Eulerian Formulation of Discrete Particle Dynamics

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Eulerian and Lagrangian Formulations

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

$$\frac{\partial}{\partial t} \int_{V} \rho dV = -\oint_{S} \rho \boldsymbol{u} \cdot d\mathbf{S}^{\mathsf{ls'}}$$
• Why?

$$\frac{\partial}{\partial t} \int_{V} \bar{\rho} \boldsymbol{u} dV = -\oint_{S} \rho \boldsymbol{u} \boldsymbol{u} \cdot d\mathbf{S} \text{and} + \mathbf{F}_{\text{surface}}$$

Insight into the molecular form of

$$\frac{\partial}{\partial t} \int_{V} \rho \mathcal{E} dV = -\oint_{S} \rho \mathcal{E} \boldsymbol{u} \cdot d\mathbf{S}$$
• The basi and cont- $\oint_{S} \boldsymbol{\Pi} \cdot \boldsymbol{u} \cdot d\mathbf{S} + \mathbf{q} \cdot$



Outline

. Introduction

- . Discrete models (molecular dynamics)
- Irving and Kirkwood (1950)
- . Eulerian Equations of motion
 - Control Volume Function
 - Reynolds' transport theorem using the control volume function
 - Application to microscopic pressure
- Results
 - Numerical simulations of Couette flow
 - Applying the method to coupling

Introduction



Discrete models (molecular dynamics)

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

$$m_i \ddot{m{r}}_i = {f F}_i = \sum_{i
eq j}^N m{f}_{ij} \qquad egin{array}{cc} \ddot{m{r}}_i
ightarrow \dot{m{r}}_i \ \dot{m{r}}_i
ightarrow m{r}_i \ \dot{m{r}}_i
ightarrow m{r}_i(t) \end{array}$$



- **Misleventa**N **Ebordansiystasetleffoed** •
 - in terms of sums High Knudsen number flows

 - Sum-presentires (stem defining agrangial ation) system
 - Crystal structures and dense fluids (correlations) How do we get an Eulerian description?
 - **Polymers**

mass_{system} =
$$\frac{1}{M} \sum_{i=1}^{M} m_i \qquad \int_{V} \rho(\mathbf{r}, t) dV = ?$$



Irving and Kirkwood (1950)

 $\alpha(\boldsymbol{r}^{N},\boldsymbol{p}^{N}) f(\boldsymbol{r}^{N},\boldsymbol{p}^{N},t) d\boldsymbol{r}^{N} d\boldsymbol{p}^{N}$ $\alpha;$ 15/0)=00 S(z-a) dx = 1 $\mathcal{S}(\mathbf{x},\mathbf{v})f(\mathbf{x},\mathbf{v})d_{\mathcal{H}}=f(\mathbf{v},\mathbf{v})_{\mathbf{v}}^{2}$ not been observed. If the preferred interpr NSPORT PROCESSE Ket Observel. If the preferred interpretation the group of Ramon hands, 769, 718, 819, and the stated to each other in much the same the state of Steras fixs da + fias The probability distril TRANSPORT PROCESSES In prilate they sity of representative points to sature or nation are sature the spectra of CO3 and CS3. tion function (relative den-ars phase space) we denote as the expectation value of the dynamical valuable $\mathcal{A} \Gamma P A$ 171.9 cm⁻¹. The band at 809.7 cm⁻¹ has been interpre 17: 9 cm⁻⁴. The band at 300.7 cm⁻¹ has been interpreted as 22×394, the rather large difference between calculated and decounted forements being standard to the communic unner as similar groups and 829 cm as 2X.995, the rather large difference between calculated and observed incomercy being accritic in the proximity is due A. Instances at House the based could be an $f(R_1, \ldots, R_N; p_1, \ldots)$ ACKROWLEDGI The writers wish to express their incented satisfying the normalization condit and observed incruency being ascrines, in the proximity to the A, fundamental. However, this hand could be an . ne writers wan to express their inconcentures. C. F. Hanmer and E. L du Pont de Nemears an to the A. Iondamental. However, this band could be an upper-stage band corresponding to S19 cm⁻¹. The interpretation of the faint sharp hand at 769.4 cm⁻¹ as an upper-stage band, 778+v⁻¹-v₋₁ scame more plauible than its interpretation as the B₁ combination, 2104-558 cm⁻¹. The faint sharp Racean hand at \$25 8(1) 2= C. F. Hammer and E. L on Pont its Nensours used Company for the samples; to Doctors Inshells and Icomes Sarle for electron difference dats; and to Dr. V. Budenet do: Mattern Doctors and a second at the Sol TRACTOROL' PROCE Jerome Karle lot electron diffraction dats; and to Dr. E. K. Phyler and the National Bureau, of Standards for $\int id\mathbf{R}_1\cdots d\mathbf{R}_N dp_1\cdots dp_N = 1$ We shall use (2.7) to derive the equations of hydro-Avanamics plausible than its interpretation as the B w combination, 2004-558 cm⁻¹. The faint sharp Raman band at \$28.5 ment has been betweeted as an unmarging band where $d\mathbf{R}_t$ stands for a volume element in the condata in the long wave-kngth region. 210+558 cm⁻¹. The faint sharp Raman band at 835. cm⁻¹ has been interpreted as an upper-stage band. 2X a07 + v₀ − v₀, rabter than as the R₂, difference band 1540-510 cm⁻¹, because the corresponding sum band water and stands for a volume element in the con-figuration space and dp a volume element in the two-non-time source of the ath weakers of schemes in time. (2.1) figuration space and dp, a volume element in the mo-mentany space of the 4th moderate f charges in time accounting on the well-become fine station III. STATISTICAL MICHANICAL MARKENSIONS FOR DENSITIES menum space of the sun molecule. ; charges a according to the well-known Liouville equation The equations of hydrodynamics (1.1), (1.2), and (1.4) are concerned with densitive in ecdancy 3-space, e.g., mass density, momentum density, and energy density. We shall now express these as the expectation values of hydramical variables over an ensemble baving distribution function f. JUNE. 1950 VULUME 15. NUMBER 6 2:0 $\frac{df}{dt} = \sum_{k=0}^{N} \left[-\frac{p_k}{m_k} \cdot \nabla \mathbf{R}_k f + \nabla \mathbf{R}_k U \cdot \nabla p_k f \right]$ The Statistical Mechanical Theory of Transport Processes. TV, The Equations of Hydrodynamics where t is the potential energy of the entire system. Any cynamical variable, $\alpha(\mathbf{R}_1, \cdots, \mathbf{R}_r; p_1, \cdots, p_N)$, $\int \cdots \int f(\mathbf{R}_1, \cdots, p_1, \cdots, f) d\mathbf{R}_1 \cdots$ has an expectation value given at time f by THE INCREAT OF CREMICAL PHYSICS is the probability per unit volume that the kth molecules be at \mathcal{R}_{k} is (e_{ij}) the expectation value of a is the integration is over all position vectors expectation value of a is a final vector. Introducing that the kth nodecut e to at fast time i_{ij} ∂ $\partial \alpha$ We thus denote by (a;j) the expectation value of a that the kth is induct of a and j inducts $j \in \{1\}$ is indeed to be and j induct of a start $j \in \{1\}$ is indeed to be and j induct of a start $(a(R_k - \gamma);j)$. Providing a does not descend on time embicitly, the α ; 81 $\overline{\partial t}$ this program is uncertain in a liquid, vantus attempts have been under to obrain a closed equation satisfies are immulify by the robustility distillution function oper immulify by the robust of molecules, One such equa-Providing a close not depend on time explosing, the rate of change of the expectation value of a ls given by 81 $\eta^{(\alpha_i,f)} \sim \left\langle \alpha_i, \frac{\partial f}{\partial t} \right\rangle = \sum_{k=1}^{N} \left[\left\langle \alpha_i, -\frac{p_k}{m_k}, p_{k_k,t} \right\rangle \right]$ $-\int \cdots \int \delta(R_{4}-t)/(R_{d_{1}}\cdots p_{d_{1}}\cdots p_{d_{1}}\cdots p_{d_{k}})dR_{t}\cdots dp_{d_{k}}$ generalization of the well-known Fokker-Planck equi HIS paper will be concerned with a der the equations of hydrodynamics from the prinkerentised antervos of assumptio Int (Re & Solt) generalization of the well-known Forker-Flanck equa-tion of stochastic theory, has been derived by Ki-tations of hydrodynamics from the prin-classical statistical mechanics. In par-distantion of continuity, the equation of the base ation of energy transport will be above the state of the 100 DI SUCCIBEN: 40075; INS 1000 university of all the smoothing the concepts of time smoothing to be a successful of the second Adde may I look Estinger = mx prof. The total that is density at r due to all audocules is thus wood ny introducing use concepts as true smoothing and a triction constant. This latter equation has been ANO + (a; V& D. Voul) . (2.4) and a metuon constant. Los after equeton na ocen applied to obtain an expression for the creas tensor By tress feneral molecular variables. applied to obtain an expression for the stress unautified to obtain an expression for the stress unautified to be stress of third velocity and, thereby, esen applied in the space of R. 10-015=0 unon in grameris of must velocity and, incertify, ex-pressions (in terms of colorniar variables) (ar co rejents of above and volume viscosity.) The same Licular, motion, and the petic part (which derived. By so doing, the $P(z; t) = \sum_{k=1}^{N} m_k (\delta(\mathbf{R}_k - z));$ density can be expressed in len oother term The stress tensor consists of a ot showr and volume viscosity. And same The m occurs in the kinetic theory of gases) a providing the integrat (dominant for a liquid) which will be expe 95 B actions of actionments emperatures (VRACIT) the system is bounded or $/N_1$ as $R_{b} \rightarrow \infty$. Likewise, since ∇R_{b} it ja .. quadrature involving the potential of interm the use compensate gradient, rears to End. (3.1) nd the locations of the quadrature involving the position of atternance to a terminate the density of pairs of molecules. The here the second state of (2.5) the coefficient of thermal connote and the uenaty of pairs of molecules. The best current density is the sum of the ismiliar kinetic part by the matin vanishes; i.e., providh mentum pa, and since / falls of others are a current density is the sum of the immitar kinetic par-and a quarkature involving the potential of inter-medicatar force and the density and current density in the configuration ensure of a voir of motionale the enfor purposes of matheaiter lines. of sufficien ly ray of Green's theorem in the most $\int p_{i\delta}(\mathbf{R}_{k}-z)/(\mathbf{R}_{i_{1}}\cdots;p_{i}\cdots;i)_{d}\mathbf{R}_{j}\cdots dp_{d'}$ an explicit expr opent, single phase malecular force and the density and current density in the configuration space of a pair of nulceulus. The re-sults were revolvably stated in the first article of this artist, when this defination are promised. To obtain explicit expressions for the pair probability density and probability current density one would in to an expression it We shall ass which interact simplicity, a single $(\alpha; \nabla \mathbf{r}_{0}U, \nabla \mathbf{p}_{0}j) = -(\nabla \mathbf{r}_{0}U, \nabla \mathbf{r}_{0})$ futures sumptions, a subject component, future system, consisting ul molecule a under central forces only. It is not difficul $\int \cdots \int \delta(R_s - t) f(R_{l_s} \cdots; p_{l_s} \cdots; j) dR_1 \cdots dp_{l_s}$ Thus, (2.4) becomes toner central reversionly. It is not component or the treatment to a multiple component or ¹ M. Dorth Ard, H. S. Green, Proc. Boy. Suc. A188, 19 (Kithowood, Buch, and Turren, J. Chern. Phys. 17, 1998 (Starwood, Stankinst, and Levingine prevariation). J. editor evaluation sensitis a more precise comparations of the frait wheat description function. To obtain explicit expressions for the pair probability density and probability current density one would in subminde most to relate the thread to consider the $\exists a; f = \tilde{\Sigma}$ (2.5) density and provability current density one would in principle need to solve the Linuville equation (Eq. (2.2)) for the probability distribution in Gibbs phase over and then perform encoded intermediate curve ·VRH Consequently, $(p_{i}(R_{i} - r), f)$ is the product of this mean momentum by the probability per unit volume that the kth molecule to at r; i.e., it is the contribution of the kth molecule to the monentum per unit volume (mass current density). The local momentum density (2.3) for the probability distribution in Gross phase space and then perious repealed laterations. Since ·Vnaif) * This work was supported by the U.S. ONE under Contract Manar 244 with the California Institute of The Souther. J. G. Kirkwood, J. Chon. Phys. 14, 301 (1946) HEV or the era momentum per unit values (mass current density), "The local momentum density N $\rho(\mathbf{r},t) = \sum \langle m_i \delta(\mathbf{r} - \mathbf{r}_i); f$ $\alpha = \sum m_i \delta \left(\boldsymbol{r} - \boldsymbol{r}_i \right)$ **Imperial College** 6 London

Selecting Functions

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

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



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

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

$$\delta(x-x_i)$$





Eulerian Equations of Motion



More information

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

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Control-volume representation of molecular dynamics

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

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Control Volume Function

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

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

$$= [H(x^{+} - x_{i}) - H(x^{-} - x_{i})]$$

$$\times [H(y^{+} - y_{i}) - H(y^{-} - y_{i})]$$

$$\times [H(z^{+} - z_{i}) - H(z^{-} - z_{i})]$$



Derivatives yields the surface flux

. Taking the Derivative of the CV function

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

• 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 can be defined

$$\frac{\partial}{\partial t} \int_{V} \rho dV, t = \frac{\partial}{\partial t} \sum_{i=1}^{N} \left\langle m_{i} \vartheta_{i} r f \right\rangle r_{i}; f \rangle$$

• Simple mathematical operations using the control volume function

$$\frac{\partial}{\partial t} \sum_{i=1}^{N} \left\langle m_{i} \vartheta_{i}; f \right\rangle = \sum_{i=1}^{N} \left\langle \frac{\boldsymbol{p}_{i}}{m_{i}} \cdot \frac{\partial m_{i} \vartheta_{i}}{\partial \boldsymbol{r}_{i}} - \boldsymbol{F}_{i} \cdot \frac{\partial m_{i} \vartheta_{i}}{\partial \boldsymbol{p}_{i}}; f \right\rangle$$
$$= \sum_{i=1}^{N} \left\langle \boldsymbol{p}_{i} \cdot \frac{\partial \vartheta_{i}}{\partial \boldsymbol{r}_{i}}; f \right\rangle$$
$$= -\sum_{i=1}^{N} \left\langle m_{i} \mathbf{v}_{i} \cdot d\boldsymbol{S}_{i}; f \right\rangle$$
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Reynolds' Transport Theorem

- Mass, momentum and energy equations
 - Mass Conservation

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

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

Momentum Balance

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

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



. Momentum Balance



. Momentum Balance









Momentum Balance

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. Momentum Balance







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Divergence of Pressure

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

$$\begin{split} \frac{d}{dt} \sum_{i=1}^{N} m_{i} \mathbf{v}_{i} \vartheta_{i} &= -\int_{V_{i}}^{N} \frac{\partial}{\partial \mathbf{r}} \cdot \rho \mathbf{u} \mathbf{u} d\mathbf{S}_{i} & \frac{\partial}{\partial t} \int_{V} \rho \mathbf{u} dV = - \oint_{V_{i}} \frac{\partial}{\partial \mathbf{r}} \rho \mathbf{u} d\mathbf{S}_{i} \\ -\frac{\partial}{\partial \mathbf{r}} \cdot \sum_{i=1}^{N} \left[\left(\mathbf{v}_{i} - +\sum_{i=1}^{N} \sum_{j \neq i}^{N} \mathbf{f}_{ij} \vartheta_{ij} + \sum_{j \neq i}^{N} \mathbf{f}_{ij} \mathbf{r}_{ij} \int_{0}^{1} \vartheta_{s} ds \right] & - + \int_{V} \frac{\partial}{\partial \mathbf{r}} \mathbf{r} \partial \mathbf{r} dV \\ - \int_{V} \frac{\partial}{\partial \mathbf{r}} \mathbf{r} \partial \mathbf{r} \partial \mathbf{r} dV = - \int_{V} \frac{\partial}{\partial \mathbf{r}} \mathbf{r} \partial \mathbf{r} \partial$$

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



$$\vartheta_{ij} = \sum_{\alpha=1}^{3} \frac{\partial}{\partial r_{\alpha}} \int_{0}^{1} \vartheta_{s} ds -$$



Surface Pressures

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

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

$$\vartheta_{ij} = \sum_{\alpha=1}^{3} \frac{\partial}{\partial r_{\alpha}} \int_{0}^{1} \vartheta_{s} ds = dS_{xij} + dS_{yij} + dS_{zij}$$

Relationship to the Boltzmann Equation



Results and Applications



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Continuum Analytical

• Simplify the momentum balance (Navier-Stokes) equation

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

• 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



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

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

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- 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



. Simulation setup

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

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

$$\frac{\partial}{\partial t} \int_{V} \rho u_{x} dV = \int_{S_{f}^{+}} \Pi_{xy} dS_{f}^{+} - \int_{S_{f}^{-}} \Pi_{xy} dS_{f}^{-}.$$

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. Simulation setup

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





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Coupling



Summary

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

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•E.R. Smith, D.M. Heyes, D. Dini, T.A. Zaki, Phys. Rev. E 85. 056705 (2012)

- Thank you for listening
 - Any Questions?

Flow past a cylinder

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



. Drag over a Carbon Nano-tube can be determined



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Shockwaves

Current work on application of control volume theory

•



Continuum Analytical Couette Flow



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

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

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

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

Lagrangian mass conservation

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

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

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

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

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