Between Kinetic Theory and Navier Stokes: Modeling Fluids at the Mesosacle

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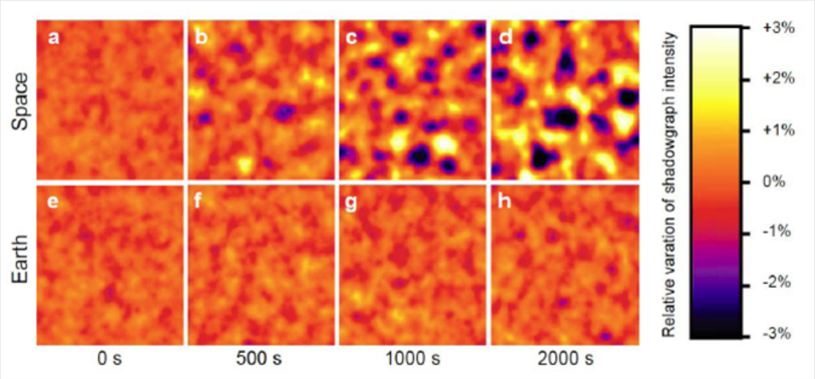
Multiscale models of fluid flow

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

- Dynamics described by set of PDEs – Navier Stokes equations
  - Mass
  - Momentum
  - Energy
  - Any additional phenomena
- 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 a different description is needed

Giant fluctuations



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Experiments show significant concentration fluctuations in zero gravity

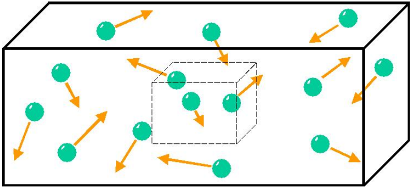
Fluctuations are reduced by gravity; cut-off wavelength proportional to $g^{-1/4}$

Vailati, *et al.*, Nature Comm., 2:290 (2011)

Thermal Fluctuations

The structures seen in experiments arise because of thermal fluctuations

- At microscopic scales, fluids are particle systems
  - Hydrodynamic variables, mass, momentum, energy, etc., correspond to averages of particle representation over representative volumes
  - Hydrodynamic variables naturally fluctuate
- In non-equilibrium settings, fluctuations lead to long-range correlations in hydrodynamic variables



Particle schemes (DSMC, MD, ...) capture statistical structure of fluctuations in macroscopic variables

- Variance of fluctuations
- Time-correlations
- Non-equilibrium behavior

But that are too expensive to use to study problems at these scales

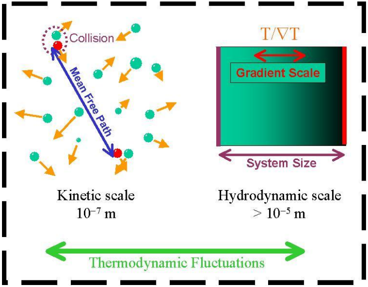
Possible approaches

Problems where fluctuations affect macroscopic dynamics can't be modeled with a deterministic continuum solver

Approaches

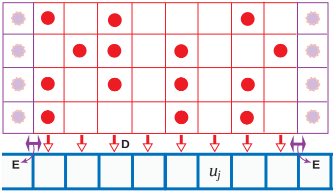
- Molecular model – correct but prohibitively expensive
- Hybrid – when detailed molecular model is needed in only a part of the domain
  - Molecular model only where needed
  - Cheaper continuum model in the bulk of the domain
  - Garcia *et al.*, JCP 1999 . . . but there's a problem
- Stochastic PDE models that incorporate fluctuations

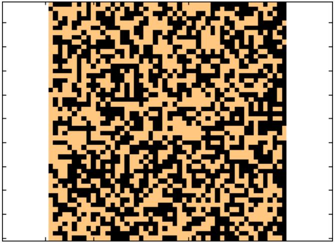
Look at fluid mechanics problems that span kinetic and hydrodynamics scales



A simple example with fluctuations

Asymmetric Excluded Random Walk:





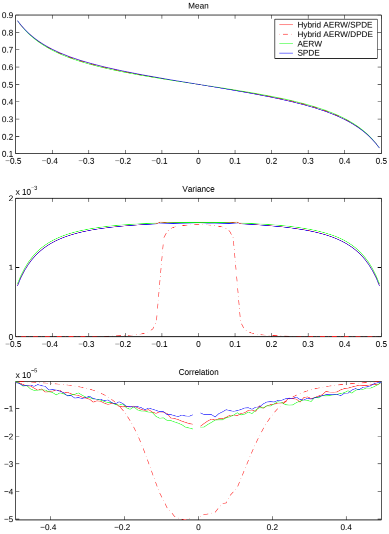
Probability of jump to the right sets the “Reynolds” number

- Mean field given by viscous Burgers’ equation

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

We can now build a hybrid algorithm for this system

AERW / Burgers'

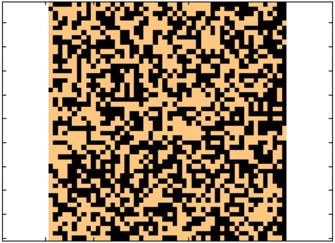


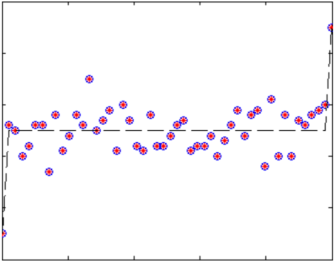
Rarefaction

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

Similar behavior observed in hybrid algorithms that combine particle algorithm with compressible Navier Stokes equations

AERW / Burgers'



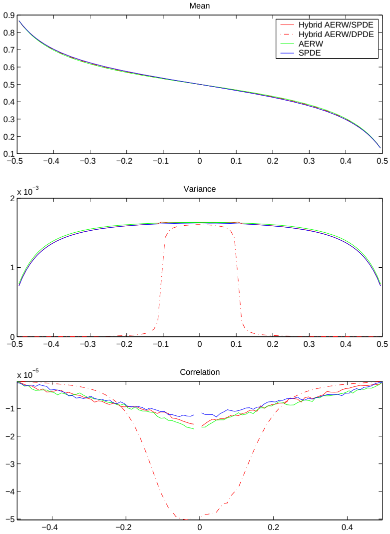


Fluctuations can be modeled by including a stochastic flux in Burgers' equation

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

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

AERW / Burgers'



Rarefaction

Adding a numerical treatment of the stochastic flux term "fixes" the problem for AERW model

How can we include the effect of fluctuations in models for fluid behavior?

How do we treat these kinds of systems numerically?

Landau-Lifshitz fluctuating Navier Stokes

Landau and Lifshitz proposed a model for continuum fluctuations in Navier-Stokes equations

- Incorporate stochastic fluxes into compressible Navier Stokes equations
- Equilibrium fluctuations known from statistical mechanics
- Magnitudes set by fluctuation dissipation balance

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

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

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

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

$$\tau = \eta(\nabla \mathbf{v} + (\nabla \mathbf{v})^T) - \frac{2}{3}\eta\, \mathbb{I}\, \nabla \cdot \mathbf{v}$$

Fluctuating Navier-Stokes

Some observations

- System is highly nonlinear
- System preserves conservation of mass, momentum and energy
- Conservation of mass is microscopically exact
- Stochastic flux of momentum reflects structure of deterministics stress tensor

Note that there are mathematical difficulties with this system

- Formally solutions would be distributions . . . we can't multiply them together
- Gaussian random noise $\rightarrow$ that the system can generate large deviations . . . but fluid equations not defined when T and ρ are negative

Think of these equations as only being applicable at a given range of spatial scales.

Only applicable on scales where unknows represent averages over at least $O(100)$ molecules.

Fluctuation dissipation balance

Consider a stochastics ODE of the form

$$du = -\lambda u dt + \alpha dB \quad u(0) = u_0$$

where dB is a Weiner process.

Without noise, solution decays to zero.

Noise term, αdB, introduces fluctuations, deterministic term, $-\lambda u$, damps the fluctuations.

Fluctuation dissipation balance charaterizes asymptotic fluctuations as $t \to \infty$.

Here

$$u(t) = e^{-\lambda t} u_0 + \alpha \int_0^t e^{\lambda(s-t)} dB(s)$$

Since the Weiner process is δ correlated in time

$$< u(T), u(T) >= \frac{1}{T} \int_0^T [e^{-2\lambda t} u_0^2 + 2\alpha e^{-\lambda t} u_0 \int_0^t e^{\lambda(s-t)} dB + \alpha^2 \int_0^t e^{2\lambda(s-t)} ds] dt$$

So

$$\lim_{T \to \infty} < u(T), u(T) >= \frac{\alpha^2}{2\lambda}$$

Stochastic PDE's

Consider system of the form

$$d\mathcal{U} = \mathcal{L}\mathcal{U}dt + \mathcal{K}dB$$

where B a Weiner process (dB 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

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

known as the dynamic structure factor

Fourier transform to obtain

$$i\omega \; d\widehat{\mathcal{U}} = \widehat{\mathcal{L}}\widehat{U}d\omega + \widehat{\mathcal{K}}d\widehat{B}$$

Then

$$S(k,\omega) = (\widehat{L} - i\omega)^{-1}(\widehat{K}\widehat{K}^*)(\widehat{L}^* + i\omega)^{-1}$$

We can also define the static structure factor

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

Static structure factor characterizes fluctuation dissipation of SPDE system

Stochastic heat equation

$$u_t = \mu u_{xx} + \sqrt{2\mu} W_x$$

Fourier transform in space and time

$$i\omega\widehat{u} = -\mu k^2 \widehat{u} + i\sqrt{2\mu} k \widehat{W}$$

Then

$$\widehat{u} = \frac{i\sqrt{2\mu} k \widehat{W}}{i\omega + \mu k^2}$$

That then give

$$S(k,\omega) = \frac{2\mu k^2}{\omega^2 + \mu^2 k^4} \qquad \text{and} \qquad S(k) = 1$$

Fluctuation dissipation relation – discrete form

For

$$\partial_t U = AU + LU + KW \quad \text{where} \qquad A = -A^* \quad \text{and} \qquad L = L^*$$

if

$$2\gamma L = -KK^*$$

then the equation satisfies a fluctuation dissipation relation with

$$S(k) = 2\gamma I \quad ,$$

which mimics the analytical form $\gamma(\mathcal{L} + \mathcal{L}^*) = -\mathcal{K}\mathcal{K}^*$

Would like to construct numerics so that

$$S^{num}(k) = 2\gamma(1 + \alpha k^{2p})$$

for small k and

$$S^{num}(k) \leq 2\gamma(1+???) \quad \text{forall } k.$$

Want approximations to differential operators with these properties discretely.

Spatial approximation

Consider finite volume discretizations where u_j^n represents average value of solution on the j^{th} cell at time t^n.

Define a discrete divergence that approximates cell-center divergence of a field defined at cell edges

$$(DF)_j = \frac{F_{j+1/2} - F_{j-1/2}}{\Delta x}$$

The adjoint to D then defines a discrete gradient at cell edges from values defined a cell centers

$$-(Gv)_{j+1/2} = (D^T v)_{j+1/2} = \frac{v_{j+1} - v_j}{\Delta x}$$

Then DG defines a cell-centered Laplacian.

This skew adjoint property is needed for discrete fluctuation dissipation balance

We will also approximate the noise by

$$\mathcal{W} = \frac{W^n_{j+1/2}}{\sqrt{\Delta t \Delta x}}$$

where $W^n_{j+1/2}$ is a normally distributed random variable and the scale approximates a δ function in space and time

Example: Stochastic heat equation

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

Explicit Euler discretizaton

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

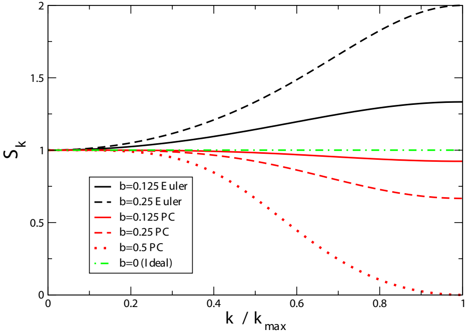
Predictor / corrector scheme

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

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

Structure factor for stochastic heat equation

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



Euler

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

Trapezoidal
Predictor/Corrector

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

Midpoint
Predictor/Corrector

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

How stochastic fluxes are treated can affect accuracy

Adding advection

What happens if we add advection to the system

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

Analytically, au_x is skew adjoint.

Upwind methods introduce artificial dissipation so that numerically the treatment of adjection is not numerically skew adjoint so we do not get discrete fluctuation dissipation balance.

Need to use centered discretizations but these can lead to stability issues as $\mu \to 0$.

RK3

We consider an alternative Runge Kutta scheme for stochastic systems $U_t = R(U, W)$

$$
\begin{aligned}
U_{i,j,k}^{n+1/3} &= U_{i,j,k}^{n} + \Delta t \mathbf{R}(U^n, W_1) \\
U_{i,j,k}^{n+2/3} &= \frac{3}{4} U_{i,j,k}^{n} + \frac{1}{4} \left[U_{i,j,k}^{n+1/3} + \Delta t \mathbf{R}(U^{n+\frac{1}{3}}, W_2) \right] \\
U_{i,j,k}^{n+1} &= \frac{1}{3} U_{i,j,k}^{n} + \frac{2}{3} \left[U_{i,j,k}^{n+2/3} + \Delta t \mathbf{R}(U^{n+\frac{2}{3}}, W_3) \right]
\end{aligned}
$$

W_i denote the random fields used in each stage of the integration.

We generate two sets of normally distributed independent Gaussian fields, W^A and W^B, and set

$$
\begin{aligned}
W_1 &= W^A + \beta_1 W^B \\
W_2 &= W^A + \beta_2 W^B \\
W_3 &= W^A + \beta_3 W^B
\end{aligned}
$$

where $\beta_1 = (2\sqrt{2} + \sqrt{3})/5$, $\beta_2 = (-4\sqrt{2} + 3\sqrt{3})/5$, and $\beta_3 = (\sqrt{2} - 2\sqrt{3})/10$.

The RK3 scheme has good stability properties, is weakly second-order accurate and is weakly third-order accurate for linear problems.

Elements of discretization of FNS – 1D

Spatial discretization – finite volume

- Stochastic fluxes generated at faces
- Standard second-order finite difference approximations for diffusion
    - Fluctuation dissipation
- Fourth-order interpolation of solution to edges

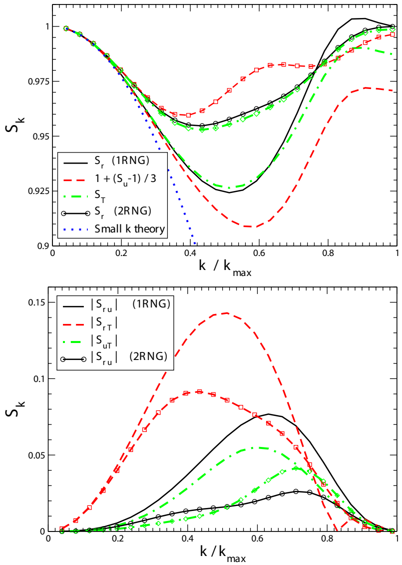
$$Q_{j+\frac{1}{2}} = \frac{7}{12}(Q_j + Q_{j+1}) - \frac{1}{12}(Q_{j-1} + Q_{j+2})$$

- Evaluate hyperbolic flux using $Q_{j+\frac{1}{2}}$
- 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



Multidimensional considerations

Standard discretizations of stress tensor in fully cell-centered finite volume approach leads to velocity correlations – can't compute divergence of stochastics stress in a way that is consistent with symmetrized gradient of velocity

$$\tau = \eta(\nabla U + (\nabla U)^T) - \frac{2}{3}\eta \mathbb{I} \nabla \cdot U$$

Rewrite stress tensor as

$$\nabla \cdot (\eta(\nabla U + (\nabla U)^T) - \frac{2}{3} \nabla \cdot (\eta \nabla \cdot U \ \mathbb{I}) = \nabla \cdot \eta \nabla U + \frac{1}{3} \nabla \cdot (\eta \mathbb{I} \ \nabla \cdot U) + \mathrm{cross} - \mathrm{terms}$$

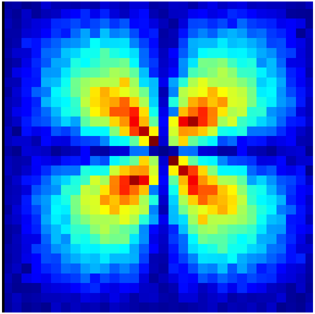
Generate noise for first term at edges and noise for second term at corners

Cross terms included in deterministic discretization but no corresponding noise.

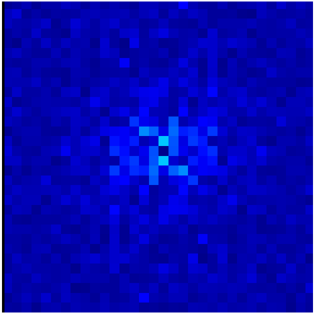
Alternative approach based on staggered grid approximation

- Easier to construct scheme with desired discrete fluctuation dissipation relation
- Harder to construct a hybrid discretization
- Balboa *et al.*

Static structure factors



Standard tensor discretization



New tensor discretization

Tests with full multicomponent model show good approximation to equilibrium covariances

Methodology validated against DSMC in non-equilibrium setting for two-component systems

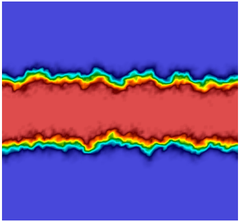
Comparison to MD simulation

Models can be validated against theory in a variety of equilibrium and non-equilibrium settings

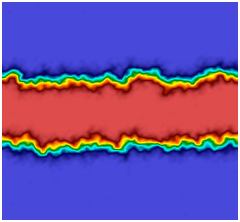
Direct comparison with particle models

Molecular dynamics

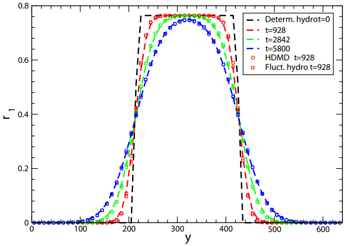
- Two-dimensional hard-disk fluid
- 128 x 128 hydrodynamics cells
- 1.25 million disks
- Average ensemble to compute effective mixing



Molecular Dynamics

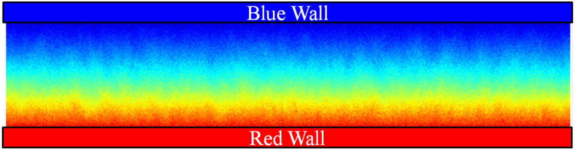


Fluctuating Navier Stokes



Essemble / horizontal average

Diffusion and fluctuations



Monotonic gas of "red" and "blue" particles in mean gradient at statistical steady state

- Nonequilibrium leads to velocity - concentration correlation
- Correlation changes effective transport equation
- Linearize, incompressible, isothermal theory

$$\hat{S}_{c,v_y} = \langle (\widehat{\delta c})(\widehat{\delta v}_y^*) \rangle \approx -[k_\perp^2 k^{-4}] \nabla c_0$$

Then

$$\langle \mathbf{j} \rangle \approx (D_0 + \Delta D) \nabla c_0 = [\ \ D_0 - (2\pi)^{-3} \int_k \hat{S}_{c,v_y} dk\ \ ] \nabla c_0$$

Fluctuating hydrodynamics results

Integrals are singular and require a molecular level cutoff

Two dimensions

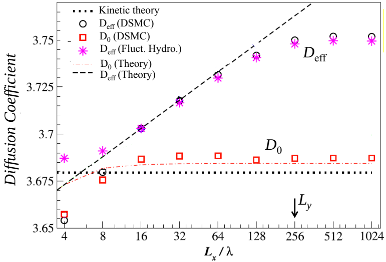
- $L_z << L_x << L_y$
- Effective diffusion $\sim ln(L_x)$

Three dimensions

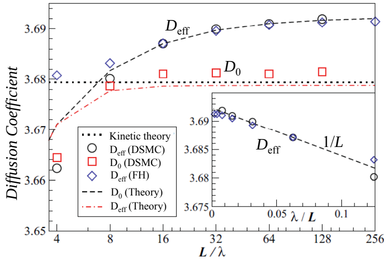
- $L_z = L_x = L << L_y$
- Effective diffusion $\sim 1/L$

DSMC confirms FNS results in both cases

Effects enhanced in liquids or when there are other physical phenomena such as reactions



2D



3D

Bells and whistles

Physics

- Multicomponent diffusion for multispecies simulations
- Reactions
- Phase transition phenomena
- Non-ideal fluid effects

Numerical models

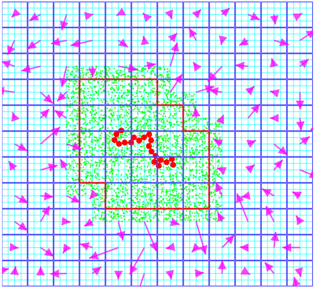
- Incompressible flow models
- Generalized low Mach number models
- Semi-implicit time-stepping schemes

Hybrid algorithm

For some applications, need to include detailed molecular effects locally. Stochastic PDE solver is not adequate

Couples a particle description to fluctuating Navier Stokes equations

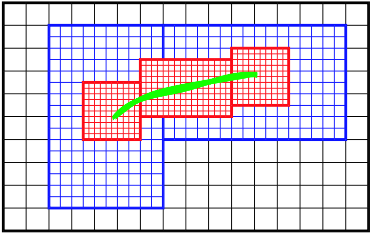
- Molecular model only where needed
- Cheaper continuum model in the bulk of the domain



Hybrid approach

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

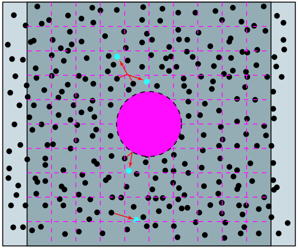
- Adaptive mesh refinement (AMR) provides a framework for such a coupling
  - AMR for fluids except change to a particle description at the finest level of the heirarchy
- Use basic AMR design paradigm for development of a hybrid method
  - How to integrate a level
  - Mapping between different representations
  - Synchronization at boundary between representations



2D adaptive grid hierarchy

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



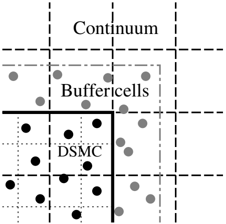
Example of flow past a sphere

Adaptive mesh and algorithm refinement

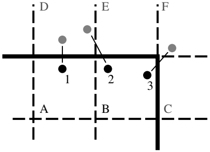
AMR approach to constructing hybrids – Garcia et al., JCP 1999

Hybrid algorithm – 2 level

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

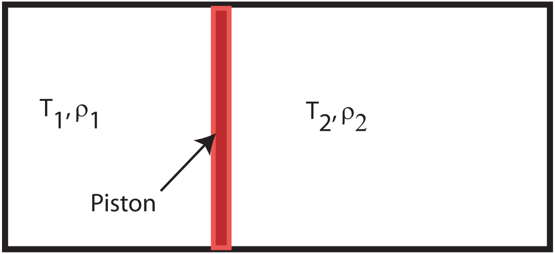


DSMC boundary conditions



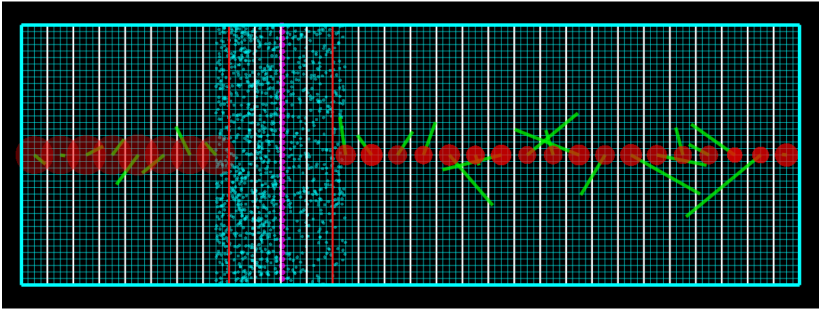
DSMC flux

Piston problem



- If $\rho_1 T_1 = \rho_2 T_2$ deterministic Navier-Stokes is in mechanical equilibrium
- Wall and piston are adiabatic boundaries
- Dynamics driven by fluctuations

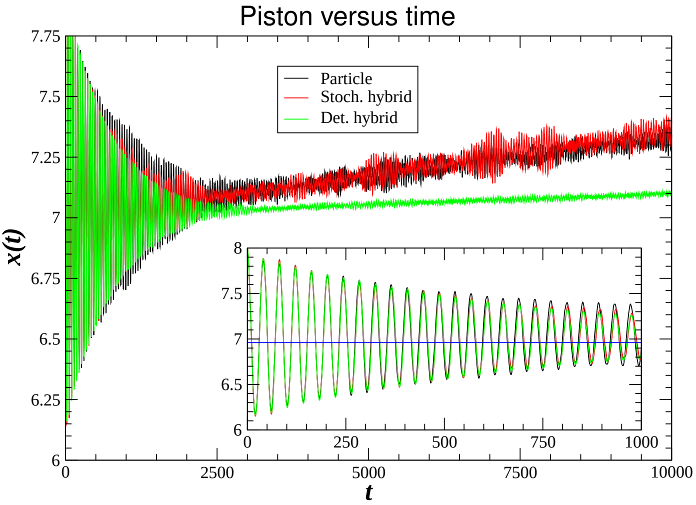
Piston dynamics



Hybrid simulation of Piston

- Small DSMC region near the piston
- Either deterministic or fluctuating continuum solver

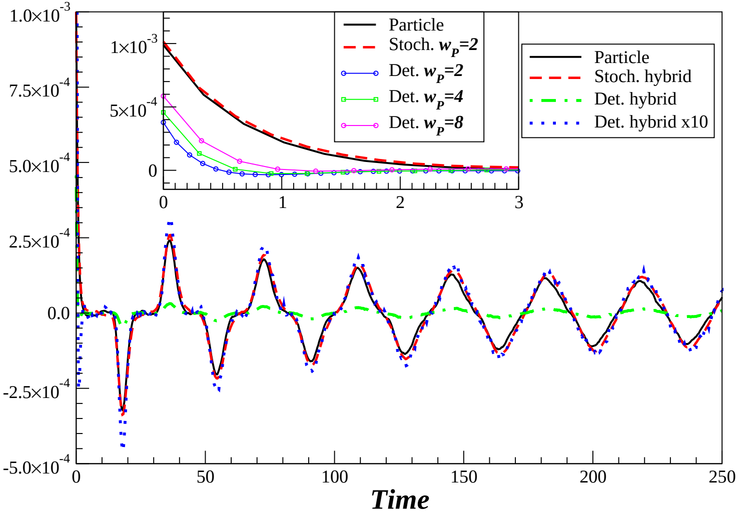
Piston position vs. time



Note: Error associated with deterministic hybrid enhanced for heavier pistons

Piston velocity autocorrelation

Start with piston at equilibrium location



Velocity Autocorrelation Function

Summary – take home messages

In non-equilibrium settings, fluctuations lead to long-range correlations in hydrodynamic behavior

- Important for a variety of phenomena at the mesoscale
- Stochastic PDE's provide effective mechanism for incorporating effect of fluctuations at those scales

Design issues for SPDE's with stochastic fluxes

- Design discrete operators to satisfy discrete fluctuation dissipation balance
- RK3 centered scheme
- Analysis of algorithms based on discrete static structure factor
- Give correct equilibrium fluctuations
- Captures enhanced diffusion in nonequilibrium mixing

Hybrid methodology for fluids – continuum model for fluctuations

- Hybridization based on adaptive mesh refinement constructs
- Continuum model – discretization of FNS equations
- Stochastic hybrid matches pure particle simulations
- Deterministic hybrids introduce spurious correlations

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