Connecting Continuous and Discrete Systems using Control Volume

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Outline

Introduction

- Continuum Mechanics & Molecular Dynamics
- Selecting function and Irving and Kirkwood (1950)
- Control Volume form

. The Control Volume Function

- Discrete Reynolds' transport theorem
- . Governing equations
- Applying the method to state coupling

. Flux Coupling and the Pressure Tensor

- Derivation of the flux form of the control volume equations
- Pressure tensor
- Coupling fluxes

Introduction



Continuum vs. Discrete

. Assumed Continuous at every point in space

. Mass Conservation

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

Momentum Balance (Newton's Law)

$$rac{\partial}{\partial t}
ho oldsymbol{u} + oldsymbol{
abla} \cdot
ho oldsymbol{u} oldsymbol{u} = oldsymbol{
abla} \cdot oldsymbol{\Pi}$$

. Energy Conservation

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



Direct Numerical Simulation of Turbulent Couette Flow

Continuum vs. Discrete

. Discrete Molecules in continuous space

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

$$m_i \ddot{m{r}}_i = {f F}_i = \sum_{i
eq j}^N m{f}_{ij}$$

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

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

where M_I is the number of molecules in volume V



Molecular Dynamics Simulation of Couette Flow

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

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

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(2.3) for the probability distribution in Gross phase space and then perious repealed laterations. Since * This work was supported by the L.S. ONR under Oxtract Ninart 24 with the California Indirity of Twelmenby, J. G. Kirkwood, J. Chun. Phys. 14, 30 (1946)

more that the activity and current activity in the configuration space of a pair of molecular. The re-sults were resolved to show the fact activity of acthe contiguration space of a pair of non-enders. The re-sults were previously stated in the first article of this arties, when this definition was promited. To obtain explicit expressions for the pair probability density and revealability expressions denotes are small in To obtain explicit expressions for the pair probability density and probability current density one would in principle need to police the Linuville equation [En. (2.3)] for the grobability distribution in Gives phase over a data then readous constant terministic Since

His paper will be concered with a derivation of the espations of hydrodynamics frem the cipies of the classical statistical mechanics. In parciples of the classical statistical mechanics, in par-ticular, the equation of continuity, the equador of motion, and the equation of energy transport will be wood ny introducing use concepts as true smoothing and a triction constant. This latter equation has been and a triction constant. Loss after equation has occar applied to obtain an expression for the stress tensor notion, and the equation of energy transport will be derived. By so doing, the stress tensor and heat current derived and be an energy to be a derived. If so doing, the stress tensor and boll current density can be expressed in terms of molecular variables. The stress service consists of a location of the location density can be expressed in terms of molecular variables. The stress tensor consists of a kinetic part (which excurs in the kinetic fueror) of gaugi and another term (dominant for a liquid) which will be expressed as a moderature involving the constraint of intermetation trommant for a neuron will be expressed as a quadrature involving the potential of intermulecular force and the second of ratio of evolution of the last quadrature involving the potential of intermalecular force and the tensity of pairs of molecules. The hert force and the uensity of pairs of molecules. The best current density is the sum of the ismiliar kinetic part current density is the arm of the forminar ungence par-and a quarketure involving the potential of inter-noicentar force and the density and current density in the content of the density and current density in

approximately by the probability distribution function in the phase space of a rair of molecules. One such equa-tion has been derived by Born and Green' using a rescalined "superposition" assumption. Another, a superposition of the next process pathware built THIS paper will be concerned with a derivation of the equations of hydrodynamics from the minireacting aperiositica assumption. Another, generalization of the well-known Fokker-Planck equigeneralization of the well-known rocker-rance coun-tion of stochastic theory, has been derived by Kjrk-100 U STOCHASTIC ID0075, DAS UPEN DETVOU DY ANTA-10000 hy introducing the concepts of time smoothing and a faction concepts of the terms concepts has been

this program is untenable for a liquid, various attempts une program se untenance sor a numa, vanous autorqua have been unde to obtain a closed equation satisfied have been made to obtain a closed equation satisfied approximately by the probability distribution function

The equations of hydrolynamics—conticulty equation, equation of easier, and repeations of energy tradpert- are derive with beam as at the classic contribution mechanics. Thereby, oppeadicular to the familiar for the system tensor with one according in terms of another analysis. In addition, the familiar terms of under the system terms of another and the system and the system terms of t

The Statistical Mechanical Theory of Transport Processes. IV. The Equations of Hydrodynamics* THE INCREAT OF CREMICAL PHYSICS J. H. IRVING AND JUNY G. EUROWOOD Gates and Crelline Jahrmierier of Chemistry No. 1343, Passdene, California (Resoluted Konsender 31, 1963).

175.9 cm⁻¹. The band at 809.7 cm⁻¹ has been interpreted 17: 9 cm⁻⁴. The band at 300.7 cm⁻¹ has been interpreted as 22×394, the rather large difference between calculated and descend forement basis at some to the second is $3X_334$, the rather large difference between calculated and observed incomency being a scriber, to the "proximity to the A_2 (undermand). However, this hand could be an unstationer band commenceding to Stutement to the A_s (undamental. However, this band could be an upper-stage band corresponding to 819 cm⁻¹. The interpretation of the faint sharp lund at 769.4 cm⁻¹ as an upper-stage band, $778 + \nu_{err} = n$ genus more blushle than its interpretation as the B_{ν} combination. Jerome Karle lot electron diffraction dats; and in Dr. E. K. Phyler and the National Bureau of Standards for cm⁻⁻ as an upper-stage band, $778+e_{1}-e_{2}$, seems more plausible than its interpretation as the B_{12} combinition 3101-552 cm⁻¹. The first show the second local second plausible than its interpretation as the H w consummation, 2104-558 cm⁻¹. The faint sharp Raman band at \$28.5 methods been been been under the unmanifold processing band lata 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

and 8.50 cm⁻¹, are related to each other in much the same manner as similar groups in the spectra of CO₂ and CS₂. The writers wish to express their inceptedness to Dr. The writers wan to express their incediedness to Dr. C. F. Hanmer and F. L can point de Nemours and C. F. Hammer and E. L Gu Pont de Nemours and Company for the samples; to Doctors Isabella and Jerone Karle for electron diffraction data; and to Dr. F. K. Budes and the Network Decomposition of Complete Long

has not been observed. If the preferred interpretations TRANSPORT PROCESSES this hot been ouserved, it the preferren interpretations are correct, the group of Raman hands, 769, 778, 819, and 829 cm², are related to each other in much the same

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applied to obtain an expression for the stress innor-linear in gradierts of third velocity and, thereby, ex-

linear in granteris of fluid velocity and, incessivy, ex-pressions (in terms of molerular variables) (or co-efficients of abeat and volume viscosity.) The same

encorns or snow and volume viscosity. Ine same equation generalized to approximate,

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atter uneariang in the temperature grausers, sens to an explicit expression for the hear current and thereby

an explicit cupression for the next current and memory to an expression for the coefficient of themal com-

ducibyly. We shall assume, for purposes of malle-natical simplicity, a single component, single place duid content conductor of molecular uplich interact

CallCal simplicity, a single component, angle page fuld system consisting ul nolecules which interact under central forces only. It is not difficult to generalize the treatment to a multicule common to emulticule

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M. USAMMAN, M. S. Creen, Proc. Roy, Suc. A188, 10 (1996). M. Boen and M. S. Creen, Proc. Roy, Suc. A188, 103 (1987). N. Elbanovol, Starkan J. Chem. J. Chem. The strain widel weather than the strain and the strain and the strain widel weather than the strain and president composation of up the effect instal disciplination function.

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Thus, (2.4) becomes

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Providing a cose not depend on time explositly, the rate of change of the expectation value of a is given by

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+ (a; VesU-Vost) . (2.4)

 $\frac{\partial}{\partial t}(\alpha_i, f) = \left(\alpha_i, \frac{\partial f}{\partial t}\right) = \sum_{k=1}^{N} \left[\left(\alpha_i, \frac{\mathbf{p}_k}{\mathbf{m}_k}\right) - \frac{\mathbf{p}_k}{\mathbf{m}_k} \right]$

By Green's theorem applied in the space of R.

providing the integrated part vanishes; i.e., providing the system is bounded or f falls off sufficiently applied as R. I. I. Kenning simo up, f is independent of applied

the gystem x bounded or f tails of sufficiently tags as $R_{k} \rightarrow \infty$. Likewise, since $\nabla R_k f$ is independent of mentum n, and since f is in or satisfies as a second

is $K_{k} \to \infty$. Likewise, since V_{k+1} is unependent meature p_{k} and since f falls off rapidly is period.

of Green's theorem in the momentum space of g

 $(\alpha; \nabla R_k U \cdot \nabla p_k f) = -\langle \nabla R_k U \cdot \nabla p_k \alpha; f \rangle$

 $\rho(\mathbf{r},t) =$

(a; - Di Part) - (Pe

Irving and Kirkwood (1950)

561-10 $S(x_n)f(x,y)dy = f(x,y)?$ The probability distribution function (relative den-as the expectation value of the dynamical variable sity of representative points in phase space) we denote $d' \int \mathcal{E}_{R}$ satisfying the normalize tion condition Sol The TRACE VEGUE POR $\int \cdots \int f d\mathbf{R}_{i} \cdots d\mathbf{R}_{i} c \hat{\mathbf{p}}_{i} \cdots d\mathbf{p}_{k'=1}$ where $d\mathbf{R}_{4}$ stands for a volume element π the conwhere $d\mathbf{R}_{t}$ stands for a volume element in the con-figuration space and $d\mathbf{p}_{t}$ a volume element in the mo-mentum space of the 4th molecule, stands in the mo-security of the society of the standard in the security of the sec (2.1) mentum space of the still molecule. ; Charges 1 according to the well-known Liouville equation

We shall use (2.7) to derive the equations of hydro- Avnomize III. STATISTICAL MICHANICAL EXPRESSIONS FOR DENSITIES The equations of hydrodynamics (1.1), (1.2), and (1.4) are concerned with densitive in endancy 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. $\frac{df}{dt} = \sum_{k=0}^{N} \left[-\frac{p_k}{m_k} \nabla \mathbf{R}_k f + \nabla \mathbf{R}_k U \cdot \nabla \mathbf{P}_k f \right]$ where U is the potential energy of the entire system. Any cynamical variable, $\alpha(\mathbf{R}_1, \dots, \mathbf{R}_n; \mathbf{R}_n; \mathbf{n}_1, \dots, \mathbf{R}_n)$, has an expectation value given at time / by $\int \cdots \int f(\mathbf{R}_1, \cdots, \mathbf{p}_l, \cdots, \mathbf{i}) d\mathbf{R}_1 \cdots$ $(\mathbf{R}_1, \dots, \mathbf{R}_k, \dots, \mathbf{d}_k)$ where the integration is over all position vectors are \mathcal{A}_k where \mathcal{A}_k and over all momental vectors. Introducing that the kih molecule be at t at time t is If the array We thus denote he (a; f) the expectation value of a that the kth in induct of a and j taken over the smartly the inner $\left(\partial(\mathbf{R}_{i} - \mathbf{y}_{i}) \right)^{n}$. Froughing a does not decord on time employible the f

instribution function f_i . The probability per unit volume that the kth molecules be as R_{a} is

 $\cdots \int \delta(\mathbf{R}_{b}-t)f(\mathbf{R}_{t_{1}}\cdots ;p_{t_{t}}\cdots ;t)d\mathbf{R}_{t}\cdots d_{t_{t_{t}}}$

others are ;

 $\langle m_i \delta \left(\boldsymbol{r} - \boldsymbol{r}_i \right); f$

The total roass density at r due to all audecules is thus

 $P(z; t) - \sum_{k=1}^{N} m_k (\delta(\mathbf{R}_k - \mathbf{r}));$

 $\int P_{i}\partial(R_{k}-r)/(R_{i_{1}}\cdots ; p_{i}\cdots ; i)dR_{i_{1}}\cdots dp_{i_{r}}$

id the locations of the

 $\int \cdots \int \delta(\mathbf{R}_{1} - \mathbf{r}) f(\mathbf{R}_{1}, \cdots, \mathbf{p}_{1}, \cdots, \mathbf{j}) d\mathbf{R}_{1} \cdots d\mathbf{p}_{N}$

at the eth molecule to the momentum per unit values (mass current decas(y), "The local momentum decasity

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it is at

(2.5)

, (2.4) becomes $\frac{\partial}{\partial t} (a; f) = \sum_{i=1}^{n} \left(\sum_{m_{e_{i}}}^{p_{e_{i}}} \nabla_{R_{i}a} - \nabla_{R_{i}} \nabla_{R_{i}a} \right) (2.7) \qquad \begin{array}{c} Consecucity, (p_{i}f)(R_{i} - t), f) \text{ is the } p_{i}(a_{i}, f) = 1 \\ mean momentum by the product of this is the product of this is the set of change of the operation value of a first the set momentum per unit volume of a first the set momentum per unit volume (mass current density). The total momentum density$

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Selecting Functions

The Dirac delta selects molecules at a point

- Infinitely high, infinitely thin peak
- Equivalent to the continuum differential formulation at a point
- Cannot be applied directly in a molecular • simulation as r_i is never exactly equal to r
 - Relaxed weighting function used*
- **Co-existence of two descriptions in same** simulation
 - Overlap used in most coupling schemes
 - Length scales comparable at interface

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

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







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

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

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

Energy Conservation

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

$$\begin{aligned} \frac{\partial}{\partial t} \int_{V} \rho \mathcal{E} dV &= -\oint_{S} \rho \mathcal{E} \boldsymbol{u} \cdot d\mathbf{S} \\ &-\oint_{S} \boldsymbol{\Pi} \cdot \boldsymbol{u} \cdot d\mathbf{S} + \mathbf{q} \cdot d\mathbf{S} \end{aligned}$$

The Control Volume (CV)

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

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

. Momentum

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

$$\int_{V} \rho \boldsymbol{u} dV = \sum_{i=1}^{N} \boldsymbol{p}_{i} \int_{V} \delta \left(\boldsymbol{r} - \boldsymbol{r}_{i} \right) dV$$

• Energy

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

The Control Volume Formulation



Control Volume Function

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

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

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

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

Derivatives yields the Surface Fluxes

. Taking the Derivative of the CV function

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

• Surface fluxes over the top and bottom surface

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



Applying the Control Volume Function

. Molecular mass in a control volume

$$\frac{d}{dt}\sum_{i=1}^{N}m_{i}\vartheta_{i} = -\sum_{i=1}^{N}m_{i}\mathbf{v}_{i}\cdot d\mathbf{S}_{i} \qquad \qquad \frac{\partial}{\partial t}\int_{V}\rho dV = -\oint_{S}\rho \boldsymbol{u}\cdot d\mathbf{S}$$

. Mathematical manipulation yields surface fluxes

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

Reynolds' Transport Theorem

. Mass, momentum and energy equations

. Mass Conservation

$$\frac{d}{dt}\sum_{i=1}^{N}m_{i}\vartheta_{i} = -\sum_{i=1}^{N}m_{i}\mathbf{v}_{i} \cdot d\boldsymbol{S}_{i}$$

Momentum Balance

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

. Energy Conservation

$$\frac{d}{dt} \sum_{i=1}^{N} e_{i}\vartheta_{i} = -\sum_{i=1}^{N} e_{i}\mathbf{v}_{i} \cdot d\mathbf{S}_{i}$$

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

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

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

$$+\mathbf{F}_{ ext{surface}}$$

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

$$-\oint_{S} \mathbf{\Pi} \cdot \boldsymbol{u} \cdot d\mathbf{S} + \mathbf{q} \cdot d\mathbf{S}_{14}$$

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







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. Momentum Balance



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Using the CV for coupling

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



$$\int_{V} \rho \boldsymbol{u} dV = \sum_{i=1}^{N} \boldsymbol{p}_{i} \vartheta_{i}$$

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

• Principle of Least Action (subject to constraint)

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

. Semi-Holonomic Constraint

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



Constraint Equation of O'Connell and Thompson (1995)

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

. Principle of Least Action (subject to constraint)

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

. Non-Holonomic Constraint

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

. Constraint Equation

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Constraint Algorithms

. Combining the CV equations of O'Connell and Thompson

$$m_{i}\ddot{\boldsymbol{q}}_{i} = \boldsymbol{F}_{i} + \frac{m_{i}\vartheta_{i}}{M_{I}} \left[\frac{d}{dt} \int_{V} \rho \boldsymbol{u} dV - \sum_{n,m}^{N} \boldsymbol{f}_{nm}\vartheta_{nm} + \sum_{n=1}^{N} m_{i}\dot{\boldsymbol{q}}_{n}\dot{\boldsymbol{q}}_{n} \cdot d\mathbf{S}_{n} \right]$$
$$+ \frac{m_{i}}{M_{I}} \left(\underbrace{\dot{\boldsymbol{q}}_{i} \cdot d\mathbf{S}_{i} - \frac{\vartheta_{i}}{M_{I}}}_{\text{Mass Flux}} \sum_{n=1}^{N} m_{n}\dot{\boldsymbol{q}}_{n} \cdot d\mathbf{S}_{n} \right) \times \underbrace{\left[\sum_{n=1}^{N} m_{n}\dot{\boldsymbol{q}}_{n}\vartheta_{n} - \int_{V} \rho \boldsymbol{u} dV \right]}_{\text{Momentum Discrepancy}}$$

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

Constraint Algorithms

. Combining the CV equations of O'Connell and Thompson

$$m_{i} \ddot{\boldsymbol{q}}_{i} = \boldsymbol{F}_{i} + \frac{m_{i} \vartheta_{i}}{M_{I}} \left[\frac{d}{dt} \int_{V} \rho \boldsymbol{u} dV - \sum_{n,m}^{N} \boldsymbol{f}_{nm} \vartheta_{nm} + \sum_{n=1}^{N} m_{i} \dot{\boldsymbol{q}}_{n} \dot{\boldsymbol{q}}_{n} \cdot d\mathbf{S}_{n} \right] \\ + \frac{m_{i}}{M_{I}} \left(\underbrace{\dot{\boldsymbol{q}}_{i} \cdot d\mathbf{S}_{i} - \frac{\vartheta_{i}}{M_{I}}}_{\text{Mass Flux}} \sum_{n=1}^{N} m_{n} \dot{\boldsymbol{q}}_{n} \cdot d\mathbf{S}_{n} \right) \times \underbrace{\left[\sum_{n=1}^{N} m_{n} \dot{\boldsymbol{q}}_{n} \vartheta_{n} - \int_{V} \rho \boldsymbol{u} dV \right]}_{\text{Momentum Discrepancy}}$$

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

$$m\ddot{\boldsymbol{q}}_{i} = \boldsymbol{F}_{i} + m\vartheta_{i} \left[\frac{D\boldsymbol{u}_{I}}{Dt} - \frac{1}{mN_{I}} \sum_{n=1}^{N} \boldsymbol{F}_{n} \vartheta_{n} \right]$$

State Coupling

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





State Coupling

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



State Coupling

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



• Flux coupling is required

Flux Coupling

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



• Flux Coupling requires significant statistical averaging

- Coupling developed for massively parallel applications to exploit high performance computers
- *E. G. Flekkøy, G. Wagner, and J. Feder, Europhys. Lett. 52, 271 (2000).

Flux Coupling and the Pressure Tensor



Flux Coupling

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



Control Volume Function

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

$$\vartheta_i \equiv \int_V \delta(\mathbf{r} - \mathbf{r}_i) \, dV$$

= $\begin{bmatrix} H(x^+ - x_i) - H(x^- - x_i) \end{bmatrix}$
× $\begin{bmatrix} H(y^+ - y_i) - H(y^- - y_i) \end{bmatrix}$
× $\begin{bmatrix} H(z^+ - z_i) - H(z^- - z_i) \end{bmatrix}$

• Replace molecular position with equation for a line

$$m{r}_i
ightarrow m{r}_i - s m{r}_{ij}$$



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

Control Volume Function

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

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

. Length of interaction inside the CV

$$\ell_{ij} = \int_{0}^{1} \vartheta_s ds$$

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



Derivatives Yield the Surface Forces

. Taking the Derivative of the CV function

$$\frac{\partial \vartheta_s}{\partial \boldsymbol{r}} \equiv \left[\delta(x^+ - x_i + sx_{ij}) - \delta(x^- - x_i + sx_{ij}) \right] \\ \times \left[H(y^+ - y_i + sy_{ij}) - H(y^- - y_i + sy_{ij}) \right] \\ \times \left[H(z^+ - z_i + sz_{ij}) - H(z^- - z_i + sz_{ij}) \right]$$

• Surface fluxes over the top and bottom surface

$$\tilde{\boldsymbol{n}} \cdot d\mathbf{S}_{ij} = \int_{0}^{1} \frac{\partial \vartheta_s}{\partial \boldsymbol{r}} ds \qquad \qquad \tilde{\boldsymbol{n}} = \begin{bmatrix} 1 & 1 & 1 \end{bmatrix}$$



Surface Pressures

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

$$\int_{V} \frac{\partial}{\partial \boldsymbol{r}} \cdot \left[P\boldsymbol{I} - \boldsymbol{\sigma}\right] dV = \frac{\partial}{\partial \boldsymbol{r}} \cdot \sum_{i=1}^{N} \left[\left(\boldsymbol{v}_{i} - \boldsymbol{u}\right) \left(\boldsymbol{v}_{i} - \boldsymbol{u}\right) \vartheta_{i} + \sum_{j \neq i}^{N} \boldsymbol{f}_{ij} \boldsymbol{r}_{ij} \int_{0}^{1} \vartheta_{s} ds \right]$$

. The derivative of $\,\vartheta_s$ gives forces over the surface - a localisation of the method of planes, (Todd et al 1995, Han Lee 2004)

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

. Kinetic







Surface Pressures

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

$$\int_{V} \frac{\partial}{\partial \boldsymbol{r}} \cdot \left[P\boldsymbol{I} - \boldsymbol{\sigma}\right] dV = \frac{\partial}{\partial \boldsymbol{r}} \cdot \sum_{i=1}^{N} \left[\left(\boldsymbol{v}_{i} - \boldsymbol{u}\right) \left(\boldsymbol{v}_{i} - \boldsymbol{u}\right) \vartheta_{i} + \sum_{j \neq i}^{N} \boldsymbol{f}_{ij} \boldsymbol{r}_{ij} \int_{0}^{1} \vartheta_{s} ds \right]$$

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

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

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

Coupling the Localised Stresses



Coupling the Surface Stresses



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State or Flux Constraint?

. Recall the coupled CV equations



. Includes both force and fluctuation terms*

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. Energy or Entropy CV equation could also be analysed/applied in a similar manner

Control Volume Coupling



Summary

- Introduced a novel mathematical function to define a control volume in a discrete system
 - Derived in a manner consistent with a continuum control volume
 - Mathematically well defined and applicable to any discrete system
- . Derivation of discrete CV conservation equation
 - Allows control volume analysis to be extended to nano-scale systems
 - The resulting equations are exactly conservative in a discrete system

Application to Coupling

- Allows both systems to be written in a consistent framework
- Averages from molecular region can be written in terms of continuum variables, e.g. surface fluxes
- Facilitates derivation of constraint algorithms using minimisation principles

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Thank you for listening

Any Questions?

Future Aims

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

Moving reference frame

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

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

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

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

Lagrangian mass conservation

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

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

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

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

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

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**44

Shockwaves

Current work on application of control volume theory

•



Flow past a cylinder

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



. Drag over a Carbon Nano-tube can be determined

