Non-linear Constitutive Relations

Fluid behaviour can be described by means of the continuity relations, which are continous statements of the conservation of mass and momentum. Unfortunately, there are too few equations for the number of unknowns, and so the system must be closed by an additional equation known as a *Constitutive Relation*. If we assume that this relation is analytic, it may be written as

$$< J >= B_0 F + B_1 F^2 + B_2 F^3 + \cdots$$

where J is a thermodynamic flux conjugate to the thermodynamic force F. B_i are the nonlinear Burnett coefficients — B_0 is the usual hydrodynamic or Navier-Stokes transport coefficient.

We will also consider the inverse relation:

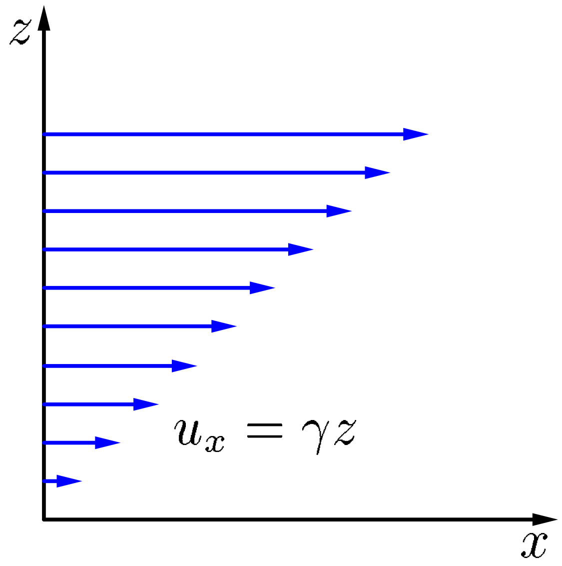
$$< F >= \mathcal{B}_0 J + \mathcal{B}_1 J^2 + \mathcal{B}_2 J^3 + \cdots$$

This can be related to the former relation by the usual inversion of a series:

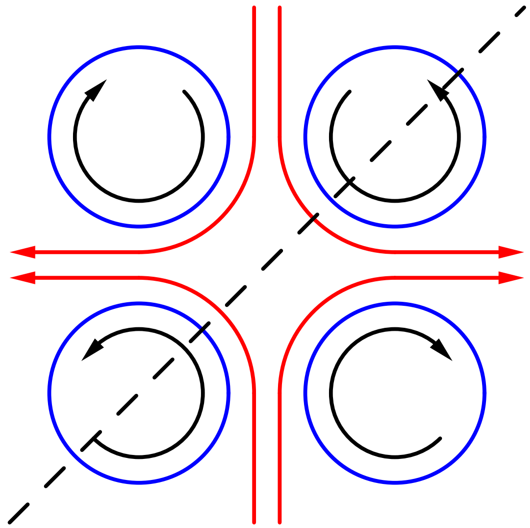
$$\mathcal{B}_0 = \frac{1}{B_0},\ \mathcal{B}_1 = -\frac{B_1}{B_0^3},\ \mathcal{B}_2 = \frac{2B_1^2}{B_0^5} - \frac{B_2}{B_0^4}$$

Shear Flow

Consider Planar Couette Shear Flow, where the velocity of the fluid u_x is proportional to the depth z of the fluid.



Nonlinear Burnett coefficients may be used to measure the difference in shearing between planar Couette flow and for example the 4 roller flow shown on the right. If one linearizes about the shear flow along the dotted line, then one cannot distinguish between 4 roller flow and planar Couette flow.



Problems with Shear Flow in Hard Spheres

In Ernst *et al.* (1978) *J. Stat. Phys.* **18**, 237–270, they show:

$$\begin{aligned} P_{xy} &= |\gamma| \ln |\gamma| \text{for hard disks} \\ P_{xy} &= -\eta\gamma + c|\gamma|^{\frac{3}{2}} \text{for hard spheres} \end{aligned}$$

So the constitutive relation is not analytic, and so $\mathcal{B}_2$ doesn't even exist!!! The reason why this happens is that coupling between hydrodynamic modes gives rise to power law contributions to the correlation functions, a phenomena known as long-time tails, discovered initially by Alder and Wainwright (1970) *Phys. Rev. A*, **1**, 18.

Can we compute these relations for systems other than hard spheres?

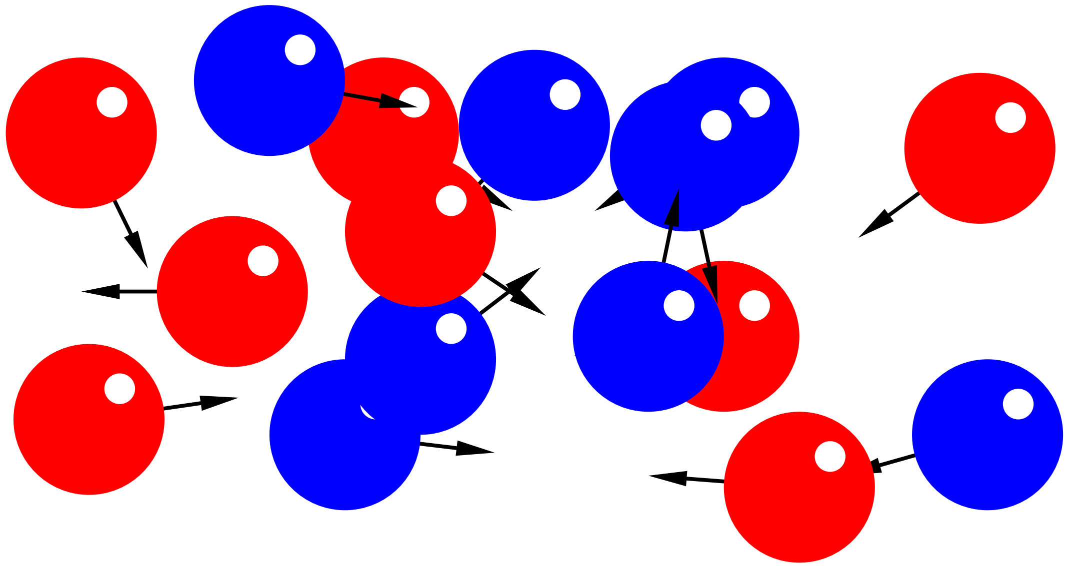
TTCF Formulation

Standish and Evans (1990), *Phys. Rev. A*, **41**,4501 develop the following Transient Time Correlation Function for $\mathcal{B}_2$.

$$\frac{3N\beta}{<\Delta J^2>^2}\int_0^\infty < F(s_J)F(0)(\Delta J^2 - <\Delta J^2>) > ds$$

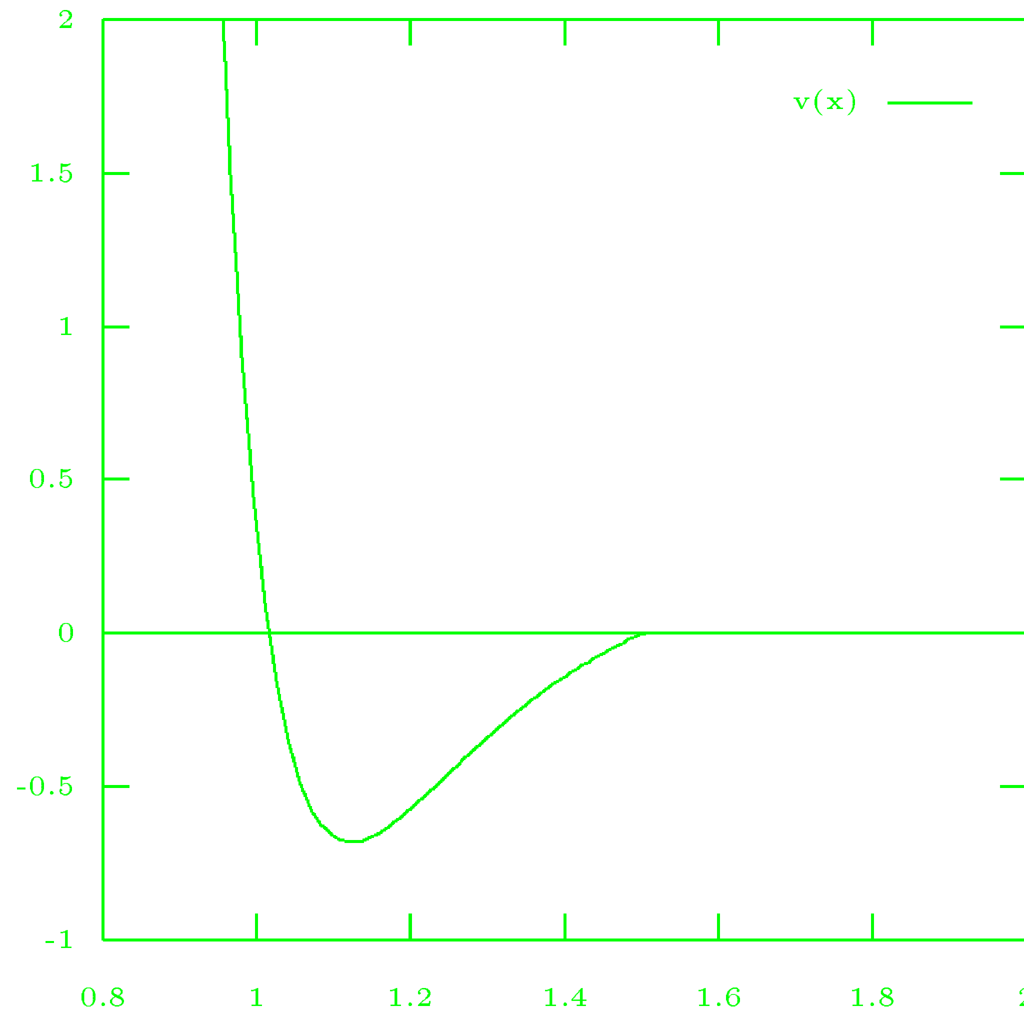
where the subscript J on s denotes that the evolution is perform at fixed or 'statted' J.

Model



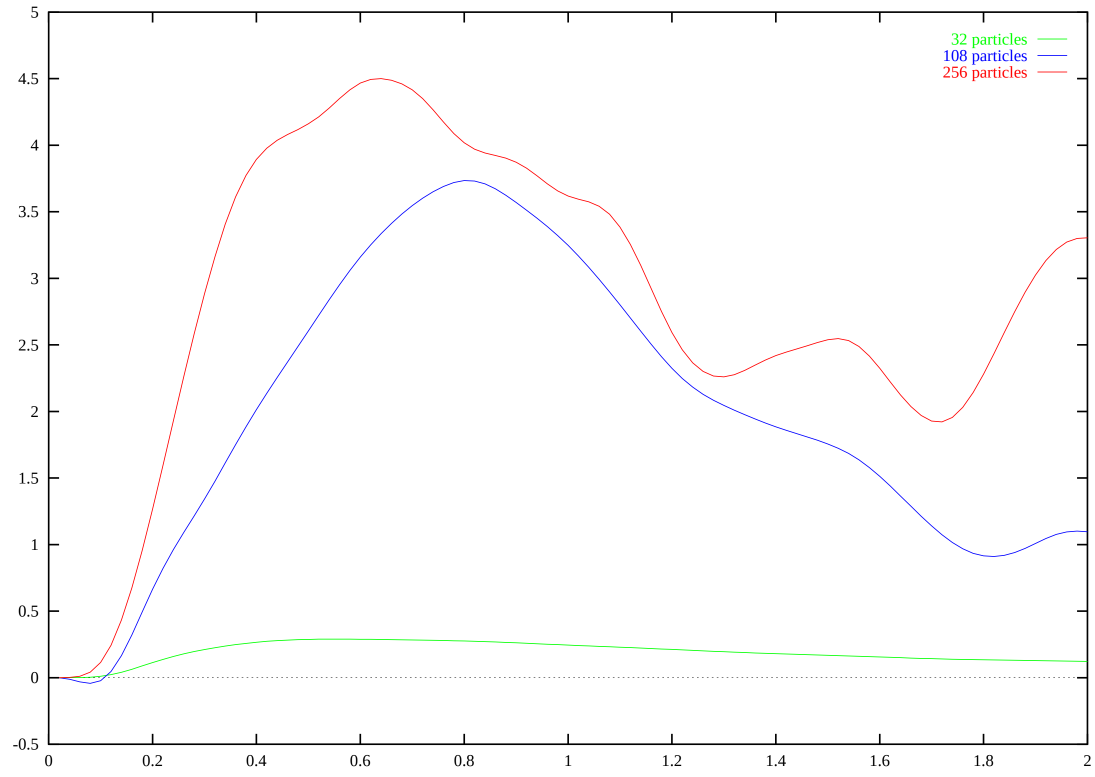
The simulation is of np particles in a box with periodic boundary conditions.

- We use a colour conductivity model, with particles interacting with a cut-off Lenard-Jones force (right), and interacting with an external field with +ve and −ve charges.
- Solve equations of motion using integrator (4th order Gear method).
- Equations of motion similar to Newton's, but with additional dissipative terms to generate particular Stat. Mech. ensembles.
- Approx. 40 SPARCstations used, each running an independent simualtion, giving approximately 120MFlops in total.



Results

$$\frac{3(Nm\beta)^3}{m}\int_0^t < \lambda(s_J)\lambda(0)(\Delta J^2 - < \Delta J^2 >) > ds$$



t

Conclusions

- The TTCF formulation appear to give finite values for the nonlinear Burnett coefficients in the thermodynamic limit (in the case of a Lenard Jones fluid under the influence of a colour field)
- Of the order of 10^9–10^{10} timesteps are required to obtain reasonable convergence. This takes of order 3 months on a 100MFlops computer for the colour conductivity model considered. Clearly, with computers being delivered now, these calculations are feasible.
- Further theoretical advances are required to rule out the possibility that long time tails cause the coefficients to diverge. The algorithm given above is linear in the parameter t, and so another possibility is to perform the calculation out to a time $t = 10$ on a GFlop computer.