Imperial College London

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Towards an exact framework for domain decomposition coupling

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Domain Decomposition

Domain decomposition coupling links continuum based computational fluid dynamics (CFD) and discrete molecular dynamics (MD) by assuming they exist at the same time and length scale. Coupled simulation of this type uses CFD to accelerate molecular simulation, with both descriptions limited to the slowest time scales of the problem. Typically the MD and CFD regions are separate with an overlaps region between them to allow the exchange of boundary conditions,

Consistent Framework & Data Exchange { **CFD→MD Boundary Condition** ; **MD→CFD Boundary Condition**

Two challenges are considered in this work:
1) Development of an exact mathematical framework to express and couple continuum and discrete systems.
2) Computational software to facilitate exchange of data for simulation on large multi-processor computers.

The motivation is coupled simulation of turbulence which requires very large scale simulations and exact coupling to exchange the complex 3D flow fields.

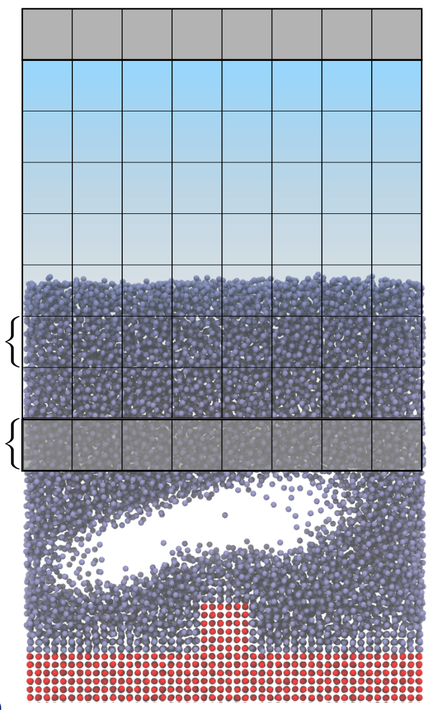


Fig 1 - Domain decomposition coupling between MD and CFD

Turbulent Flow

Perhaps the greatest motivation for domain decompositional coupling is to explore large scale and complex non-equilibrium flows which are prohibitively expensive with MD simulation alone.
It is just possible to simulate turbulent flow with Molecular Dynamics. This requires about 300,000,000 molecules to provide a Reynolds number of 400. The resulting molecular simulation shows turbulent structures and statistics which agree well with experimental results.
As large computing resources are required for MD studies of this type, coupled simulation is ideally placed to answer open questions in turbulence research.

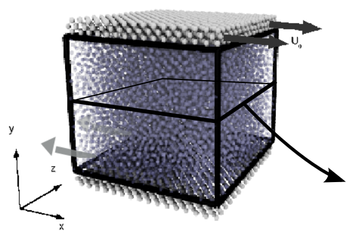


Fig x. MD Couette schematic with central plane used for contours

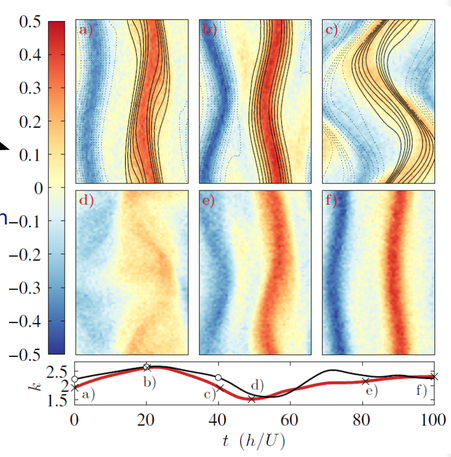


Fig 2c. Contour plots of u velocity on the x z plane at the centreline for MD (colors) and CFD (black contours with positive (—) and negative (· · ·), separated by 0.1). The times of the six contour plots, (a)–(f), are denoted on the bottom line plot (CFD (◦) and MD (×)) showing the evolution of whole domain turbulent kinetic energy k

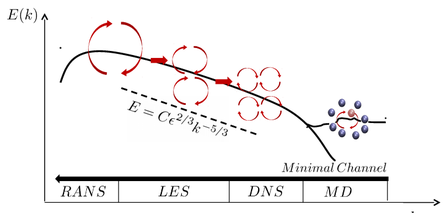


Fig 2a - Energy cascade including molecule region

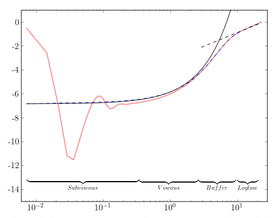


Fig 2b - Law of the wall with molecular stacking

CPL library

CPL library is open-source software designed to couple two massively parallel codes.

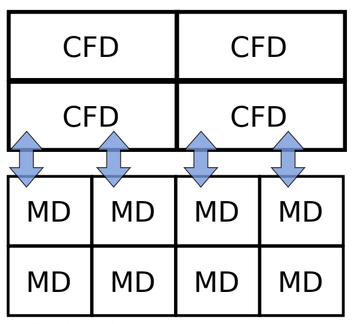


Fig 3a - Local communication between processors

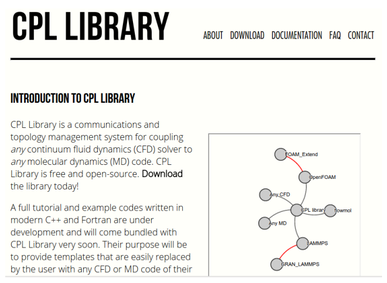


Fig 3b - Snapshot of CPL library website with tree diagram of coupled software

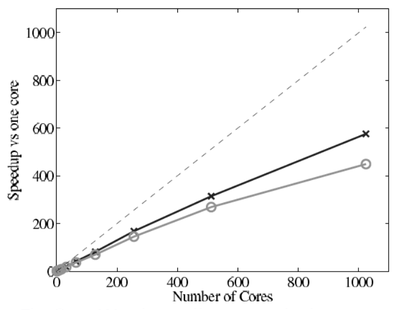


Fig 3c - Weak scaling coupled case (◦), MD alone (×) and ideal (--)

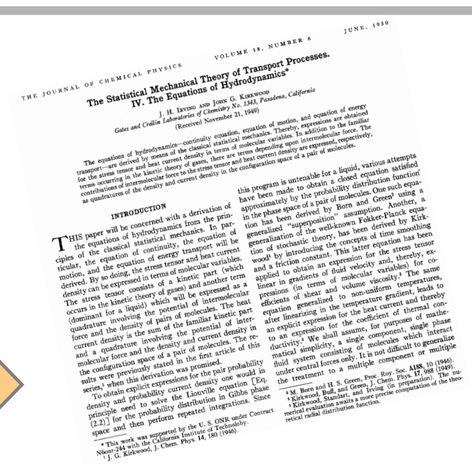
Key Features include:

- Optimal scaling for coupled cases with only local communication between processors which physically overlap.
- Shared library run in the mpmd model: mpiexec -n 16 ./cfd : -n 256 ./md maintaining the scope of the two coupled codes
- Minimal functional interface with clear documentation and a range of examples.
- Bindings available for Fortran, C++ and python with coupling supported between software written in different programming languages.
- Sockets for a number of open-source CFD and MD codes available.

CPL www.cpl-library.org

Work with David Trevelyan, Eduardo Ramos Fernandez and Lucian Anton

Mathematical Framework



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

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(Received November 21, 1949)

The equations of hydrodynamics—continuity equation, equation of motion, and equation of energy transport—are derived by means of the classical statistical mechanics. Thereby, expressions are obtained for the stress tensor and heat current density in terms of molecular variables. In addition to the familiar terms occurring in the kinetic theory of gases, there are terms depending upon intermolecular force. The correspondence of intermolecular force to the stress tensor and heat current density is expressed, respectively, as conservations of the density and current density in the configuration space of a pair of molecules.

INTRODUCTION

THIS paper will be concerned with a derivation of the equations of hydrodynamics from the principles of the classical statistical mechanics. In particular, the equation of continuity, the equation of motion, and the equation of energy transport will be derived. By so doing, the stress tensor and heat current density can be expressed in terms of molecular variables. The stress tensor consists of a kinetic part (which occurs in the kinetic theory of gases) and another term (dominant for a liquid) which will be expressed as a quadrature involving the potential of intermolecular force and the density of pairs of molecules. The heat current density is the sum of the familiar kinetic part and a quadrature involving the potential of intermolecular force and the density in the configuration space of a pair of molecules. The results were previously stated in the first article of this series,[1] when this derivation was promised.

To obtain explicit expressions for the pair probability density and probability current density one would in principle need to solve the Liouville equation [Eq. (2.2)] for the probability distribution in Gibbs phase space and then perform repeated integrations. Since this program is untenable for a liquid, various attempts have been made to obtain a closed equation satisfied approximately by the probability distribution function in the phase space of a pair of molecules. One such equation has been derived by Born and Green[2] using a generalization of the well-known Fokker-Planck equation of stochastic theory, has been derived by Kirkwood[3] by introducing the concepts of time smoothing and a friction constant. This latter equation has been applied to obtain an expression for the stress tensor linear in gradients of fluid velocity and, thereby, expressions of shear and volume viscosity.[4] The same equation generalized to non-uniform temperatures, after linearizing in the temperature gradient and thereby an explicit expression for the coefficient of thermal conductivity.[5] We shall assume, for purposes of mathematical simplicity, a single component, single phase fluid system consisting of molecules which interact under central forces only. It is not difficult to generalize the treatment to a multiple component or multiple

* This work was supported by the U. S. ONR under Contract Nonr-244 with the California Institute of Technology.
[1] J. G. Kirkwood, J. Chem. Phys. 14, 180 (1946).
[2] M. Born and H. S. Green, Proc. Roy. Soc. A188, 10 (1946).
[3] Kirkwood, Buff, and Green, J. Chem. Phys. 17, 988 (1949).
[4] Kirkwood, Romberg, and Irving, (in preparation). The numerical evaluation a more precise computation of the theoretical radial distribution function.

Starting with the Irving and Kirkwood (1950) definition of density in term of microscopic quantities,

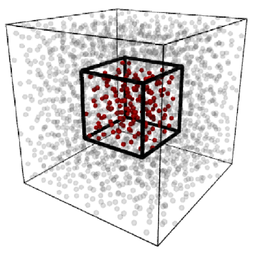
$$\rho(\boldsymbol{r},t)=\sum_{i=1}^{N}\left\langle m_i\delta\left(\boldsymbol{r}-\boldsymbol{r}_i\right);f\right\rangle$$

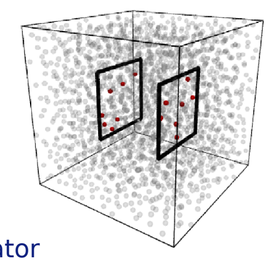
Integrate exactly over a control volume so the requirement of pointwise agreement between descriptions is no longer essential,

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

Formal integration, shown here for a cube, results in a combination of Heaviside functionals which isolate molecules in the volume,

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





A similar functional can also be obtained for the interaction operator between two molecules (the IK operator).

Evaluating the derivative with respect to a given direction gives a function which selects all crossings over surfaces,

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

Using this control volume functional, it is then possible to define the control volume form of the mass, momentum and energy equations but in a molecular system. As these equations are for volumes, they are exactly conservative and equivalent in both systems. This allows both MD and CFD to be expressed in the same mathematical form.

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

$$\frac{d}{dt}\sum_{i=1}^{N}m_i\mathbf{v}_i\vartheta_i=-\sum_{i=1}^{N}m_i\mathbf{v}_i\mathbf{v}_i\cdot d\mathbf{S}_i+\frac{1}{2}\sum_{i,j}^{N}\boldsymbol{f}_{ij}\mathbf{n}\cdot d\mathbf{S}_{ij}\qquad\frac{\partial}{\partial t}\int_V\rho\boldsymbol{u}dV=-\oint_S\rho\boldsymbol{u}\boldsymbol{u}\cdot d\mathbf{S}-\oint_S\boldsymbol{\Pi}\cdot d\mathbf{S}$$

Molecular Surface Stresses

The above derivation provides a mathematical form of surface stress/flux which is linked exactly to evolution of momentum inside the control volume.

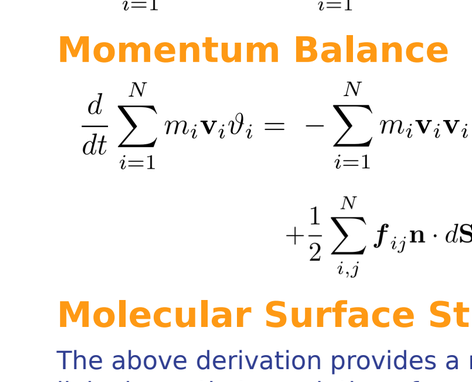
$$-\oint_S\boldsymbol{\Pi}\cdot d\mathbf{S}=-\sum_{i=1}^{N}m_i\left(\boldsymbol{v}_i-\boldsymbol{u}\right)\left(\boldsymbol{v}_i-\boldsymbol{u}\right)\cdot d\mathbf{S}_i+\frac{1}{2}\sum_{i,j}^{N}\boldsymbol{f}_{ij}\mathbf{n}\cdot d\mathbf{S}_{ij}$$

The surface crossing terms are equivalent to a localised form of the method of planes stress.

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

Constrained Dynamics

Using the control volume framework with Gauss' principle of least constraint we derive a method for control of momentum in a localised region of the domain. Iteration ensures exact momentum control by cancelling the MD fluxes and replacing,



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

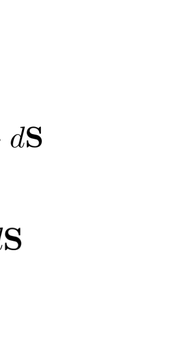
$\frac{1}{2}\sum_{i,j}^{N}\boldsymbol{f}_{ij}\mathbf{n}\cdot d\mathbf{S}_{ij}$ Interactions cross surface

All fluxes cancelled and cosine applied

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

$\sum_{i=1}^{N}m_i\boldsymbol{v}_i\vartheta_i$

Time evolution of momentum in the control volume is set here to be exactly equal to a cosine function.



The sum of fluxes gives the appropriate evolution in time. However, the individual surface fluxes on a control volume can be controlled individually to allow complex flow fields which still satisfy the required sum. The constraint therefore unifies flux and state coupling, allowing complex flow coupling.

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

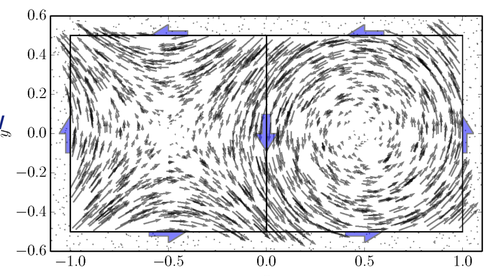


Fig 4 - Turbulence like elongation and rotation applied to a molecular control volume