Finite-Volume Schemes for Fluctuating Hydrodynamics

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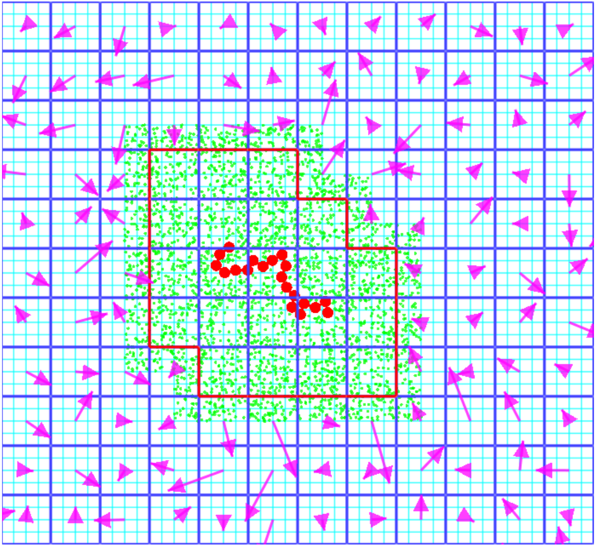
Outline

Micro- and nano-hydrodynamics

- 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**.

Particle/Continuum Hybrid Approach



Fluctuating Hydrodynamics

- We consider stochastic transport equations (conservation laws) [2] of the form

$$\partial_t \mathbf{U} = -\boldsymbol{\nabla} \cdot [\mathbf{F}(\mathbf{U}) - \mathcal{Z}] = -\boldsymbol{\nabla} \cdot [\mathbf{F}_H(\mathbf{U}) - \mathbf{F}_D(\boldsymbol{\nabla}\mathbf{U}) - \mathbf{B}(\mathbf{U})\boldsymbol{\mathcal{W}}],$$

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

$$\left\langle \boldsymbol{\mathcal{W}}(\mathbf{r}, t)\boldsymbol{\mathcal{W}}^{\star}(\mathbf{r}', t') \right\rangle = \delta(t - t')\delta(\mathbf{r} - \mathbf{r}').$$

- 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*!).

Euler Method for Advection-Diffusion Equation

- Consider the **stochastic advection-diffusion equation** in one dimension

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

- Simple Euler time integrator

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

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

$$\alpha = \frac{c\Delta t}{\Delta x} \text{ and } \beta = \frac{\mu \Delta t}{\Delta x^2} = \frac{\alpha}{r}.$$

Linear Additive-Noise SPDEs

- Consider the general linear SPDE

$$\mathbf{U}_t = \mathbf{L}\mathbf{U} + \mathbf{K}\mathcal{W},$$

  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**, $\widehat{\mathbf{U}}(\mathbf{k}, \omega)$, where the covariance is the **spectrum**.
- We focus on the static or **spatial spectrum** (static structure factor matrix)

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

  but the analysis can be extended to the **spatio-temporal spectrum** $\mathbf{S}(\mathbf{k}, \omega)$ (dynamic structure factor matrix).

Spatio-Temporal Discretization

- **Finite-volume discretization** of the field

$$\mathbf{U}_j(t) = \frac{1}{\Delta x} \int_{(j-1)\Delta x}^{j\Delta x} \mathbf{U}(x,t)dx$$

- General numerical method given by a **linear recursion**

$$\mathbf{U}_j^{n+1} = (\mathbf{I} + \mathbf{L}_j \Delta t)\, \mathbf{U}^n + \Delta t \mathbf{K}_j \mathcal{W}^n = (\mathbf{I} + \mathbf{L}_j \Delta t)\, \mathbf{U}^n + \sqrt{\frac{\Delta t}{\Delta x}} \mathbf{K}_j \mathbf{W}^n$$

- 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**.

Stochastic Consistency and Accuracy

- Use the **discrete Fourier transform (DFT)** to convert the iteration to Fourier space.
- Analysis will be focused on the **discrete static spectrum**

$$\mathbf{S}_k = V \left\langle \widehat{\mathbf{U}}_k \left(\widehat{\mathbf{U}}_k \right)^\star \right\rangle = \mathbf{S}(k) + O\left(\Delta t^{p_1} k^{p_2}\right),$$

  for a **weakly consistent** scheme.
- For fluctuating hydrodynamics equations we have a **spatially-white** field at equilibrium, $\mathbf{S}(\mathbf{k}) = \mathbf{I}$.
- The remainder term quantifies the *stochastic accuracy* for **large wavelengths ($\Delta k = k\Delta x \ll 1$) and small frequencies ($\Delta\omega = \omega\Delta t \ll 1$)**.

Discrete Fluctuation-Dissipation Balance

- A straightforward calculation **[3]** gives

$$\left(\mathbf{I}+\Delta t\widehat{\mathbf{L}}_k\right)\mathbf{S}_k\left(\mathbf{I}+\Delta t\widehat{\mathbf{L}}_k^\star\right)-\mathbf{S}_k=-\Delta t\widehat{\mathbf{K}}_k\widehat{\mathbf{K}}_k^\star.$$

- For small Δt

$$\widehat{\mathbf{L}}_k\mathbf{S}_k^{(0)}+\mathbf{S}_k^{(0)}\widehat{\mathbf{L}}_k^\star=-\widehat{\mathbf{K}}_k\widehat{\mathbf{K}}_k^\star,$$

and thus $\mathbf{S}_k^{(0)}=\lim_{\Delta t\to 0}\mathbf{S}_k=\mathbf{I}$ iff **discrete fluctuation-dissipation balance** [4, 5] holds

$$\widehat{\mathbf{L}}_k+\widehat{\mathbf{L}}_k^\star=-\widehat{\mathbf{K}}_k\widehat{\mathbf{K}}_k^\star.$$

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

"**On the Accuracy of Explicit Finite-Volume Schemes for Fluctuating Hydrodynamics**", by A. Donev, E. Vanden-Eijnden, A. L. Garcia, and J. B. Bell, CAMCOS, 2010 [**arXiv:0906.2425**]

Spatial Discretization

$$\partial_t \mathbf{U} = -\boldsymbol{\nabla} \cdot [\mathbf{F}(\mathbf{U}) - \mathcal{Z}] = \boldsymbol{\nabla} \cdot \left[-\mathbf{A}\mathbf{U} + \mu \boldsymbol{\nabla} \mathbf{U} + \sqrt{2\mu} \mathcal{W} \right]$$

- The conservative discretization,

$$\Delta \mathbf{U}_j = (\partial_t \mathbf{U}_j)\, \Delta t = -\frac{\Delta t}{\Delta x} \mathbf{A} \left(\mathbf{U}_{j+\frac{1}{2}} - \mathbf{U}_{j-\frac{1}{2}} \right),$$

$$+ \frac{\mu \Delta t}{\Delta x} \left(\boldsymbol{\nabla}_{j+\frac{1}{2}} - \boldsymbol{\nabla}_{j-\frac{1}{2}} \right) \mathbf{U} + \frac{\sqrt{2\mu\Delta t}}{\Delta x^{3/2}} \left(\mathbf{W}_{j+\frac{1}{2}} - \mathbf{W}_{j-\frac{1}{2}} \right)$$

  satisfies the discrete fluctuation-dissipation balance if:

  - The discrete divergence $\mathbf{D} \equiv \boldsymbol{\nabla}\cdot$ and gradient $\mathbf{G} \equiv \boldsymbol{\nabla}$ operators are **dual**, $\mathbf{D}^\star = -\mathbf{G}$,

$$\boldsymbol{\nabla}_{j+\frac{1}{2}} \mathbf{U} = \Delta x^{-1} \left(\mathbf{U}_{j+1} - \mathbf{U}_j \right).$$

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

$$\mathbf{U}_{j+\frac{1}{2}} = \frac{7}{12} \left(\mathbf{U}_j + \mathbf{U}_{j+1} \right) - \frac{1}{12} \left(\mathbf{U}_{j-1} + \mathbf{U}_{j+2} \right).$$

Runge-Kutta (RK3) Method

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

$$\begin{aligned}
\mathbf{U}_j^{n+\frac{1}{3}} &= \mathbf{U}_j^n + \Delta\mathbf{U}_j(\mathbf{U}^n, \mathbf{W}_1) \\
\mathbf{U}_j^{n+\frac{2}{3}} &= \frac{3}{4}\mathbf{U}_j^n + \frac{1}{4}\left[\mathbf{U}_j^{n+\frac{1}{3}} + \Delta\mathbf{U}_j(\mathbf{U}_j^{n+\frac{1}{3}}, \mathbf{W}_2)\right] \\
\mathbf{U}_j^{n+1} &= \frac{1}{3}\mathbf{U}_j^n + \frac{2}{3}\left[\mathbf{U}_j^{n+\frac{2}{3}} + \Delta\mathbf{U}_j(\mathbf{U}^{n+\frac{2}{3}}, \mathbf{W}_3)\right].
\end{aligned}$$

- Two random numbers per cell per time step

$$\begin{aligned}
\mathbf{W}_1 &= \mathbf{W}_A - \sqrt{3}\mathbf{W}_3 \\
\mathbf{W}_2 &= \mathbf{W}_A + \sqrt{3}\mathbf{W}_3
\end{aligned}$$

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]:

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

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

$$\boldsymbol{\sigma} = \left[\eta(\boldsymbol{\nabla}\mathbf{v} + \boldsymbol{\nabla}\mathbf{v}^T) - \frac{\eta}{3}(\boldsymbol{\nabla}\cdot\mathbf{v})\,\mathbf{I}\right] \text{ and } \boldsymbol{\xi} = \mu\boldsymbol{\nabla}T$$

$$\boldsymbol{\Sigma} = \sqrt{2k_B\bar{\eta}\bar{T}}\left[\boldsymbol{\mathcal{W}}_T + \sqrt{\frac{1}{3}}\mathcal{W}_V\mathbf{I}\right] \text{ and } \boldsymbol{\Xi} = \sqrt{2\bar{\mu}k_B\bar{T}^2}\,\boldsymbol{\mathcal{W}}_S$$

RK3 Method in 1D

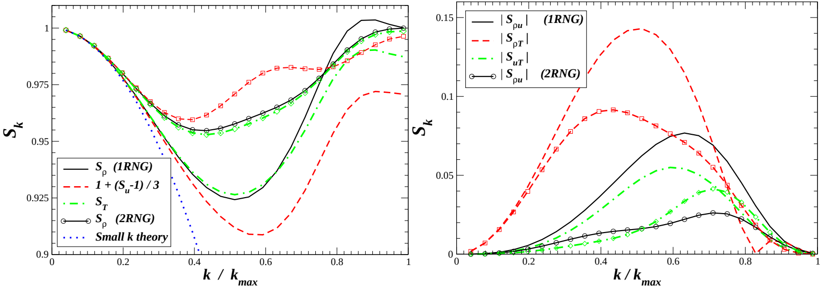


Figure: RK3 for 1D LLNS system for $\alpha = 0.5$, $\beta = 0.2$ and $\gamma = 0.1$.

Three Dimensions

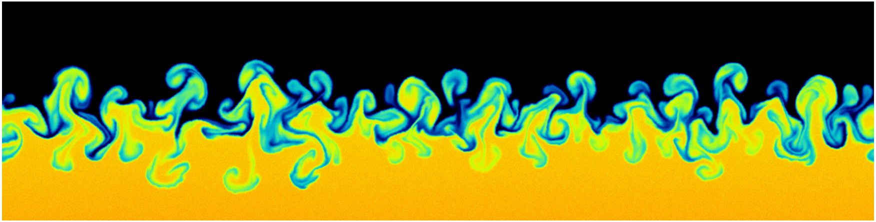
- In 3D, for **compressible flows**, the diffusive velocity portion of the LLNS equations is

$$\begin{aligned}\mathbf{v}_t &= \eta\left[\boldsymbol{\nabla}^2\mathbf{v}+\frac{1}{3}\boldsymbol{\nabla}\left(\boldsymbol{\nabla}\cdot\mathbf{v}\right)\right]+\sqrt{2\eta}\left[\left(\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{W}}_T\right)+\sqrt{\frac{1}{3}}\boldsymbol{\nabla}\mathcal{W}_V\right]\\ &= \eta\left(\mathbf{D}_T\mathbf{G}_T+\frac{1}{3}\mathbf{G}_V\mathbf{D}_V\right)\mathbf{v}+\sqrt{2\eta}\left(\mathbf{D}_T\boldsymbol{\mathcal{W}}_T+\sqrt{\frac{1}{3}}\mathbf{G}_V\mathcal{W}_V\right).\end{aligned}$$

- To obtain discrete fluctuation-dissipation balance, we require discrete **tensorial** divergence and gradient operators $\mathbf{G}_T=-\mathbf{D}_T^\star$, and **vectorial** divergence and gradient $\mathbf{G}_V=-\mathbf{D}_V^\star$.
- Use **MAC** (marker-and-cell) second-order centered discretizations for the tensorial operators (D_T : faces $\rightarrow$ cells), as in incompressible projection methods on staggered grids.
- Use **Fortin** discretization for vectorial operators (D_V : corners$\rightarrow$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

$$\begin{aligned}\mathbf{v}_t &= \eta\boldsymbol{\nabla}^2\mathbf{v} + \sqrt{2\eta}\left(\boldsymbol{\nabla}\cdot\boldsymbol{\mathcal{W}}_T\right)\\ \boldsymbol{\nabla}\cdot\mathbf{v} &= 0,\end{aligned}$$

  which is equivalent to

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

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

$$\mathcal{P} = \mathbf{I} - \mathbf{G}_V\left(\mathbf{D}_V\mathbf{G}_V\right)^{-1}\mathbf{D}_V, \text{ equivalently, } \hat{\mathcal{P}} = \mathbf{I} - \hat{\mathbf{k}}\hat{\mathbf{k}}^T.$$

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

Spatial Discretization

- Consider a stochastic projection scheme,

$$\mathbf{v}^{n+1} = \mathbb{P}\left\{\left[\mathbf{I} + \eta \mathbf{D}_T \mathbf{G}_T \Delta t + O\left(\Delta t^2\right)\right] \mathbf{v}^n + \sqrt{2\eta\Delta t}\mathbf{D}_T \boldsymbol{\mathcal{W}}_T\right\}.$$

- The difficulty is the discretization of the projection operator $\mathbb{P}$ [7]:

$$\textbf{Exact} \text{ (idempotent): } \mathbb{P}_0 = \mathbf{I} - \mathbf{G}_V \left(\mathbf{D}_V \mathbf{G}_V\right)^{-1} \mathbf{D}_V$$

$$\textbf{Approximate} \text{ (non-idempotent): } \widetilde{\mathbb{P}} = \mathbf{I} - \mathbf{G}_V \mathbf{L}_V^{-1} \mathbf{D}_V$$

- Our analysis indicates that the stochastic forcing should projected using an exact projection, even if the velocities are approximately projected: **mixed exact-approximate projection** method under development...

Exact vs. Approximate Projection

$$\text{If } \mathbb{P} = \mathbb{P}_0 \text{ then } \mathbf{S}_k = \mathbb{P}_0 + O\left(\Delta t^2\right).$$
$$\text{If } \mathbb{P} = \widetilde{\mathbb{P}} \text{ then } \mathbf{S}_k = \mathbb{P}_0 + O\left(\Delta t\right).$$

- 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 $\mathbf{S}_k = \mathbb{P}_0 \mathbf{S}_k^{(ad)}$, is

$$\mathbf{v}^{n+1} = \widetilde{\mathbb{P}} \left[\mathbf{I} + \eta \mathbf{D}_T \mathbf{G}_T \Delta t + O\left(\Delta t^2\right) \right] \mathbf{v}^n + \sqrt{2\eta \Delta t} \mathbb{P}_0 \mathbf{D}_T \boldsymbol{\mathcal{W}}_T.$$

- **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.

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