UNIVERSITÄT SIEGEN

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MASTERARBEIT

Fluctuation Hydrodynamics

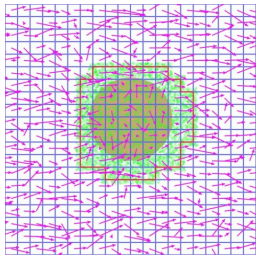
Direct Simulation Monte Carlo vs. CFD

Stochastic vs. Deterministic

Description of the problem :

With the increased interest in nanofluidics and microfluidics, it has become necessary to develop tools for hydrodynamic calculations at the atomistic scale. Numerical schemes based on a particle representation of a fluid inherently include spontaneous fluctuations due to the irregular dynamics of the particles. To incorporate thermal fluctuations into macroscopic hydrodynamics, Landau and Lifshitz introduced an extended form of the compressible Navier–Stokes equations obtained by adding white-noise stochastic flux terms to the standard deterministic equations (Landau–Lifshitz Navier–Stokes equations). These equations incorporate thermal fluctuations into macroscopic hydrodynamics by the addition of white- noise fluxes whose magnitudes are set by a fluctuation-dissipation relation. Question: *Is it necessary to use stochastic PDEs in the continuum region given that the particle region has fluctuations?* Answer: *YES!*

First test is the calculation of the Brownian motion of a spherical particle.



$$\partial \mathbf{U}/\partial t + \nabla \cdot \mathbf{F} = \nabla \cdot \mathbf{D} + \nabla \cdot \mathbf{S}$$

Hyperbolic Fluxes Parabolic Fluxes Stochastic Fluxes

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

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

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

Tasks:

- **Hydrodynamic fluctuations**
  - understanding of finite-volume methods for Landau–Lifshitz Navier–Stokes stochastic equations
    - Direct simulation Monte Carlo (DSMC) solver for 3D flows
      - **foamDSMC** - a DSMC solver for flow application based on OpenFOAM
  - CFD – pseudo-spectral code, Fourier-Fourier-Chebyshev (the coding is done for hydrodynamic fluctuations in this numerical code, student just needs to understand it with our help).
- **Application: Brownian motion** in plane Couette flow

Required qualifications :

- Basic knowledge in C, FORTRAN and MATLAB;
- Basics of fluid dynamics;
- Basic knowledge of stochastic processes, random numbers, etc.