
Eulerian Formulation of Discrete Particle Dynamics

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Eulerian and Lagrangian Formulations

- Lagrangian follows a fixed collection of fluid
- Eulerian watches flow through a fixed volume

- **We Want**

$$\frac{\partial}{\partial t} \int_V \rho dV = - \oint_S \rho \mathbf{u} \cdot d\mathbf{S}$$

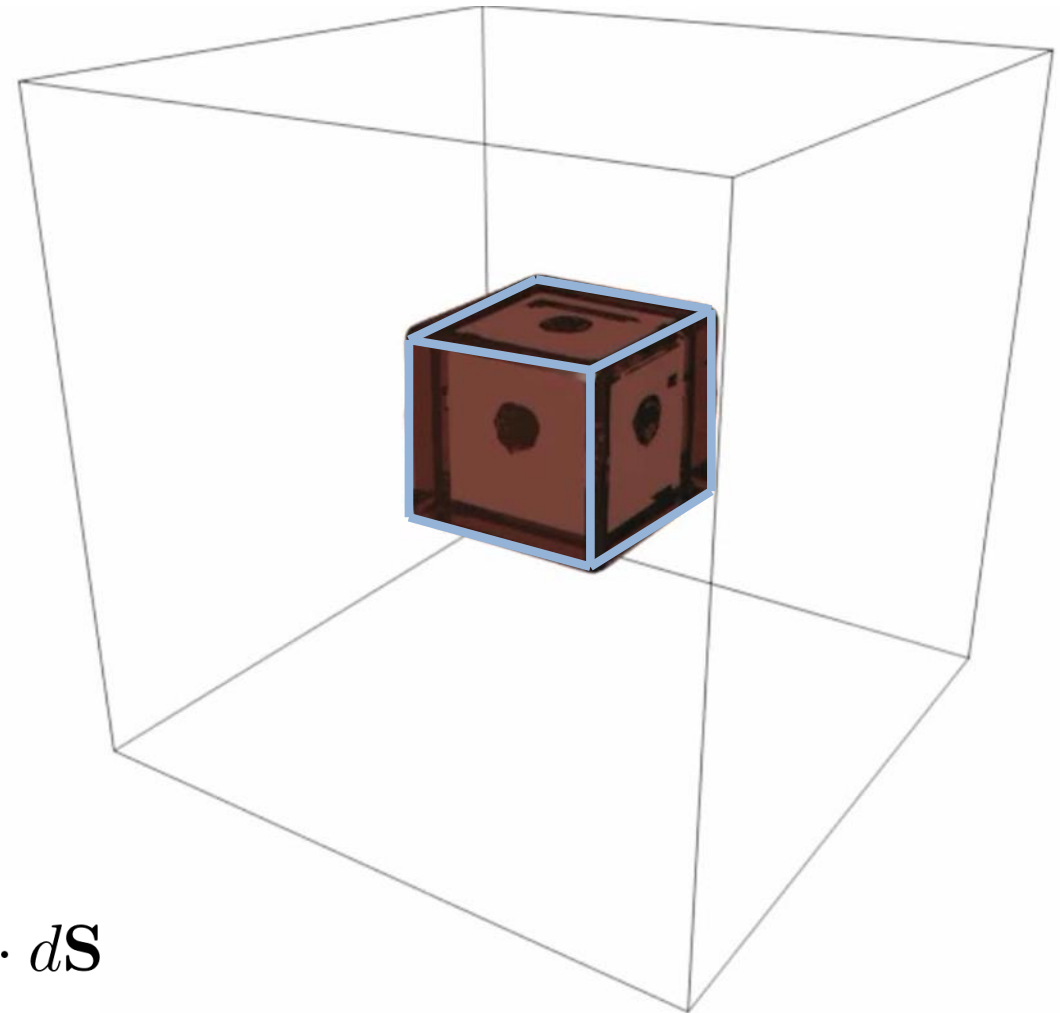
- **Why?**

$$\frac{\partial}{\partial t} \int_V \rho \mathbf{u} dV = - \oint_S \rho \mathbf{u} \mathbf{u} \cdot d\mathbf{S} + \mathbf{F}_{\text{surface}}$$

- Insight into the molecular form of

$$\frac{\partial}{\partial t} \int_V \rho \mathcal{E} dV = - \oint_S \rho \mathcal{E} \mathbf{u} \cdot d\mathbf{S}$$

- The basic and continuity equation
- $$\oint_S \mathbf{\Pi} \cdot \mathbf{u} \cdot d\mathbf{S} + \mathbf{q} \cdot d\mathbf{S}$$



Outline

- **Introduction**

- Discrete models (molecular dynamics)
- Irving and Kirkwood (1950)

- **Eulerian Equations of motion**

- Control Volume Function
- Reynolds' transport theorem using the control volume function
- Application to microscopic pressure

- **Results**

- Numerical simulations of Couette flow
- Applying the method to coupling

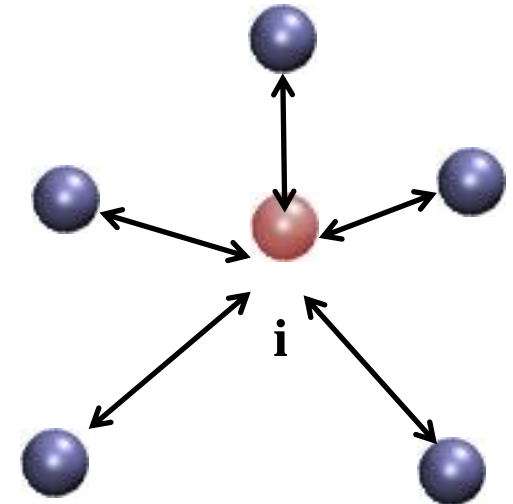
Introduction

Discrete models (molecular dynamics)

Discrete Molecules in continuous space

- Governed by Newton's Law for an N-body system
- Point particles with pairwise interactions only

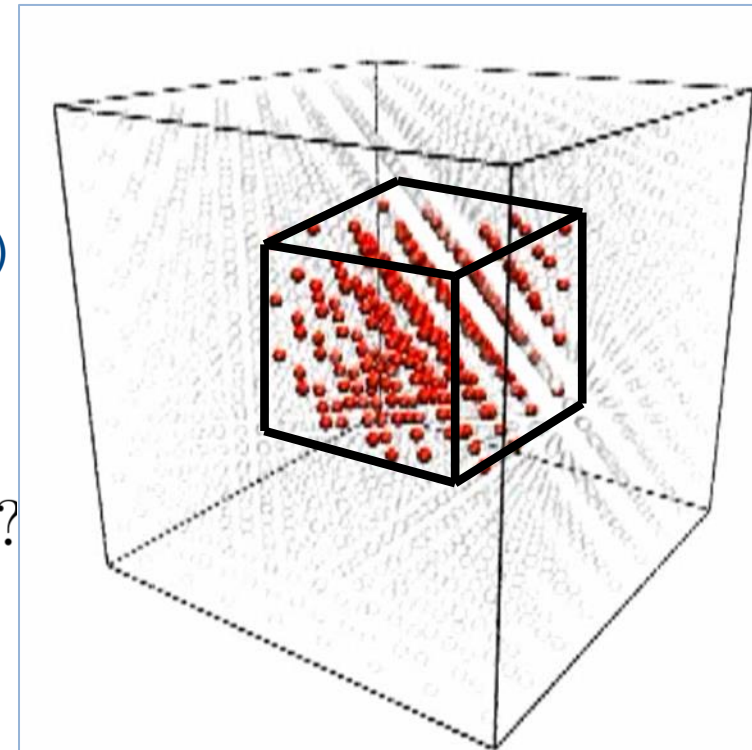
$$m_i \ddot{\mathbf{r}}_i = \mathbf{F}_i = \sum_{i \neq j}^N \mathbf{f}_{ij} \quad \begin{array}{l} \ddot{\mathbf{r}}_i \rightarrow \dot{\mathbf{r}}_i \\ \dot{\mathbf{r}}_i \rightarrow \mathbf{r}_i(t) \end{array}$$



Discrete N-body systems defined in terms of sums

- High Knudsen number flows
- Sum over entire system defines Lagrangian system
- Multi-phase fluids (phase change and nucleation)
- Crystal structures and dense fluids (correlations)
- How do we get an Eulerian description?
- Polymers

$$\text{mass}_{system} = \frac{1}{M} \sum_{i=1}^M m_i \quad \int_V \rho(\mathbf{r}, t) dV = ?$$



Irving and Kirkwood (1950)

$$\langle \alpha; f \rangle \equiv \int \dots \int \alpha(\mathbf{r}^N, \mathbf{p}^N) f(\mathbf{r}^N, \mathbf{p}^N, t) d\mathbf{r}^N d\mathbf{p}^N$$

$$\frac{\partial}{\partial t} \langle \alpha; f \rangle = \sum_{i=1}^N \left\langle \frac{\partial \alpha}{\partial r_i} \cdot \mathbf{F}_i + \frac{\partial \alpha}{\partial p_i} \cdot \dot{\mathbf{p}}_i; f \right\rangle$$

$$\alpha = \sum_{i=1}^N m_i \delta(\mathbf{r} - \mathbf{r}_i)$$

$$\rho(\mathbf{r}, t) = \sum_{i=1}^N \langle m_i \delta(\mathbf{r} - \mathbf{r}_i); f \rangle$$

TRANSPORT PROCESSES

has not been observed. If the preferred interpretation is that the group of Raman bands, 769, 778, 819, and 829 cm^{-1} , are related to each other in much the same manner as similar groups in the spectra of CO_2 and CS_2 .

ACKNOWLEDGMENTS

The writers wish to express their indebtedness to Dr. C. F. Hamner and E. L. du Pont de Nemours and Company for the samples; to Doctors Isabella and Jerome Kafke for electron diffraction data; and to Dr. E. K. Plyler and the National Bureau of Standards for data in the long wave-length region.

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The Statistical Mechanical Theory of Transport Processes. I. The Equations of Hydrodynamics*

J. D. Kirkwood and J. G. Kirkwood

Chemical Laboratories, University of California, San Diego, California (Received November 21, 1949)

INTRODUCTION

THIS paper will be concerned with a derivation of the equations of hydrodynamics from the principles of the statistical mechanics of transport. In particular, the equations of energy transport will be derived. By so doing, the stress tensor and heat current density can be expressed in terms of molecular variables. The stress tensor consists of a convective term which occurs in the kinetic theory of gases and another term (dominant for a liquid) which will be expressed as a quadrature involving the potential of intermolecular force and the density of the sum of the potential of intercurrent density involving the density and current density in the configuration space of a pair of molecules.

This program is unfeasible for a liquid, various attempts have been made to obtain a closed equation satisfied by a pair of molecules. One such equation has been derived by Debye and Green* using a "superposition" assumption. Another generalization of the well-known Fokker-Planck equation of stochastic theory, has been derived by Kirkwood¹ by introducing the concepts of time smoothing and a friction constant. This latter equation has been applied to obtain an expression for the stress tensor and a friction constant (in terms of molecular variables) for a nonuniform temperature, and thereby generalized to non-uniform temperatures, and an explicit expression for the coefficient of thermal conductivity.² We shall assume, for purposes of mathematical simplicity, a single component, single phase fluid system consisting of molecules which interact under central forces only. It is not difficult to generalize the treatment to a multiple component of molecules.

* This work was supported by the U. S. ONR under Contract N00r-244 with the California Institute of Technology. J. G. Kirkwood, J. Chem. Phys. 14, 50 (1946).

TRANSPORT PROCESSES I

The probability distribution function (relative density of representative points in phase space) we denote by

$$f(\mathbf{R}_1, \dots, \mathbf{R}_N; \mathbf{p}_1, \dots, \mathbf{p}_N, t)$$

satisfying the normalization condition

$$\int \dots \int f(\mathbf{R}_1, \dots, \mathbf{R}_N; \mathbf{p}_1, \dots, \mathbf{p}_N, t) d\mathbf{R}_1 \dots d\mathbf{R}_N d\mathbf{p}_1 \dots d\mathbf{p}_N = 1 \quad (2.1)$$

where $d\mathbf{R}_i$ stands for a volume element in the configuration space and $d\mathbf{p}_i$ a volume element in the momentum space of the i th molecule. f changes in time according to the well-known Liouville equation

$$\frac{df}{dt} = \sum_{i=1}^N \left[\frac{p_i}{m_i} \cdot \nabla_{\mathbf{R}_i} f + \nabla_{\mathbf{p}_i} U \cdot \nabla_{\mathbf{p}_i} f \right] \quad (2.2)$$

where U is the potential energy of the entire system. Any dynamical variable, $\alpha(\mathbf{R}_1, \dots, \mathbf{R}_N; \mathbf{p}_1, \dots, \mathbf{p}_N, t)$ has an expectation value given at time t by

$$\langle \alpha; f \rangle = \int \dots \int \alpha(\mathbf{R}_1, \dots, \mathbf{R}_N; \mathbf{p}_1, \dots, \mathbf{p}_N, t) f(\mathbf{R}_1, \dots, \mathbf{R}_N; \mathbf{p}_1, \dots, \mathbf{p}_N, t) d\mathbf{R}_1 \dots d\mathbf{R}_N d\mathbf{p}_1 \dots d\mathbf{p}_N \quad (2.3)$$

We thus denote by $\langle \alpha; f \rangle$ the expectation value of α for a distribution function f . (It is merely the inner product of α and f taken over phase space.) Providing α does not depend on time explicitly, the rate of change of the expectation value of α is given by

$$\frac{d}{dt} \langle \alpha; f \rangle = \left\langle \frac{\partial \alpha}{\partial t} + \sum_{i=1}^N \left[\frac{p_i}{m_i} \cdot \nabla_{\mathbf{R}_i} \alpha + \nabla_{\mathbf{p}_i} U \cdot \nabla_{\mathbf{p}_i} \alpha \right] \right\rangle \quad (2.4)$$

By Green's theorem applied in the space of \mathbf{R}_i

$$\left\langle \frac{\partial \alpha}{\partial t} + \sum_{i=1}^N \left[\frac{p_i}{m_i} \cdot \nabla_{\mathbf{R}_i} \alpha + \nabla_{\mathbf{p}_i} U \cdot \nabla_{\mathbf{p}_i} \alpha \right] \right\rangle = \sum_{i=1}^N \int \dots \int \left[\frac{p_i}{m_i} \cdot \nabla_{\mathbf{R}_i} \alpha + \nabla_{\mathbf{p}_i} U \cdot \nabla_{\mathbf{p}_i} \alpha \right] f(\mathbf{R}_1, \dots, \mathbf{R}_N; \mathbf{p}_1, \dots, \mathbf{p}_N, t) d\mathbf{R}_1 \dots d\mathbf{R}_N d\mathbf{p}_1 \dots d\mathbf{p}_N \quad (2.5)$$

providing the integrated part vanishes, i.e., providing the system is bounded or f falls off sufficiently rapidly as $\mathbf{R}_i \rightarrow \infty$. Likewise, since $\nabla_{\mathbf{p}_i} U$ is independent of \mathbf{p}_i and since f falls off rapidly as $\mathbf{p}_i \rightarrow \infty$, we use Green's theorem in the momentum space and it yields

$$\frac{d}{dt} \langle \alpha; f \rangle = \sum_{i=1}^N \int \dots \int \left[\frac{p_i}{m_i} \cdot \nabla_{\mathbf{R}_i} \alpha + \nabla_{\mathbf{p}_i} U \cdot \nabla_{\mathbf{p}_i} \alpha \right] f(\mathbf{R}_1, \dots, \mathbf{R}_N; \mathbf{p}_1, \dots, \mathbf{p}_N, t) d\mathbf{R}_1 \dots d\mathbf{R}_N d\mathbf{p}_1 \dots d\mathbf{p}_N \quad (2.5)$$

Thus, (2.4) becomes

$$\frac{d}{dt} \langle \alpha; f \rangle = \sum_{i=1}^N \int \dots \int \left[\frac{p_i}{m_i} \cdot \nabla_{\mathbf{R}_i} \alpha + \nabla_{\mathbf{p}_i} U \cdot \nabla_{\mathbf{p}_i} \alpha \right] f(\mathbf{R}_1, \dots, \mathbf{R}_N; \mathbf{p}_1, \dots, \mathbf{p}_N, t) d\mathbf{R}_1 \dots d\mathbf{R}_N d\mathbf{p}_1 \dots d\mathbf{p}_N \quad (2.7)$$

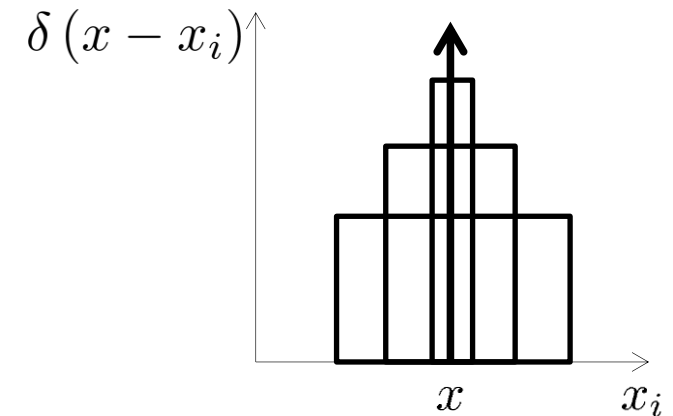
Consequently, $\langle \mathbf{p}_i \delta(\mathbf{R}_i - \mathbf{r}); f \rangle$ is the product of this mean momentum by the probability per unit volume that the i th molecule be at \mathbf{r} ; i.e., it is the contribution of the i th molecule to the momentum per unit volume (mass current density). The total momentum density

Selecting Functions

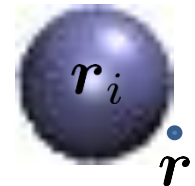
- **The Dirac delta selects molecules at a point**

- Infinitely high, infinitely thin peak
- Equivalent to the continuum differential formulation at a point

$$\rho(\mathbf{r}, t) = \sum_{i=1}^N \left\langle m_i \delta(\mathbf{r} - \mathbf{r}_i); f \right\rangle$$

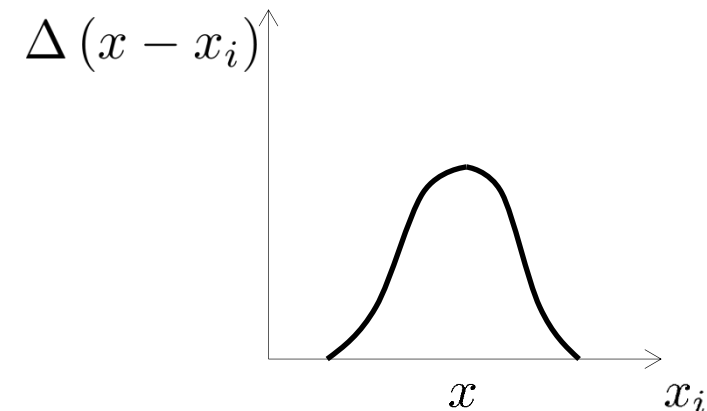


- **Cannot be applied directly in a molecular simulation as \mathbf{r}_i is never exactly equal to \mathbf{r}**



- **Relaxed weighting function used by Hardy(1981), Hoover (2009), Murdoch (2010) and others**

$$\rho(\mathbf{r}, t) \neq \sum_{i=1}^N \left\langle m_i \Delta(\mathbf{r} - \mathbf{r}_i); f \right\rangle$$



Eulerian Equations of Motion

More information

- Further details of mathematics and numerical simulations are available in the recently published paper in *Physical Review E*

PHYSICAL REVIEW E 85, 056705 (2012)

Control-volume representation of molecular dynamics

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A molecular dynamics (MD) parallel to the control volume (CV) formulation of fluid mechanics is developed by integrating the formulas of Irving and Kirkwood [J. Chem. Phys. 18, 817 (1950)] over a finite cubic volume of molecular dimensions. The Lagrangian molecular system is expressed in terms of an Eulerian CV, which yields an equivalent to Reynolds' transport theorem for the discrete system. This approach casts the dynamics of the molecular system into a form that can be readily compared to the continuum equations. The MD equations of motion are reinterpreted in terms of a Lagrangian-to-control-volume (\mathcal{LCV}) conversion function ϑ_i for each molecule i . The \mathcal{LCV} function and its spatial derivatives are used to express fluxes and relevant forces across the control surfaces. The relationship between the local pressures computed using the volume average [Lutsko, J. Appl. Phys. 64, 1152 (1988)] techniques and the method of planes [Todd *et al.*, Phys. Rev. E 52, 1627 (1995)] emerges naturally from the treatment. Numerical experiments using the MD CV method are reported for equilibrium and nonequilibrium (start-up Couette flow) model liquids, which demonstrate the advantages of the formulation. The CV formulation of the MD is shown to be exactly conservative and is, therefore, ideally suited to obtain macroscopic properties from a discrete system.

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PACS number(s): 05.20.-y, 47.11.Mn, 31.15.xv

Control Volume Function

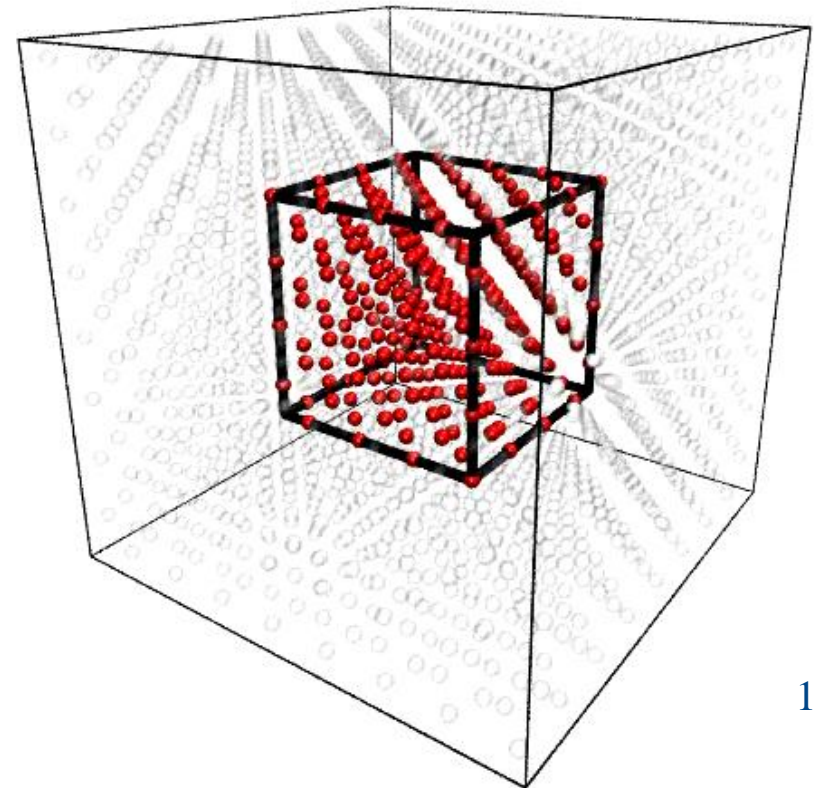
- The Control Volume function is the integral of the Dirac delta function in 3 Dimensions

$$\vartheta_i \equiv \int_{x^-}^{x^+} \int_{y^-}^{y^+} \int_{z^-}^{z^+} \delta(x_i - x) \delta(y_i - y) \delta(z_i - z) dx dy dz$$

$$= [H(x^+ - x_i) - H(x^- - x_i)]$$

$$\times [H(y^+ - y_i) - H(y^- - y_i)]$$

$$\times [H(z^+ - z_i) - H(z^- - z_i)]$$



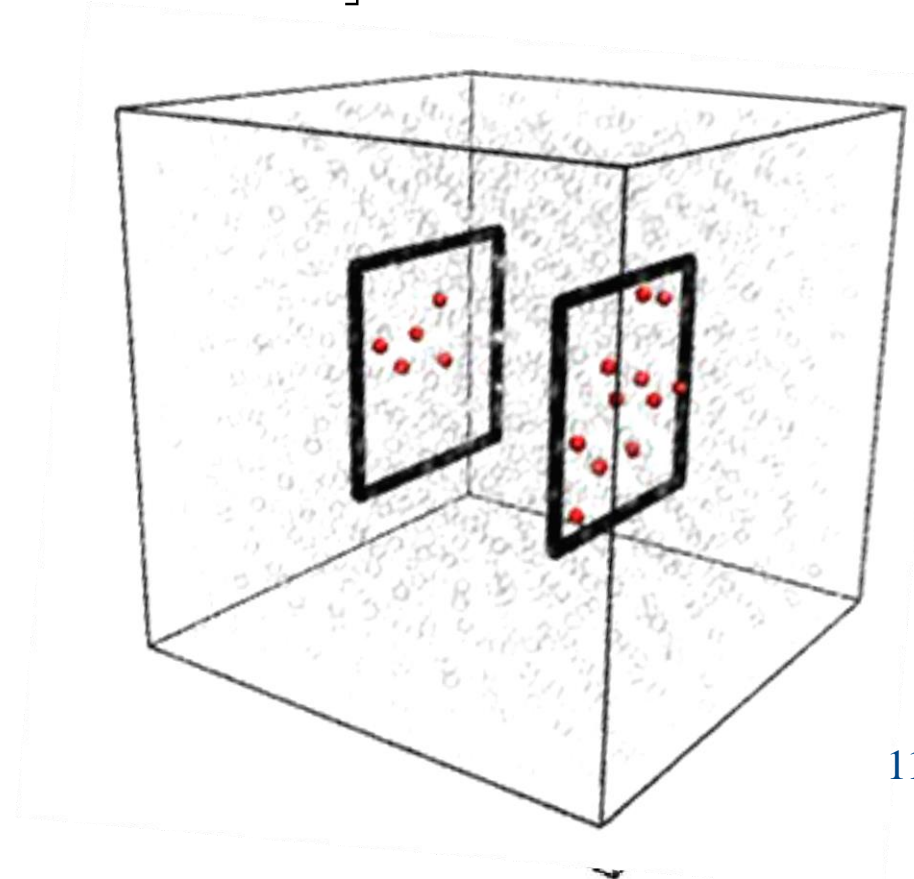
Derivatives yields the surface flux

- Taking the Derivative of the CV function

$$\begin{aligned} dS_{ix} &\equiv -\frac{\partial \vartheta_i}{\partial x_i} = [\delta(x^+ - x_i) - \delta(x^- - x_i)] \\ &\quad \times [H(y^+ - y_i) - H(y^- - y_i)] \\ &\quad \times [H(z^+ - z_i) - H(z^- - z_i)] \end{aligned}$$

- Surface fluxes over the top and bottom surface

$$dS_{ix} = dS_{ix}^+ - dS_{ix}^-$$



Applying the Control Volume Function

- Molecular mass in a control volume can be defined

$$\frac{\partial}{\partial t} \int_V \rho dV, t = \frac{\partial}{\partial t} \sum_{i=1}^N \left\langle m_i \vartheta_i(\mathbf{r}_i); f \right\rangle$$

- Simple mathematical operations using the control volume function

$$\begin{aligned} \frac{\partial}{\partial t} \sum_{i=1}^N \left\langle m_i \vartheta_i; f \right\rangle &= \sum_{i=1}^N \left\langle \frac{\mathbf{p}_i}{m_i} \cdot \frac{\partial m_i \vartheta_i}{\partial \mathbf{r}_i} - \mathbf{F}_i \cdot \frac{\partial m_i \vartheta_i}{\partial \mathbf{p}_i}; f \right\rangle \\ &= \sum_{i=1}^N \left\langle \mathbf{p}_i \cdot \frac{\partial \vartheta_i}{\partial \mathbf{r}_i}; f \right\rangle \\ &= - \sum_{i=1}^N \left\langle m_i \mathbf{v}_i \cdot d\mathbf{S}_i; f \right\rangle \end{aligned}$$

Reynolds' Transport Theorem

- Mass, momentum and energy equations

- Mass Conservation

$$\frac{d}{dt} \sum_{i=1}^N m_i \vartheta_i = - \sum_{i=1}^N m_i \mathbf{v}_i \cdot d\mathbf{S}_i$$

$$\frac{\partial}{\partial t} \int_V \rho dV = - \oint_S \rho \mathbf{u} \cdot d\mathbf{S}$$

- Momentum Balance

$$\begin{aligned} \frac{d}{dt} \sum_{i=1}^N m_i \mathbf{v}_i \vartheta_i = & - \sum_{i=1}^N m_i \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i \\ & + \sum_{i=1}^N \sum_{j \neq i}^N \mathbf{f}_{ij} \vartheta_{ij} \end{aligned}$$

$$\begin{aligned} \frac{\partial}{\partial t} \int_V \rho \mathbf{u} dV = & - \oint_S \rho \mathbf{u} \mathbf{u} \cdot d\mathbf{S} \\ & + \mathbf{F}_{\text{surface}} \end{aligned}$$

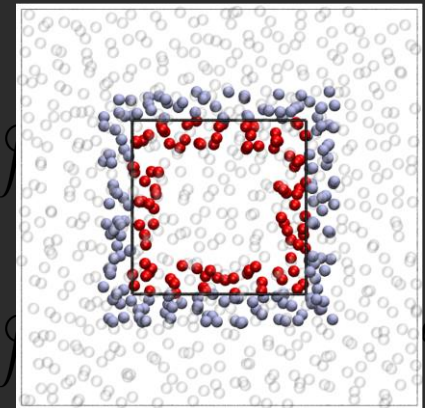
- The difference between two control volume functions for i and j

$$\frac{d}{dt} \sum_{i=1}^N e_i \vartheta_i = - \sum_{i=1}^N e_i \mathbf{v}_i \cdot d\mathbf{S}_i$$

$$\vartheta_{ij} \equiv \vartheta_i - \vartheta_j$$

$$+ \frac{1}{2} \sum_{i=1}^N \sum_{i \neq j}^N \frac{\mathbf{p}_i}{m_i} \cdot \mathbf{f}_{ij} \vartheta_{ij}$$

$$\frac{\partial}{\partial t} \int_V \rho \mathcal{E} dV = - \oint_S \rho \mathcal{E} \mathbf{u} \cdot d\mathbf{S} + \dots$$

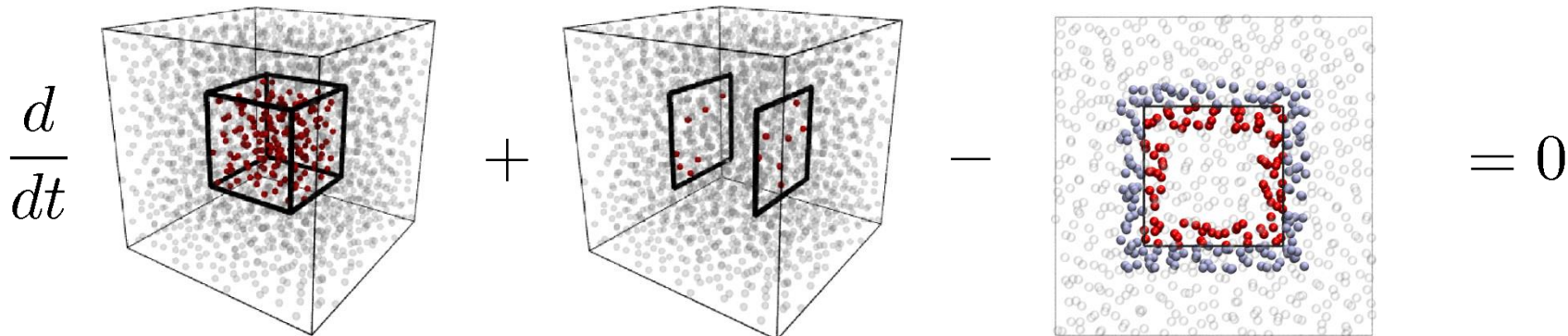


dS

Testing Momentum Balance

• Momentum Balance

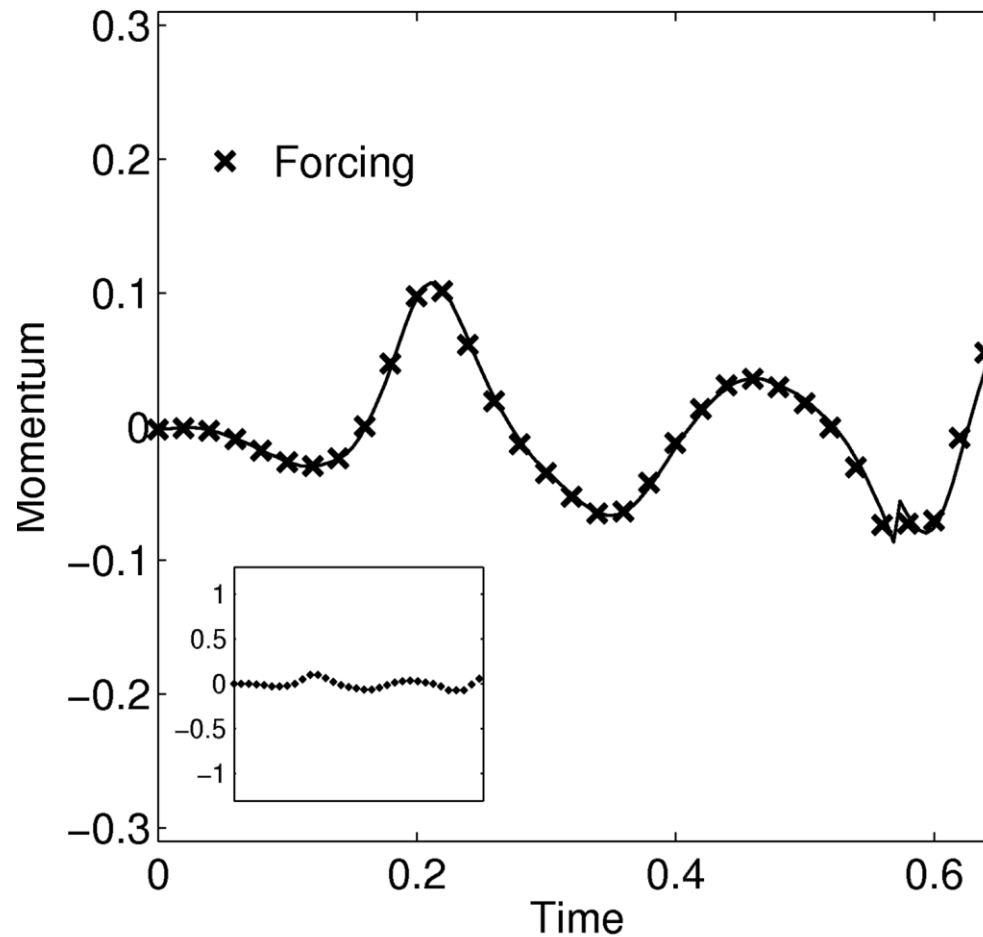
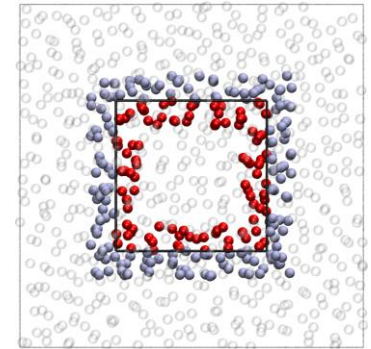
$$\underbrace{\frac{d}{dt} \sum_{i=1}^N m_i \dot{\mathbf{r}}_i \vartheta_i}_{\text{Accumulation}} + \underbrace{\sum_{i=1}^N m \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i}_{\text{Advection}} - \underbrace{\sum_{i=1}^N \sum_{j \neq i}^N \mathbf{f}_{ij} \vartheta_{ij}}_{\text{Forcing}} = 0$$



Testing Momentum Balance

- Momentum Balance

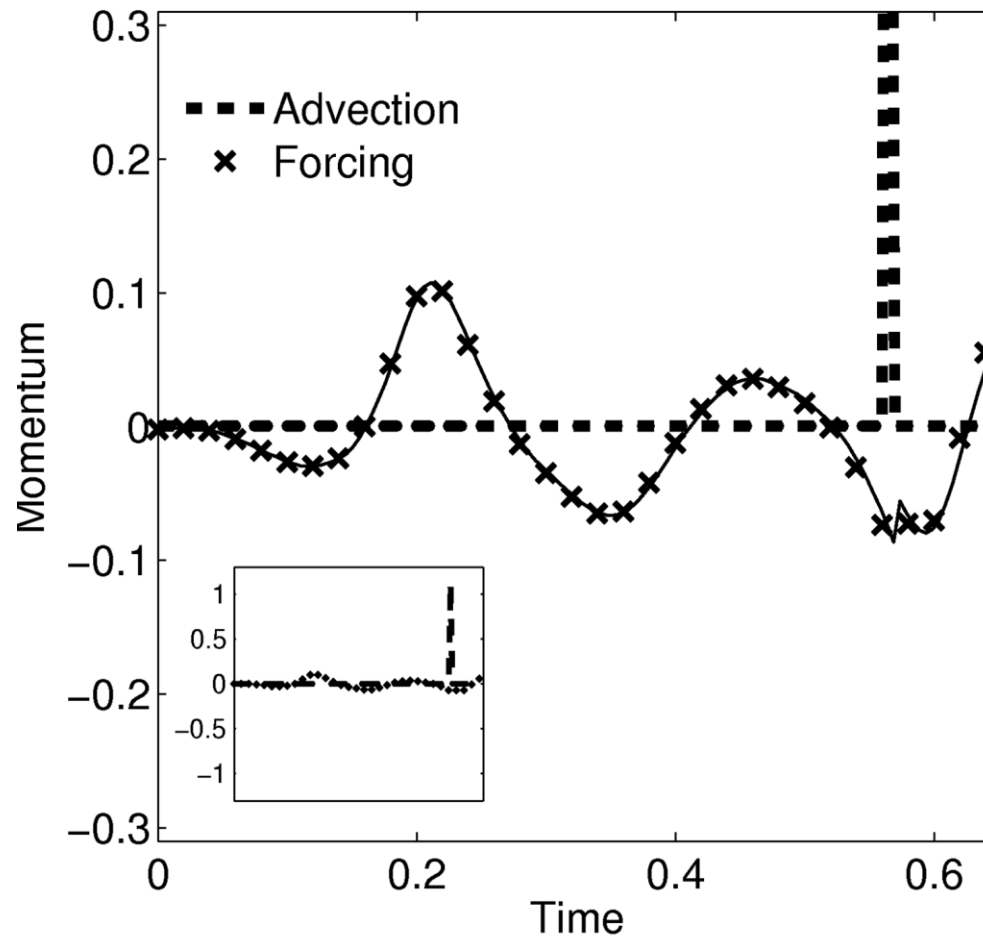
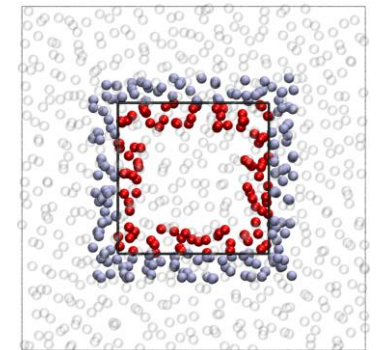
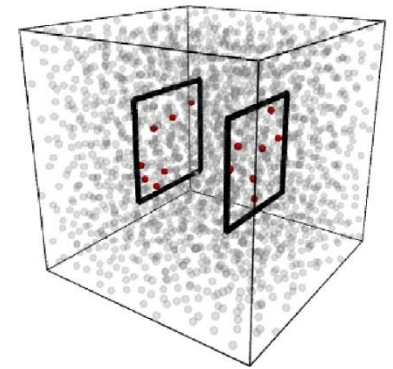
$$\underbrace{\sum_{i=1}^N \sum_{j \neq i}^N \mathbf{f}_{ij} \vartheta_{ij}}_{\text{Forcing}}$$



Testing Momentum Balance

• Momentum Balance

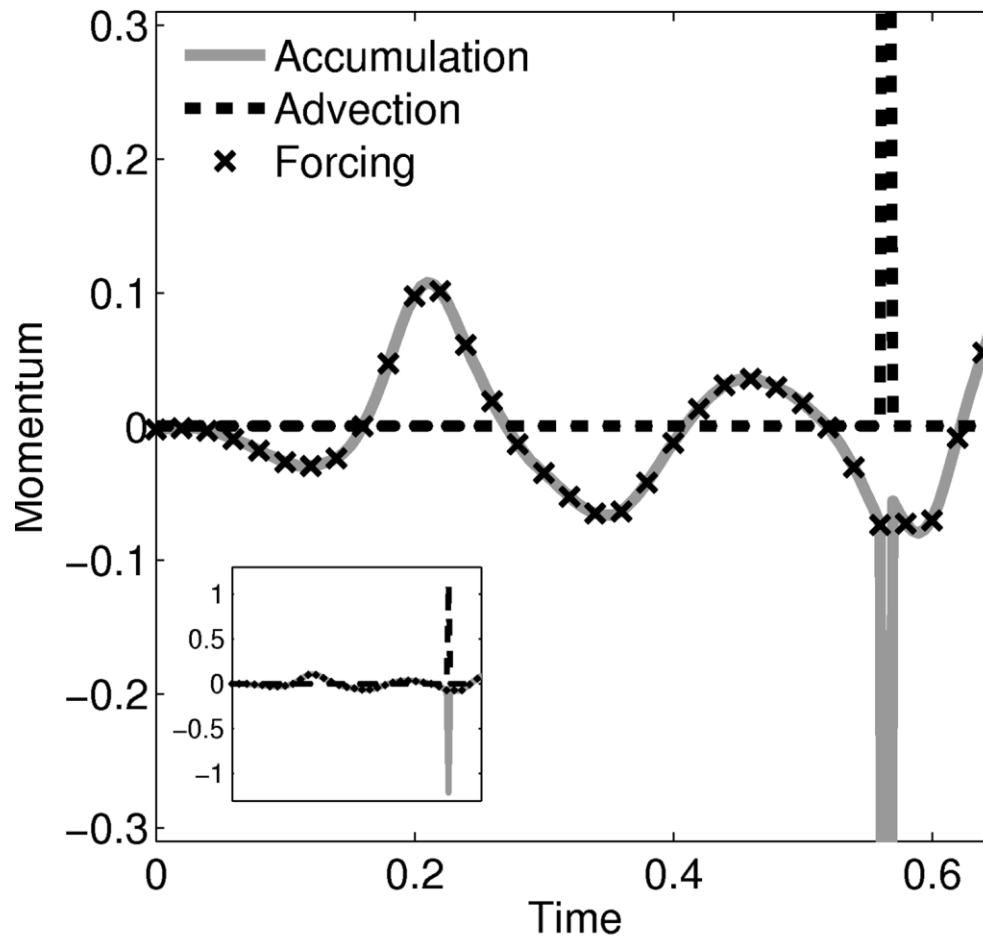
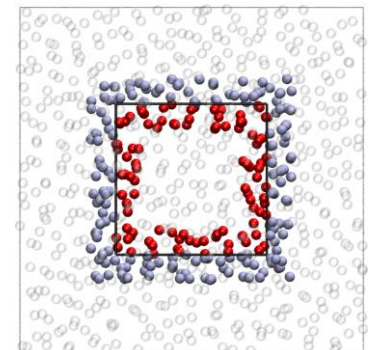
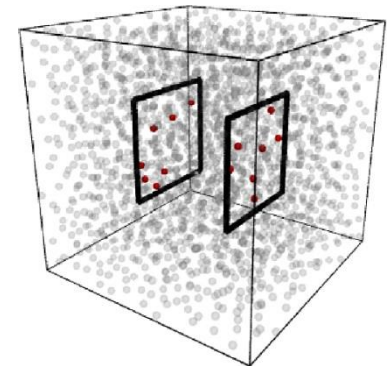
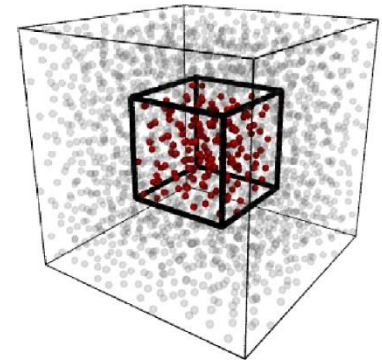
$$-\underbrace{\sum_{i=1}^N m_i \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i}_{\text{Advection}} + \underbrace{\sum_{i=1}^N \sum_{j \neq i}^N \mathbf{f}_{ij} \vartheta_{ij}}_{\text{Forcing}}$$



Testing Momentum Balance

• Momentum Balance

$$\underbrace{\frac{d}{dt} \sum_{i=1}^N m_i \mathbf{v}_i \vartheta_i}_{\text{Accumulation}} = - \underbrace{\sum_{i=1}^N m_i \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i}_{\text{Advection}} + \underbrace{\sum_{i=1}^N \sum_{j \neq i}^N \mathbf{f}_{ij} \vartheta_{ij}}_{\text{Forcing}}$$

 $\frac{d}{dt}$


Divergence of Pressure

- The momentum balance equation can be re-written in terms of the divergence of pressure

- Momentum Balance

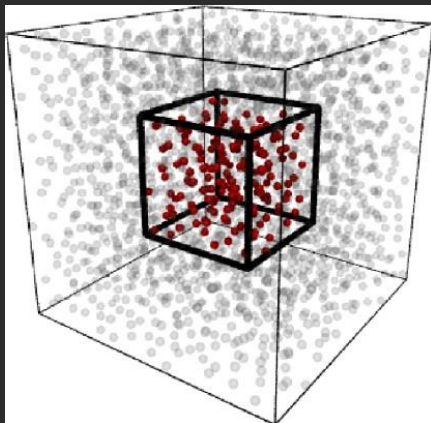
$$\frac{d}{dt} \sum_{i=1}^N m_i \mathbf{v}_i \vartheta_i = - \int_{V_1}^N \frac{\partial}{\partial \mathbf{r}} \cdot \rho \mathbf{u} d\mathbf{S}_i$$

$$\frac{\partial}{\partial t} \int_V \rho \mathbf{u} dV = - \oint_{\partial V} \frac{\partial}{\partial \mathbf{r}} \rho \mathbf{u} \cdot d\mathbf{S}$$

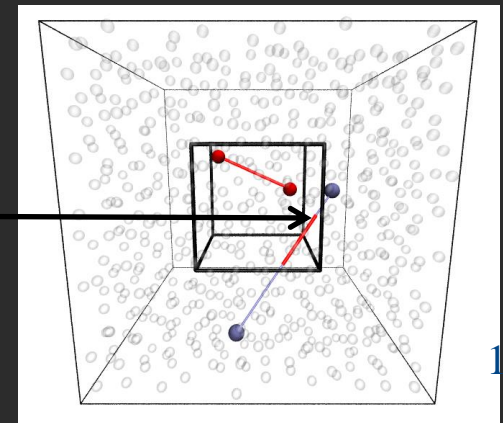
$$- \frac{\partial}{\partial \mathbf{r}} \cdot \sum_{i=1}^N \left[(\mathbf{v}_i - \mathbf{u}) + \sum_{i=1}^N \sum_{j \neq i} \mathbf{f}_{ij} \vartheta_{ij} + \sum_{j \neq i} \mathbf{f}_{ij} \mathbf{r}_{ij} \int_0^1 \vartheta_s ds \right]$$

$$+ \int_V \frac{\partial}{\partial \mathbf{r}} \Pi dV$$

- Volume Average Form of Lutsko (1988) & Cormier et al (2001)



$$\vartheta_{ij} = \sum_{\alpha=1}^3 \frac{\partial}{\partial r_\alpha} \int_0^1 \vartheta_s ds$$



Surface Pressures

- The momentum balance equation can be re-written in terms of pressure over the control volume surfaces

- Momentum Balance

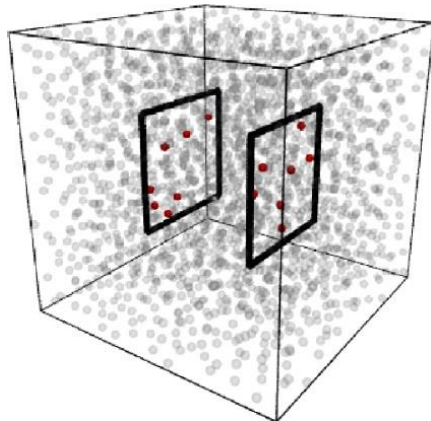
$$\frac{d}{dt} \sum_{i=1}^N m_i \mathbf{v}_i \vartheta_i = - \oint_S \rho \mathbf{u} \mathbf{u} \cdot d\mathbf{S}$$

$$\frac{\partial}{\partial t} \int_V \rho \mathbf{u} dV = - \oint_S \rho \mathbf{u} \mathbf{u} \cdot d\mathbf{S}$$

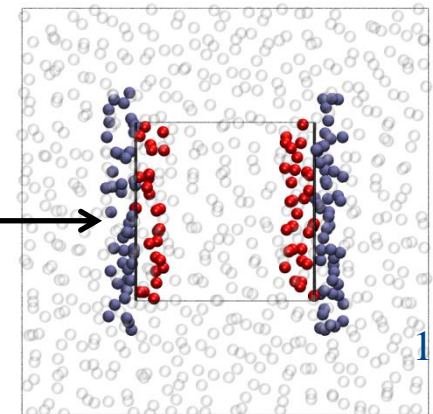
$$-\frac{\partial}{\partial r} \cdot \left[\sum_{i=1}^N \sum_{j=1}^N \left[(\mathbf{v}_i - \mathbf{u})(\mathbf{v}_i - \mathbf{u}) \vartheta_i d\mathbf{S}_i \sum_{j \neq i}^N \sum_{i=1}^N \sum_{j \neq i}^N \int_0^1 f_{ij} r_{ij} \int_{ij} \vartheta_s d\mathbf{S}_{ij} \right] \right]$$

$$- \int_V \nabla \cdot \left[\frac{\partial \mathbf{H}}{\partial r} \cdot d\mathbf{S} \right] dV$$

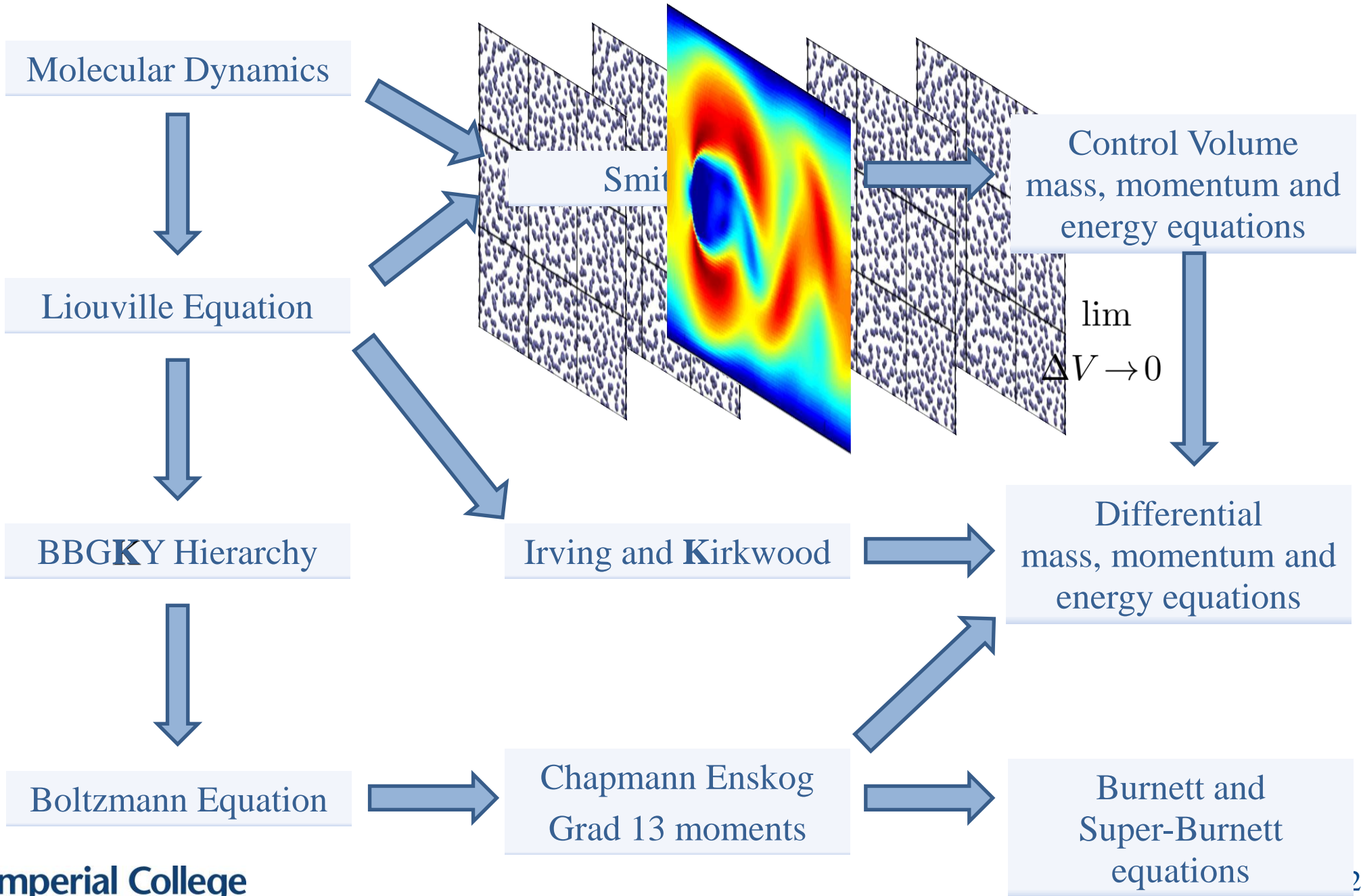
- The derivative of ϑ_s is the forces acting over the surface
a localisation of the method of planes (Todd et al 1995)



$$\vartheta_{ij} = \sum_{\alpha=1}^3 \frac{\partial}{\partial r_{\alpha}} \int_0^1 \vartheta_s ds = dS_{xij} + dS_{yij} + dS_{zij}$$



Relationship to the Boltzmann Equation



Results and Applications

Unsteady Couette Flow

Continuum Analytical

- Simplify the momentum balance (Navier-Stokes) equation

$$\frac{\partial}{\partial t} \mathbf{u} + \cancel{\nabla \cdot \mathbf{u} \mathbf{u}} = \frac{1}{\rho} \cancel{\nabla P} + \frac{\mu}{\rho} \nabla^2 \mathbf{u}$$

- Solve the 1D unsteady diffusion equation.

$$\frac{\partial u_x}{\partial t} = \frac{\mu}{\rho} \frac{\partial^2 u_x}{\partial y^2}$$

- With Boundary Conditions

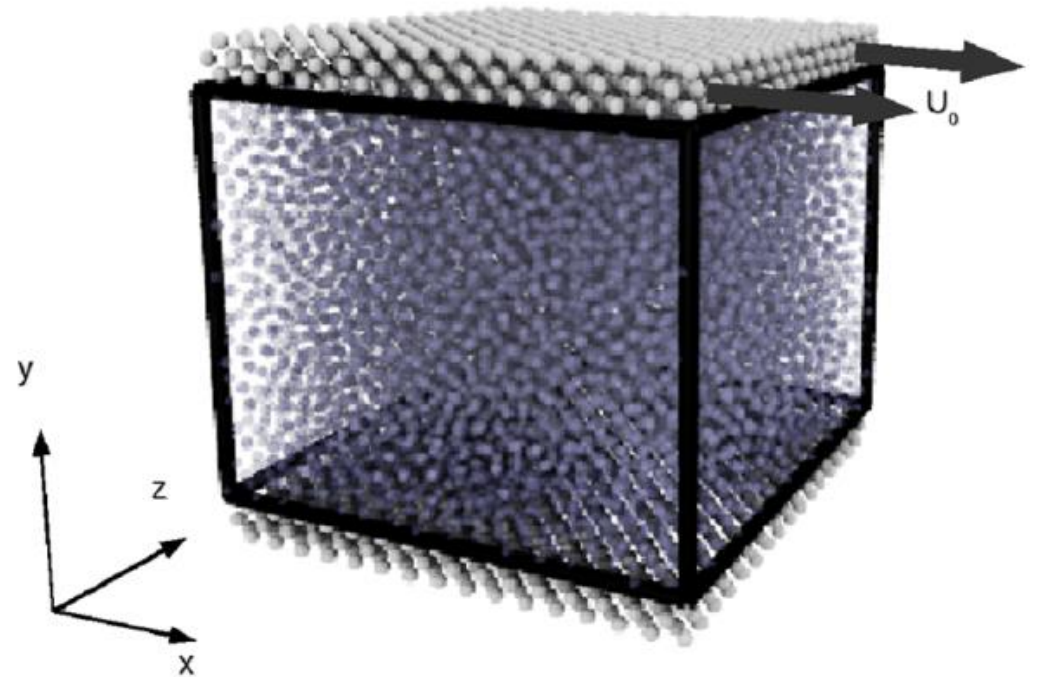
$$u_x(0, t) = 0$$

$$u_x(L, t) = U_0$$

$$u_x(y, 0) = 0$$

Molecular Dynamics

- Fixed bottom wall, sliding top wall with both thermostatted



Unsteady Couette Flow

Continuum Analytical

- Simplify the control volume momentum balance equation

$$\frac{\partial}{\partial t} \int_V \rho \mathbf{u} dV = - \oint_S \rho \mathbf{u} \mathbf{u} \cdot d\mathbf{S} - \oint_S P \mathbf{I} \cdot d\mathbf{S} + \oint_S \boldsymbol{\sigma} \cdot d\mathbf{S}$$

- Simplifies for a single control volume

$$\frac{\partial}{\partial t} \int_V \rho u_x dV = \int_{S_y^+} \sigma_{xy} dS_f^+ - \int_{S_y^-} \sigma_{xy} dS_f^-$$

- With Boundary Conditions

$$u_x(0, t) = 0$$

$$u_x(L, t) = U_0$$

$$u_x(y, 0) = 0$$

Molecular Dynamics

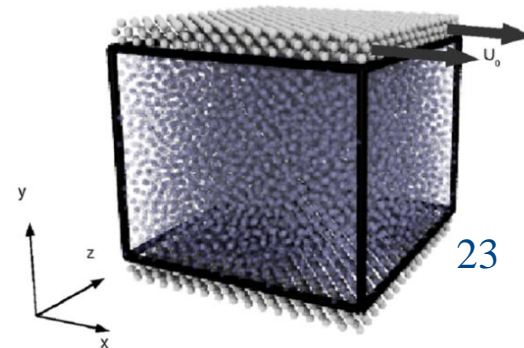
- Discrete form of the Momentum balance equation

$$\frac{d}{dt} \sum_{i=1}^N m_i \mathbf{v}_i \vartheta_i = - \oint_S \rho \mathbf{u} \mathbf{u} \cdot d\mathbf{S} - \sum_{i=1}^N (\mathbf{v}_i - \mathbf{u})(\mathbf{v}_i - \mathbf{u}) \cdot d\mathbf{S}_i - \sum_{i=1}^N \sum_{j \neq i}^N \zeta_{ij} \cdot d\mathbf{S}_{ij}$$

- Simplifies for a single control volume

$$\frac{d}{dt} \sum_{i=1}^N m_i \mathbf{v}_i \vartheta_i = \sum_{i,j} f_{xij} dS_{yij}^+ - \sum_{i,j} f_{xij} dS_{yij}^-$$

- Fixed bottom wall, sliding top wall with both thermostatted



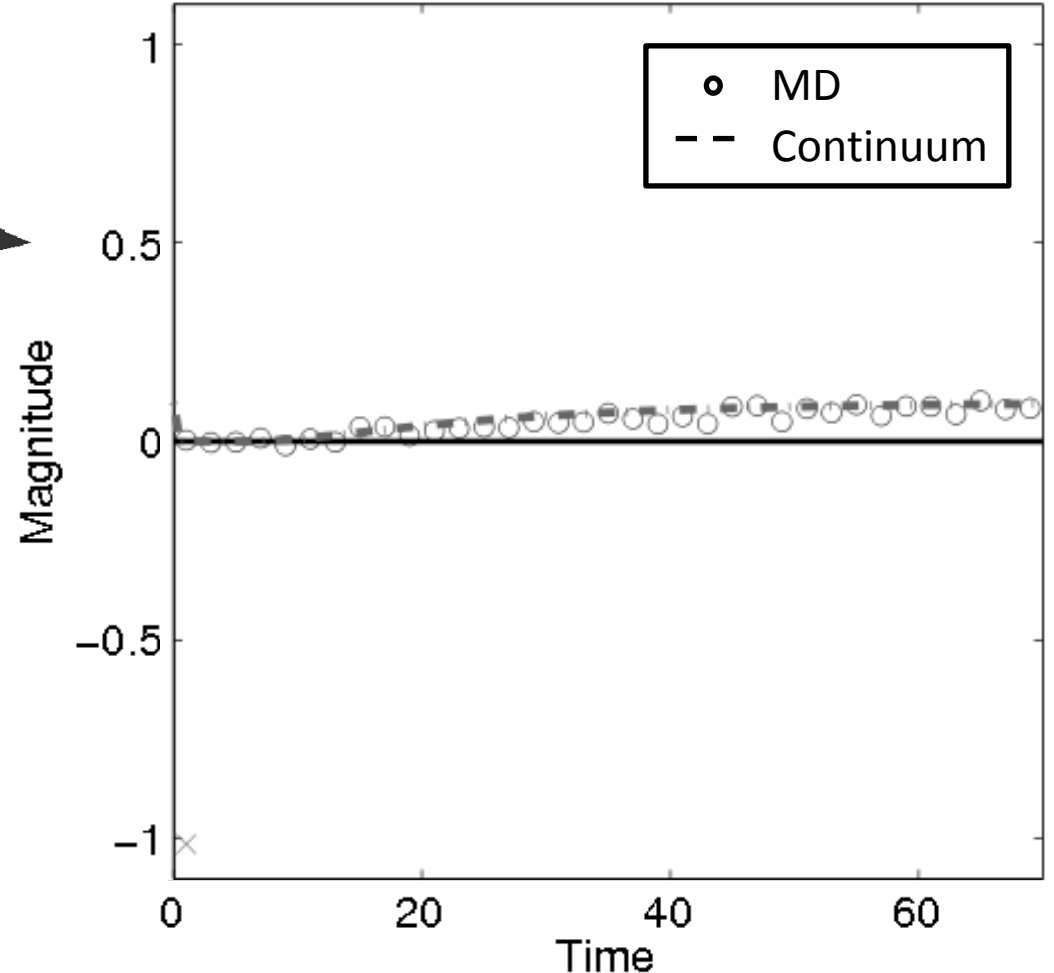
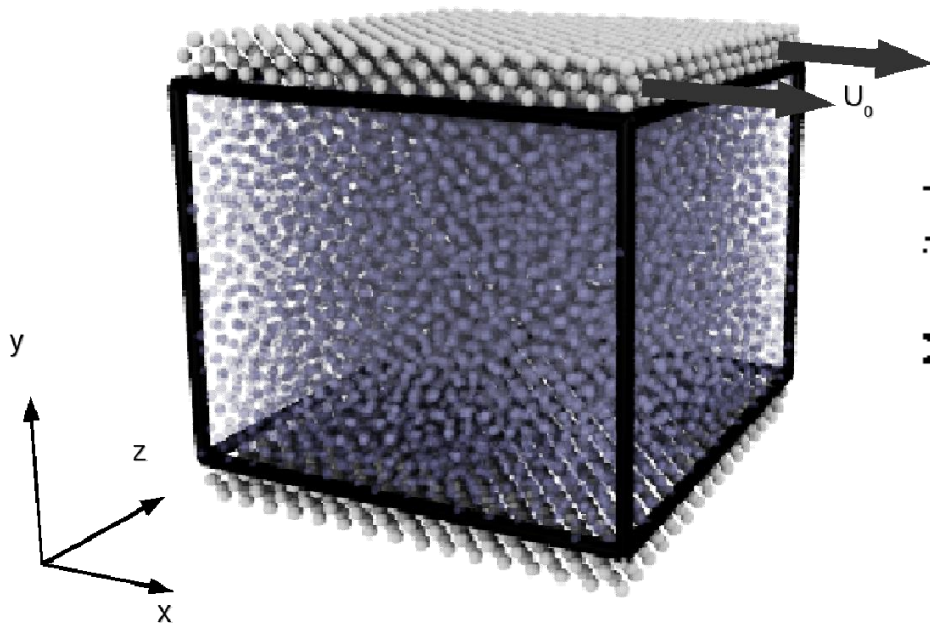
Unsteady Couette Flow

Simulation setup

- Starting Couette flow
- Wall thermostat: Nosé-Hoover
- Averages are computed over 1000 time steps and 8 realizations

$$\frac{d}{dt} \sum_{i=1}^N m_i \mathbf{v}_i \vartheta_i = \sum_{i,j} f_{xij} dS_{yij}^+ - \sum_{i,j} f_{xij} dS_{yij}^-$$

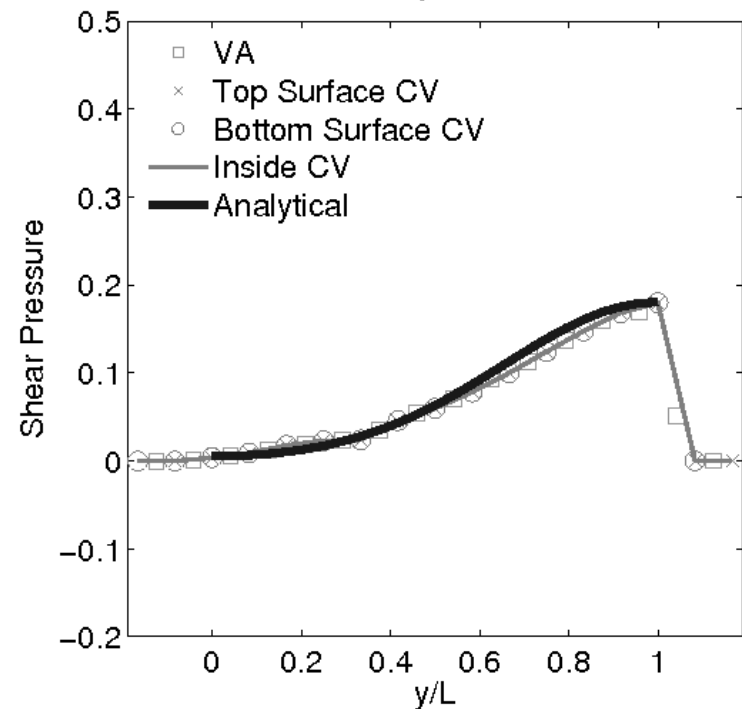
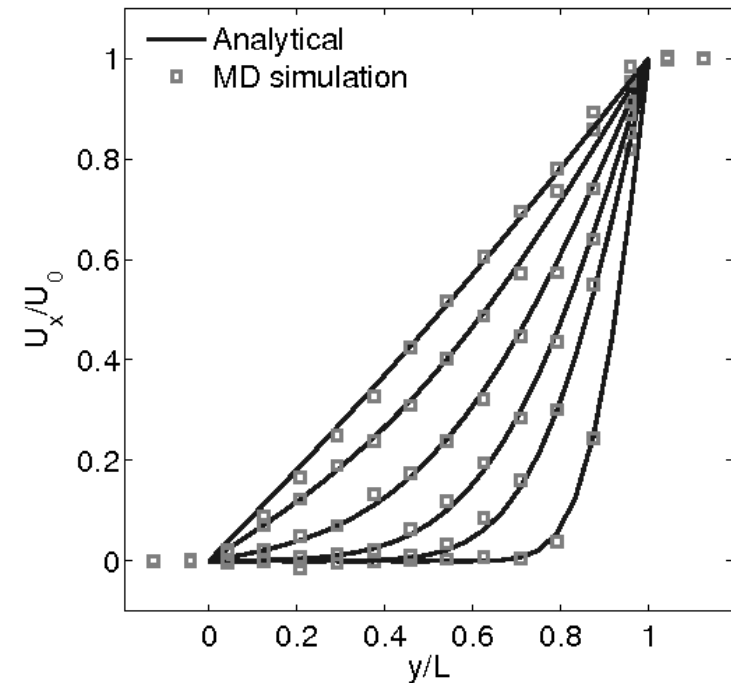
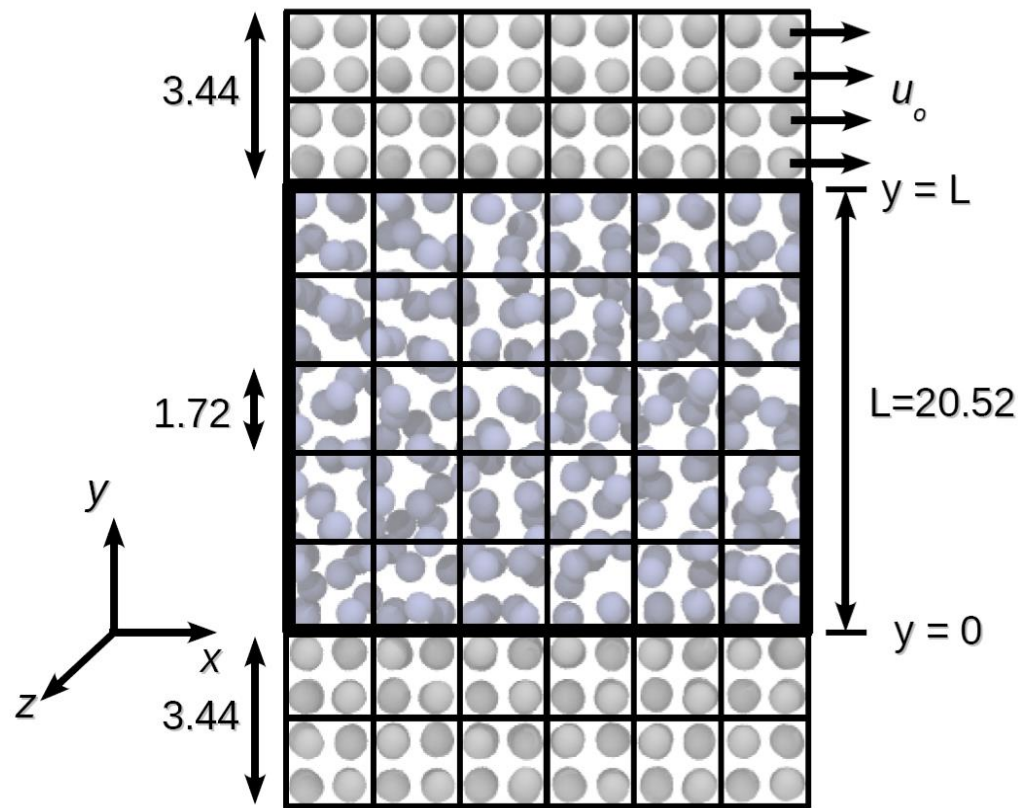
$$\frac{\partial}{\partial t} \int_V \rho u_x dV = \int_{S_f^+} \Pi_{xy} dS_f^+ - \int_{S_f^-} \Pi_{xy} dS_f^-$$



Unsteady Couette Flow

Simulation setup

- Starting Couette flow
- Wall thermostat: Nosé-Hoover
- Averages are computed over 1000 time steps and 8 realizations



Coupling

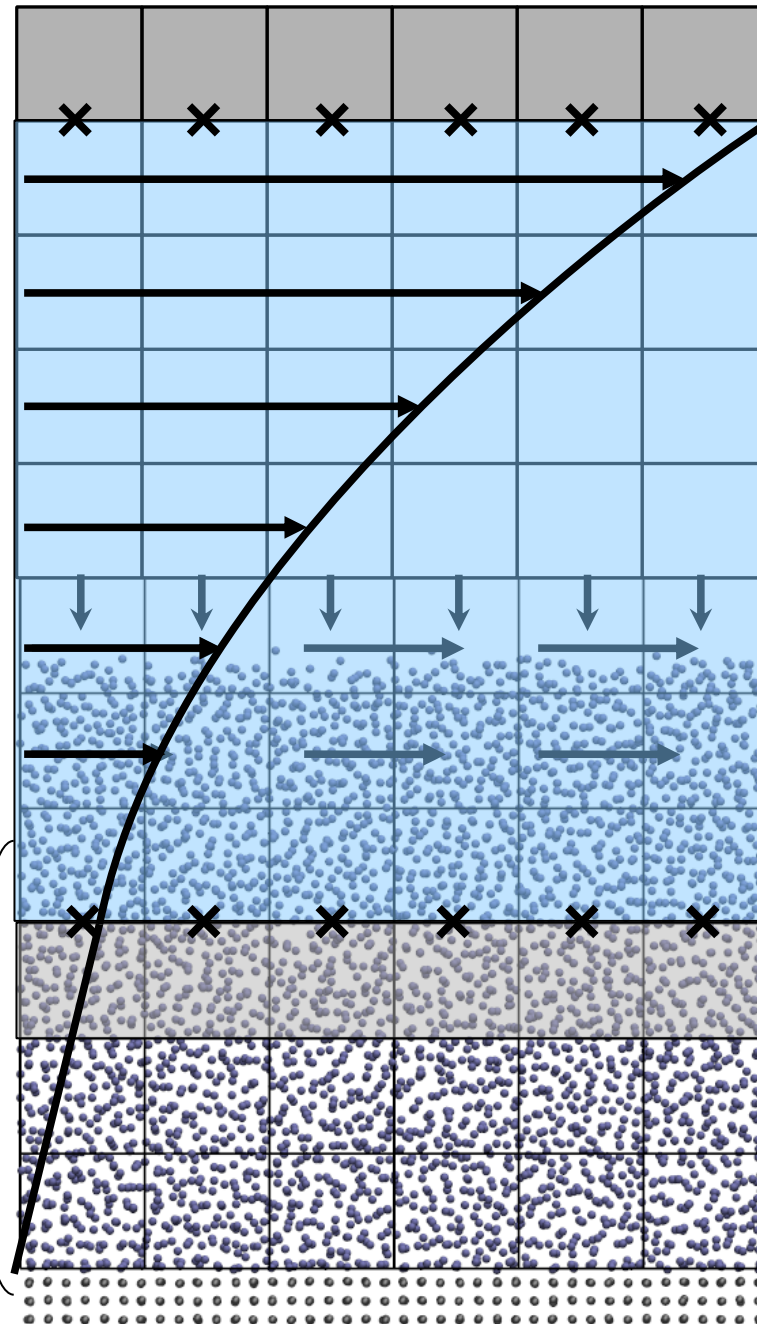
$$\frac{d}{dt} \sum_{i=1}^N m_i \mathbf{v}_i \vartheta_i = - \oint_S \rho \mathbf{u} \mathbf{u} \cdot d\mathbf{S}$$

$$- \sum_{i=1}^N (\mathbf{v}_i - \mathbf{u}) (\mathbf{v}_i - \mathbf{u}) \cdot d\mathbf{S}_i$$

$$- \sum_{i=1}^N \sum_{j \neq i}^N \mathbf{S}_{ij} \cdot d\mathbf{S}_{ij}$$

• **Molecular Equations**

$$m \ddot{\mathbf{r}}_i = \sum_{j \neq i}^N \mathbf{f}_{ij}$$



$$\rho \mathbf{u} = \rho \mathbf{U}_0$$

• **Continuum Equations**

$$\frac{\partial}{\partial t} \int_V \rho \mathbf{u} dV = - \oint_S \rho \mathbf{u} \mathbf{u} \cdot d\mathbf{S}$$

$$- \oint_S \mathbf{\Pi} \cdot d\mathbf{S}$$

Summary

- **Introduced a novel mathematical function to defines a control volume in a discrete system**
 - Derived in a manner consistent with a continuum form of the control volume
 - Mathematically well defined and applicable to any discrete system
- **Reynolds' transport theorem is extended beyond the continuum**
 - Allows control volume analysis to be extended to nano-scale systems
 - The resulting equations are exactly conservative in a discrete system
- **The resulting formulation has a number of applications**
 - Give a consistent and intuitive form of molecular pressure - connecting two widely used descriptions in the literature
 - Semi-analytical solution to problems like Couette flow
 - Facilitates a rigorous derivation of coupling strategies

References/Acknowledgments

• References

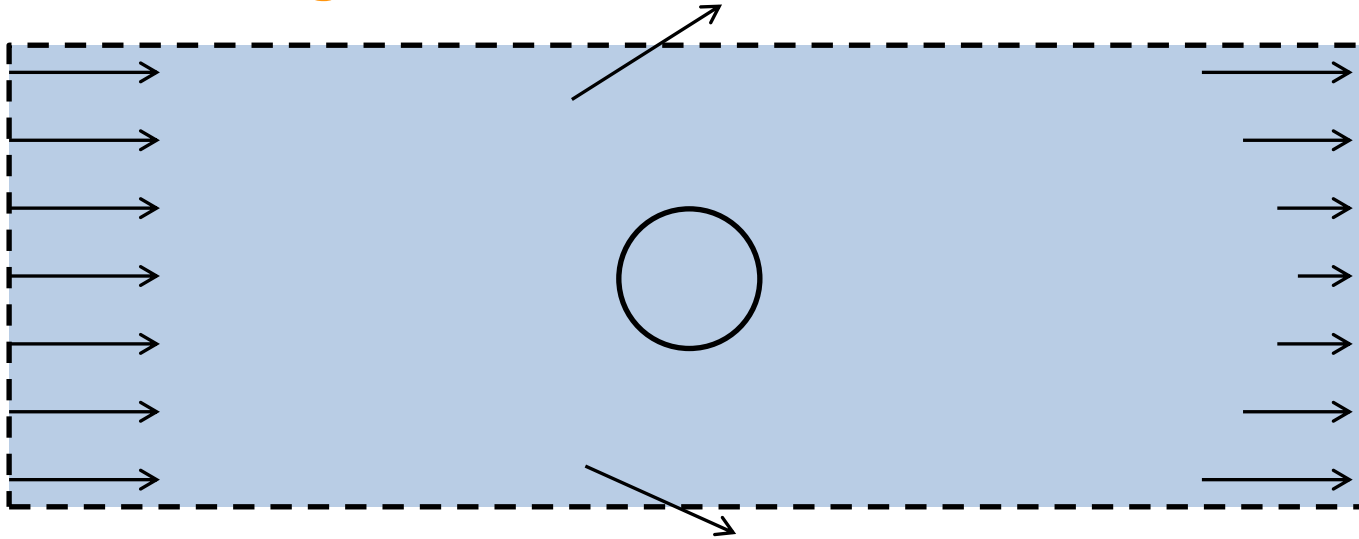
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• **Thank you for listening**

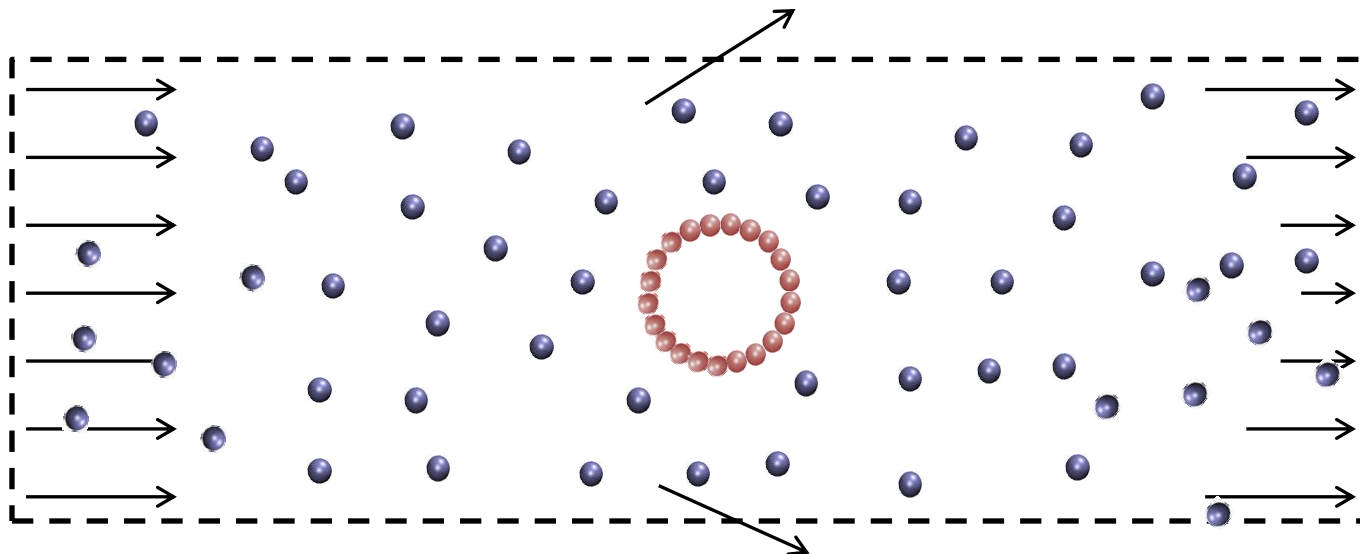
• **Any Questions?**

Flow past a cylinder

- Use of the momentum conservation of the control volume to determine the drag coefficient

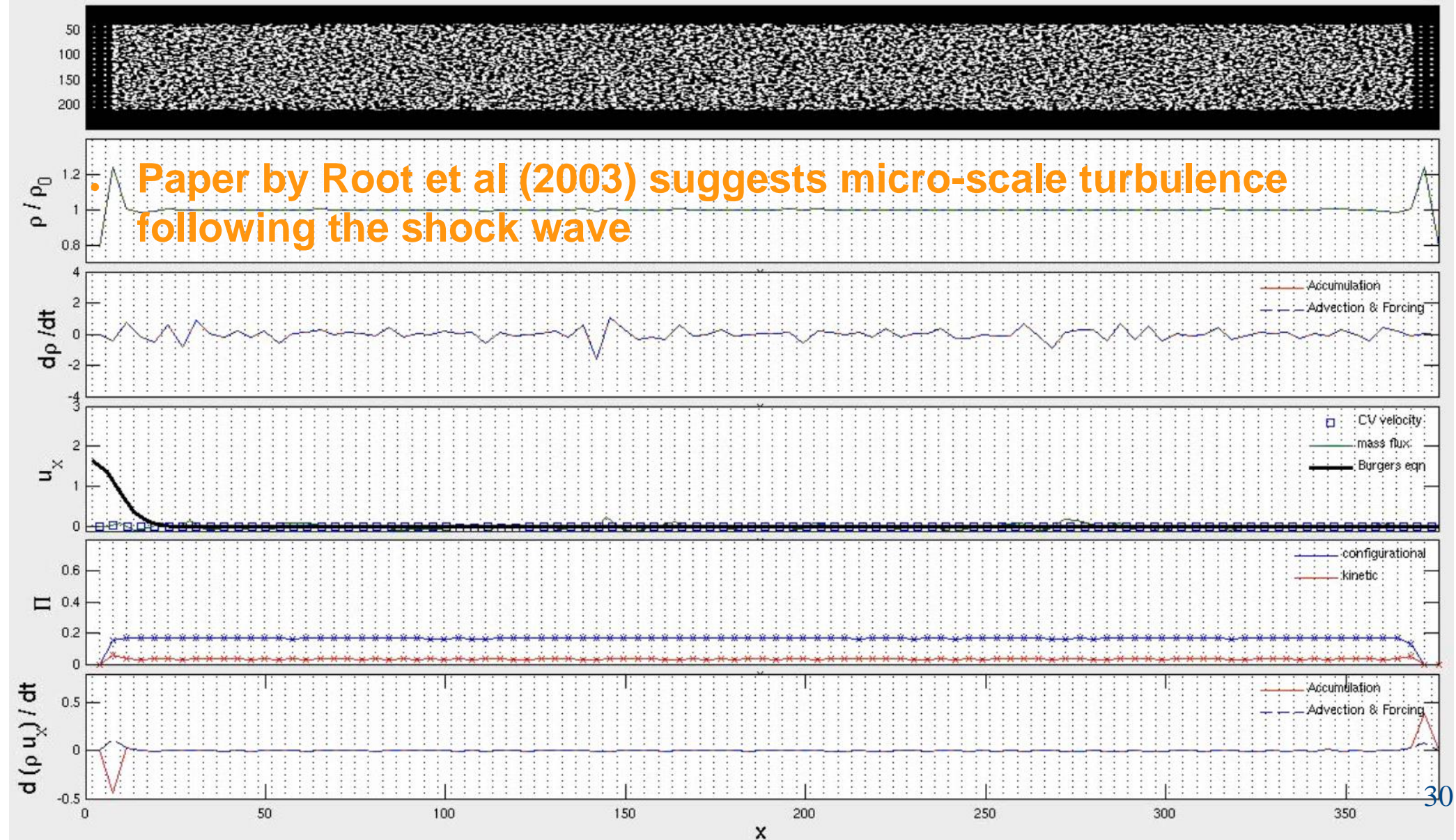


- Drag over a Carbon Nano-tube can be determined

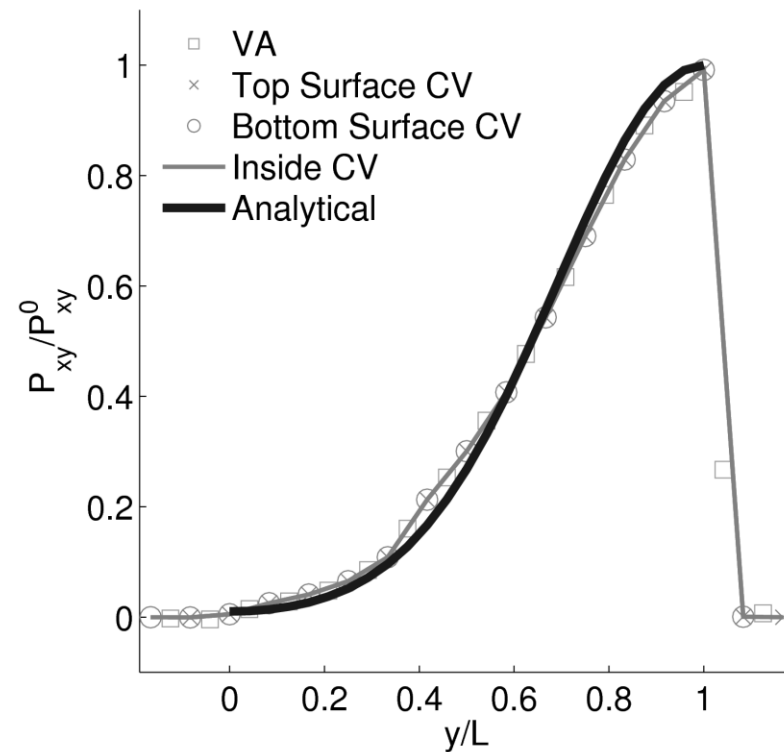
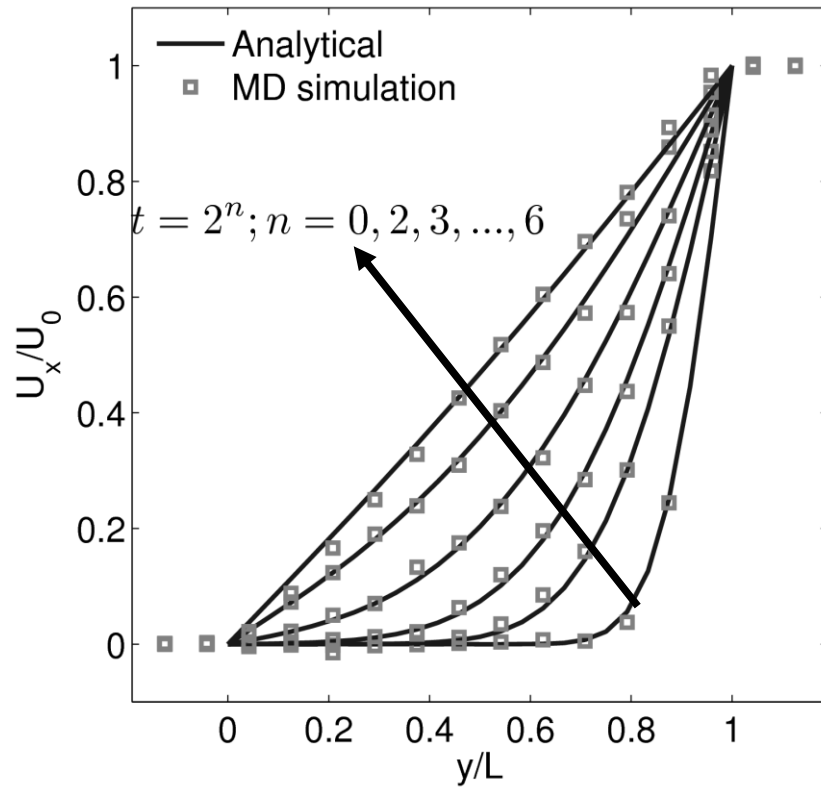


Shockwaves

- Current work on application of control volume theory



Continuum Analytical Couette Flow



$$u_x(y, t) = \begin{cases} U_0 & y = L \\ \sum_{n=1}^{\infty} u_n(t) \sin\left(\frac{n\pi y}{L}\right) & 0 < y < L \\ 0 & y = 0 \end{cases}$$

$$\Pi_{xy}(y, t) = \frac{\mu U_0}{L} \left[1 + 2 \sum_{n=1}^{\infty} (-1)^n e^{-\frac{\lambda_n \mu t}{\rho}} \cos\left(\frac{n\pi y}{L}\right) \right]$$

Where, $\lambda_n = \left(\frac{n\pi}{L}\right)^2$ and $u_n(t) = \frac{2U_0(-1)^n}{n\pi} \left(e^{-\frac{\lambda_n \mu t}{\rho}} - 1\right)$

Moving reference frame

- Why the continuum form of Reynolds' transport theorem has a partial derivative but the discrete is a full derivative

- Eulerian mass conservation

$$\vartheta_i = \vartheta_i(\mathbf{r}_i(t), \mathbf{r})$$

$$\frac{d}{dt} \sum_{i=1}^N m_i \vartheta_i = - \sum_{i=1}^N m_i \mathbf{v}_i \cdot d\mathbf{S}_i$$

$$\frac{\partial}{\partial t} \int_V \rho dV = - \oint_S \rho \mathbf{u} \cdot d\mathbf{S}$$

- Lagrangian mass conservation

$$\vartheta_i = \vartheta_i(\mathbf{r}_i(t), \mathbf{r}(t))$$

$$\frac{d}{dt} \sum_{i=1}^N m_i \vartheta_i = - \sum_{i=1}^N m_i (\mathbf{v}_i + \bar{\mathbf{u}}) \cdot d\mathbf{S}_i$$

$$\frac{d}{dt} \int_V \rho dV = \oint_S \rho (\mathbf{u} - \bar{\mathbf{u}}) \cdot d\mathbf{S}$$

$$\bar{\mathbf{u}} \cdot d\mathbf{S}_i = \frac{d\mathbf{r}}{dt} \cdot \frac{d\vartheta_i}{d\mathbf{r}}$$

$$\oint_S \rho \mathbf{u} \cdot d\mathbf{S} - \oint_S \rho \bar{\mathbf{u}} \cdot d\mathbf{S} = 0$$