Finite Volume Methods for Fluctuating Hydrodynamics

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Outline

- Giant fluctuations
- Landau-Lifshitz fluctuating Navier Stokes equations
- Numerical methods for stochastic PDE's
- Fluctuations and diffusion
- Hybrid algorithms
- Conclusions

Multi-scale models of fluid flow

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

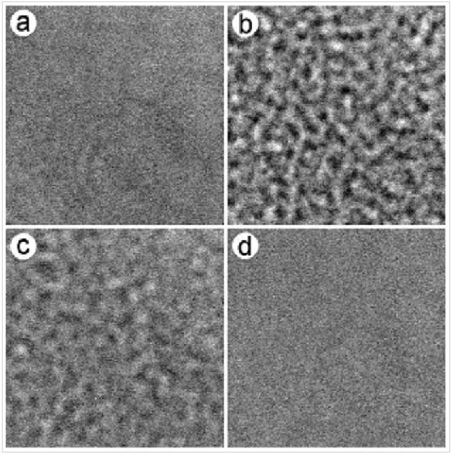
- Dynamics described by set of PDEs.
- Well-established numerical methods (finite difference, finite elements, etc.) for solving these PDEs.
- Hydrodynamic PDEs are accurate over a broad range of length and time scales.

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

When is the continuum description of a fluid not accurate?

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

Giant fluctuations



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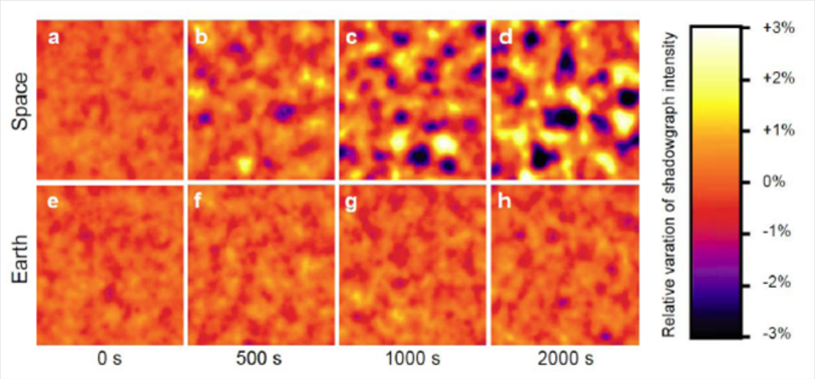
Experimental images of light scattering from the interface between two miscible fluids

Images show formation of giant fluctuations in diffusive mixing

Vailati and Giglio, Nature 390,262 (1997)

Additional experiments



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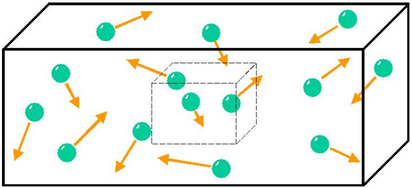
Experiments show significant concentration fluctuations in zero gravity

Fluctuations are reduced by gravity with a cut-off wavelength proportional to g

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

Hydrodynamic Fluctuations



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

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

Can we capture fluctuations at the continuum level and model giant fluctuations

Landau-Lifshitz fluctuating Navier Stokes

Landau and Lifshitz proposed model for fluctuations at the continuum level

- Incorporate stochastic fluxes into compressible Navier Stokes equations
- Magnitudes set by fluctuation dissipation balance

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

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

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

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

Note that there are mathematical difficulties with this system

Numerical methods for stochastic PDE's

Capturing fluctuations 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

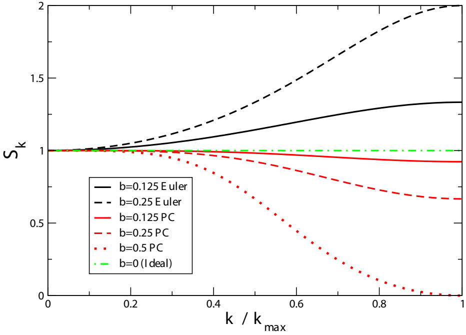
$$u_j^{n+1} = u_j^n + \frac{\mu \Delta t}{\Delta x^2}\left(u_{j-1}^n - 2u_j^n + u_{j+1}^n\right) + \sqrt{2\mu}\frac{\Delta t^{1/2}}{\Delta x^{3/2}}\left(W_{j+\frac{1}{2}}^n - W_{j-\frac{1}{2}}^n\right)$$

Predictor / corrector scheme

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

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

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 – fully cell-centered

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

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

  - Evaluate hyperbolic flux using $U_{j+\frac{1}{2}}$
  - Adequate representation of fluctuations in density flux

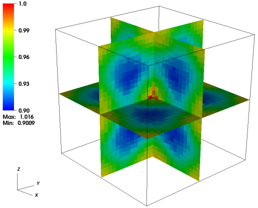
Temporal discretization

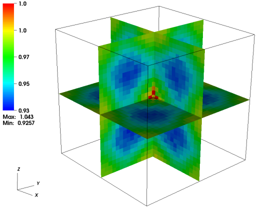
- Low storage TVD 3^{rd} order Runge Kutta
- Care with evaluation of stochastic fluxes can improve accuracy

Multidimensional considerations

Basic cell-centered 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
- Alternative approach based on staggered grid approximation
  - Easier to construct scheme with desired discrete fluctuation dissipation relation
  - Harder to construct a hybrid discretization
  - See Balboa *et al.*, submitted for publication

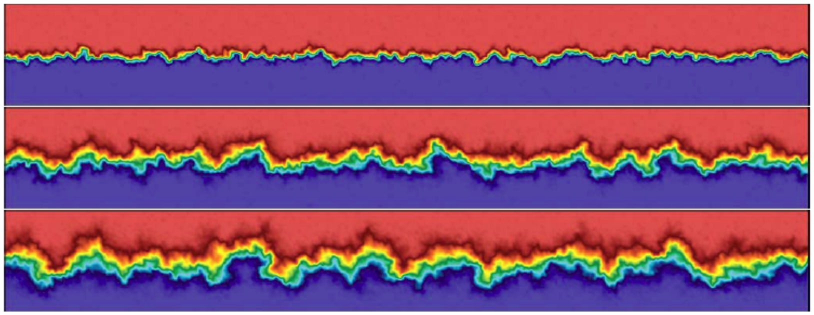




Donev *et al.*, CAMCoS, 5:149-157 (2010).

Fluctuations and mixing

Snapshots of the concentration during diffusive mixing
($t = 1, 4, 10$)

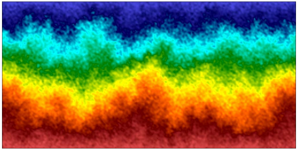


- Two species are identical
- Interface is initially perfectly flat
- Closed box (periodic in x) with no external forcing
- This is not a hydrodynamic instability

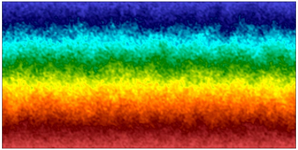
Effect of gravity

- Heavy (red) and light (blue) particles with density ratio 4
- Non-equilibrium: Establish a concentration gradient by imposing concentration boundary conditions at top and bottom
- Long-time simulations show formation of giant fluctuations with no gravity
- Adding gravity suppresses the fluctuations
- Qualitatively in agreement with experimental observations

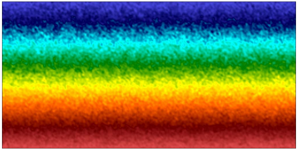
Donev *et al.*, J. Stat. Mech. 2011:P06014 (2011)
Donev *et al.*, PRL, 106(20):204501(2011)



$g = 0$

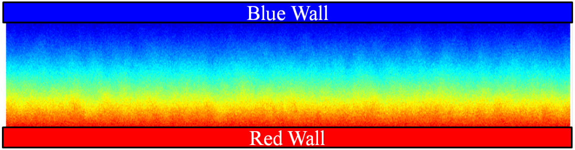


$g = 0.1g_0$



$g = g_0$

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

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

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

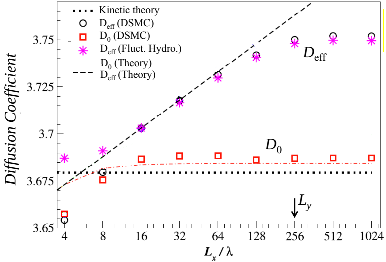
- $L_z << L_x << L_y$
- Effective diffusion $\sim ln(L_x)$

Three dimensions

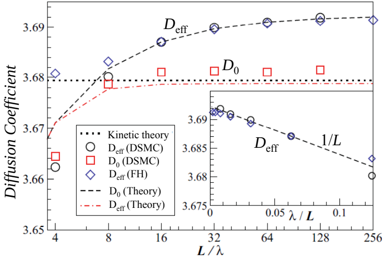
- $L_z = L_x = L << L_y$
- Effective diffusion $\sim 1/L$

DSMC confirms FNS results in both cases

System size dependence of enhanced diffusion is related to the range of power law behavior in the VACF of fluid particles in finite systems and observed finite size effects in MD simulations



2D



3D

Summary

Correlation of fluctuations that leads to enhanced diffusion can also lead to macroscale observables in diffusive mixing (giant fluctuations)

- Effect is relatively small in gases
- Signficantly enhanced for liquids or additional physics such as reactions
- Fluctuations can play a key role in the design of microfluidic devices

Numerical methodology for fluctuating Navier Stokes equations

- Higer-order centered discretization of advection (skew adjoint)
- Second-order centered approximation of diffusion (self adjoint)
- RK3 centered scheme
- Resulting discretization satisfies discrete fluctuation dissipation result
- Discretization designed to have well-behaved discrete static structure factors
- FNS solver is able to capture enhancement of diffusion resulting from fluctuations

Future directions

- Fluctuations in low Mach number flows
- Fluctuations in reacting systems

Hybrid approach

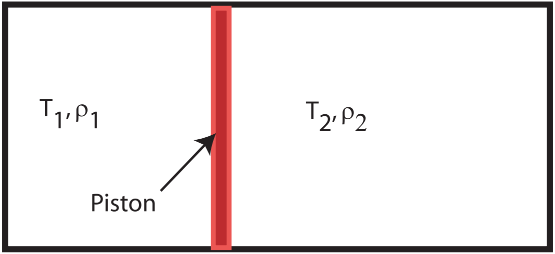
Develop a hybrid algorithm for fluid mechanics that couples a particle description to a continuum description

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

- AMR provides a framework for such a coupling
  - AMR for fluids except change to a particle description at the finest level of the heirarchy

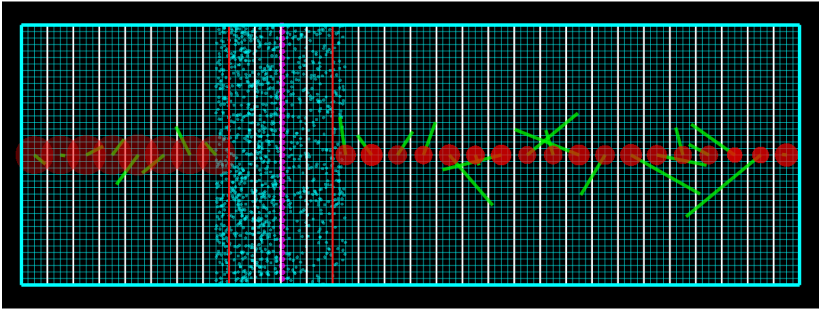
- Use basic AMR design paradigm for development of a hybrid method

Piston problem



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

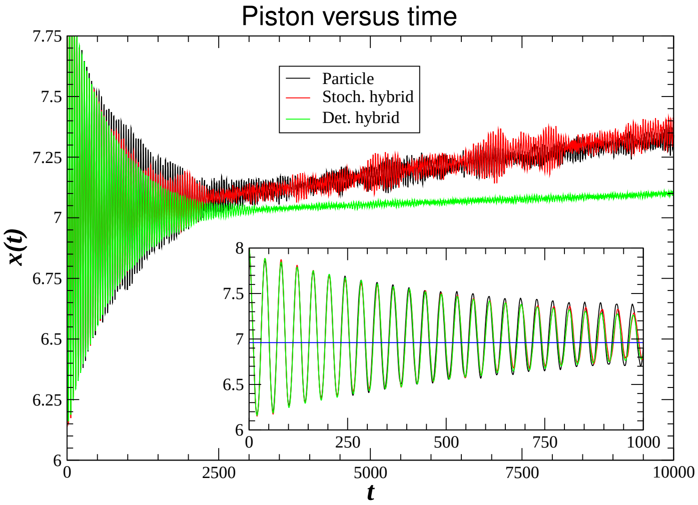
Piston dynamics



Hybrid simulation of Piston

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

Piston position vs. time



Note: Error associated with deterministic hybrid enhanced for heavier pistons