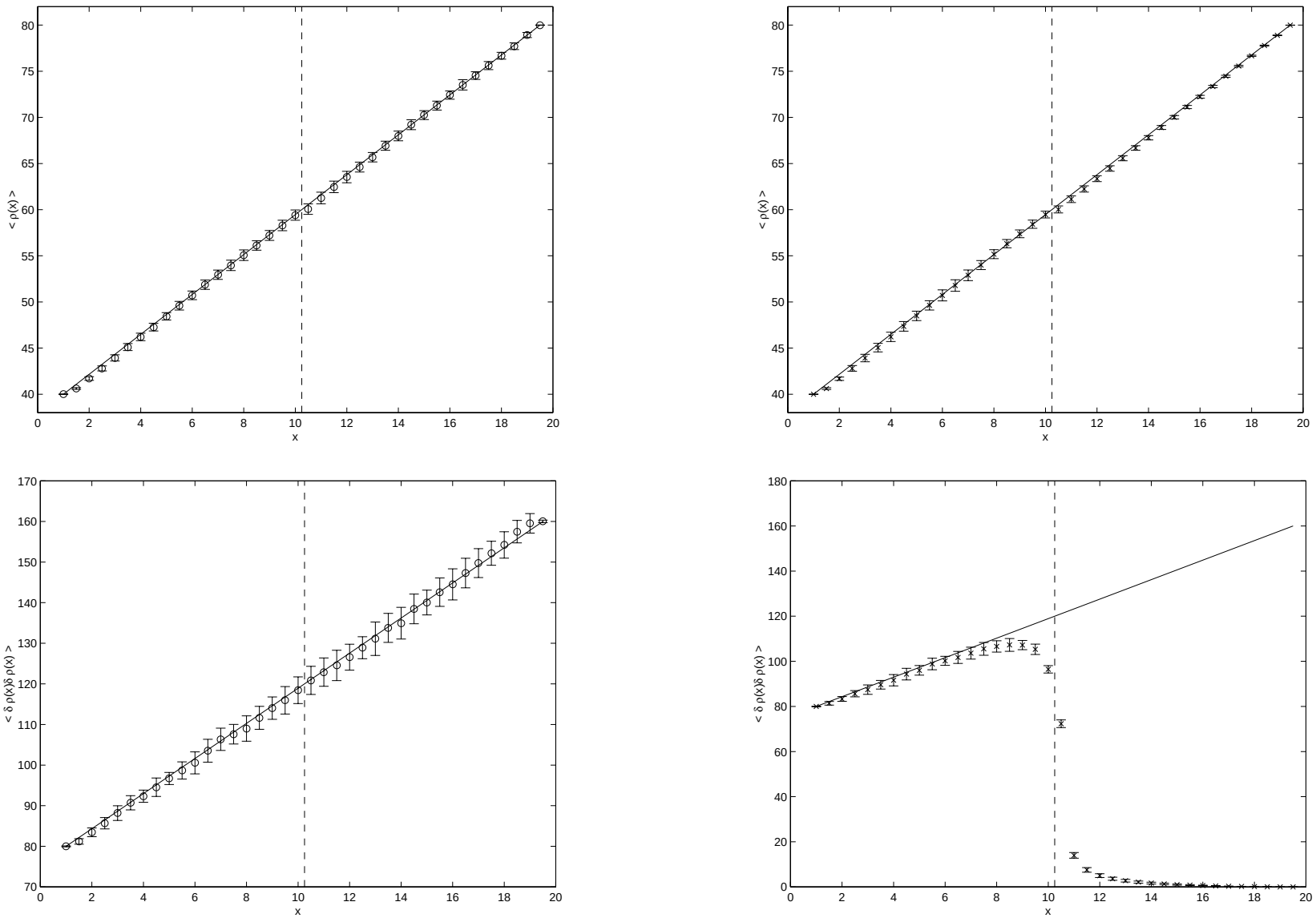
Particle / SPDE



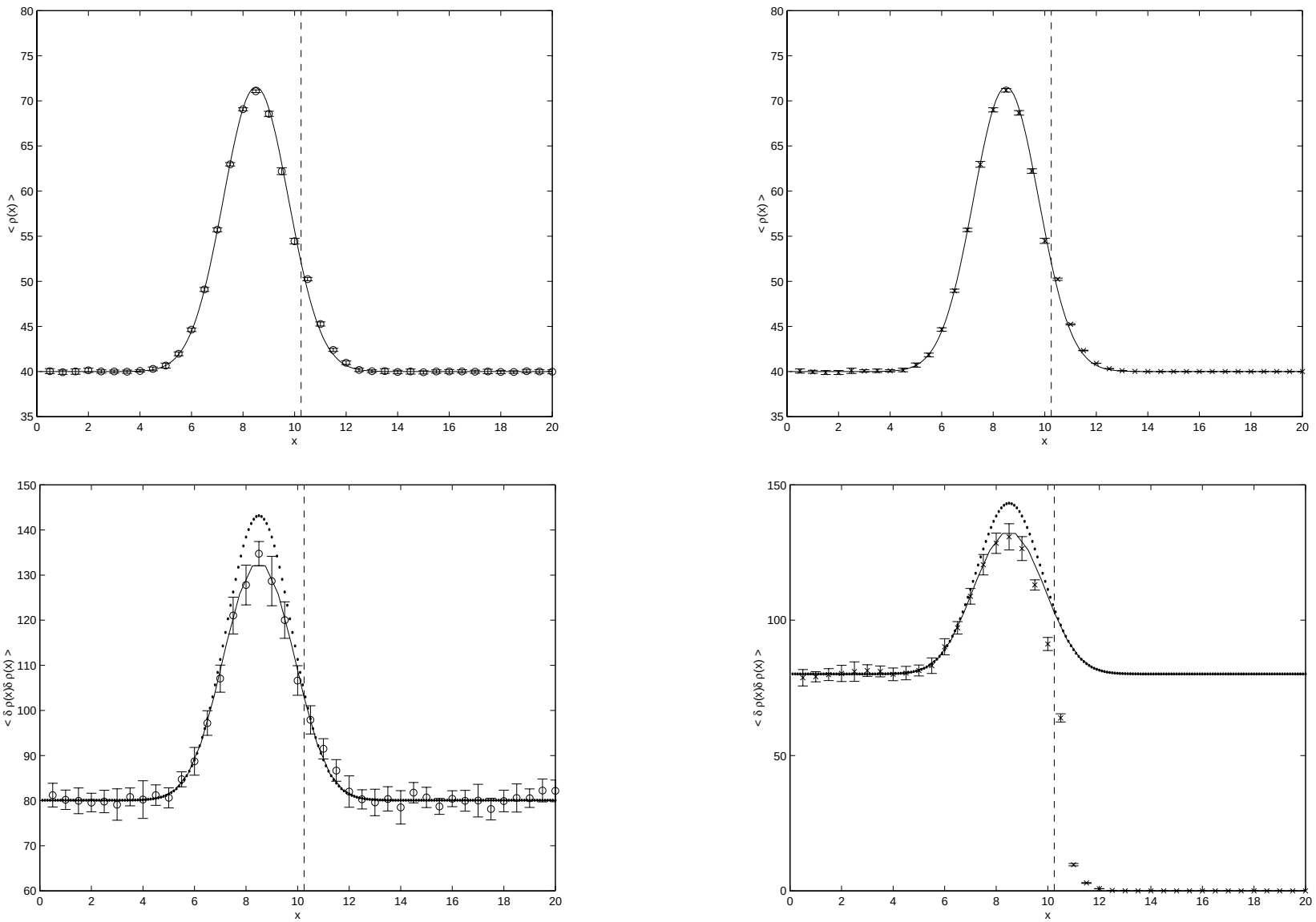
Particle / PDE



Linear Diffusion: Density Gradient



Linear Diffusion: Time Dependent Particle-SPDE Hybrid



Linear Diffusion

$$\begin{aligned}\rho_{i;n+1} &= \rho_{i;n} + \frac{D\Delta t}{\Delta x^2}\left(\rho_{i+1;n} + \rho_{i-1;n} - 2\rho_{i;n}\right) \\ &- \sqrt{\frac{D\Delta t}{\Delta x^3}}\left(\sqrt{\bar{\rho}_{i;n} + \bar{\rho}_{i+1;n}}\,\Re_{i;n} - \sqrt{\bar{\rho}_{i;n} + \bar{\rho}_{i-1;n}}\,\Re_{i-1;n}\right)\end{aligned} \quad (9$$

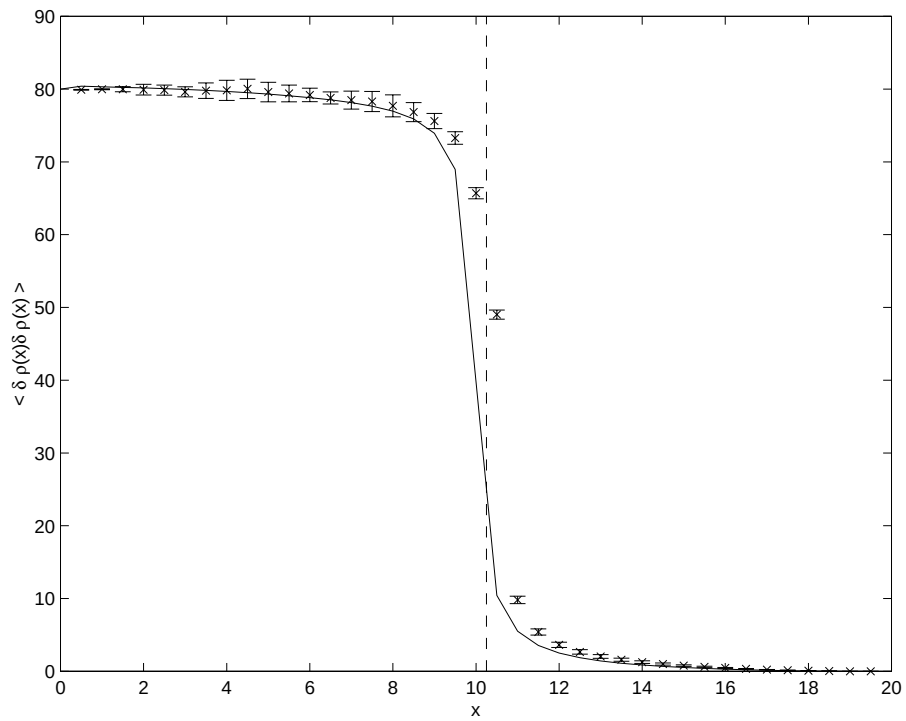
$$A_{i;n} = \begin{cases} 2D\bar{\rho}_{i;n} & i \leq M/2 \\ 0 & \text{otherwise} \end{cases} \quad (10$$

$$
\begin{aligned}
4\left(1-\frac{D\Delta t}{\Delta x^2}\right)G_{i,j} \quad &- \quad \left(1-\frac{2D\Delta t}{\Delta x^2}\right)(G_{i,j+1}+G_{i,j-1}+G_{i+1,j}+G_{i-1} \\
&- \quad \frac{D\Delta t}{\Delta x^2}(G_{i+1,j+1}+G_{i+1,j-1}+G_{i-1,j+1}+G_{i-1,j} \\
=\frac{1}{\Delta x}(B_iB_j\delta_{i,j} \quad &- \quad B_iB_{j-1}\delta_{i,j-1}-B_{i-1}B_j\delta_{i-1,j}+B_{i-1}B_{j-1}\delta_{i-1,}
\end{aligned}
$$

$$
\begin{aligned}
&B_iB_j\delta_{i,j}-B_iB_{j-1}\delta_{i,j-1}-B_{i-1}B_j\delta_{i-1,j}+B_{i-1}B_{j-1}\delta_{i-1,j-1} \\
&\quad = 4\bar{\rho}_{i;n}\delta_{i,j}-(\bar{\rho}_{i;n}\delta_{i,j+1}+\bar{\rho}_{i;n}\delta_{i,j-1}+\bar{\rho}_{i+1;n}\delta_{i+1,j}+\bar{\rho}_{i-1;n}\delta_{i-}(1
\end{aligned}
$$

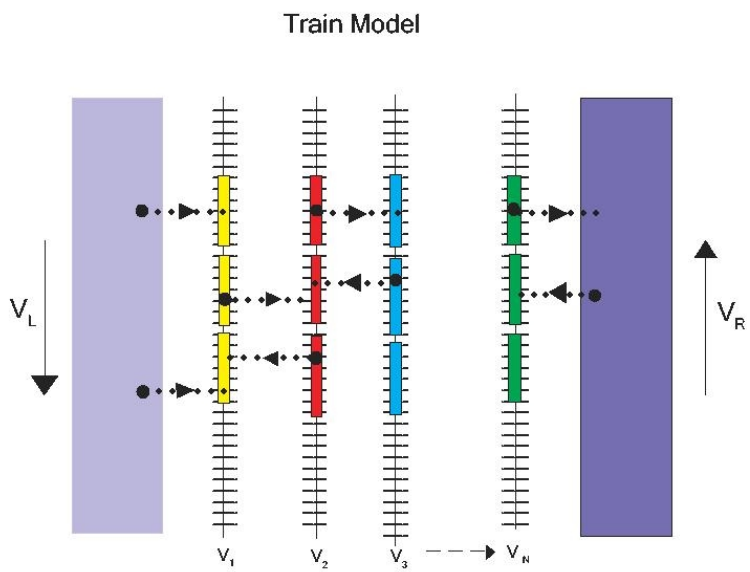
$$B_i = \begin{cases} \sqrt{\bar{\rho}_{i;n} + \bar{\rho}_{i+1;n}} & i < M/2 \\ \sqrt{\bar{\rho}_{i;n}} & i = M/2 \\ 0 & \text{otherwise} \end{cases} \qquad (1$$

Linear Diffusion: Numerical Analysis

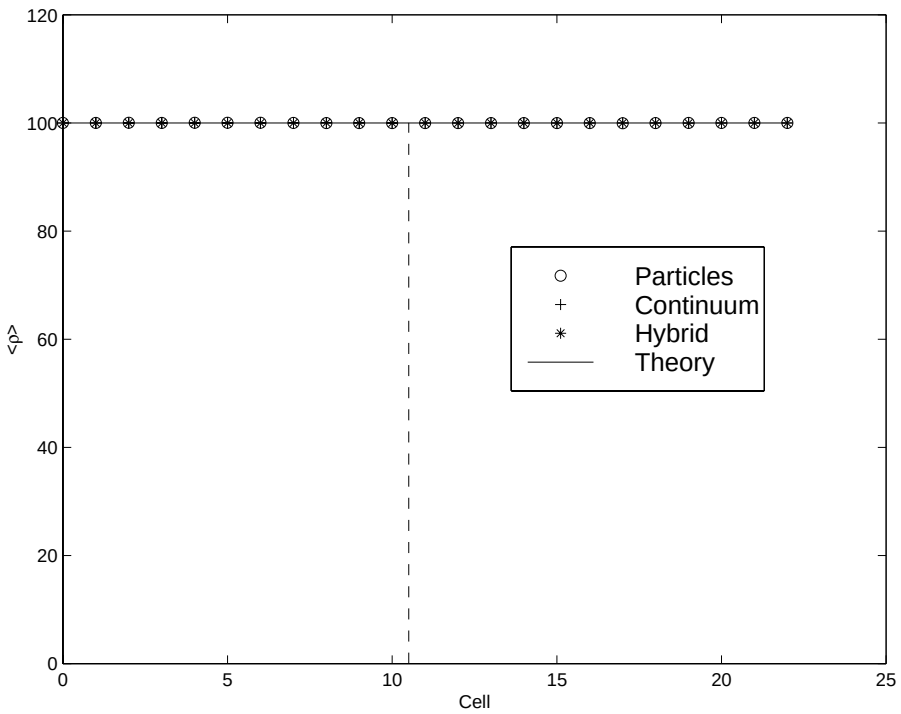


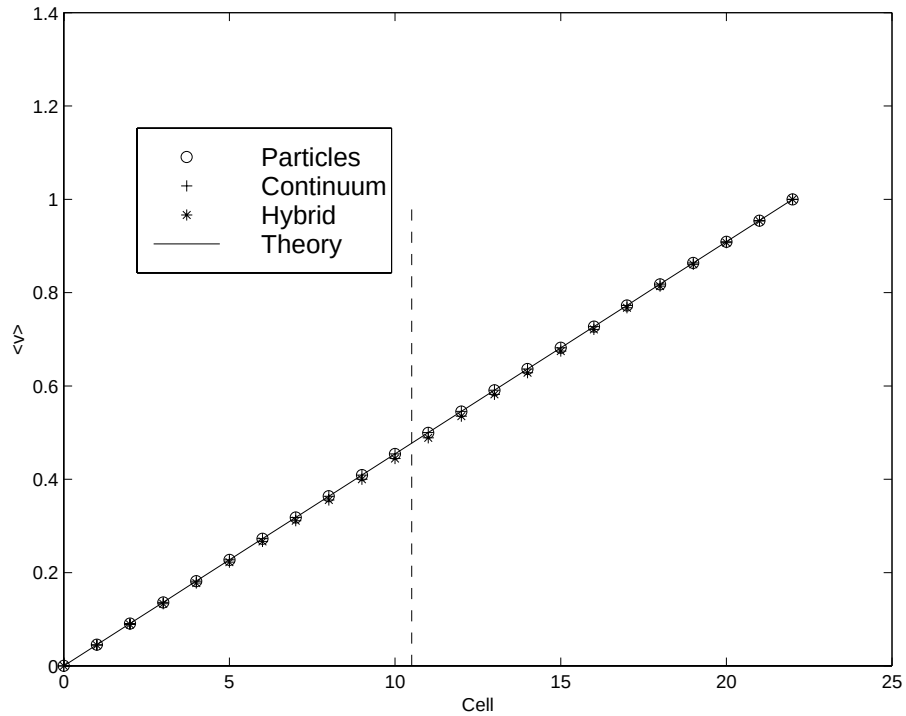
Transport with Correlations: The Train Model

- Long Range Velocity-Velocity Correlations
- "A Simple Model for Nonequilibrium Fluctuations in a Fluid", F. Baras, M. Malek Mansour and A. Garcia, Am. J. Phys. 64 1488 (1996)

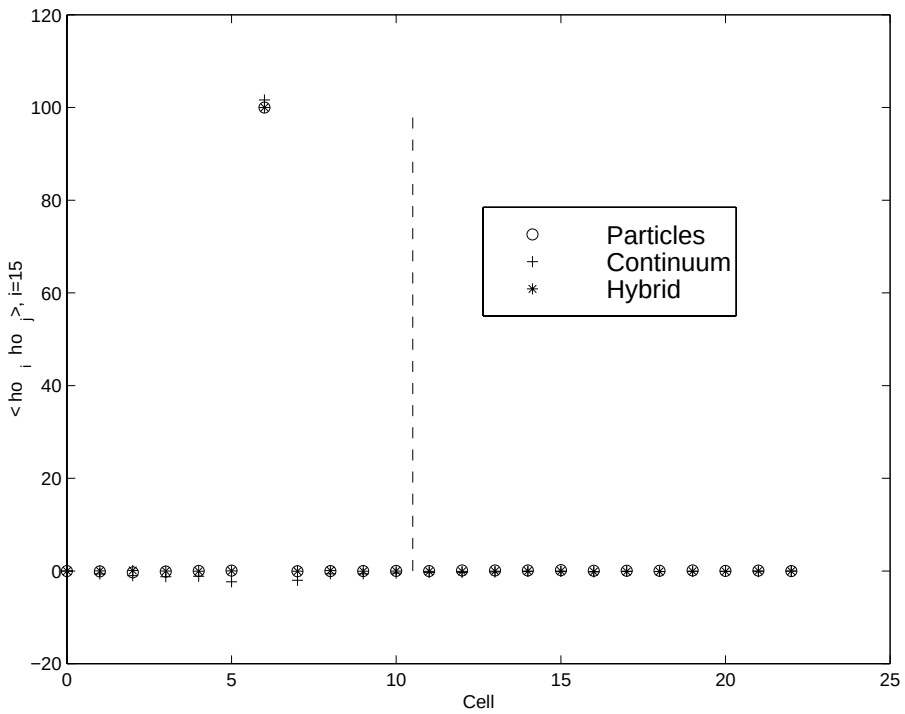


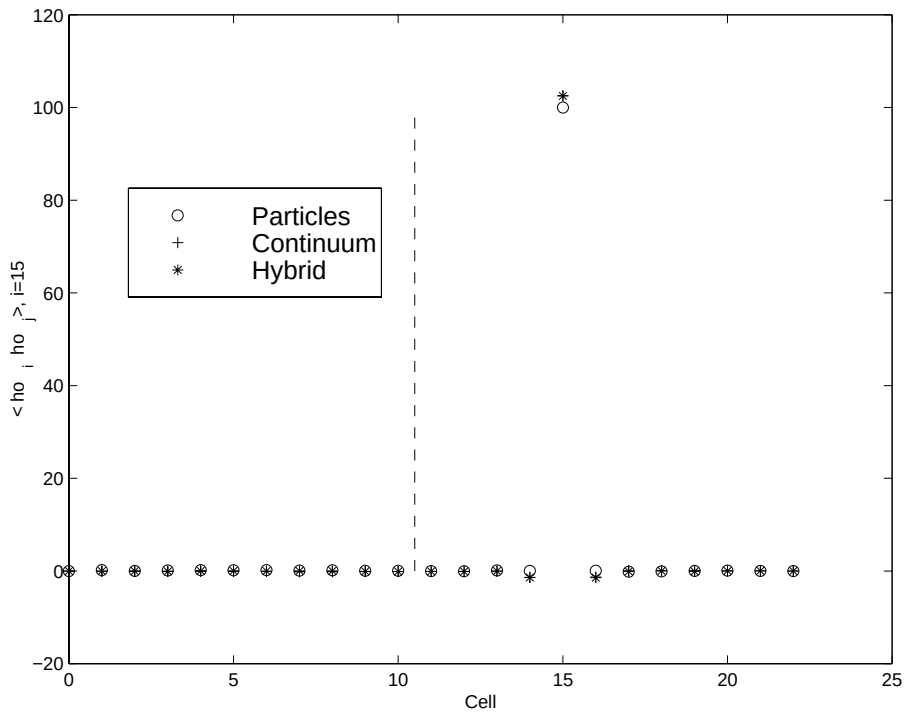
Transport with Correlations: Velocity Gradient, Fully Stochastic





Transport with Correlations: Velocity Gradient Fully Stochastic





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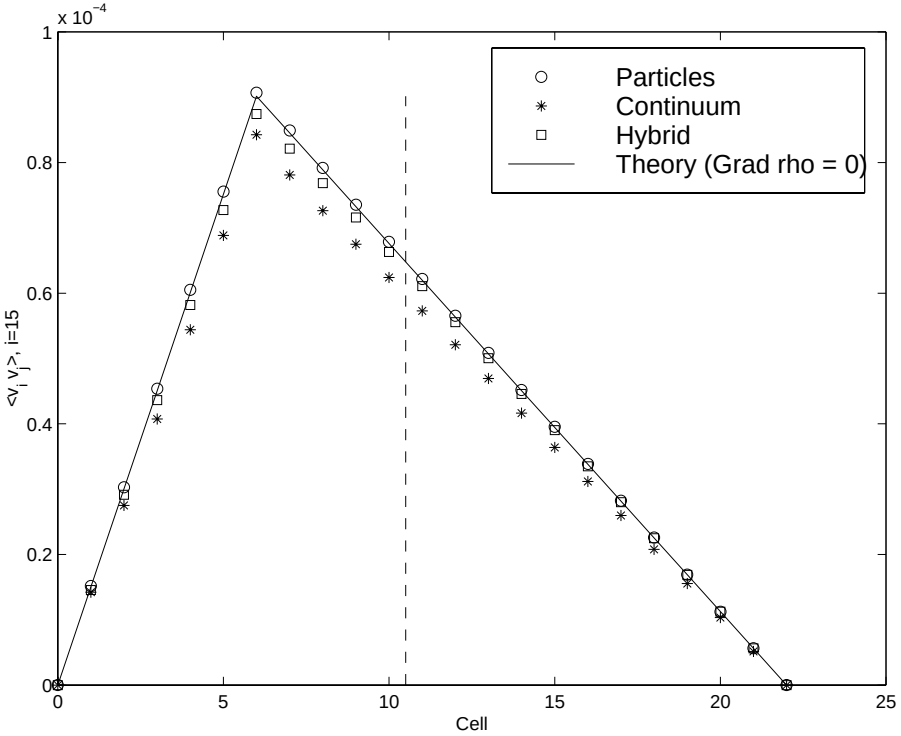
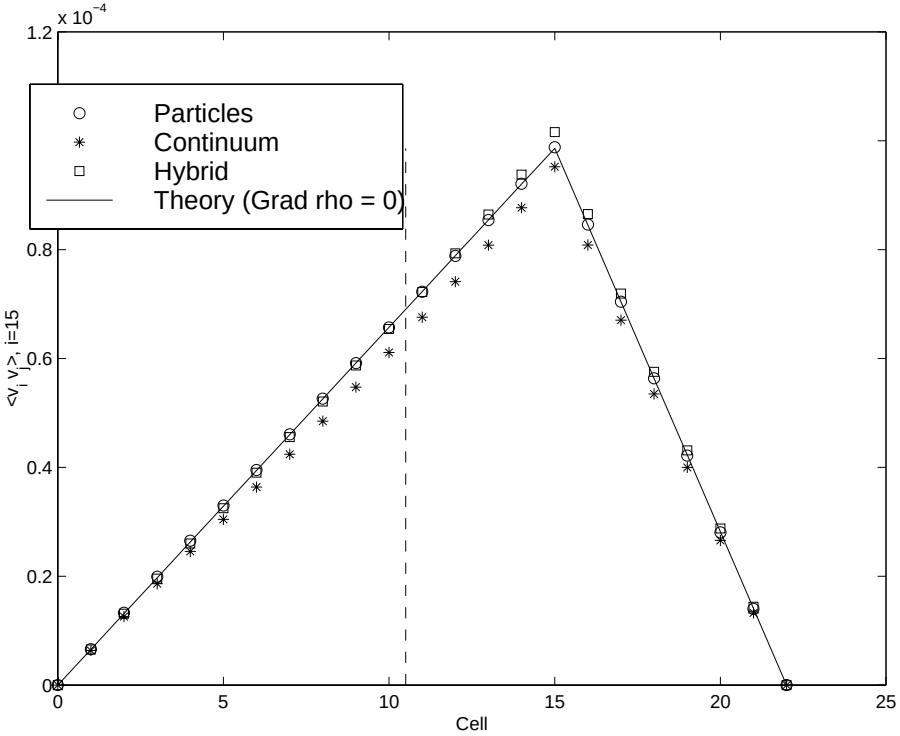
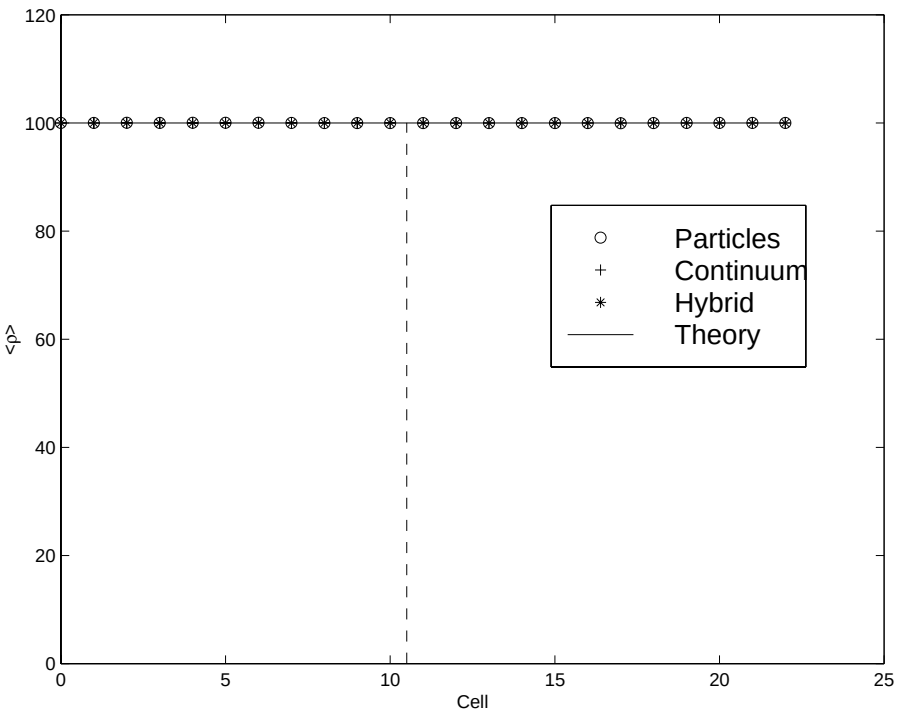
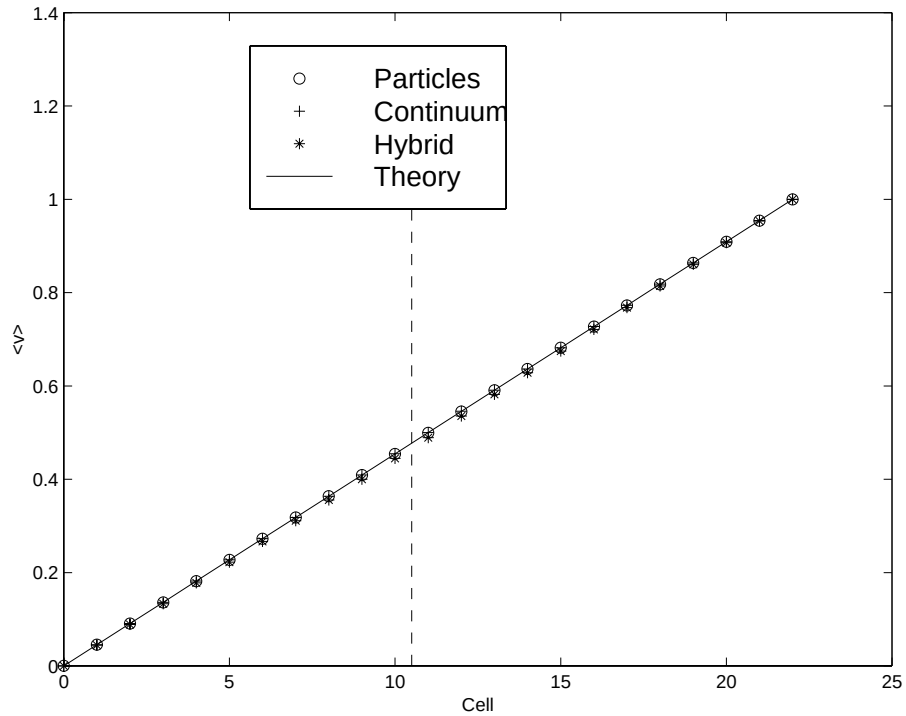




Transport: Velocity Gradient Half-Stochastic





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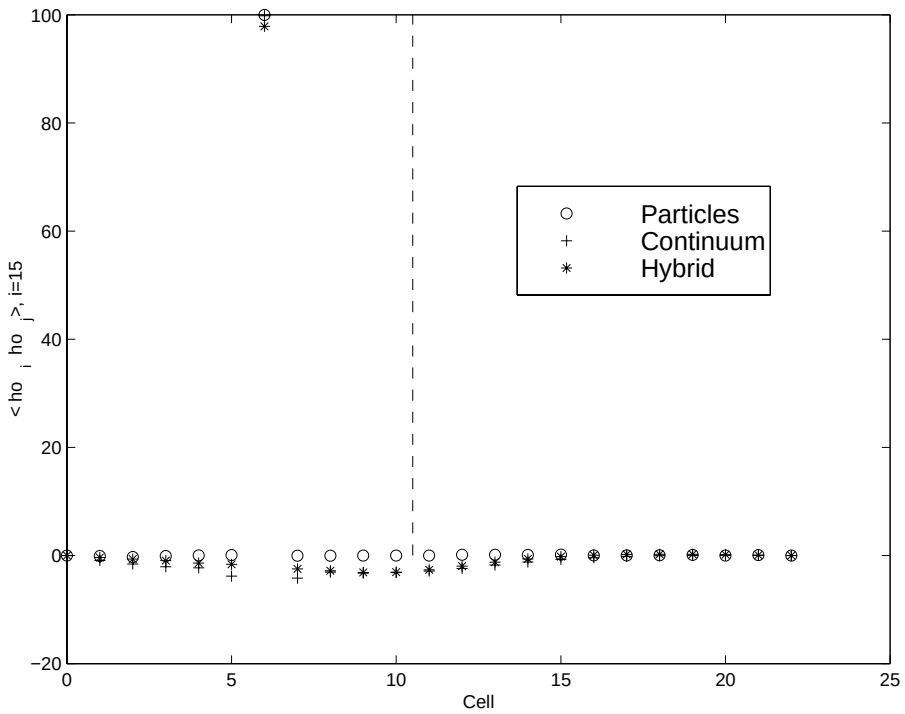

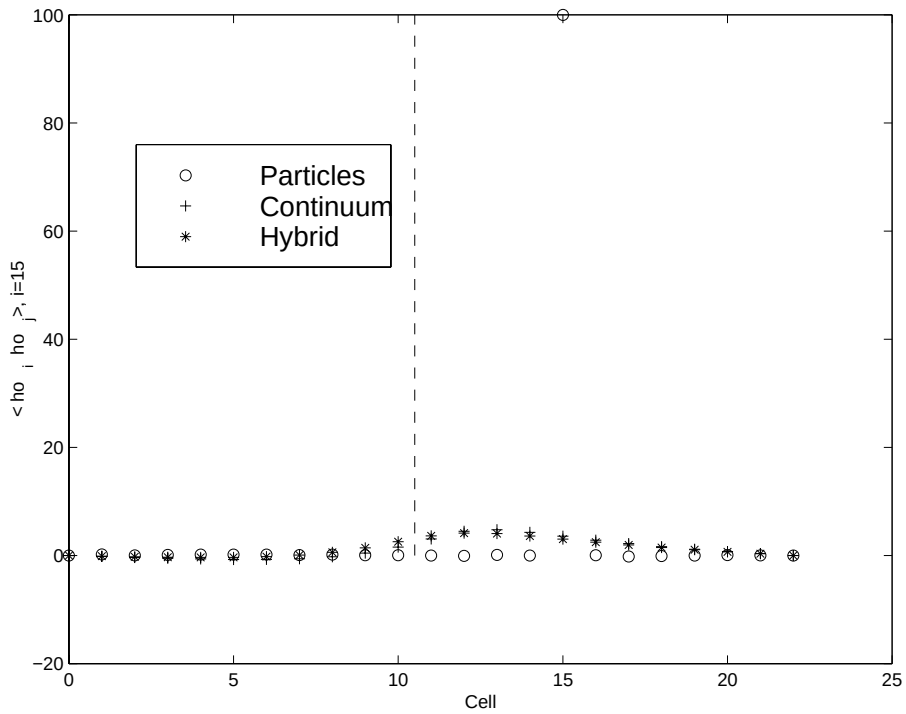

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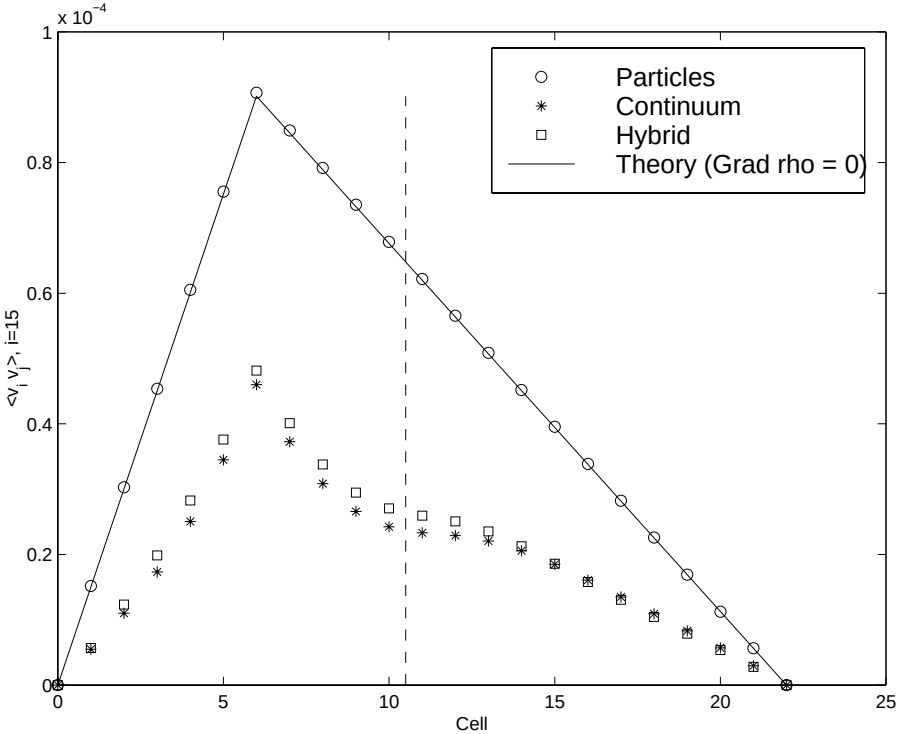
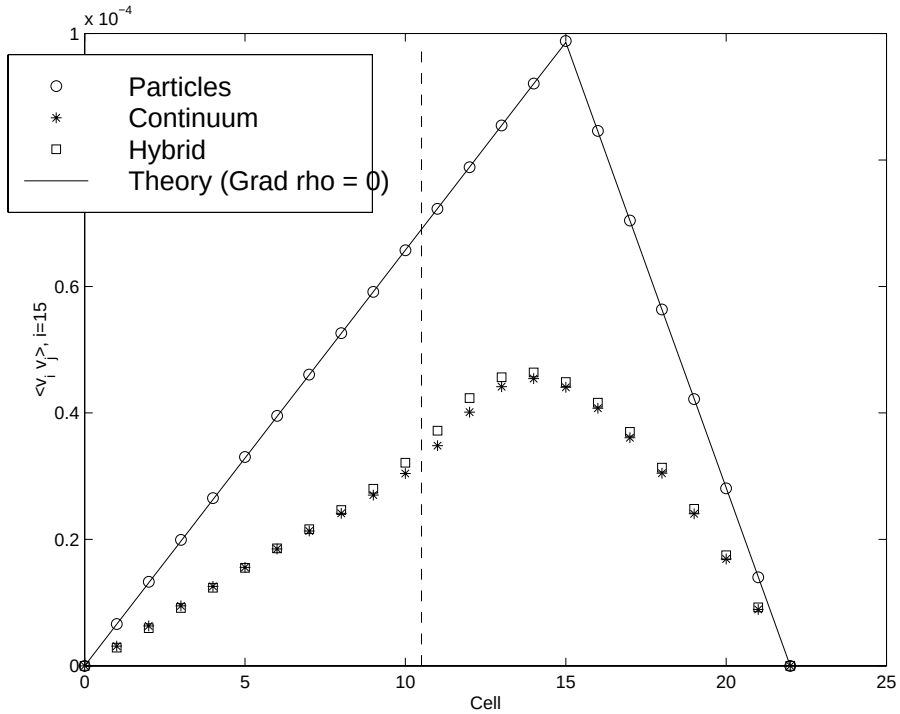
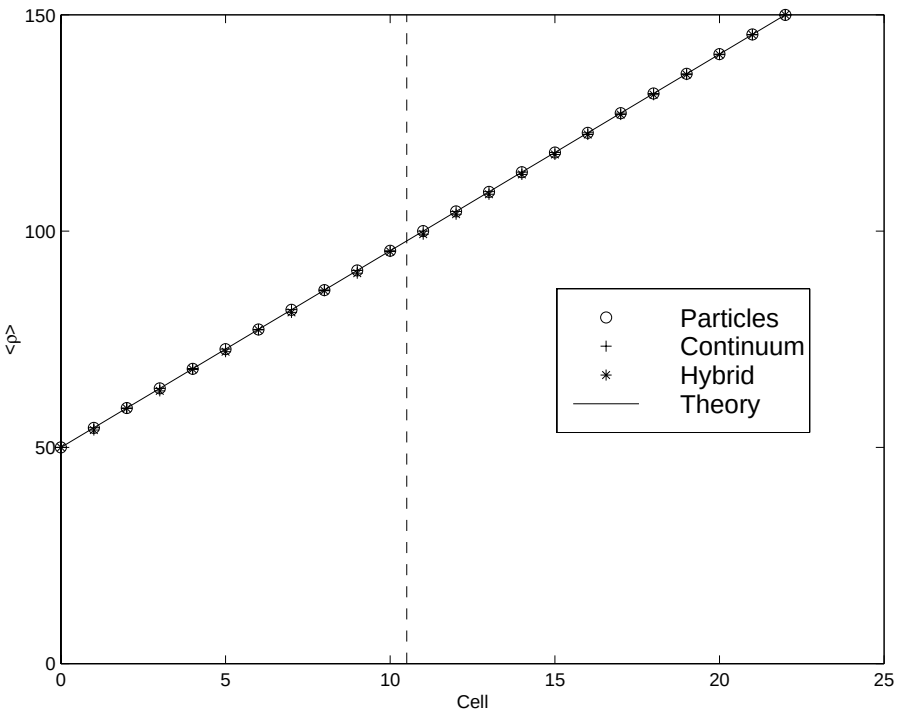
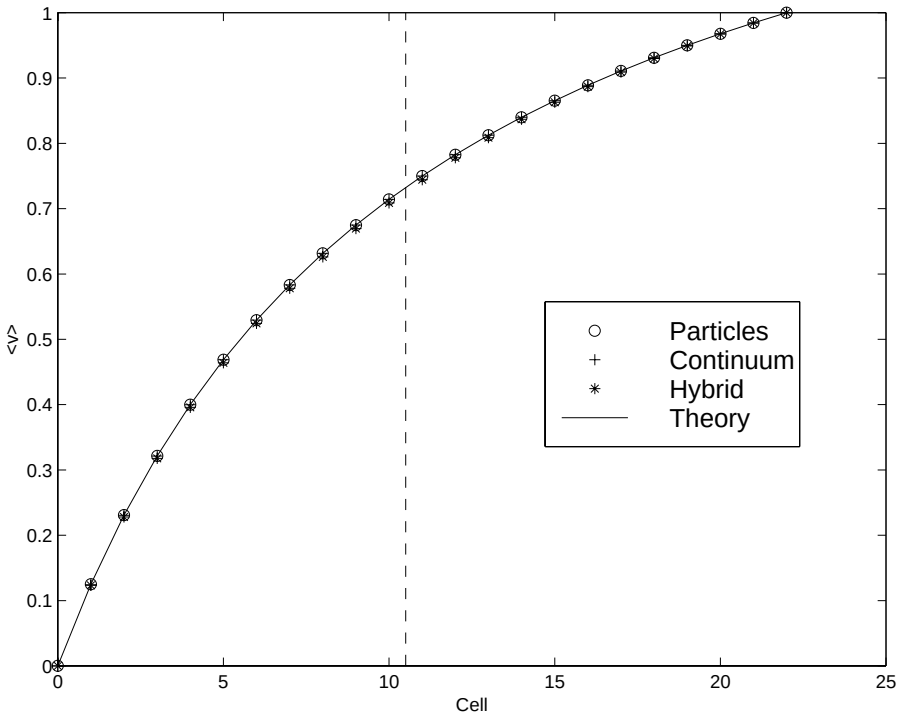




Transport: Velocity & Density Gradient Fully Stochastic





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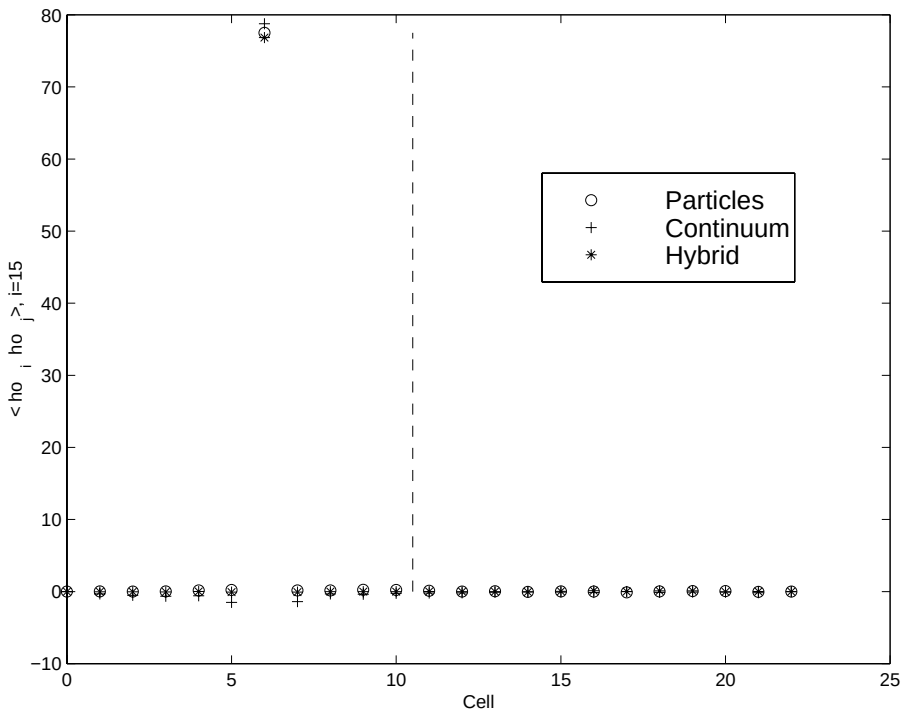

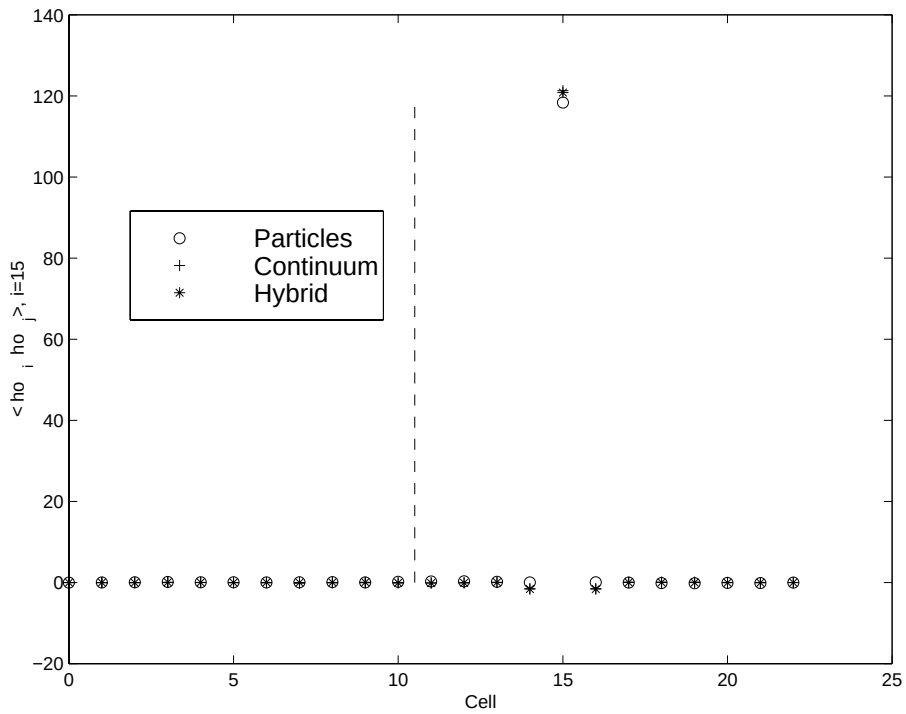

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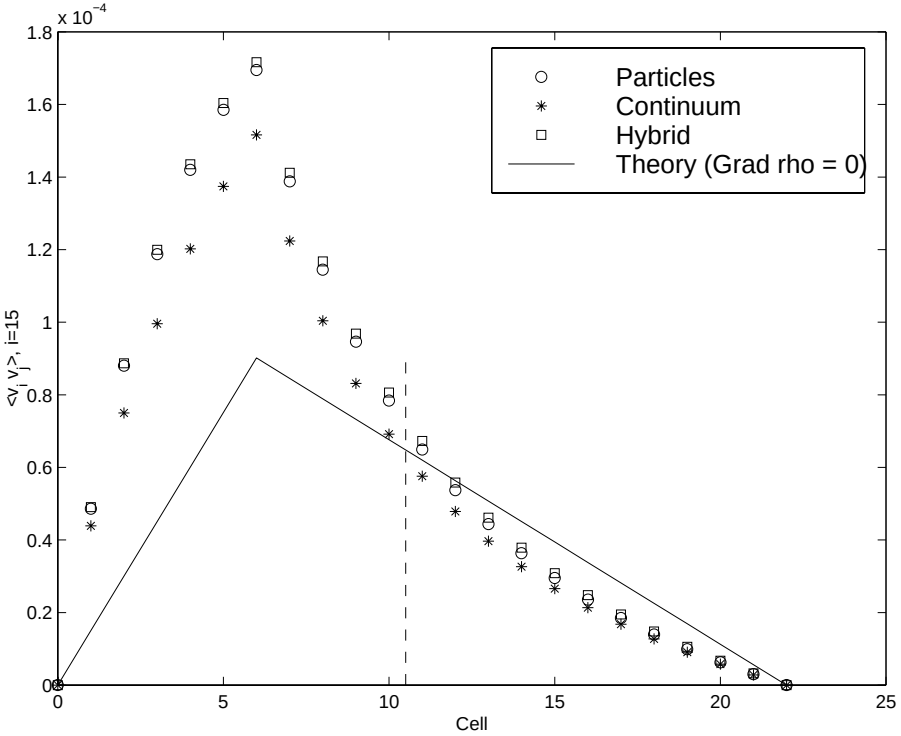
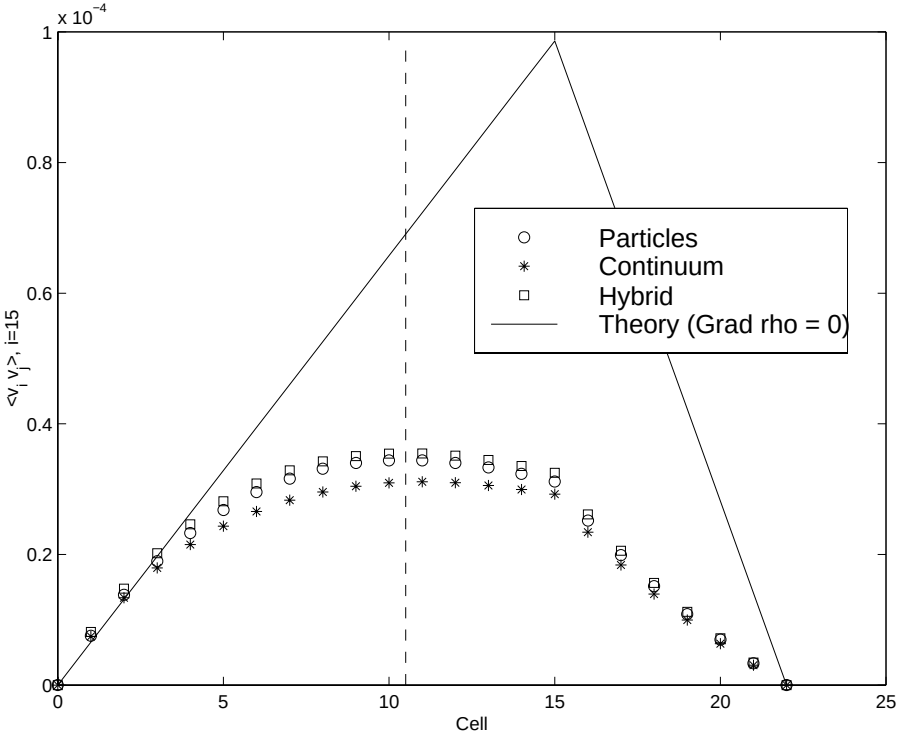
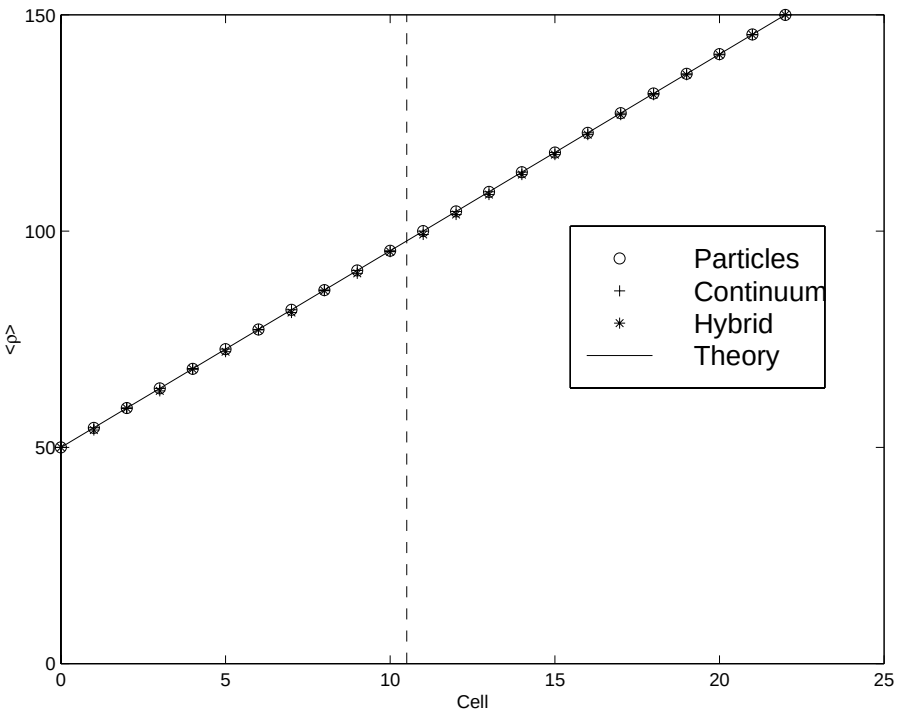
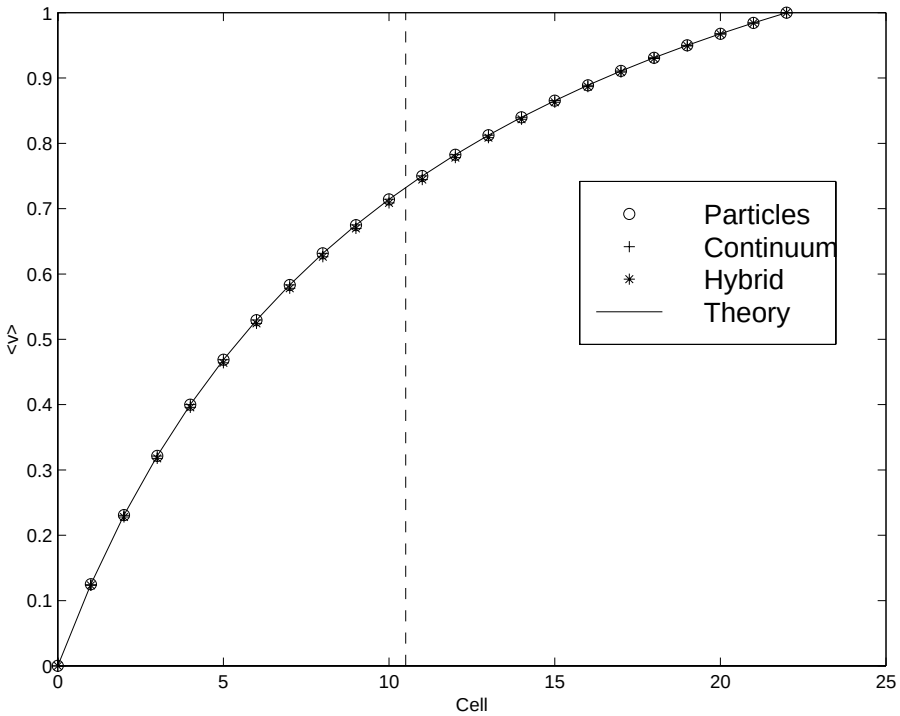




Transport: Velocity & Density Gradient Half-Stochastic





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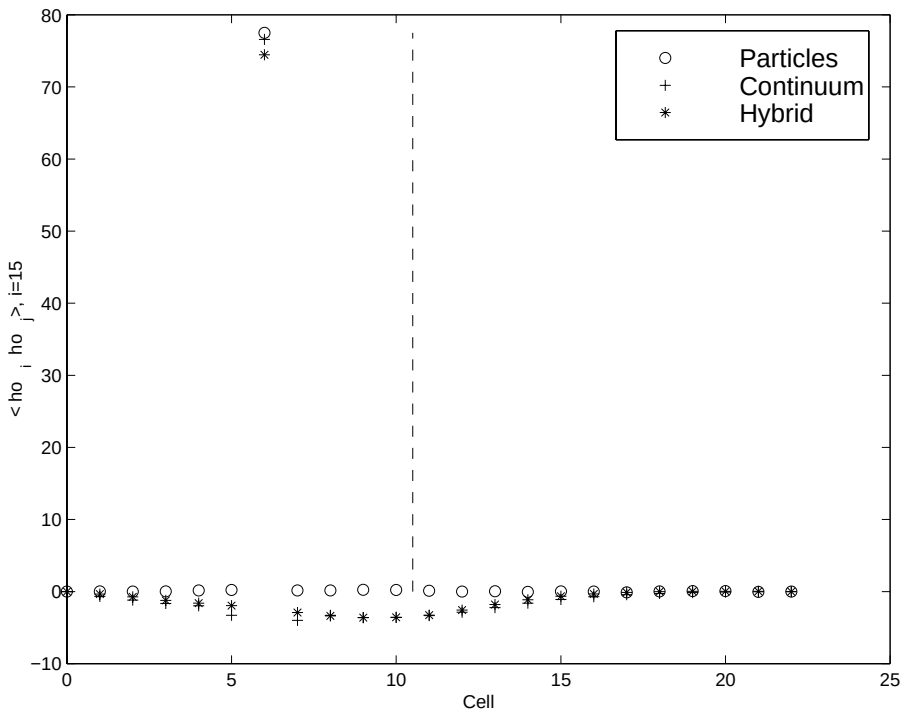

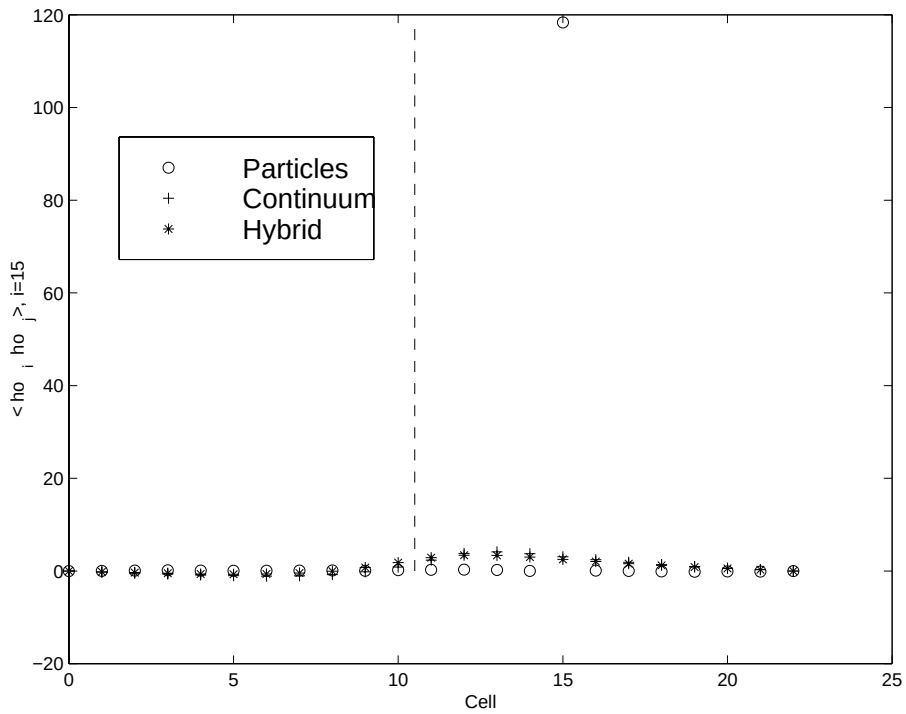

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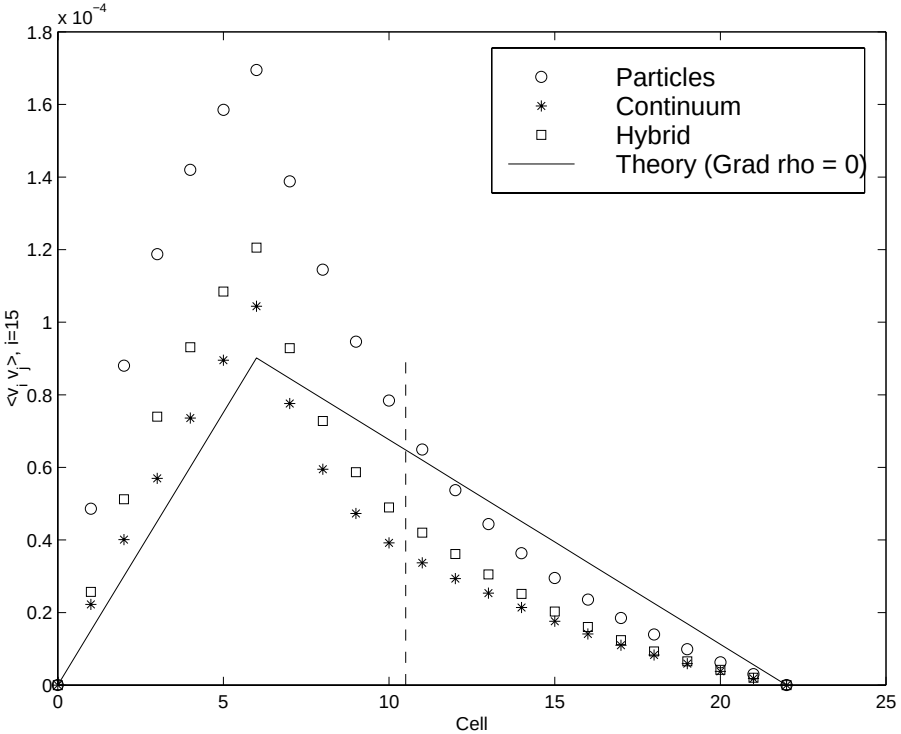
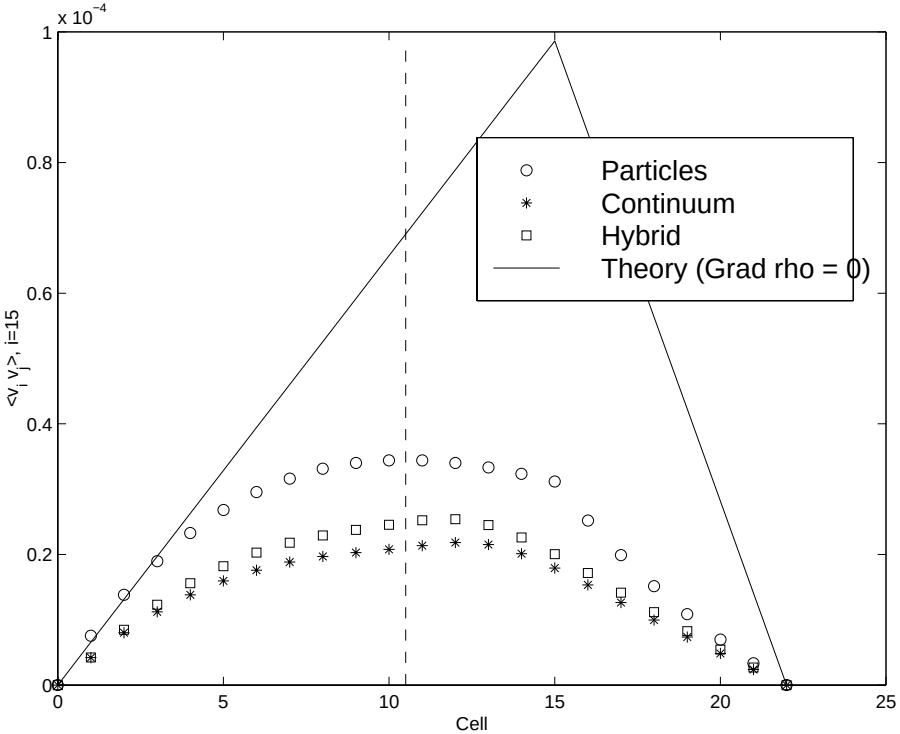
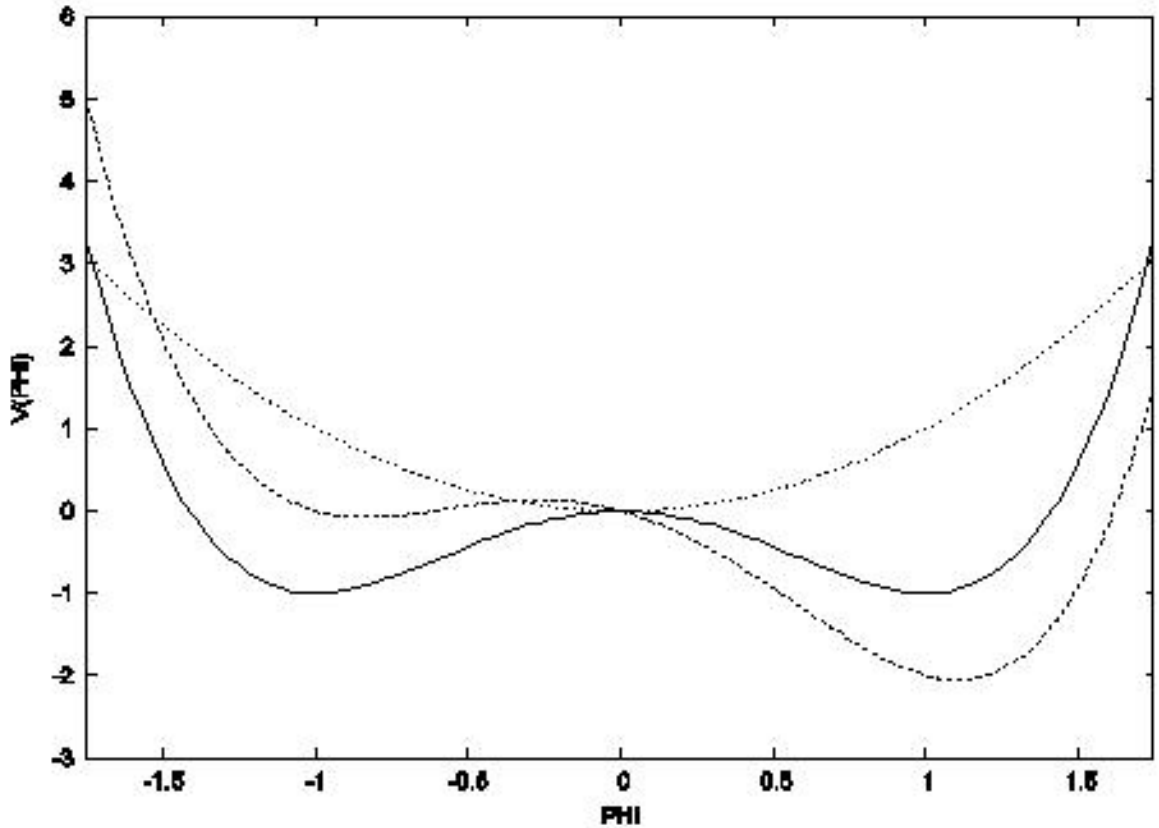




Phase Ordering Dynamics

$$\partial_t \varphi = D\Delta\varphi - V'(\phi)^3 + \eta$$



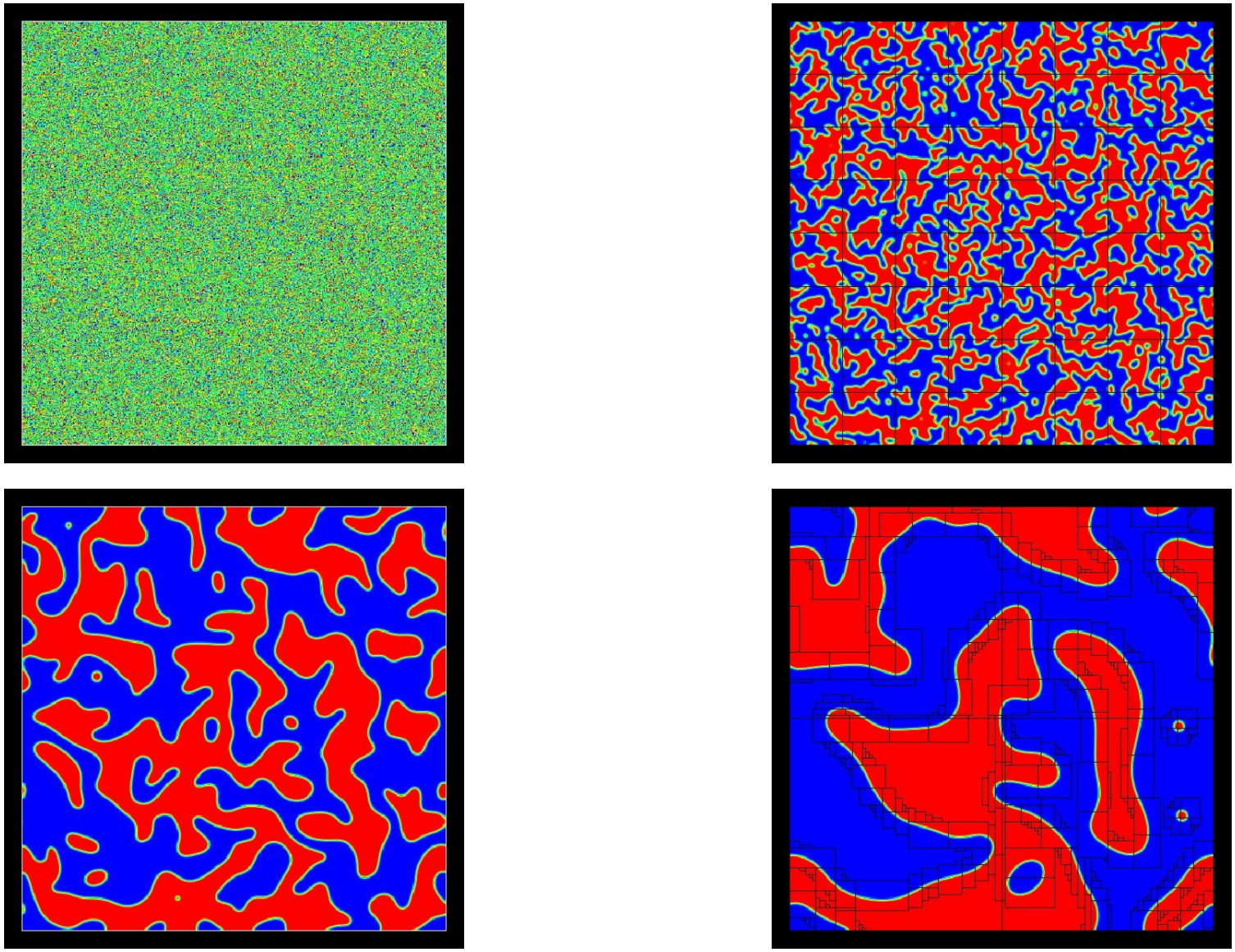
Parting Thoughts

APPLICATION AREAS:

- Materials Science: defect modeling, structural phase transitions, nucleation
- Condensed Matter Physics: soft-matter dynamics, quantum transport in nanodevices
- Fluid Dynamics: instabilities, interface motion, nanoscale fluidics
- Numerical Analysis: coupled stochastic/deterministic PDEs stochastic Adaptive Mesh Refinement
- Plasma Physics: kinetic theory coupled to MHD, space weather
- Dynamics on Networks: queueing, coupling discrete-event simulations to (S)PDEs / stochastic fluid eqn's to optimize performance

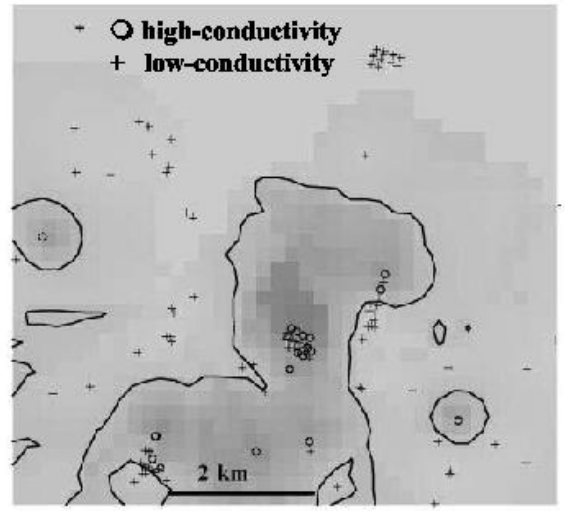
- STRONG SUGGESTIONS
- For some problems SPDE's may be unavoidable
- Need for numerical analysis (Stochastic Methods)
- Careful testing in nonlinear systems

Parting Thoughts: Stochastic AMR



SPDE Approach to Uncertainty Quantification

- Consider a physical process $\mathcal{N}_{\{p\}}u = f$
  - System parameters $p_i = p(\boldsymbol{x}_i)$, $i = 1, \ldots, N$
  - System states $u_j = u(\boldsymbol{x}_j)$, $j = 1, \ldots, M$



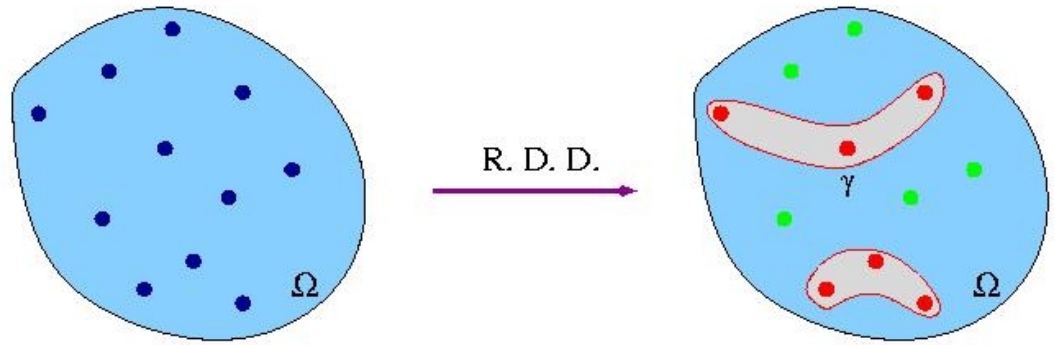
- Modeling steps

1. Use data to construct a probabilistic description of $\{p\}$
2. Solve SPDEs to obtain a probabilistic description of u
3. Assimilate $u_j = u(\boldsymbol{x}_j)$ to refine prior distributions

State of the Art

- Real systems are characterized by
  - Non-stationary (statistically inhomogeneous)
  - Multi-modal
  - Large variances
  - Complex correlation structures
- Standard SPDE techniques require
  - Stationarity (statistically homogeneity)
  - Small variances
  - Simple correlation structures (Gaussian, exponential)
  - Uni-modality
- Our goal is
  - to incorporate realistic statistical parameterizations
  - to enhance predictive power
  - to improve computational efficiency

Random Domain Decompositions for SPDEs



$p(\{\Pi\})$

Multi-modal distributions
High variances
Complex correlation structures

$p(\{\Pi\}, \Gamma)$

Uni-modal distributions
Low variances
Simple correlation structures