SIMULATING AND COMPARING ALTERNATIVE FORMULATIONS OF THE BOLTZMANN EQUATION

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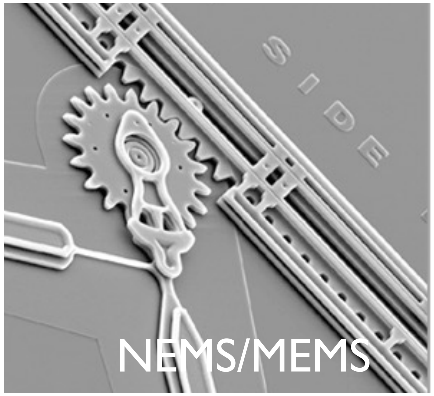
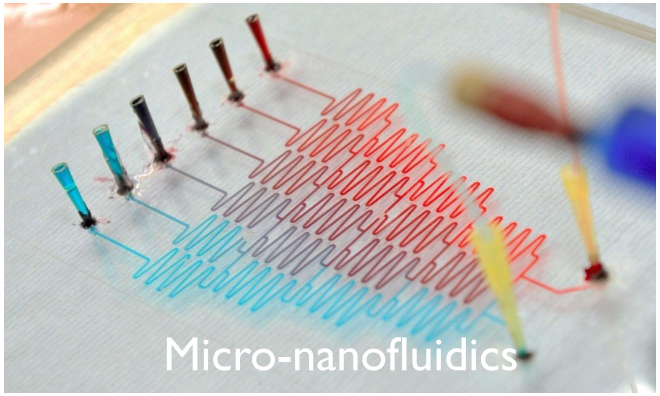
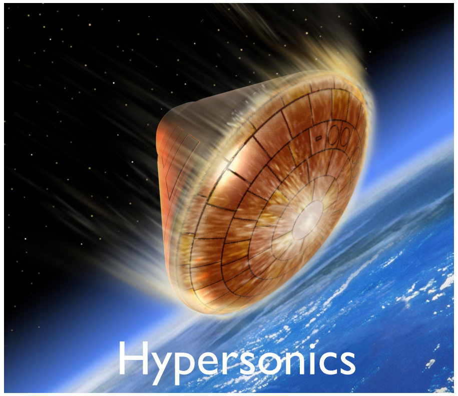
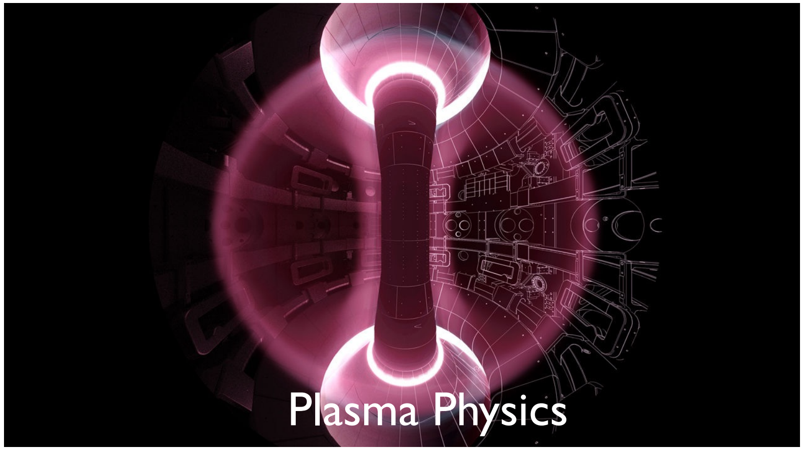
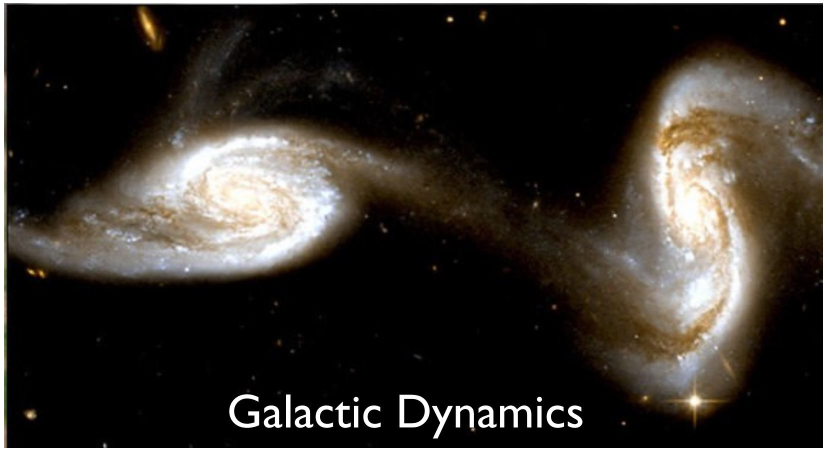
APPLICATIONS











BACKGROUND

- The Navier-Stokes equations rely on the continuum hypothesis[1], such that the fluid intensive property functions are well behaved (often C^∞)
- Knudsen number $Kn = \lambda/L$ is the ratio of the mean free path of particle over the characteristic length
    - measures the degree to which the state locally departs from equilibrium
    - $Kn = 0 \implies$ local equilibrium $\implies$ Euler Equations
    - $Kn \lesssim 0.01 \implies$ sufficiently continuous $\implies$ Navier-Stokes
- For non-continuum flows and any Kn, need a new governing equation derived from first principles: e.g. the Boltzmann Equation

[1] Pierre Lermusiaux, *Recitation Navier-Stokes*, MIT 2.29 (2021)

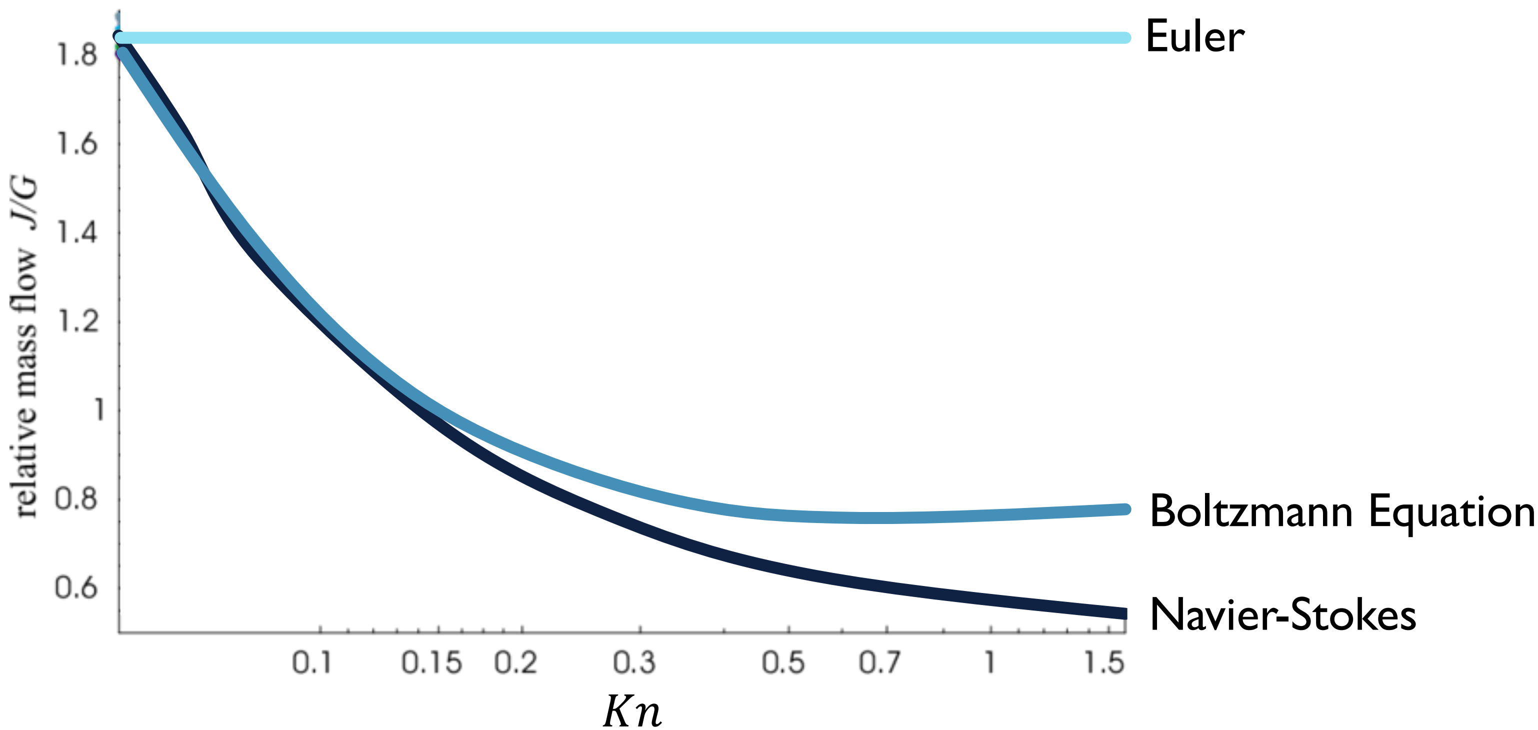
BOLTZMANN EQUATION

- The Boltzmann Equation is a $(6+1)-$dimensional PDE that describes the evolution of the single particle distribution function (pdf) $f(\boldsymbol{x}, \boldsymbol{c}, t)$ of a gas

$$\frac{\partial f}{\partial t} + \boldsymbol{c} \cdot \frac{\partial f}{\partial \boldsymbol{x}} + \frac{\boldsymbol{F}}{m} \cdot \frac{\partial f}{\partial \boldsymbol{c}} = \frac{1}{Kn} Q(f, f) \qquad \text{(Eq 1)}$$

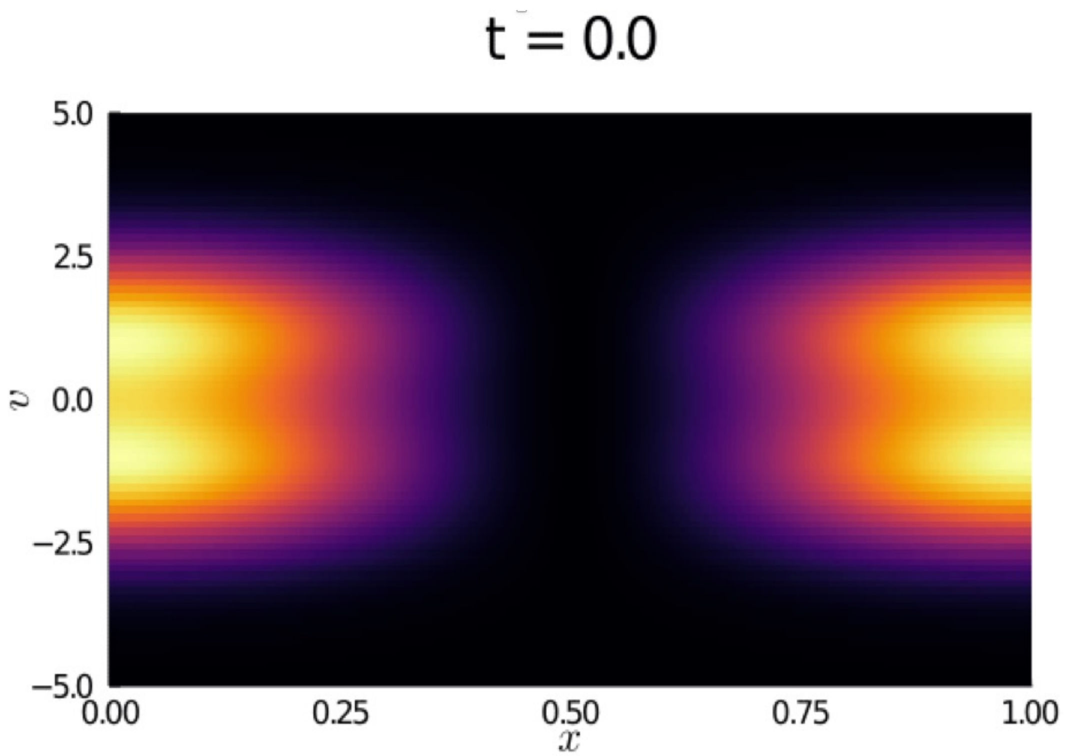
- In the ballistic regime $Kn \gg 1,$ Eq 1 approximately only depends on LHS
- In the diffusive regime $Kn \ll 1,$ Eq 1 is collision dominated and thus close to local equilibrium
    - Chapman-Enskog derives the Euler and Navier-Stokes as the zeroth and first order correction in a perturbative expansion $f = f^{(0)} + Kn\, f^{(1)} + \mathcal{O}(Kn^2)$
- For $0.1 \lesssim Kn \lesssim 10$ only the Boltzmann Equation (or Molecular Dynamics) is appropriate

EXAMPLE 1



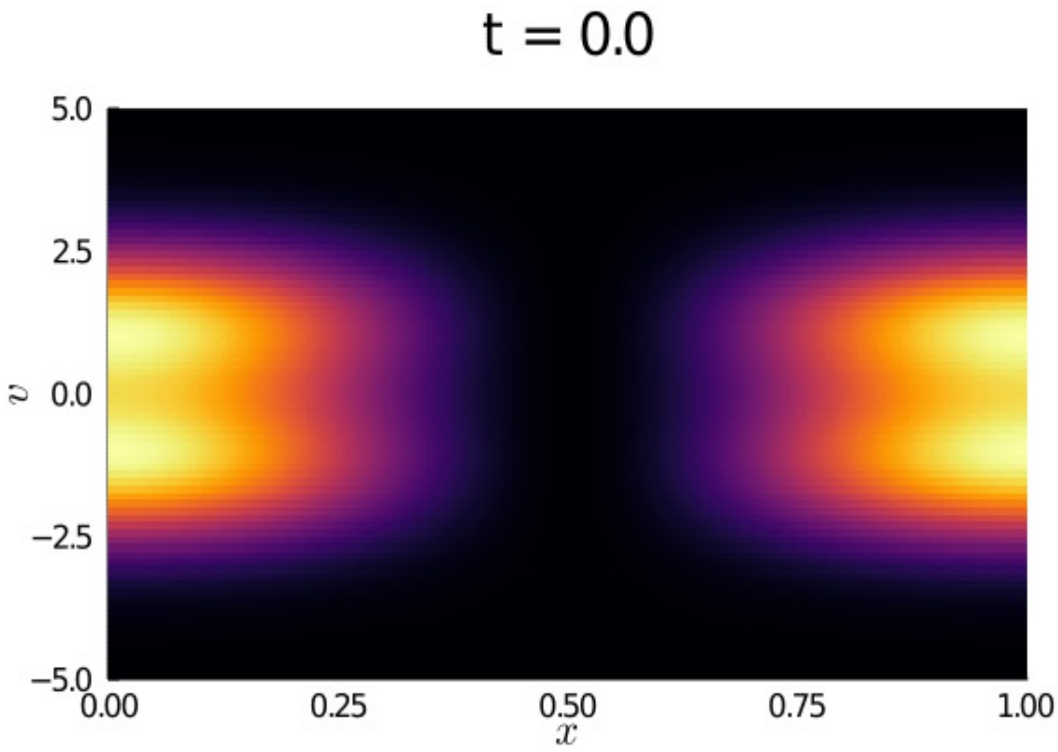
[2] Adapted from Henning Struchtrup and Manuel Torrilhon, *Higher-Order Effects in Rarefied Channel Flows*, 10.1103/PhysRevE.78.046301 (2008)

EXAMPLE II



[3] Evan Massaro, *Hermite Spectral Method for the Boltzmann Equation*, MIT 18.336 (2020)

EXAMPLE II



[3] Evan Massaro, *Hermite Spectral Method for the Boltzmann Equation*, MIT 18.336 (2020)

NUMERICAL METHODS I

- Two body collision integral

$$Q(f,f)=\int_{\mathbb{R}^3}\int_{\mathbb{S}^2}\left[f\left(\mathbf{v}'\right)f\left(\mathbf{v}_*'\right)-f(\mathbf{v})f\left(\mathbf{v}_*\right)\right]\mathcal{B}(\cos\theta,g)d\mathbf{\Omega}d\mathbf{v}_*$$

- Evaluating this integral is difficult due to the high dimensionality and nonlinearity
- Fast spectral method is use to discretize space and the polar angles
- Flux reconstruction in space computed within the Lagrange polynomial basis

$$l_p=\prod_{q=0,q\neq p}^{m}\left(\frac{r-r_q}{r_p-r_q}\right) \qquad \hat{f}^\delta=\sum_{p=0}^{m}\hat{f}_p^\delta l_p \qquad \hat{F}^{\delta D}=\sum_{p=0}^{m}\hat{F}_p^{\delta D}l_p$$

[4] Tianbai Xiao, A Flux Reconstruction Kinetic Scheme for the Boltzmann Equation, arxiv.org/pdf/2103.10371.pdf (2021)

NUMERICAL METHODS II

- Spectral representation

$$\hat{f}^{\delta}(t,\mathbf{r},\mathbf{v}) = \sum_{k=-N/2}^{N/2-1} \hat{f}_k^{\delta}(t,\mathbf{r}) \exp\left(i\xi_k \cdot \mathbf{v}\right)$$

$$\hat{Q}_k^{\delta} = \sum_{l,m=-N/2,(l+m=k)}^{N/2-1} \hat{f}_l^{\delta} \hat{f}_m^{\delta} [\beta(l,m) - \beta(m,m)]$$

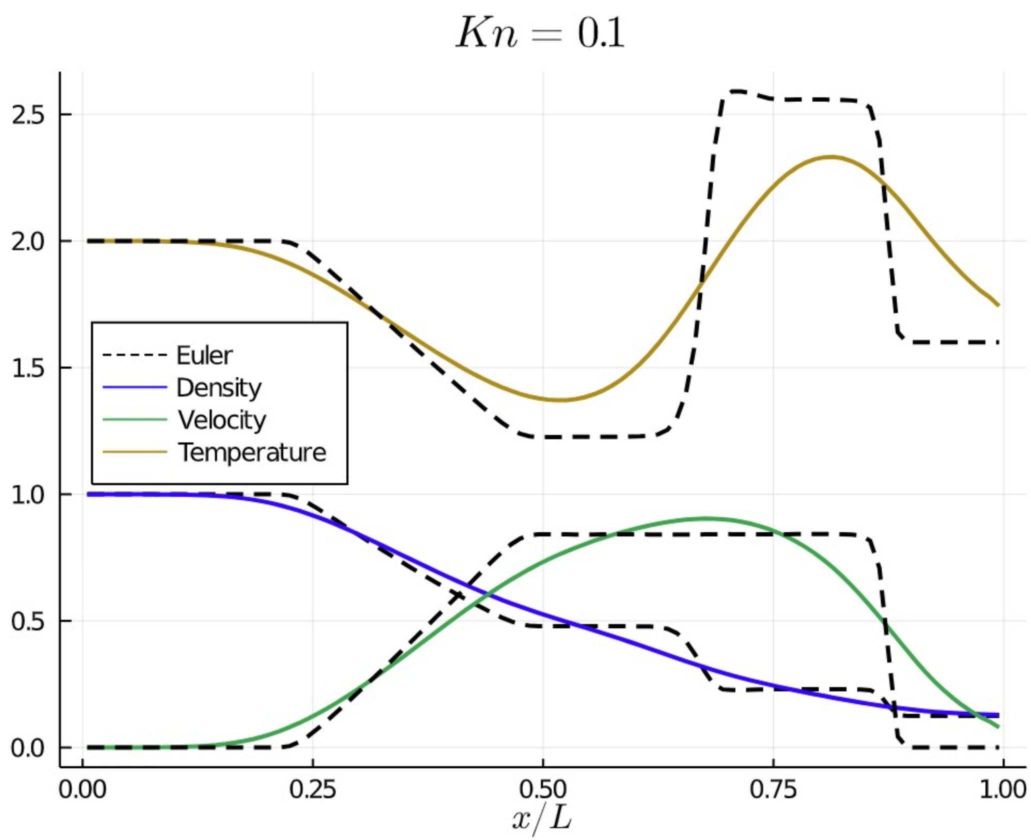
$$\beta(l,m) = 4 \int \left[\int_0^R \rho \cos\left(\rho \xi_l \cdot \mathbf{e}\right) d\rho \right] \left[\int \delta\left(\mathbf{e} \cdot \mathbf{e}'\right) \int_0^R \rho' \Theta \cos\left(\rho' \xi_m \cdot \mathbf{e}'\right) d\rho' d\mathbf{e}' \right] d\mathbf{e}$$

$$\frac{\partial \hat{f}_{i,j}^{\delta}}{\partial t} = -\nabla_{\mathbf{r}} \cdot \hat{\mathbf{F}}_{i,j}^{\delta} + \hat{Q}_{i,j}^{\delta} = \hat{C}_{i,j}^{\delta}$$

- Use singly diagonally implicit Runge–Kutta (SDIRK) for time integration

[4] Tianbai Xiao, A Flux Reconstruction Kinetic Scheme for the Boltzmann Equation, arxiv.org/pdf/2103.10371.pdf (2021)

SOD SHOCK TUBE



[4] Code based in Kinetic.jl, https://xiaotianbai.com/Kinetic.jl/dev (2021)

ERROR ANALYSIS

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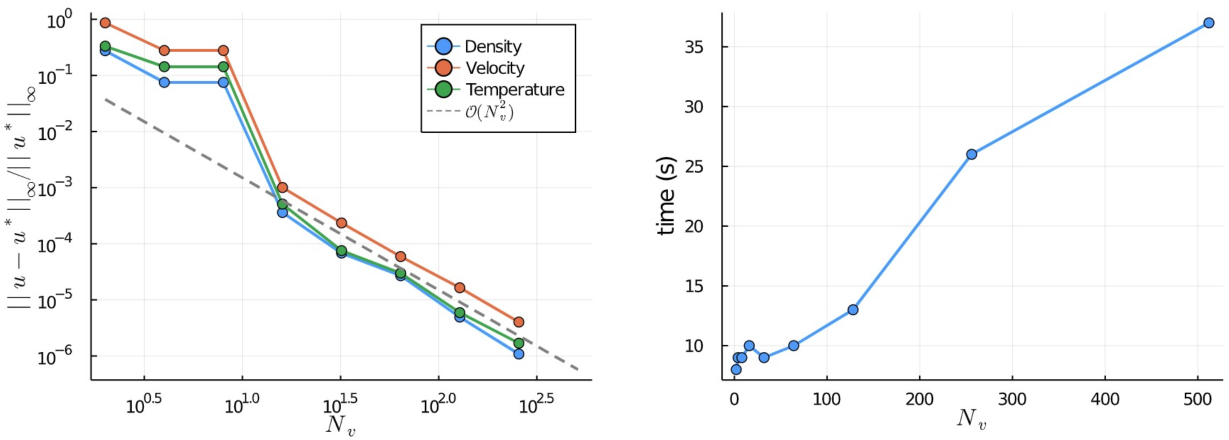

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