Linking the Continuous and the Discrete

Coupling Molecular Dynamics to Continuum Fluid Mechanics

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Outline

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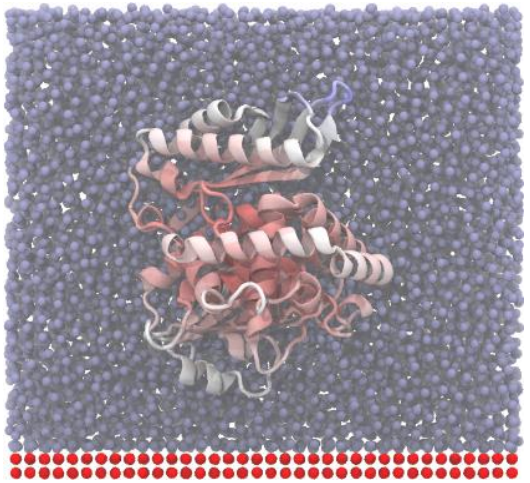
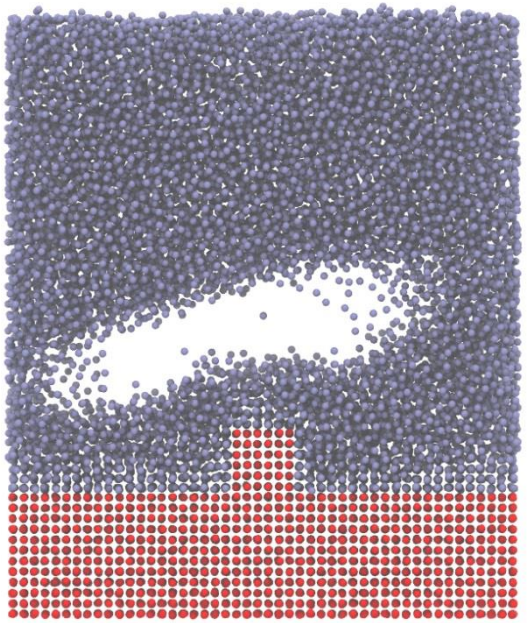
  - Motivation for coupling
  - Molecular dynamics (MD)
  - Computational fluid dynamics (CFD)
- **Mathematical Formulation for Coupling**
  - Irving and Kirkwood (1950)
  - The control volume function
  - Coupling using Hamilton's principle
- **Computational Developments**
  - The molecular dynamics solver
  - The computational fluid dynamics solver
  - The CPL_Library (open source)

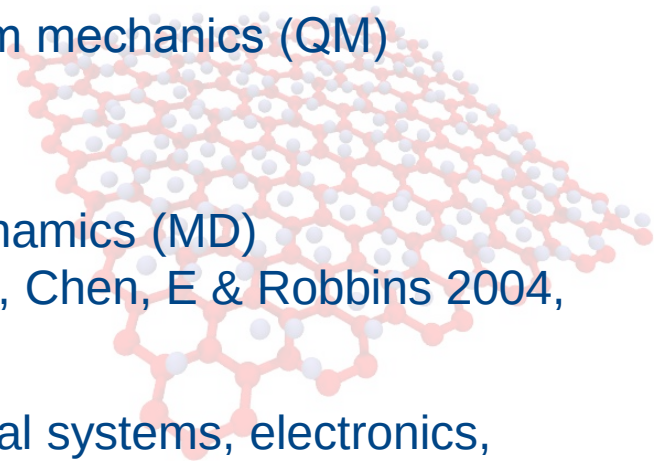




Introduction

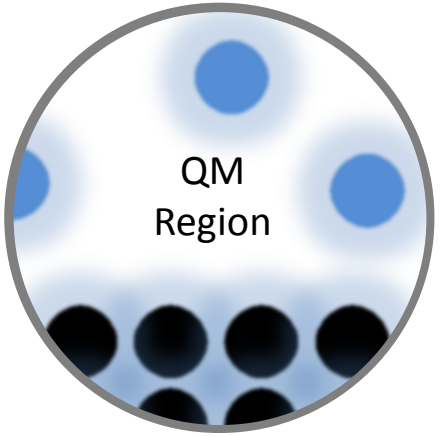
Motivation

- **Modern engineering problems require sub-continuum models**
  - Quantum mechanics is limited to very small systems
  - Even Molecular dynamics is still prohibitively expensive
  - Multi-scale coupling overcomes these limitations by linking to cheaper methods
  - Quantum mechanics ↔ Molecular dynamics (MD) (Karplus, Levitt and Warshel)
- **Multi-scale coupling has been employed since the 1970's (Curtin & Miller 2003) in solid mechanics modelling (*e.g.* for crack tips)**
  - Essential to fully capture both the complicated detail in the crack and the impact on the wider system
  - Continuum ↔ Molecular mechanics (MM) ↔ Quantum mechanics (QM)
- **Classical coupling for fluids is less mature**
  - Computational fluid dynamics (CFD) ↔ Molecular dynamics (MD) (O'Connell & Thompson 1995, Flekkøy et al 2000, Nie, Chen, E & Robbins 2004, Delgado-Buscalioni & Coveney, 2004)
  - Important for *e.g.* flow over carbon allotropes, biological systems, electronics, chemical reactions and combustion



Motivation

- **Long term goal is to seamlessly link various scales of modelling**
  - Fine/coarse graining as required based on the problem of interest
  - Dynamic resource allocation and load balancing on multi-core architectures



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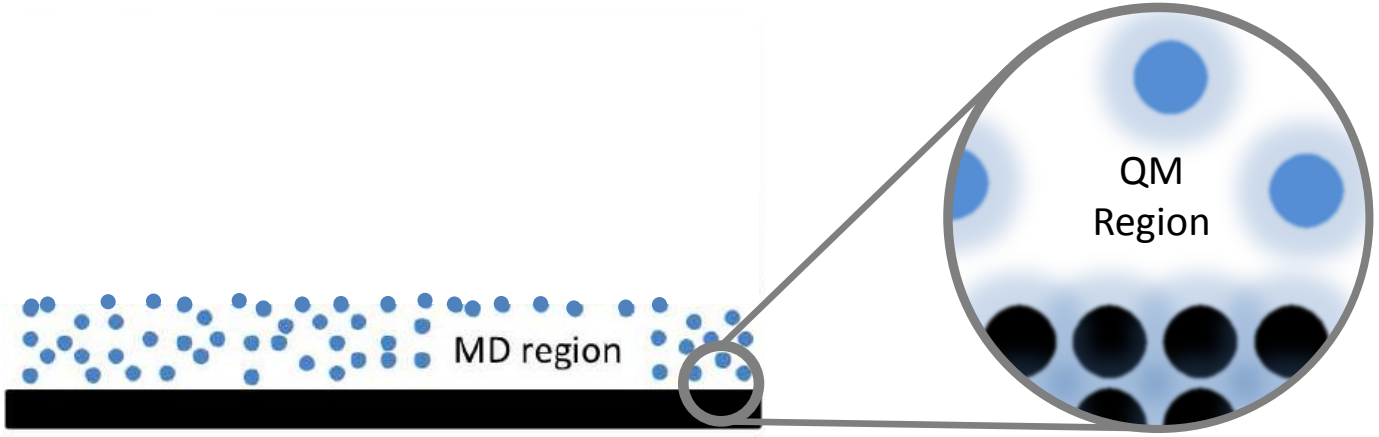

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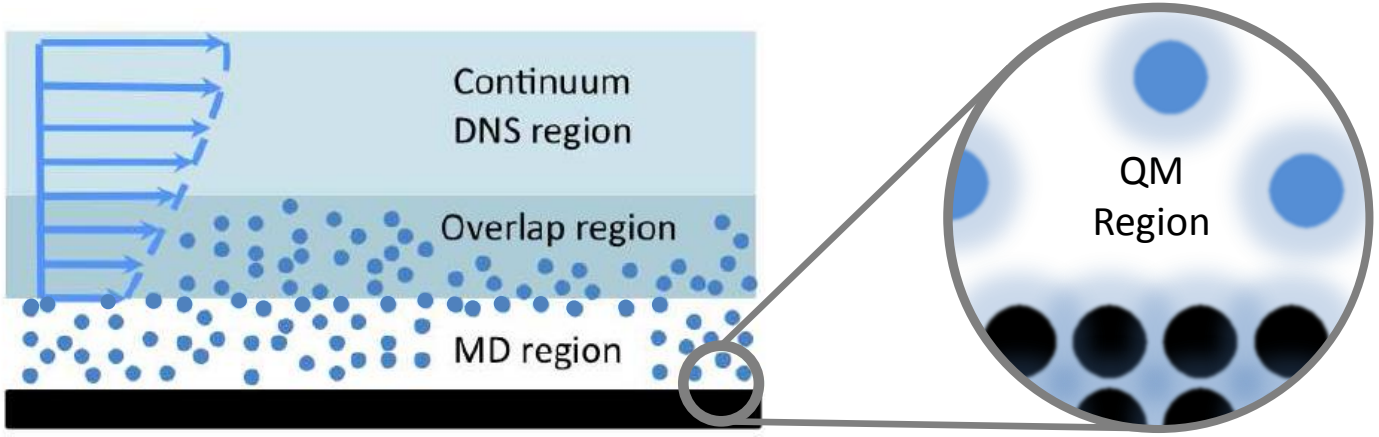

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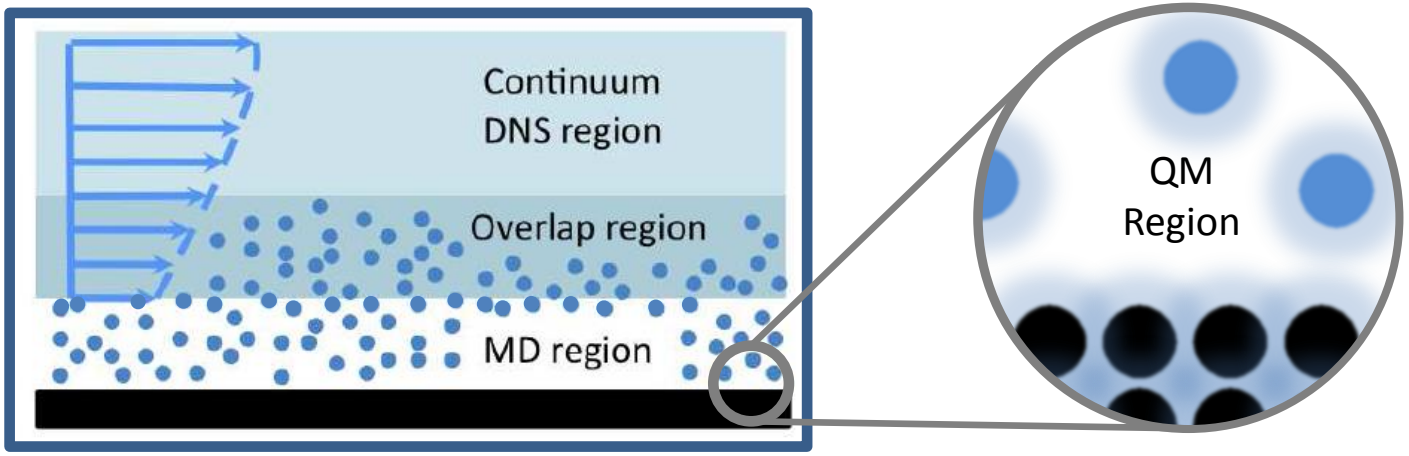
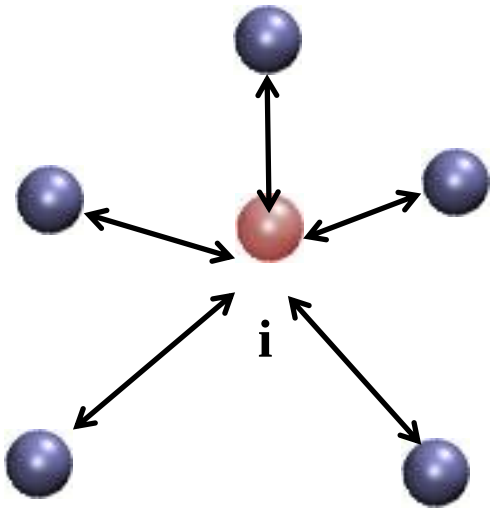


- **Solving similar and relevant problems to quantum mechanics**
  - Relationship between the mathematical framework used to describe a continuous field and a discrete system (The Dirac delta function)
  - Ensuring the dynamics agree in both systems in a physically meaningful manner
  - Interfacing of computational solvers and data exchange
  - Extend the range of quantum modelling, via MD-CFD coupling

Discrete Models (Molecular Dynamics)

- **Discrete molecules in continuous space**
  - Molecular position evolves continuously in time
  - Position and velocity from acceleration

$$\ddot{\boldsymbol{r}}_i \longrightarrow \dot{\boldsymbol{r}}_i$$
$$\dot{\boldsymbol{r}}_i \longrightarrow \boldsymbol{r}_i(t)$$

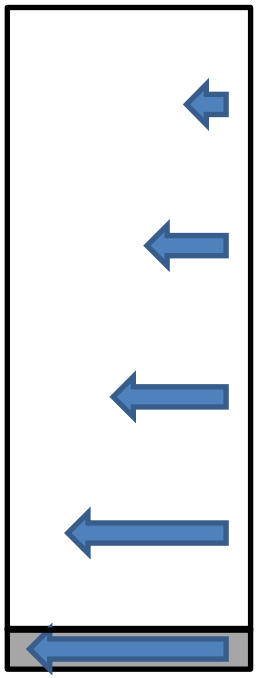


- **Acceleration obtained from forces**
  - Governed by Newton's law for an N-body system
  - Point particles with pairwise interactions only

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

$$\Phi(r_{ij}) = 4\epsilon \left[\left(\frac{\ell}{r_{ij}} \right)^{12} - \left(\frac{\ell}{r_{ij}} \right)^{6} \right]$$

Discrete Models (Molecular Dynamics)



Molecular Dynamics Simulation of Couette Flow

Continuum Field Equations

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

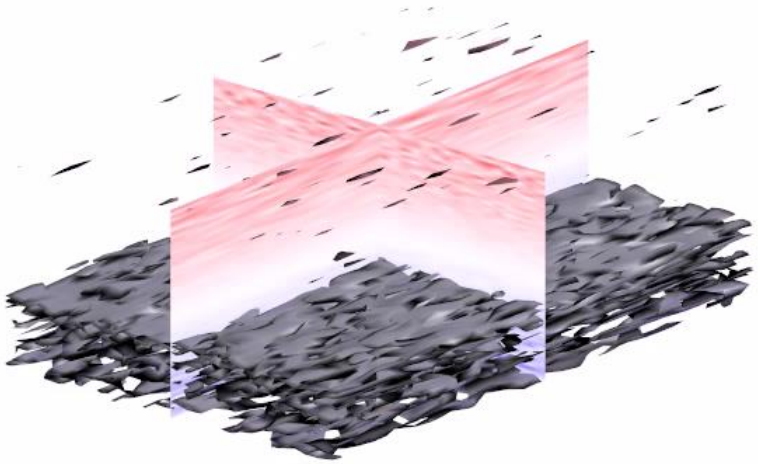
$$\frac{\partial \rho}{\partial t} = -\boldsymbol{\nabla} \cdot \rho \boldsymbol{u}$$

  - 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

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

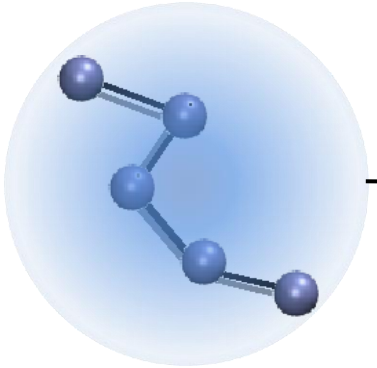


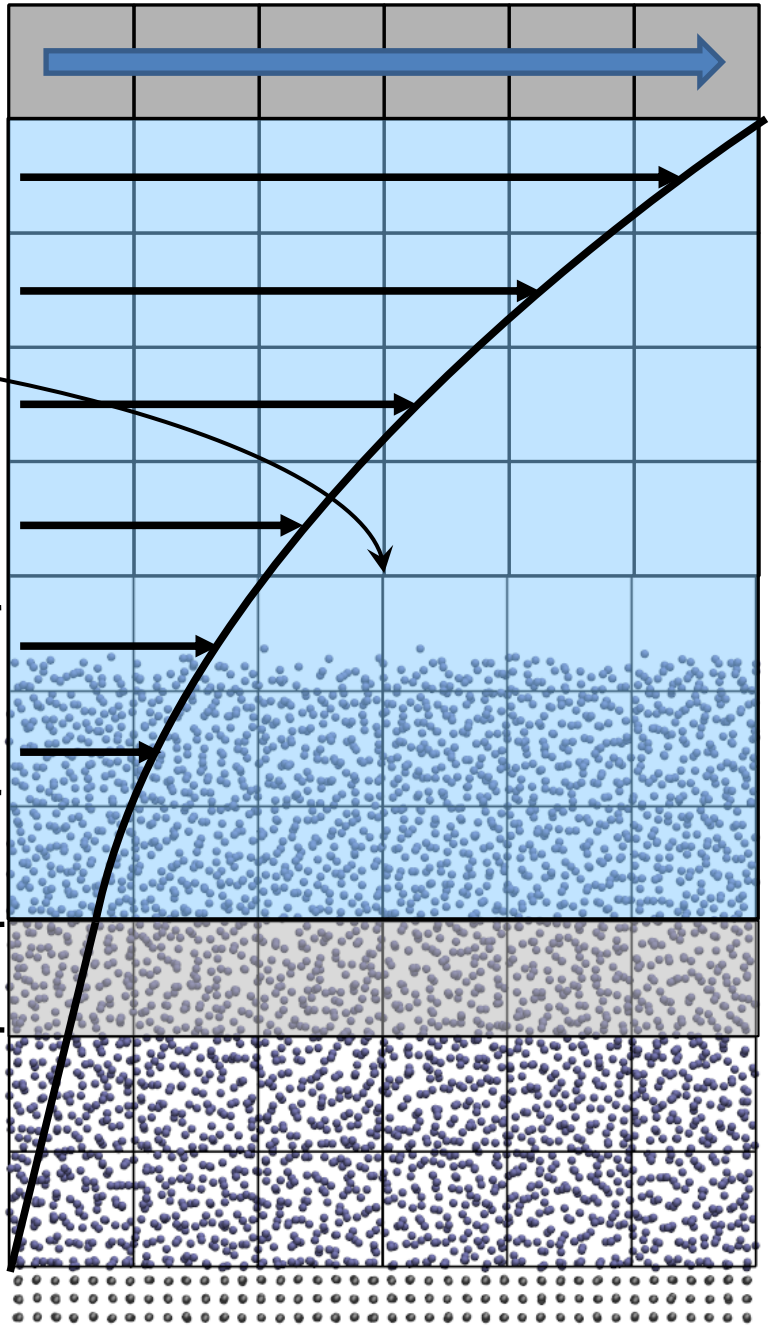
Direct Numerical Simulation of Turbulent Couette Flow

Mathematical Formulation for Coupling

Coupling Schematic

Insertion of molecules





Consistent Framework

CFD→MD Boundary condition

MD→CFD Boundary condition

$$m_i\ddot{\boldsymbol{r}}_i = \mathbf{F}_i \overset{?}{\Longleftrightarrow} \frac{\partial}{\partial t}\rho\boldsymbol{u} + \boldsymbol{\nabla}\cdot\rho\boldsymbol{u}\boldsymbol{u} = \boldsymbol{\nabla}\cdot\boldsymbol{\Pi}$$

Irving and Kirkwood (1950)

$$\left\langle \alpha; f \right\rangle \equiv \int \cdots \int \alpha(\boldsymbol{r}^N, \boldsymbol{p}^N) f(\boldsymbol{r}^N, \boldsymbol{p}^N, t) d\boldsymbol{r}^N d\boldsymbol{p}^N$$

$$\frac{\partial}{\partial t}\left\langle \alpha; f \right\rangle = \sum_{i=1}^{N} \left\langle \frac{\boldsymbol{p}_i}{m_i} \cdot \frac{\partial \alpha}{\partial \boldsymbol{r}_i} + \boldsymbol{F}_i \cdot \frac{\partial \alpha}{\partial \boldsymbol{p}_i}; f \right\rangle$$

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

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

Irving and Kirkwood (1950) cont.

- **Density in the molecular system is defined**

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

- **Time evolution from the Irving and Kirkwood procedure**

$$\frac{\partial}{\partial t}\left\langle \alpha;f\right\rangle=\sum_{i=1}^{N}\left\langle \frac{\boldsymbol{p}_i}{m_i}\cdot\frac{\partial\alpha}{\partial\boldsymbol{r}_i}-\boldsymbol{F}_i\cdot\frac{\partial\alpha}{\partial\boldsymbol{p}_i};f\right\rangle \qquad \alpha=\sum_{i=1}^{N}m_i\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right)$$

$$\frac{\partial}{\partial t}\sum_{i=1}^{N}\left\langle m_i\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right);f\right\rangle=\sum_{i=1}^{N}\left\langle \frac{\boldsymbol{p}_i}{m_i}\cdot\frac{\partial}{\partial\boldsymbol{r}_i}m_i\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right)\right.$$

$$\left.-\boldsymbol{F}_i\cdot\frac{\partial}{\partial\boldsymbol{p}_i}m_i\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right);f\right\rangle$$

$$=-\frac{\partial}{\partial\boldsymbol{r}}\cdot\sum_{i=1}^{N}\left\langle \boldsymbol{p}_i\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right);f\right\rangle$$

Mass Conservation Equation

- **Continuum mass conservation**

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

- **Molecular Equivalent**

$$\underbrace{\frac{\partial}{\partial t} \sum_{i=1}^{N} \left\langle m_i \delta \left(\boldsymbol{r} - \boldsymbol{r}_i \right) ; f \right\rangle}_{\rho} = -\boldsymbol{\nabla} \cdot \underbrace{\sum_{i=1}^{N} \left\langle \boldsymbol{p}_i \delta \left(\boldsymbol{r} - \boldsymbol{r}_i \right) ; f \right\rangle}_{\rho \boldsymbol{u}}$$

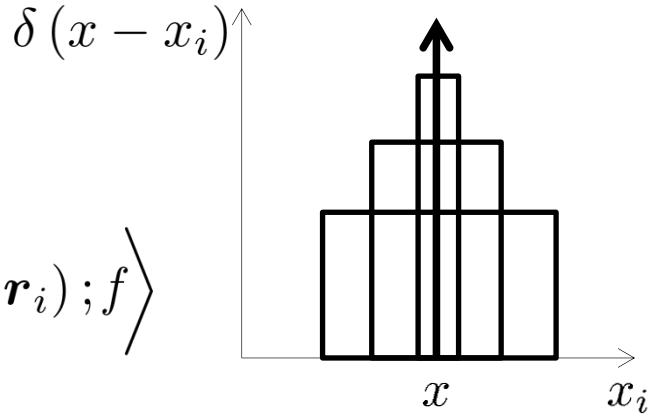
- **Similarly for the time evolution of momentum (and beyond)**

$$\frac{\partial}{\partial t} \rho \boldsymbol{u} = -\boldsymbol{\nabla} \cdot \left[\rho \boldsymbol{u} \boldsymbol{u} + \boldsymbol{\Pi} \right]$$

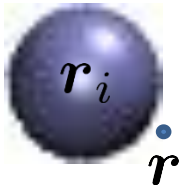
Selecting Functions

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

$$\nabla \cdot \boldsymbol{A} \equiv \lim_{V \to 0} \frac{1}{V} \oint_S \boldsymbol{A} \cdot d\mathbf{S} \qquad \rho(\boldsymbol{r}, t) = \sum_{i=1}^{N} \left\langle m_i \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right); f \right\rangle$$

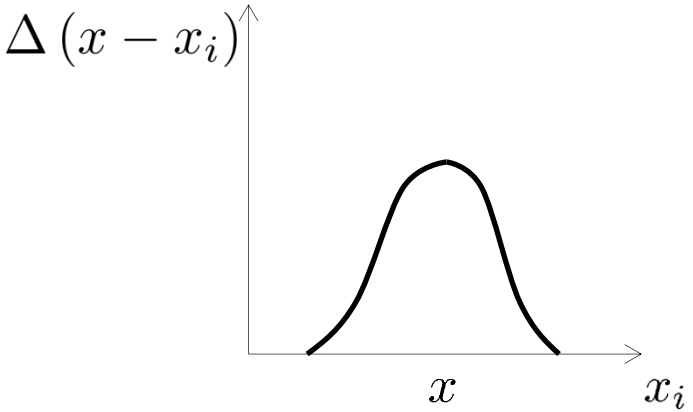


- **In a molecular simulation r is never exactly equal to r_i**
  - Other difficulties with the Dirac delta function



- **Relaxed weighting functions**
  - By Hardy(1981), Hoover (2009), Murdoch (2010) and others

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



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The Control Volume (CV)

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

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

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

  - Momentum Balance (Newton's Law)

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

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

  - Energy Conservation

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

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

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

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

Control Volume Function

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

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

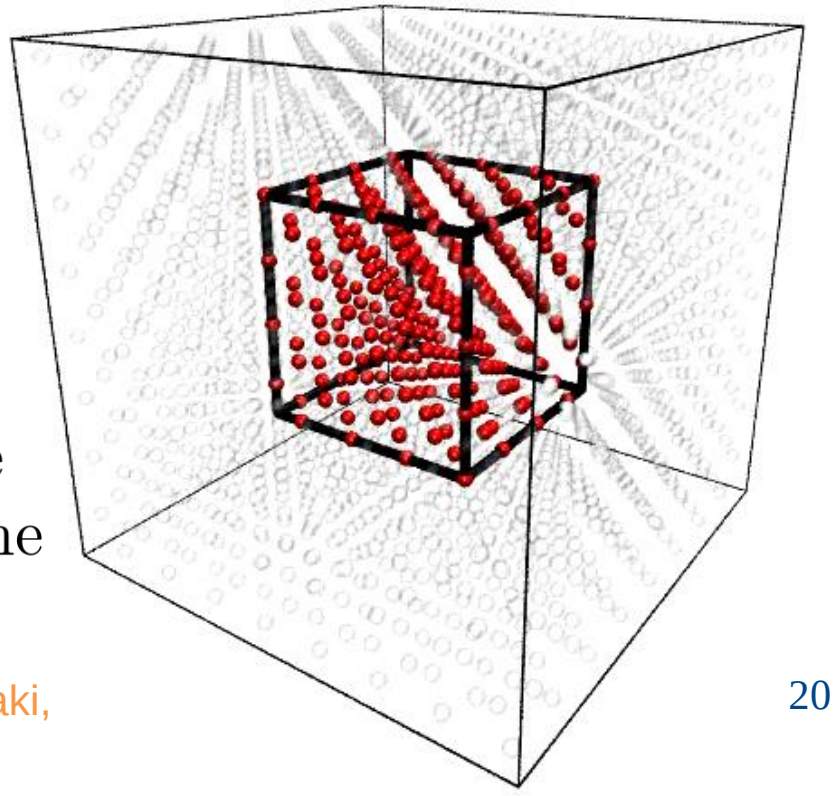
$$= \left[H(x^+ - x_i) - H(x^- - x_i)\right]$$

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

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

- **Or in words**

$$\vartheta \equiv \begin{cases} 1 & \text{if molecule is inside volume} \\ 0 & \text{if molecule is outside volume} \end{cases}$$



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**

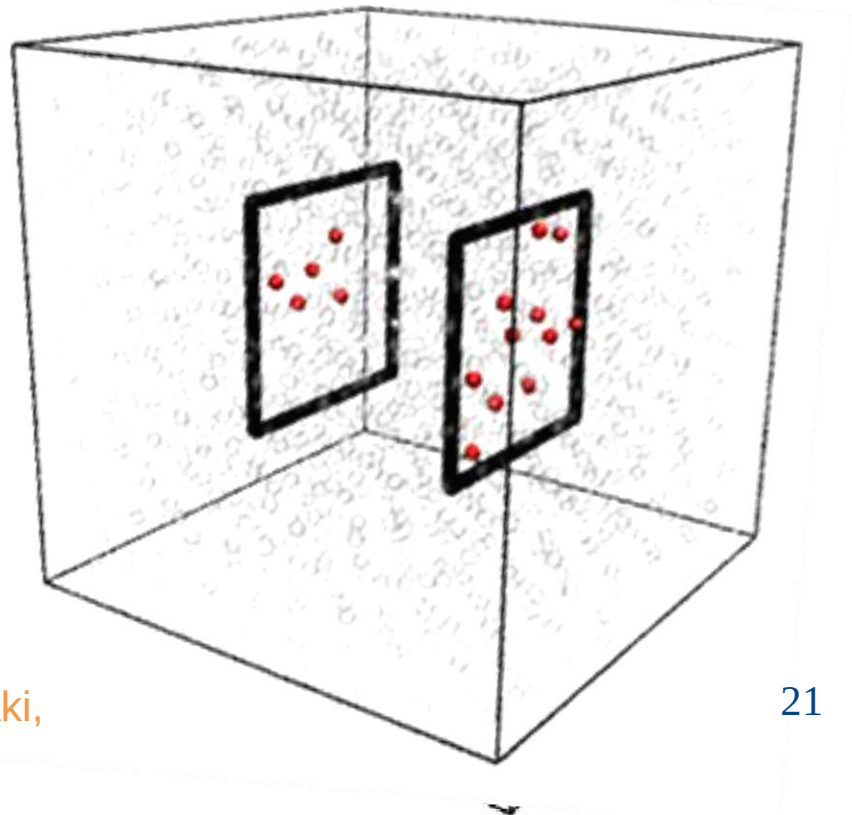
$$dS_{ix} \equiv -\frac{\partial \vartheta_i}{\partial x_i} = \left[\delta(x^+ - x_i) - \delta(x^- - x_i)\right] \times \left[H(y^+ - y_i) - H(y^- - y_i)\right] \times \left[H(z^+ - z_i) - H(z^- - z_i)\right]$$

- **Vector form defines six surfaces**

$$d\mathbf{S}_i = \boldsymbol{i} dS_{xi} + \boldsymbol{j} dS_{yi} + \boldsymbol{k} dS_{zi}$$

- **Or in words**

$$d\mathbf{S}_i \equiv \begin{cases} \infty & \text{if molecule on surface} \\ 0 & \text{otherwise} \end{cases}$$



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Applying the Control Volume Function

- **Molecular mass in a control volume can be defined**

$$\frac{\partial}{\partial t}\int_V \rho dV = \frac{\partial}{\partial t}\sum_{i=1}^{N}\left\langle m_i\vartheta_i; f\right\rangle \qquad \frac{\partial}{\partial t}\int_V \rho dV = -\oint_S \rho \boldsymbol{u}\cdot d\mathbf{S}$$

- **Simple mathematical operations using the control volume function**

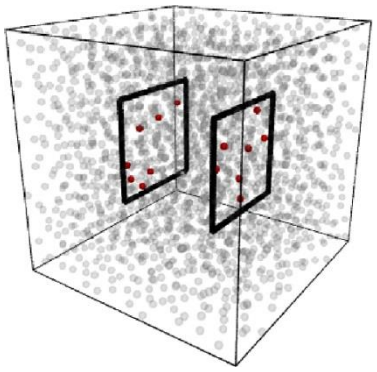
$$\frac{\partial}{\partial t}\left\langle \alpha; f\right\rangle = \sum_{i=1}^{N}\left\langle \frac{\boldsymbol{p}_i}{m_i}\cdot\frac{\partial\alpha}{\partial \boldsymbol{r}_i} - \boldsymbol{F}_i\cdot\frac{\partial\alpha}{\partial \boldsymbol{p}_i}; f\right\rangle \qquad \alpha = \sum_{i=1}^{N} m_i\vartheta_i$$

$$\frac{\partial}{\partial t}\sum_{i=1}^{N}\left\langle m_i\vartheta_i; f\right\rangle = \sum_{i=1}^{N}\left\langle \frac{\boldsymbol{p}_i}{m_i}\cdot\frac{\partial m_i\vartheta_i}{\partial \boldsymbol{r}_i} - \boldsymbol{F}_i\cdot\frac{\partial m_i\vartheta_i}{\partial \boldsymbol{p}_i}; f\right\rangle$$

$$= \sum_{i=1}^{N}\left\langle \boldsymbol{p}_i\cdot\frac{\partial\vartheta_i}{\partial \boldsymbol{r}_i}; f\right\rangle$$

$$= -\sum_{i=1}^{N}\left\langle \boldsymbol{p}_i\cdot d\boldsymbol{S}_i; f\right\rangle$$

$3\times$



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

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = -\sum_{i=1}^{N} m_i \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i + \frac{1}{2}\sum_{i,j}^{N} \boldsymbol{f}_{ij}\vartheta_{ij}$$

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

  - Energy Conservation

$$\frac{d}{dt}\sum_{i=1}^{N} e_i \vartheta_i = -\sum_{i=1}^{N} e_i \mathbf{v}_i \cdot d\mathbf{S}_i + \frac{1}{2}\sum_{i=1}^{N}\sum_{i\neq j}^{N} \frac{\mathbf{p}_i}{m_i} \cdot \boldsymbol{f}_{ij}\vartheta_{ij}$$

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

Reynolds' Transport Theorem

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

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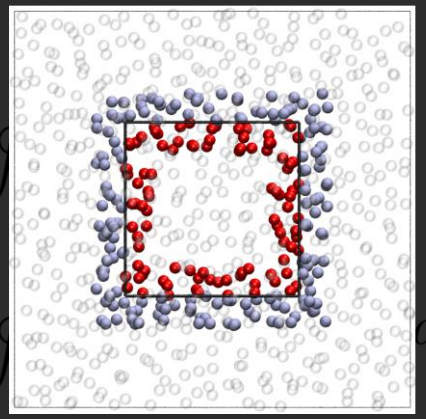
$$\frac{\partial}{\partial t}\int_V \rho\mathcal{E}dV = -\oint \ldots - \oint \ldots d\mathbf{S}$$

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

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

- **This is the IK operator for a CV**

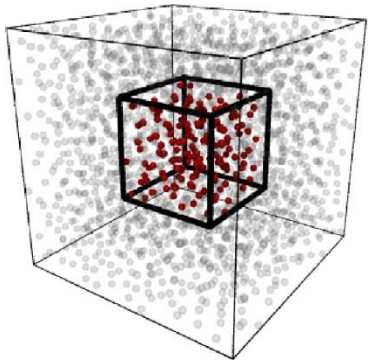


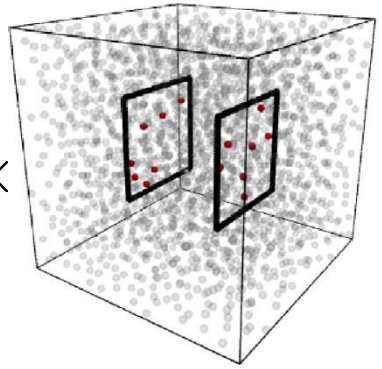
Testing Momentum Balance

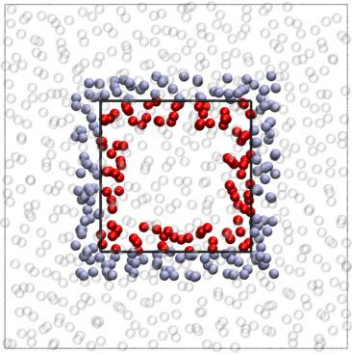
- **Momentum Balance**

$$\underbrace{\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i =}_{\text{Accumulation}} \quad + \underbrace{\sum_{i=1}^{N} m \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i}_{\text{Advection}} \quad - \underbrace{\frac{1}{2}\sum_{i,j}^{N} \boldsymbol{f}_{ij} \vartheta_{ij}}_{\text{Forcing}} \quad = 0$$

$$\frac{d}{dt} \quad + \; 3\times \quad - \quad = 0$$







The Pressure Tensor

- **Continuum Control Volume equations in terms of the pressure tensor**

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

$$\mathbf{F}_{\text{surface}} = -\frac{\partial}{\partial \boldsymbol{r}}\cdot\int_V \boldsymbol{\Pi} dV \qquad -\oint_S \boldsymbol{\Pi}\cdot d\boldsymbol{S}$$

- **Molecular Control Volume equations in terms of the pressure tensor**

Volume Average
(Lutsko 1988 & Cormier et al 2001)

$$\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = -\sum_{i=1}^{N} m_i \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i + \frac{1}{2}\sum_{i,j}^{N} \boldsymbol{f}_{ij}\vartheta_{ij}$$

$$\frac{1}{2}\sum_{i,j}^{N} \boldsymbol{f}_{ij}\vartheta_{ij} = -\frac{\partial}{\partial \boldsymbol{r}}\cdot\frac{1}{2}\sum_{i,j}^{N} \boldsymbol{f}_{ij}\boldsymbol{r}_{ij}\int_0^1 \vartheta_s ds \qquad -\frac{1}{4}\sum_{i,j}^{N} \boldsymbol{\varsigma}_{ij}\cdot d\mathbf{S}_{ij}$$

Method of planes
(Todd et al 1995, Han & Lee 2004)

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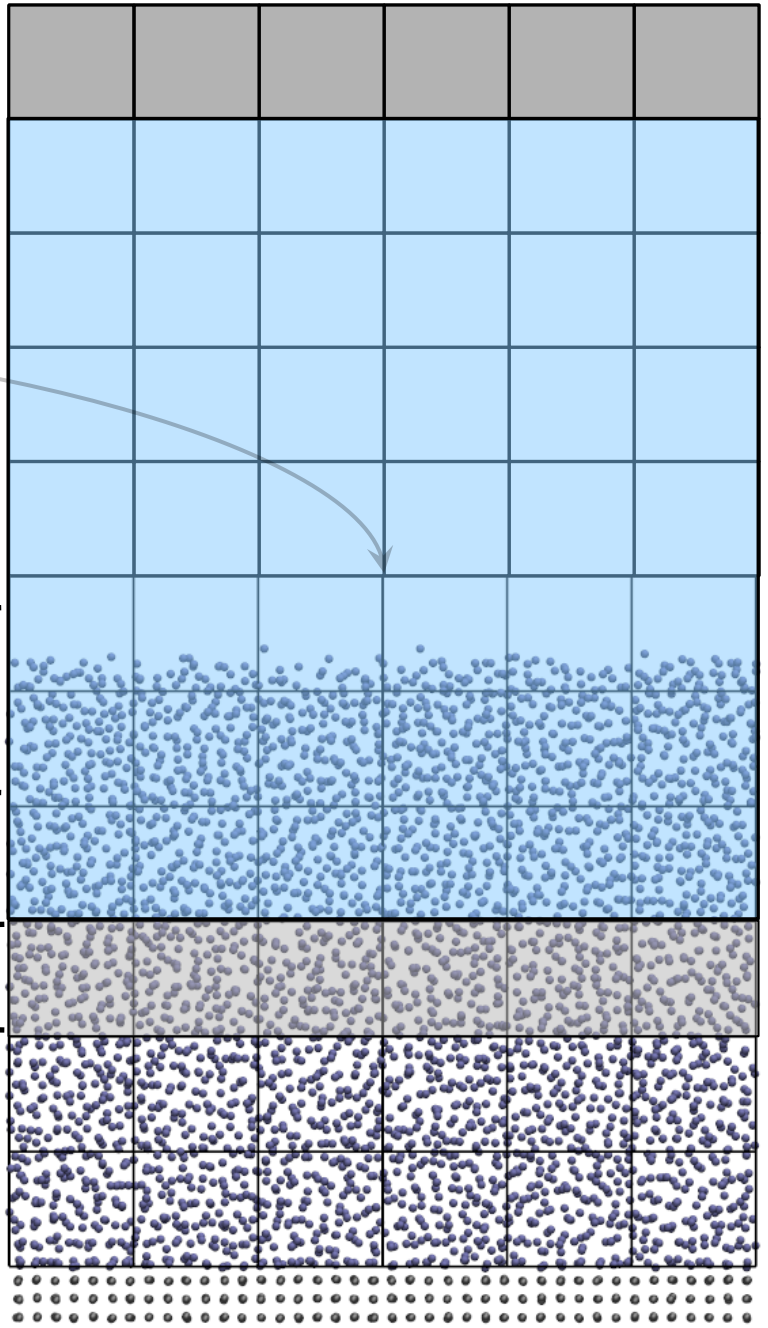
Coupling Using the Control Volume

Insertion of molecules



CFD→MD Boundary condition

Consistent Framework ✓

MD→CFD Boundary condition

Coupling Using the Control Volume

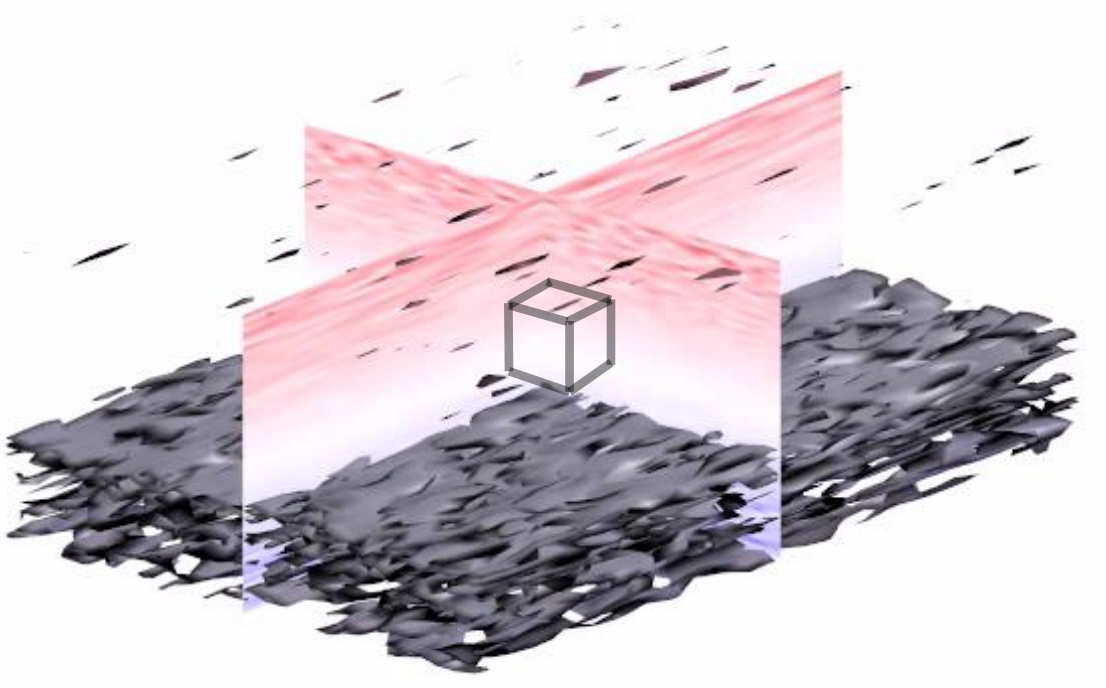
- **We now have an equivalent description in both regions**
  - Momentum or stresses inside an arbitrary control volume in both domains

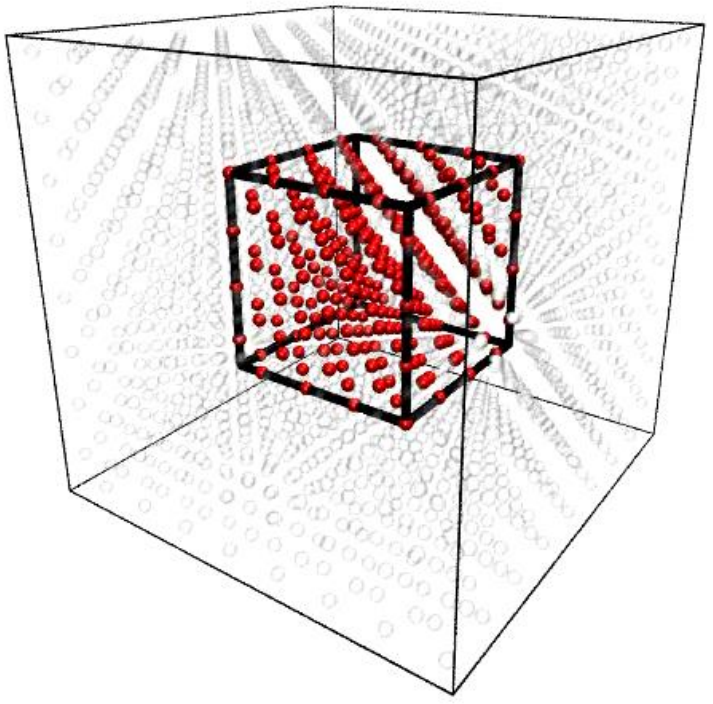
$$\int_V \rho u dV = \sum_{i=1}^{N} m_i \dot{\boldsymbol{r}}_i \vartheta_i$$

$$\oint_S \boldsymbol{\Pi} \cdot d\boldsymbol{S} = \frac{1}{4} \sum_{i,j}^{N} \boldsymbol{\varsigma}_{ij} \cdot d\mathbf{S}_{ij}$$

State Coupling : O'Connell & Thompson (1995), Nie, Chen, E & Robbins (2004)

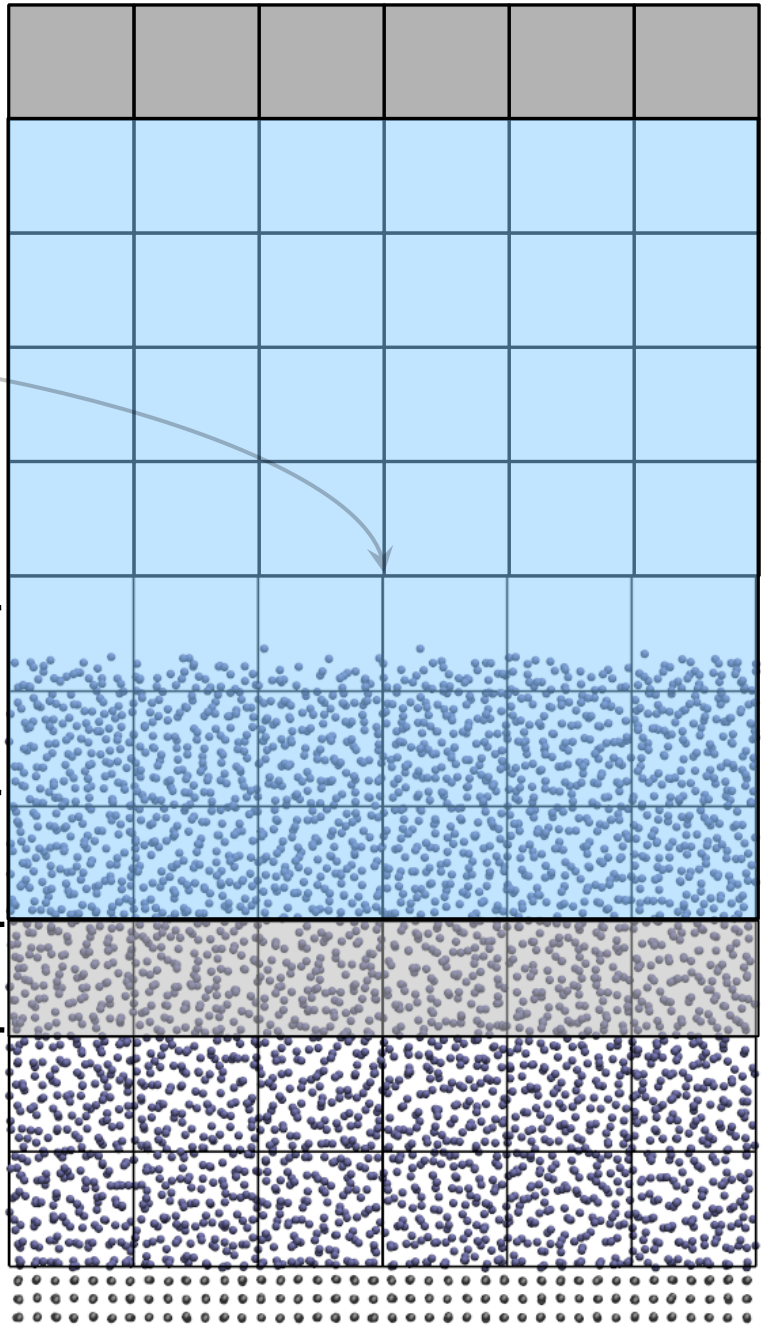
Flux Coupling: Flekkøy et al (2000), Delgado-Buscalioni & Coveney, (2004)





Coupling Using the Control Volume

Insertion of molecules



CFD→MD Boundary condition

Consistent Framework ✓

MD→CFD Boundary condition ✓

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

Constrained Control Volume

- **Non-unique solution**
  - Continuum field properties must specify N molecules
- **Hamilton's principle (subject to a constraint)**
  - As close as possible to the true trajectory
  - Used in the first fluids coupling scheme (O'Connell and Thompson 1995)

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

- **But now we want to apply a constraint localised using the control volume function**
  - CV function takes care of the localisation for us

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

Principle of least action

- **The Euler-Lagrange equation is applicable**
  - As the constraint is semi-holonomic (Flannery 2004,2011)

$$\frac{d}{dt}\frac{\partial \mathcal{L}_c}{\partial \dot{q}_i} - \frac{\partial \mathcal{L}_c}{\partial q_i} = 0 \qquad \mathcal{L}_c = \mathcal{L} + \boldsymbol{\lambda} \cdot \boldsymbol{g}$$

- **Written in terms of canonical momentum and its time derivative**

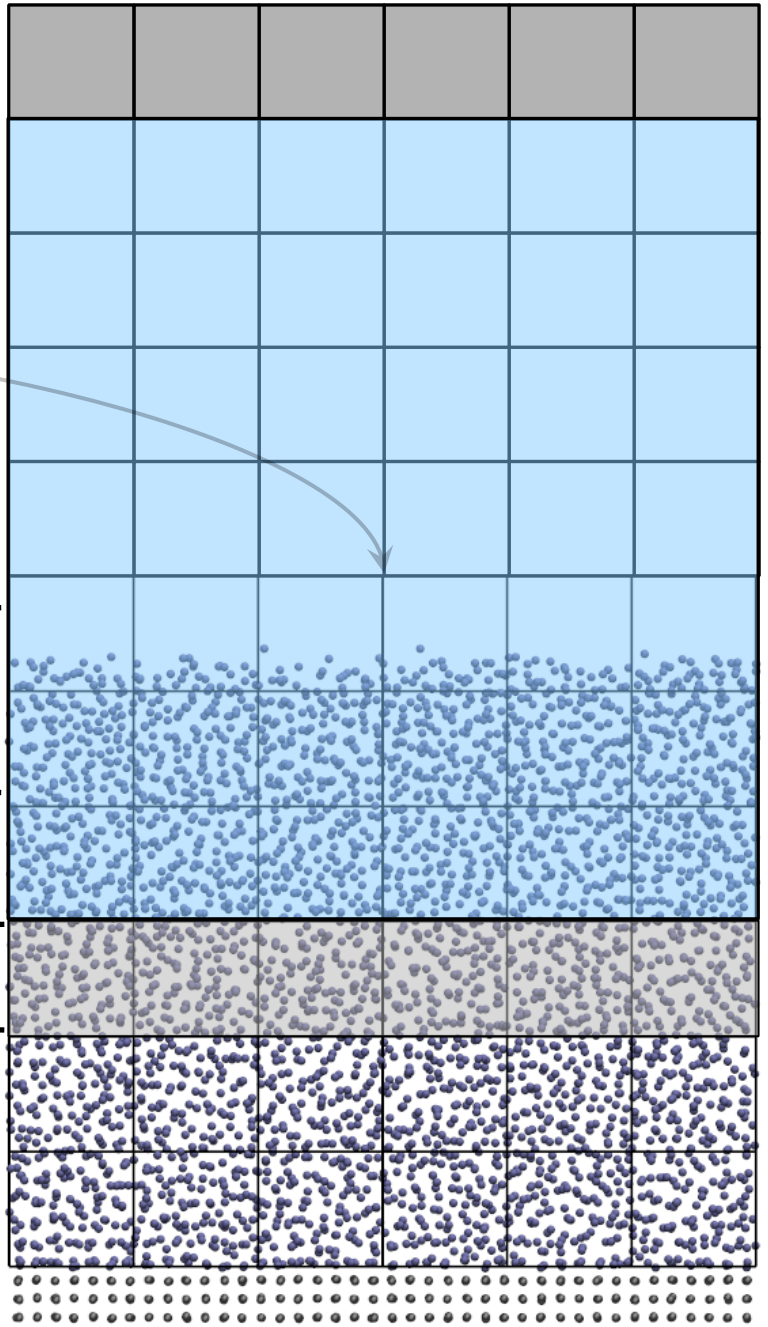
$$p_i = \frac{\partial \mathcal{L}_c}{\partial \dot{q}_i}$$

$$\dot{p}_i = \frac{\partial \mathcal{L}_c}{\partial q_i}$$

- **To give equations of motions**
  - Applying the MD boundary condition based on Hamilton's principle
  - Localised to a region in space (courtesy of the CV function)
  - No energy added to the system when applied correctly (i.e. with the CV function)

Coupling Using the Control Volume

Insertion of molecules

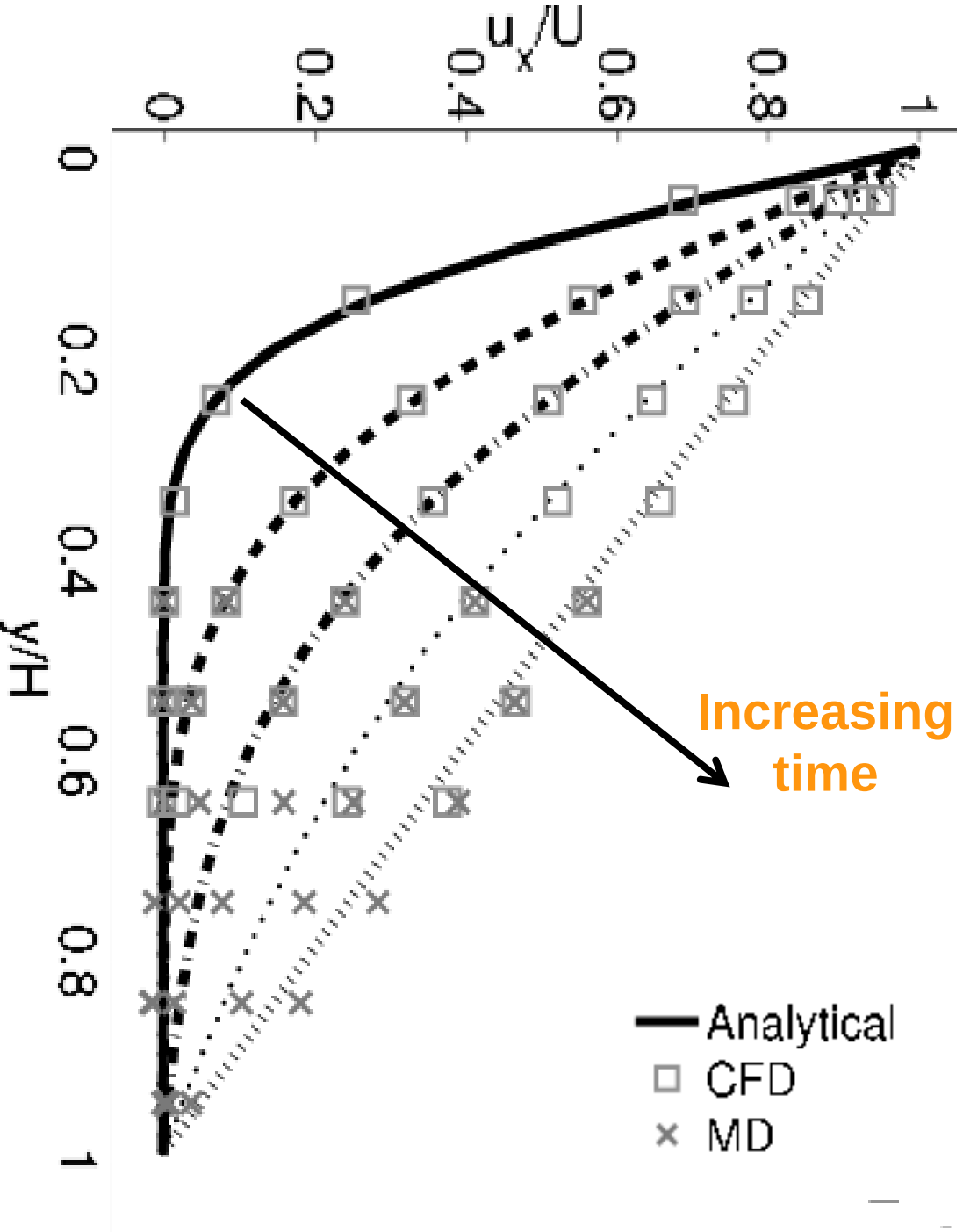


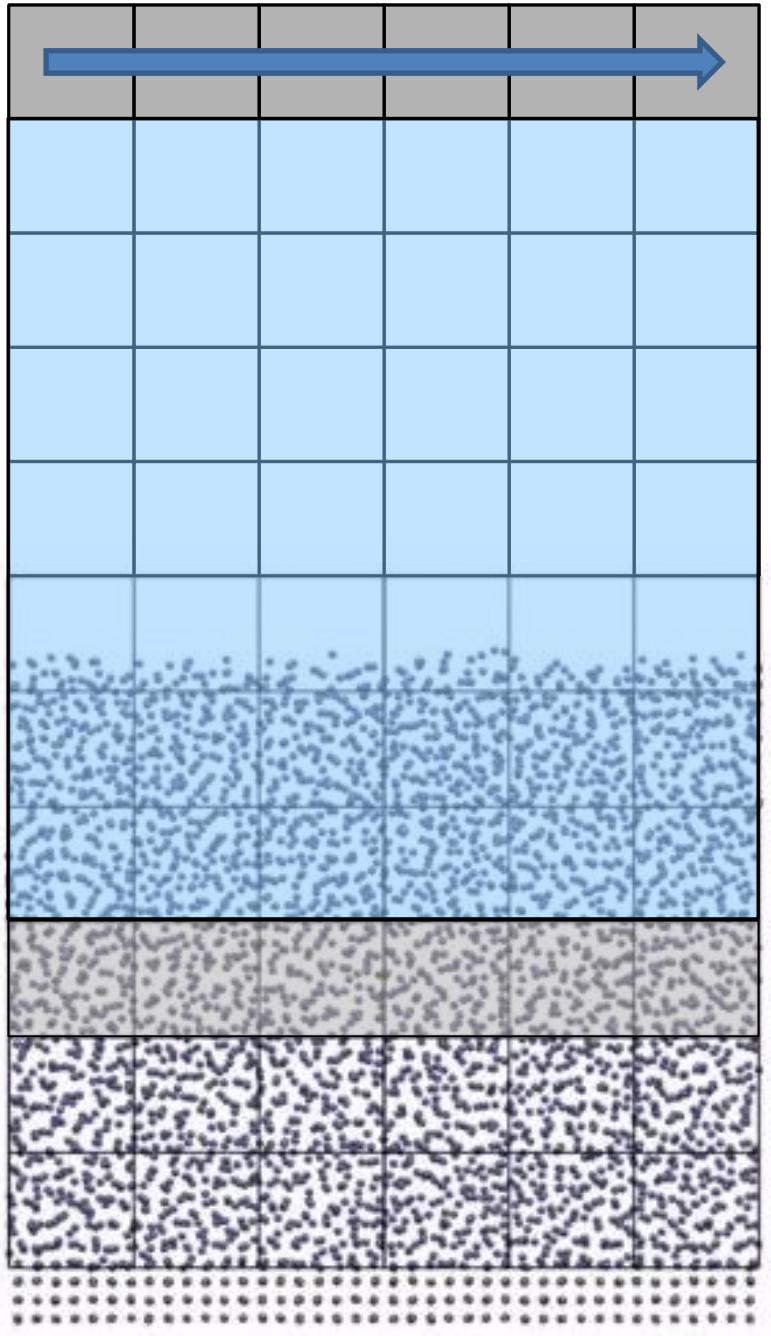
CFD→MD Boundary condition ✓

MD→CFD Boundary condition ✓

Consistent Framework ✓

Coupling Results

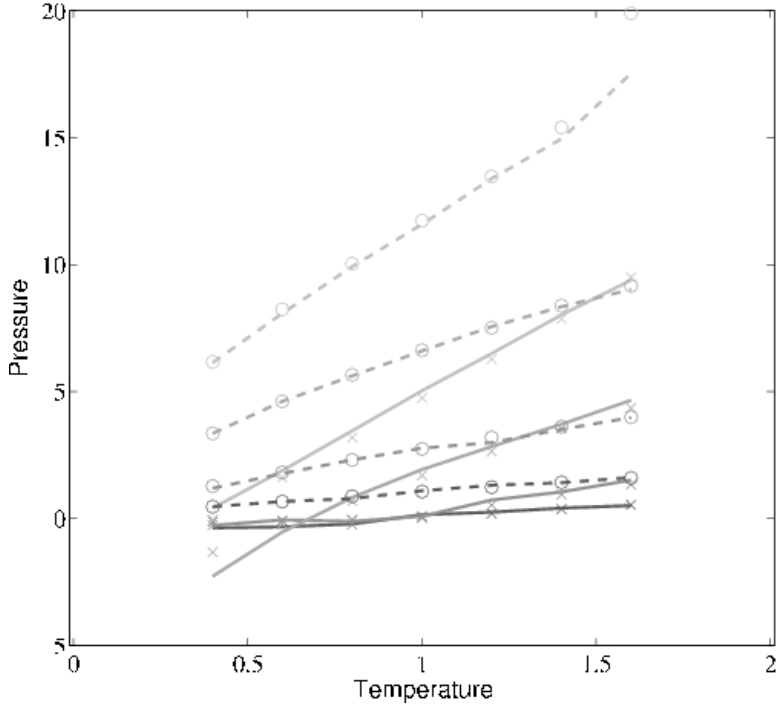


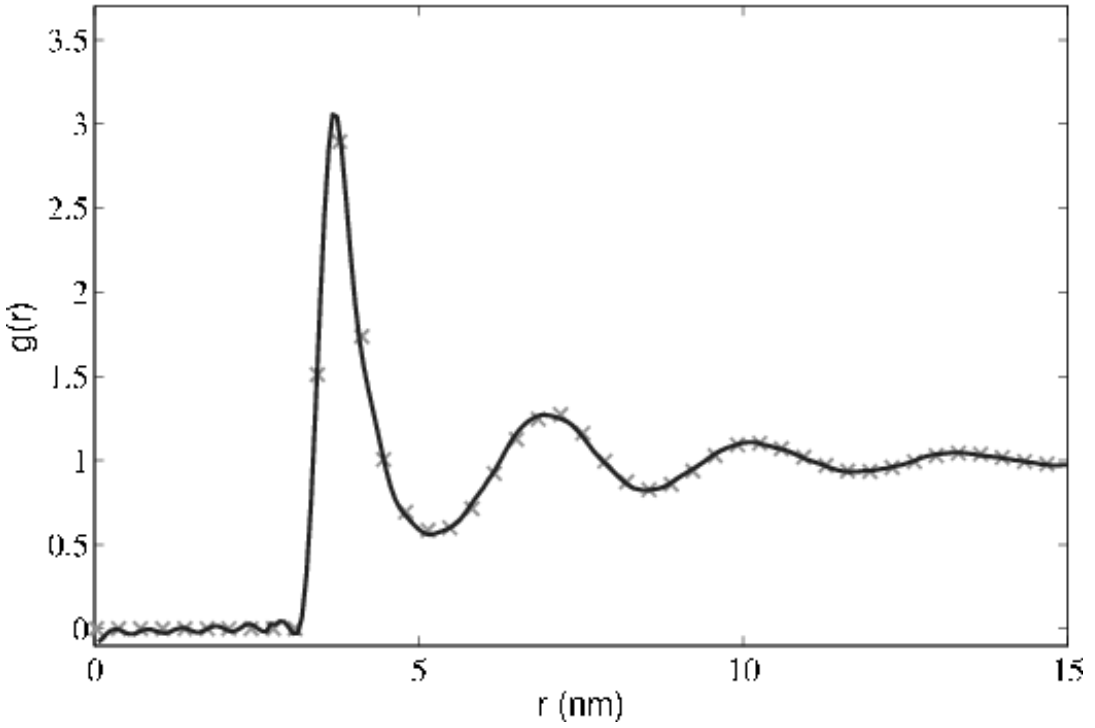


Computing Developments

Molecular Dynamics Solver

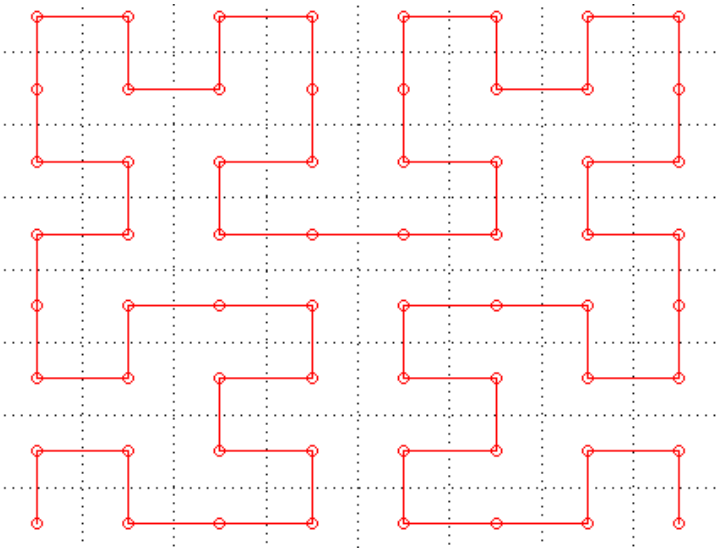
- **New parallel molecular dynamics (MD) code**
  - Fortran 90 (including ‘modern’ 2003 features and python wrappers)
  - Optimised for non-equilibrium molecular dynamics and linking to CFD
- **A range of verification tests using experimental data and literature benchmarks**
  - Phase diagrams
  - Radial Distribution Function (related to the scattering function)



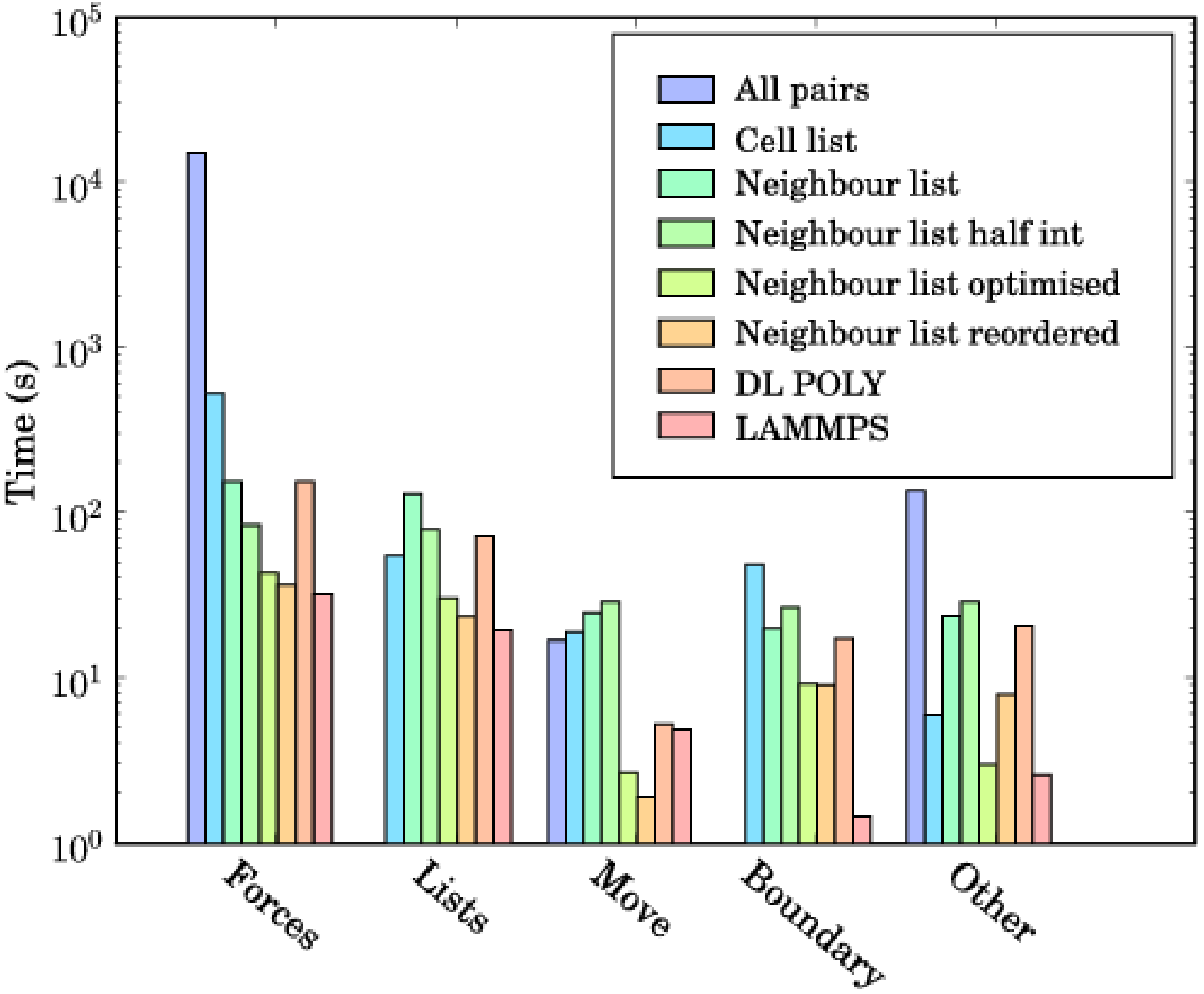


MD Computing – Serial optimisations

- **All pairs simulation uses local cell/neighbour lists**
  - N^2 calculation reduced to order N
  - Linked lists are used in order to manipulate data
  - Result in non-contiguous data access
- **Hilbert curve sorting improves cache efficiency of operations**
  - Improvement becomes greater on larger systems
  - Some tuning required
- **Heaviside function implemented in assembly language**
  - cmplesd xmm1,xmm0 #Check input less than 0.0; true=zeros, false=ones
  - movsd xmm0,xmm2 #Save 1.0 into xmm0
  - andpd xmm0,xmm1 #AND 1.0 with all zeros/ones

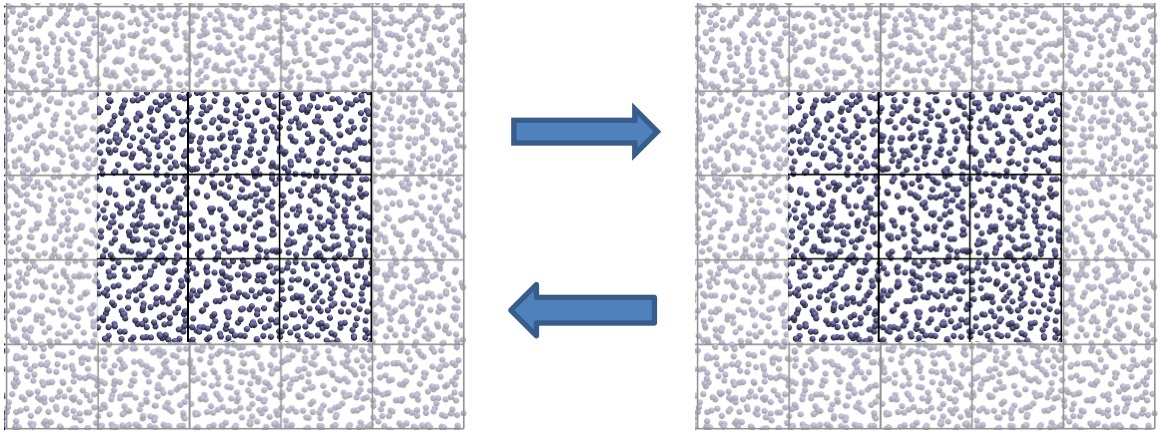


MD Computing – Serial optimisations



MD Computing – Parallel optimisations

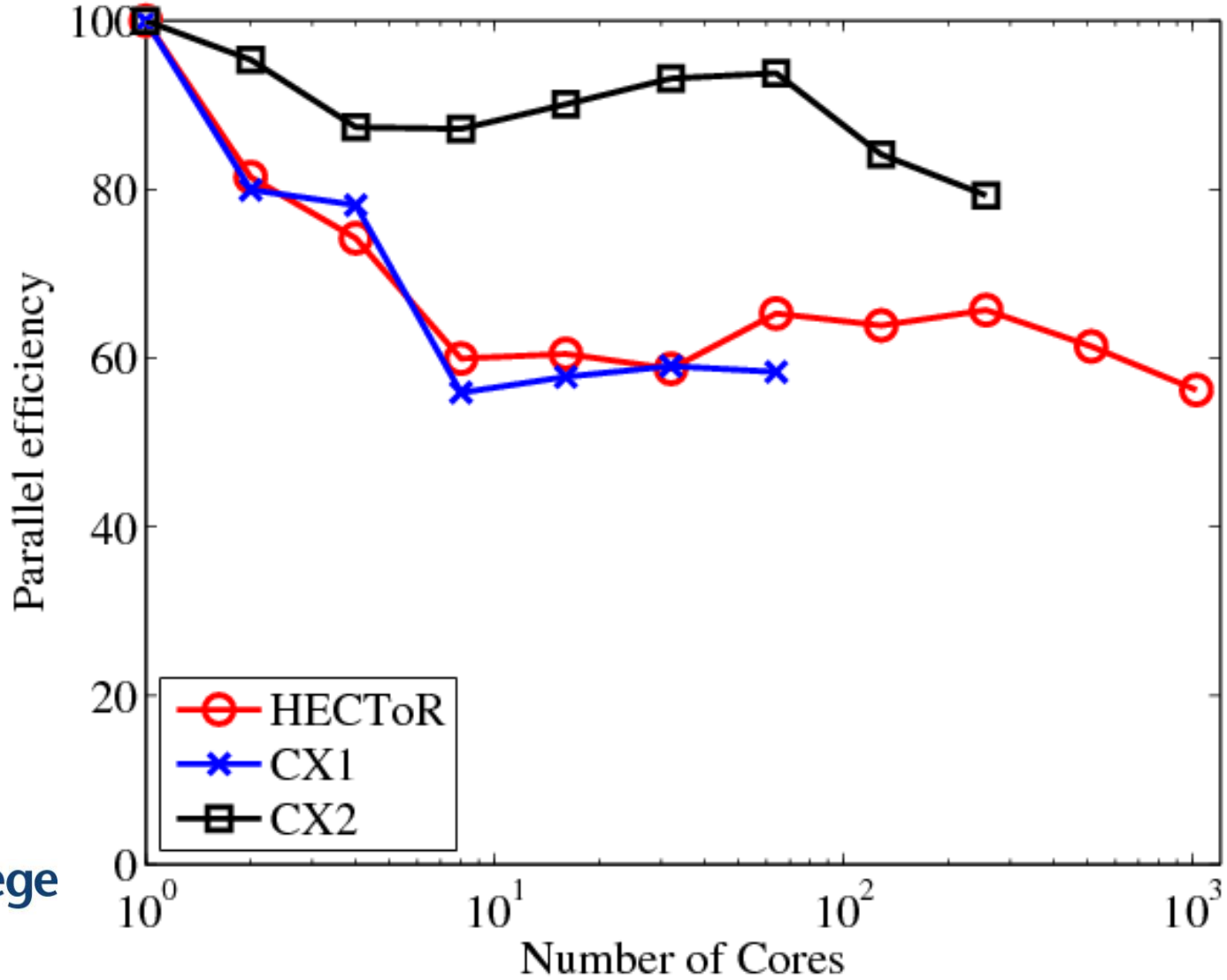
- **Localisations lends itself to parallel computing using MPI**
  - Spatial decomposition employed
  - Halo cells (ghost molecules) are used to link adjacent regions



- **Halo exchange of variable amounts of data**
  - MPI_Send, MPI_Probe and MPI_Recv employed
- **CUDA implementation developed but found to be too inflexible to justify the speedup (especially in parallel)**
  - 30x speedup reported if entire code on GPU (Anderson et al 2008)
  - Speedup negated by transfer, multi-GPU implementation challenging

MD Computing – Parallel optimisations

- **Strong scaling vs 1 core with 3,322,336 molecules**
  - On HECToR and Imperial's supercomputers CX1/CX2
  - Efficiency of 90% when comparing 1024 cores to 8 cores



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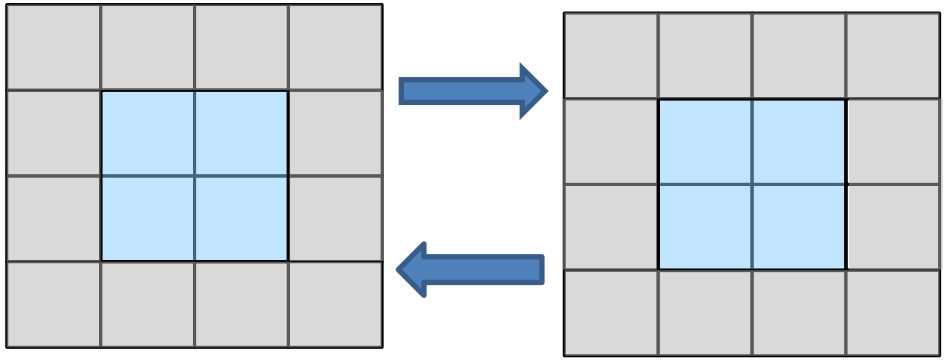
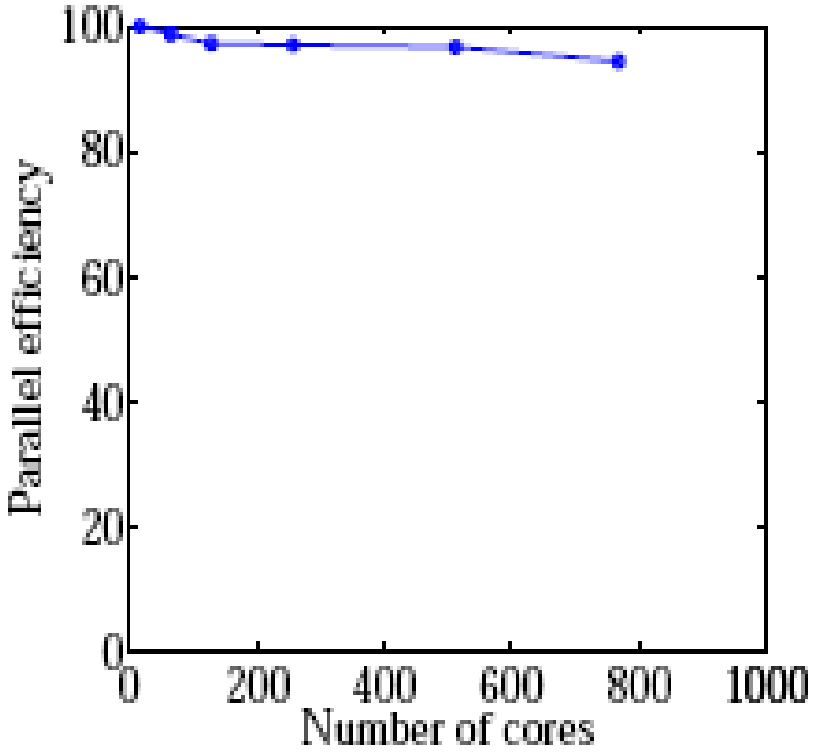
Computational Fluid Dynamics

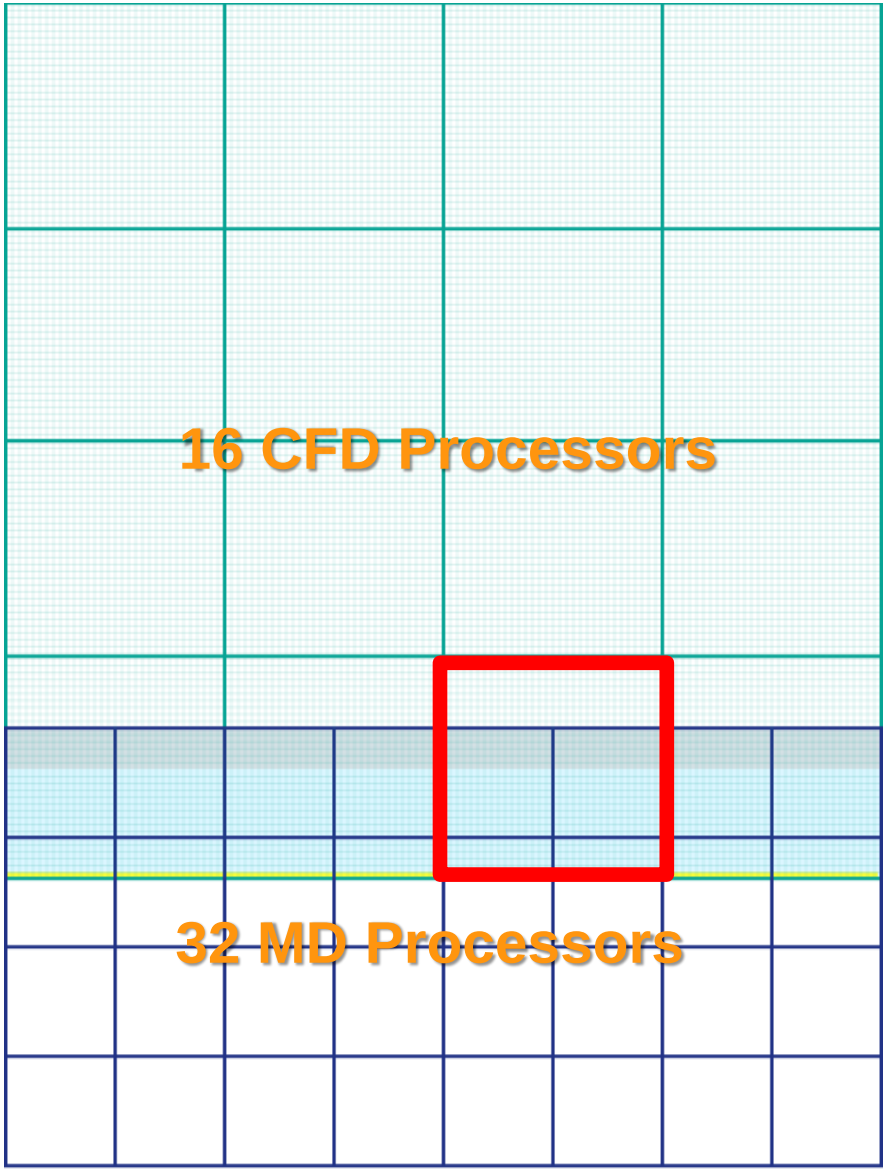
- **Fortran finite volume (FV) Direct Numerical Simulation (DNS)**
  - Highly optimised algorithm used in simulation of turbulence
  - Fully parallelised using MPI (halo cells) with good scalability in benchmark tests
  - Extensively tested and verified (Zaki & Durbin, 2005, 2006)





CPL_LIBRARY Overview

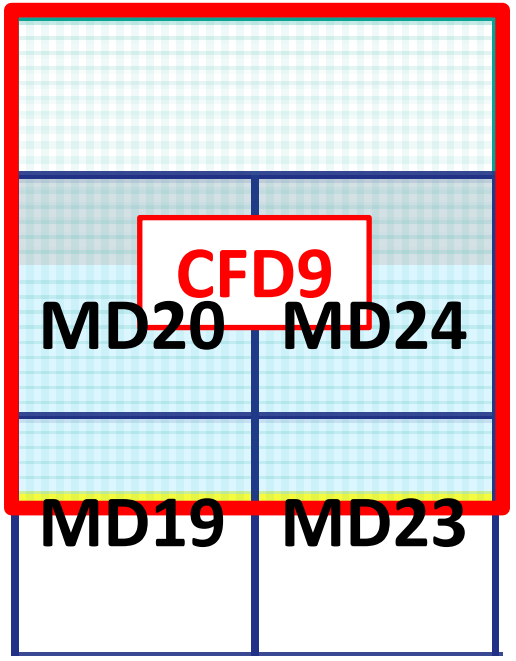
- **Based on the MPI module**
  - Designed in collaboration with Numerical Algorithms Group (NAG)
  - Lightweight and efficient library to preserve the scaling of the two codes
  - API using pure Fortran functions, unit tested and inclusive of error checking
- **Framework is general**
  - Exchange any arbitrary data arrays per continuum cell
  - Allows, in principle, the coupling of any continuum code to any molecular code
  - MPMD implementation enforces separate scope of the two solvers



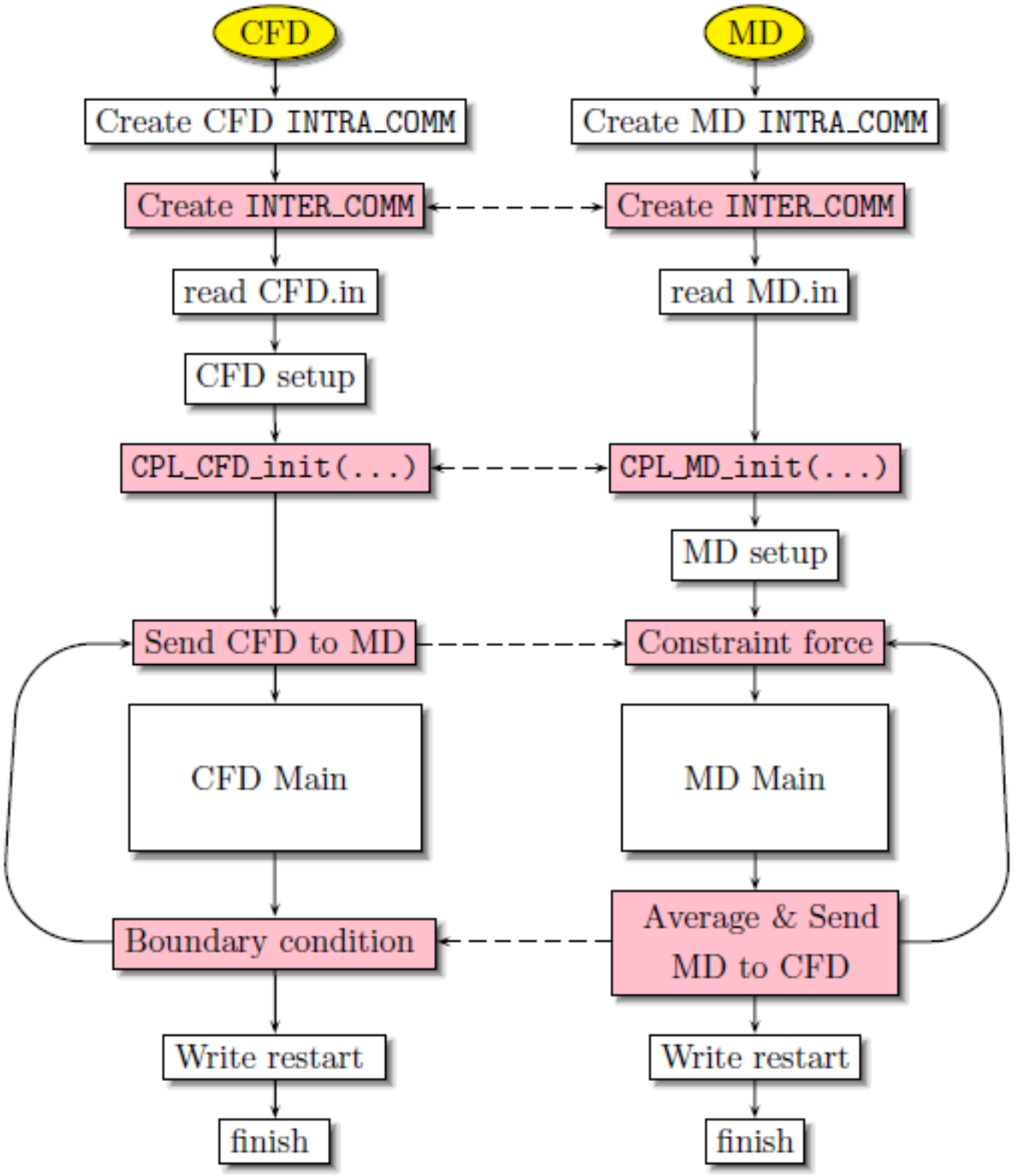
mpiexec –n 32./md.exe : -n 16 ./cfd.exe

CPL_LIBRARY Key Routines

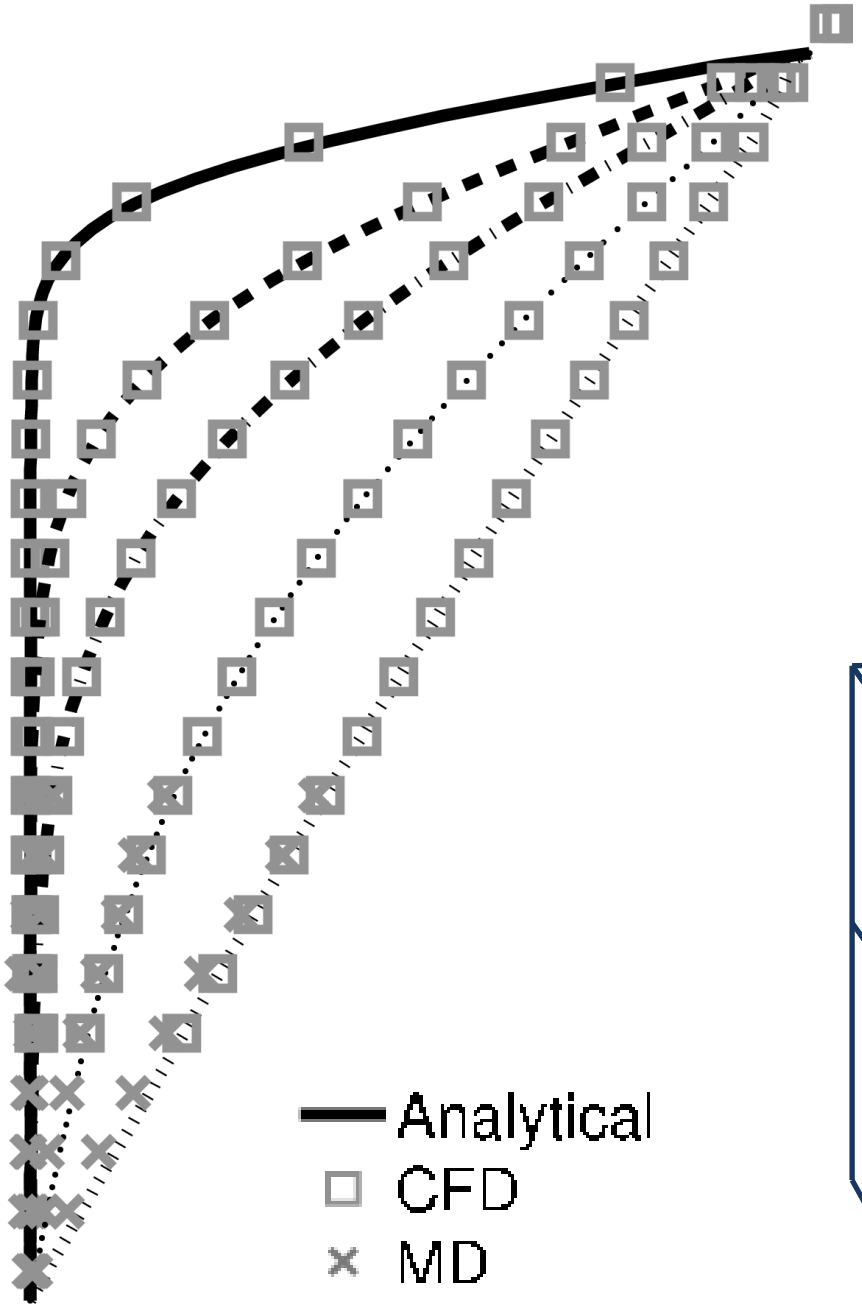
- **Setup**
  - CPL_create_comm – Split intra-comms and create inter-comms
  - CPL_CFD_init / CPL_MD_init –Define mapping between domains. Every processor stores a copy of all mappings, communicators and both solvers processor topology
- **Exchange**
  - CPL_send / CPL_recv – Send and receive data between overlapping processors on the coupling interface
  - CPL_gather / CPL_scatter – Gather/scatter operations implemented efficiently on dedicated communicators linking coupled processors
- **Enquiry**
  - CPL_get – Return copies of protected library internal data
  - CPL_cart_coord – Coordinate of any processor on either solver
  - CPL_COMM_rank – Rank of processor in specified communicator
  - CPL_extents – extents of cells on current processor

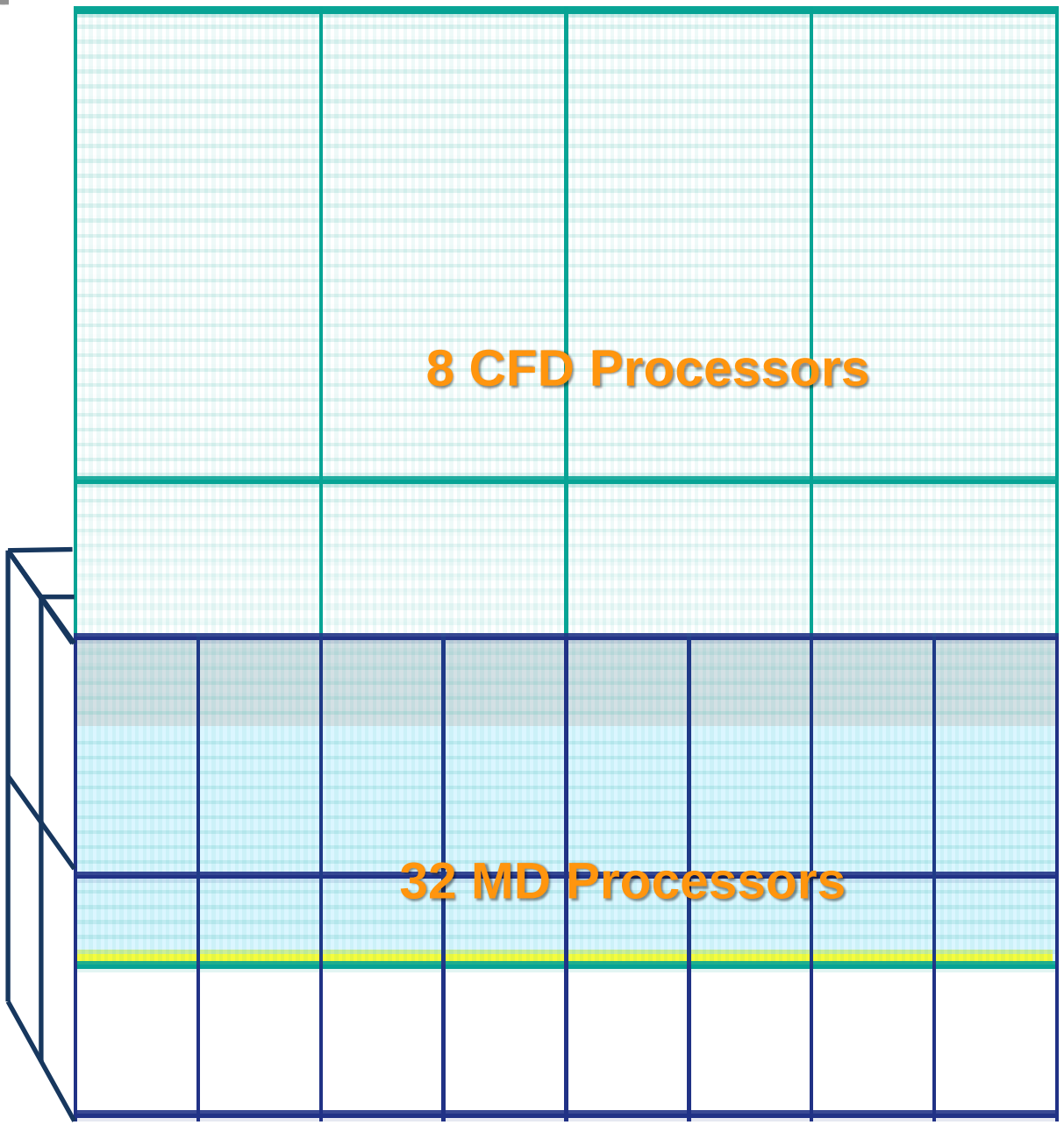


CPL_LIBRARY Schematic

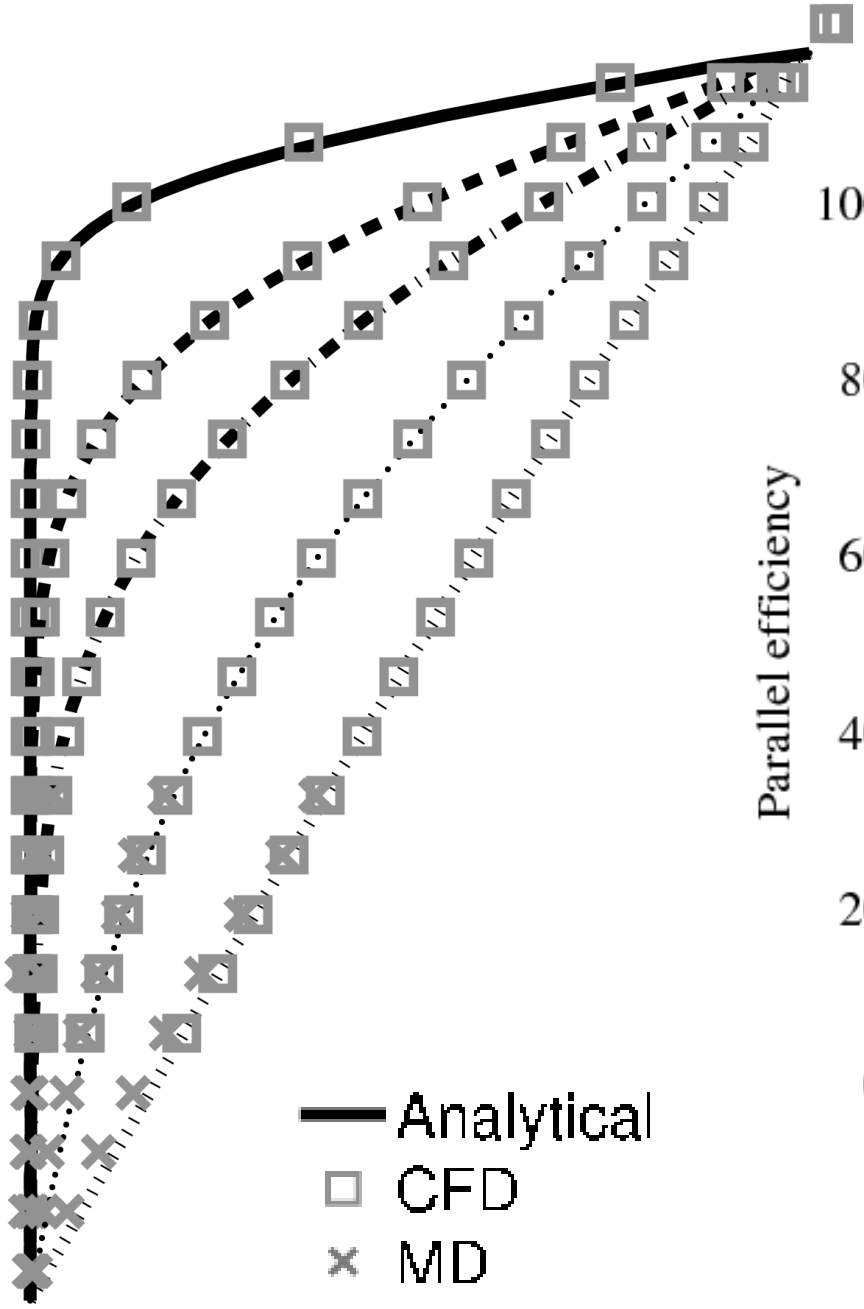


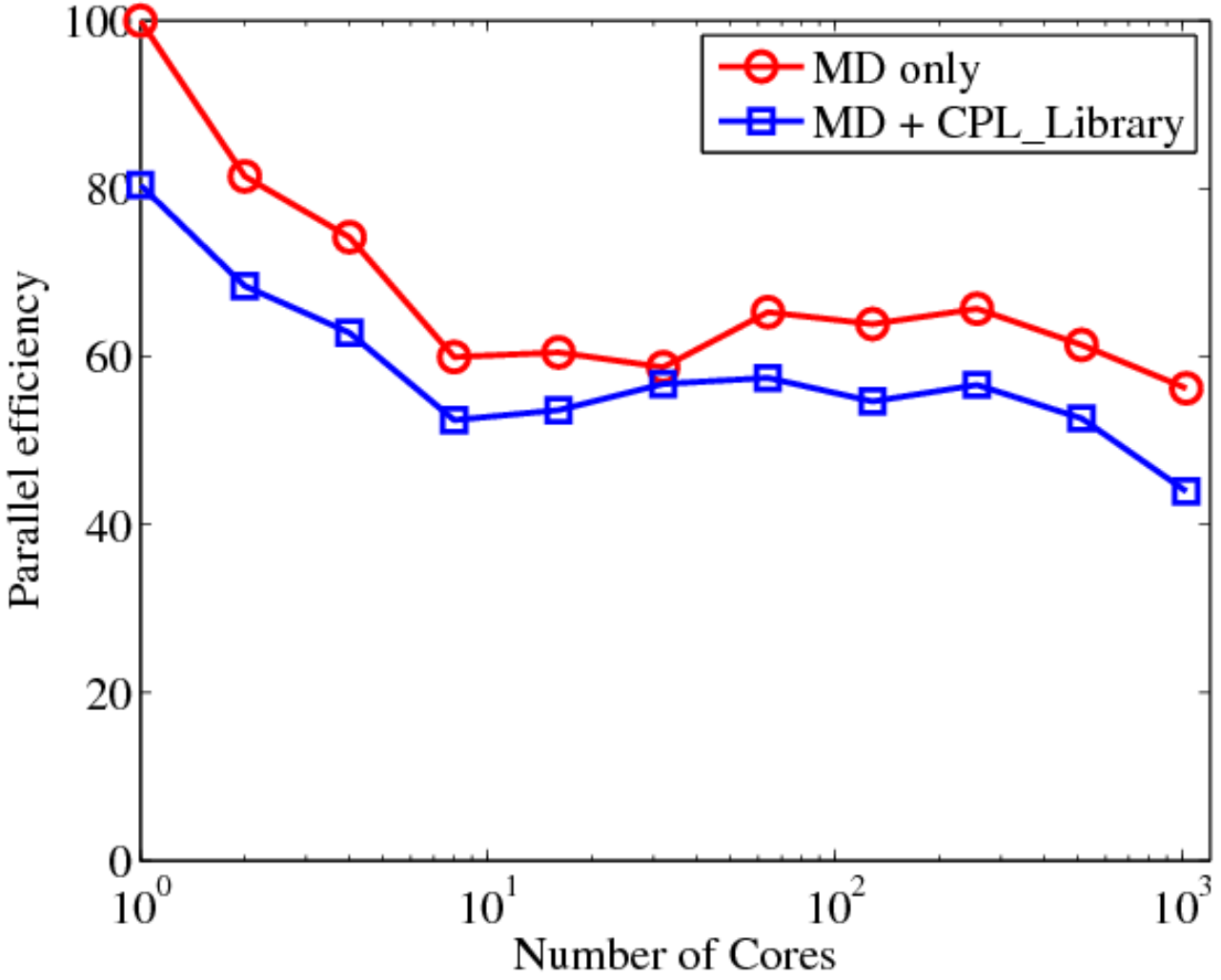
CPL_Library results





CPL_Library results





Conclusions

- **Multi-scale coupling is essential for modern engineering**
  - Implementation of molecular dynamics (and quantum mechanics) where essential and a continuum model to extend to engineering scales
- **Consistent framework for coupling fluid descriptions**
  - Control volume (CV) function expresses continuum and discrete systems in an equivalent formulation (rigours backing to existing coupling)
  - Hamilton's principle, with the CV function, provides a constraint which ensures the descriptions in both domains agree
  - Verified using test cases with known analytical solutions
- **Computational developments**
  - Extensive serial and parallel optimisations applied to the molecular dynamics solver
  - CPL_library is an open source library to facilitates the exchange of data between two coupled codes (https://code.google.com/p/cpl-library/)
  - Verified with test cases on a range of processor topologies

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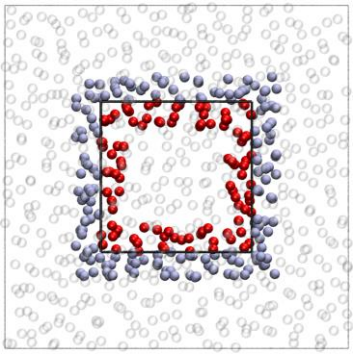
- Mr David Trevelyan
- Dr Lucian Anton (NAG)

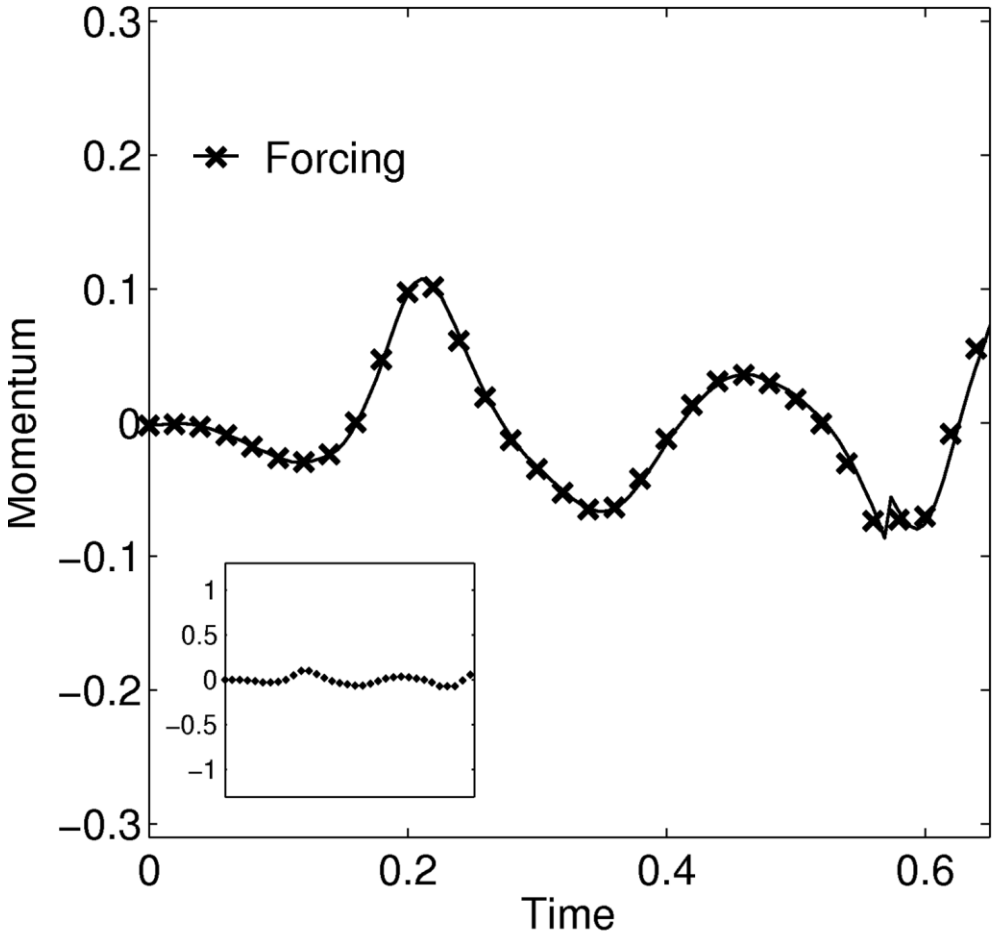
Extra Material

Testing Momentum Balance

- **Momentum Balance**

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

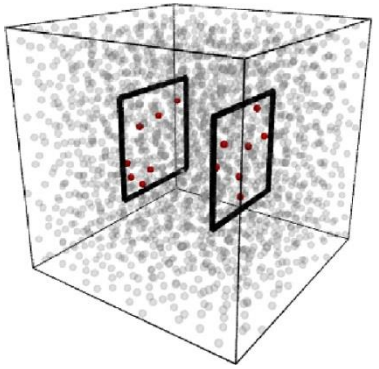


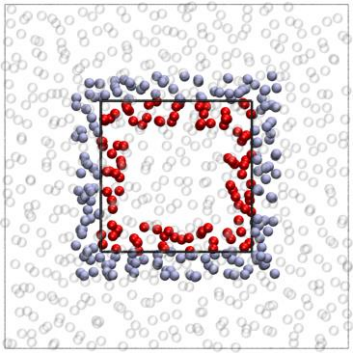


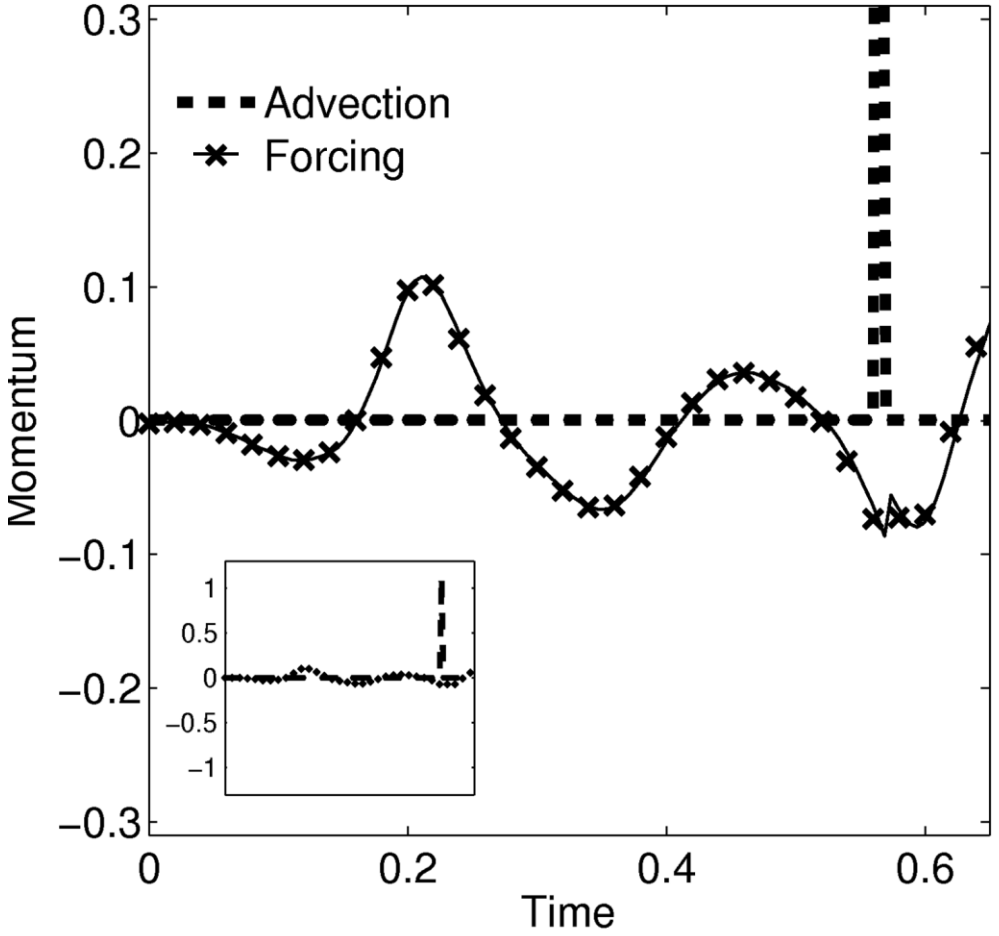
Testing Momentum Balance

- **Momentum Balance**

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





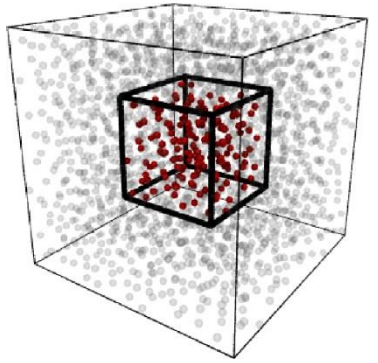


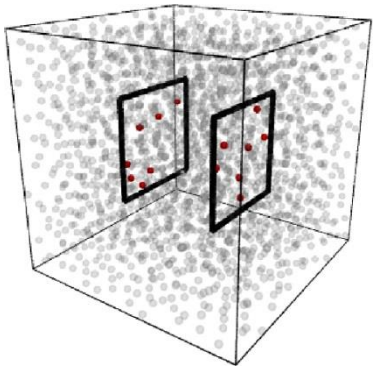
Testing Momentum Balance

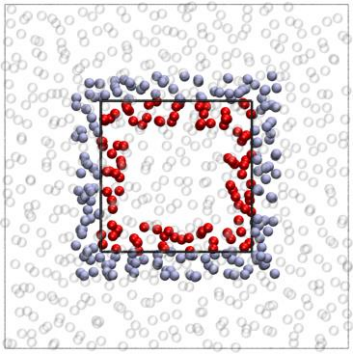
- **Momentum Balance**

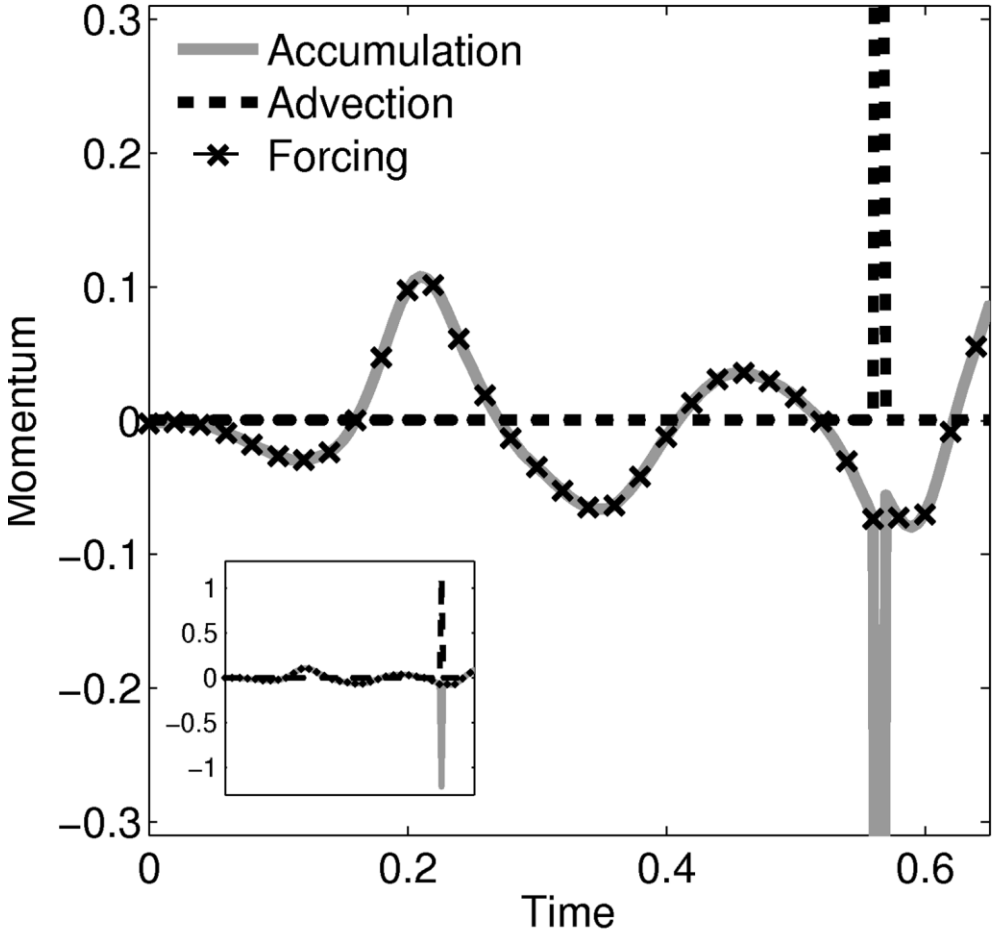
$$\underbrace{\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i}_{\text{Accumulation}} = \underbrace{-\sum_{i=1}^{N} m_i \mathbf{v}_i \mathbf{v}_i \cdot d\boldsymbol{S}_i}_{\text{Advection}} + \underbrace{\sum_{i=1}^{N}\sum_{j\neq i}^{N} \mathbf{f}_{ij}\vartheta_{ij}}_{\text{Forcing}}$$

$\frac{d}{dt}$









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Control Volume Function (revisited)

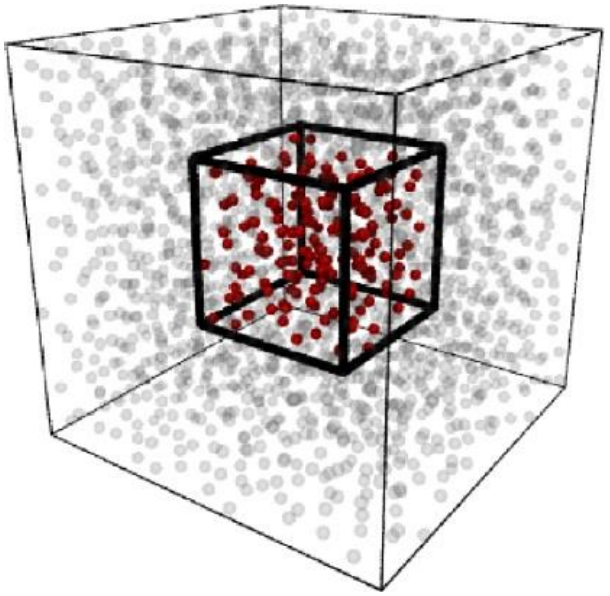
- **The Control volume function is the integral of the Dirac delta function in 3 dimensions**

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

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

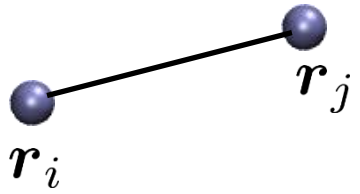
$$\times \left[H(y^+ - y_i) - H(y^- - y_i)\right]$$

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



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

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



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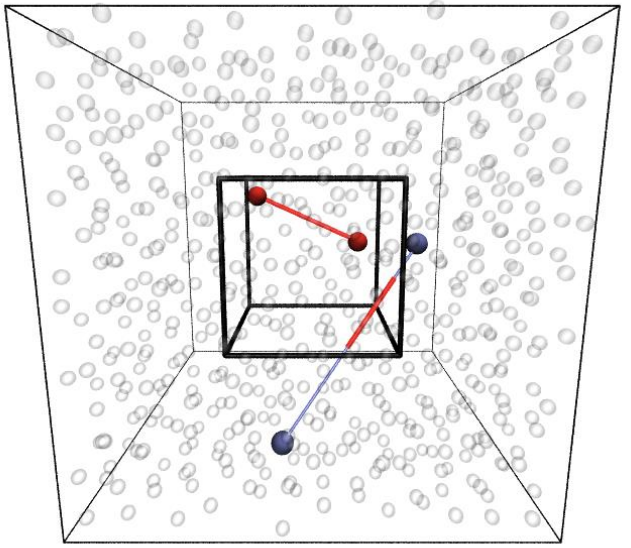
For full details, please see
E.R. Smith, D.M. Heyes, D. Dini, T.A. Zaki, Phys. Rev. E 85. 056705 (2012)

Control Volume Function (revisited)

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

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



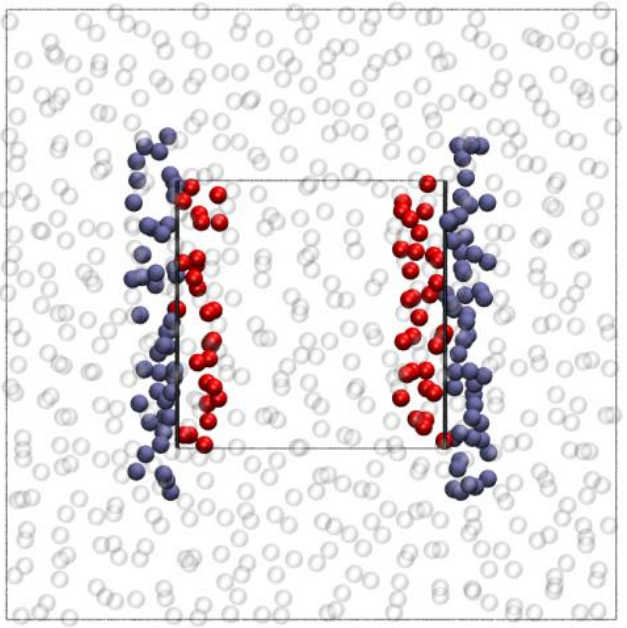
- **Length of interaction inside the CV**

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

Derivatives Yield the Surface Forces

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

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



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

$$dS_{xij} \equiv \int_0^1 \frac{\partial \vartheta_s}{\partial x} ds = dS^+_{xij} - dS^-_{xij}$$

$$dS^+_{xij} = \frac{1}{2} \underbrace{\left[sgn(x^+ - x_i) - sgn(x^+ - x_j)\right]}_{MOP} \boxed{S_{xij}}$$

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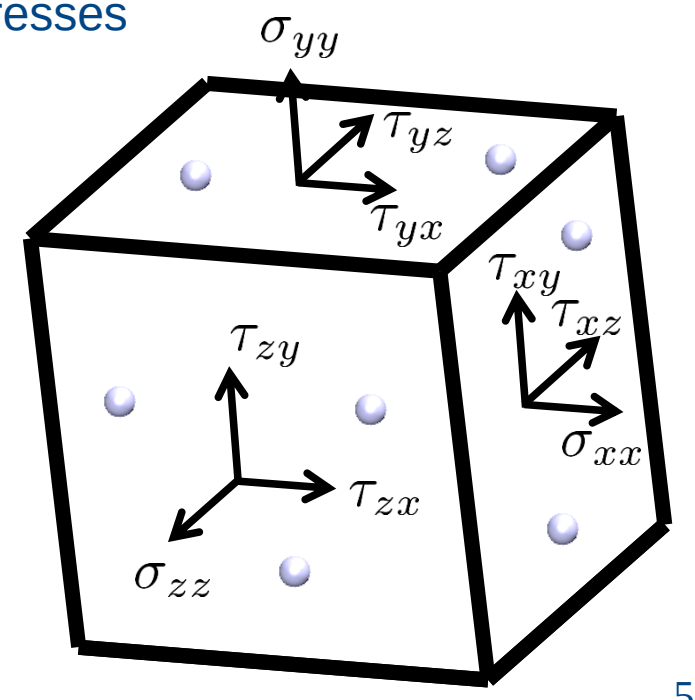
More on the Pressure Tensor

- **Extensive literature on the form of the molecular stress tensor**
  - No unique solution Schofield, Henderson (1988)
  - Two key forms in common use – Volume Average (Lutsko, 1988) and Method of Planes (Todd et al 1995)
- **Link provided between these descriptions**
  - Through formal manipulation of the functions
  - Exposes the relationship between the molecular stresses and the evolution of momentum
- **In the limit the Dirac delta form of Irving and Kirkwood (1950) is obtained**
  - This suggests the same limit is not possible in the molecular system
  - Arbitrary stress based on the volume of interest



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

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

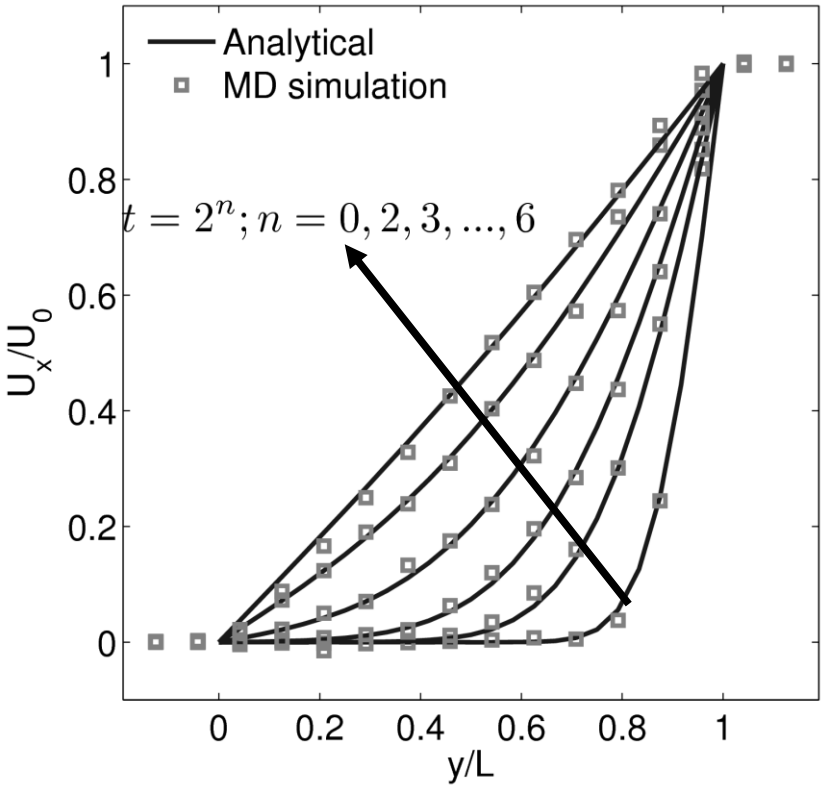
$$\frac{d}{dt}\sum_{i=1}^{N} m_i\vartheta_i = -\sum_{i=1}^{N} m_i\left(\mathbf{v}_i + \overline{\boldsymbol{u}}\right)\cdot d\boldsymbol{S}_i$$

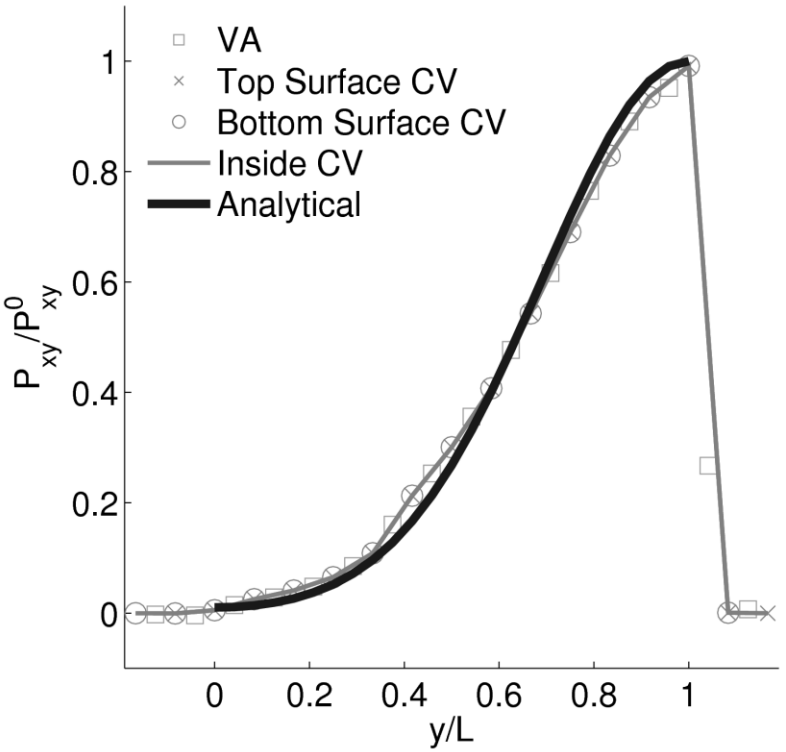
$$\frac{d}{dt}\int_V \rho dV = \oint_S \rho\left(\boldsymbol{u} - \overline{\boldsymbol{u}}\right)\cdot d\boldsymbol{S}$$

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

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

Continuum Analytical Couette Flow





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

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

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

Unsteady Couette Flow

- **Continuum Analytical**
  - Simplify the momentum balance (Navier-Stokes) equation

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

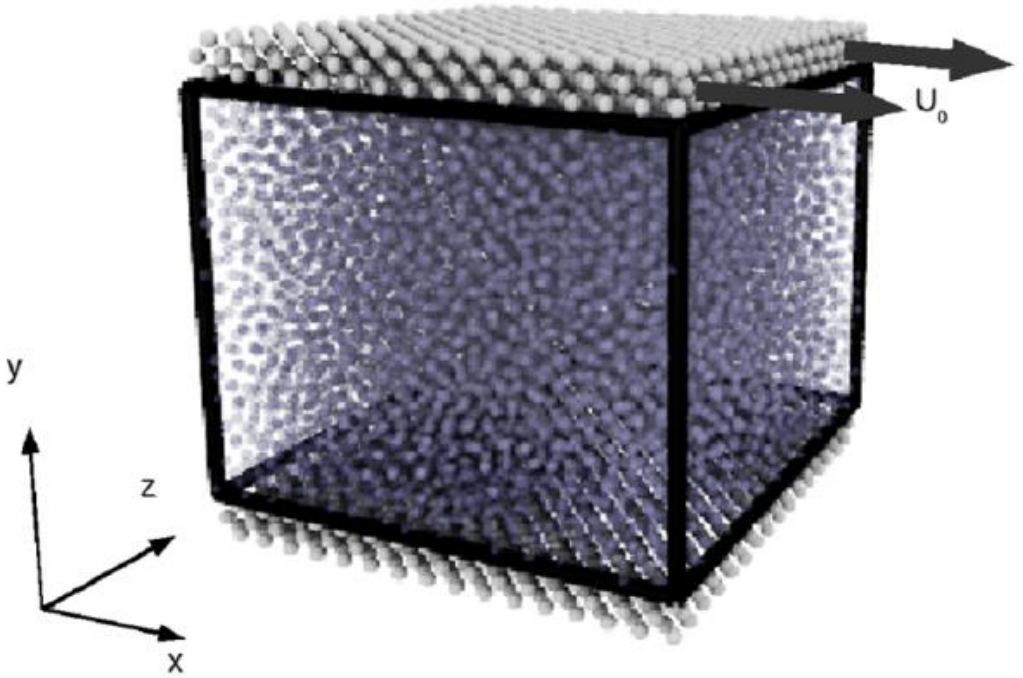
  - Solve the 1D unsteady diffusion equation.

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

  - 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

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

  - Simplifies for a single control volume

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

  - With Boundary Conditions

$$u_x(0,t) = 0$$
$$u_x(L,t) = U_0$$
$$u_x(y,0) = 0$$

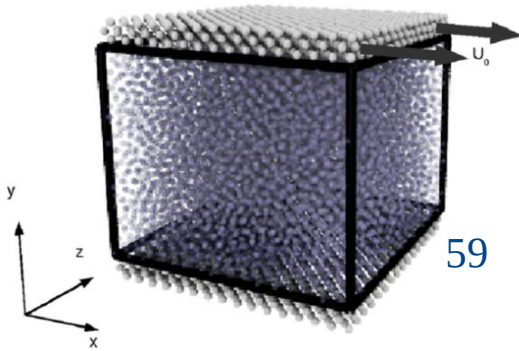
- **Molecular Dynamics**
  - Discrete form of the Momentum balance equation

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

  - Simplifies for a single control volume

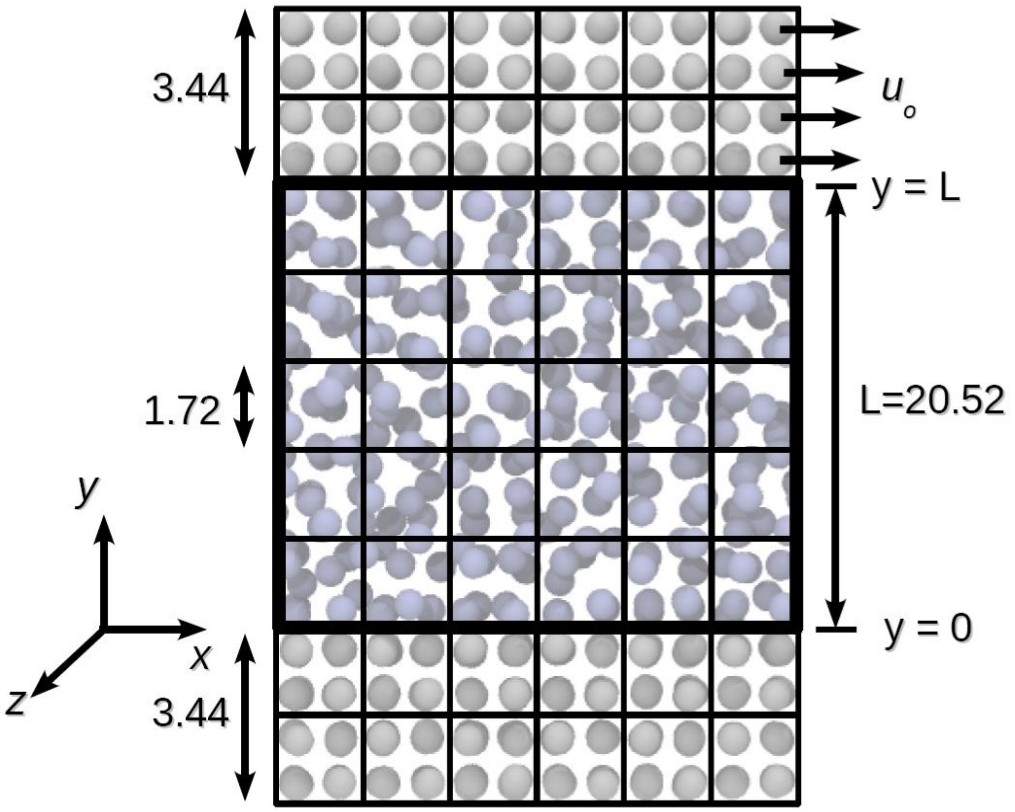
$$\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i = \sum_{i,j}^{N} f_{xij} dS_{yij}^+ - \sum_{i,j}^{N} f_{xij} dS_{yij}^-$$

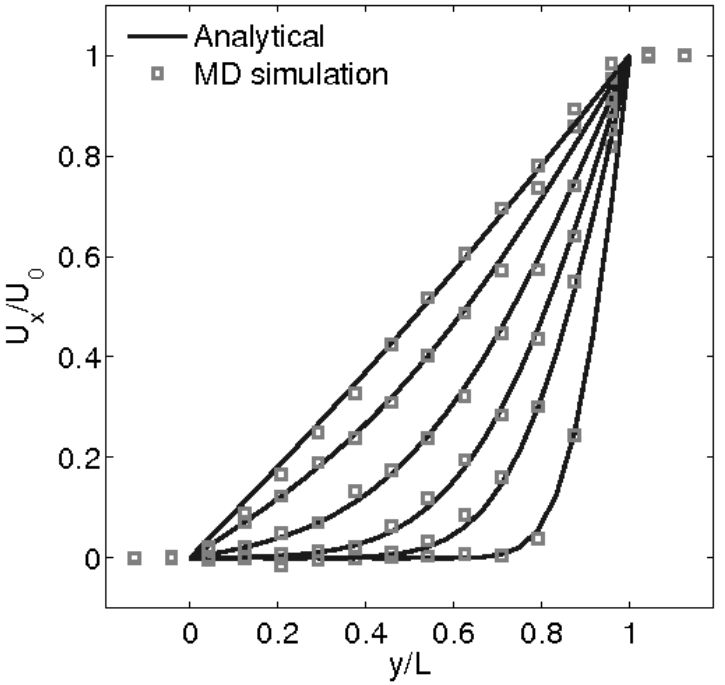
  - Fixed bottom wall, sliding top wall with both thermostatted

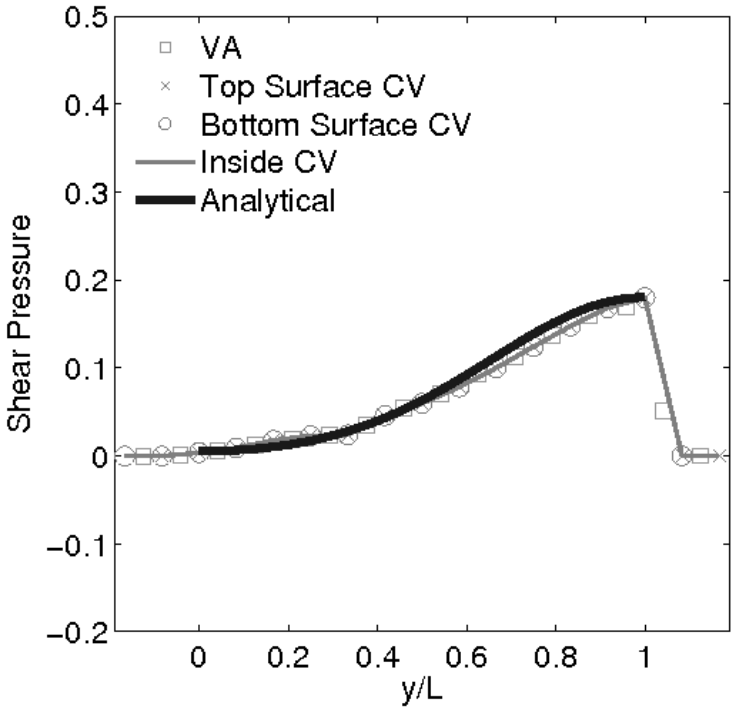


Unsteady Couette Flow

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

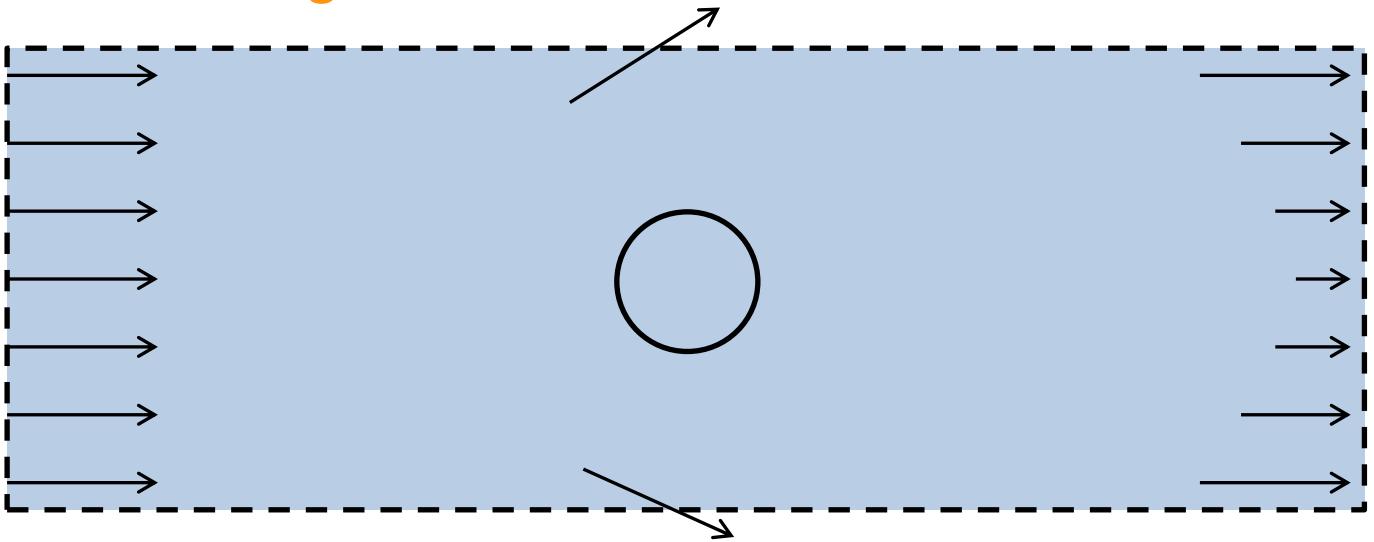






Flow past a cylinder

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



- Drag over a Carbon Nano-tube can be determined