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**!
- Another important feature of small-scale flows, not discussed here, is **surface/boundary effects** (e.g., slip in the contact line problem).

Stochastic Conservation Laws

- Formally, we consider the continuum field of **conserved quantities** for a two-fluid mixture,

$$\mathbf{U}(\mathbf{r}, t) = \begin{bmatrix} \rho \\ \mathbf{j} \\ e \\ \rho_1 \end{bmatrix} = \begin{bmatrix} \rho \\ \rho \mathbf{v} \\ c_v \rho T + \rho v^2/2 \\ \rho c \end{bmatrix},$$

  where the primitive variables are density ρ, velocity $\mathbf{v}$, temperature T, and concentration c.

- Here we consider **Langevin-type models**, following Landau and Lifshitz:
  Postulate a **white-noise stochastic flux** term in the usual Navier-Stokes-Fourier equations with magnitude determined from the **fluctuation-dissipation balance** condition.

The SPDEs of Fluctuating Hydrodynamics

- Due to the **microscopic conservation** of mass, momentum and energy,

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

  where the flux is broken into a **hyperbolic**, **diffusive**, and a **stochastic flux**.

- Here $\boldsymbol{\mathcal{W}}$ is spatio-temporal **white noise**, i.e., a Gaussian random field with covariance

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

- A simple example is the one-dimensional **stochastic Burgers equation**

$$u_t = -c\left[u\left(1-u\right)\right]_x + \mu u_{xx} + \sqrt{2\mu u\left(1-u\right)}\mathcal{W}_x.$$

Compressible Fluctuating Navier-Stokes

Neglecting viscous heating, the equations of **compressible fluctuating hydrodynamics** in primitive variables are

$$\begin{aligned} D_t\rho &= -\,\rho\left(\boldsymbol{\nabla}\cdot\mathbf{v}\right) \\ \rho\left(D_t\mathbf{v}\right) &= -\,\boldsymbol{\nabla}P + \boldsymbol{\nabla}\cdot\left(\eta\overline{\boldsymbol{\nabla}}\mathbf{v} + \boldsymbol{\Sigma}\right) \\ \rho c_v\left(D_t T\right) &= -\,P\left(\boldsymbol{\nabla}\cdot\mathbf{v}\right) + \boldsymbol{\nabla}\cdot\left(\kappa\boldsymbol{\nabla}T + \boldsymbol{\Xi}\right) \\ \rho\left(D_t c\right) &= \boldsymbol{\nabla}\cdot\left[\rho\chi\left(\boldsymbol{\nabla}c\right) + \boldsymbol{\Psi}\right], \end{aligned} \tag{1}$$

where $D_t\square = \partial_t\square + \mathbf{v}\cdot\boldsymbol{\nabla}\left(\square\right)$ is the advective derivative,

$$\overline{\boldsymbol{\nabla}}\mathbf{v} = \left(\boldsymbol{\nabla}\mathbf{v} + \boldsymbol{\nabla}\mathbf{v}^T\right) - 2\left(\boldsymbol{\nabla}\cdot\mathbf{v}\right)\mathbf{I}/3,$$

the heat capacity c_v, and the pressure is $P = \rho\left(k_B T/m\right)$.
The transport coefficients are the **viscosity** η, $\nu = \eta/\rho$, **thermal conductivity** κ, and the **mass diffusion coefficient** χ.

Incompressible Fluctuating Navier-Stokes

- Ignoring density and temperature fluctuations, equations of **incompressible isothermal fluctuating hydrodynamics** are

$$\begin{aligned}
\partial_t \mathbf{v} =& -\mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v} - \boldsymbol{\nabla}\pi + \nu\boldsymbol{\nabla}^2\mathbf{v} + \rho^{-1}\left(\boldsymbol{\nabla}\cdot\boldsymbol{\Sigma}\right) \qquad (2)\\
\boldsymbol{\nabla}\cdot\mathbf{v} =& 0\\
\partial_t c =& -\mathbf{v}\cdot\boldsymbol{\nabla}c + \chi\boldsymbol{\nabla}^2 c + \rho^{-1}\left(\boldsymbol{\nabla}\cdot\boldsymbol{\Psi}\right), \qquad (3)
\end{aligned}$$

- Note that because of incompressibility:

$$\mathbf{v}\cdot\boldsymbol{\nabla}c = \boldsymbol{\nabla}\cdot(c\mathbf{v}) \text{ and } \mathbf{v}\cdot\boldsymbol{\nabla}\mathbf{v} = \boldsymbol{\nabla}\cdot\left(\mathbf{v}\mathbf{v}^T\right).$$

Stochastic Forcing

- The **fluctuation-dissipation balance principle** determines

$$\boldsymbol{\Sigma} = \sqrt{2\eta k_B T}\,\boldsymbol{\mathcal{W}}^{(\mathbf{v})}$$
$$\boldsymbol{\Psi} = \sqrt{2m\chi\rho\, c(1-c)}\,\boldsymbol{\mathcal{W}}^{(c)},$$

  where the $\boldsymbol{\mathcal{W}}$'s denote white random tensor/vector fields.

- Adding stochastic fluxes to the **non-linear** NS equations produces **ill-behaved stochastic PDEs** (solution is too irregular).
- For now, we will simply **linearize** the equations around a **steady state** $\mathbf{U}_0$ that is in **thermodynamic equilibrium** (no dissipative fluxes),

$$\mathbf{U} = \langle \mathbf{U} \rangle + \delta\mathbf{U} = \mathbf{U}_0 + \delta\mathbf{U}.$$

Linear Additive-Noise SPDEs

- Consider the **stochastic advection-diffusion equation** for a scalar filed, e.g., concentration, at **equilibrium**:

$$c_t = -\mathbf{v} \cdot \boldsymbol{\nabla} c + \chi \boldsymbol{\nabla}^2 c + \boldsymbol{\nabla} \cdot \left(\sqrt{2\chi} \boldsymbol{\mathcal{W}} \right) = \boldsymbol{\nabla} \cdot \left[-c\mathbf{v} + \chi \boldsymbol{\nabla} c + \sqrt{2\chi} \boldsymbol{\mathcal{W}} \right]$$

$$c_t = \boldsymbol{\mathcal{D}} \left[-c\mathbf{v} + \chi \boldsymbol{\mathcal{G}} c + \sqrt{2\chi} \boldsymbol{\mathcal{W}} \right],$$

  where $\mathbf{v}$ denotes the mean (reference) **background flow field**, $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$.

- In a more general setting, we want to solve:

$$\partial_t \boldsymbol{\mathcal{U}} = \boldsymbol{\mathcal{A}} \boldsymbol{\mathcal{U}} - \boldsymbol{\mathcal{L}} \boldsymbol{\mathcal{U}} + \sqrt{2 \boldsymbol{\mathcal{L}}} \cdot \boldsymbol{\mathcal{W}},$$

  where the **advection** $\boldsymbol{\mathcal{A}}$ and the **viscous friction operator** $\boldsymbol{\mathcal{L}}$ are constant linear operators.

Structure factor

- The solution is a *generalized process*, whose **equilibrium distribution** (long-time limit, invariant measure) is a *stationary Gaussian process*.
- This Gaussian process is fully characterized by the covariance

$$\boldsymbol{\mathcal{C}}(t) = \left\langle \boldsymbol{\mathcal{U}}(t')\boldsymbol{\mathcal{U}}^{\star}(t'+t) \right\rangle .$$

- Of particular importance is the **covariance of a snapshot** of the fluctuating field,

$$\boldsymbol{\mathcal{S}}(\mathbf{r},\mathbf{r}') = \boldsymbol{\mathcal{C}}(t=0) = \langle \boldsymbol{\mathcal{U}}\boldsymbol{\mathcal{U}}^{\star} \rangle \succeq \mathbf{0},$$

which depends on the basis used to represent $\boldsymbol{\mathcal{U}}$.

- In **Fourier space** the equilibrium distribution is characterized by the **static spectrum** or **static structure factor**,

$$\boldsymbol{\mathcal{S}}(\mathbf{k},\mathbf{k}') = \left\langle \widehat{\boldsymbol{\mathcal{U}}}(\mathbf{k})\widehat{\boldsymbol{\mathcal{U}}}^{\star}(\mathbf{k}') \right\rangle .$$

Fluctuation-Dissipation Balance

$$\partial_t \boldsymbol{\mathcal{U}} = \boldsymbol{\mathcal{A}}\boldsymbol{\mathcal{U}} - \boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{U}} + \sqrt{2\boldsymbol{\mathcal{L}}} \cdot \boldsymbol{\mathcal{W}}$$

- It is important that **advection** by an incompressible velocity field **is skew-adjoint**

$$\boldsymbol{\mathcal{A}}^\star = -\boldsymbol{\mathcal{A}},$$

while the **viscous dissipation is self-adjoint**,

$$\boldsymbol{\mathcal{L}} = -\boldsymbol{\mathcal{D}}\boldsymbol{\mathcal{G}} = \boldsymbol{\mathcal{D}}\boldsymbol{\mathcal{D}}^\star \succeq \mathbf{0}.$$

- Using Ito calculus it is easy to write an equation for $d\boldsymbol{\mathcal{S}} = \mathbf{0}$:

$$\boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{S}} + \boldsymbol{\mathcal{S}}\boldsymbol{\mathcal{L}}^\star = \boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{S}} + \boldsymbol{\mathcal{S}}\boldsymbol{\mathcal{L}} = 2\boldsymbol{\mathcal{L}}\delta(\mathbf{r} - \mathbf{r}')$$

leading to the continuum **fluctuation-dissipation balance** condition

$$\boldsymbol{\mathcal{S}}(\mathbf{r}, \mathbf{r}') = \mathbf{I}\delta\left(\mathbf{r} - \mathbf{r}'\right) \text{ and } \boldsymbol{\mathcal{S}}(\mathbf{k}, \mathbf{k}') = \mathbf{I}\delta\left(\mathbf{k} - \mathbf{k}'\right).$$

Dynamics of Fluctuations

- A snapshot of the fluctuating field $\boldsymbol{\mathcal{U}}$ looks like white noise in space.
- We consider the **fluctuation-dissipation balance** the **most important** property of the continuum equations:
  The equations of fluctuating hydrodynamics preserve the Gibbs-Boltzmann distribution.
- The temporal evolution is, however, not white in time.
- In the Fourier domain, the **dynamic structure factor** is

$$\boldsymbol{\mathcal{S}}(\mathbf{k},\omega)=\left\langle\widehat{\boldsymbol{\mathcal{U}}}(\mathbf{k}',\omega')\widehat{\boldsymbol{\mathcal{U}}}^{\star}(\mathbf{k},\omega)\right\rangle=\delta\left(\mathbf{k}-\mathbf{k}'\right)\delta\left(\omega-\omega'\right)$$
$$\left[2\left(\widehat{\boldsymbol{\mathcal{A}}}-\widehat{\boldsymbol{\mathcal{L}}}-i\omega\right)^{-1}\left(\widehat{\boldsymbol{\mathcal{L}}}\right)\left(-\widehat{\boldsymbol{\mathcal{A}}}-\widehat{\boldsymbol{\mathcal{L}}}+i\omega\right)^{-1}\right],$$

which follows directly from the space-time $(\mathbf{k},\omega)$ Fourier transform of the SPDE.

Stochastic Advection-Diffusion Equation

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

$$c_t = -v c_x + \chi c_{xx} + \sqrt{2\chi}\mathcal{W}_x.$$

- Simple **conservative (finite-volume) scheme**:

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

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

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

Finite-Volume Scheme

$$c_t = \boldsymbol{\mathcal{D}} \left[-c\mathbf{v} + \chi \boldsymbol{\mathcal{G}} c + \sqrt{2\chi} \boldsymbol{\mathcal{W}} \right]$$

- Generic **explicit** step of a **finite-volume scheme**

$$\mathbf{c}^{n+1} = \mathbf{c}^n + \mathbf{D} \left[\left(-\mathbf{V}\mathbf{c}^n + \mathbf{G}\mathbf{c}^n \right) \Delta t + \sqrt{2\Delta t} \mathbf{W}^n \right],$$

  where $\mathbf{D}$ is a discrete vector divergence, $\mathbf{G}$ is a discrete scalar gradient.
- Here $\mathbf{W}^n$ is a vector of random normal variates generated independently at each time step.
- The advection operator $\mathbf{V} \equiv \mathbf{V}(\mathbf{v})$ denotes a discretization of the advective fluxes.
- Note that for **implicit schemes** the discrete operators will themselves be functions of Δt, but not to leading order.

Discrete Fluctuation-Dissipation Balance

- 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.
- For these SPDEs, it is natural to define **weak convergence** based on the **second moments** and focus on the equilibrium distribution.
- Consider a uniform grid. Grid spacing Δx is an artificial length scale: all modes are equally strong at equilibrium.
- We want the discrete solution to satisfy **disrete fluctuation-dissipation balance** [1]

$$\mathbf{S}^{(0)} = \lim_{\Delta t \to 0} \mathbf{S} = \lim_{\Delta t \to 0} \langle \mathbf{c}\mathbf{c}^\star \rangle = \mathbf{I}.$$

"*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, 5(2):149-197, 2010** [arXiv:0906.2425]

Discrete Diffusion

- **Strict local conservation** should be maintained, that is, $\mathbf{D}$: faces $\to$ cells:

$$\nabla \cdot \mathbf{v} \to (\mathbf{D}\mathbf{v})_{i,j} = \Delta x^{-1} \left(\mathbf{v}^{(x)}_{i+\frac{1}{2},j} - \mathbf{v}^{(x)}_{i-\frac{1}{2},j} \right) + \Delta y^{-1} \left(\mathbf{v}^{(y)}_{i,j+\frac{1}{2}} - \mathbf{v}^{(y)}_{i,j-\frac{1}{2}} \right).$$

- This means that the stochastic fluxes (white noise) $\mathbf{W}$ must be generated on the **faces of the grid**.
- The **discrete divergence** and **gradient** operators should be **duals**, $\mathbf{D}^{\star} = -\mathbf{G}$, giving $\mathbf{G}$: cells $\to$ faces:

$$(\nabla c)_x \to (\mathbf{G}\mathbf{c})^{(x)}_{i+\frac{1}{2},j} = \Delta x^{-1} \left(c_{i+1,j} - c_{i,j} \right).$$

- This gives the standard discretization for the negative Laplacian $\mathbf{L} = -\mathbf{D}\mathbf{G}$, $\mathbf{L}$: cells $\to$ cells:

$$(\mathbf{L}\mathbf{c})_{i,j} = -\left[\Delta x^{-2} \left(c_{i-1,j} - 2c_{i,j} + c_{i+1,j} \right) + \Delta y^{-2} \left(c_{i,j-1} - 2c_{i,j} + c_{i,j+1} \right) \right.$$

Discrete Advection

- We assume that the background flow is **discretely-divergence free**, $\mathbf{D}\mathbf{v} = \mathbf{0}$. Otherwise it cannot be in equilibrium!
- The advection should be **constant-preserving**,

$$(\mathbf{D}\mathbf{V})\,\mathbf{1} = \mathbf{0}.$$

- The mapping $\mathbf{V}(\mathbf{v})$: cells $\rightarrow$ faces should be such that advection is **skew-adjoint**,

$$[(\mathbf{D}\mathbf{V})\,\mathbf{c}] \cdot \mathbf{w} = -\mathbf{c} \cdot [(\mathbf{D}\mathbf{V})\,\mathbf{w}]\,,$$

  since advection does not dissipate but only transports fluctuations.
- Note that artificial viscosity, upwinding, Godunov methods, limiters, and the like, are all out of consideration!

Skew-Adjoint Advection

- The skew-adjointness property has proven useful in **turbulence modeling** since skew-symmetric advection conserves kinetic energy [2].
- For uniform grids a very simple construction works:

$$(c\mathbf{v})_x \rightarrow (\mathbf{Vc})^{(x)}_{i+\frac{1}{2},j} = v^{(x)}_{i+\frac{1}{2},j}\bar{c}_{i+\frac{1}{2},j}.$$

- Simple averaging can be used to interpolate scalars from cells to faces, for example,

$$\bar{c}_{i+\frac{1}{2},j} = \frac{1}{2}\left(c_{i+1,j} + c_{i,j}\right).$$

- If $\mathbf{c} = \mathbf{1}$ is constant, then $\bar{\mathbf{c}} = \mathbf{1}$ as well, and thus this advection is constant preserving:

$$\mathbf{DV1} = \mathbf{Dv} = \mathbf{0}$$

Skew-Adjointness

- The advection discretization simplifies because $\mathbf{D}\mathbf{v}=\mathbf{0}$,

$$\begin{aligned}(\mathbf{DVc})_{i,j} =&\Delta x^{-1}\left(v^{(x)}_{i+\frac{1}{2},j}c_{i+1,j}-v^{(x)}_{i-\frac{1}{2},j}c_{i-1,j}\right)+\\ &\Delta y^{-1}\left(v^{(y)}_{i,j+\frac{1}{2}}c_{i,j+\frac{1}{2}}-v^{(y)}_{i,j-\frac{1}{2}}c_{i,j-\frac{1}{2}}\right)+c_{i,j}\left(\mathbf{D}\mathbf{v}\right)_{i,j}.\end{aligned}$$

- In one dimension, it is easy to show that this form of advection is skew-adjoint,

$$(\mathbf{Vc})_i=\Delta x^{-1}\left(v_{i+\frac{1}{2}}c_{i+1}-v_{i-\frac{1}{2}}c_{i-1}\right).$$

- All that is needed is to discretize the **advection flow field** on the **faces** of the **c** grid.
- One can use a **staggered** grid (**v** lives on faces), or a **collocated** (cell-centered) grid (**v** lives at cell centers).

Compressible Isothermal Equations

$$\rho_t = -\boldsymbol{\nabla} \cdot (\rho \mathbf{v})$$

$$(\rho c)_t = \rho c_t + c \rho_t = \boldsymbol{\nabla} \cdot \left[-c \left(\rho \mathbf{v} \right) + \rho \chi \left(\boldsymbol{\nabla} c \right) + \sqrt{2\chi} \widetilde{\boldsymbol{\mathcal{W}}} \right]$$

$$\text{Or the usual } \rho c_t = -\left(\rho \mathbf{v} \right) \boldsymbol{\nabla} c + \boldsymbol{\nabla} \cdot \left[\rho \chi \left(\boldsymbol{\nabla} c \right) + \sqrt{2\chi} \widetilde{\boldsymbol{\mathcal{W}}} \right]$$

- All scalar fields are discretized in the same manner, let's just call it **cell-centered**.
- It is important to use the same advection discretization for all scalars, since the term $c \rho_t$ ought to cancel $-c \left[\boldsymbol{\nabla} \cdot (\rho \mathbf{v}) \right]$.
- Notice that the "advection field" is now the background (mean) momentum field, $\mathbf{j} = \rho \mathbf{v}$, and it has to be discretely divergence-free

$$\langle \boldsymbol{\nabla} \cdot (\rho \mathbf{v}) \rangle = \boldsymbol{\nabla} \cdot \langle \rho \mathbf{v} \rangle = \langle \rho \rangle_t = 0.$$

Boundary Conditions

- Consider Dirichlet or von-Neumann conditions for c at the wall $x = 0$,

$$c(x=0) = 0 \text{ or } \frac{\partial c}{\partial x}|_{x=0} = 0.$$

- Advection velocity must be parallel to a wall, so we do not need to worry about it:

$$\mathbf{c}^{n+1} = \mathbf{c}^n + \mathbf{D}\left[\mathbf{G}\mathbf{c}^n \Delta t + \sqrt{2\Delta t}\mathbf{W}^n\right].$$

- We want to keep **D** the usual **conservative difference** of facial fluxes.

Staggered Boundary Conditions

- The main issue is when the faces of the grid are on the wall, that is, when $\mathbf{W}_{1/2,j}$ is on the boundary itself.
- The gradient $\mathbf{G}$ is chosen to be consistent with boundary conditions, for example,

$$(\mathbf{Gc})_{1/2,j} = \begin{cases} 0 & \text{for von-Neumann} \\ 2c_{1,j}/\Delta x & \text{for Dirichlet } (c_{-1,j} = -c_{1,j}) \end{cases}$$

- Note that the Laplacian $\mathbf{L} = -\mathbf{DG}$ is formally only first-order accurate for Dirichlet, but this is OK.
- For Dirichlet conditions $\mathbf{D}^{\star} \neq -\mathbf{G}$, so the DFDB condition is violated near the walls, $\mathbf{S}^{(0)} \neq \mathbf{I}$.

Boundary Stochastic Stresses

- We have to add some correlations between stochastic fluxes on the faces near the wall.
- The generalized discrete fluctuation-dissipation balance condition is

$$\mathbf{L} + \mathbf{L}^\star = 2\mathbf{D}\langle \mathbf{W}\mathbf{W}^\star \rangle \mathbf{D}^\star = 2\mathbf{D}\mathbf{C}_\mathbf{W}\mathbf{D}^\star,$$

  and for periodic systems $\mathbf{C}_\mathbf{W} = \mathbf{I}$ worked.
- An explicit 1D calculation gives the simple **fix for boundaries**:
  - For von Neumann just set $\mathbf{W}_{1/2,j} = 0$ (gives desired conservation!).
  - For Dirichlet set $\mathbf{W}_{1/2,j} = \sqrt{2}r$, where r is a unit normal variate.

Finite Time Steps

$$\partial_t \mathcal{U} = -\mathcal{L}\mathcal{U} + \sqrt{2\mathcal{L}} \cdot \mathcal{W}$$

- In the linear setting, any temporal discretization is a **linear iteration** of the form:

$$\mathbf{U}^{n+1} = \left[\mathbf{M}\left(\Delta t\right)\right]\mathbf{U}^{n} + \left[\mathbf{N}\left(\Delta t\right)\right]\mathbf{W}^{n}.$$

- A simple calculation shows that the **discrete covariance**

$$\mathbf{S} = \langle \mathbf{U}\mathbf{U}^{\star} \rangle = \mathbf{S}^{(0)} + (\Delta t)\,\Delta\mathbf{S} + O\left(\Delta t^{2}\right)$$

satisfies the linear system of equations

$$\mathbf{M}\mathbf{S}\mathbf{M}^{\star} - \mathbf{S} = -\mathbf{N}\mathbf{N}^{\star}.$$

Stochastic Accuracy

- The analysis can be done explicitly in **Fourier space** for **periodic BCs**:
  One small linear system per wavenumber:

$$\widehat{\mathbf{M}}\widehat{\mathbf{S}}\widehat{\mathbf{M}}^{\star} - \widehat{\mathbf{S}} = -\widehat{\mathbf{N}}\widehat{\mathbf{N}}^{\star}.$$

- We want $\widehat{\mathbf{S}}(\mathbf{k}, \omega)$ to converge to the continuum one for **large wavelengths** ($k\Delta x \ll 1$) and **small frequencies** ($\omega\Delta t \ll 1$).
- Of course we want to preserve second-order temporal accuracy for the deterministic case.
- But we also want to achieve $\mathbf{S}^{(0)} = \mathbf{I}$ and $\Delta\mathbf{S} = \mathbf{0}$, i.e., **second-order accurate static covariance**:

$$\mathbf{S} = \mathbf{I} + O\left(\Delta t^2\right).$$

Predictor-Corrector Method

- The usual **predictor-corrector** method works:

$$\mathbf{U}^{\star} = \mathbf{U}^{n} + \left[\left(\mathbf{L}\mathbf{U}^{n} \right) \Delta t + \sqrt{2 \Delta t}\, \mathbf{L}\mathbf{W}_1 \right],$$

$$\mathbf{U}^{n+1} = \frac{1}{2} \left\{ \mathbf{U}^{n} + \mathbf{U}^{\star} + \left[\left(\mathbf{L}\mathbf{U}^{\star} \right) \Delta t + \sqrt{2 \Delta t}\, \mathbf{L}\mathbf{W}_2 \right] \right\}.$$

- We have a choice whether to take $\mathbf{W}_1 = \mathbf{W}_2$ or use two independent random numbers per time step.
- Formally it is better to take $\mathbf{W}_1$ and $\mathbf{W}_2$ independent, but in practice it seems to depend on the equation and method.
- In any Runge-Kutta integrator one has choices with the how to modify the random numbers from stage to stage.
- To get **stability for small viscosit**y we need at least three-stage Runge-Kutta.

Runge-Kutta (RK3) Method

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

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

- Two random numbers per cell per time step works best for the stochastic advection-diffusion equation:

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

Crank-Nicolson

- It turns out that **Crank-Nicolson** gives perfect covariances for **any time step**, $\mathbf{S} = \mathbf{I}$:

$$\mathbf{L}_1 \mathbf{U}^{n+1} = \mathbf{U}^n + \left[\left(\mathbf{L}_2 \mathbf{U}^n \right) + \sqrt{2 \Delta t}\, \mathbf{L} \mathbf{W} \right],$$

$$\mathbf{L}_1 = \mathbf{I} - \frac{\Delta t}{2} \mathbf{L} \text{ and } \mathbf{L}_2 = \mathbf{I} + \frac{\Delta t}{2} \mathbf{L}.$$

- This is because of the special property:

$$\mathbf{L}_2^2 - \mathbf{L}_1^2 = 2 \Delta t\, \mathbf{L}.$$

- Of course, doing **advection semi-implicitly** may lead to numerical difficulties.

Collocated Grid

- First consider the simplified velocity equation

$$\mathbf{v}_t = -\mathbf{v} \cdot \boldsymbol{\nabla} \mathbf{v} + \nu \boldsymbol{\nabla}^2 \mathbf{v} + \boldsymbol{\nabla} \cdot \left(\sqrt{2\eta} \boldsymbol{\mathcal{W}} \right)$$

- Observe that each of the velocity components follows the usual stochastic advection-diffuson equation:

$$v_t^{(x)} = \boldsymbol{\mathcal{D}} \left[-v^{(x)} \mathbf{v} + \nu \boldsymbol{\mathcal{G}} v^{(x)} + \sqrt{2\nu} \boldsymbol{\mathcal{W}}^{(x)} \right],$$
$$v_t^{(y)} = \boldsymbol{\mathcal{D}} \left[-v^{(y)} \mathbf{v} + \nu \boldsymbol{\mathcal{G}} v^{(y)} + \sqrt{2\nu} \boldsymbol{\mathcal{W}}^{(y)} \right].$$

- In a **collocated** spatial discretization the velocities (or momenta densities) are discretized on the same grid as the scalars (density, concentration), and are advected/diffused in exactly the same way.

Staggered Grid

- For a **staggered** spatial discretization, $v^{(x)}$ lives on its own grid, shifted from the scalar grid by $\Delta x/2$ along the x axis (work with Florencio Balboa).
- The stresses (fluxes) live on the faces of the shifted grid:
  - The **diagonal components** of the stresses live at the **cell centers** (i, j).
  - The **off-diagonal components** of the stresses live at the **nodes** of the grid $(i + \frac{1}{2}, j + \frac{1}{2})$.
- This applies to the stochastic stress as well:
  Generate two random numbers for each cell center, $W_{i,j}^{(x)}$ and $W_{i,j}^{(y)}$, as well as two random numbers for each node of the grid, $W_{i+\frac{1}{2},j+\frac{1}{2}}^{(x)}$ and $W_{i+\frac{1}{2},j+\frac{1}{2}}^{(y)}$.

Advection for Staggered Grid

- The skew-adjoint advection scheme relies on defining **face-centered** advection velocities what are discretely divergence-free.
- We can obtain these by faces $\rightarrow$ (cells,nodes) **interpolation**, for example, to advect $\mathbf{v}^{(x)}$ we use averaging:

$$\begin{aligned} \left(v_x^{(x)}\right)_{i,j} &= \frac{1}{2}\left(v_{i-\frac{1}{2},j}^{(x)} + v_{i+\frac{1}{2},j}^{(x)}\right) \\ \left(v_y^{(x)}\right)_{i+\frac{1}{2},j+\frac{1}{2}} &= \frac{1}{2}\left(v_{i,j+\frac{1}{2}}^{(y)} + v_{i+1,j+\frac{1}{2}}^{(y)}\right). \end{aligned}$$

- It is not hard to verify that this advection field is discretely divergence-free if $\mathbf{v}$ is:

$$\left(\mathbf{D}^{(x)}\mathbf{v}^{(x)}\right)_{i+\frac{1}{2},j} = \frac{1}{2}\left[(\mathbf{D}\mathbf{v})_{i,j} + (\mathbf{D}\mathbf{v})_{i+1,j}\right] = \mathbf{0}.$$

Compressible Equations

- For **compressible flows**, the diffusive part of the velocity equation is:

$$\rho \mathbf{v}_t = \boldsymbol{\nabla} \cdot \left[\eta \left(\boldsymbol{\nabla} \mathbf{v} + \boldsymbol{\nabla} \mathbf{v}^T - \frac{2}{3} \left(\boldsymbol{\nabla} \cdot \mathbf{v} \right) \mathbf{I} \right) + \sqrt{2 \eta k_B T} \, \boldsymbol{\mathcal{W}} \right].$$

- The original formulation by Landau-Lifshitz constructed $\boldsymbol{\mathcal{W}}$ to be a **traceless symmetric tensor**:

$$\langle \mathcal{W}_{ij}(\mathbf{r}, t) \mathcal{W}^{\star}_{kl}(\mathbf{r}', t') \rangle = \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{3}\delta_{ij}\delta_{kl}/3 \right) \delta(t - t')\delta(\mathbf{r} - \mathbf{r}').$$

- This implies that there are correlations between the diagonal components, and also correlations between the off-diagonal components.
- For a **staggered grid**, this poses no problem:
  - The diagonal $\mathcal{W}_{ii}$ lives at cell centers, and can be generated to add to zero (traceless).
  - The off-diagonal part of $\boldsymbol{\mathcal{W}}$ lives at the nodes, and can be generated to be symmetric.

Collocated Compressible Equations

- For a **collocated grid**, however, there are diagonal and off-diagonal components on each face of the grid. But we cannot put correlations between **random numbers on different faces**!
- Instead, we can rewrite the equations as follows:

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

- We need 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 the same **MAC** discretization as before for $\mathbf{G}_T$: cells $\rightarrow$ faces, giving the usual discrete Laplacian.
- Use **Fortin** discretization for $\mathbf{D}_V$: cells$\rightarrow$corners, as in approximate projection methods.

Collocated Compressible Code

- We have designed a numerical scheme for the LLNS equations that satisfies discrete fluctuation-dissipation balance and has good temporal accuracy.
- We have developed a parallel three dimensional two species **compressible fluctuating hydrodynamics code** (LBL).

Spontaneous Rayleigh-Taylor mixing of two gases

Incompressible Flows

- For **isothermal incompressible flows**, ignoring advection, the fluctuating velocities follow

$$\partial_t \mathbf{v} = \mathcal{P}\mathbf{w} = \mathcal{P}\left[\nu\boldsymbol{\nabla}^2\mathbf{v} + \boldsymbol{\nabla}\cdot\left(\sqrt{2\nu}\boldsymbol{\mathcal{W}}\right)\right] = -\mathcal{P}\left[\boldsymbol{\mathcal{L}}\mathbf{v} + \sqrt{2\boldsymbol{\mathcal{L}}}\,\boldsymbol{\mathcal{W}}\right]$$

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

- Here $\mathcal{P}$ is the **orthogonal projection** onto the space of divergence-free velocity fields, and it **self-adjoint** and **idempotent**, $\mathcal{P}^2 = \mathcal{P}$,

$$\mathcal{P} = \mathcal{P}^\star = \mathbf{I} - \mathcal{G}\left(\mathcal{D}\mathcal{G}\right)^{-1}\mathcal{D}.$$

- This requires solving a **Poisson problem**

$$\boldsymbol{\nabla}^2\phi = \left(\mathcal{D}\mathcal{G}\right)\phi = \boldsymbol{\nabla}\cdot\mathbf{w},$$

with von-Neumann conditions at stick walls, where $\mathbf{v} = 0$,

$$\boldsymbol{\nabla}\phi\cdot\mathbf{n} = \mathbf{w}\cdot\mathbf{n}.$$

Continuum Fluctuation-Dissipation Balance

- The static covariance at equilibrium is determined from

$$\mathcal{P}\mathcal{L}\mathcal{S} + \mathcal{S}\mathcal{L}\mathcal{P}^{\star} = 2\mathcal{P}\mathcal{L}\mathcal{P}^{\star} \quad \Rightarrow \quad \mathcal{S} = \mathcal{P}$$

- For **periodic BCs**, in Fourier space,

$$\hat{\mathcal{S}} = \hat{\mathcal{P}} = \mathbf{I} - \hat{\mathbf{k}}\hat{\mathbf{k}}^T$$

showing that the velocity variance is reduced by one degree of freedom due to the incompressibility constraint:

$$\text{Trace}\,\hat{\mathcal{S}} = \text{Trace}\,\hat{\mathcal{P}} = d - 1.$$

- For non-periodic conditions, one must **diagonalize the operators** in a suitable basis set (following E and Liu).

Projection Methods

- Consider a stochastic **projection scheme**,

$$\mathbf{v}^{n+1} = \mathbb{P}\left\{[\mathbf{I} + \mathbf{L}\,\Delta t]\,\mathbf{v}^n + \sqrt{2\Delta t\,\mathbf{L}}\mathbf{W}\right\}.$$

- Here the iteration matrices are

$$\mathbf{M} = \mathbb{P}\left[\mathbf{I} + \mathbf{L}\,\Delta t\right] \text{ and } \mathbf{N} = \mathbb{P}\sqrt{2\Delta t\,\mathbf{L}}.$$

- Recall that $\mathbf{S}$ is the solution to the **DFDB condition**:

$$\mathbf{M}\mathbf{S}\mathbf{M}^\star - \mathbf{S} = -\mathbf{N}\mathbf{N}^\star,$$

which can be expanded in powers of Δt.

Spatial Discretization

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

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

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

- For cell-centered discretizations, there are significant **disadvantages** to using exact projection due to **subgrid decoupling** (multigrid, mesh refinement, Low Mach).
- We define **discrete fluctuation-dissipation balance** to be

$$\mathbf{S} = \mathbb{P}_0 + O\left(\Delta t\right),$$

which at least gives the right velocity variance,

$$\text{Trace}\,\widehat{\mathbb{P}}_0 = \text{Trace}\,\widehat{\boldsymbol{\mathcal{P}}} = d - 1$$

.

Approximate Projection

- Observe that $\mathbb{P}_0\widetilde{\mathbb{P}} = \widetilde{\mathbb{P}}\mathbb{P}_0 = \mathbb{P}_0$ for the Almgren projection [3].
- It turns out that one has to use **exact projections** at least once:

$$\mathbf{v}^{n+1} = \widetilde{\mathbb{P}}\left[\mathbf{I} + \mathbf{L}\,\Delta t\right]\mathbf{v}^n + \mathbb{P}_0\left(\sqrt{2\Delta t}\,\mathbf{L}\mathbf{W}\right).$$

- To see this, plug $\mathbf{S} = \mathbb{P}_0 + O\left(\Delta t\right)$ into DFDB condition:

$$O\left(\Delta t^0\right): \quad \widetilde{\mathbb{P}}\mathbb{P}_0\widetilde{\mathbb{P}} - \mathbb{P}_0 = \mathbb{P}_0 - \mathbb{P}_0 = \mathbf{0}$$

$$O\left(\Delta t^1\right): \quad \mathbb{P}_0\mathbf{L}^{\star}\widetilde{\mathbb{P}} + \widetilde{\mathbb{P}}\mathbf{L}\mathbb{P}_0 = 2\mathbb{P}_0\mathbf{L}\mathbb{P}_0$$

- For periodic systems, all operators commute, and the $O\left(\Delta t\right)$ terms work out, but not obvious for non-periodic systems.

Exact Projection on Staggered Grid

- For exact projections, there is no problem, and in fact simple predictor-corrector (with two projections per step) would give the desired $\mathbf{S} = \mathbb{P}_0 + O\left(\Delta t^2\right)$.
- Exact **MAC projection** is easy to do on a **staggered grid**.
- We (with Thomas Fai, Boyce Griffith, Charles Peskin) are now implementing **staggered** grid schemes for incompressible fluctuating hydrodynamics.
- For **non-periodic** systems there are well-known problems with boundary conditions for projection methods in the deterministic context.
- Getting **second-order** deterministic accuracy with one (exact) projection per time step, without messing up DFDB, seems harder.

Stokes Solver on Staggered Grid

- One can avoid projection entirely and directly do a **Stokes solver**, as implemented in IBAMR code.
- The method of Boyce Griffith [4], neglecting advection, solves the semi-implicit problem:

$$\begin{bmatrix} \left(\mathbf{I} - \frac{\Delta t}{2}\mathbf{L}\right) & \mathbf{G}\Delta t \\ -\mathbf{D}\Delta t & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{v}^{n+1} \\ \phi \end{bmatrix} = \begin{bmatrix} \left(\mathbf{I} + \frac{\Delta t}{2}\mathbf{L}\right)\mathbf{v}^{n} + \sqrt{2\Delta t}\,\mathbf{L}\mathbf{W} \\ \phi \end{bmatrix}$$

- A standard projection method is used as a **preconditioner** for this solver.
- To get second order accuracy for (weak) advection, one can use two iterations ala **predictor-corrector**, or perhaps **Adams-Bashforth**.

Low-Mach Number Equations

- Eliminate acoustics from the full LLNS system using low Mach number asymptotics [5], $P = P_0 + \pi$,

$$P_{EOS}(\rho, c, T) = P_0 = \text{const.}$$

- **Formally** treating the white noise as a regular forcing gives the **low Mach fluctuating hydrodynamics** equations:

$$\begin{aligned}
D_t\rho &= -\rho\boldsymbol{\nabla}\cdot\mathbf{v} \\
\rho\left(D_t\mathbf{v}\right) &= -\boldsymbol{\nabla}\pi + \eta\boldsymbol{\nabla}^2\mathbf{v} + \boldsymbol{\nabla}\cdot\boldsymbol{\Sigma} \\
\rho c_p\left(D_t T\right) &= \mu\boldsymbol{\nabla}^2 T + \boldsymbol{\nabla}\cdot\boldsymbol{\Xi}, \\
\boldsymbol{\nabla}\cdot\mathbf{v} &= \alpha\left(\rho c_p\right)^{-1}\left(\mu\boldsymbol{\nabla}^2 T + \boldsymbol{\nabla}\cdot\boldsymbol{\Xi}\right),
\end{aligned}$$

  where α is the thermal expansion coefficient, and π is the *non-thermodynamic pressure* π.

- One ought to do derive this more carefully though since there may be **missing terms**.

Isothermal Low-Mach Equations

- For an *isothermal* **miscible mixture** of two fluids, the low Mach approximation leads to a **non-homogeneous constraint** on the velocity divergence,

$$\rho \boldsymbol{\nabla} \cdot \mathbf{v} = -\beta \boldsymbol{\nabla} \cdot \left[\rho \chi \boldsymbol{\nabla} c + \boldsymbol{\Psi} \right],$$

  where $\beta = \rho^{-1} \left(\partial \rho / \partial c \right)_{P_0, T_0}$ is the solutal expansion coefficient.
- The **incompressible approximation** $\boldsymbol{\nabla} \cdot \mathbf{v} = 0$ is only applicable to isothermal mixtures of **nearly identical** ($\beta \approx 0$) or **immiscible fluids** ($\chi = 0$).
- To model some experiments on **giant fluctuations** we need to handle this case.
- John Bell et al. have developed **collocated low Mach projection**-type schemes.
- There seem to be few **low Mach staggered** schemes out there...

Stochastic Accuracy Out of Equilibrium

- Consider the simplest non-equilibrium model, where there is an imposed concentration gradient:

$$(\delta c)_t + \mathbf{v} \cdot \boldsymbol{\nabla} c_0 = -\chi \boldsymbol{\nabla}^2 (\delta c) + \sqrt{2\chi k_B T} \left(\boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{W}}_c \right)$$
$$\rho \mathbf{v}_t = \eta \boldsymbol{\nabla}^2 \mathbf{v} - \boldsymbol{\nabla} \pi + \sqrt{2\eta k_B T} \left(\boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{W}}_{\mathbf{v}} \right) \text{ and } \boldsymbol{\nabla} \cdot \mathbf{v} = 0$$

- Solve in Fourier space to obtain the **static structure factors** between velocity and concentration fluctuations:

$$\widehat{S}_{c,v_\parallel}(\mathbf{k}) = \langle (\widehat{\delta c})(\widehat{v}_\parallel^\star) \rangle \sim -\left(k_\perp^2 k^{-4} \right) \| \boldsymbol{\nabla} c_0 \| ,$$

which is a **power-law of the wavenumber** k.

- At equilibrium we wanted the discrete spectra to be white, i.e., independent of k, to mimic the continuum. What about non-white spectra?

Future Directions

- Develop **staggered** schemes for **compressible** fluctuating hydrodynamics.
- Develop numerical schemes for **incompressible** and **Low-Mach Number** fluctuating hydrodynamics.
- **AMR**: DFDB balance at **coarse-fine mesh interfaces** for compressible and incompressible collocated and staggered schemes.
- (Discrete) fluctuation-dissipation in systems **out of equilibrium**.
- **Direct fluid-structure coupling** between fluctuating hydrodynamics and microstructure (**stochastic immersed boundary method** [6]).
- Ultimately we desire an **Adaptive Mesh and Algorithm Refinement** (AMAR) framework that couples a particle model (**micro**), with compressible fluctuating Navier-Stokes (**meso**), and incompressible or low Mach fluctuating hydro (**macro**).

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