A Heterogeneous Multiscale Model for Plasma Simulation

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INTRODUCTION

Many plasma physics systems require molecular-level detail to resolve, but have large domains that preclude molecular dynamics simulations even on state of the art computers. Examples include inertial confinement fusion, warm dense matter, and streaming cold plasmas.

There is demand for simulations with molecular resolution that are computationally tractable. We use the heterogeneous multiscale method to construct such a hybrid method with a theoretical and computational connection between scales.

We couple a macroscopic kinetic description to a microscopic molecular description of the same system. The multiscale simulation runs with statistical data drawn from the microscopic as needed.

MODELS

The full system is described by particles with positions \( \{ r_i \} \) and velocities \( \{ v_i \} \), interacting with potential \( U_{ij} \) according to the Hamiltonian

\[
H(\mathbf{r}, \mathbf{v}, t) = \sum_i \frac{m_i \mathbf{v}_i^2}{2} + \sum_{i<j} U_{ij}(r_{ij}, r_i, r_j).
\]

The macroscopic observables are the distribution functions \( f_k(r, v, t) \), modeled using the kinetic Vlasov-BGK equation with internal potential \( \phi \) from the charge density of particles. Thus,

\[
\frac{\partial f_k}{\partial t} + \mathbf{v} \cdot \nabla f_k = \sum_{i \neq k} \frac{f_i - f_k}{\tau_k} + \sum_i \frac{F_{ik}}{m_k} \mathbf{v} \cdot \nabla \phi[f_i] = \frac{f_k - f_k}{\tau_k} + \sum_i \frac{F_{ik}}{m_k} \mathbf{v} \cdot \nabla \phi[f_i].
\]

As this MD simulation runs, we collect data on ion trajectories and interactions. Unfortunately, the relaxation timescales are phenomenological parameters, and do not have a closed-form expression in terms of statistics of molecular quantities. We compute \( \tau_k \) by forcing the rate of entropy production due to each species in the cell to match for both models.

CONCLUSIONS

This heterogeneous multiscale method allows us to simulate large plasma systems that require molecular-level detail. The mathematical rigor allows us to characterize the model’s strengths and limitations. Local updates of relaxation timescales are highly parallelizable, and we are able to adaptively update only the cells that require it. The result is an efficient and accurate hybrid method for plasma simulation that pushes the boundary of simulation sizes. This will lead to new understandings of inertial confinement fusion experiments and other plasma applications.

MULTISCALE CONNECTION

The domain is discretized into finite volume cells over which we approximate the distribution of each particle species as piecewise constant. Each \( f_k \) is evolved according to its BGK-Vlasov equation, provided accurate relaxation times \( \tau_k \) for each species pair. Relaxation timescales in BGK can be derived explicitly only in very simple cases. Otherwise, they are handled in an ad hoc manner. Our method improves upon this practice by statistically deriving this quantity from small, brief molecular dynamics simulations.

When we decide to update \( \tau_k \) for the finite volume cell \( \Omega \) located at \( r \), we simulate an MD cell \( \omega \) embedded within the cell of interest. The multiscale cell is much smaller than the macroscopic cell. This MD simulation is populated with particles such that each species of particle has velocity distribution and density consistent with their \( f_k \) in \( \Omega \). Periodic boundary conditions simulate a homogeneous environment for the MD simulation.

The entropy of species \( k \) in \( \Omega \) is defined as

\[
H_{\text{BT}}^k(t) = -\int f_k \log(f_k) \, dv.
\]

where the \( r \) integral is over \( \Omega \) and the \( v \) integral is over all velocities. Because \( f_k \) is defined as the expected value of the microscopic distribution function \( N_k \), the MD interpretation of the entropy is

\[
H_{\text{BT}}^k(t) = -\int \langle N_k \rangle \log(\langle N_k \rangle) \, dv.
\]

We can calculate the rates of change of these quantities due to collisional effects. Both can be decomposed into self-contributions, and contributions from interactions with other species. Setting the corresponding terms equal yields

\[
\frac{dH_{\text{BT}}^k}{dt} = -\frac{1}{\tau_k} \int (f_k^\text{eq} - f_k) \log(f_k) \, dv.
\]

The rate of change of \( H_{\text{BT}}^k \) can be computed as

\[
\frac{dH_{\text{BT}}^k}{dt} = -\sum_{i \neq k} \int \langle F_{ik} \rangle \mathbf{v} \cdot \nabla \langle f_i \rangle \, dv.
\]

Given the MD state, we solve the matching conditions for \( \tau_k \) and \( \tau_k \) in a least-squares sense to account for noise and possible linear dependence. This will tell us how to choose relaxation rates to match the collisional entropy production between scales. The key assumptions of this method are:

- The relaxation timescales change slowly relative to both the BGK and MD variables
- The collision term is a local quantity and its effects can be computed from a small homogeneous MD simulation
- Robust MD statistics can be computed
- The MD state is consistent with the macroscopic variables

MOLECULAR INITIALIZATION

The MD system must be initialized consistently with the macroscopic cell. To match each density \( n_i \), we initialize each species with \( n_i V_r \) particles. Because the kinetic system has no knowledge of the two-particle correlation function, we cannot reproduce the proper correlations, so the initial configuration will heat. To counteract this, we equilibrate using a Langevin thermostat.

RESULTS

Hydrogen (dotted) and aluminum (solid) ions undergoing temperature relaxation. HMM (blue) accurately tracks MD trajectories (green) much better than pure kinetic models (red and purple).

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