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

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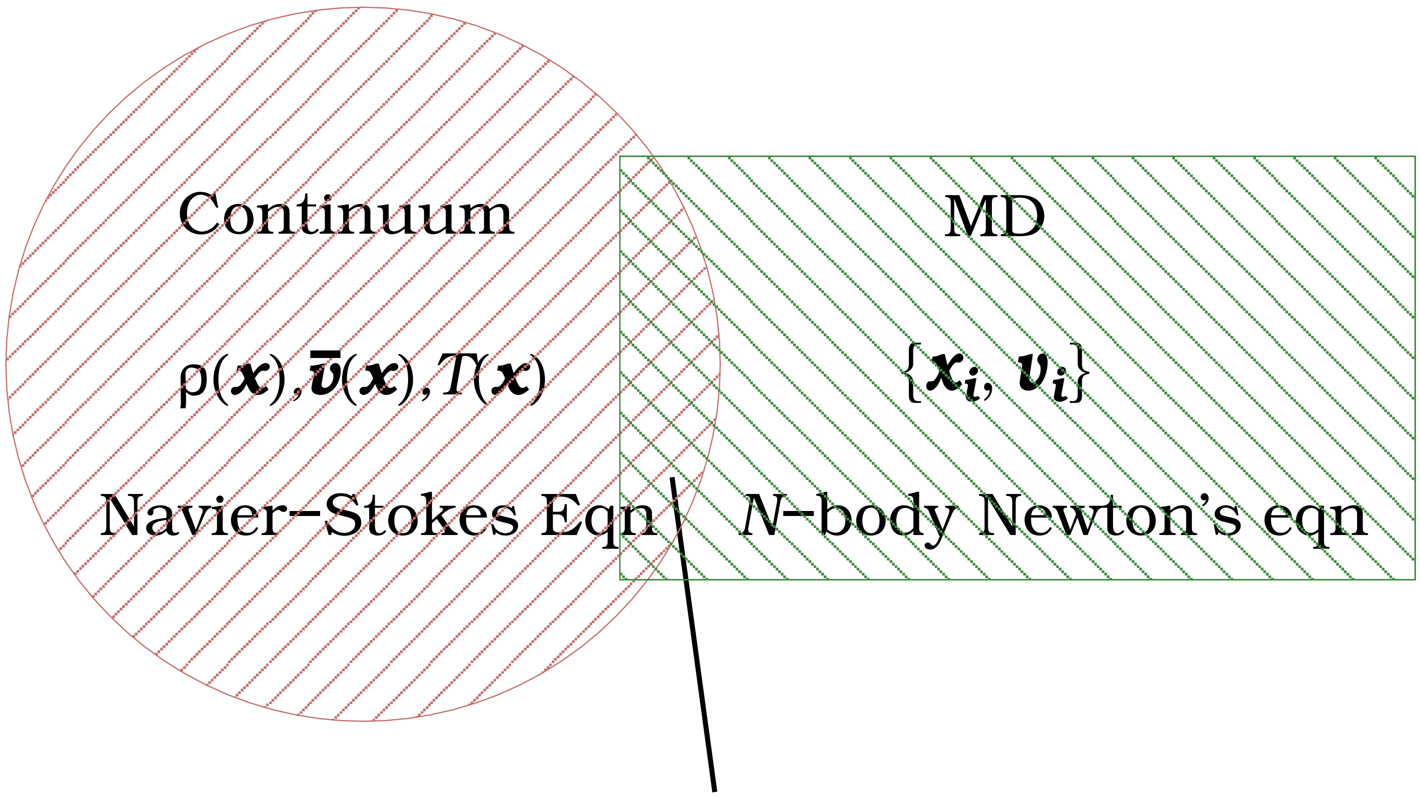
Theoretical Challenges to Linking Continuum with MD

- *Different* **degrees of freedom**
- *Different* **evolution**



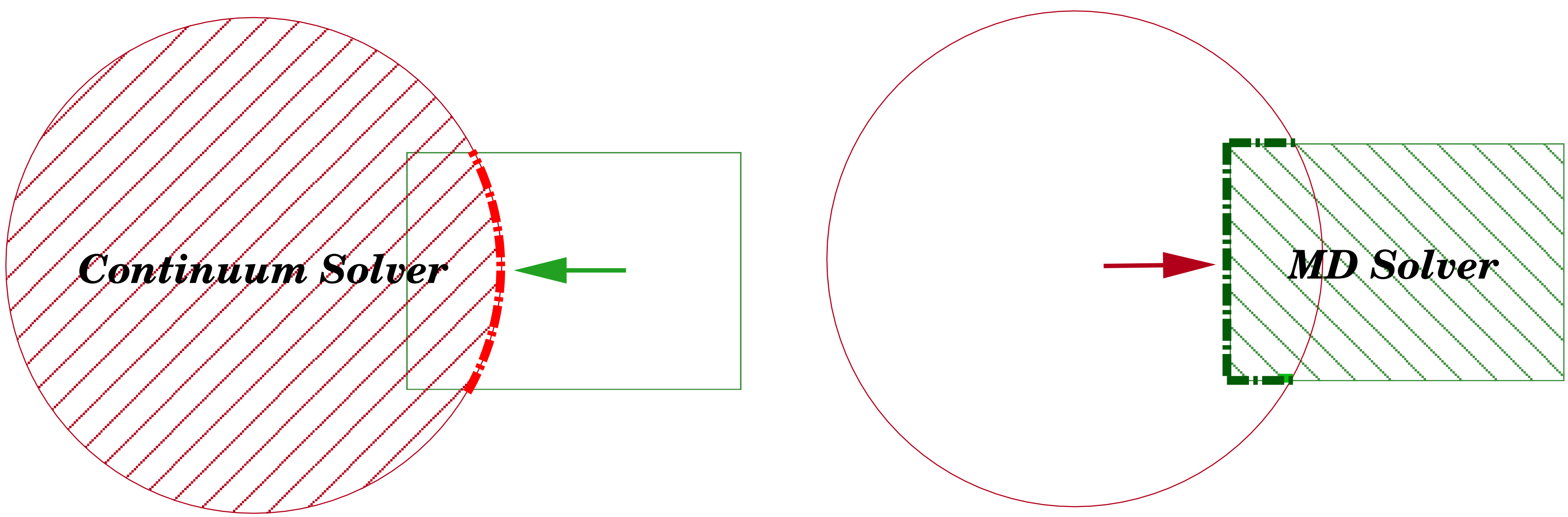
$$dP = f(\boldsymbol{x},\boldsymbol{v})\,d\boldsymbol{x}\,d\boldsymbol{v} = \frac{\rho(\boldsymbol{x})\,d\boldsymbol{x}}{(2\pi T(\boldsymbol{x}))^{3/2}} \exp\left(\frac{-|\boldsymbol{v}-\bar{\boldsymbol{v}}(\boldsymbol{x})|^2}{2T(\boldsymbol{x})}\right) d\boldsymbol{v} + f^{(2)}$$

<u>The Bridge is **Particle Distribution Function**</u>

*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.



Easier Job: **Continuum** ⟵ **MD** *i.e.*, $\{\boldsymbol{x_i}, \boldsymbol{v_i}\} \longrightarrow \rho(\boldsymbol{x}), \boldsymbol{v}(\boldsymbol{x}), T(\boldsymbol{x})$

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

Thermodynamic Field Estimator

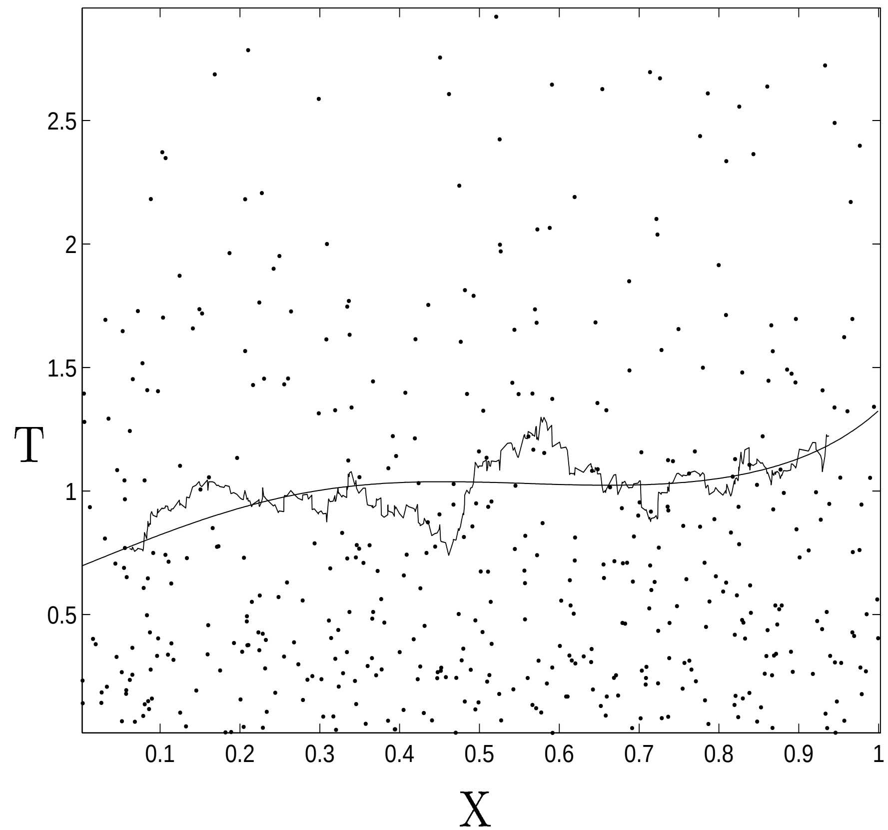
- Maximum Likelihood Inference

  $\max\left(\prod_i P(\boldsymbol{x_i}, \boldsymbol{v_i} | \rho, \bar{\boldsymbol{v}}, T) \right)$

- Basis expansion of target fields in Chebyshev polynomials

- CG optimization of coeffcients

Example **1**
Heat Conduction MD Simulation

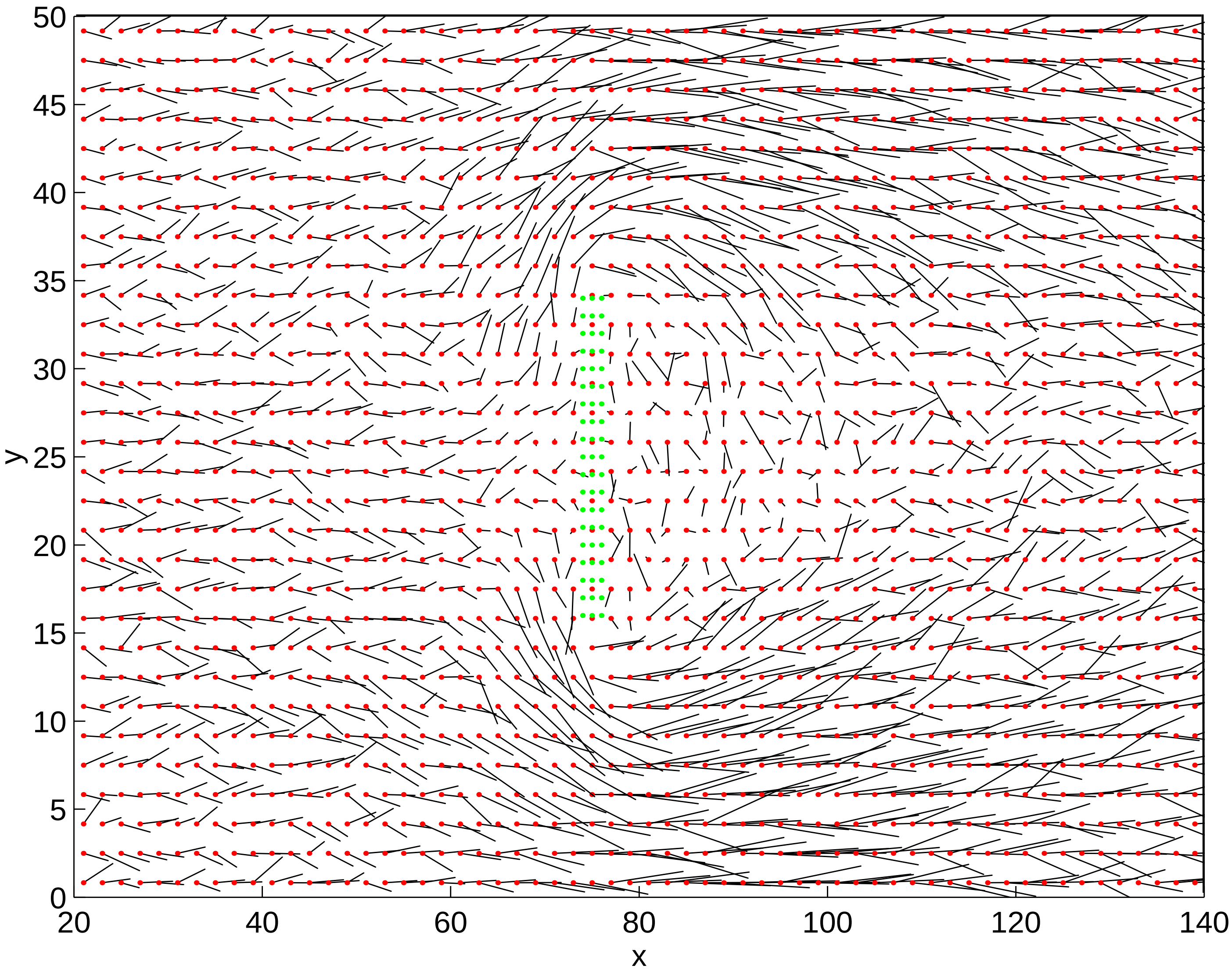


Properties: 1. smooth 2. maximal utilization of given information
3. value at any point depends on **all** data

Example **2a**

MD simulation of fluids flowing by a solid–wall barrier in midstream

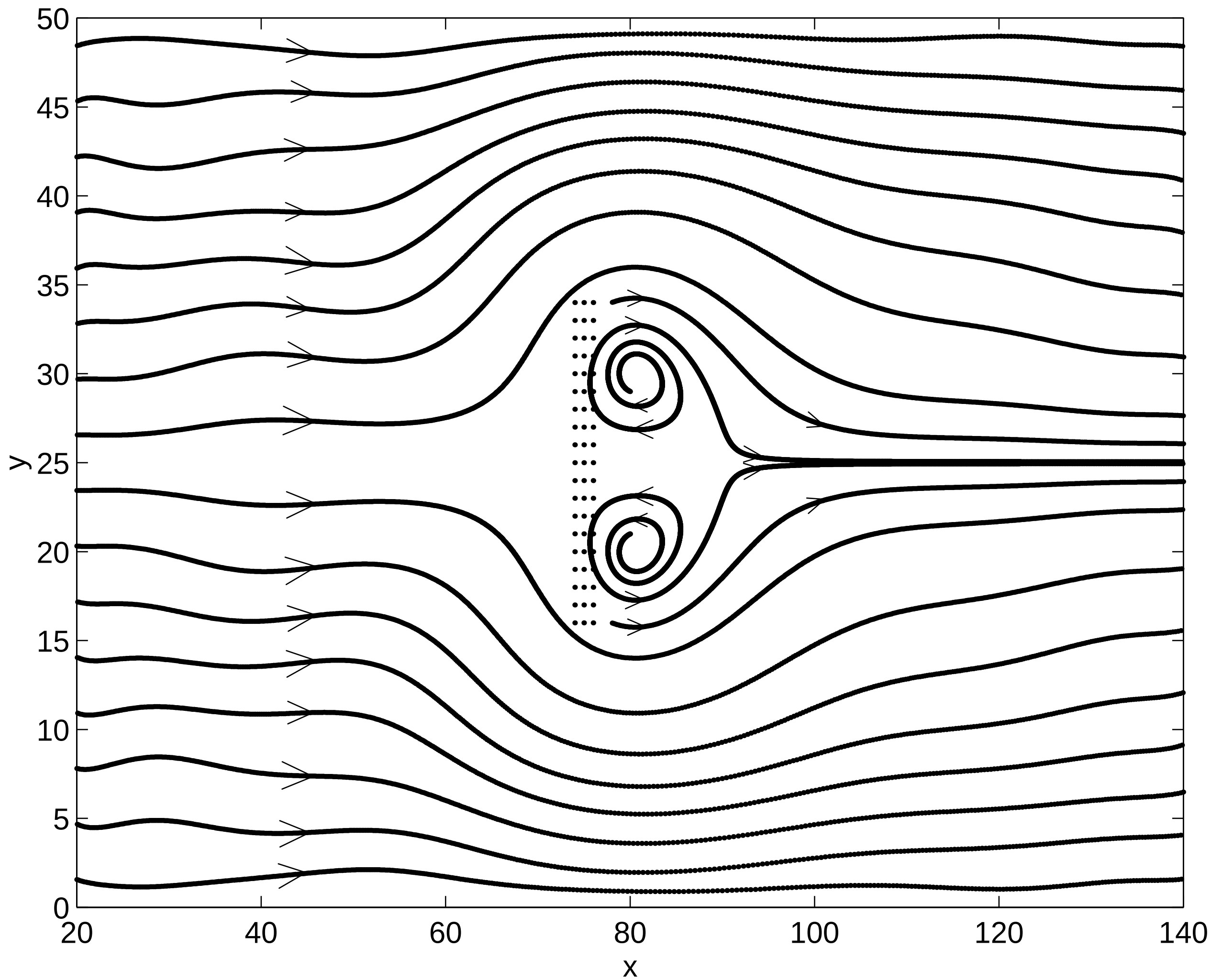
- 60 x 30 bin–averaging
- Not well–characterized
- Streamlines not available



Example **2b**

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

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



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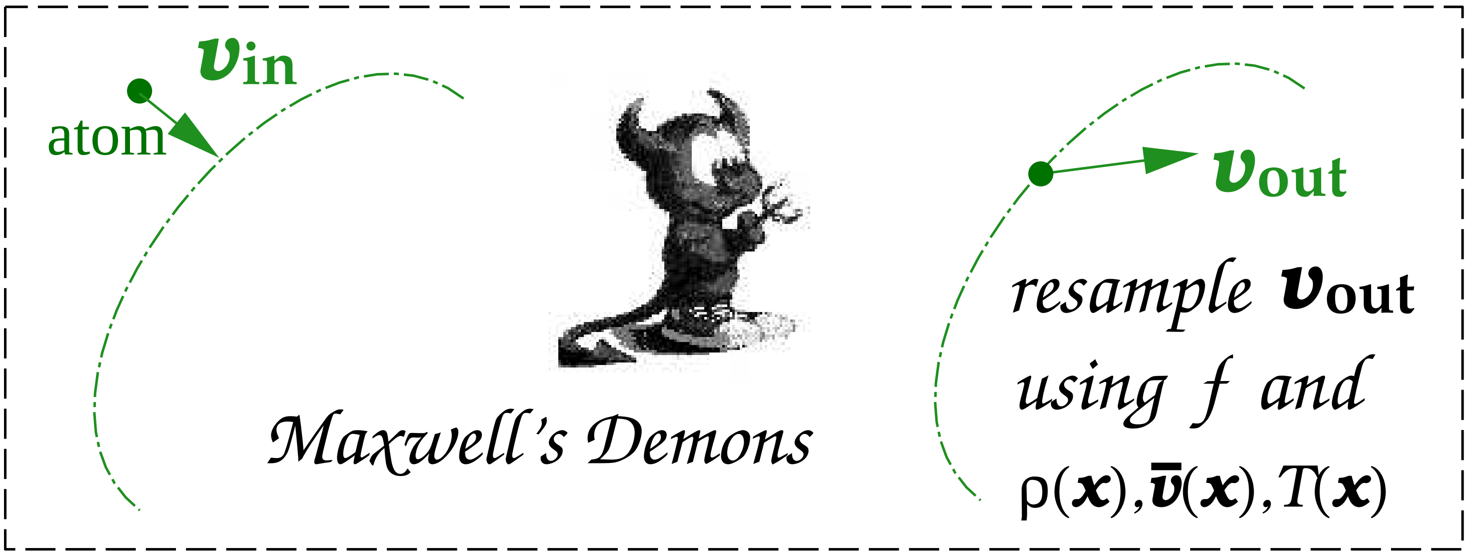
More Difficult Job: Continuum fields → MD

Demand $\{\boldsymbol{x}_i, \boldsymbol{v}_i\}$ to satisfy the **distribution** $f(\boldsymbol{x},\boldsymbol{v})$ specified by $\rho(\boldsymbol{x}),\bar{\boldsymbol{v}}(\boldsymbol{x}),T(\boldsymbol{x})$ on the boundary.

$\boldsymbol{v}_{\text{in}}$ may $\notin f$



but $\boldsymbol{v}_{\text{out}}$ will

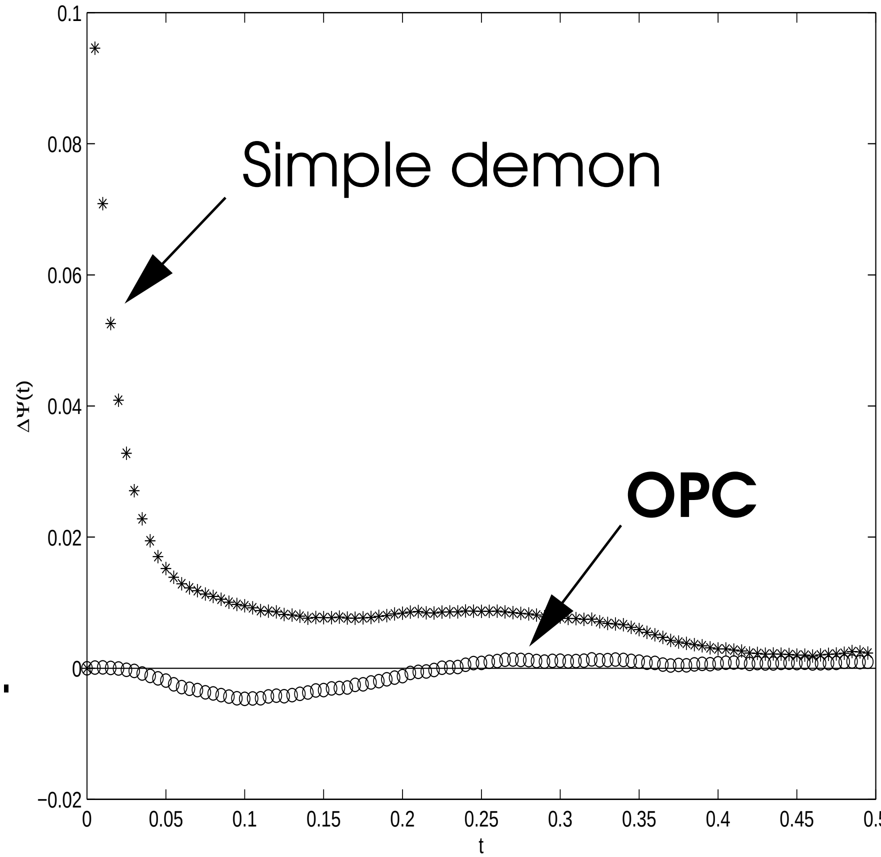
But for MD result to be ***exact***, atoms should evolve ***naturally*** without ***feeling*** artificial disturbance. ∴ ~~*Maxwell's Demons*~~

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 $f(Y)$
- **OPC** is the **unique** $X \blacktriangleright Y$ transform. that ***minimizes*** $\overline{|Y-X|^2}$

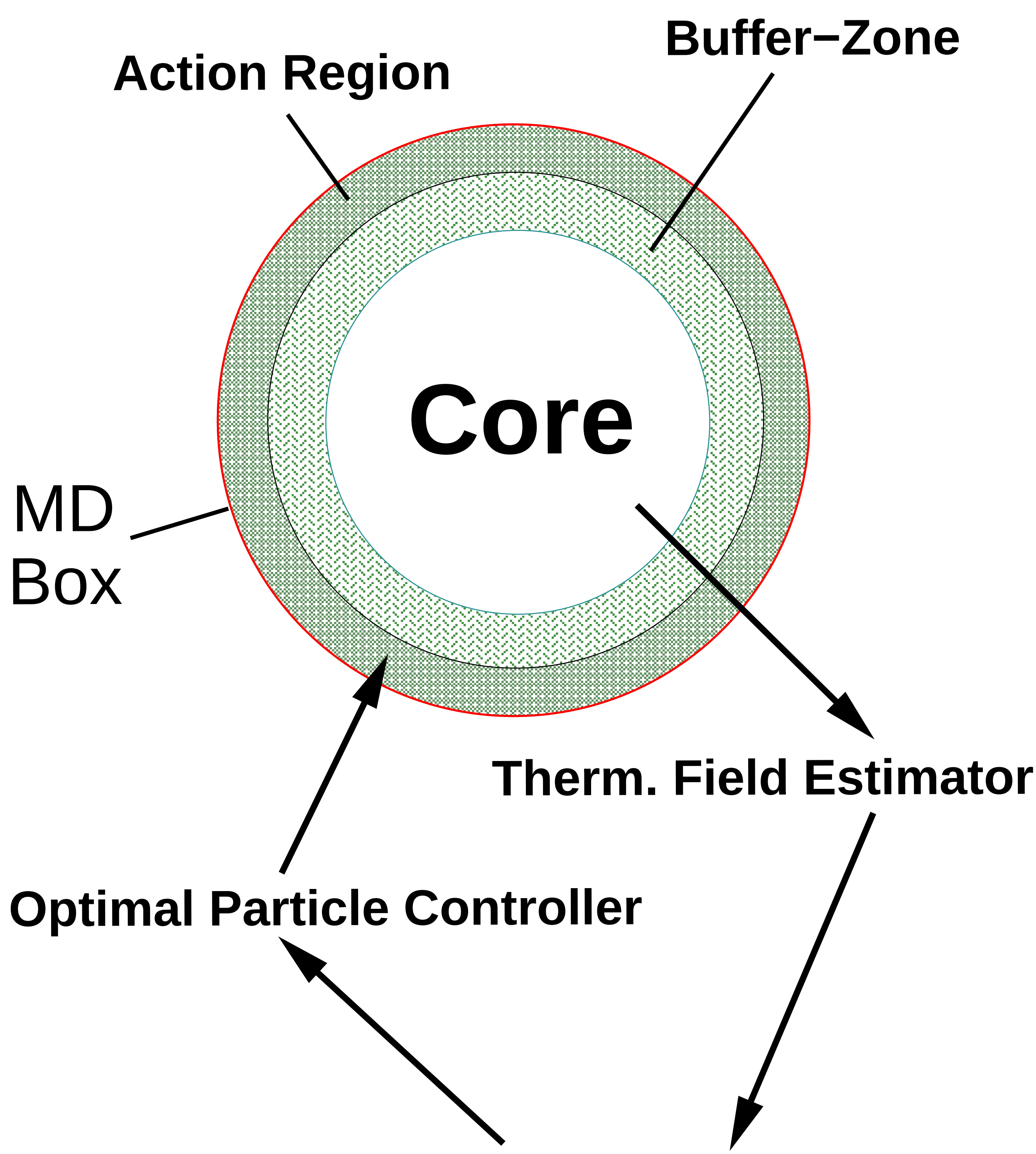
$\Delta\Psi(t)$ in Couette Flow Simulation



Evidence: particle **velocity auto−correlation** function $\Psi(t) = \dfrac{\langle \boldsymbol{v}(t)\boldsymbol{v}(0)\rangle}{\langle \boldsymbol{v}(0)\boldsymbol{v}(0)\rangle}$

Molecular Chaos in Fluids

✓ Particle dynamics

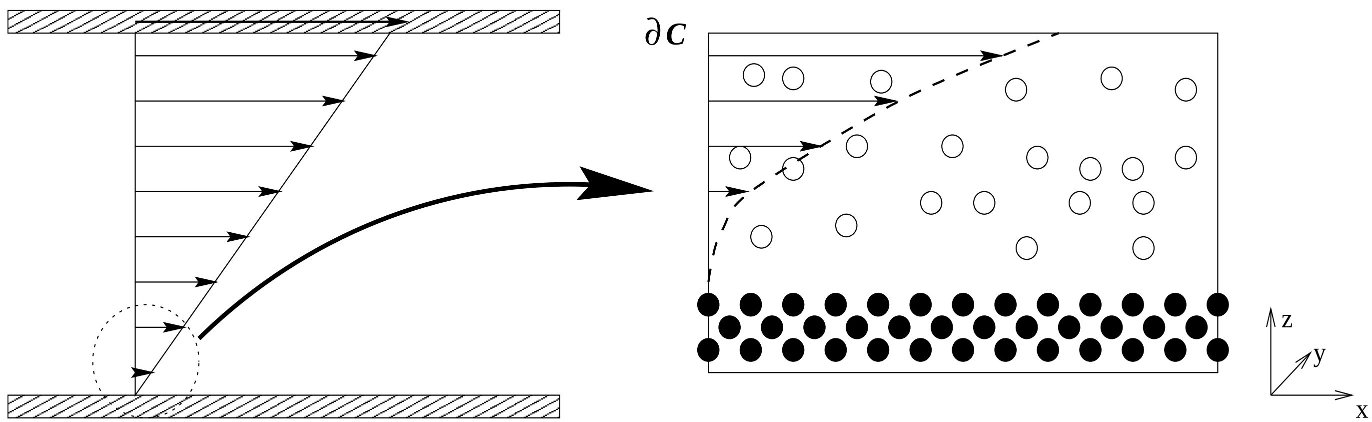


Feedback Control Algorithm

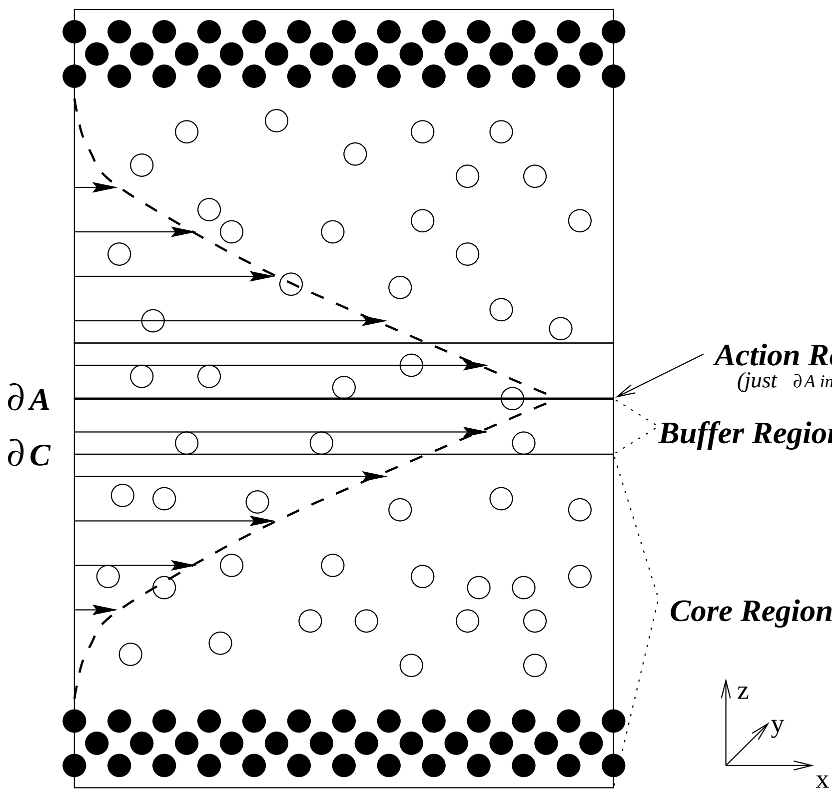
✓ BC

Coupled Continuum–MD Simulation of Couette Flow

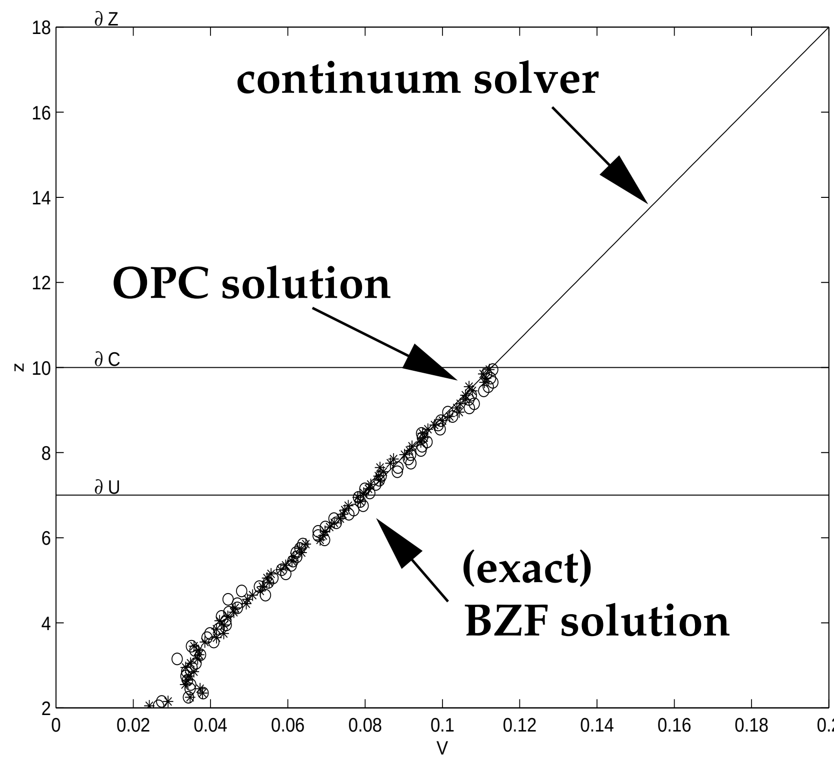
1. Problem



2. Buffer–Zone Feedback Method



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



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