Modeling of Fluctuations in Algorithm Refinement Methods

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Outline

- Hybrid algorithms
  - Motivation
  - Approach
- Role of fluctuations
  - Burgers' equation example
- Landau-Lifshitz Navier Stokes equations
- Numerical methods for stochastic PDE's
- Hybrid algorithms for fluids
- Examples
- Conclusions

Multi-scale models of fluid flow

Most computations of fluid flows use a continuum representation (density, pressure, etc.) for the fluid.

- Dynamics described by set of PDEs.
- Well-established numerical methods (finite difference, finite elements, etc.) for solving these PDEs.
- Hydrodynamic PDEs are accurate over a broad range of length and time scales.

But at some scales the continuum representation breaks down and more physics is needed

When is the continuum description of a gas not accurate?

- Discreteness of collisions and fluctuations are important
  - Micro-scale flows, surface interactions, complex fluids
  - Particles / macromolecules in a flow
  - Biological / chemical processes

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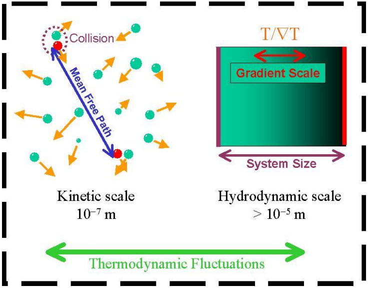
Hybrid methods

Look at fluid mechanics problems that span kinetic and hydrodynamics scales

Approaches

- Molecular description – correct but expensive
- Continuum CFD – cheap but doesn't model correct physics
- Hybrid – Use different models for the physics in different parts of the domain
  - Molecular model only where needed
  - Cheaper continuum model in the bulk of the domain



Hybrid approach

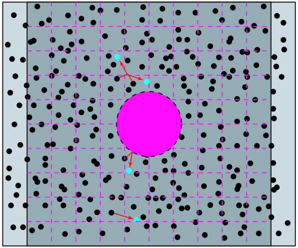
Develop a hybrid algorithm for fluid mechanics that couples a particle description to a continuum description

- AMR provides a framework for such a coupling
  - AMR for fluids except change to a particle description at the finest level of the heirarchy
- Use basic AMR design paradigm for development of a hybrid method
  - How to integrate a level
  - How to synchronize levels

DSMC

Discrete Simulation Monte Carlo (DSMC) is a leading numerical method for molecular simulations of dilute gases

- Initialize system with particles
- Loop over time steps
  - Create particles at open boundaries
  - Move all the particles
  - Process particle/boundary interactions
  - Sort particles into cells
  - Select and execute random collisions
  - Sample statistical values



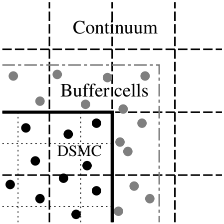
Example of flow past a sphere

Adaptive mesh and algorithm refinement

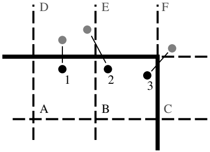
AMR approach to constructing hybrids – Garcia et al., JCP 1999

Hybrid algorithm – 2 level

- Advance continuum CNS solver
  - Accumulate flux F_C at DSMC boundary
- Advance DMSC region
  - Interpolation – Sampling from Chapman-Enskog distribution
  - Fluxes are given by particles crossing boundary of DSMC region
- Synchronize
  - Average down – moments
  - Reflux $\delta F = -\Delta t A F_C + \sum_p F_p$

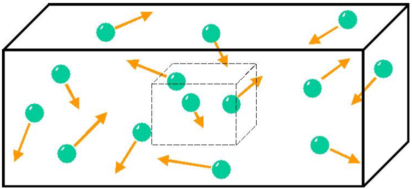


DSMC boundary conditions



DSMC flux

Hydrodynamic Fluctuations



Given particle positions and velocities, measure macroscopic variables

- These quantities naturally fluctuate
- Particle scheme:
  - Capture variance of fluctuations
  - Predict time-correlations at hydrodynamic scale
  - Predict non-equilibrium fluctuations hydrodynamic scale

Fluctuations at continuum level

How do molecular-scale fluctuations interact with the continuum?

Can / should we capture fluctuations at the continuum level?

Do they matter?

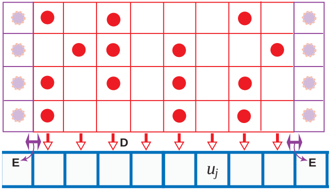
This has been investigated for a number of models

- Diffusion
- ”Train” model
- Burgers’ equation

Example: Burgers’ equation – Bell et al. JCP, 2007.

AERW / Burgers'

Asymmetric Excluded Random Walk:



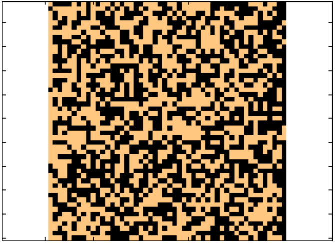
Probability of jump to the right sets the "Reynolds" number

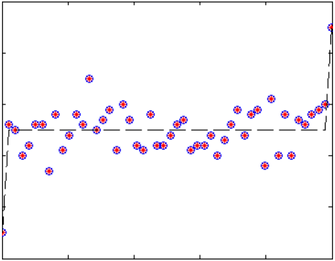
- Mean field given by viscous Burgers' equation
- Stochastic flux models fluctuation behavior

$$u_t + c((u(1-u))_x = \epsilon u_{xx} + \mathcal{S}_x$$

Stochastic flux is zero-mean Gaussian uncorrelated in space and time with magnitude from fluctuation dissipation theorem

AERW / Burgers'

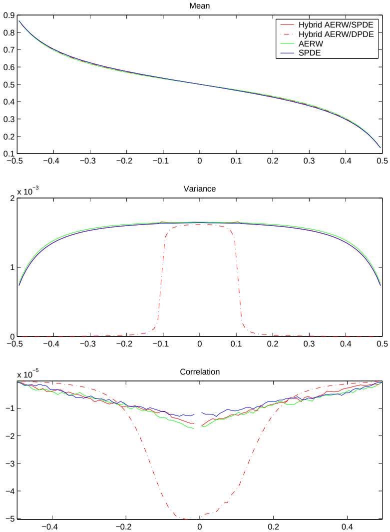




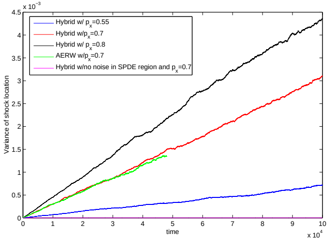
Simple numerical ideas work well

- Second-order Godunov for advective flux
- Standard finite difference approximation of viscosity
- Explicitly add stochastic flux

AERW / Burgers'



Rarefaction



Shock Drift

Failure to include the effect of fluctuations at the continuum level disrupts correlations in the particle region

Landau-Lifshitz fluctuating Navier Stokes

What about fluid dynamics?

- Can we model fluctuations at the continuum level?
- Do they matter in this context?

$$\partial \mathbf{U}/\partial t + \nabla \cdot \mathbf{F} = \nabla \cdot \mathbf{D} + \nabla \cdot \mathbf{S} \quad \text{where} \quad \mathbf{U} = \begin{pmatrix} \rho \\ \mathbf{J} \\ E \end{pmatrix}$$

$$\mathbf{F} = \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v}\mathbf{v} + P\mathbf{I} \\ (E+P)\mathbf{v} \end{pmatrix} \; \mathbf{D} = \begin{pmatrix} 0 \\ \tau \\ \kappa \nabla T + \tau \cdot \mathbf{v} \end{pmatrix} \; \mathbf{S} = \begin{pmatrix} 0 \\ \mathcal{S} \\ \mathcal{Q} + \mathbf{v} \cdot \mathcal{S} \end{pmatrix},$$

$$\langle \mathcal{S}_{ij}(\mathbf{r},t)\mathcal{S}_{k\ell}(\mathbf{r}',t')\rangle = 2k_B\eta T \left(\delta^K_{ik}\delta^K_{j\ell} + \delta^K_{i\ell}\delta^K_{jk} - \tfrac{2}{3}\delta^K_{ij}\delta^K_{k\ell}\right)\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'),$$

$$\langle \mathcal{Q}_i(\mathbf{r},t)\mathcal{Q}_j(\mathbf{r}',t')\rangle = 2k_B\kappa T^2\delta^K_{ij}\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'),$$

LLNS Discretization

Experience with Burger's equations suggests adding a stochastic flux to a standard second-order scheme captures fluctuations reasonably well.

This is not the case with LLNS

	$\langle \delta\rho^2 \rangle$	$\langle \delta J^2 \rangle$	$\langle \delta E^2 \rangle$
Exact value	2.35×10^{-8}	13.34	2.84×10^{10}
MacCormack	2.01×10^{-8}	13.31	2.61×10^{10}
PPM	1.97×10^{-8}	13.27	2.58×10^{10}
DSMC	2.35×10^{-8}	13.21	2.78×10^{10}
Error MacCormack	-14.3%	-0.3%	-8.4%
Error PPM	-16.0%	-0.5%	-9.4%
Error DSMC	0.0%	-1.0%	-2.1%

Mass conservation is microscopically exact. There is no diffusion or fluctuation term in the mass conservation equation

Numerical methods for stochastic PDE's

Accurately capturing fluctuations in a hybrid algorithm requires accurate methods for PDE's with a stochastic flux.

$$\partial_t U = LU + KW$$

where W is spatio-temporal white noise

We can characterize the solution of these types of equations in terms of the invariant distribution, given by the covariance

$$S(k,t) =< \hat{U}(k,t')\hat{U}^*(k,t'+t) >= \int_{-\infty}^{\infty} e^{i\omega t} S(k,\omega) d\omega$$

where

$$S(k,\omega) =< \hat{U}(k,\omega)\hat{U}^*(k,\omega) >$$

is the dynamic structure factor

We can also define the static structure factor

$$S(k) = \int_{-\infty}^{\infty} S(k,\omega) d\omega$$

Fluctuation dissipation relation

For

$$\partial_t U = LU + KW$$

if

$$L + L^* = -KK^*$$

then the equation satisfies a fluctuation dissipation relation and

$$S(k) = I$$

The linearized LLNS equations are of the form

$$\partial_t U = -\nabla \cdot (AU - C\nabla U - BW)$$

When $BB^* = 2C$, then the fluctuation dissipation relation is satisfied and the equilibrium distribution is spatially white with $S(k) = 1$

Discretization design issues

Consider discretizations of

$$\partial_t U = -\nabla \cdot (AU - C\nabla U - BW)$$

of the form

$$\partial_t U = -D(AU - CGU - BW)$$

Scheme design criteria

1. Discretization of advective component DA is skew adjoint; i.e., $(DA)^* = -DA$
2. Discrete divergence and gradient are skew adjoint: $D = -G^*$
3. Discretization without noise should be relatively standard
4. Should have “well-behaved” discrete static structure factor
   - $S(k) \approx 1$ for small k; i.e. $S(k) = 1 + \alpha k^p + h.o.t$
   - $S(k)$ not too large for all k. (Should $S(k) \leq 1$ for all k?)

Example: Stochastic heat equation

$$u_t = \mu u_{xx} + \sqrt{2\mu}\mathcal{W}_x$$

Explicit Euler discretizaton

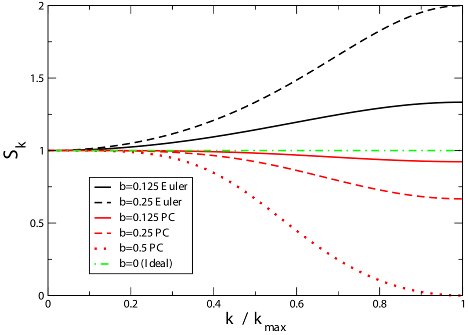
$$u_j^{n+1} = u_j^n + \frac{\mu \Delta t}{\Delta x^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right) + \sqrt{2\mu}\frac{\Delta t^{1/2}}{\Delta x^{3/2}}\left(W_{j+\frac{1}{2}}^n - W_{j-\frac{1}{2}}^n\right)$$

Predictor / corrector scheme

$$\tilde{u}_j^n = u_j^n + \frac{\mu \Delta t}{\Delta x^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right) + \sqrt{2\mu}\frac{\Delta t^{1/2}}{\Delta x^{3/2}}\left(W_{j+\frac{1}{2}}^n - W_{j-\frac{1}{2}}^n\right)$$

$$\begin{aligned} u_j^{n+1} &= \frac{1}{2}\left[u_j^n + \tilde{u}_j^n + \frac{\mu \Delta t}{\Delta x^2}\left(\tilde{u}_{j-1}^n - 2\tilde{u}_j^n + \tilde{u}_{j+1}^n\right)\right. \\ &+ \left.\sqrt{2\mu}\frac{\Delta t^{1/2}}{\Delta x^{3/2}}\left(W_{j+\frac{1}{2}}^n - W_{j-\frac{1}{2}}^n\right)\right] \end{aligned}$$

Structure factor for stochastic heat equation



Euler

$$S(k) = 1 + \beta k^2/2$$

Predictor/Corrector

$$S(k) = 1 - \beta^2 k^4/4$$

PC2RNG:

$$S(k) = 1 + \beta^3 k^6/8$$

How stochastic fluxes are treated can effect accuracy

Elements of discretization of LLNS – 1D

Spatial discretization

- Stochastic fluxes generated at faces
- Standard finite difference approximations for diffusion
  - Fluctuation dissipation
- Higher-order reconstruction based on PPM

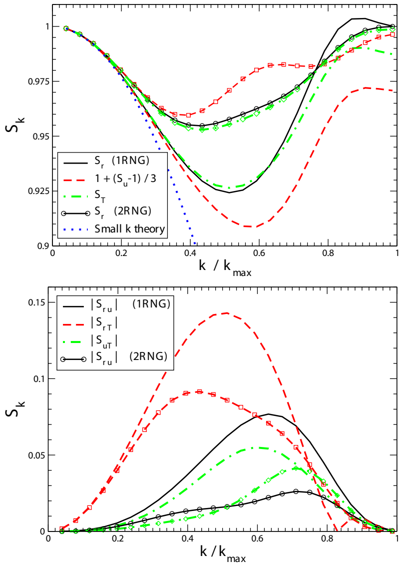
$$U_{J+½} = \frac{7}{12}(U_j + U_{j+1)} - \frac{1}{12}(U_{j-1} + U_{j+2})$$

  - Evaluate hyperbolic flux using $U_{j+½}$
  - Adequate representation of fluctuations in density flux

Temporal discretization

- Low storage TVD 3^{rd} order Runge Kutta
- Care with evaluation of stochastic fluxes can improve accuracy

Structure factor for LLNS in 1D



Discretization for LLNS

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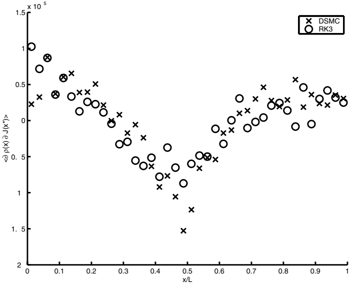
Exact value	2.35×10^{-8}	13.34	2.84×10^{10}
PPM	1.97×10^{-8}	13.27	2.58×10^{10}
RK3	2.29×10^{-8}	13.54	2.82×10^{10}
Error PPM	-16.0%	-0.5%	-9.4%
Error for RK3	-2.5%	1.5%	-0.7%

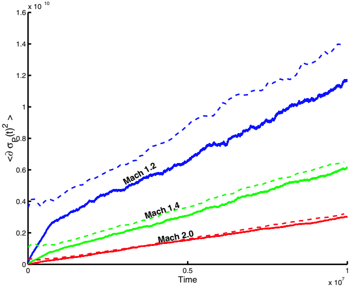
Basic scheme has been generalized to 3D and two component mixtures

- Additional complication is correlation between elements of stochastic stress tensor
- Several standard discretization approaches do not correctly respect these correlations
  - Do not satisfy discrete fluctuation dissipation relation
  - Leads to spurious correlations
- Alternative approach based on randomly selecting faces on which to impose correlation
  - Preserves correlation structure in 2D and 3D

SPDE versus DSMC

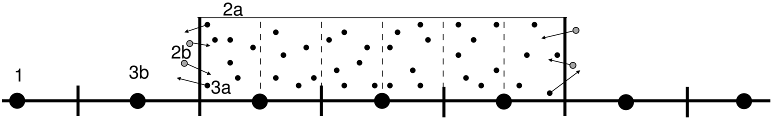


Correlation of density and momentum in a thermal gradient



Shock drift

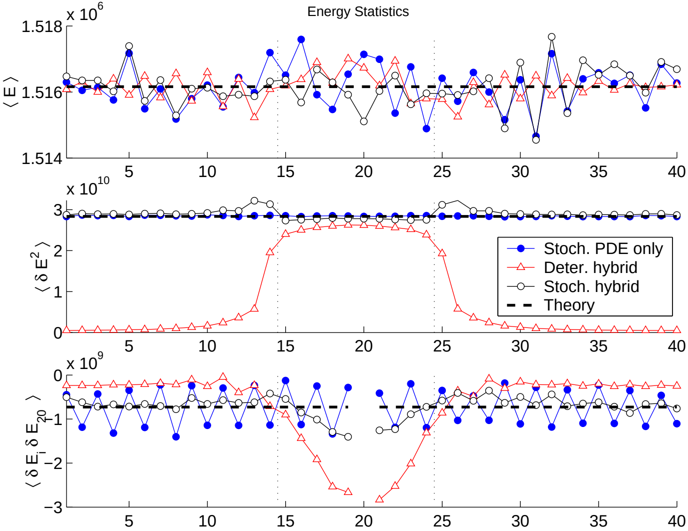
Hybrid Issues



- Maxwellian versus Chapman Enskog
  - Measuring gradients for C-E is problematic
  - Maxwellian typically gives better results in hybrid
- Refinement criterion
  - Use smoothed gradient – width based on noise magnitude
  - Potentially use breakdown parameter to guide refinement

Equilibrium

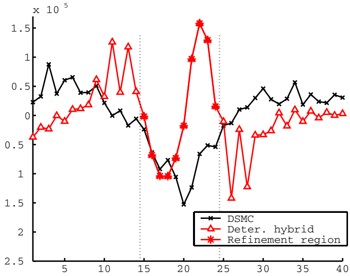
Does deterministic PDE treatment affect fluctuations for fluid simulations?



Non-equilibrium

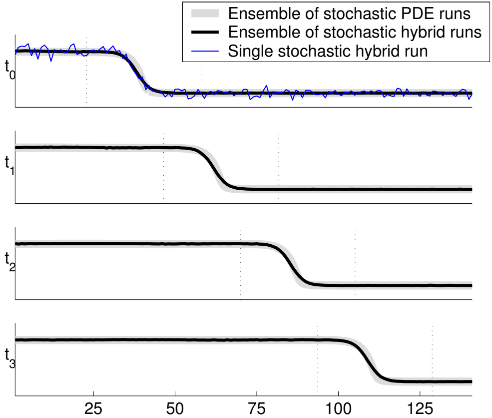
Look at correlations in the presence of a thermal gradient

Stochastic hybrid



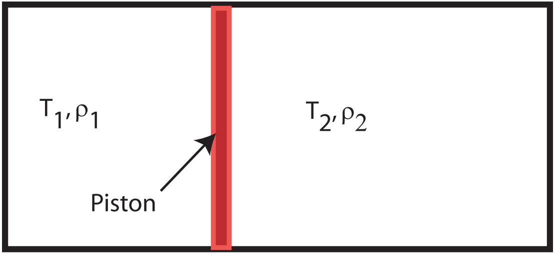
Deterministic hybrid

Shock propagation



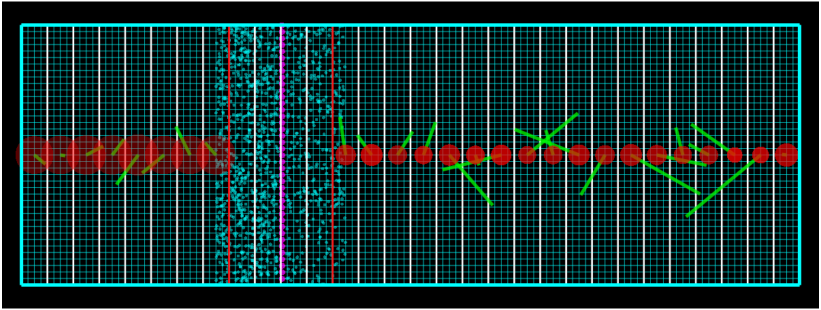
Propagation of refined shock

Piston problem



- $\rho_1 T_1 = \rho_2 T_2$
- Wall and piston are adiabatic boundaries
- Dynamics driven by fluctuations

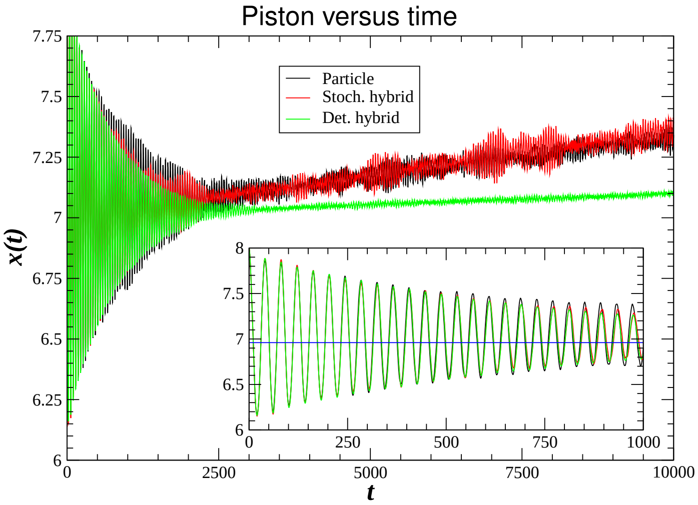
Piston dynamics



Hybrid simulation of Piston

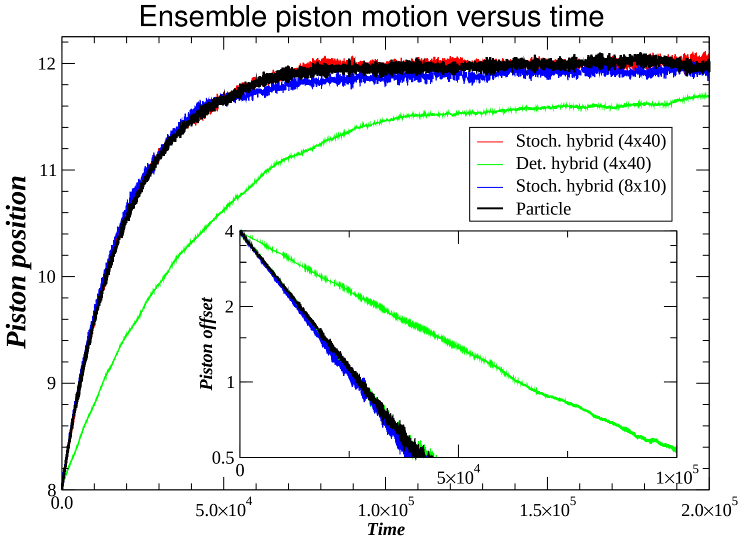
- Small DSMC region near the piston
- I-DSMC – see Donev talk

Piston position vs. time



Note: Error associated with deterministic hybrid enhanced for heavier pistons

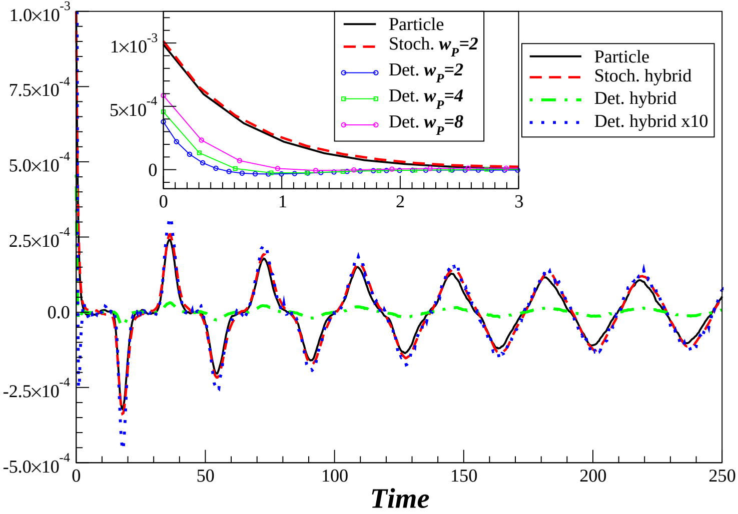
Averge piston position vs. time



Note: Some sensitivity to mesh used for continuum simulation

Piston velocity autocorrelation

Start with piston at equilibrium location



Velocity Autocorrelation Function

Summary

Failing to include fluctuations at the continuum level in a hybrid model can pollute the microscopic model

Hybrid methodology for capturing fluctuations

- Microscopic model – DSMC
- Continuum model – discretization of LLNS equations
  - RK3 centered scheme
  - Captures equilibrium fluctuations
- Hybridization based on adaptive mesh refinement constructs

Future issues

- Numerics / Mathematics
  - Mathematical structure of systems
  - Criterion for evaluating schemes / hybrids
  - Stochastic analogs of limiting – robustness
  - Fluctuations in low Mach number flows
- Physics
  - Reacting systems
  - Complex fluids