Finite-Volume Schemes for Fluctuating Hydrodynamics

Aleksandar Donev

Luis W. Alvarez Fellow, Lawrence Berkeley National Laboratory

&

Eric Vanden-Eijnden, Courant Institute, NYU

Jonathan Goodman, Courant Institute, NYU

Alejandro L. Garcia, San Jose State University

John B. Bell, Lawrence Berkeley National Laboratory

1This work performed in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

SIAM MS10 Conference

May 21, 2010
Flows of fluids (gases and liquids) through micro- (µm) and nano-scale (nm) structures has become technologically important, e.g., micro-fluidics, microelectromechanical systems (MEMS).

Biologically-relevant flows also occur at micro- and nano- scales.

Essential distinguishing feature from “ordinary” CFD: thermal fluctuations! Fluctuations impact Brownian motion and instabilities.

It is necessary to include thermal fluctuations in continuum solvers in particle-continuum hybrids [1].

The flows of interest often include suspended particles: colloids, polymers (e.g., DNA), blood cells, bacteria: complex fluids.
Introduction

Particle/Continuum Hybrid Approach
We consider stochastic transport equations (conservation laws) [2] of the form

\[
\partial_t U = - \nabla \cdot \left[ F(U) - \mathcal{Z} \right] = - \nabla \cdot \left[ F_H(U) - F_D(\nabla U) - B(U) \mathcal{W} \right],
\]

where \( B(U) \) is a scaling matrix for the spatio-temporal white noise \( \mathcal{W} \), i.e., a Gaussian random field with covariance

\[
\langle \mathcal{W}(r, t) \mathcal{W}^*(r', t') \rangle = \delta(t - t') \delta(r - r').
\]

The white noise forcing models intrinsic thermal fluctuations as originally proposed by Landau-Lifshitz [2].

These equations are interpreted in a finite-volume (finite-dimensional) context, which is well-defined for the linearized equations (but nonlinear equations are problematic!).
Consider the **stochastic advection-diffusion equation** in one dimension

\[ u_t = -cu_x + \mu u_{xx} + \sqrt{2\mu} W_x. \]

**Simple Euler time integrator**

\[
\begin{align*}
    u_j^{n+1} &= u_j^n - \alpha (u_{j+1}^n - u_{j-1}^n) \\
    &\quad + \beta (u_{j-1}^n - 2u_j^n + u_{j+1}^n) + \sqrt{2\beta} \Delta x^{-1/2} \left( W_{j+1/2}^n - W_{j-1/2}^n \right)
\end{align*}
\]

**Dimensionless (CFL) time steps control the stability and the accuracy**

\[
\alpha = \frac{c \Delta t}{\Delta x} \quad \text{and} \quad \beta = \frac{\mu \Delta t}{\Delta x^2} = \frac{\alpha}{r}.
\]
Consider the general linear SPDE

$$U_t = LU + KW,$$

where the generator $L$ and the filter $K$ are linear operators.

The solution is a generalized process, which in the long-time limit is a stationary Gaussian process, fully characterized by its covariance.

SPDEs like this are best studied in Fourier wavevector-frequency space, $\hat{U}(k, \omega)$, where the covariance is the spectrum.

We focus on the static or spatial spectrum (static structure factor matrix)

$$S(k) = \lim_{t \to \infty} V \left\langle \hat{U}(k, t)\hat{U}^*(k, t) \right\rangle,$$

but the analysis can be extended to the spatio-temporal spectrum $S(k, \omega)$ (dynamic structure factor matrix).
Spatio-Temporal Discretization

- **Finite-volume discretization** of the field
  \[ U_j(t) = \frac{1}{\Delta x} \int_{(j-1)\Delta x}^{j\Delta x} U(x, t) \, dx \]

- General numerical method given by a **linear recursion**
  \[ U_{j}^{n+1} = (I + L_j \Delta t) U^n + \Delta t K_j W^n = (I + L_j \Delta t) U^n + \sqrt{\frac{\Delta t}{\Delta x}} K_j W^n \]

- The classical PDE concepts of consistency and stability **continue to apply** for the mean solution of the SPDE, i.e., the **first moment** of the solution.

- However, the classical concepts of convergence do not translate to the stochastic context!

- For SPDEs, it is natural to focus on the **second moments**.
Use the **discrete Fourier transform (DFT)** to convert the iteration to Fourier space.

Analysis will be focused on the **discrete static spectrum**

\[
S_k = V \langle \hat{U}_k (\hat{U}_k)^* \rangle = S(k) + O(\Delta t^{p_1} k^{p_2}) ,
\]

for a **weakly consistent** scheme.

For fluctuating hydrodynamics equations we have a **spatially-white** field at equilibrium, \( S(k) = 1 \).

The remainder term quantifies the **stochastic accuracy** for **large wavelengths** \( (\Delta k = k \Delta x \ll 1) \) and **small frequencies** \( (\Delta \omega = \omega \Delta t \ll 1) \).
A straightforward calculation \cite{3} gives

\[(I + \Delta t \hat{L}_k) S_k \left( I + \Delta t \hat{L}_k^* \right) - S_k = -\Delta t \hat{K}_k \hat{K}_k^*.\]

For small $\Delta t$

\[\hat{L}_k S_k^{(0)} + S_k^{(0)} \hat{L}_k^* = -\hat{K}_k \hat{K}_k^*,\]

and thus $S_k^{(0)} = \lim_{\Delta t \to 0} S_k = I$ iff discrete fluctuation-dissipation balance \cite{4, 5} holds

\[\hat{L}_k + \hat{L}_k^* = -\hat{K}_k \hat{K}_k^*.\]

Use the method of lines: first choose a spatial discretization consistent with the discrete fluctuation-dissipation balance condition, and then choose a temporal discretization.

\[
\partial_t U = -\nabla \cdot [F(U) - \mathcal{E}] = \nabla \cdot \left[ -AU + \mu \nabla U + \sqrt{2\mu} \mathcal{W} \right]
\]

- The conservative discretization,

\[
\Delta U_j = (\partial_t U_j) \Delta t = -\frac{\Delta t}{\Delta x} A \left( U_{j+\frac{1}{2}} - U_{j-\frac{1}{2}} \right),
\]

\[
+ \frac{\mu \Delta t}{\Delta x} \left( \nabla j_{+\frac{1}{2}} - \nabla j_{-\frac{1}{2}} \right) U + \frac{\sqrt{2\mu \Delta t}}{\Delta x^{3/2}} \left( W_{j+\frac{1}{2}} - W_{j-\frac{1}{2}} \right)
\]
satisfies the discrete fluctuation-dissipation balance if:

- The discrete divergence \( D \equiv \nabla \cdot \) and gradient \( G \equiv \nabla \) operators are dual, \( D^* = -G \),

\[
\nabla j_{+\frac{1}{2}} U = \Delta x^{-1} (U_{j+1} - U_j).
\]

- \( DA \) is skew-adjoint, \( (DA)^* = DA \), i.e., the cell-to-face interpolation is centered (\textit{no upwinding!}),

\[
U_{j+\frac{1}{2}} = \frac{7}{12} (U_j + U_{j+1}) - \frac{1}{12} (U_{j-1} + U_{j+2}).
\]
Runge-Kutta (RK3) Method

- Adapted a standard TVD **three-stage Runge-Kutta** temporal integrator and optimized the stochastic accuracy:

\[
U_{j}^{n+\frac{1}{3}} = U_{j}^{n} + \Delta U_{j}(U^{n}, W_{1})
\]

\[
U_{j}^{n+\frac{2}{3}} = \frac{3}{4} U_{j}^{n} + \frac{1}{4} \left[ U_{j}^{n+\frac{1}{3}} + \Delta U_{j}(U_{j}^{n+\frac{1}{3}}, W_{2}) \right]
\]

\[
U_{j}^{n+1} = \frac{1}{3} U_{j}^{n} + \frac{2}{3} \left[ U_{j}^{n+\frac{2}{3}} + \Delta U_{j}(U_{j}^{n+\frac{2}{3}}, W_{3}) \right].
\]

- Two random numbers per cell per time step

\[
W_{1} = W_{A} - \sqrt{3}W_{3}
\]

\[
W_{2} = W_{A} + \sqrt{3}W_{3}
\]

gives third-order temporal stochastic accuracy

\[
S_{k} = 1 - \frac{r}{24} \alpha^{3} \Delta k^{2} - \frac{24 + r^{2}}{288r} \alpha^{3} \Delta k^{4} + \text{h.o.t.}
\]
Landau-Lifshitz Navier-Stokes Equations

Complete single-species fluctuating hydrodynamic equations [6]:

\[ \mathbf{U}(r, t) = [\rho, \mathbf{j}, e]^T = [\rho, \rho \mathbf{v}, c_v \rho \mathbf{T} + \frac{\rho v^2}{2}]^T \]

\[ \mathbf{F}_H = \begin{bmatrix} \rho \mathbf{v} \\ \rho \mathbf{v}^T + P(\rho, T) \mathbf{I} \\ (e + P)\mathbf{v} \end{bmatrix}, \quad \mathbf{F}_D = \begin{bmatrix} 0 \\ \sigma \\ \sigma \cdot \mathbf{v} + \xi \end{bmatrix}, \quad \mathbf{Z} = \begin{bmatrix} 0 \\ \Sigma \\ \Sigma \cdot \mathbf{v} + \Xi \end{bmatrix} \]

\[ \sigma = \begin{bmatrix} \eta (\nabla \mathbf{v} + \nabla \mathbf{v}^T) - \frac{\eta}{3} (\nabla \cdot \mathbf{v}) \mathbf{I} \end{bmatrix} \text{ and } \xi = \mu \nabla T \]

\[ \Sigma = \sqrt{2k_B \bar{\eta} T} \left[ \mathcal{W}_T + \sqrt{\frac{1}{3}} \mathcal{W}_V \mathbf{I} \right] \text{ and } \Xi = \sqrt{2\bar{\mu}k_B T^2} \mathcal{W}_S \]
Figure: RK3 for 1D LLNS system for $\alpha = 0.5$, $\beta = 0.2$ and $\gamma = 0.1$. 
In 3D, for **compressible flows**, the diffusive velocity portion of the LLNS equations is

\[
\mathbf{v}_t = \eta \left[ \nabla^2 \mathbf{v} + \frac{1}{3} \nabla (\nabla \cdot \mathbf{v}) \right] + \sqrt{2} \eta \left[ (\nabla \cdot \mathbf{W}_T) + \sqrt{\frac{1}{3}} \nabla \mathbf{W}_V \right]
\]

\[
= \eta \left( D_T G_T + \frac{1}{3} G_V D_V \right) \mathbf{v} + \sqrt{2} \eta \left( D_T \mathbf{W}_T + \sqrt{\frac{1}{3}} G_V \mathbf{W}_V \right).
\]

To obtain discrete fluctuation-dissipation balance, we require discrete **tensorial** divergence and gradient operators \( G_T = -D_T^* \), and **vectorial** divergence and gradient \( G_V = -D_V^* \).

Use **MAC** (marker-and-cell) second-order centered discretizations for the tensorial operators \( D_T : \text{faces} \rightarrow \text{cells} \), as in incompressible projection methods on staggered grids.

Use **Fortin** discretization for vectorial operators \( D_V : \text{corners} \rightarrow \text{cells} \), as in approximate projection methods.
Implementation

We have implemented a three dimensional two species compressible fluctuating RK3 code, parallelized with the help of Michael J. Lijewski.

Spontaneous Rayleigh-Taylor mixing of two gases

- Future work: Use existing AMR framework to do mesh refinement.
- Special spatial discretization of the stochastic fluxes is necessary to satisfy the fluctuation-dissipation balance at coarse-fine interfaces [4].
Incompressible Flows

- In 3D, for **isothermal incompressible flows**, the fluctuating velocities follow

\[ \mathbf{v}_t = \eta \nabla^2 \mathbf{v} + \sqrt{2\eta} (\nabla \cdot \mathbf{W}_T) \]
\[ \nabla \cdot \mathbf{v} = 0, \]

which is equivalent to

\[ \mathbf{v}_t = \mathcal{P} \left[ \eta \nabla^2 \mathbf{v} + \sqrt{2\eta} (\nabla \cdot \mathbf{W}_T) \right], \]

where \( \mathcal{P} \) is the orthogonal projection onto the space of divergence-free velocity fields

\[ \mathcal{P} = \mathbf{I} - \mathbf{G}_V (\mathbf{D}_V \mathbf{G}_V)^{-1} \mathbf{D}_V, \quad \text{equivalently,} \quad \hat{\mathcal{P}} = \mathbf{I} - \hat{\mathbf{k}} \hat{\mathbf{k}}^T. \]

- Since \( \mathcal{P} \) is idempotent, \( \mathcal{P}^2 = \mathcal{P} \), the equilibrium spectrum is \( S(k) = \mathcal{P} \).
Incompressible Fluctuating Hydrodynamics

Spatial Discretization

Consider a stochastic projection scheme,

\[
v^{n+1} = P \left\{ \left[ I + \eta D_T G_T \Delta t + O(\Delta t^2) \right] v^n + \sqrt{2\eta \Delta t} D_T \mathcal{W}_T \right\}.
\]

The difficulty is the discretization of the projection operator \( P \) [7]:

Exact (idempotent): \( P_0 = I - G_V (D_V G_V)^{-1} D_V \)

Approximate (non-idempotent): \( \tilde{P} = I - G_V L_V^{-1} D_V \)

Our analysis indicates that the stochastic forcing should be projected using an exact projection, even if the velocities are approximately projected: **mixed exact-approximate projection method** under development...
If $P = P_0$ then $S_k = P_0 + O(\Delta t^2)$.
If $P = \tilde{P}$ then $S_k = P_0 + O(\Delta t)$.

- For cell-centered discretizations, there are significant disadvantages to using exact projection due to subgrid decoupling (multigrid, mesh refinement, Low Mach).
- A potential compromise, leading to $S_k = P_0 S_k^{(ad)}$, is

$$v^{n+1} = \tilde{P} \left[ I + \eta DTGT \Delta t + O(\Delta t^2) \right] v^n + \sqrt{2\eta \Delta t} P_0 DTW^T.$$  

- Special multigrid is required for exact projections even on uniform grids. With periodic boundaries one can use FFTs instead.
Conclusions and Future Work

- We have developed a framework for analysis of numerical methods for fluctuating hydrodynamics, based on looking at spectra as a function of wavenumber and wavefrequency.
- By focusing on the stochastic advection-diffusion equation, we developed an explicit three-stage Runge-Kutta scheme for the (compressible) LLNS equations of fluctuating hydrodynamics that is robust at large time steps.
- We have developed a two-species mixture parallel RK3D code that uses a mixed MAC/Fortin spatial discretization (AMR in the future).
- The fluctuating hydrodynamic solver has been used in a hybrid method [1].
- For incompressible fluctuating hydrodynamics, a mixed approximate-exact projection approach is under development.
- In the future, we will explore the full Low Mach Number fluctuating hydrodynamic equations, including temperature and density fluctuations.
A hybrid particle-continuum method for hydrodynamics of complex fluids.

J. L. Lebowitz, E. Presutti, and H. Spohn.
Microscopic models of hydrodynamic behavior.

On the Accuracy of Explicit Finite-Volume Schemes for Fluctuating Hydrodynamics.

P. J. Atzberger.

P. J. Atzberger.

J. B. Bell, A. Garcia, and S. A. Williams.

A. S. Almgren, J. B. Bell, and W. G. Szymczak.
A numerical method for the incompressible Navier-Stokes equations based on an approximate projection.