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A Control Volume Study of the Pressure Tensor across a Liquid-Vapour Interface

By Edward Smith

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Overview

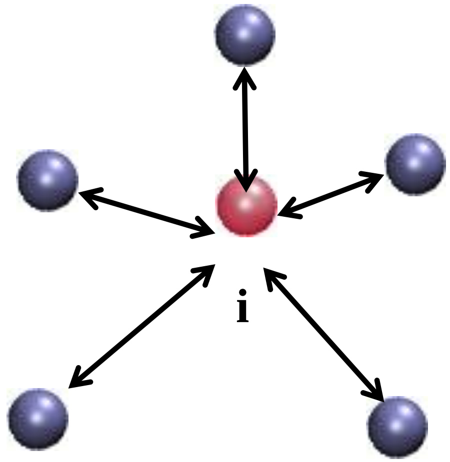
- Molecular Dynamics
- The control volume functional
- Liquid-vapour interfaces and the intrinsic surface
- Defining a control volume based on the liquid-vapour interface
- Expressions for density, pressure and surface tension
- Results and extensions

Molecular Dynamics

Molecular Dynamics

Discrete molecules in continuous space

- Molecular position evolves continuously in time
- Position and velocity from acceleration



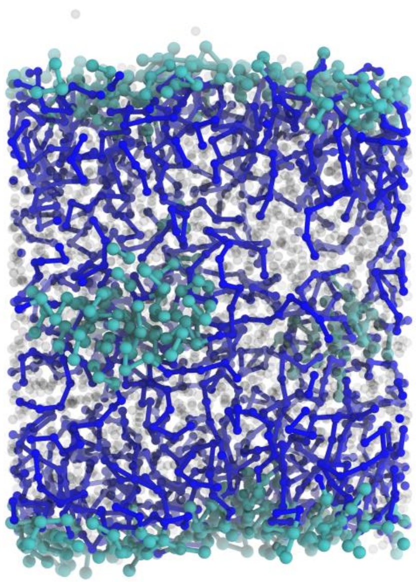
$$\ddot{\boldsymbol{r}}_i \rightarrow \dot{\boldsymbol{r}}_i$$
$$\dot{\boldsymbol{r}}_i \rightarrow \boldsymbol{r}_i(t)$$

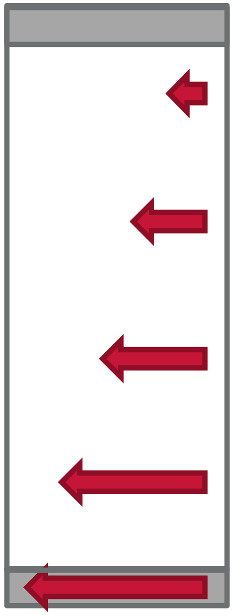
Acceleration obtained from forces

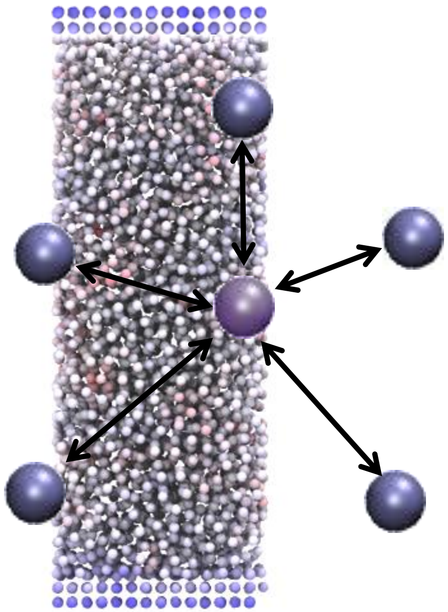
- Governed by Newton’s law for an N-body system
- Point particles with pairwise interactions only

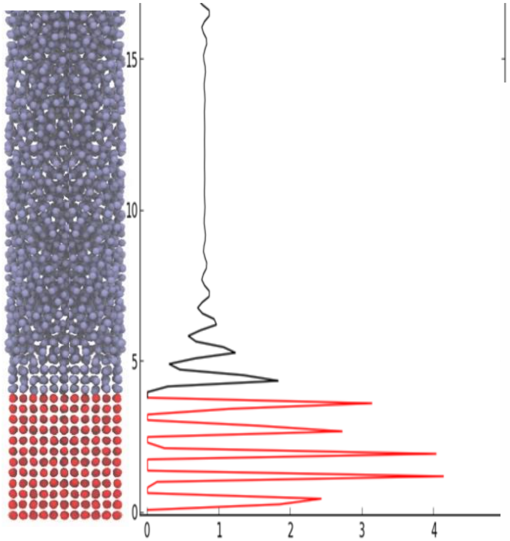
$$m_i \ddot{\boldsymbol{r}}_i = \mathbf{F}_i = \sum_{i \neq j}^{N} \boldsymbol{f}_{ij} \qquad \Phi(r_{ij}) = 4\epsilon \left[\left(\frac{\ell}{r_{ij}} \right)^{12} - \left(\frac{\ell}{r_{ij}} \right)^{6} \right]$$

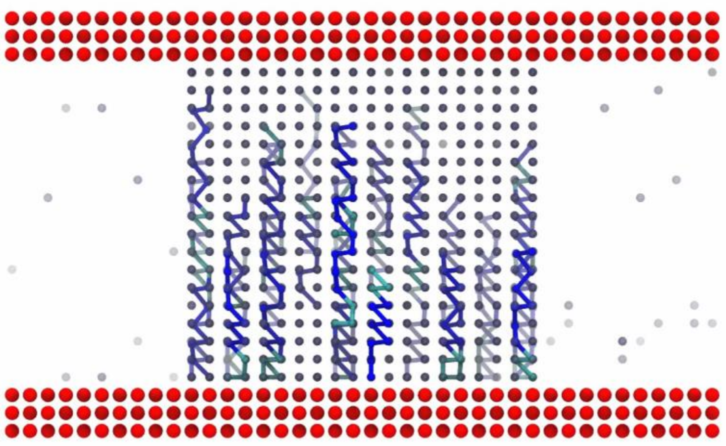
Molecular Dynamics

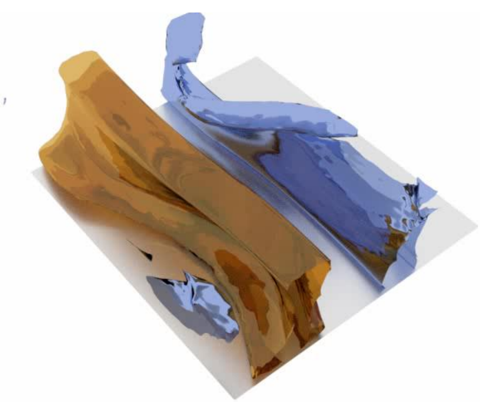












Molecular Simulation of Interfaces

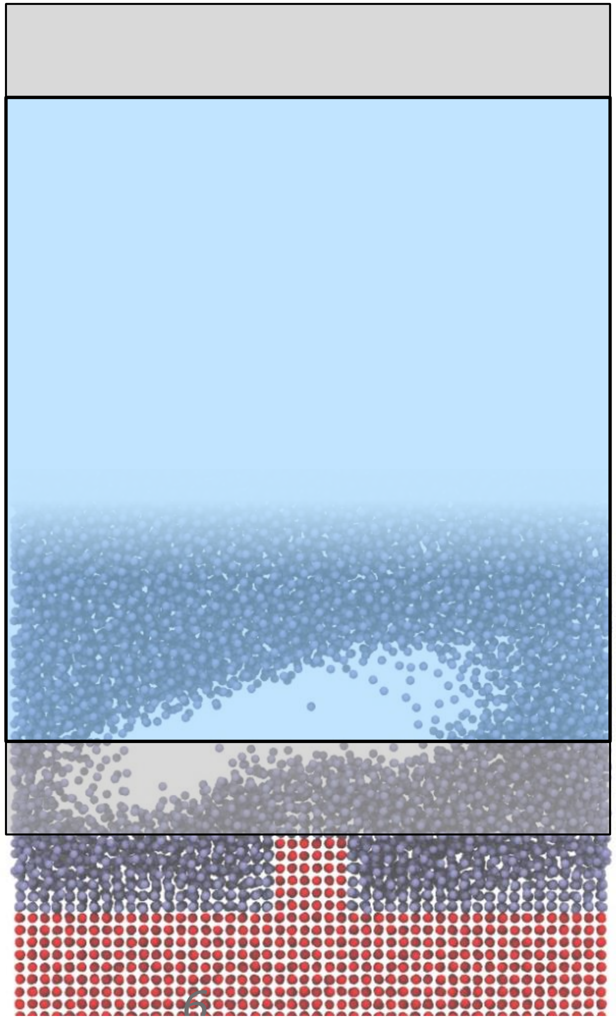
- Assumes continuous fields

$$\frac{\partial}{\partial t}\rho\boldsymbol{u} + \boldsymbol{\nabla}\cdot\rho\boldsymbol{u}\boldsymbol{u} = \boldsymbol{\nabla}\cdot\boldsymbol{\Pi} \text{ and } \gamma, C, \mathrm{T}$$

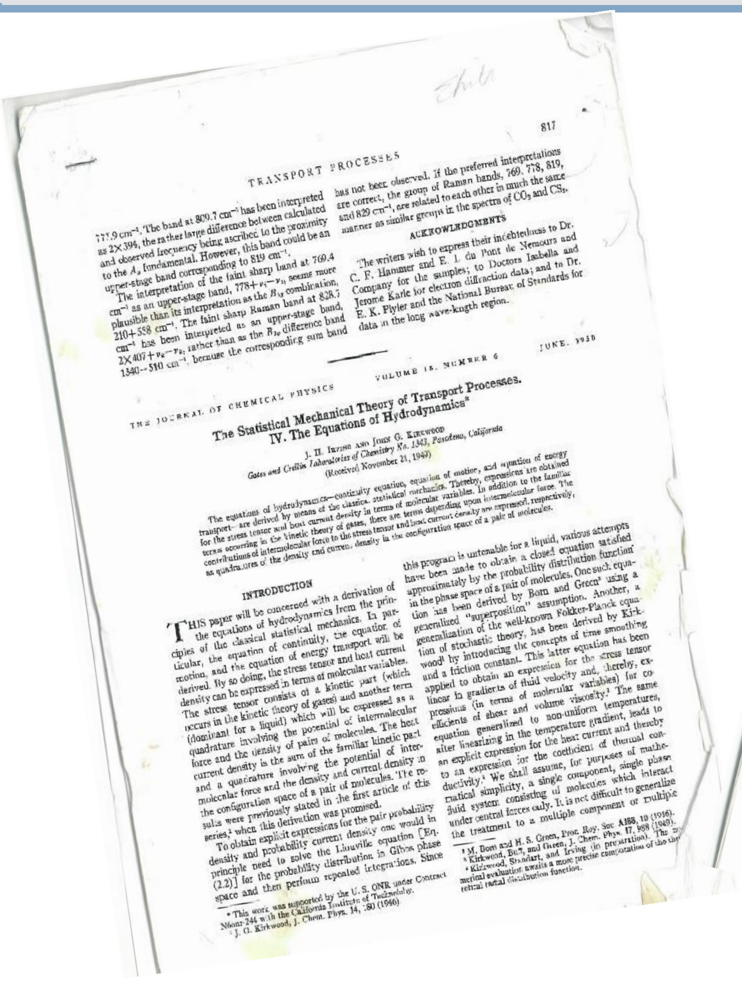
How do we get continuum values from the molecular system?

- Discrete molecules

$$m_i\ddot{\boldsymbol{r}}_i = \mathbf{F}_i \text{ for all i in N}$$



Irving and Kirkwood (1950)



TRANSPORT PROCESSES 817

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

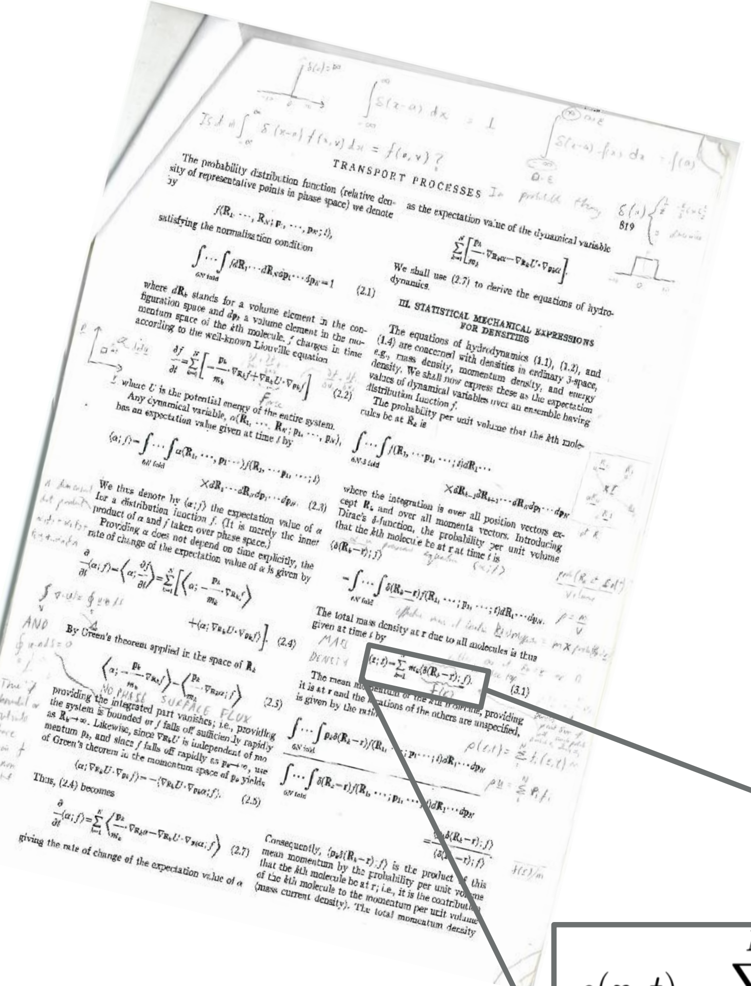
The Statistical Mechanical Theory of Transport Processes. IV. The Equations of Hydrodynamics*

J. H. Irving and John G. Kirkwood

Gates and Crellin Laboratories of Chemistry, No. 1343, Pasadena, California

(Received November 21, 1949)

INTRODUCTION



TRANSPORT PROCESSES 819

II. STATISTICAL MECHANICAL EXPRESSIONS FOR DENSITIES

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

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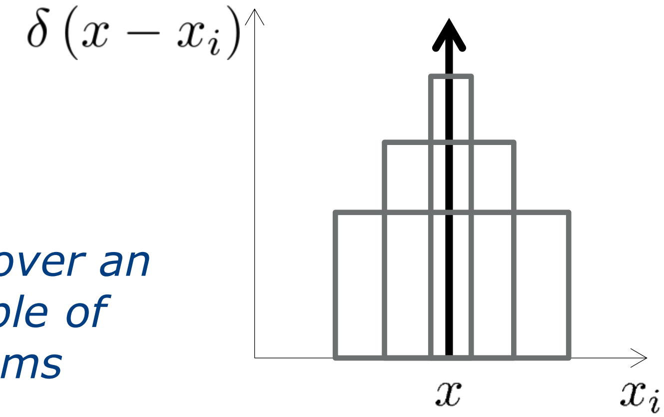
Irving and Kirkwood (1950)



*Continuum density field valid at any point, **r**, in space*

Mass of each molecule

Average over an ensemble of systems

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

Sum over all molecules

*Delta function is only non-zero if molecule i's position $\boldsymbol{r}_i$ is exactly at **r***

The Dirac delta infinitely high, infinitely thin peak. Formally equivalent to the continuum differential formulation

BUT

No molecule is ever exactly at a point

Irving and Kirkwood (1950)

- The Dirac delta is key to express continuum equivalents in MD

Density

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

Momentum

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

Energy

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

Kinetic Pressure

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

Configurational Stress

$$\boldsymbol{\Pi}^c = \frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \boldsymbol{f}_{ij} \boldsymbol{r}_{ij} \int_0^1 \delta \big(\boldsymbol{r} - \underbrace{\boldsymbol{r}_i + s \boldsymbol{r}_{ij}}_{\boldsymbol{r}_s} \big) ds$$

The infamous IK operator in integral form

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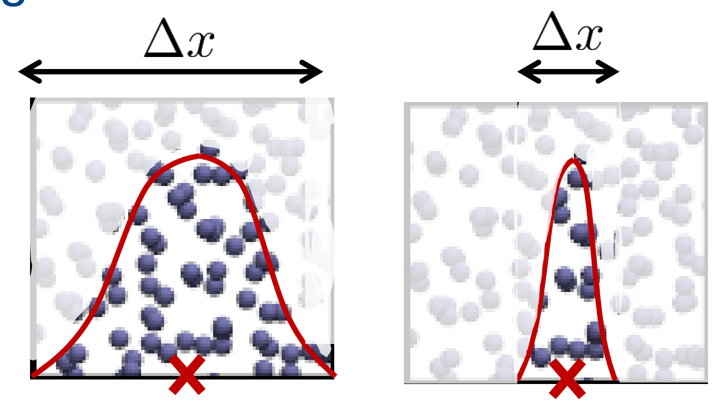
Problems with the Dirac Delta Function

- Irving and Kirkwood (1950) express field based quantities using the Dirac delta functional and ensemble averages

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



$$\delta(x) = \lim_{\Delta x \to 0} \frac{1}{\Delta x} e^{x^2/\Delta x^2}$$

- No ensemble – purely mechanical

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

- Without ensemble:
  - Dirac delta formally correct but no molecule ever at point r
- A relaxation of the Dirac delta is no longer formally correct
  - A discrete system can only be approximately represented using a continuous field – the weak form avoid this problem

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The Control Volume Functional

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Control Volume (Weak) Form

- The "weak formulation" give the equations in integrated form

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

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

- Integration of the Dirac delta in three dimensions

$$\int_V \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right) dV = \int_{z^-}^{z^+} \int_{y^-}^{y^+} \int_{x^-}^{x^+} \delta\left(x - x_i\right) \delta\left(y - y_i\right) \delta\left(z - z_i\right) dx dy dz$$

$$x^+ = x + \frac{\Delta x}{2} \qquad x^- = x - \frac{\Delta x}{2} \quad \text{etc}$$

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Integrating the Dirac delta functional gives a combination of Heaviside functionals, which can:

- *Be mathematically manipulated to give fluxes and forces*
- *Be implemented directly in MD codes*
- *Be linked to the continuum control volume.*

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The Control Volume Functional

- The Control volume functional is the formal integral of the Dirac delta functional in 3 dimensions (3D top hat or box car function)

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

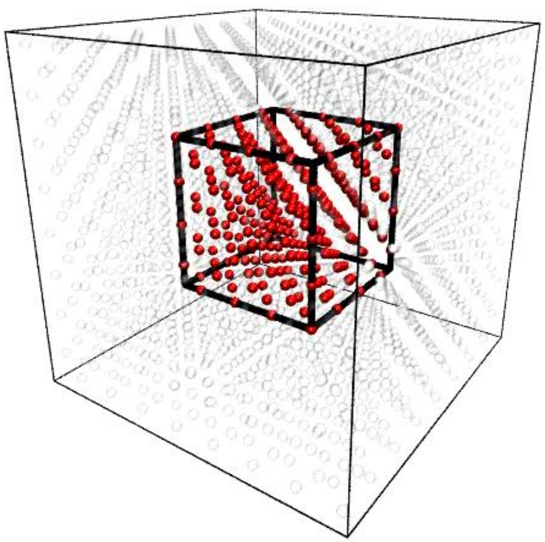
$$= \left[H(x^+ - x_i) - H(x^- - x_i)\right]$$

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

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

- In words

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



The Control Volume Functional

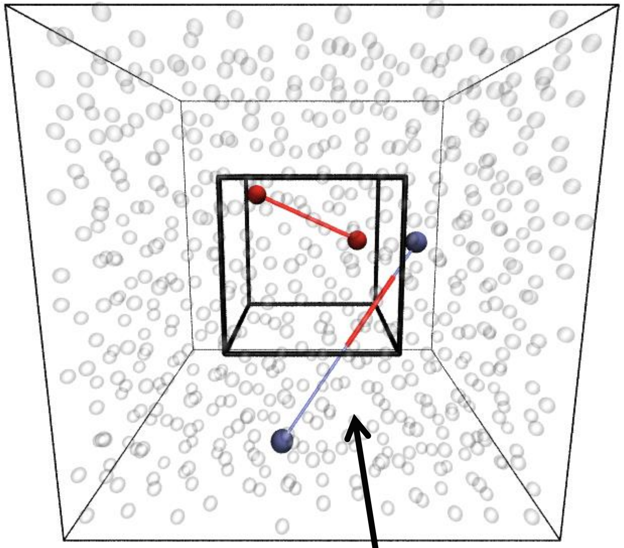
- The Control volume functional is the formal integral of the Dirac delta functional in 3 dimensions (3D top hat or box car function)

$$\vartheta_s \equiv \int_V \delta(\mathbf{r} - \mathbf{r}_s) dV =$$

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

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

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



- In words

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

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

Control Volume form of Irving and Kirkwood (1950)

- The control volume functional can express continuum equivalents in MD

Density

$$\int \rho dV = \sum_{i=1}^{N} m_i \vartheta_i$$

Momentum

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

Energy

$$\int \rho \mathcal{E} dV = \sum_{i=1}^{N} e_i \vartheta_i$$

Kinetic Pressure

$$\int \boldsymbol{\Pi}^k dV = \sum_{i=1}^{N} m_i \boldsymbol{v}_i \boldsymbol{v}_i \vartheta_i$$

Configurational Stress

$$\int_V \boldsymbol{\Pi}^c dV = \frac{1}{2} \sum_{i=1}^{N} \sum_{j \neq i}^{N} \boldsymbol{f}_{ij} \boldsymbol{r}_{ij} \int_0^1 \vartheta_s ds$$

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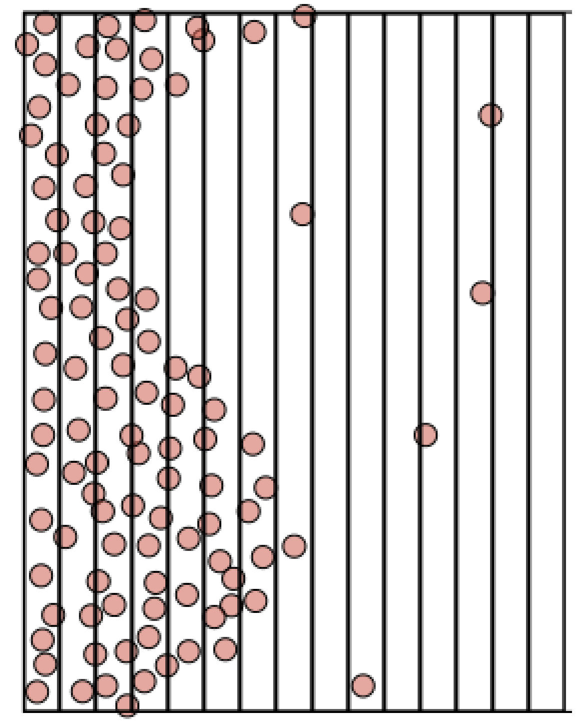
Applied to Density

- Density in a cubic control volume

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

$$= \sum_{i=1}^{N} m_i \left[H\left(x^+ - x_i\right) - H\left(x^- - x_i\right)\right]$$
$$\times \left[H(y^+ - y_i) - H(y^- - y_i)\right]$$
$$\times \left[H(z^+ - z_i) - H(z^- - z_i)\right]$$

- Assume a periodic domain in y and z



Applied to Density

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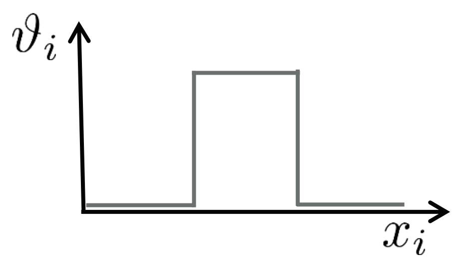

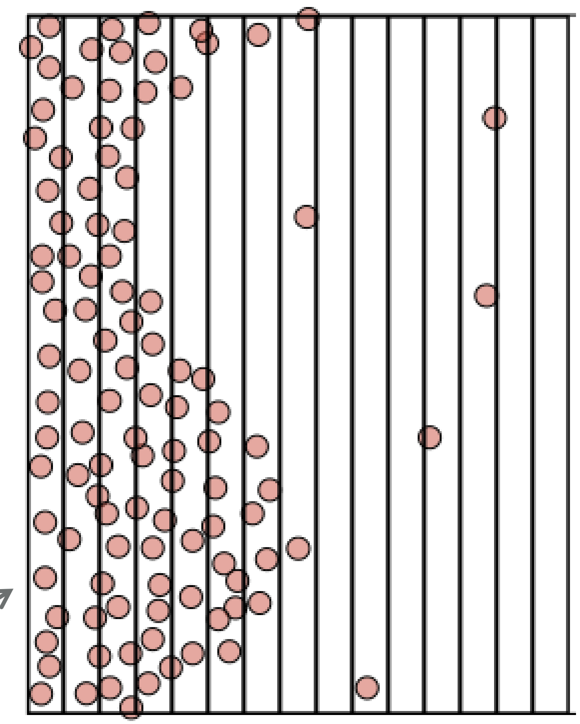

- Top hat function selects molecules inside a volume. Domain is therefore split into uniform bins in x

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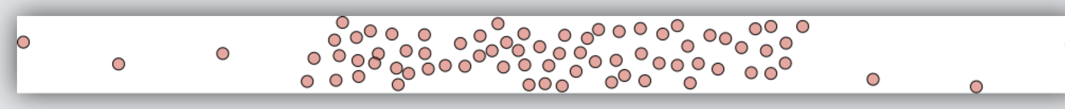
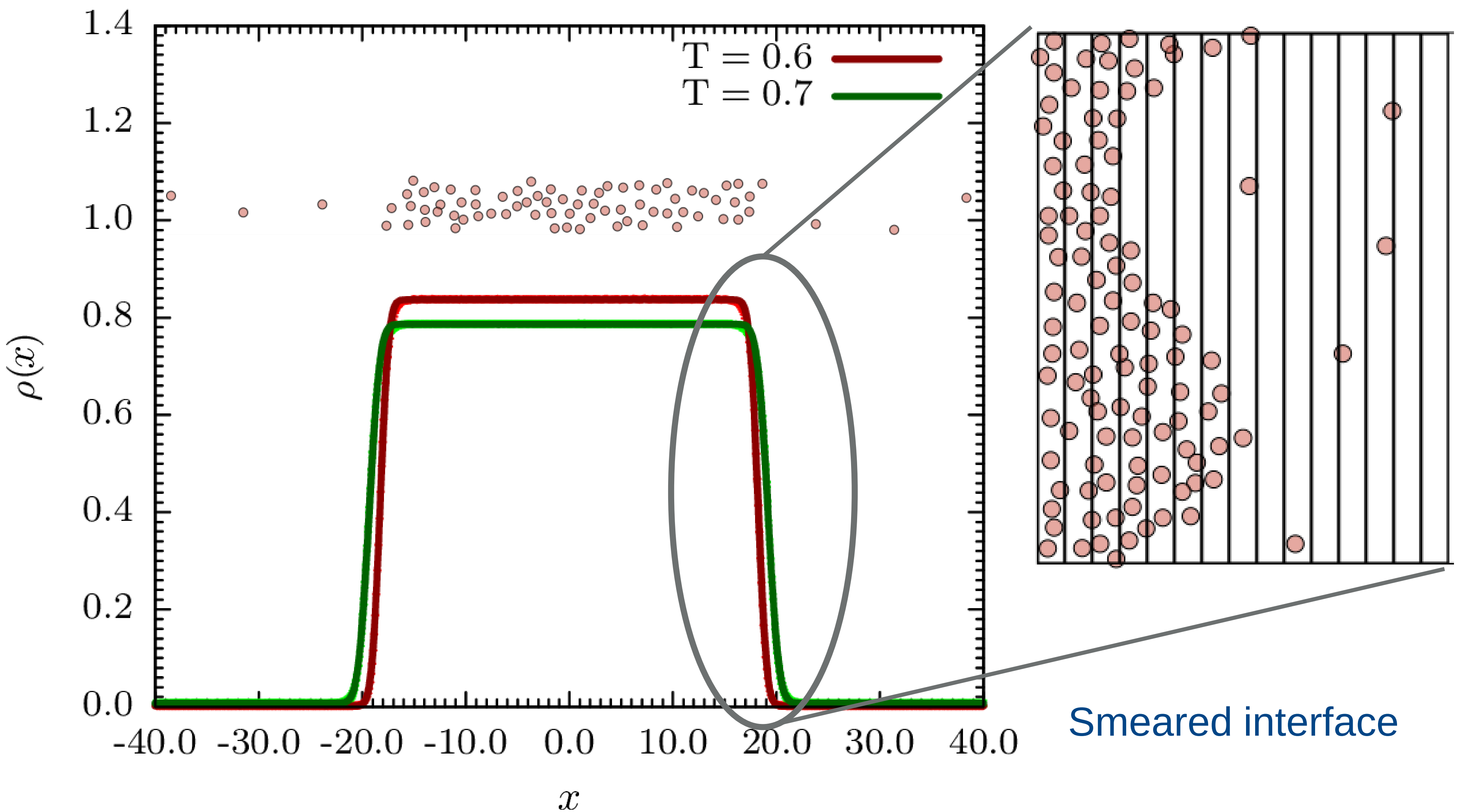
Results for Density





Smeared interface

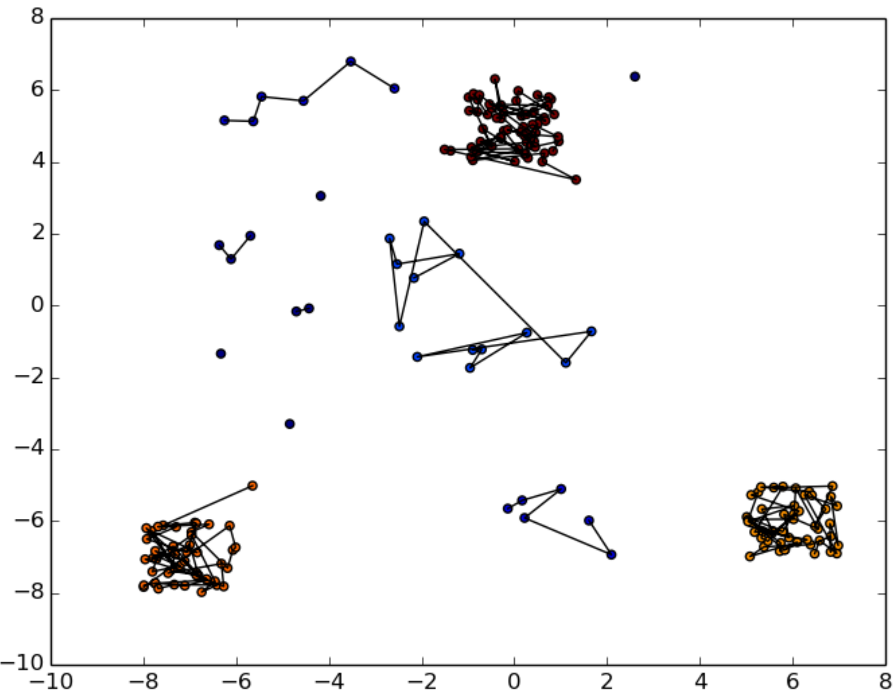
Summary so Far...

- We want to get quantities such as density, pressure and surface tension from an MD system
- Irving Kirkwood (1950) provides this but is based on the Dirac delta functional and ensemble averages (valid for interfaces, non-equilibrium systems, flow fields, complex molecules?)
- By using the control volume (weak) form, we avoid the Dirac delta and get a useful operator valid arbitrarily far from equilibrium
- We will now apply this to an interface

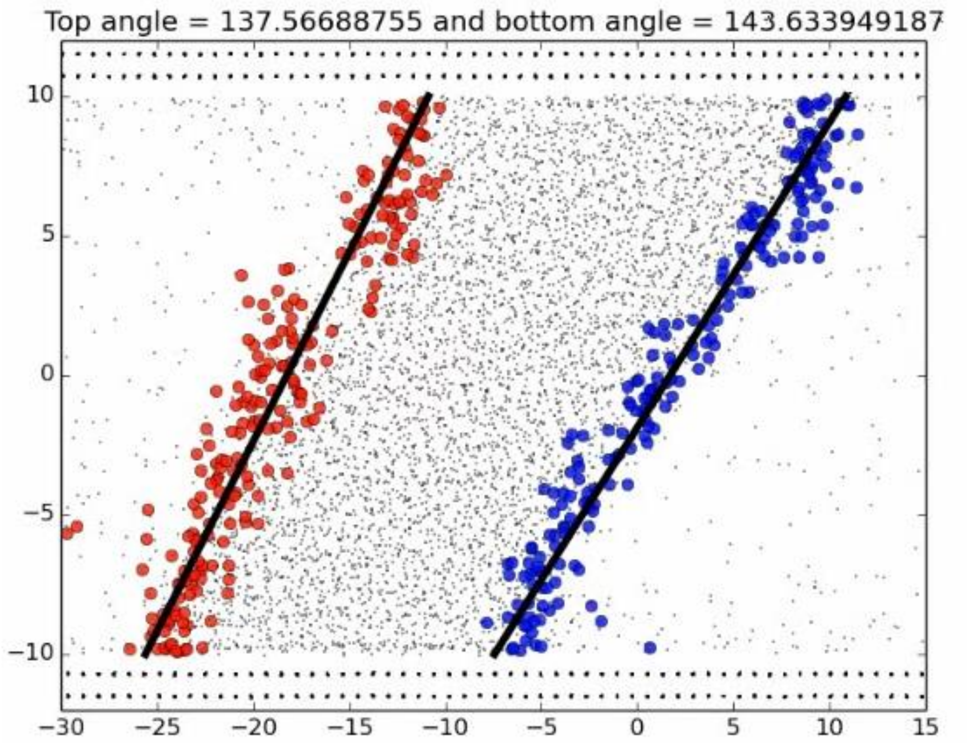
The Control Volume for an Intrinsic Surface

Cluster analysis and surface fitting

Cluster analysis

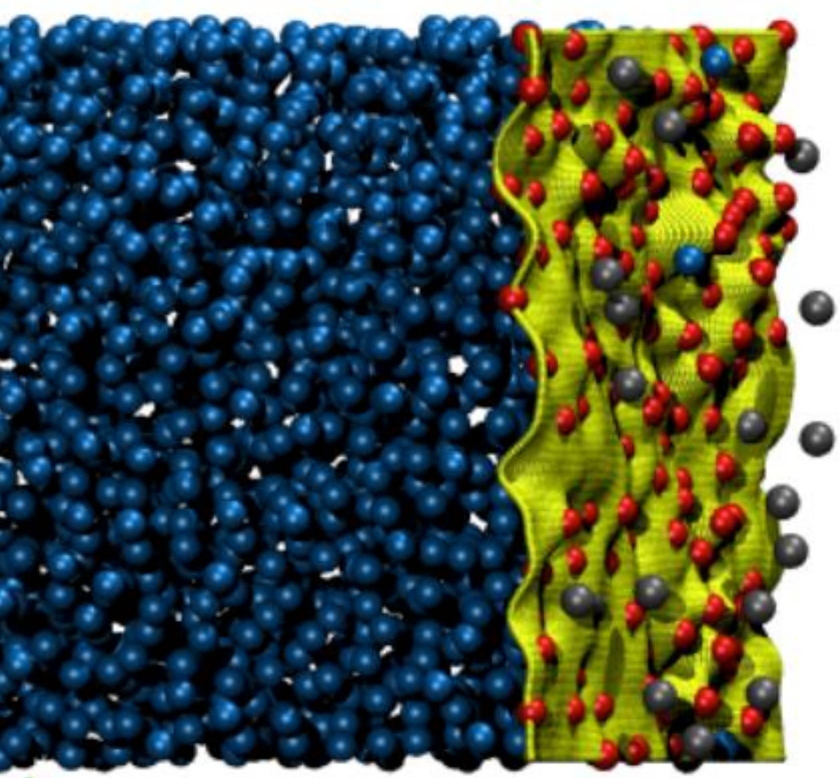


Finding the fluid-liquid interface



Intrinsic surface

- Intrinsic Surface by minimising a penalty function



$$W = \frac{1}{2}\sum_{i=1}^{N_s}(x_i - \xi(y,z))^2 + \lambda C$$

$$\xi(y,z) = \sum_{\mu,\nu} a_{\mu\nu} f_\mu(x) f_\nu(y)$$

Function of sines and cosines

Chacon & Tarazona (2003) PRL 91, 166103

An Intrinsic Control Volume Functional

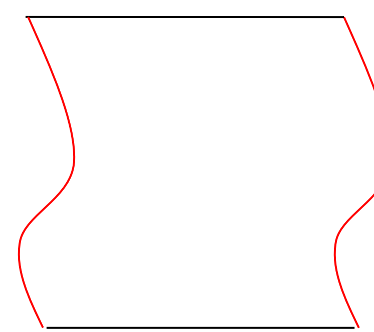
- The Control volume functional is the formal integral of the Dirac delta functional in 3 dimensions (3D top hat or box car function)

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

$$= \left[H\left(x^+ + \xi(y_i, z_i) - x_i\right) - H\left(x^- + \xi(y_i, z_i) - x_i\right)\right]$$

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

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



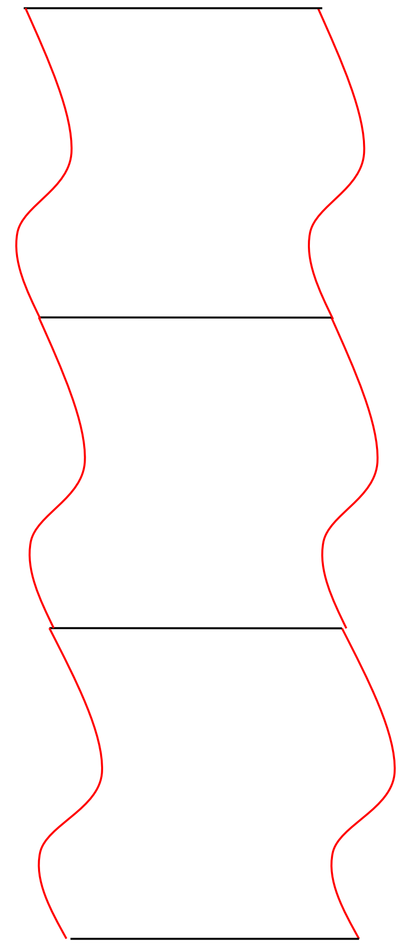
- In words

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

An Intrinsic Control Volume Functional

- Assume a periodic domain in y and z with a surface which is equal at the top and bottom (correct as sines and cosines)

$$\vartheta_i = \left[H\left(x^+ + \xi - x_i\right) - H\left(x^- + \xi - x_i\right)\right]$$
$$\times \left[H(y^+ - y_i) - H(y^- - y_i)\right]$$
$$\times \left[H(z^+ - z_i) - H(z^- - z_i)\right]$$



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An Intrinsic Control Volume Functional

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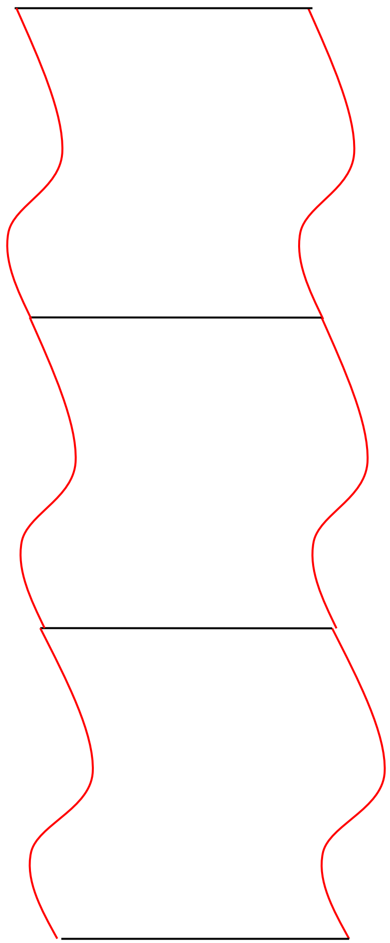
$$\vartheta_i = \left[H\left(x^{+} + \xi - x_i\right) - H\left(x^{-} + \xi - x_i\right) \right]$$



- In words

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

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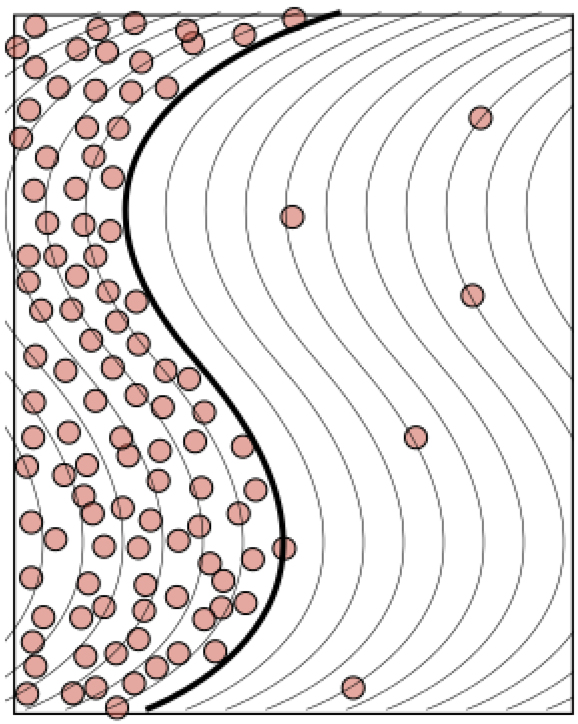
Applied to Density

- Density in a control volume based on the intrinsic surface

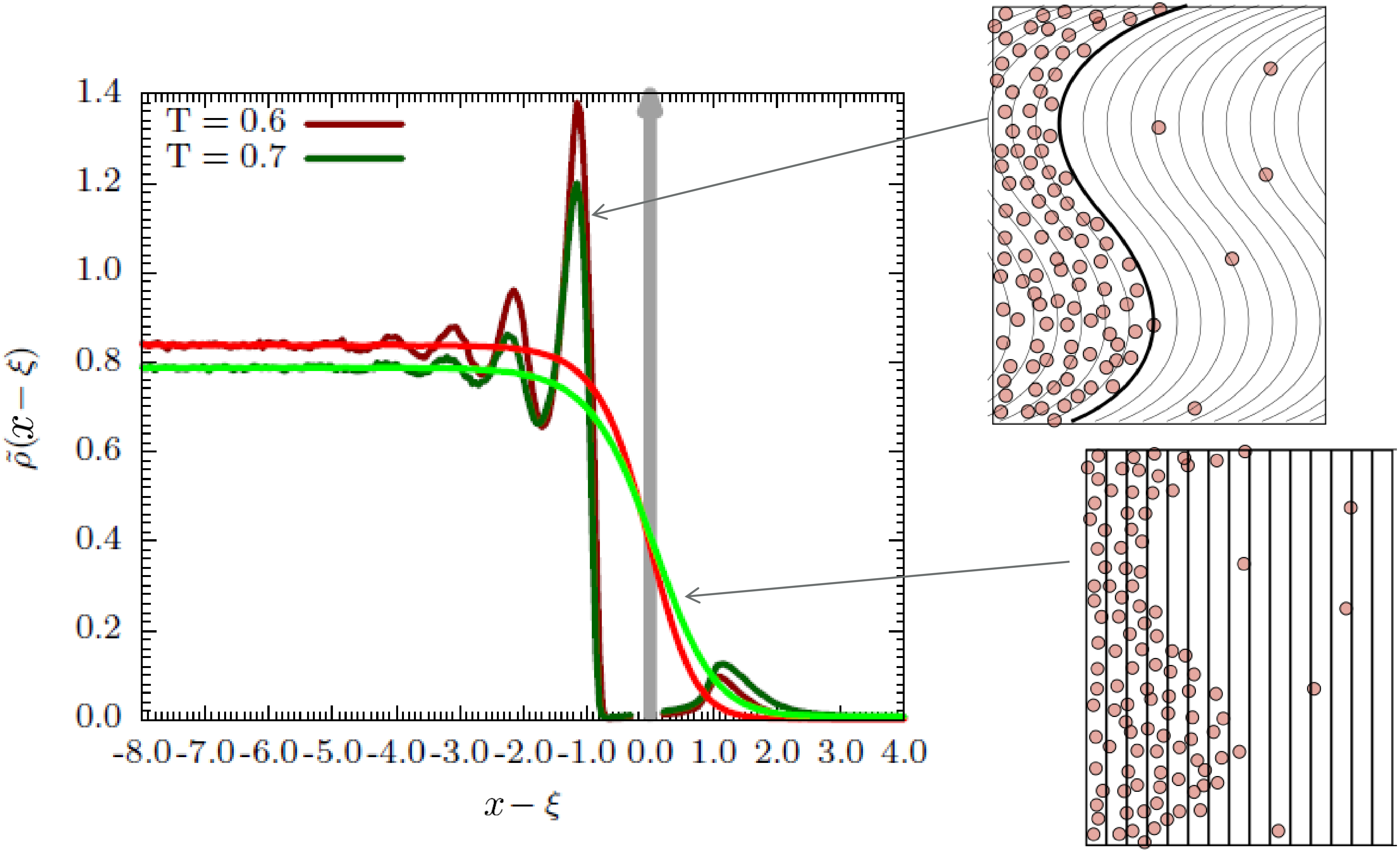
$$\int_{\tilde{V}} \rho(\boldsymbol{r}, t) dV = \sum_{i=1}^{N} m_i \int_V \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right) dV$$

$$= \sum_{i=1}^{N} m_i \left[H\left(x^+ + \xi - x_i\right) - H\left(x^- + \xi - x_i\right) \right]$$



Results

Results for Density

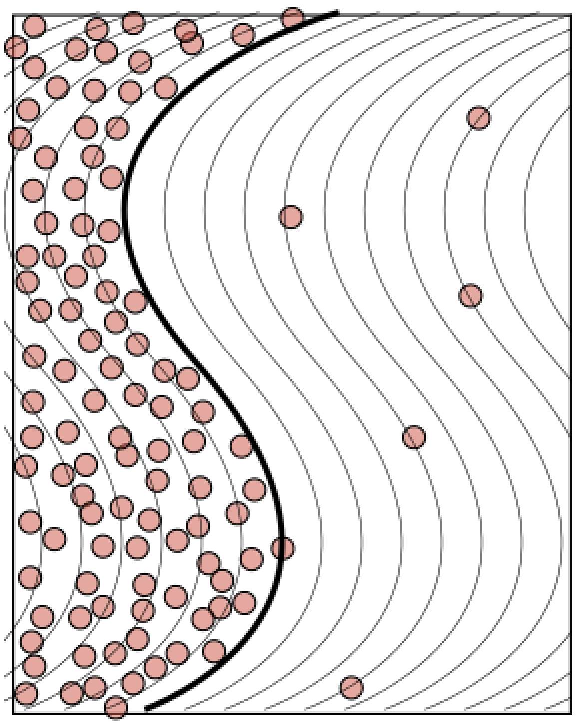


Applied to Density

- Density in a control volume based on the intrinsic surface

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

$$= \sum_{i=1}^{N} m_i \left[H\left(x^{+} + \xi - x_i\right) - H\left(x^{-} + \xi - x_i\right)\right]$$



- Which in the limit of zero width gives the definition of intrinsic density

$$\tilde{\rho}(x-\xi) = \lim_{\Delta x \to 0} \frac{1}{\Delta x \Delta y \Delta z} \sum_{i=1}^{N} m_i \vartheta_i$$

$$= \frac{1}{A} \sum_{i=1}^{N} m_i \delta\left(x + \xi - x_i\right)$$

Recall $x^{+} = x + \Delta x \quad x^{-} = x - \Delta x$ and $\delta(x) \equiv \lim_{\Delta x \to 0} \frac{H(x+\Delta x) - H(x-\Delta x)}{\Delta x}$

Pressure and Surface Tension

- The surface tension is given by the following expression

$$\gamma = \int_{-\infty}^{\infty} \left[\Pi_N(x) - \Pi_T(x) \right] dx$$

- Obtained by the integral of the difference in normal pressure and tangential pressure over an interface. For our convention:

$$\Pi_N = \Pi_{xx} \text{ and } \Pi_T = \Pi_{yy} = \Pi_{zz}$$

- Therefore, pressure is an essential quantity in fluid-fluid surface physics. Made up of kinetic and configurational part

$$\mathbf{\Pi} = \mathbf{\Pi}^k + \mathbf{\Pi}^c$$

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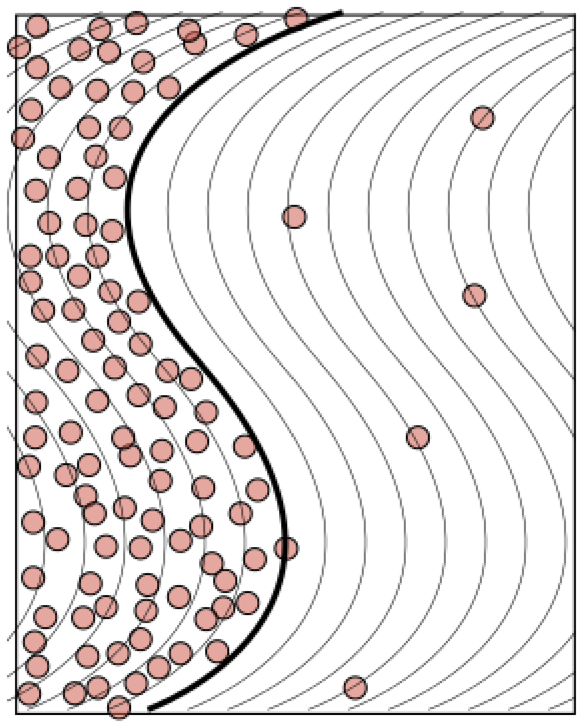
Applied to Kinetic Pressure

- Kinetic Pressure in a control volume based on the intrinsic surface

$$\int_{\tilde{V}} \mathbf{\Pi}^k dV = \sum_{i=1}^{N} m_i \boldsymbol{v}_i \boldsymbol{v}_i \int_{\tilde{V}} \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right) dV$$

$$= \sum_{i=1}^{N} m_i \boldsymbol{v}_i \boldsymbol{v}_i \left[H\left(x^+ + \xi - x_i\right) - H\left(x^- + \xi - x_i\right) \right]$$



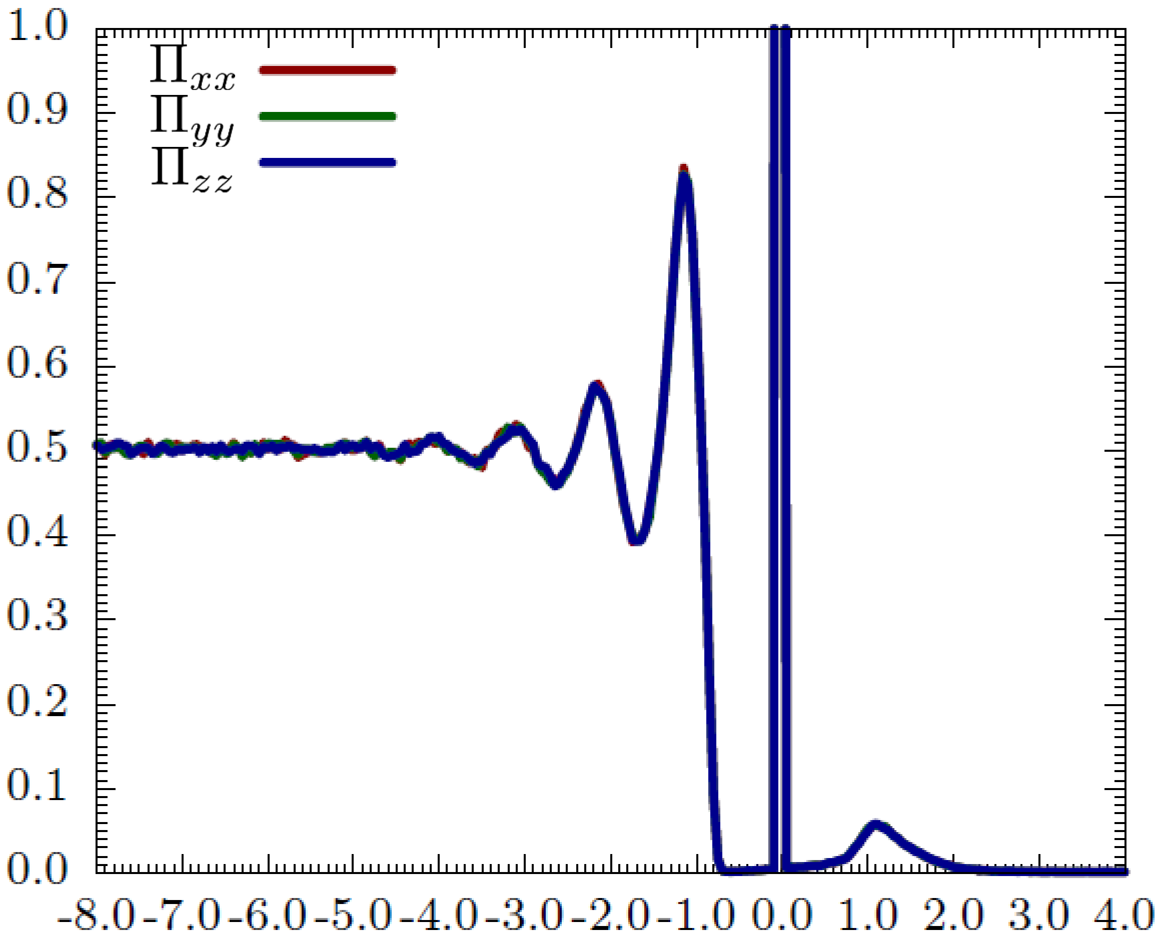
- This is a nine component tensor but only direct components are non zero
- We can define an intrinsic Pressure as with density

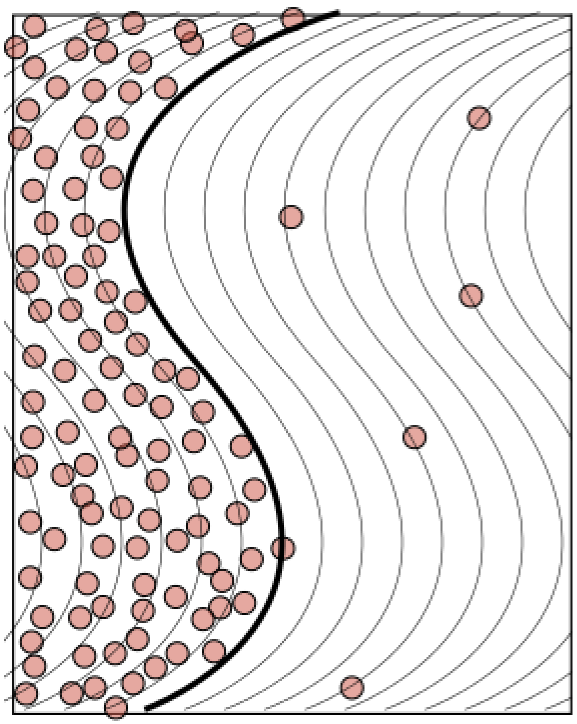
$$\tilde{\mathbf{\Pi}}^k = \frac{1}{A} \sum_{i=1}^{N} m_i \boldsymbol{v}_i \boldsymbol{v}_i \delta\left(x^+ + \xi - x_i\right)$$

Results for Kinetic Pressure

$$\gamma = \int_{-\infty}^{\infty} \left[\Pi_{xx} - \Pi_{yy} \right] dx = 0$$

Kinetic Pressure in volumes at distance from a surface



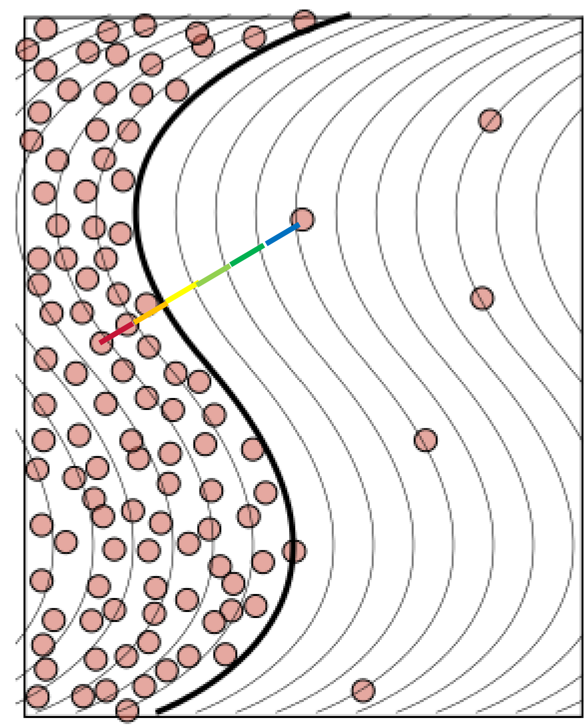


Applied to Stress

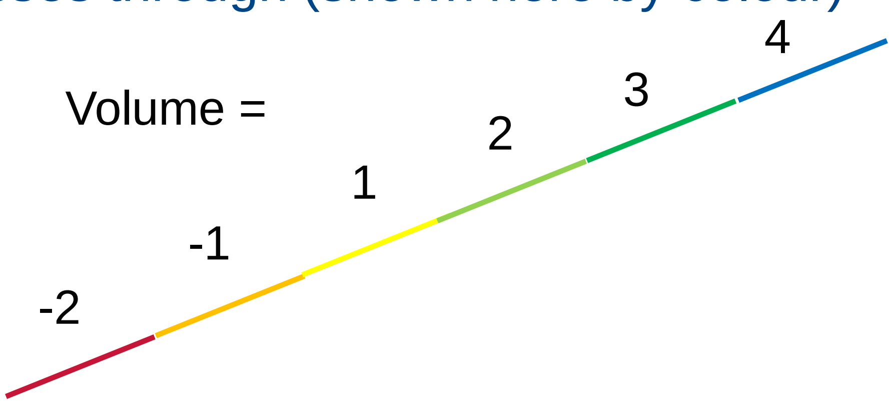
- Stress in a control volume based on the intrinsic surface

$$\int_V \tilde{\mathbf{\Pi}}^c dV = \sum_{i,j}^{N} \boldsymbol{f}_{ij} \boldsymbol{r}_{ij} \int_0^1 \vartheta_s ds$$

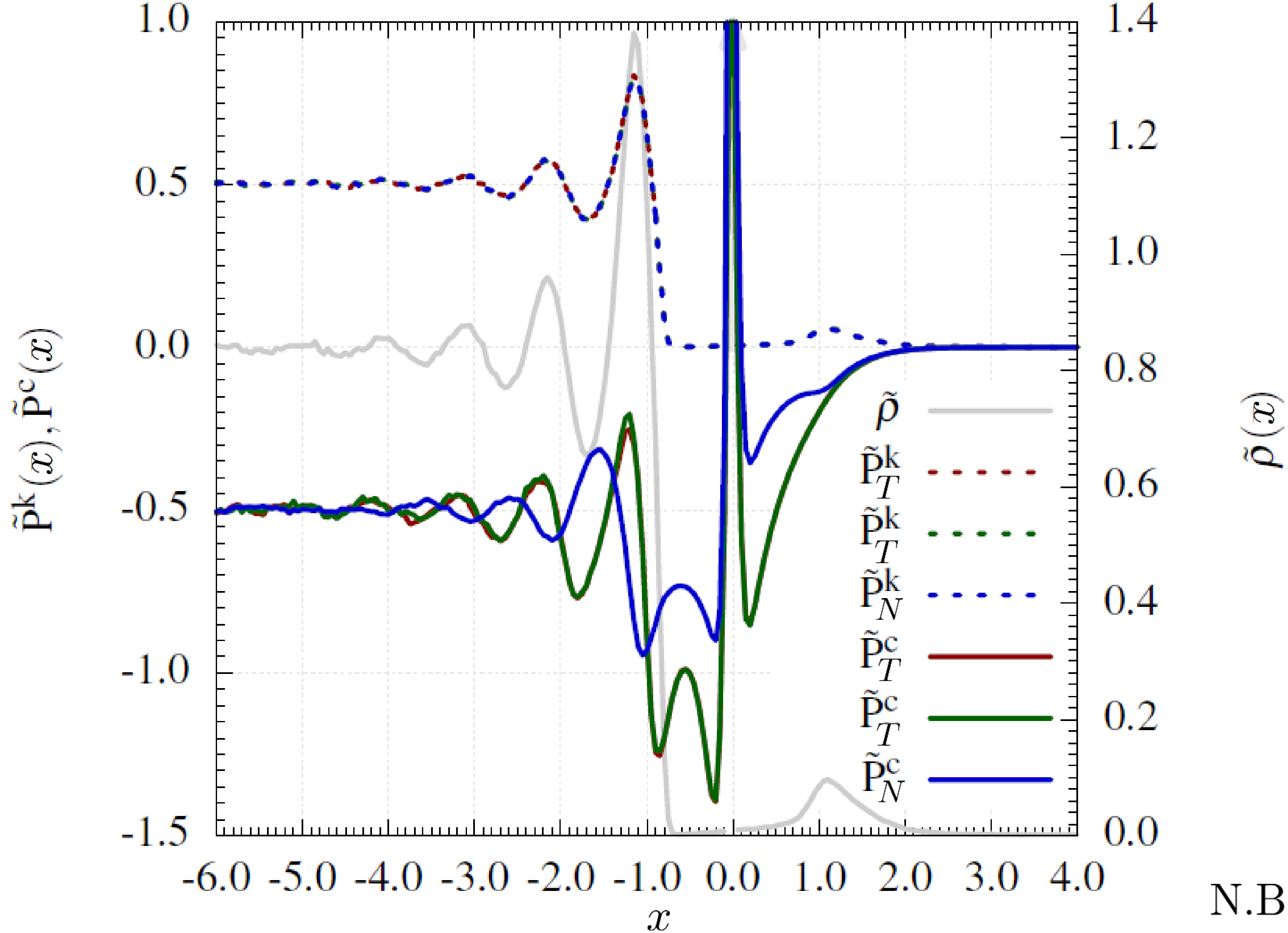
$$\vartheta_s = [\ H(x^+ + \xi(y_s, z_s) - x_s) \\ -H(x^- + \xi(y_s, z_s) - x_s)]$$



- Line of interaction split over every volume it passes through (shown here by colour)



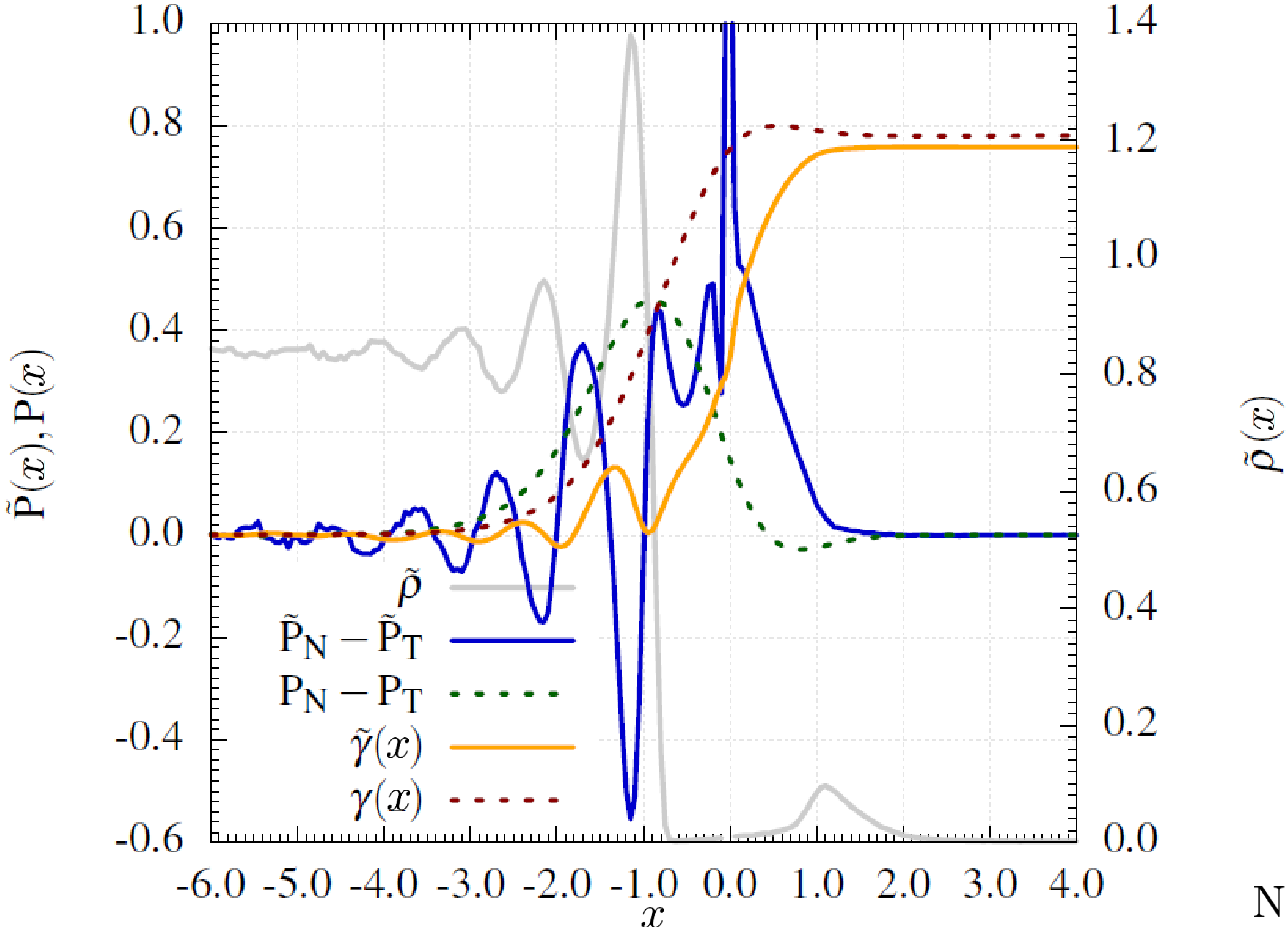
Results for Stress



N.B. $\Pi \equiv P$

Results for Surface Tension

$$\gamma = \int_{-\infty}^{x} [\Pi_N - \Pi_T]\, dx$$



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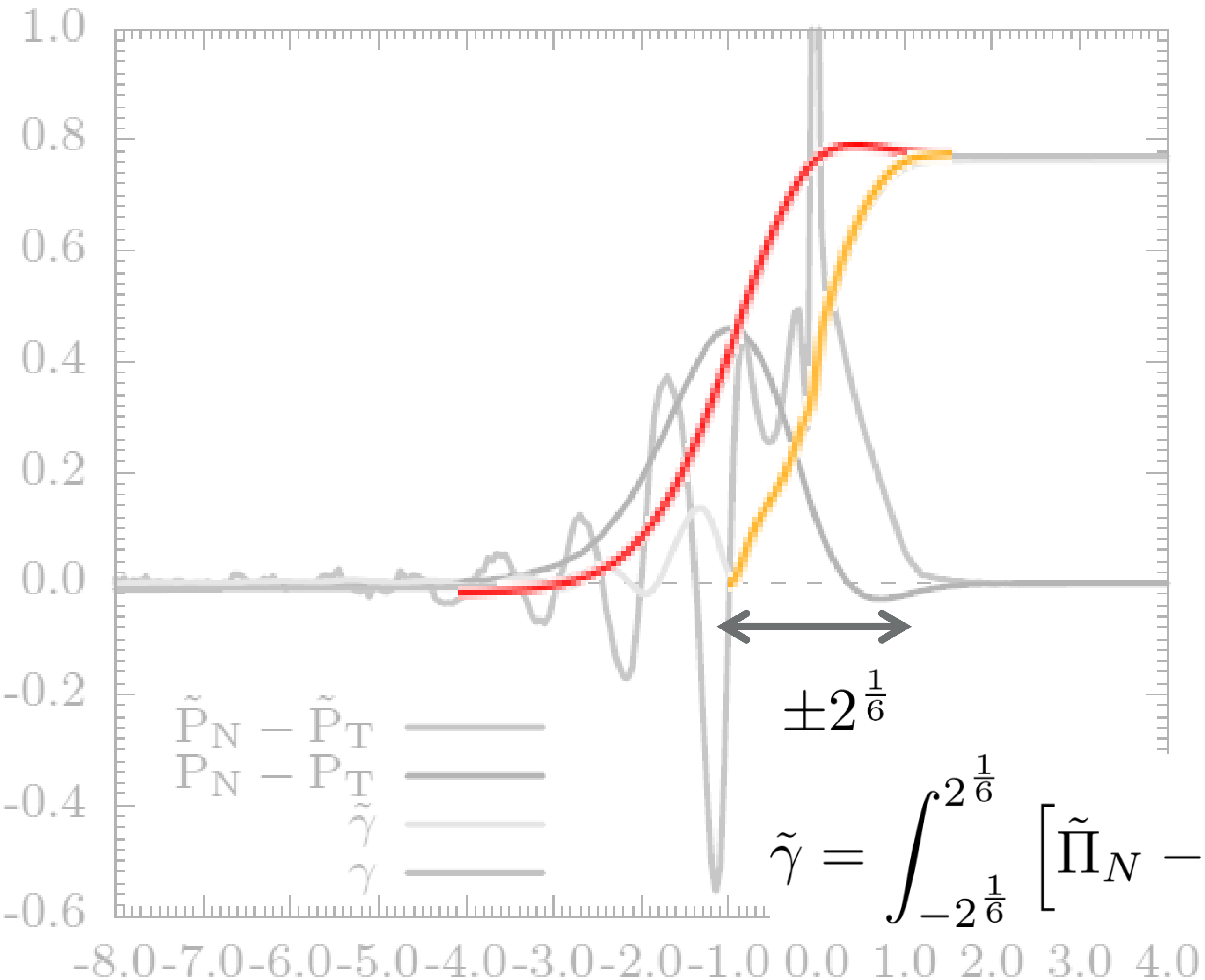
Results for Surface Tension



$$\tilde{\gamma} = \int_{-2^{\frac{1}{6}}}^{2^{\frac{1}{6}}} \left[\tilde{\Pi}_N - \tilde{\Pi}_T \right] dx$$

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Extensions

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A Grid of Intrinsic Control Volumes

- The Control Volume integral in 3D

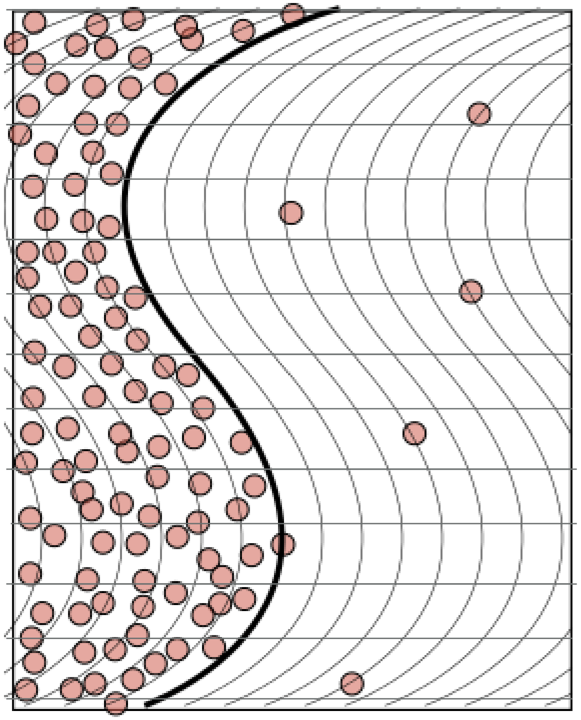
$$\vartheta_i \equiv \int_{z^-}^{z^+} \int_{y^-}^{y^+} \int_{x^-+\xi(y,z)}^{x^++\xi(y,z)} \delta\left(x - x_i\right) \delta\left(y - y_i\right) \delta\left(z - z_i\right) dxdydz$$

$$= \left[H\left(x^+ + \xi(y_i, z_i) - x_i\right) - H\left(x^- + \xi(y_i, z_i) - x_i\right)\right]$$

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

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

- Lots of volumes forming a 3D grid fitted to a surface



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

Control Volume Form

- The "weak formulation" expressed the equations in integrated form

$$\int_V \rho(\boldsymbol{r},t)dV = \sum_{i=1}^{N} m_i \int_V \delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right)dV = \sum_{i=1}^{N} m_i \vartheta_i \equiv \sum_{i\in\text{Cell}}^{N_{\text{Cell}}} m_i$$

$$\frac{d}{dt}\int_V \rho(\boldsymbol{r},t)dV = \sum_{i=1}^{N} m_i \frac{d\vartheta_i}{dt} = \sum_{i=1}^{N} m_i \frac{d\boldsymbol{r}_i}{dt}\cdot\frac{d\vartheta_i}{dr_i} = \sum_{i=1}^{N} m_i \boldsymbol{v}_i \cdot d\mathbf{S}_i$$

Control Volume Extension

Taking the Derivative of the CV function

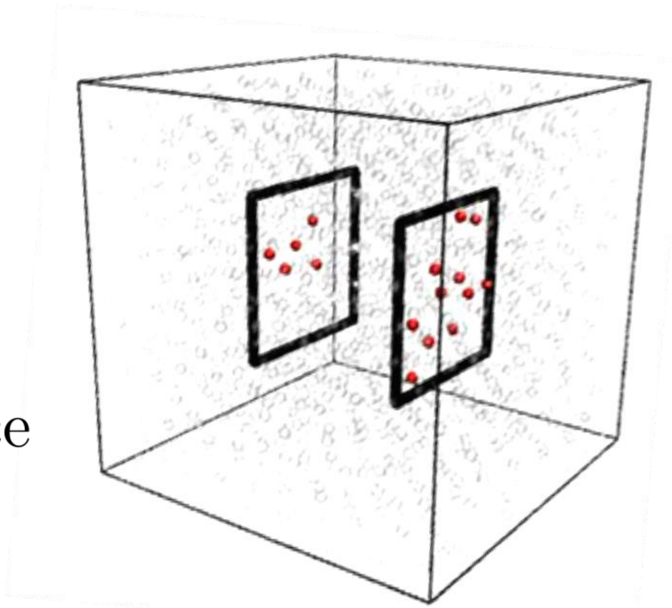
$$dS_{ix} \equiv -\frac{\partial \vartheta_i}{\partial x_i} = \left[\delta(x^+ - x_i) - \delta(x^- - x_i)\right] \times \left[H(y^+ - y_i) - H(y^- - y_i)\right] \times \left[H(z^+ - z_i) - H(z^- - z_i)\right]$$

Vector form defines six surfaces

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

Or in words

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



Control Volume Form

- The “weak formulation” expressed the equations in integrated form

$$\int_V \rho(\boldsymbol{r},t)dV = \sum_{i=1}^{N} m_i \int_V \delta\left(\boldsymbol{r} - \boldsymbol{r}_i\right) dV = \sum_{i=1}^{N} m_i \vartheta_i \equiv \sum_{i \in \text{Cell}}^{N_{\text{Cell}}} m_i$$

$$\frac{d}{dt}\int_V \rho(\boldsymbol{r},t)dV = \sum_{i=1}^{N} m_i \frac{d\vartheta_i}{dt} = \sum_{i=1}^{N} m_i \frac{d\boldsymbol{r}_i}{dt} \cdot \frac{d\vartheta_i}{d\boldsymbol{r}_i} = \sum_{i=1}^{N} m_i \boldsymbol{v}_i \cdot d\mathbf{S}_i$$

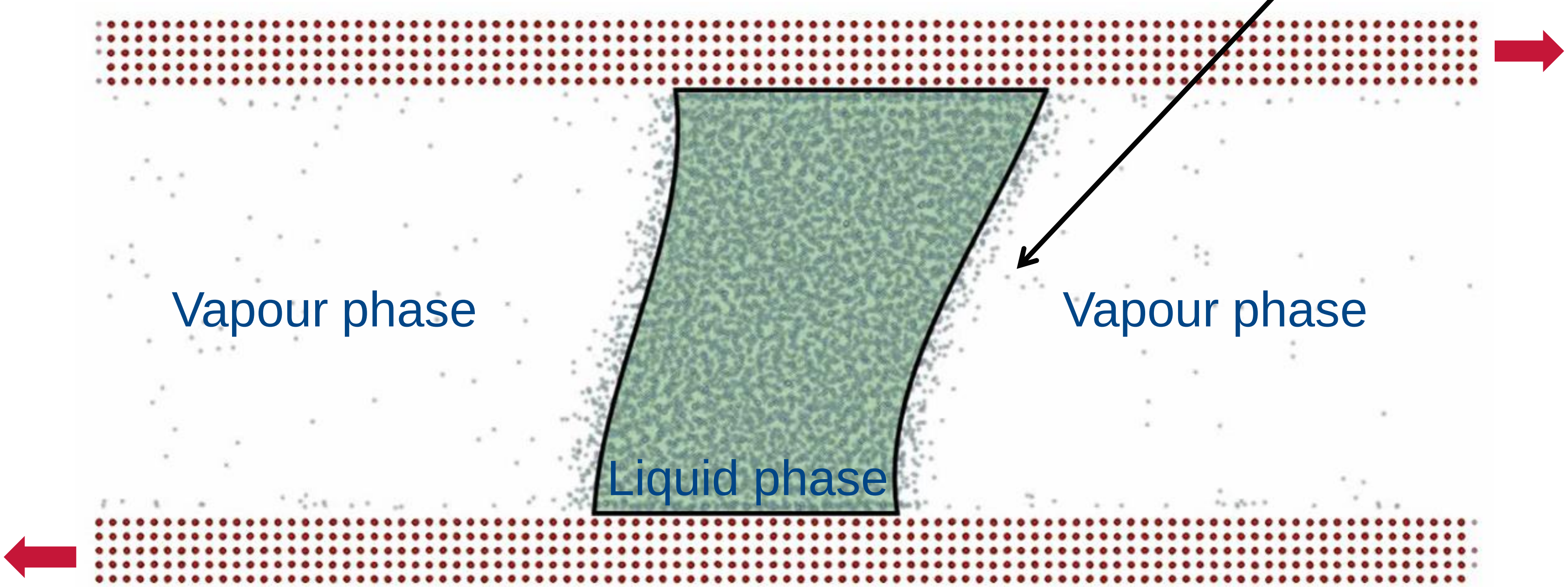
- Integrating the Dirac delta function exactly provides a combination of Heaviside functions, which can:
  - Be mathematically manipulated to give fluxes and forces
  - Be implemented directly in MD codes
  - Be linked to the continuum control volume/finite volume equations as they are now expressed in the same form

Surface Curvature

- Derivative now includes terms for moving surface, curvature, etc

$$dS_{xi}^{+} = \left[\dot{x} - \dot{x}_i + \dot{y}_i \frac{\partial \xi^+}{\partial y_i} + \dot{z}_i \frac{\partial \xi^+}{\partial z_i} + \frac{\partial \xi^+}{\partial t} \right] \delta\left(x^+ + \xi^+ - x_i\right)$$
$$\times \left[H\left(y^+ - y_i\right) - H\left(y^- - y_i\right) \right]$$
$$\times \left[H\left(z^+ - z_i\right) - H\left(z^- - z_i\right) \right]$$

- Allows MOP stresses to be obtained on arbitrary surfaces



Sliding Solid walls (tethered)

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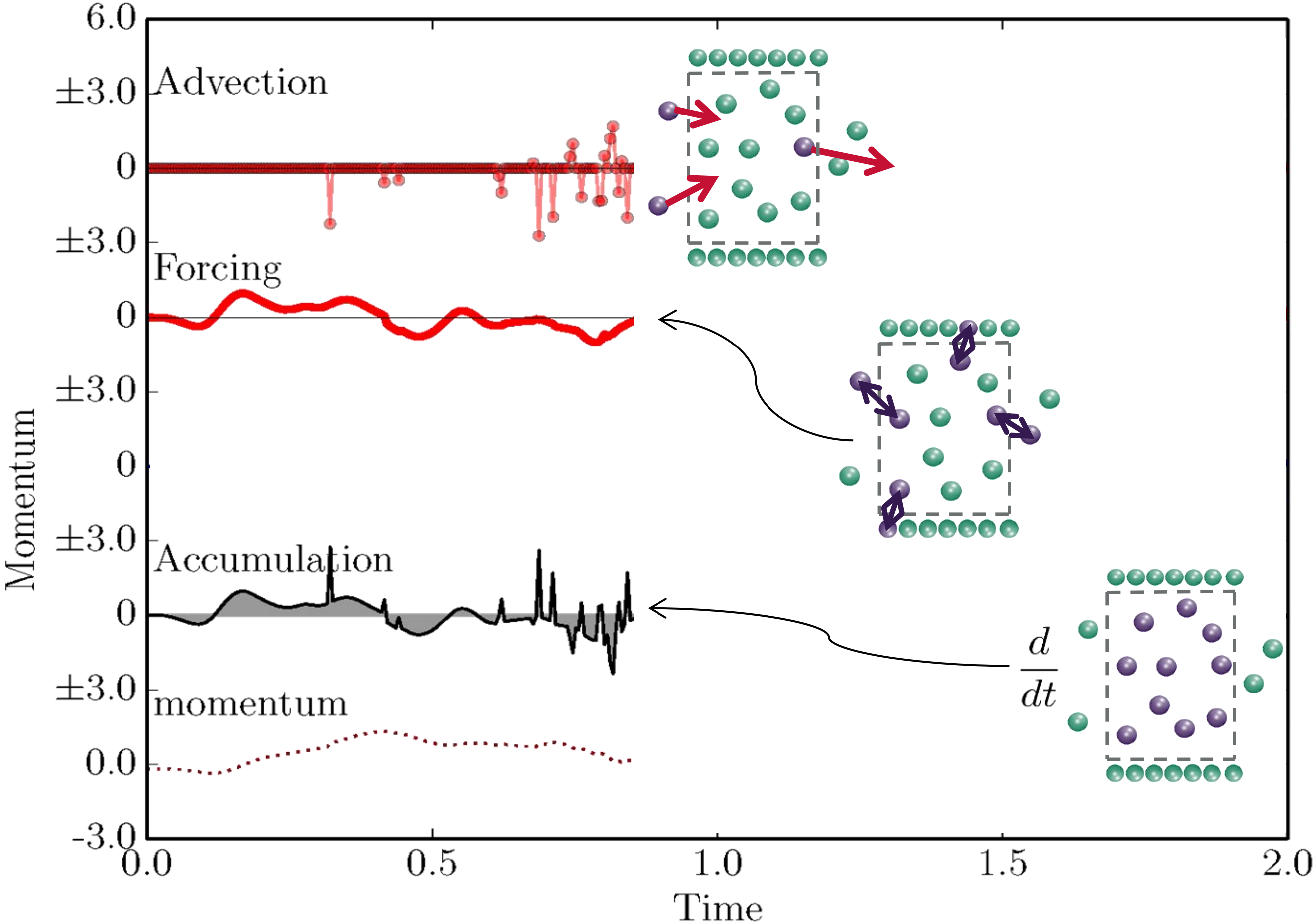
Exact Conservation for a cubic CV

Accumulation = Forcing + Advection + surface

Momentum evolution from integral of Accumulation



Method of Planes on 6 surfaces

$$\underbrace{\sum_{i=1}^{N} m_i \mathbf{v}_i \mathbf{v}_i \cdot d\mathbf{S}_i}_{\textit{Advection}}$$

$$\underbrace{-\frac{1}{2}\sum_{i,j}^{N} \boldsymbol{f}_{ij}\mathbf{n} \cdot d\mathbf{S}_{ij}}_{\textit{Forcing}}$$

$$\underbrace{\frac{d}{dt}\sum_{i=1}^{N} m_i \mathbf{v}_i \vartheta_i}_{\textit{Accumulation}}$$

Possible Insights and Applications

- Concentration gradients on the fluid surface could be measured with a grid of surface volumes
  - Explore Marangoni type flows
  - Measure bulk and surface interchange of complex molecules
- Track hydrodynamic instabilities and the interplay with the surface itself
- The exact balance could allow us to work backward in the exploration of unknown processes
- Explore a range of process which are inherently non-local, non-equilibrium and unsteady

Summary

- We want to get quantities such as density, pressure, surface tension, etc from an MD system
- Irving Kirkwood (1950) integrated over a control volume gives a useful operator valid arbitrarily far from equilibrium
- By defining this volume following a fluid-fluid interface we obtain insights into the interface
- The control volume operator formalises typical averaging and provides a useful framework to explore moving interfaces in detail

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Thank you

Questions?

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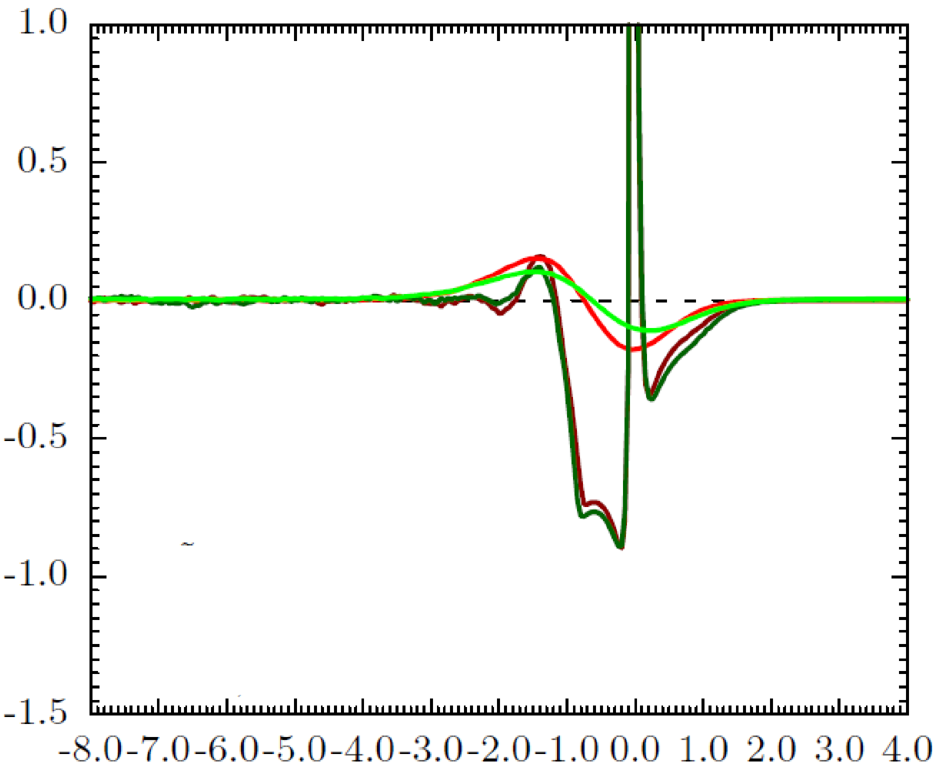
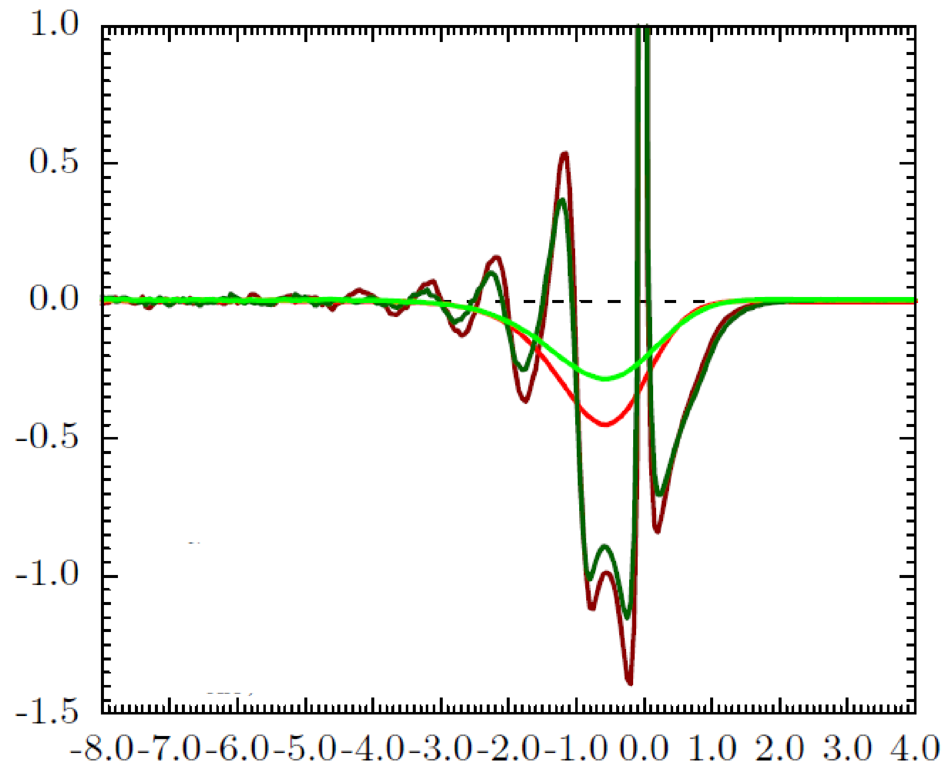
Results for Stress

Normal Stress



Tangential Stress



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Results for Surface Tension

$$\gamma = \int_{-\infty}^{x} [\Pi_N - \Pi_T] \, dx$$