Coupling Continuum to MD in Fluid Simulation:
Thermodynamic Field Estimator
Optimal Particle Controller
Buffer-Zone Feedback

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Theoretical Challenges to Linking Continuum with MD

- Different degrees of freedom
- Different evolution

\[ dP = f(x, v) dx dv = \frac{\rho(x) dx}{(2\pi T(x))^{3/2}} \exp\left(\frac{-|v - \bar{v}(x)|^2}{2T(x)}\right) dv + f^{(2)} \]

The Bridge is **Particle Distribution Function**
Practical Challenges: How to **Determine** and **Apply** BC

**Two** Kinds of BC Applications

Once we know both ← and → without **invalidating** the intrinsic mechanisms of either solvers, a unified solution can be brought by the **Schwarz Iteration** procedure. We will show that generally **exact solution** exists for steady-state fluid at **finite** $T$. 

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**MD Solver**

**Continuum Solver**

**Continuum result** ← MD result

**Continuum result** → MD
Easier Job: Continuum $\xrightarrow{MD}$

Bin-averaging is bad, neglects spatial coherency of data.

**Thermodynamic Field Estimator**

- Maximum Likelihood Inference
  \[
  \max \left( \prod_i P(x_i, v_i | \rho, \bar{v}, T) \right)
  \]

- Basis expansion of target fields in Chebyshev polynomials

- CG optimization of coefficients

Properties:
1. smooth
2. maximal utilization of given information
3. value at any point depends on all data

Example 1
Heat Conduction MD Simulation
Example 2a

- 60 x 30 bin-averaging
- Not well-characterized
- Streamlines not available

MD simulation of fluids flowing by a solid-wall barrier in midstream
Example 2b

- 9 x 9 spatial basis
- Continuous streamlines
- Vortex formation
- Re = $10^1$

After applying **TFE** to the same particle data

More Difficult Job: Continuum fields → [MD]

Demand \( \{x_i, v_i\} \) to satisfy the distribution \( f(x,v) \) specified by \( \rho(x), \bar{v}(x), T(x) \) on the boundary.

But for MD result to be exact, atoms should evolve naturally without feeling artificial disturbance. \( \therefore \) Maxwell's Demons

Is this possible?
**Optimal Particle Controller:** a more sophisticated demon who inflicts *least* disturbance on *particle dynamics* while applying a desired *boundary distribution*.

- incoming random variables \(\{X\}\) with distribution \(g(X)\)
- the desired distribution is \(f(X)\)
- replace \(X\)'s by \(Y\)'s such that \(Y\) satisfies distribution \(f(Y)\)
- \(\text{OPC}\) is the unique \(X \rightarrow Y\) transform.
  that *minimizes* \(|Y-X|^2\)

**Evidence:** particle *velocity auto-correlation* function \(\Psi(t) = \frac{\langle \mathbf{v}(t) \mathbf{v}(0) \rangle}{\langle \mathbf{v}(0) \mathbf{v}(0) \rangle}\)
Molecular Chaos in Fluids

- Particle dynamics

Action Region

Buffer-Zone

Core

MD Box

Therm. Field Estimator

Optimal Particle Controller

Feedback Control Algorithm

✓ BC
1. Problem

\[ \frac{\partial c}{\partial y} \]

2. Buffer–Zone Feedback Method

3. Result: correct BC + dynamics = Exact solution at finite \( T \).

- **Coupled Continuum–MD Simulation of Couette Flow**

- **Action Region A** (just \( \delta x \) in this figure)
- **Buffer Region B**
- **Core Region C**

- **continuum solver**
- **OPC solution**
- **(exact) BZF solution**
Conclusion:

- Exact steady-state solution = correct BC + Particle dynamics.
- Obtainable in fluids due to molecular chaos, using Buffer-Zone Feedback and novel tools such as TFE and OPC.

Open Question:

How do we get exact solutions for solids at finite $T$?

- Long range order
- Phonons almost do not decay