Connecting Continuous and Discrete Systems using Control Volume

Edward Smith

Collaborating with:
D. M. Heyes, D. Dini, T. A. Zaki

Mechanical Engineering
Imperial College London

Imperial College London

Outline

- **Introduction**
  - Continuum Mechanics & Molecular Dynamics
  - Selecting function and Irving and Kirkwood (1950)
  - Control Volume form
- **The Control Volume Function**
  - Discrete Reynolds' transport theorem
  - Governing equations
  - Applying the method to state coupling
- **Flux Coupling and the Pressure Tensor**
  - Derivation of the flux form of the control volume equations
  - Pressure tensor
  - Coupling fluxes

Introduction

Continuum vs. Discrete

- **Assumed Continuous at every point in space**
  - Mass Conservation

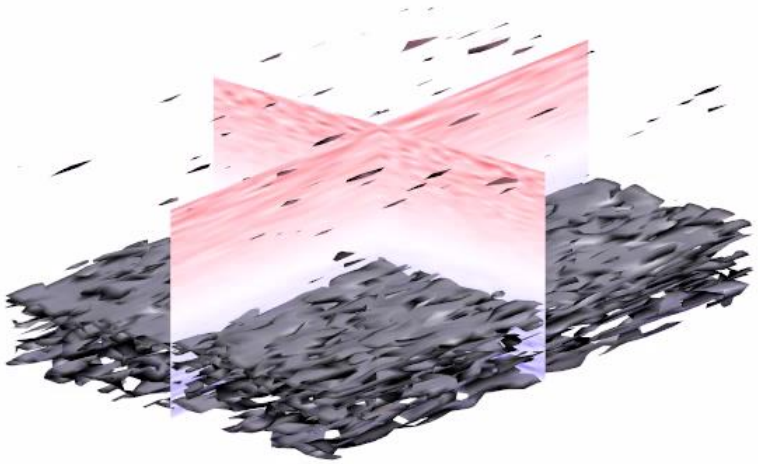
$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot \rho \boldsymbol{u}$$

  - Momentum Balance (Newton's Law)

$$\frac{\partial}{\partial t} \rho \boldsymbol{u} + \boldsymbol{\nabla} \cdot \rho \boldsymbol{u} \boldsymbol{u} = \boldsymbol{\nabla} \cdot \boldsymbol{\Pi}$$

  - Energy Conservation

$$\frac{\partial}{\partial t} \rho \mathcal{E} dV = -\boldsymbol{\nabla} \cdot [\rho \mathcal{E} \boldsymbol{u} + \boldsymbol{\Pi} \cdot \boldsymbol{u} + \mathbf{q}]$$

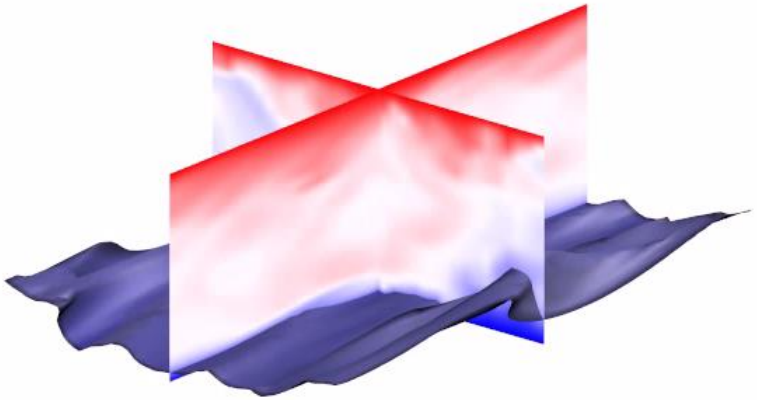


Direct Numerical Simulation of Turbulent Couette Flow

Continuum vs. Discrete

- **Discrete Molecules in continuous space**
  - Governed by Newton's Law for an N-body system
  - Point particles with pairwise interactions

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



Molecular Dynamics Simulation of Couette Flow

- **Average required to obtain the continuous field**
  - How do we get an Eulerian description?

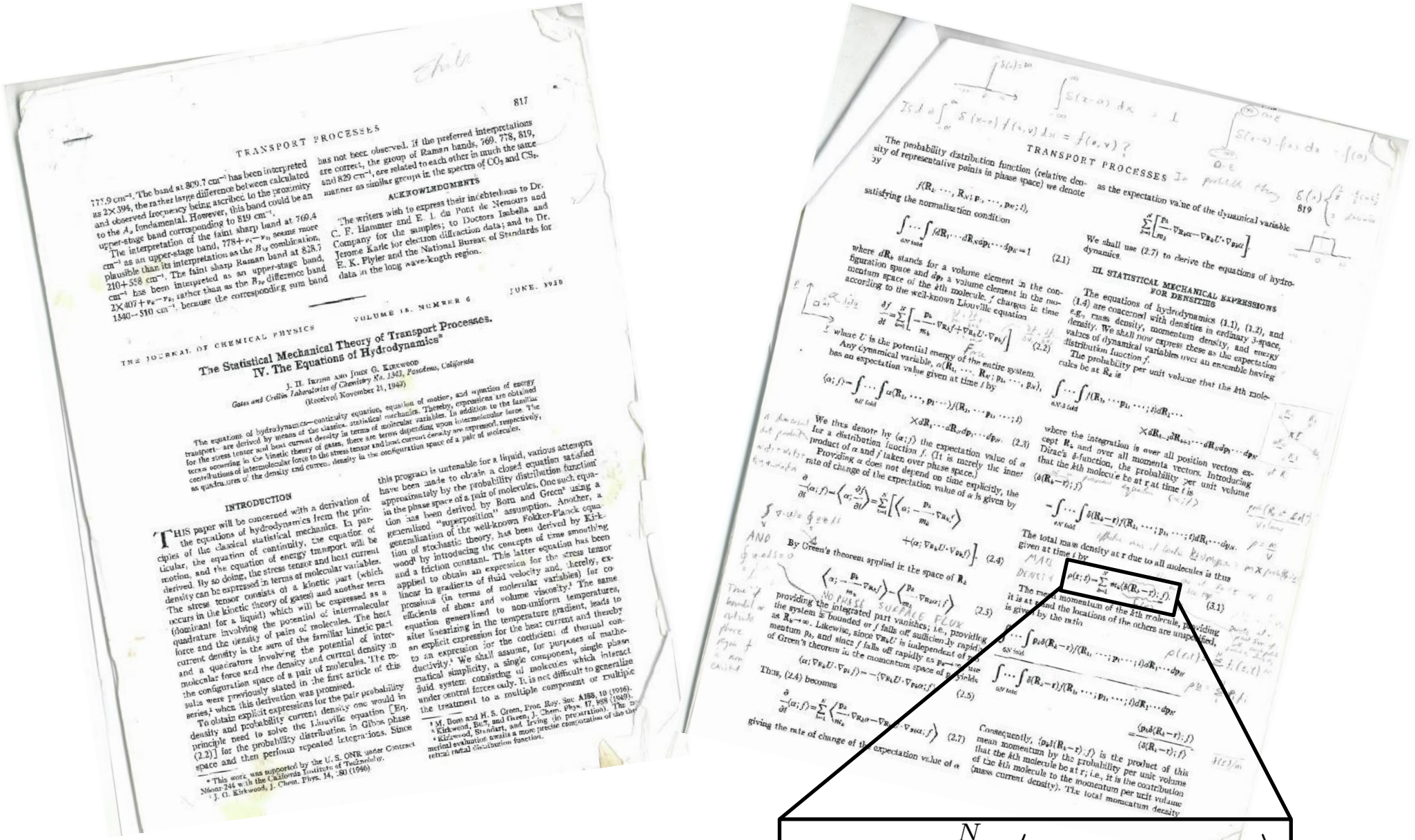
$$\rho = \frac{1}{V} \sum_{i=1}^{M_I} m_i$$

where M_I is the number of molecules in volume V

$$\rho = \frac{1}{V} \sum_{i \in S} m_i$$

where $S = \{i | \boldsymbol{r}^- < \boldsymbol{r}_i < \boldsymbol{r}^+\}$

Irving and Kirkwood (1950)



THE JOURNAL OF CHEMICAL PHYSICS VOLUME 18, NUMBER 6 JUNE, 1950

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

J. H. IRVING AND JOHN G. KIRKWOOD
Gates and Crellin Laboratories of Chemistry No. 1343, Pasadena, California
(Received November 21, 1949)

TRANSPORT PROCESSES

817

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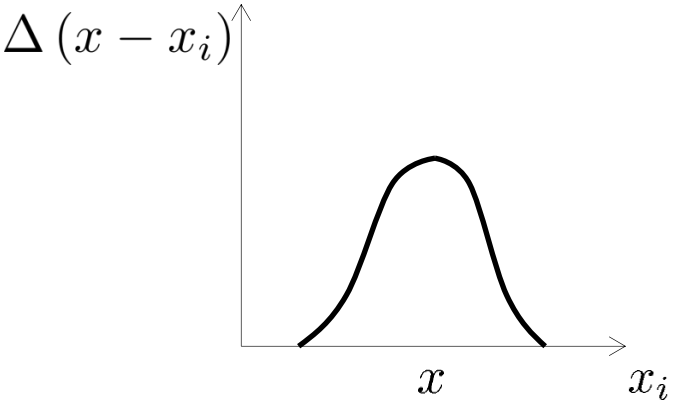
$$\rho(\boldsymbol{r},t)=\sum_{i=1}^{N}\left\langle m_i\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right);f\right\rangle$$

Selecting Functions

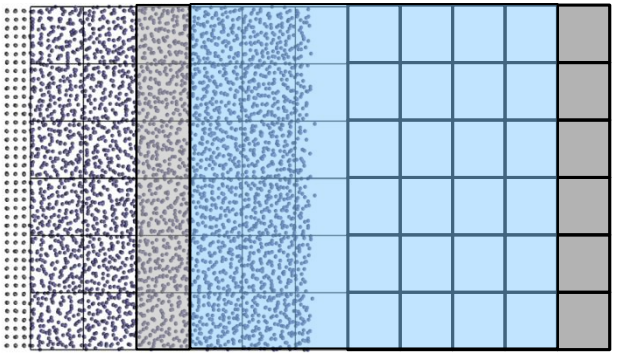
- **The Dirac delta selects molecules at a point**
  - Infinitely high, infinitely thin peak
  - Equivalent to the continuum differential formulation at a point

$$\rho(\boldsymbol{r},t)=\sum_{i=1}^{N} m_i \delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right)$$

- **Cannot be applied directly in a molecular simulation as $\boldsymbol{r}_i$ is never exactly equal to $\boldsymbol{r}$**
  - Relaxed weighting function used*



- **Co-existence of two descriptions in same simulation**
  - Overlap used in most coupling schemes
  - Length scales comparable at interface



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* E.g. by Hardy(1981), Hoover (2009), Murdoch (2010)

The Control Volume (CV)

- **A finite volume with fluxes and forces acting over its surfaces**
  - Mass Conservation

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

  - Momentum Balance (Newton's Law

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

  - Energy Conservation

$$\frac{\partial}{\partial t}\rho \mathcal{E} dV = -\boldsymbol{\nabla} \cdot [\rho \mathcal{E} \boldsymbol{u} + \boldsymbol{\Pi} \cdot \boldsymbol{u} + \mathbf{q}] \qquad \frac{\partial}{\partial t}\int_V \rho \mathcal{E} dV = -\oint_S \rho \mathcal{E} \boldsymbol{u} \cdot d\mathbf{S} - \oint_S \boldsymbol{\Pi} \cdot \boldsymbol{u} \cdot d\mathbf{S} + \mathbf{q} \cdot d\mathbf{S}$$

The Control Volume (CV)

- **Writing the molecular system in terms of control volumes**
  - Mass

$$\rho = \sum_{i=1}^{N} m_i \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right) \qquad \int_V \rho dV = \sum_{i=1}^{N} m_i \int_V \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right) dV$$

  - Momentum

$$\rho \boldsymbol{u} = \sum_{i=1}^{N} \boldsymbol{p}_i \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right) \qquad \int_V \rho \boldsymbol{u} dV = \sum_{i=1}^{N} \boldsymbol{p}_i \int_V \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right) dV$$

  - Energy

$$\rho \mathcal{E} = \sum_{i=1}^{N} e_i \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right) \qquad \int_V \rho \mathcal{E} dV = \sum_{i=1}^{N} e_i \int_V \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right) dV$$

The Control Volume Formulation

Control Volume Function

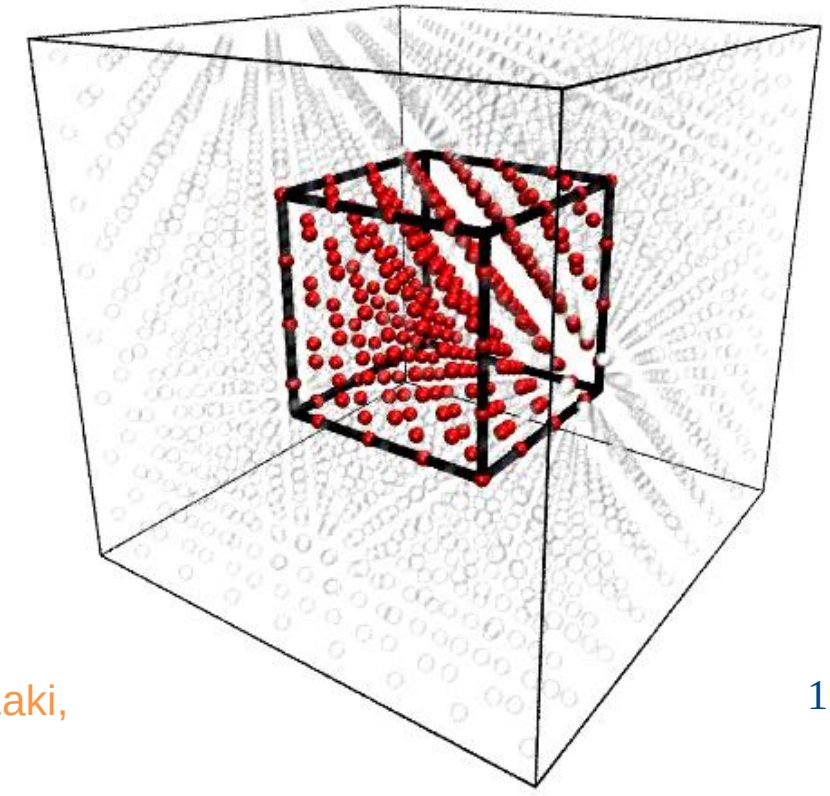
- **The Control volume function is the integral of the Dirac delta function in 3 dimensions**

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

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

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

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



For full details, please see
E.R. Smith, D.M. Heyes, D. Dini, T.A. Zaki,
Phys. Rev. E 85. 056705 (2012)

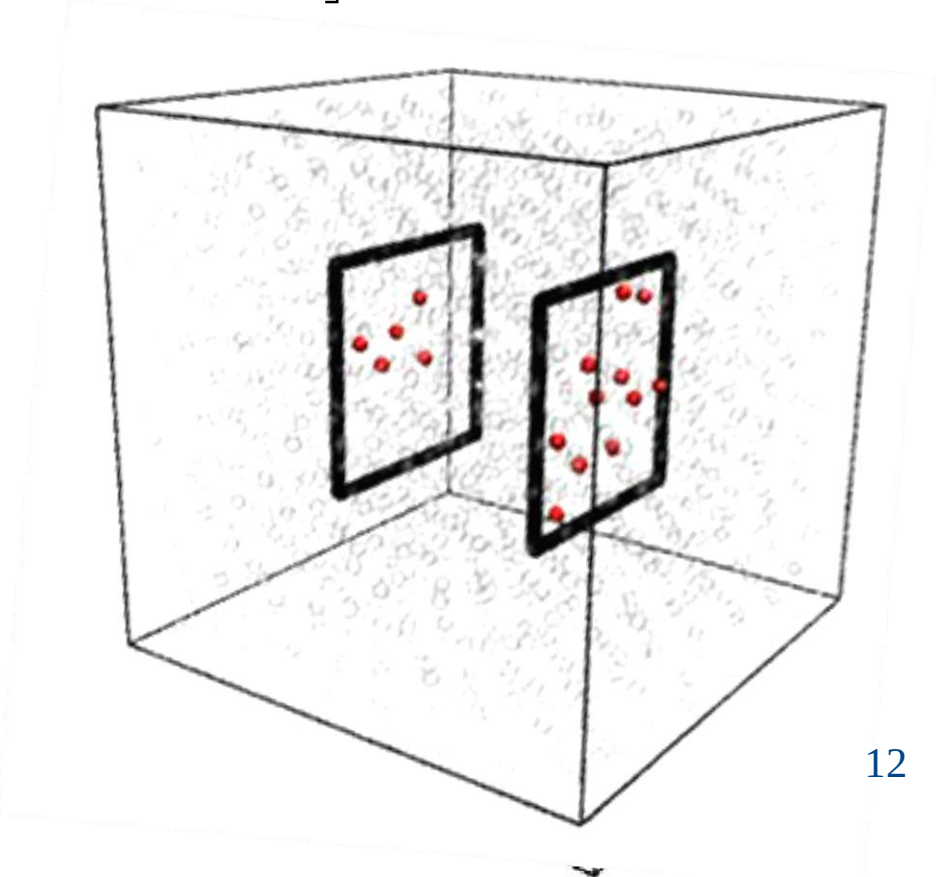
Derivatives yields the Surface Fluxes

- **Taking the Derivative of the CV function**

$$dS_{ix} \equiv -\frac{\partial \vartheta_i}{\partial x_i} = \left[\delta(x^+ - x_i) - \delta(x^- - x_i)\right] \times \left[H(y^+ - y_i) - H(y^- - y_i)\right] \times \left[H(z^+ - z_i) - H(z^- - z_i)\right]$$

- **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**

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

- **Mathematical manipulation yields surface fluxes**

$$\frac{d}{dt}\sum_{i=1}^{N} m_i\vartheta_i = \sum_{i=1}^{N}\left(\vartheta_i\frac{d}{dt}m_i + m_i\frac{d}{dt}\vartheta_i\right)$$

$$= \sum_{i=1}^{N} m_i\frac{d\boldsymbol{r_i}}{dt}\cdot\frac{d}{d\boldsymbol{r_i}}\vartheta_i$$

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

Reynolds' Transport Theorem

- **Mass, momentum and energy equations**
  - Mass Conservation

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

  - Momentum Balance

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = -\sum_{i=1}^{N} m_i \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i + \sum_{i=1}^{N}\sum_{j\neq i}^{N} \mathbf{f}_{ij}\vartheta_{ij} \qquad \frac{\partial}{\partial t}\int_V \rho \boldsymbol{u} dV = -\oint_S \rho \boldsymbol{u}\boldsymbol{u} \cdot d\mathbf{S} + \mathbf{F}_{\text{surface}}$$

  - Energy Conservation

$$\frac{d}{dt}\sum_{i=1}^{N} e_i \vartheta_i = -\sum_{i=1}^{N} e_i \mathbf{v}_i \cdot d\mathbf{S}_i + \frac{1}{2}\sum_{i=1}^{N}\sum_{i\neq j}^{N} \frac{\mathbf{p}_i}{m_i} \cdot \boldsymbol{f_{ij}}\vartheta_{ij} \qquad \frac{\partial}{\partial t}\int_V \rho \mathcal{E} dV = -\oint_S \rho \mathcal{E}\boldsymbol{u} \cdot d\mathbf{S} - \oint_S \boldsymbol{\Pi} \cdot \boldsymbol{u} \cdot d\mathbf{S} + \mathbf{q} \cdot d\mathbf{S}$$

Reynolds' Transport Theorem

- **Mass, momentum and energy equations**
  - Mass Conservation

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

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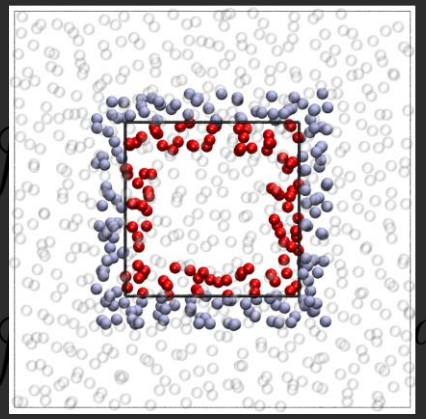
$$\frac{d}{dt}\sum_{i=1}^{N} e_i \vartheta_i = -\sum_{i=1}^{N} e_i \mathbf{v}_i \cdot d\mathbf{S}_i + \frac{1}{2}\sum_{i=1}^{N}\sum_{i\neq j}^{N} \frac{\mathbf{p}_i}{m_i} \cdot \boldsymbol{f}_{ij}\vartheta_{ij} \qquad \frac{\partial}{\partial t}\int_V \rho \mathcal{E} dV = -\oint \; - \oint \; d\mathbf{S}$$

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

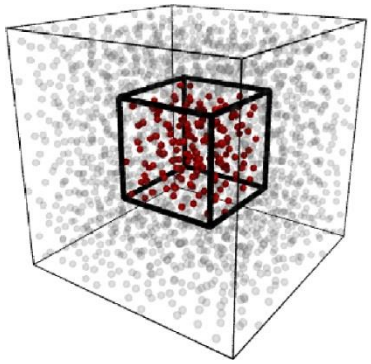
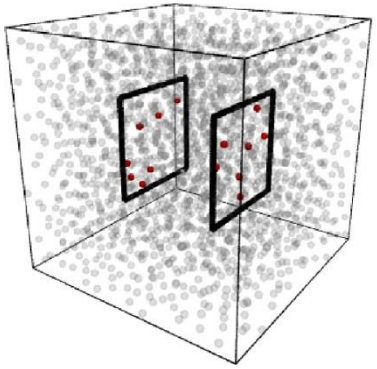
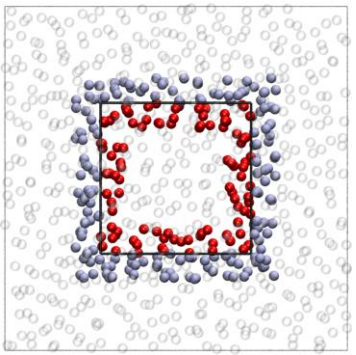
$$\vartheta_{ij} \equiv \vartheta_i - \vartheta_j$$



Testing Momentum Balance

- **Momentum Balance**

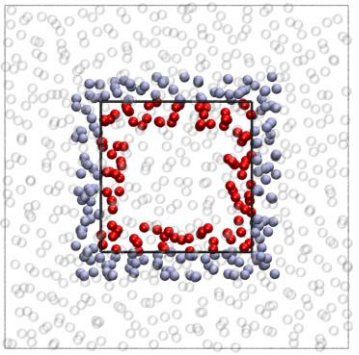
$$\underbrace{\frac{d}{dt}\sum_{i=1}^{N} m_i \dot{\mathbf{r}}_i \vartheta_i}_{\textit{Accumulation}} + \underbrace{\sum_{i=1}^{N} m \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i}_{\textit{Advection}} - \underbrace{\sum_{i=1}^{N}\sum_{j\neq i}^{N} \mathbf{f}_{ij}\vartheta_{ij}}_{\textit{Forcing}} = 0$$

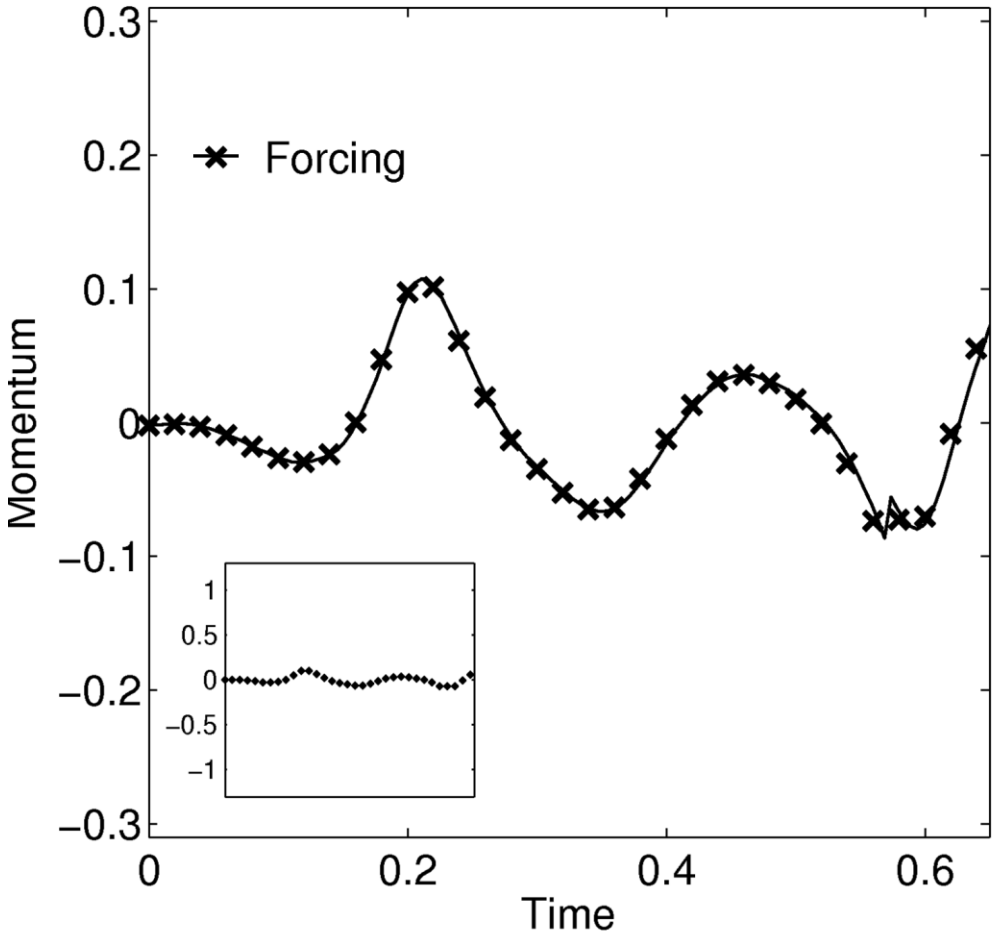
$$\frac{d}{dt}$$  +  −  $= 0$

Testing Momentum Balance

- **Momentum Balance**

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

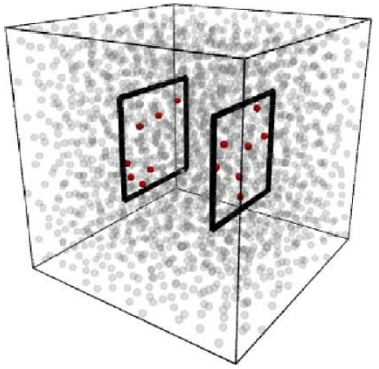


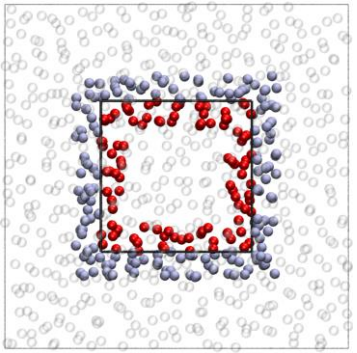


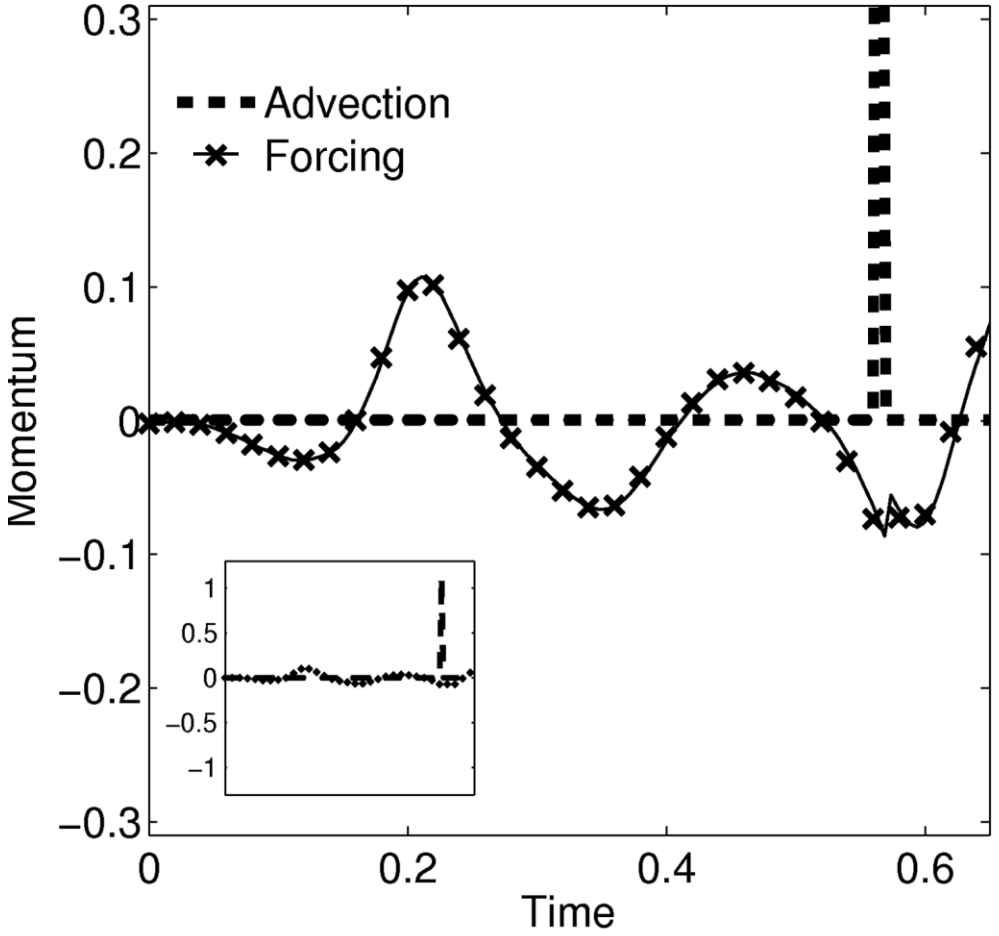
Testing Momentum Balance

- **Momentum Balance**

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





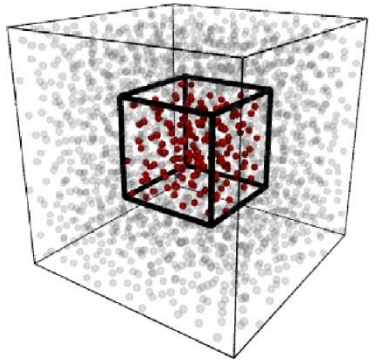


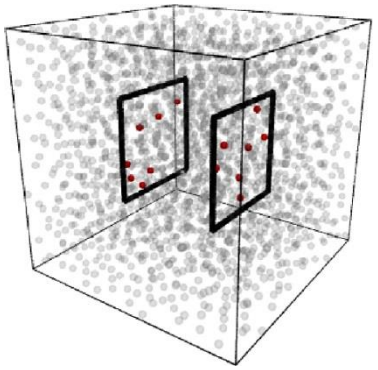
Testing Momentum Balance

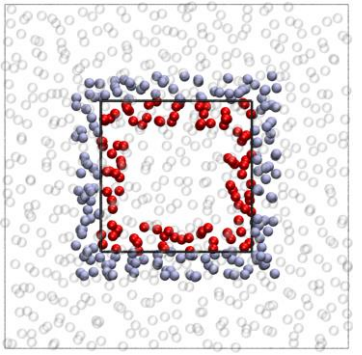
- **Momentum Balance**

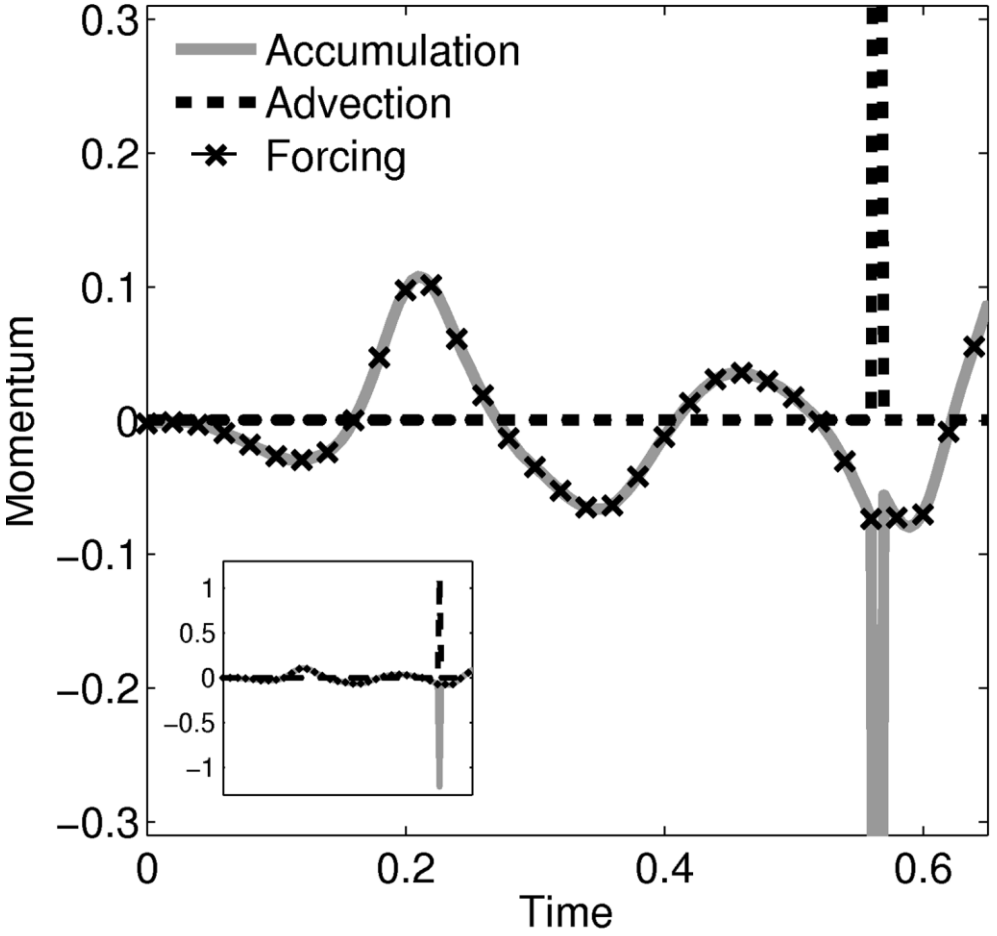
$$\underbrace{\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i}_{\text{Accumulation}} = \underbrace{-\sum_{i=1}^{N} m_i \mathbf{v}_i \mathbf{v}_i \cdot d\boldsymbol{S}_i}_{\text{Advection}} + \underbrace{\sum_{i=1}^{N}\sum_{j\neq i}^{N} \mathbf{f}_{ij}\vartheta_{ij}}_{\text{Forcing}}$$

$\frac{d}{dt}$









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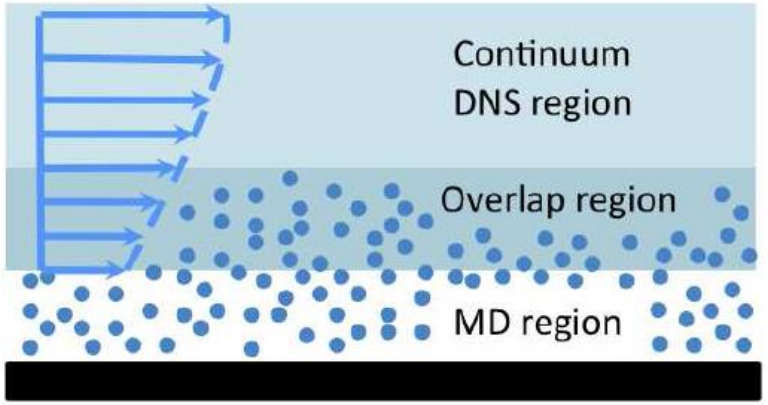
Using the CV for coupling

- **Layout of a typical coupled simulation**
  - Separate MD and CFD regions with Overlap region between
  - MD averages give CFD boundary conditions
  - CFD values used to apply a constraint to MD
- **Control Volume can be used to**
  - Average values from MD
  - Apply a constraint to any arbitrary CV
- **Constraint is non-unique**
  - Hamilton's principle is one of the most fundamental formulations of mechanics
  - Used to apply physically meaningful constraints



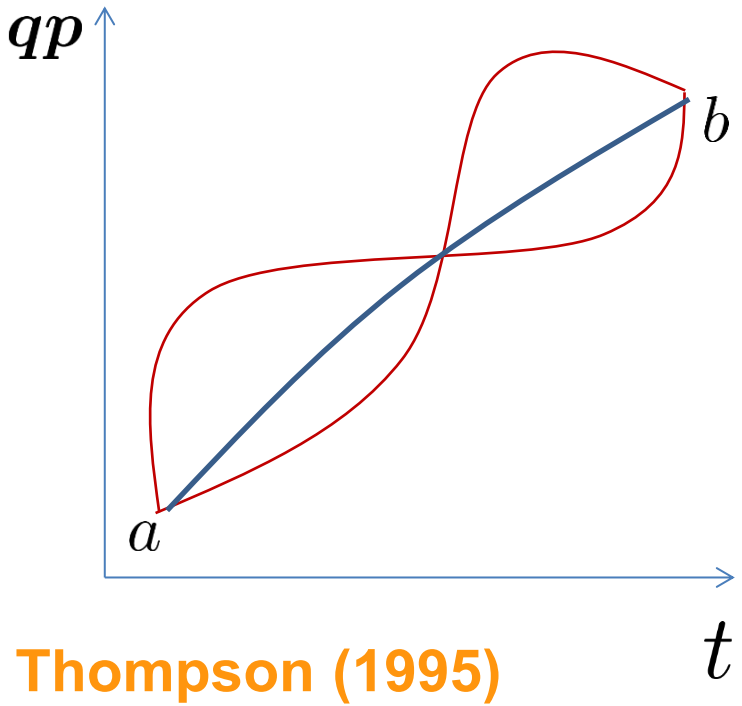
$$\int_V \rho \boldsymbol{u} dV = \sum_{i=1}^{N} \boldsymbol{p}_i \vartheta_i$$

$$\delta A = \delta \int_a^b \mathcal{L} dt = 0$$

Constraint Algorithms

- **Principle of Least Action (subject to constraint)**

$$\delta A_c = \delta \int_a^b (\mathcal{L} + \lambda g)\, dt = 0$$



- **Semi-Holonomic Constraint**

$$g(\dot{\boldsymbol{q}}_i) = \sum_{i \in S} \boldsymbol{p}_i - M_I \boldsymbol{u}_I = 0$$

- **Constraint Equation of O'Connell and Thompson (1995)**

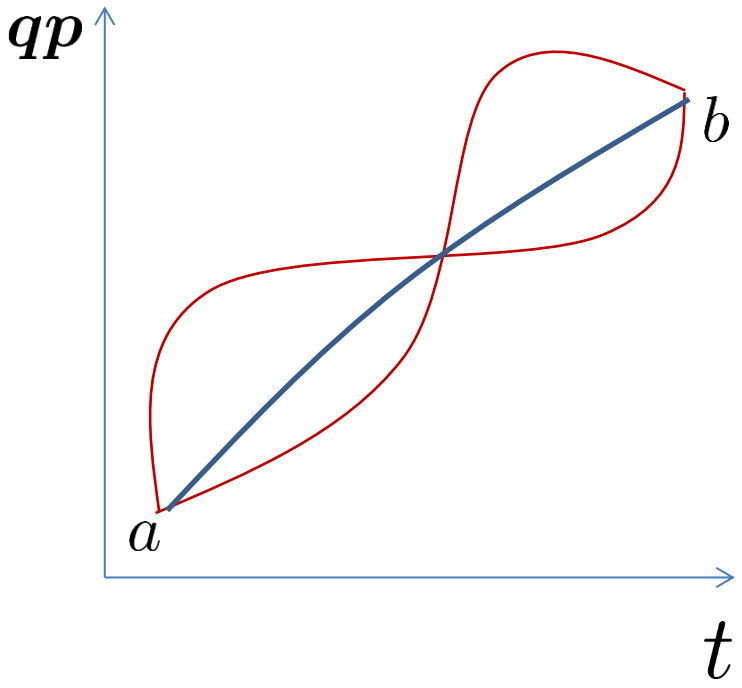
$$m_i \dot{\boldsymbol{q}}_i = \boldsymbol{p}_i - \frac{1}{mN_I} \left[\sum_{i \in S} \boldsymbol{p}_i - M_I \boldsymbol{u}_I \right]$$

$$\dot{\boldsymbol{p}}_i = \boldsymbol{F}_i$$

Constraint Algorithms

- **Principle of Least Action (subject to constraint)**

$$\delta A_c = \delta \int_a^b (\mathcal{L} + \lambda g)\, dt = 0$$



- **Non-Holonomic Constraint**

$$g(\boldsymbol{q}_i, \boldsymbol{p}_i) = \sum_{i=1}^{N} \boldsymbol{p}_i \vartheta_i - \int_V \rho \boldsymbol{u} dV = 0$$

- **Constraint Equation**

$$\left.\begin{aligned} m_i \dot{\boldsymbol{q}}_i &= \boldsymbol{p}_i - \frac{m_i \vartheta_i}{M_I} \left[\sum_{n=1}^{N} \boldsymbol{p}_n \vartheta_n - \int_V \rho \boldsymbol{u} dV \right] \\ \dot{\boldsymbol{p}}_i &= \boldsymbol{F}_i \\ \text{Where } M_I &\equiv \sum_{n=1}^{N} m_n \vartheta_n \end{aligned}\right\} \; m_i \ddot{\boldsymbol{q}}_i = \boldsymbol{F}_i + \boldsymbol{F}_i^C$$

Constraint Algorithms

- **Combining the CV equations of O'Connell and Thompson**

$$m_i\ddot{\boldsymbol{q}}_i = \boldsymbol{F}_i + \frac{m_i\vartheta_i}{M_I}\left[\frac{d}{dt}\int_V \rho\boldsymbol{u}dV - \overbrace{\sum_{n,m}^{N}\boldsymbol{f}_{nm}\vartheta_{nm}}^{\mathbf{F}_{\text{surface}}} + \overbrace{\sum_{n=1}^{N} m_i\dot{\boldsymbol{q}}_n\dot{\boldsymbol{q}}_n\cdot d\mathbf{S}_n}^{\text{Momentum Flux}}\right]$$

$$+\frac{m_i}{M_I}\underbrace{\left(\dot{\boldsymbol{q}}_i\cdot d\mathbf{S}_i - \frac{\vartheta_i}{M_I}\sum_{n=1}^{N} m_n\dot{\boldsymbol{q}}_n\cdot d\mathbf{S}_n\right)}_{\text{Mass Flux}} \times \underbrace{\left[\sum_{n=1}^{N} m_n\dot{\boldsymbol{q}}_n\vartheta_n - \int_V \rho\boldsymbol{u}dV\right]}_{\text{Momentum Discrepancy}}$$

- **Surface forces only are included in the constraint**
  - The CV is effectively isolated (no forces) from the rest of the system
- **Extra terms due to molecular flux**
  - Molecules crossing the surface result in extra forces

Constraint Algorithms

- **Combining the CV equations of O'Connell and Thompson**

$$m_i\ddot{\boldsymbol{q}}_i = \boldsymbol{F}_i + \frac{m_i\vartheta_i}{M_I}\left[\frac{d}{dt}\int_V \rho\boldsymbol{u}dV - \overbrace{\sum_{n,m}^{N}\boldsymbol{f}_{nm}\vartheta_{nm}}^{\mathbf{F}_{\text{surface}}} + \overbrace{\sum_{n=1}^{N} m_i\dot{\boldsymbol{q}}_n\dot{\boldsymbol{q}}_n\cdot d\mathbf{S}_n}^{\text{Momentum Flux}}\right]$$

$$+\frac{m_i}{M_I}\underbrace{\left(\dot{\boldsymbol{q}}_i\cdot d\mathbf{S}_i - \frac{\vartheta_i}{M_I}\sum_{n=1}^{N} m_n\dot{\boldsymbol{q}}_n\cdot d\mathbf{S}_n\right)}_{\text{Mass Flux}} \times \underbrace{\left[\sum_{n=1}^{N} m_n\dot{\boldsymbol{q}}_n\vartheta_n - \int_V \rho\boldsymbol{u}dV\right]}_{\text{Momentum Discrepancy}}$$

- **Negligible surface flux and average mass/velocity inside volume yields Nie, Chen, E and Robbins (2004) coupling**

$$m\ddot{\boldsymbol{q}}_i = \boldsymbol{F}_i \;+\; m\vartheta_i\left[\frac{D\boldsymbol{u}_I}{Dt} - \frac{1}{mN_I}\sum_{n=1}^{N}\boldsymbol{F}_n\,\vartheta_n\right]$$

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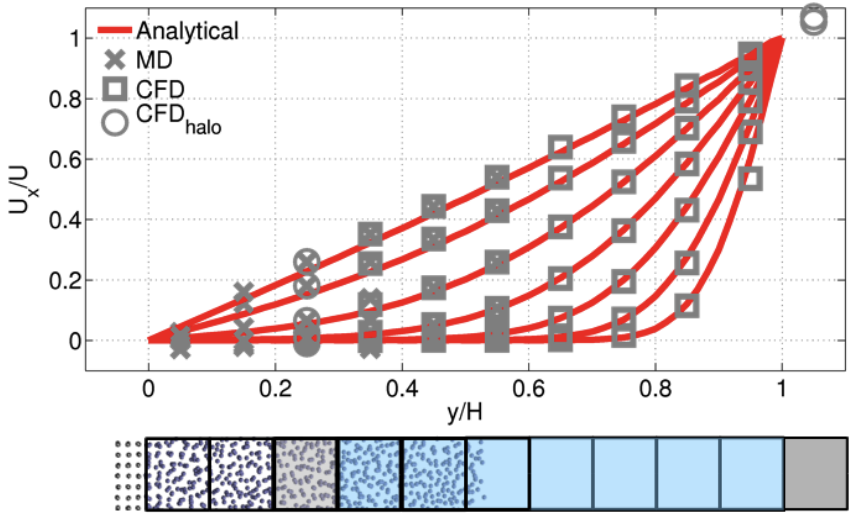
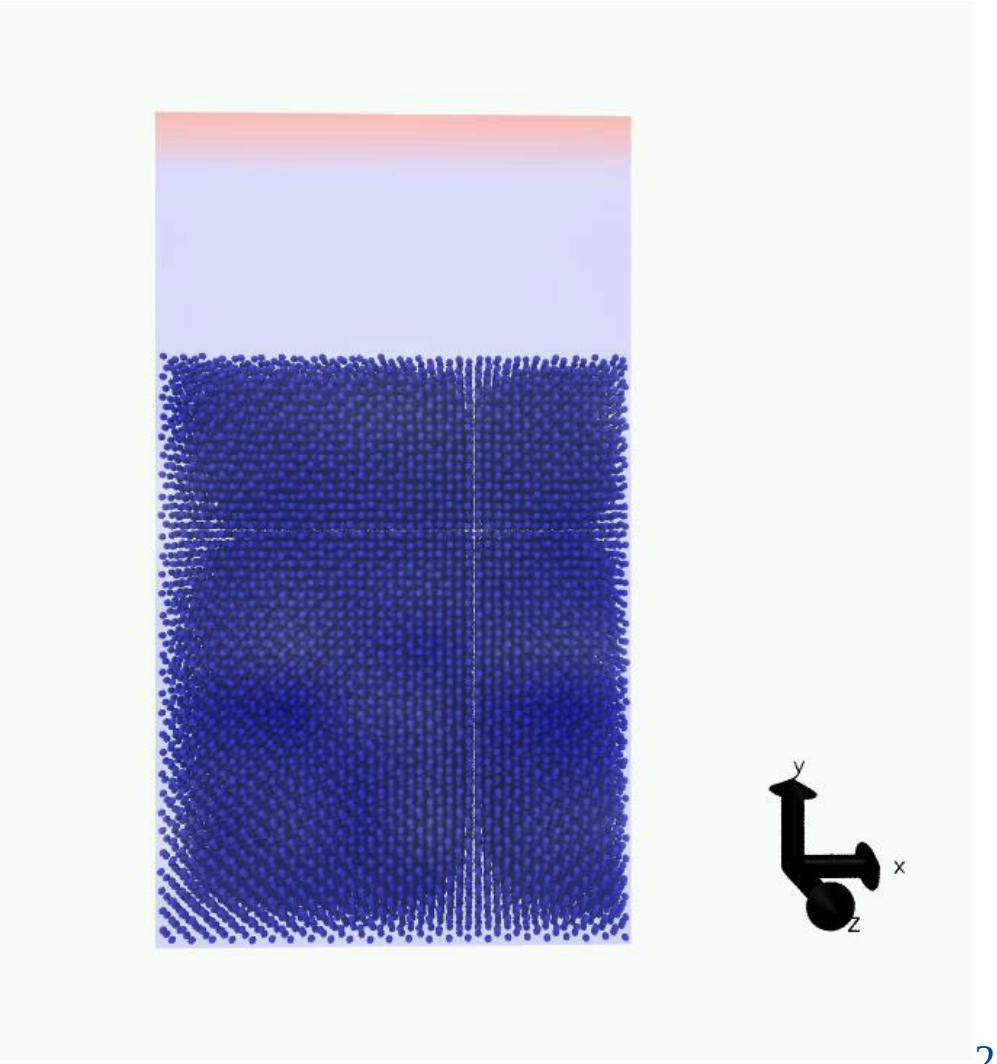
State Coupling

- **Continuum-MD coupling using state variables shows good agreement in the velocity profiles**

$$\mu_{\mathrm{MD}} = \mu_{\mathrm{CFD}} = 2.14$$

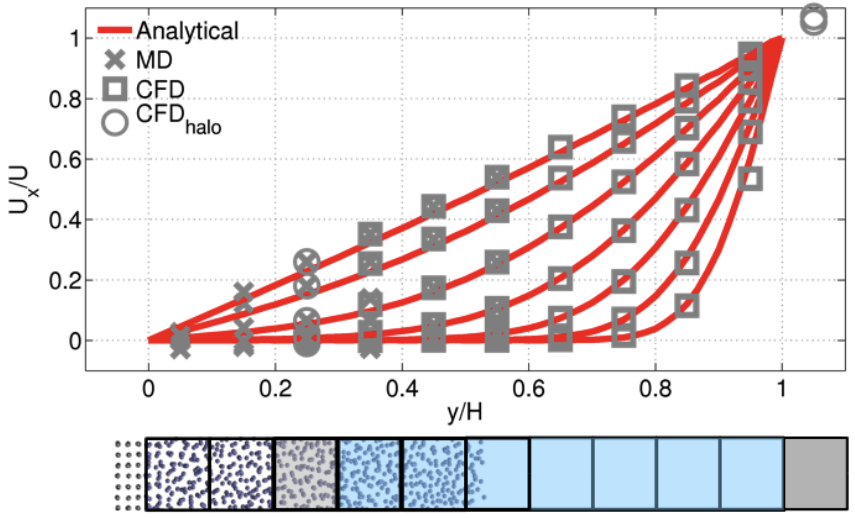




State Coupling

- **Continuum-MD coupling using state variables shows good agreement in the velocity profiles**

$\mu_{\mathrm{MD}} = \mu_{\mathrm{CFD}} = 2.14$



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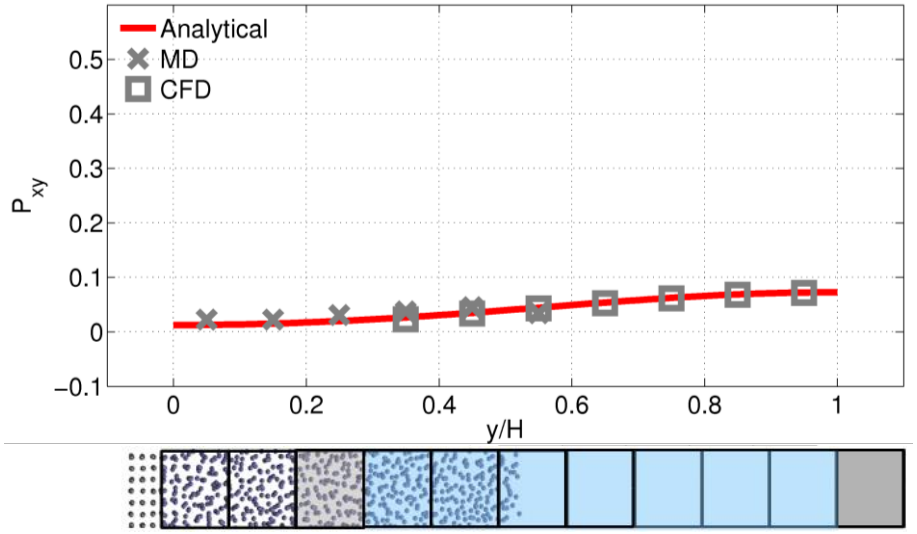
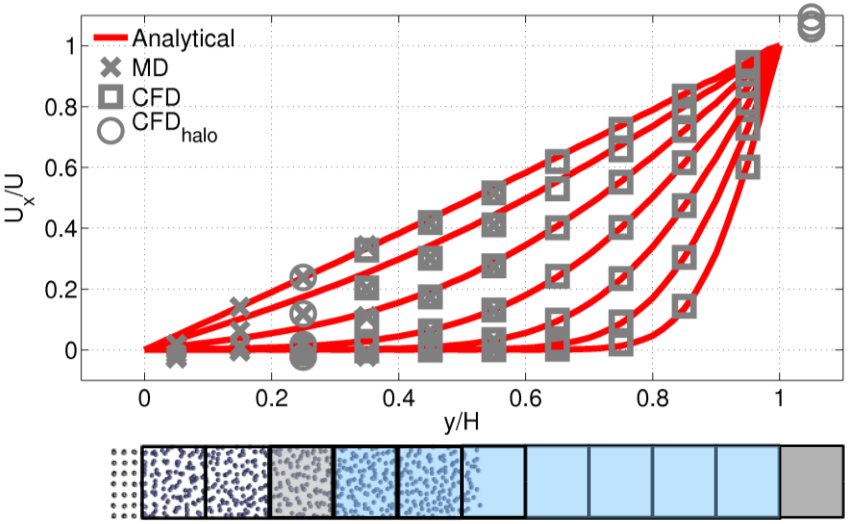


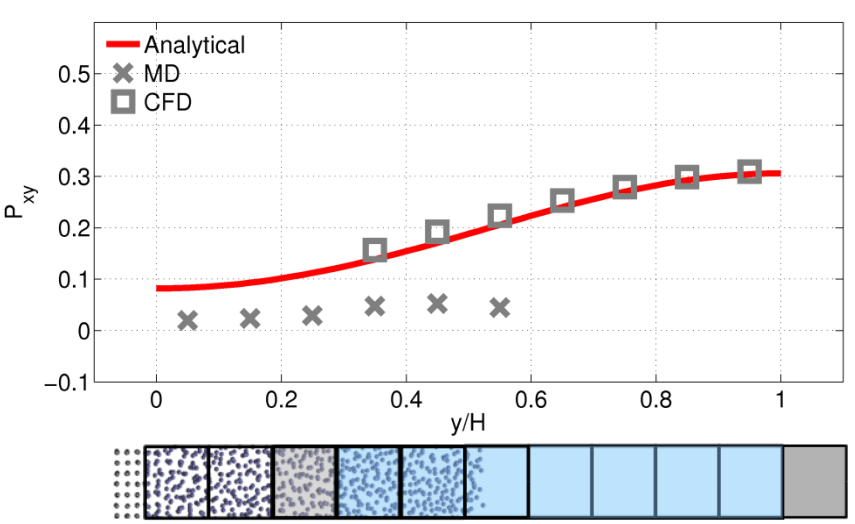
State Coupling

- **Continuum-MD coupling using state variables shows good agreement in the velocity profiles**
  - However, a mismatch in the stress can occur at the interface
  - Unless both regions have a constant viscosity, fluxes are not coupled despite agreement of velocity profile

$\mu_{\mathrm{MD}} = 2.14 \quad \mu_{\mathrm{CFD}} = 10$



$\mu_{\mathrm{MD}} = 2.14 \quad \mu_{\mathrm{CFD}} = 10$

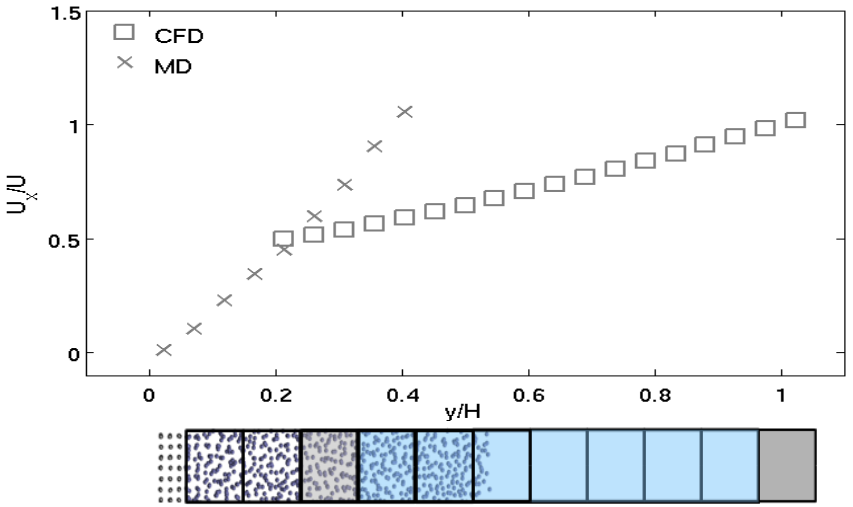


- **Flux coupling is required**

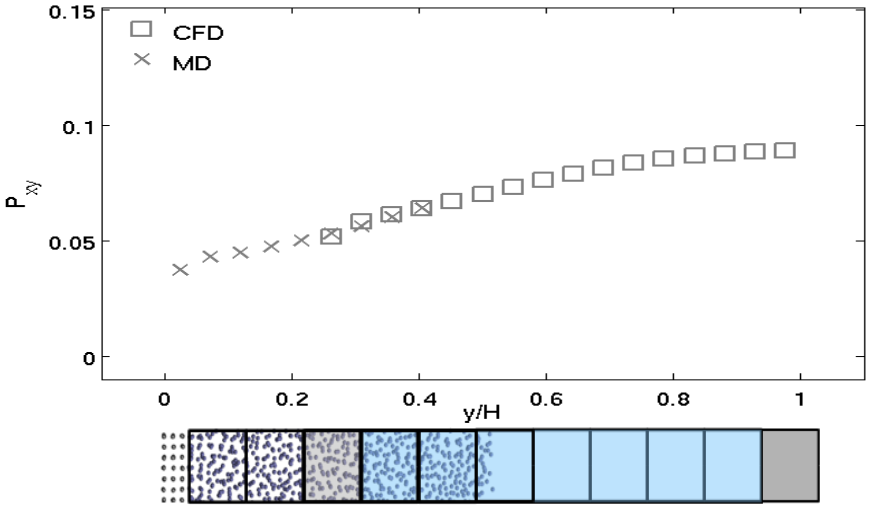
Flux Coupling

- **Continuum-MD coupling using flux variables shows good agreement in the stress profiles***
  - A mismatch in the velocity occurs at the interface
  - Analogous to the interface between two immiscible fluids

$\mu_{\mathrm{MD}} = 2.14 \quad \mu_{\mathrm{CFD}} = 10$



$\mu_{\mathrm{MD}} = 2.14 \quad \mu_{\mathrm{CFD}} = 10$



- **Flux Coupling requires significant statistical averaging**
  - Coupling developed for massively parallel applications to exploit high performance computers

- ***E. G. Flekkøy, G. Wagner, and J. Feder, Europhys. Lett. 52, 271 (2000).**

Flux Coupling and the Pressure Tensor

Flux Coupling

- **Flux Coupling requires the equations of motion in terms of stresses and fluxes**

- **Surface Forces**

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

- **Divergence of stress**

$$\frac{\partial}{\partial t}\int_V \rho \boldsymbol{u} dV = -\int_V \frac{\partial}{\partial \boldsymbol{r}}\cdot \rho \boldsymbol{u}\boldsymbol{u} - \int_V \frac{\partial}{\partial \boldsymbol{r}}\cdot\left[P\boldsymbol{I}-\boldsymbol{\sigma}\right] dV$$

- **Surface Stresses**

$$\frac{\partial}{\partial t}\int_V \rho \boldsymbol{u} dV = -\oint_S \rho \boldsymbol{u}\boldsymbol{u}\cdot d\boldsymbol{S} - \oint_S \left[P\boldsymbol{I}-\boldsymbol{\sigma}\right]\cdot d\boldsymbol{S}$$

Control Volume Function

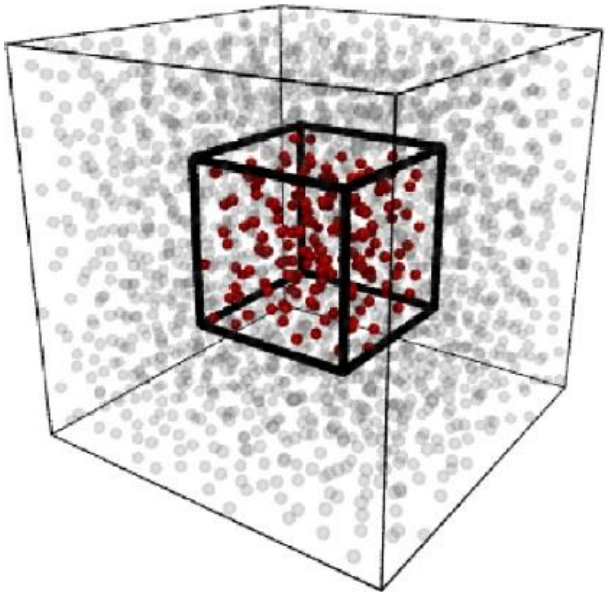
- **The Control volume function is the integral of the Dirac delta function in 3 dimensions**

$$\vartheta_i \equiv \int_V \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right) dV$$

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

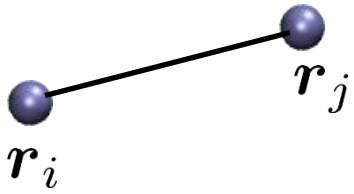
$$\times \left[H(y^+ - y_i) - H(y^- - y_i)\right]$$

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



- **Replace molecular position with equation for a line**

$$\boldsymbol{r}_i \rightarrow \boldsymbol{r}_i - s\boldsymbol{r}_{ij}$$



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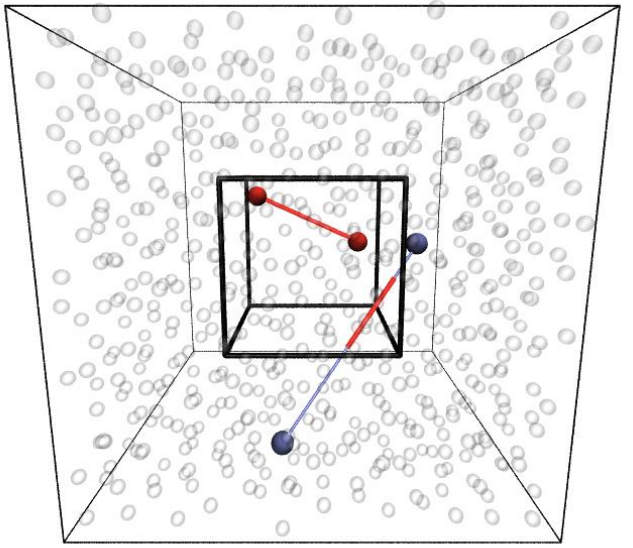
For full details, please see
E.R. Smith, D.M. Heyes, D. Dini, T.A. Zaki, Phys. Rev. E 85. 056705 (2012)

Control Volume Function

- **The Control volume function is the integral of the Dirac delta function in 3 dimensions**

$$\vartheta_s \equiv \int_V \delta(\mathbf{r} - \mathbf{r}_i + s\mathbf{r}_{ij})dV =$$
$$\left[H(x^+ - x_i + sx_{ij}) - H(x^- - x_i + sx_{ij})\right]$$
$$\times \left[H(y^+ - y_i + sy_{ij}) - H(y^- - y_i + sy_{ij})\right]$$
$$\times \left[H(z^+ - z_i + sz_{ij}) - H(z^- - z_i + sz_{ij})\right]$$



- **Length of interaction inside the CV**

$$\ell_{ij} = \int_0^1 \vartheta_s ds$$

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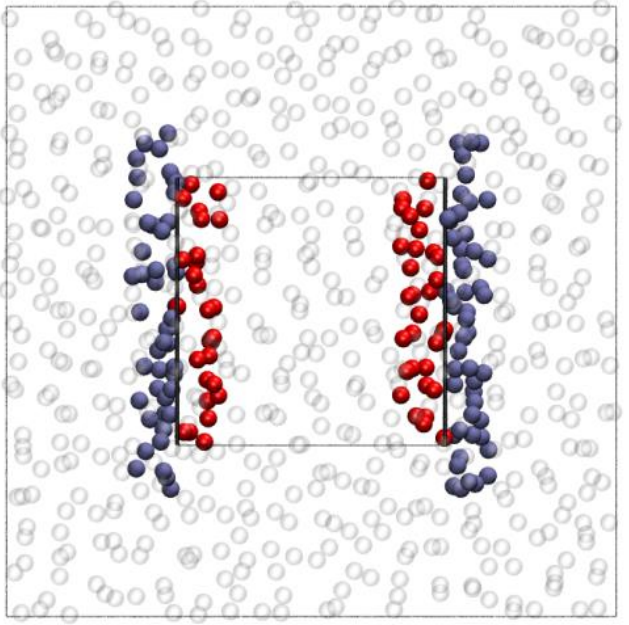
For full details, please see
E.R. Smith, D.M. Heyes, D. Dini, T.A. Zaki, Phys. Rev. E 85. 056705 (2012)

Derivatives Yield the Surface Forces

- **Taking the Derivative of the CV function**

$$\frac{\partial \vartheta_s}{\partial \boldsymbol{r}} \equiv \left[\, \delta(x^+ - x_i + s x_{ij}) \;-\; \delta(x^- - x_i + s x_{ij})\right]$$
$$\times \left[H(y^+ - y_i + s y_{ij}) \;-\; H(y^- - y_i + s y_{ij})\right]$$
$$\times \left[H(z^+ - z_i + s z_{ij}) \;-\; H(z^- - z_i + s z_{ij})\right]$$



- **Surface fluxes over the top and bottom surface**

$$\tilde{\boldsymbol{n}} \cdot d\mathbf{S}_{ij} = \int_0^1 \frac{\partial \vartheta_s}{\partial \boldsymbol{r}} ds \qquad \tilde{\boldsymbol{n}} = [1 \;\; 1 \;\; 1]$$

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Surface Pressures

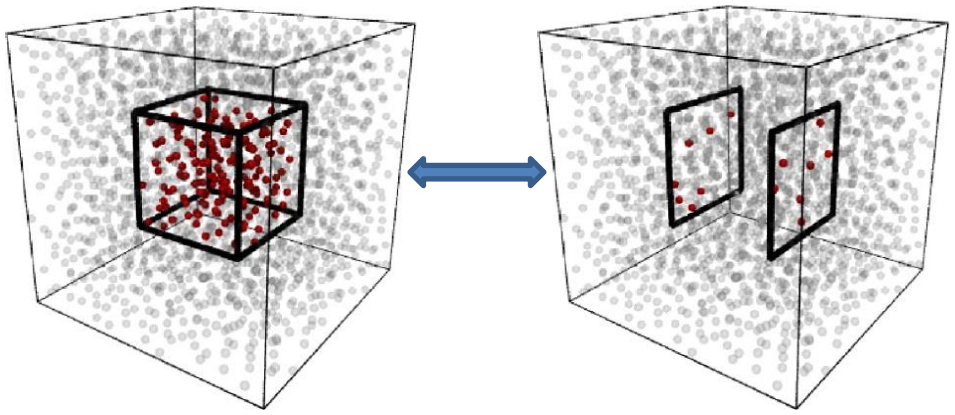
- **Volume Average Form of Lutsko (1988) & Cormier et al (2001)**

$$\int_V \frac{\partial}{\partial \boldsymbol{r}} \cdot [P\boldsymbol{I} - \boldsymbol{\sigma}]\, dV = \frac{\partial}{\partial \boldsymbol{r}} \cdot \sum_{i=1}^{N} \left[(\boldsymbol{v}_i - \boldsymbol{u})(\boldsymbol{v}_i - \boldsymbol{u})\, \vartheta_i + \sum_{j \neq i}^{N} \boldsymbol{f}_{ij} \boldsymbol{r}_{ij} \int_0^1 \vartheta_s ds \right]$$

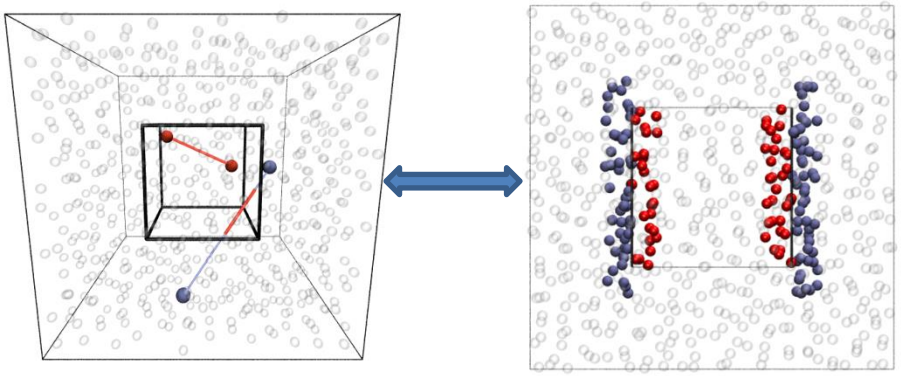
- **The derivative of ϑ_s gives forces over the surface - a localisation of the method of planes, (Todd et al 1995, Han Lee 2004)**

$$\oint_S [P\boldsymbol{I} - \boldsymbol{\sigma}] \cdot d\boldsymbol{S} = \sum_{i=1}^{N} \left[(\boldsymbol{v}_i - \boldsymbol{u})(\boldsymbol{v}_i - \boldsymbol{u}) \cdot d\boldsymbol{S}_i + \sum_{j \neq i}^{N} \boldsymbol{f}_{ij} \tilde{\boldsymbol{n}} \cdot d\boldsymbol{S}_{ij} \right]$$

- **Kinetic**



- **Configurational**



Surface Pressures

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

$$\int_V \frac{\partial}{\partial \boldsymbol{r}} \cdot [P\boldsymbol{I} - \boldsymbol{\sigma}]\, dV = \frac{\partial}{\partial \boldsymbol{r}} \cdot \sum_{i=1}^{N} \left[(\boldsymbol{v}_i - \boldsymbol{u})(\boldsymbol{v}_i - \boldsymbol{u})\, \vartheta_i + \sum_{j \neq i}^{N} \boldsymbol{f}_{ij} \boldsymbol{r}_{ij} \int_0^1 \vartheta_s ds \right]$$

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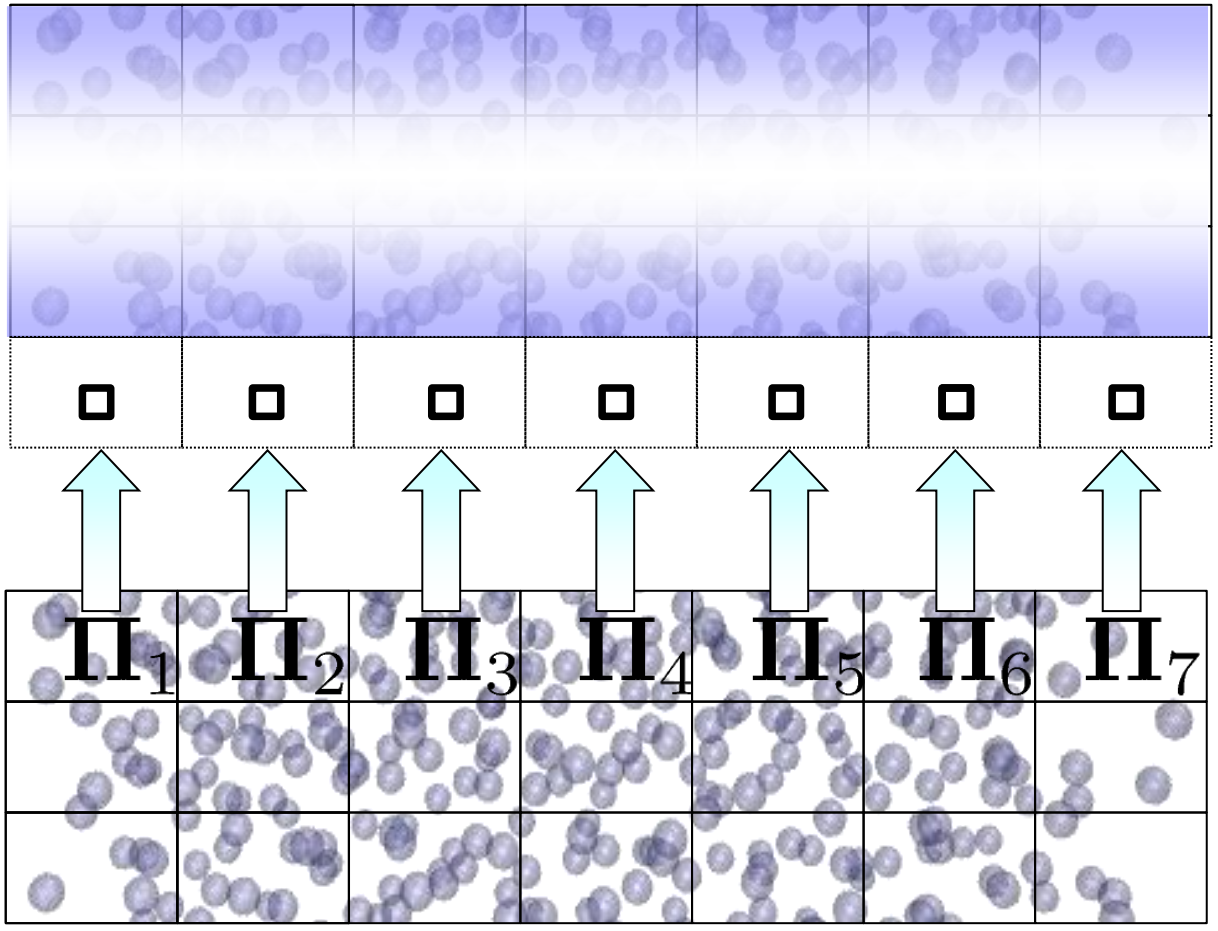
$$\oint_S [P\boldsymbol{I} - \boldsymbol{\sigma}] \cdot d\boldsymbol{S} = \sum_{i=1}^{N} \left[(\boldsymbol{v}_i - \boldsymbol{u})(\boldsymbol{v}_i - \boldsymbol{u}) \cdot d\boldsymbol{S}_i + \sum_{j \neq i}^{N} \boldsymbol{f}_{ij} \tilde{\boldsymbol{n}} \cdot d\boldsymbol{S}_{ij} \right]$$

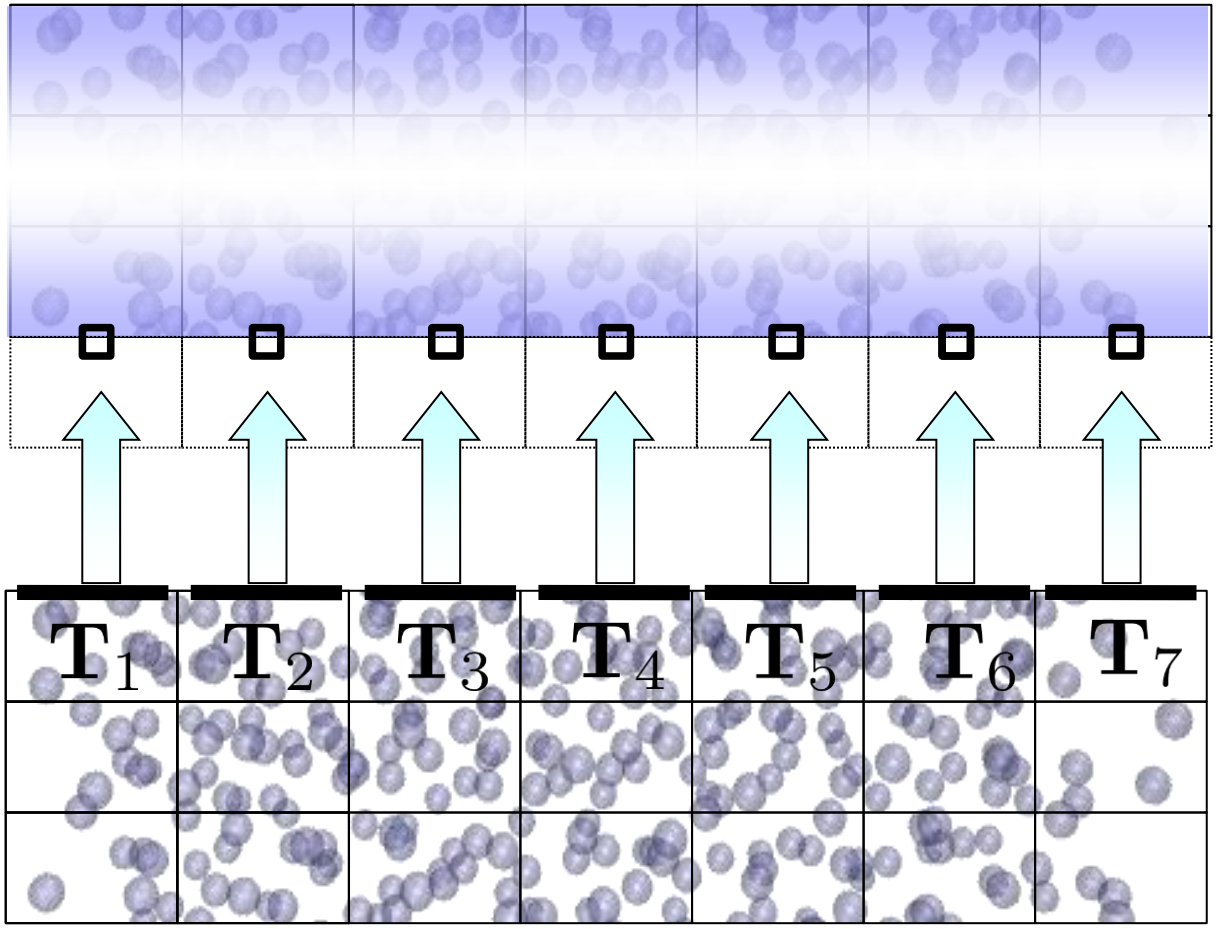
- **Stress tensor is non-unique but link shown between**
  - Volume Average (Lutsko, 1988) and Method of Planes (Todd et al 1995)
- **Exact relationship between surface flux/stress form and momentum change inside the control volume**
  - Conservation can be used to obtain unknown values
  - Most appropriate form of the non-unique stress tensor for coupling

Coupling the Localised Stresses



$$\boldsymbol{\Pi} = \sum_{i=1}^{N} \left[(\boldsymbol{v}_i - \boldsymbol{u})(\boldsymbol{v}_i - \boldsymbol{u})\vartheta_i + \sum_{j \neq i}^{N} \boldsymbol{f}_{ij}\boldsymbol{r}_{ij} \int_0^1 \vartheta_s ds \right]$$

Coupling the Surface Stresses



$$\mathbf{T} = \sum_{i=1}^{N} \left[(\boldsymbol{v}_i - \boldsymbol{u})(\boldsymbol{v}_i - \boldsymbol{u}) \cdot d\boldsymbol{S}_{yi}^{+} + \sum_{j \neq i}^{N} \boldsymbol{f}_{ij} \tilde{\boldsymbol{n}} \cdot d\boldsymbol{S}_{ij}^{+} \right]$$

State or Flux Constraint?

- **Recall the coupled CV equations**

$$m_i\ddot{\boldsymbol{q}}_i = \boldsymbol{F}_i + \frac{m_i\vartheta_i}{M_I}\left[\frac{d}{dt}\int_V \rho\boldsymbol{u}dV - \overbrace{\sum_{n,m}^{N}\boldsymbol{f}_{nm}\vartheta_{nm}}^{\mathbf{F}_{\text{surface}}} + \overbrace{\sum_{n=1}^{N} m_i\dot{\boldsymbol{q}}_n\dot{\boldsymbol{q}}_n\cdot d\mathbf{S}_n}^{\text{Momentum Flux}}\right]$$

$$+\frac{m_i}{M_I}\underbrace{\left(\dot{\boldsymbol{q}}_i\cdot d\mathbf{S}_i - \frac{\vartheta_i}{M_I}\sum_{n=1}^{N} m_n\dot{\boldsymbol{q}}_n\cdot d\mathbf{S}_n\right)}_{\text{Mass Flux}} \times \underbrace{\left[\sum_{n=1}^{N} m_n\dot{\boldsymbol{q}}_n\vartheta_n - \int_V \rho\boldsymbol{u}dV\right]}_{\text{Momentum Discrepancy}}$$

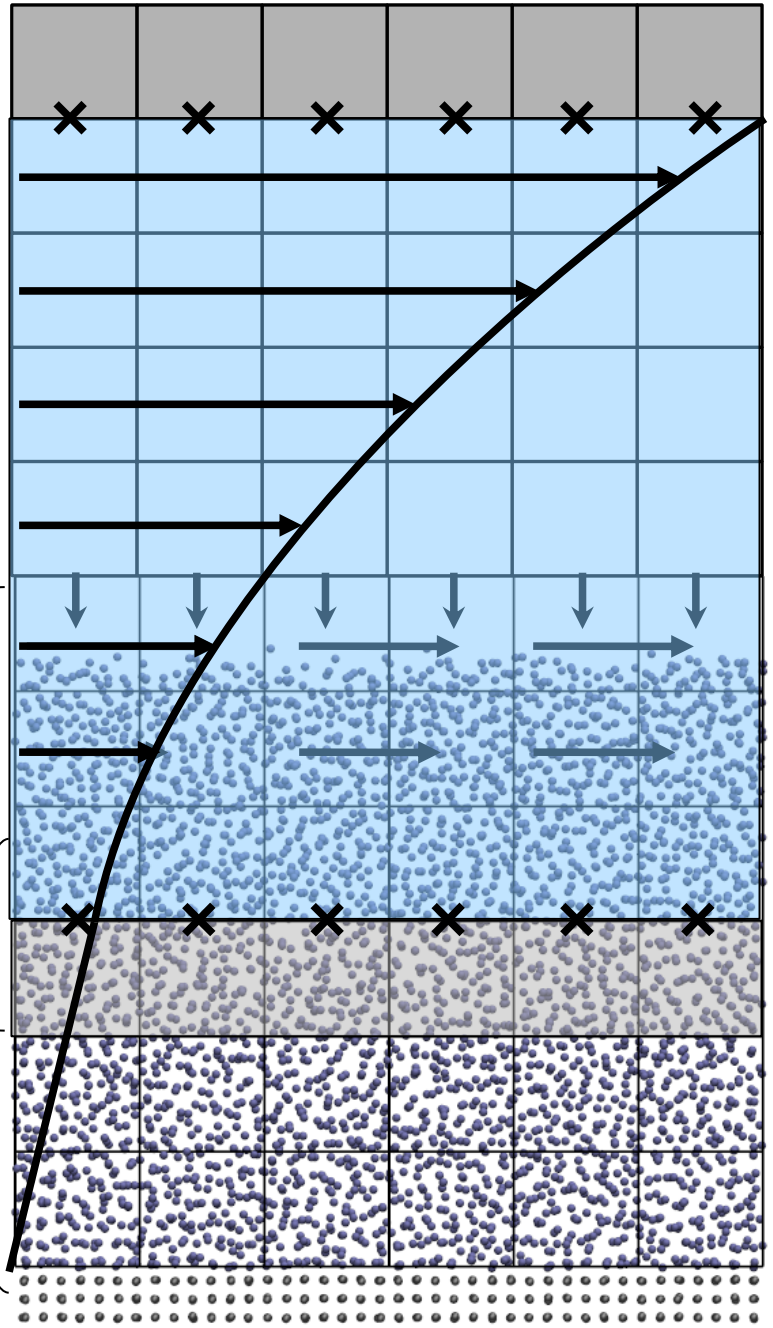
$$\overbrace{-\oint_S[\rho\boldsymbol{u}\boldsymbol{u}+P\boldsymbol{I}-\boldsymbol{\sigma}]\cdot d\boldsymbol{S}}$$

- **Includes both force and fluctuation terms***
- **Energy or Entropy CV equation could also be analysed/applied in a similar manner**
- * *Flekkoy, Delgado-Buscalioni and Coveney (2005)

Control Volume Coupling

- **Molecular Equations**

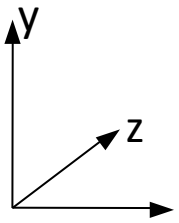
$$\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = -\oint_S \rho \boldsymbol{u}\boldsymbol{u}\cdot d\boldsymbol{S} - \sum_{i=1}^{N}(\boldsymbol{v}_i-\boldsymbol{u})(\boldsymbol{v}_i-\boldsymbol{u})\cdot d\boldsymbol{S}_i - \sum_{i=1}^{N}\sum_{j\neq i}^{N}\varsigma_{ij}\cdot d\boldsymbol{S}_{ij}$$



$$\rho u = \rho U_0$$

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

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



- **Continuum Equations**

Summary

- **Introduced a novel mathematical function to define a control volume in a discrete system**
  - Derived in a manner consistent with a continuum control volume
  - Mathematically well defined and applicable to any discrete system
- **Derivation of discrete CV conservation equation**
  - Allows control volume analysis to be extended to nano-scale systems
  - The resulting equations are exactly conservative in a discrete system
- **Application to Coupling**
  - Allows both systems to be written in a consistent framework
  - Averages from molecular region can be written in terms of continuum variables, e.g. surface fluxes
  - Facilitates derivation of constraint algorithms using minimisation principles

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- **References**

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Thank you for listening

Any Questions?

Future Aims

- **We have the mathematical framework to express both systems consistently**
  - Matching control volumes in both regions
  - Surface fluxes and stress in the CFD and MD are equivalent
- **Apply the extended CV constraint equations to derived exactly conservative coupling**
  - Total coupled system is exactly conservative
  - Energy and entropy changes can be evaluated exactly
- **Large scale coupling simulation**
  - Flexible computational coupling framework already developed for parallel MD and CFD codes
  - Simulate very large and highly non-linear problems using coupled molecular and continuum systems

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

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

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

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

  - Lagrangian mass conservation

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

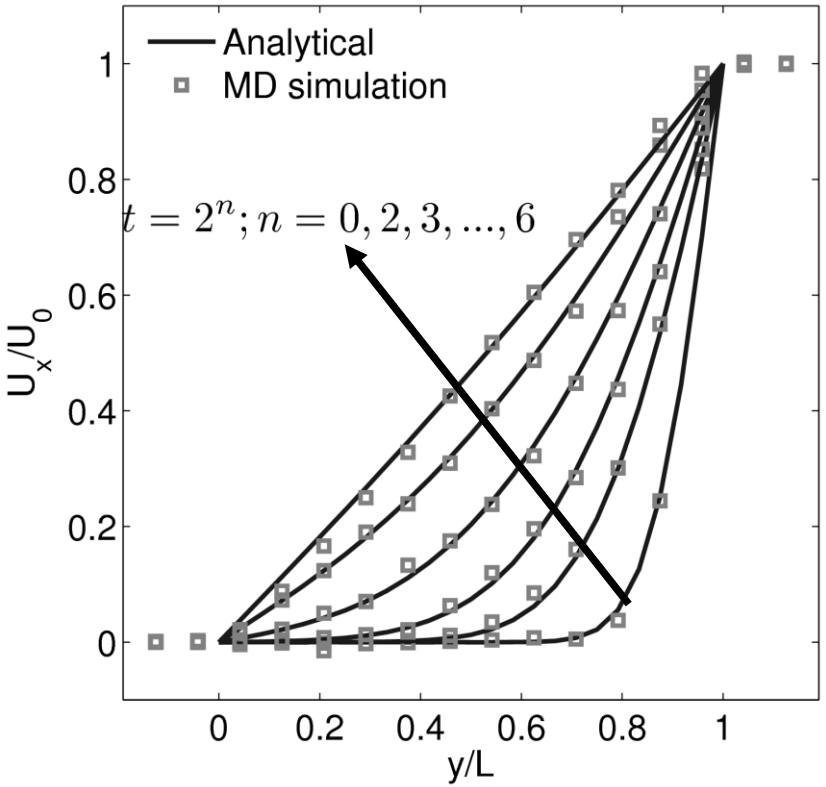
$$\frac{d}{dt}\sum_{i=1}^{N} m_i\vartheta_i = -\sum_{i=1}^{N} m_i\left(\mathbf{v}_i + \overline{\boldsymbol{u}}\right)\cdot d\boldsymbol{S}_i$$

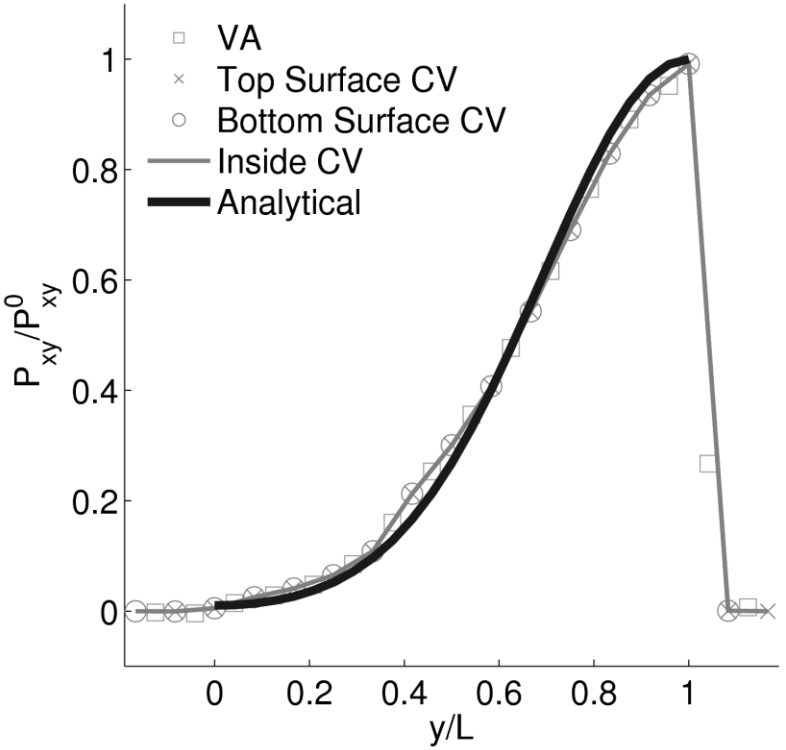
$$\frac{d}{dt}\int_V \rho dV = \oint_S \rho\left(\boldsymbol{u} - \overline{\boldsymbol{u}}\right)\cdot d\boldsymbol{S}$$

$$\overline{\boldsymbol{u}}\cdot d\boldsymbol{S}_i = \frac{d\boldsymbol{r}}{dt}\cdot\frac{d\vartheta_i}{d\boldsymbol{r}}$$

$$\oint_S \rho\boldsymbol{u}\cdot d\boldsymbol{S} - \oint_S \rho\overline{\boldsymbol{u}}\cdot d\boldsymbol{S} = 0$$

Continuum Analytical Couette Flow





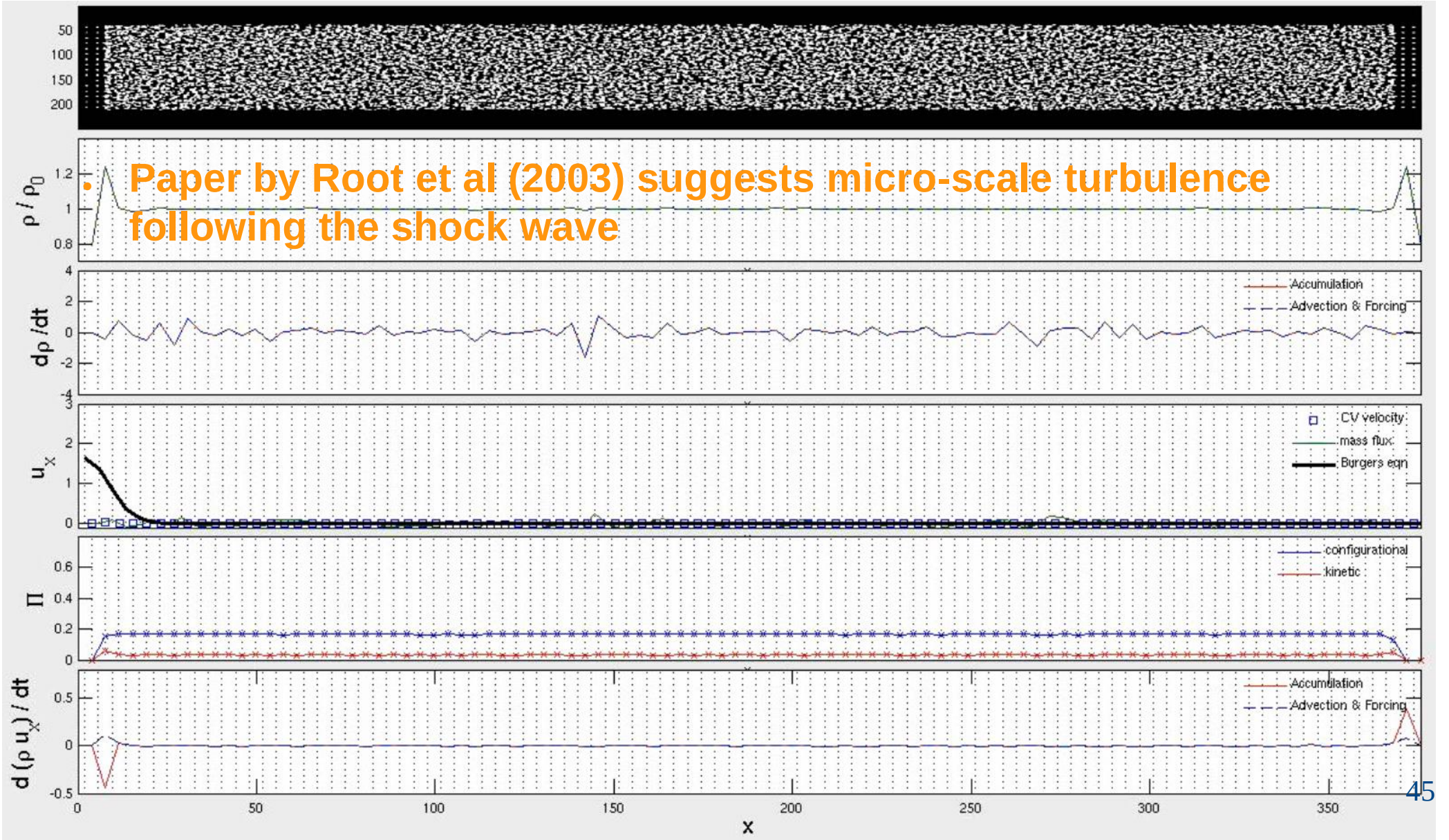
$$u_x(y,t) = \begin{cases} U_0 & y = L \\ \sum_{n=1}^{\infty} u_n(t) sin\left(\frac{n\pi y}{L}\right) & 0 < y < L \\ 0 & y = 0 \end{cases}$$

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

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

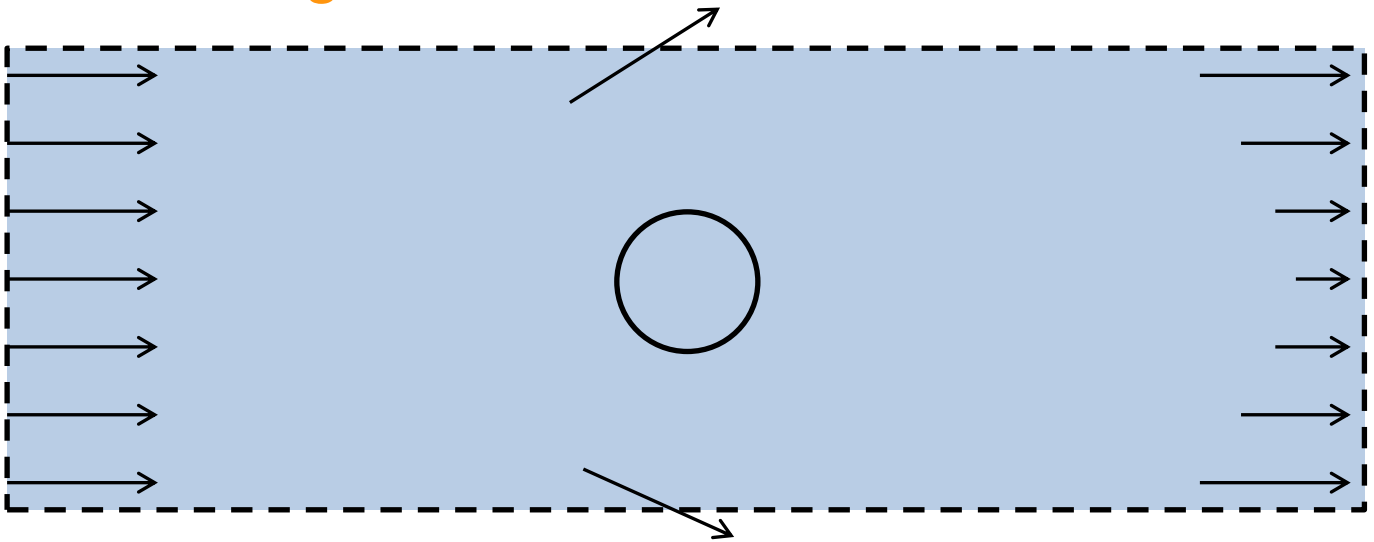
Shockwaves

- Current work on application of control volume theory



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