Numerical Methods for Fluctuating Hydrodynamics

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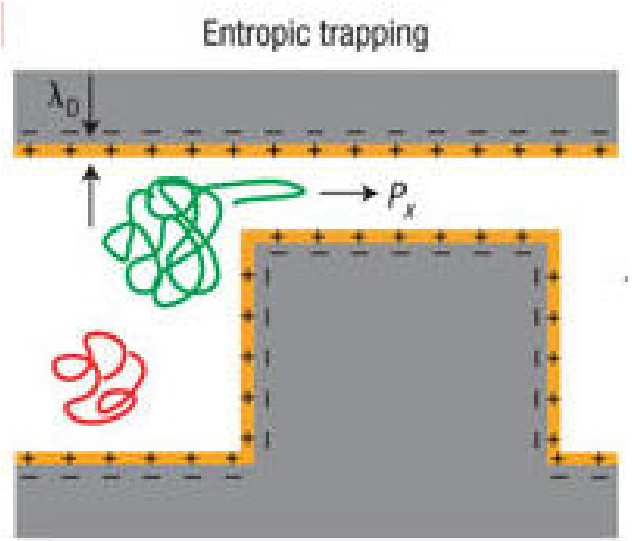
Outline

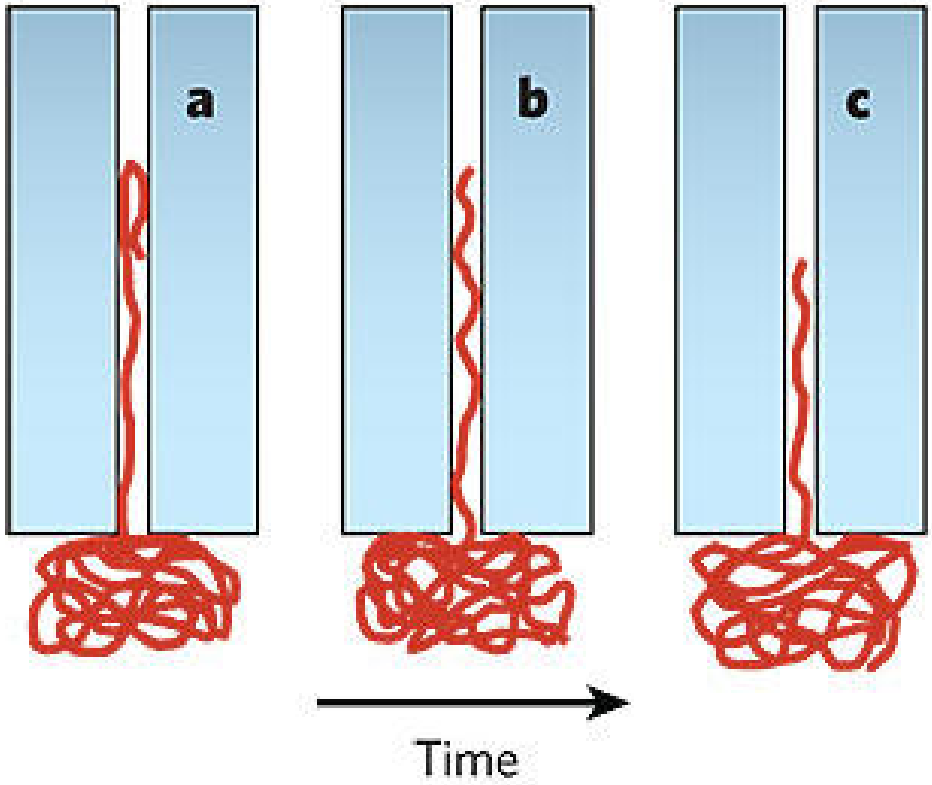
Micro- and nano-hydrodynamics

- 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.
- The flows of interest often include **suspended particles**: colloids, polymers (e.g., DNA), blood cells, bacteria: **complex fluids**.
- Essential distinguishing feature from "ordinary" CFD: **thermal fluctuations**!

Example: DNA Filtering



Fu et al., Nature Nanotechnology 2 (2007)



H. Craighead, Nature 442 (2006)

Example: Droplet Formation

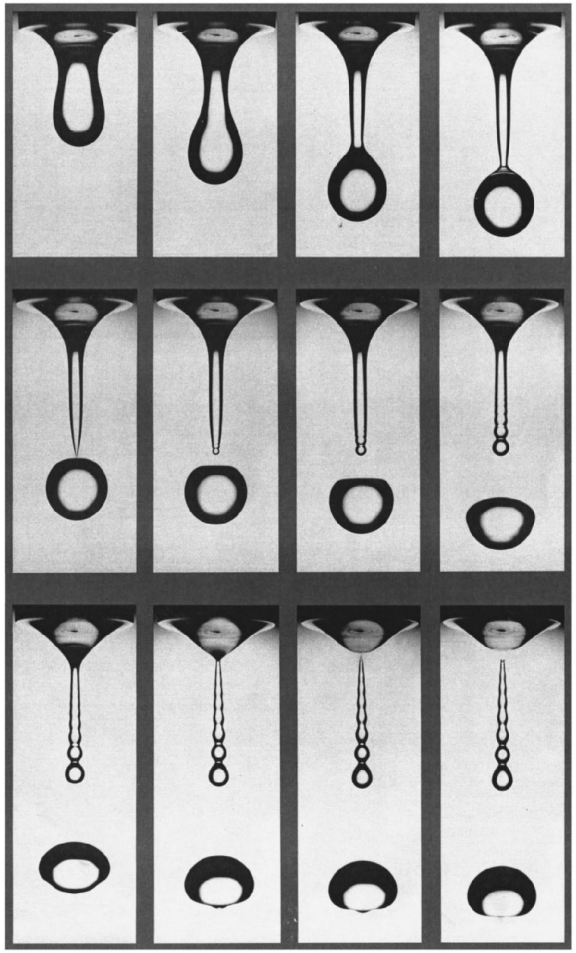
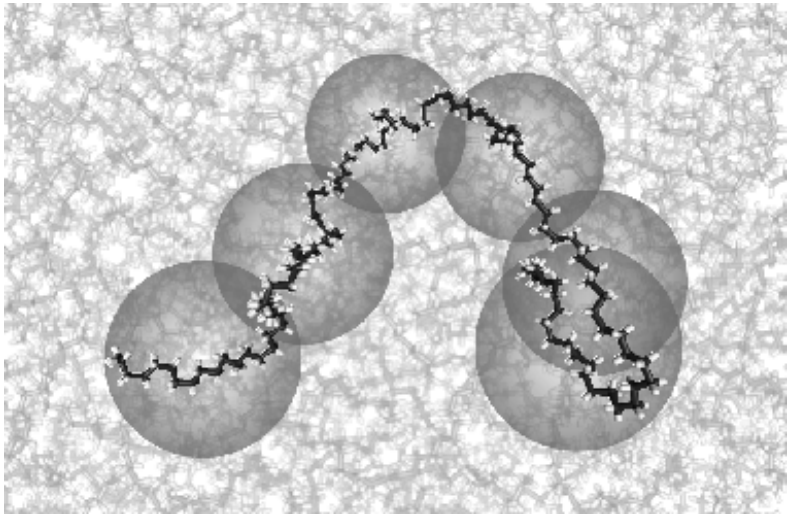


Figure: From *Jens Eggers, Reviews of Modern Physics*, 69, 1997 (see also *M. Moseler and U. Landman, Science*, 2000)

Example: Polymer chains



Johan Padding, Cambridge

- Consider modeling of a polymer chain in a flowing solution, for example, DNA in a micro-array.
- The detailed structure of the polymer chain is usually **coarse-grained** to a model of spherical **beads**.

The issue: **How to coarse grain the fluid (solvent) and couple it to the suspended structures?**

Molecular Dynamics

- At the particle level, the state of the fluid is characterized by the set of molecular *positions*, $\mathbf{R}(t) = \{\mathbf{r}_1(t), \mathbf{r}_2(t), \cdots, \mathbf{r}_N(t)\} \in \mathbb{R}^{3N}$.
- The most direct and accurate way to simulate the microscopic dynamics of fluids is **Molecular Dynamics (MD)**, i.e., solving Newton's equations of motion:

$$m_i \ddot{\mathbf{r}}_i = m_i \dot{\mathbf{v}}_i = \sum_j \mathbf{f}_{ij}(\mathbf{r}_{ij})$$

- Standard (time-driven) molecular dynamics:
  All of the particles are displaced *synchronously* in small *time steps* Δt, calculating positions and forces on each particle at every time step.
- For hard spheres, one can use **asynchronous event-driven MD**:
  Spheres are *advected* along straight lines until they *collide* with another sphere and exchange momentum and energy.

"*Asynchronous Event-Driven Particle Algorithms*", by A. Donev, **SIMULATION, 85(4):229-242, 2009**, [cs.OH/0703096] [1].

Deterministic Molecular Dynamics

- Most of the computation is "wasted" on computing detailed (exact) trajectories of fluid particles (water molecules)!
- Over longer times it is **hydrodynamics** (*local momentum* and energy **conservation**) and **fluctuations** (Brownian motion) that matter.
- We need to coarse grain the fluid model further: *Replace deterministic interactions with stochastic ones.*

MNG

"*Stochastic Event-Driven Molecular Dynamics*", A. Donev, A. L. Garcia and B. J. Alder, **J. Comp. Phys., 227(4):2644-2665, 2008** [2]

Stochastic Molecular Dynamics

- **Stochastic conservative collisions** of randomly chosen nearby solvent particles, as in Direct Simulation Monte Carlo (DSMC).
- Can think of this as the hard-sphere equivalent of Dissipative Particle Dynamics (DPD).
- Binary DSMC collisions can be replaced with *multiparticle collisions* (MPCD/SRD).

MNG

"*Stochastic Hard-Sphere Dynamics for Hydrodynamics of Non-Ideal Fluids*", by A. Donev, A. L. Garcia and B. J. Alder, **Phys. Rev. Lett. 101:075902 (2008)** [arXiv:0803.0359, arXiv:0908.0510], [3]

Isotropic DSMC

- Define a simplified continuous Markov-chain microscopic dynamics for our *stochastic particle system*:
  - *Particles move ballistically in-between collisions,* $\dot{\mathbf{r}}_i = \mathbf{v}_i = const.$
  - *While two particles* i *and* j *are less than a diameter* D *apart,* $r_{ij} \leq D$, *there is a probability rate* $\chi D^{-1} K_c(\mathbf{v}_{ij}, \mathbf{r}_{ij})$ *for them to collide and change velocities without changing their positions.*
  - *Upon collision, the center-of-mass velocity does not change, while the relative velocity is drawn from a probability density* $P_c(\mathbf{v}'_{ij}; \mathbf{v}_{ij}, \mathbf{r}_{ij})$, $\left\| \mathbf{v}'_{ij} \right\| = \| \mathbf{v}_{ij} \|$.
- This Markov chain can be simulated using a Kinetic Monte Carlo (KMC) algorithm we call the **Isotropic Direct Simulation Monte Carlo** (I-DSMC).
- The I-DSMC fluid is a **viscous ideal gas** (structureless fluid), but by biasing collisions structure can be introduced.

Where we are now

- We have a serial implementation of many variants of DSMC-inspired algorithms for a single-species fluid, including a mixed deterministic-stochastic MD framework.
- We have a preliminary **parallel DSMC code for mixtures** of species.
- We still need to **parallelize the I-DSMC algoritm** (difficulty in synchronizing random event lists)
- We still need to include chemical reactions in the algorithms (**reactive mixtures**).

Coarse-Graining: Microscopic to Macroscopic

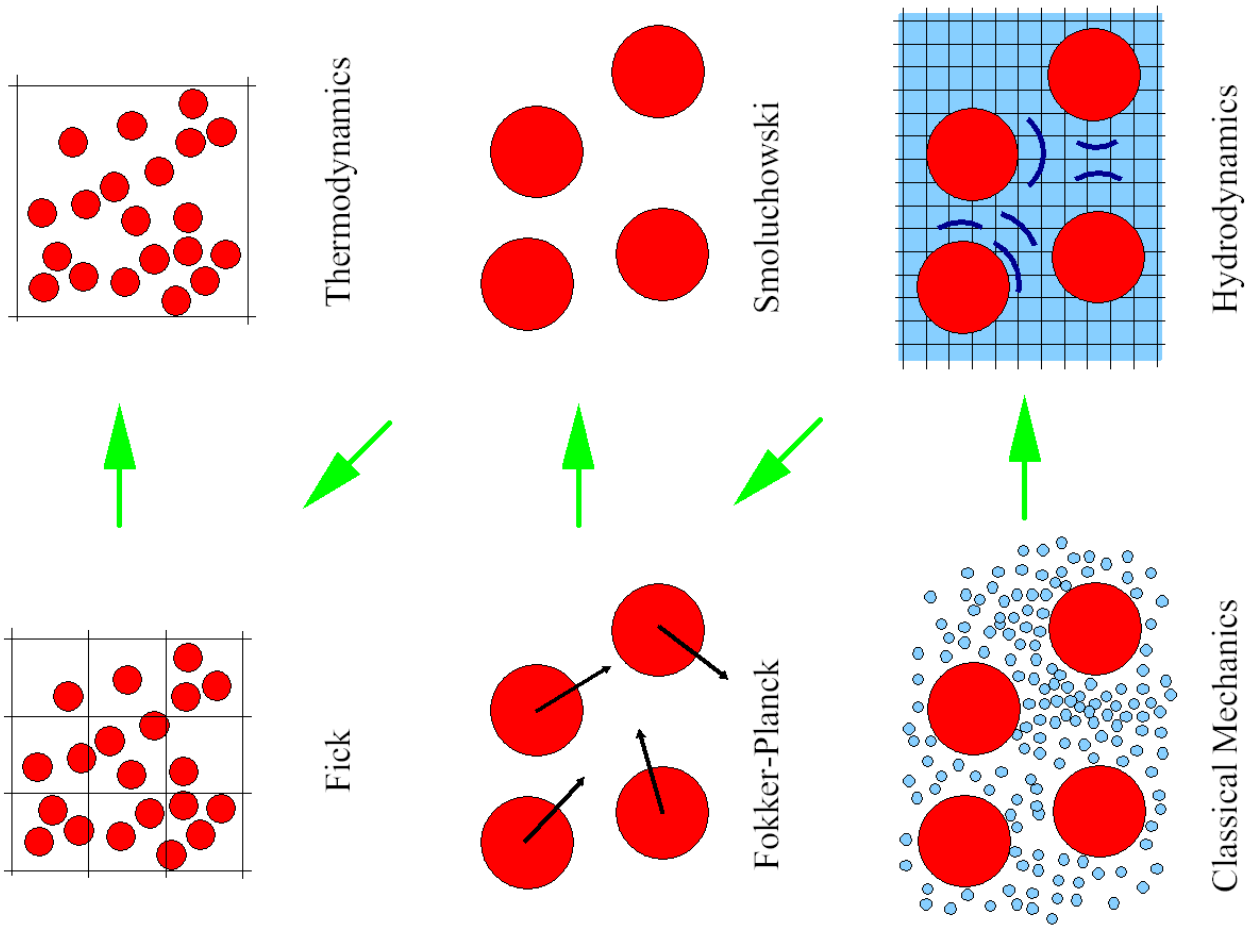


Figure: Levels of coarse graining according to Pep Español, "Statistical Mechanics of Coarse-Graining"

The Need for Coarse-Graining

- In order to examine the time-scales involved, we focus on a fundamental problem:
  A single spherical **bead** *of size a and density* ρ' *suspended in a stationary fluid with density* ρ and viscosity η (**Brownian walker**).
- The isssue: Wide **separation of timescales occurs** *between the timescales of microscopic and macroscopic* processes as the bead becomes much bigger than the mean free path λ of the solvent particles.
- Typical bead sizes are nm (nano-colloids, short polymers) or μm (colloids, DNA), while typical atomistic sizes are $0.1nm$.

Estimates from Fluid Dynamics

- Classical picture for the following dissipation process: *Push a sphere suspended in a liquid with initial velocity* $V_{th} \approx \sqrt{kT/M}$, $M \approx \rho' a^3$, *and watch how the velocity decays:*
  - **Sound waves** are generated from the sudden compression of the fluid and they take away a fraction of the kinetic energy during a **sonic time** $t_{sonic} \approx a/c$, where c is the (adiabatic) sound speed.
  - **Viscous dissipation** then takes over and slows the particle *non-exponentially* over a **viscous time** $t_{visc} \approx \rho a^2/\eta$, where η is the shear viscosity.
  - **Thermal fluctuations** get similarly dissipated, but their constant presence pushes the particle diffusively over a **diffusion time** $t_{diff} \approx a^2/D$, where $D \sim kT/(a\eta)$.

Timescale Estimates

- The mean collision time is $t_{coll} \approx \lambda / v_{th} \sim \eta / (\rho c^2)$, where the thermal velocity is $v_{th} \approx \sqrt{\frac{kT}{m}}$, for water

$$t_{coll} \sim 10^{-15} s = 1 fs$$

- The **sound time**

$$t_{sonic} \sim \begin{cases} 1ns \text{ for } a \sim \mu m \\ 1ps \text{ for } a \sim nm \end{cases}, \text{ with gap } \frac{t_{sonic}}{t_{coll}} \sim \frac{a}{\lambda} \sim 10^2 - 10^5$$

Estimates contd...

- **Viscous time** estimates

$$t_{visc} \sim \begin{cases} 1\mu s \text{ for } a \sim \mu m \\ 1ps \text{ for } a \sim nm \end{cases}, \text{ with gap } \frac{t_{visc}}{t_{sonic}} \sim \sqrt{C}\frac{a}{\lambda} \sim 1 - 10^3$$

- Finally, the **diffusion time** can be estimated to be

$$t_{diff} \sim \begin{cases} 1s \text{ for } a \sim \mu m \\ 1ns \text{ for } a \sim nm \end{cases}, \text{ with gap } \frac{t_{diff}}{t_{visc}} \sim \frac{a}{\phi R} \sim 10^3 - 10^6$$

which can now reach **macroscopic timescales**!

Continuum Models of Fluid Dynamics

- Formally, we consider the continuum field of **conserved quantities**

$$\mathbf{U}(\mathbf{r},t)=\begin{bmatrix}\rho\\ \mathbf{j}\\ e\end{bmatrix}\cong\widetilde{\mathbf{U}}(\mathbf{r},t)=\sum_i\begin{bmatrix}m_i\\ m_i\boldsymbol{\upsilon}_i\\ m_i\upsilon_i^2/2\end{bmatrix}\delta\left[\mathbf{r}-\mathbf{r}_i(t)\right],$$

  where the symbol $\cong$ means that $\mathbf{U}(\mathbf{r},t)$ approximates the true atomistic configuration $\widetilde{\mathbf{U}}(\mathbf{r},t)$ over **long length and time scales**.
- Formal coarse-graining of the microscopic dynamics has been performed to derive an **approximate closure** for the macroscopic dynamics [4].
- Here we consider more phenomenological **Langevin equations** formed by postulating a random flux term in the usual Navier-Stokes-Fourier equations with magnitude determined from the **fluctuation-dissipation balance** condition, following Landau and Lifshitz.

The SPDEs of Fluctuating Hydrodynamics

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

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

  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

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

- Prototype example is the (linear) **stochastic advection-diffusion equation** in one dimension

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

- More relevant but also problematic is the (nonlinear) **stochastic Burgers equation**

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

Landau-Lifshitz Navier-Stokes (LLNS) Equations

Complete single-species fluctuating hydrodynamic equations:

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

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

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

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

Problems with the LLNS equations

- Solving them numerically requires paying attention to **discrete fluctuation-dissipation balance**, in addition to the usual deterministic difficulties!
- It is not clear whether the Navier-Stokes equations apply at **nano-scales**.
- Adding stochastic fluxes to the **non-linear** NS equations produces **ill-behaved stochastic PDEs** (solution is too irregular).
- Mathematically-rigorous limit theorems only give the **linearized fluctuations** around the nonlinear mean, which lacks important physics.
- Fluctuations at scales smaller than the atomistic correlation length and time should be renormalized to account for discreteness of matter (recall *ultra-violet catastrophe*).

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*, whose **equilibrium distribution** (long-time limit, invariant measure) is a *stationary* **Gaussian process**.
- In **Fourier space** the equilibrium distribution is characterized by the **static spectrum**,

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

- For fluctuating hydrodynamics equations we have a **spatially-white** field at equilibrium, $\mathbf{S}(\mathbf{k}) = \mathbf{I}$.

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**

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

- 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.
- For these SPDEs, it is natural to define **weak convergence** based on the **second moments** and focus on the equilibrium distribution.

Stochastic Consistency and Accuracy

- Use the **discrete Fourier transform (DFT)** to separate wavenumbers, as usual.
- 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.
- The remainder term quantifies the *stochastic accuracy* for **large wavelengths ($\Delta k = k\Delta x \ll 1$) and small frequencies ($\Delta\omega = \omega\Delta t \ll 1$)**.
- Note that classical CFD is not meant to deal with such irregular fields, for which all modes are equally strong.

"*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] [5]

Discrete Fluctuation-Dissipation Balance

- Recall our numerical scheme

$$\widehat{\mathbf{U}}_k^{n+1} = \left[\mathbf{I} + \Delta t \widehat{\mathbf{L}}_k(\Delta t)\right] \widehat{\mathbf{U}}_k^n + \sqrt{\frac{\Delta t}{\Delta x}} \left[\widehat{\mathbf{K}}_k(\Delta t)\right] \widehat{\mathbf{W}}_k.$$

- A straightforward calculation **[5]** gives

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

- Thus $\mathbf{S}_k^{(0)} = \lim_{\Delta t \to 0} \mathbf{S}_k = \mathbf{S}(k) = \mathbf{I}$ iff **discrete fluctuation-dissipation balance** holds

$$\widehat{\mathbf{L}}_k^{(0)} + \left(\widehat{\mathbf{L}}_k^{(0)}\right)^\star = -\widehat{\mathbf{K}}_k^{(0)} \left(\widehat{\mathbf{K}}_k^{(0)}\right)^\star. \tag{1}$$

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

Compressible Fluctuating Hydrodynamics

- 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

- Future work: Use existing AMR framework to do **mesh refinement** (fluctuation-dissipation balance at coarse-fine interfaces [6]).

Incompressible Approximation

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

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

  which is equivalent to

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

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

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

- 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,

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

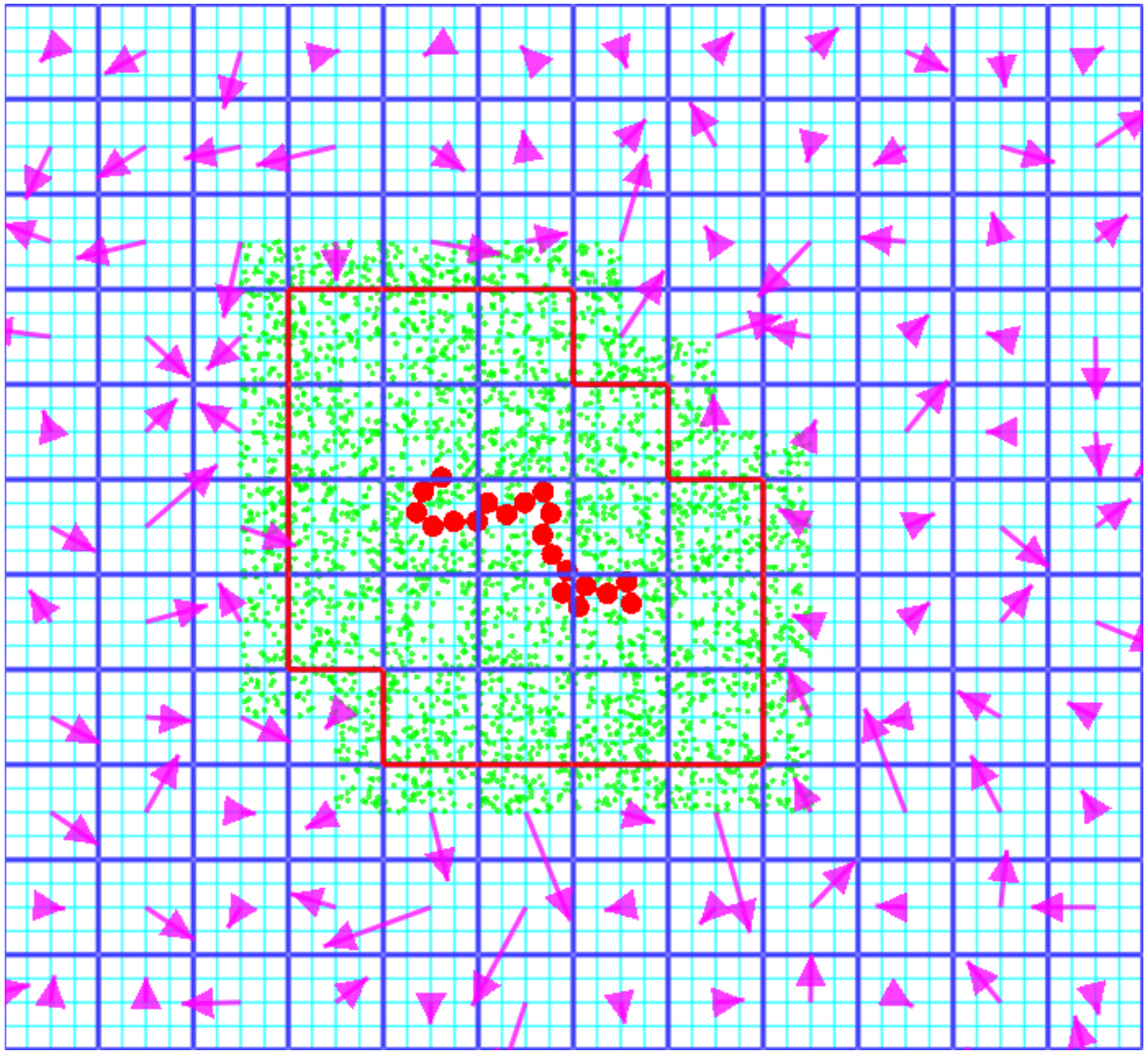
- The difficulty is the discretization of the projection operator $\mathbb{P}$:

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

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

- 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.

Particle/Continuum Hybrid Approach



Solute-Solvent Coupling using Particles

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- Split the domain into a **particle** and a **continuum (hydro) subdomains**, with timesteps $\Delta t_H = K \Delta t_P$.
- Hydro solver is a simple explicit **(fluctuating) compressible LLNS** code and is *not aware* of particle patch.
- The method is based on Adaptive Mesh and Algorithm Refinement (AMAR) methodology for conservation laws and ensures **strict conservation** of mass, momentum, *and* energy.

Continuum-Particle Coupling

- Each macro (hydro) cell is either **particle or continuum**. There is also a **reservoir region** surrounding the particle subdomain.
- The coupling is roughly of the **state-flux** form:
  - The continuum solver provides *state boundary conditions* for the particle subdomain via reservoir particles.
  - The particle subdomain provides *flux boundary conditions* for the continuum subdomain.
- The fluctuating hydro solver is **oblivious** to the particle region: Any conservative explicit finite-volume scheme can trivially be substituted.
- The coupling is greatly simplified because the particle fluid is ideal (no internal structure): **No overlap region**.

"*A hybrid particle-continuum method for hydrodynamics of complex fluids*", A. Donev and J. B. Bell and A. L. Garcia and B. J. Alder, **SIAM J. Multiscale Modeling and Simulation 8(3):871-911, 2010** [7]

Hybrid Algorithm

Steps of the coupling algorithm:

1. The hydro solution is computed everywhere, including the **particle patch**, giving an estimated total flux $\mathbf{\Phi}_H$.
2. **Reservoir particles** are *inserted* at the boundary of the particle patch based on *Chapman-Enskog distribution* from kinetic theory, accounting for *both* collisional and kinetic viscosities.
3. Reservoir particles are *propagated* by Δt and *collisions* are processed (including virtual particles!), giving the total particle flux $\mathbf{\Phi}_p$.
4. The hydro solution is overwritten in the particle patch based on the particle state $\mathbf{u}_p$.
5. The hydro solution is corrected based on the more accurate flux, $\mathbf{u}_H \leftarrow \mathbf{u}_H - \mathbf{\Phi}_H + \mathbf{\Phi}_p$.

The adiabatic piston problem

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Relaxation Toward Equilibrium

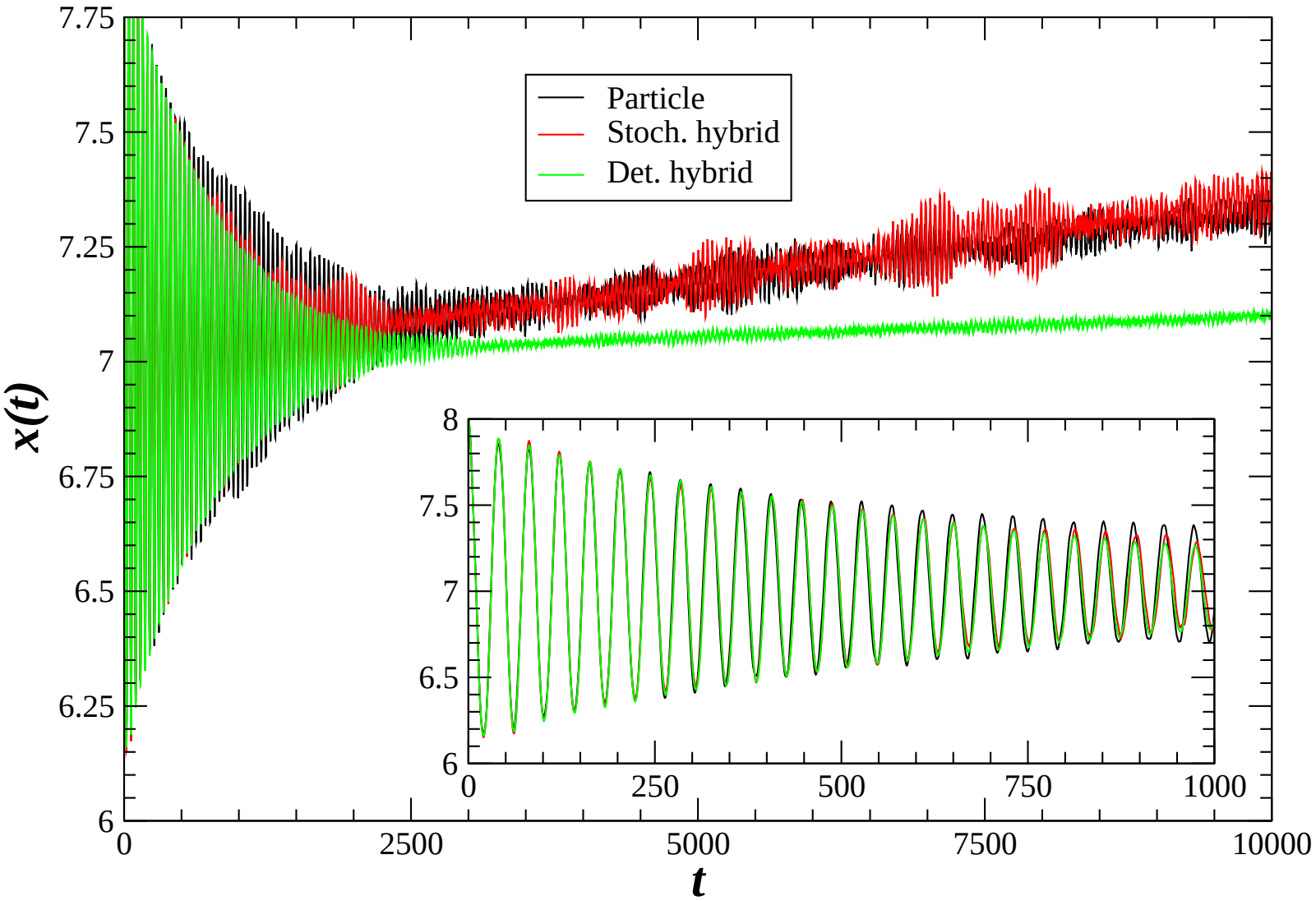


Figure: Massive rigid piston ($M/m = 4000$) not in mechanical equilibrium.

VACF for Piston

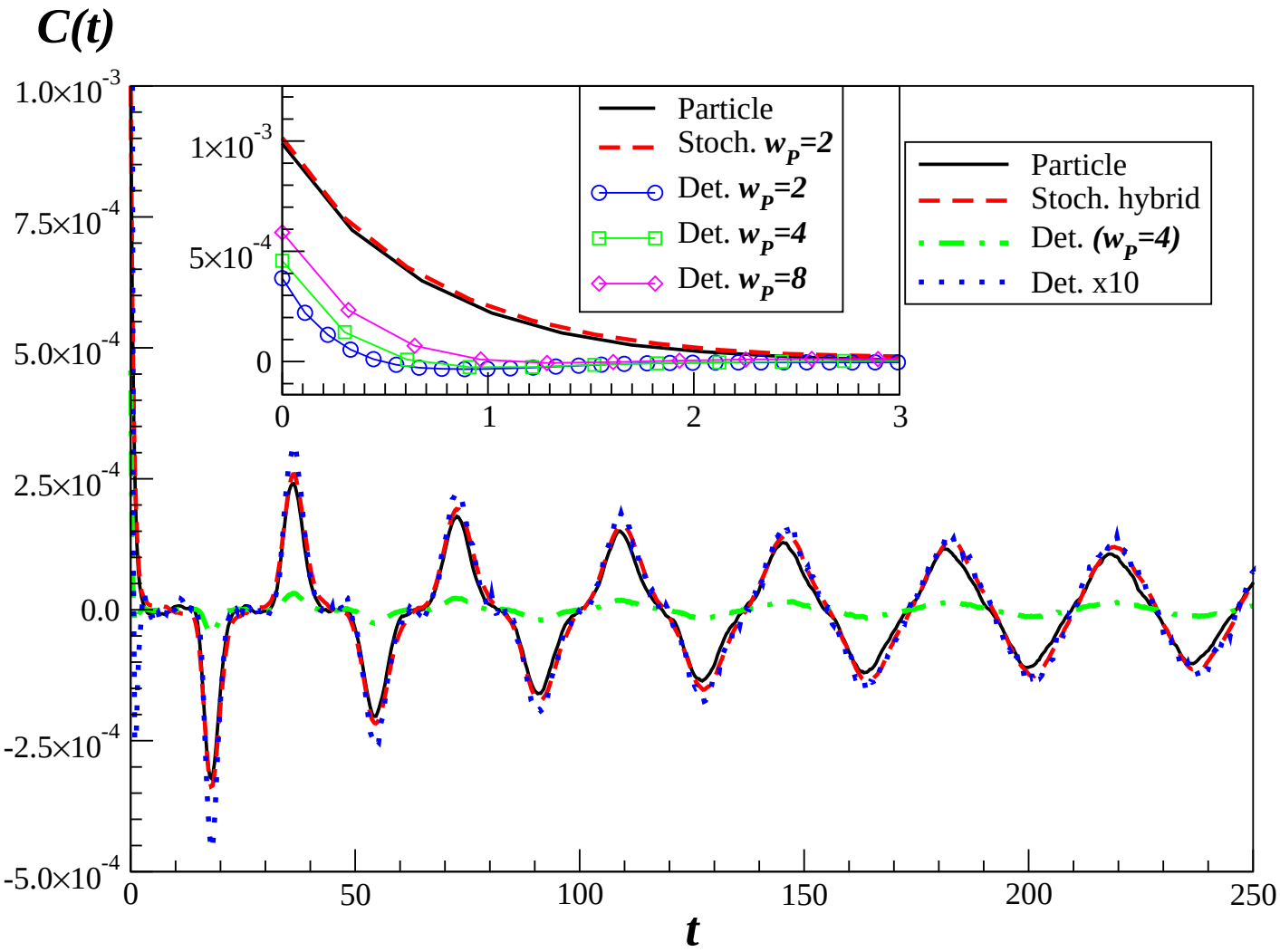


Figure: The VACF for a rigid piston of mas $M/m = 1000$ at thermal equilibrium.

Fluctuations in the presence of gradients

- At **equilibrium**, hydrodynamic fluctuations have non-trivial temporal correlations, but there are no spatial correlations between any variables.
- When macroscopic gradients are present, however, **long-ranged correlated fluctuations** appear.
- Consider a **binary mixture** of fluids and consider **concentration fluctuations** around a steady state $c_0(\mathbf{r})$:

$$c(\mathbf{r}, t) = c_0(\mathbf{r}) + \delta c(\mathbf{r}, t)$$

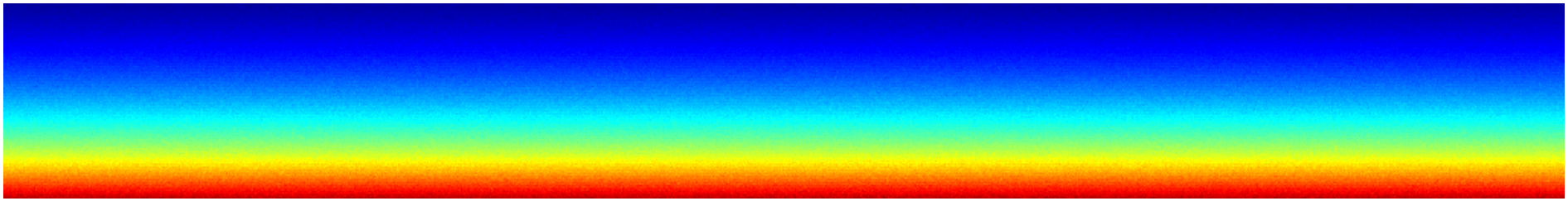
- The concentration fluctuations are **advected by the random velocities $\mathbf{v}(\mathbf{r}, t)$**, approximately:

$$(\delta c)_t + \mathbf{v} \cdot \boldsymbol{\nabla} c_0 = D \boldsymbol{\nabla}^2 (\delta c) + \sqrt{2 D k_B T} \, (\boldsymbol{\nabla} \cdot \boldsymbol{\mathcal{W}}_c)$$

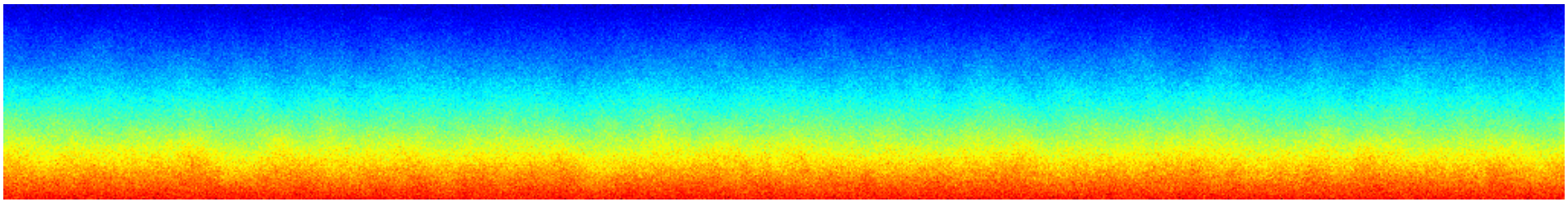
- The velocity fluctuations drive and amplify the concentration fluctuations leading to so-called **giant fluctuations**.

Equilibrium versus Non-Equilibrium

Results obtained using our fluctuating continuum compressible solver.



Concentration for a mixture of two (heavier red and lighter blue) fluids at **equilibrium**, in the presence of gravity.



No gravity but a similar **non-equilibrium** concentration gradient is imposed via the boundary conditions.

Giant Fluctuations during diffusive mixing

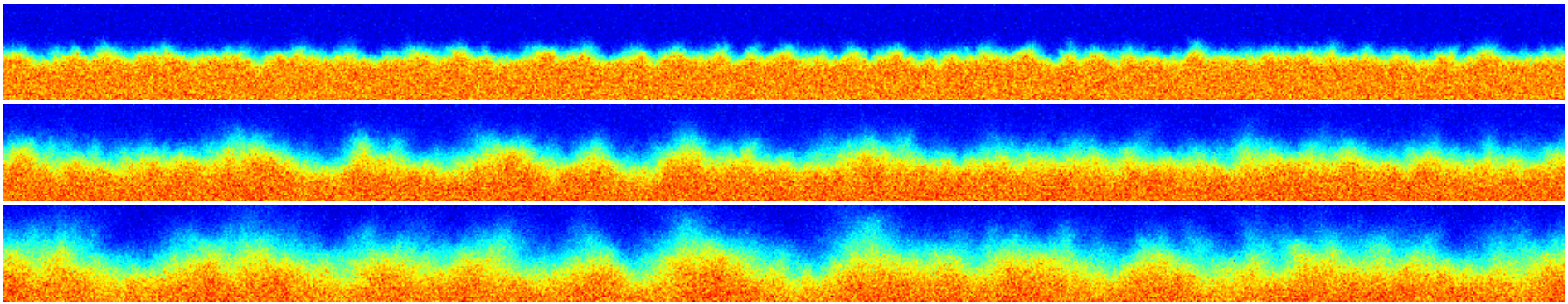


Figure: Snapshots of the concentration during the diffusive mixing of two fluids (red and blue) at $t = 1$ (top), $t = 4$ (middle), and $t = 10$ (bottom), starting from a flat interface (phase-separated system) at $t = 0$.

Giant Fluctuations in 3D

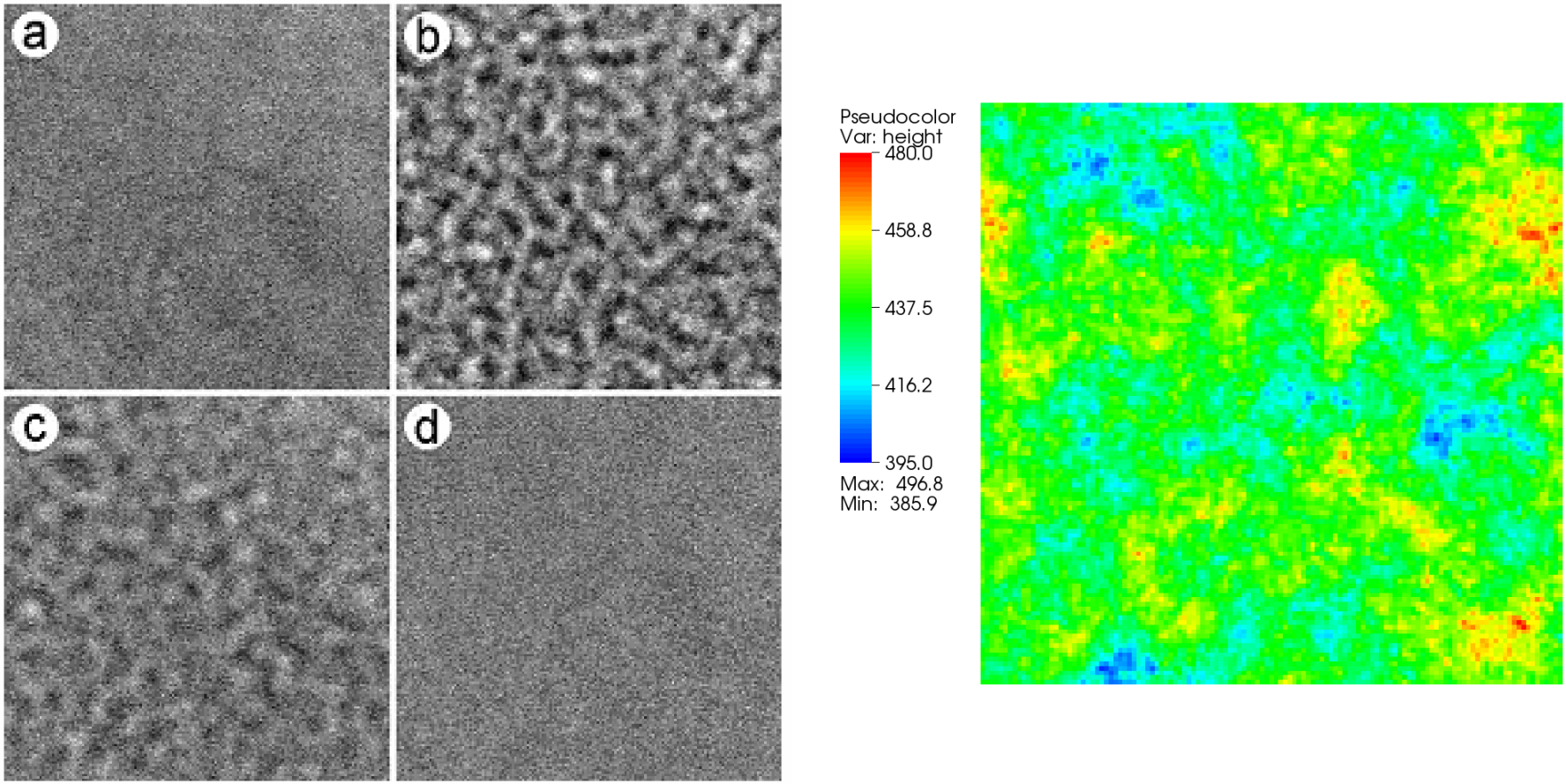


Figure: (Left) Experimental images (1mm side) of scaterring from the interface between two miscible fluids (A. Vailati & M. Giglio, Nature 1997 [8]). (Right) Snapshot of the interface in a computational simulation without gravity.

Conclusions

- **Coarse-grained particle methods** can be used to accelerate hydrodynamic calculations at small scales.
- Designing numerical methods for fluctuating hydrodynamics requires attention to **discrete fluctuation-dissipation balance**, in addition to the usual (deterministic) stability and accuracy considerations.
- **Hybrid particle continuum methods** closely reproduce purely particle simulations at a fraction of the cost.
- It is **necessary to include fluctuations** in the continuum subdomain in hybrid methods.
- **Advection by the fluctuating velocities** fields leads to some very interesting physics and mathematics, such as giant fluctuations.

Future Directions

- Improve and implement in a public-domain code the stochastic **particle methods** (parallelize, add chemistry, analyze theoretically).
- Develop numerical schemes for **incompressible** and **Low-Mach Number** fluctuating hydrodynamics.
- Theoretical work on the **equations of fluctuating hydrodynamics**: regularization, renormalization, systematic coarse-graining.
- **Direct fluid-structure coupling** between fluctuating hydrodynamics and microstructure (solute beads).
- Ultimately we require 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 CFD (**macro**).

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