Coupling Continuum to Molecular Dynamics Simulation:

Reflecting Particle Method

Thermodynamic Field Estimator

Optimal Particle Controller.

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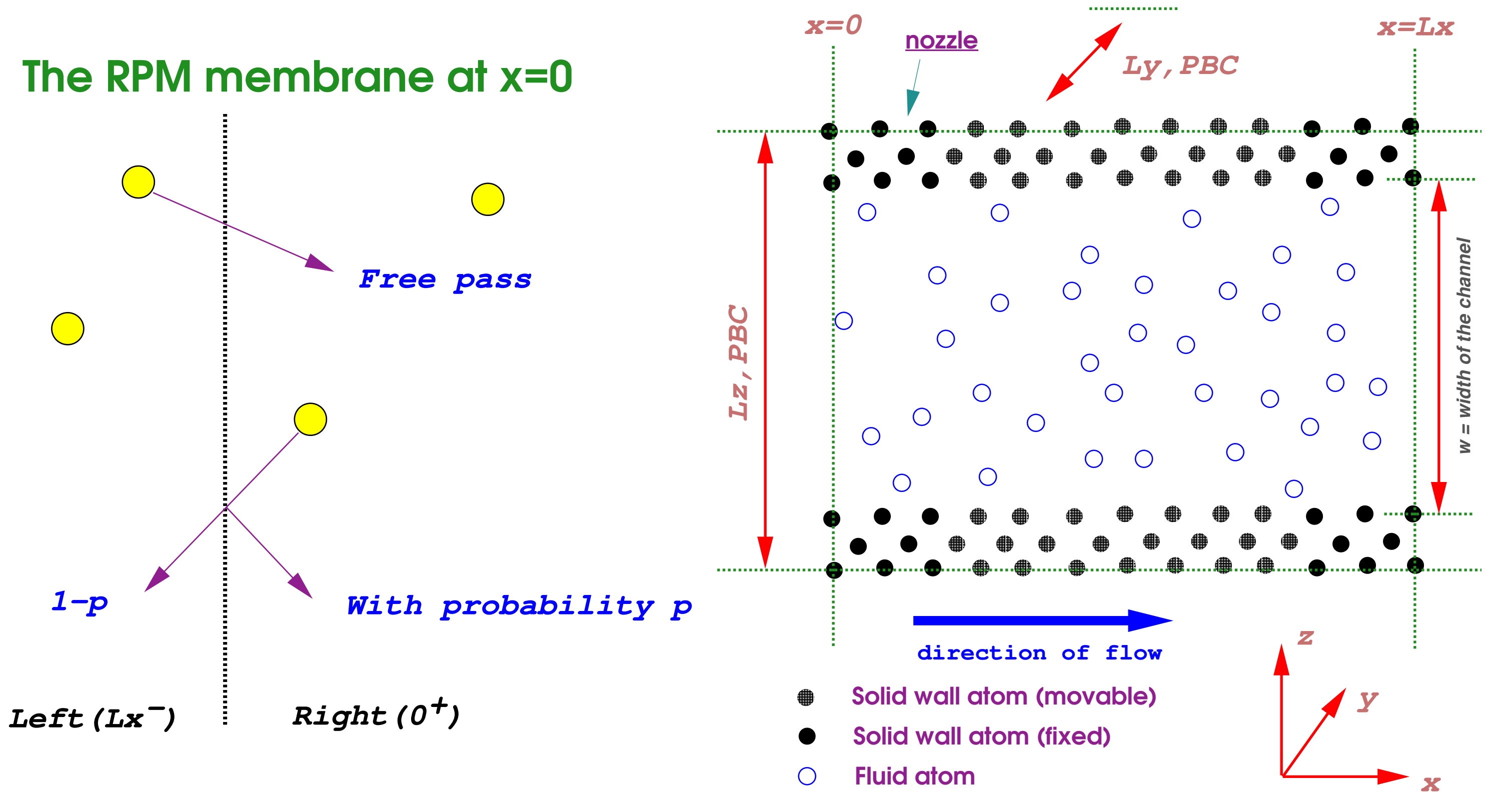
Abstract:

We present a general approach for coupling continuum to molecular dynamics simulation. Macroscopic thermodynamic field (temperature, velocity) **boundary conditions** *can be coupled to a MD system while* **minimally** *disturbing particle dynamics of the system. And by acting far away from the region of interest through a* **feedback control** *mechanism, we can even eliminate that disturbance. The field estimator serves as the* **detector** *of the control loop, based on Maximum Likelihood Inference, which infers smooth instantaneous thermodynamic fields from particle data; The* **optimal** *particle controller, defined through an implicit relation* $\mathcal{T}_3(X \to Y)$: $\int_{-\infty}^{X} f(\xi)d\xi = \int_{-\infty}^{Y} g(\eta)d\eta$*, can be proven to come up to the required task with* **least** *disturbance to particle dynamics; The reflecting particle method (RPM) is a (funny) way to drive fluid flow in MD by employing selectively reflecting "***Maxwell's demons***" at ends of the cell. Under steady flow, heat generated by viscous dissipation inside the fluid is to be balanced with the* **entropy/information** *input by the demons, for which we estimate analytically and has been explicitly verified.*

Reflecting Particle Method to Drive Fluid Flow:



Consider a Poiseuille (pipe/channel) flow scenario: fluid comes in with pressure P_{in} and exits with pressure P_{out}. $\Delta P = P_{\text{in}} - P_{\text{out}} > 0$ is what drives the fluid flow.

- **How do we set up the pressure head ΔP in MD ?**

$$\textbf{Continuum description}: \ \rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) = -\nabla P + \mu\nabla^2\mathbf{v} + \rho\mathbf{g}$$

In steady state, $\frac{\partial \mathbf{v}}{\partial t} = 0$ and $\rho\mathbf{g}$ is usually negligible, which means the fluid in concern is *only pushed by other fluids.*

In order to simulate such flows in MD, we have to make sure that in the **region of interest** $\mathcal{D}$, the fluid atoms are not affected on by artificial forces of any kind, and that the local dynamics of particles should be the same **as in nature**. The desired flow should only be achieved by applying appropriate **boundary conditions/actions** far from $\mathcal{D}$ (could be artificial). Because of molecular chaos, the disturbance to particle dynamics due to artificial action on the boundary will decay rapidly (in a few mean free paths) as it approaches $\mathcal{D}$. In a sense we want to build a **feedback control** system: certain flow conditions are desired in $\mathcal{D}$, yet we can not directly act on $\mathcal{D}$ because it will invariably disturb the local particle dynamics. Thus it would be ideal if by **acting far away**, we can achieve the **desired** flow conditions in $\mathcal{D}$, because then local particle dynamics will also be preserved. In fact, the fluid atoms will **not** be able to distinguish any difference from "reality" inside $\mathcal{D}$, and how the flow is set up has become irrelevant.

Mechanism: A bunch of "Maxwell's demons" sit on a membrane at $x = 0$: they are such that if an atom crosses $x = 0$ from **left** ($x = L_X^-$) **to right** ($x = 0^+$), it passes through without hindrance; but if it crosses $x = 0$ from **right to left**, then it could be elasticly reflected with probability p. The membrane is otherwise transparent in the sense that particles on two sides can interact.

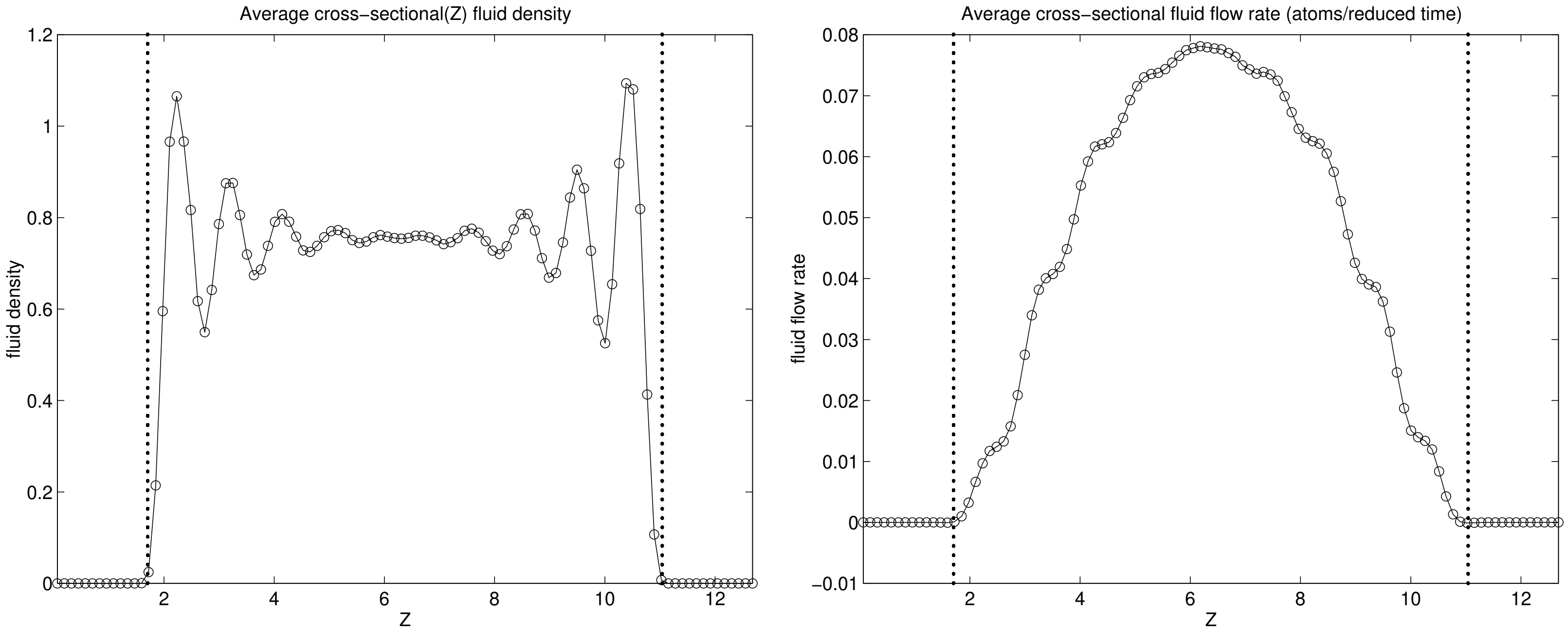
Our method is simple and effective. It

- conserves number of particles (so steady flow is possible)
- conserves total energy (no need for temperature rescaling in the system)
- reaches steady state gracefully.

But most importantly, particle dynamics (except in regions near the membrane) are preserved[1], and we recover the Navier-Stokes equation in continuum limit (the so-called gravity method does not). However it is an **implicit** method, i.e., ΔP is an "output" (a function of p and geometry) rather than being specified. For ΔP to serve as input, we need to have a **feedback control mechanism**.

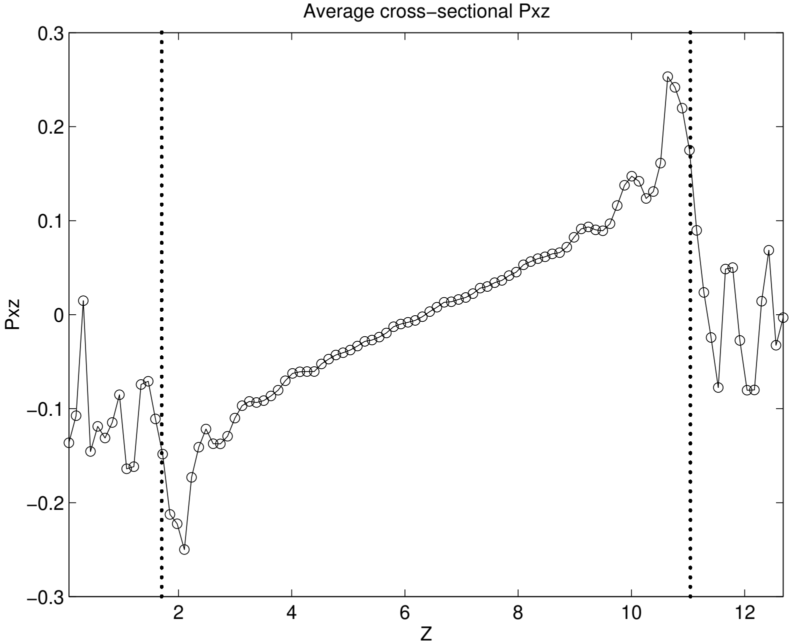
[1] A fluid atom in midstream has no way to tell whether the local pressure gradient is set up by RPM or by neighbor's kid's water gun.

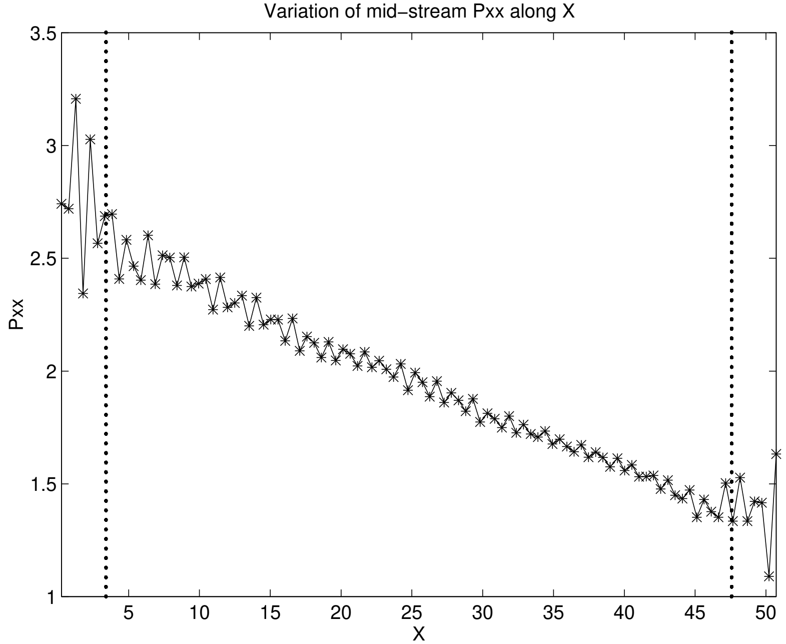
RPM Works: ($xyz = 51.0 \times 5.1 \times 12.7$, 1783 fluid atoms, 900 wall atoms, $\rho = 0.81$, $T = 1.1$, $p_{reflect} = 1.$)



Density and flowrate profile of fluid atoms in cross-section z. The dotted lines indicate the positions of fluid-solid interfaces. The characteristic time and length scales of the fluid and solid atoms are made equal, so "no-slip" condition is seen to hold very well near the interface. The flowrate profile is in rough accord with the parabolic shape predicted by Navier-Stokes equation for incompressible fluids.

RPM Works...





Shear stress τ_{xz} profile in z, and midstream pressure τ_{xx} along x. The objective of setting up pressure difference between two ends of the channel is indeed realized by RPM.

- Using the obtained total flowrate and pressure gradient, we can infer the fluid shear viscosity, *assuming* the continuum description to hold everywhere. It gives $\mu = 2.47$, in fair agreement with $\mu = 2.14$, as predicted by bulk liquid simulation[a] at the same condition.

[a] S. T. O'Connell and P. A. Thompson, Phys. Rev. E **52**, 5792 (1995).

Demons vs Heat:

Facts:

– Demons don't do work (by selectively reflecting), so system energy stays constant.

– Heat is *generated* by viscous action inside fluid bulk[a]. The rate, as calculated by continuum description, is

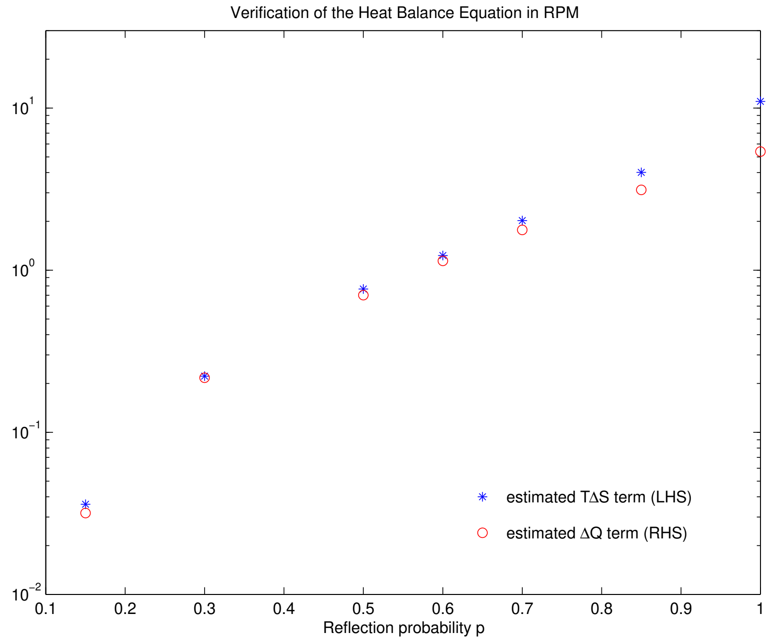
$$\frac{dQ}{dt} = \int \tau_{ij} v_{i,j} d\Omega = \frac{L_X L_Y w^3}{12\mu} \left(\frac{\Delta P}{\Delta x}\right)^2$$

– Steady state is observed to be reached. The system does not heat up.

[a] Other dissipative sources may exist, such as "stick-slip" motion at fluid-solid interfaces. In our examples it should be negligible.

- **Q: Where does the heat go?**
- **A:** $\Delta Q = T\Delta S$.The demons reduce system entropy by selectively reflecting atoms at $x = 0$.
- **Q: How do we calculate this ΔS?**
- **A:** Let f_1/f_2 be the rate of particles hitting $x = 0$ from left/right when the system reaches steady state. If the demons do *not* act, then in a unit period of time, the parameters specifying the membrane system is f_1 and f_2, which correspond to $\Omega_1 = \frac{(f_1+f_2)!}{f_1!f_2!}$ ways of crossing (micro-states); after the demons interfere it becomes $\Omega_2 = \frac{(f_1+f_2)!}{(f_1+pf_2)!((1-p)f_2)!}$, as *the system can not distinguish between atoms which hit from the right and then get reflected and atoms which originally hit from the left.* Thus we arrive at the following **heat balance equation:**

$$k_{\mathrm{B}}T\log\frac{\Omega_1}{\Omega_2}=k_{\mathrm{B}}T\left\{f_1\log(1+\frac{pf_2}{f_1})+pf_2\log(p+\frac{f_1}{f_2})+f_2(1-p)\log(1-p)\right\}=\frac{L_XL_Yw^3}{12\mu}\left(\frac{\Delta P}{\Delta x}\right)^2$$



This balance has been explicitly verified using data obtained from our MD simulations. The difference (in numerical value) between LHS and RHS is usually within 15%, which is extremely good agreement[2] considering all the assumptions made. The fact that LHS is consistently a bit higher than RHS is in the right direction because fluids near the membrane are more "turbulent" and the continuum dissipation kernel tends to underestimate.

[2] In a much bigger system ($76.5\times 10.2\times 20.4$) run with 10179 fluid atoms and 2700 wall atoms, LHS and RHS are found to agree within 1%.

Thermodynamic Field Estimator:

Basic Assumption:

At any given instant, there exist continuous, *slowly varying* thermodynamic fields $\{\rho(\mathbf{x}), T(\mathbf{x}), \bar{\mathbf{v}}(\mathbf{x})\}$, such that particles conform to single-particle distribution function of

$$dP = f_{\mathrm{M}}\left(\mathbf{x}, \mathbf{v} | \{\rho(\mathbf{x}), T(\mathbf{x}), \bar{\mathbf{v}}(\mathbf{x}\}\right) d\mathbf{x} d\mathbf{v} = \frac{\rho(\mathbf{x})}{(2\pi T(\mathbf{x}))^{D/2}} \exp\left(-\frac{|\mathbf{v} - \bar{\mathbf{v}}(\mathbf{x})|^2}{2T(\mathbf{x})}\right) d\mathbf{x} d\mathbf{v}.$$

Inverse problem:

Given a set of particle data, $\{(\mathbf{x}_i, \mathbf{v}_i), i = 1..N\}$, how can we obtain the "actual" set of continuous functions $\{\rho(\mathbf{x}), T(\mathbf{x}), \bar{\mathbf{v}}(\mathbf{x})\}$, such as required for drawing streamlines in fluid flow?

- **Usual answer:** Divide the geometry into bins and average over each bin.

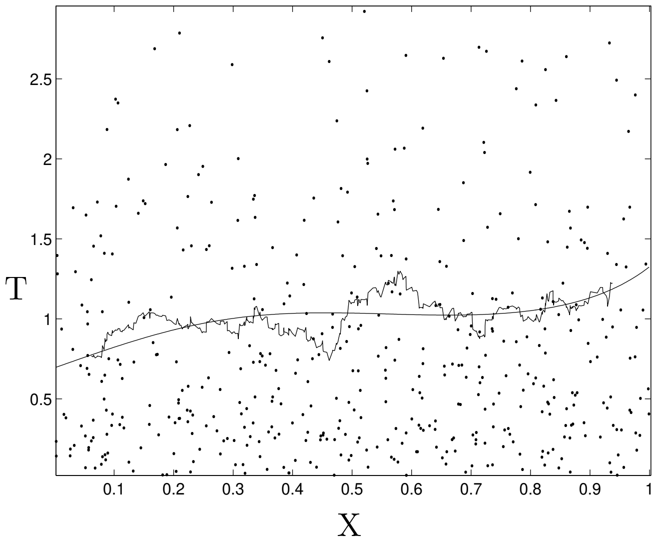
- **Shortcomings:** We neglect spatial correlations between particle data, implied by the fact that the "actual" fields should be **continuous** and **slowly varying**. For this reason we often face the choice between spatial resolution and statistical accuracy, especially when data are scarce and expensive.

$\Rightarrow$ *Is it the best we can do? Are we maximally utilizing the information?*

Maximum Likelihood Inference: Given a set of independent data (sample) points $\{(\mathbf{x}_i, \mathbf{v}_i), i = 1..N\}$, the "most probable" fields $\{\rho(\mathbf{x}), T(\mathbf{x}), \bar{\mathbf{v}}(\mathbf{x})\}$ are which maximizes

$$P = \prod_{i=1}^{N} f_{\mathrm{M}}\left(\mathbf{x}_i, \mathbf{v}_i | \{\rho(\mathbf{x}), T(\mathbf{x}), \mathbf{v}(\mathbf{x})\}\right)$$

In actual implementation we expand the fields in a certain spatial basis and optimize the coefficients using conjugate gradient minimizer. The spatial basis usually consist of low order polynomials (Chebyshev), which is equivalent to assigning "priors" to fields with slow spatial variations.

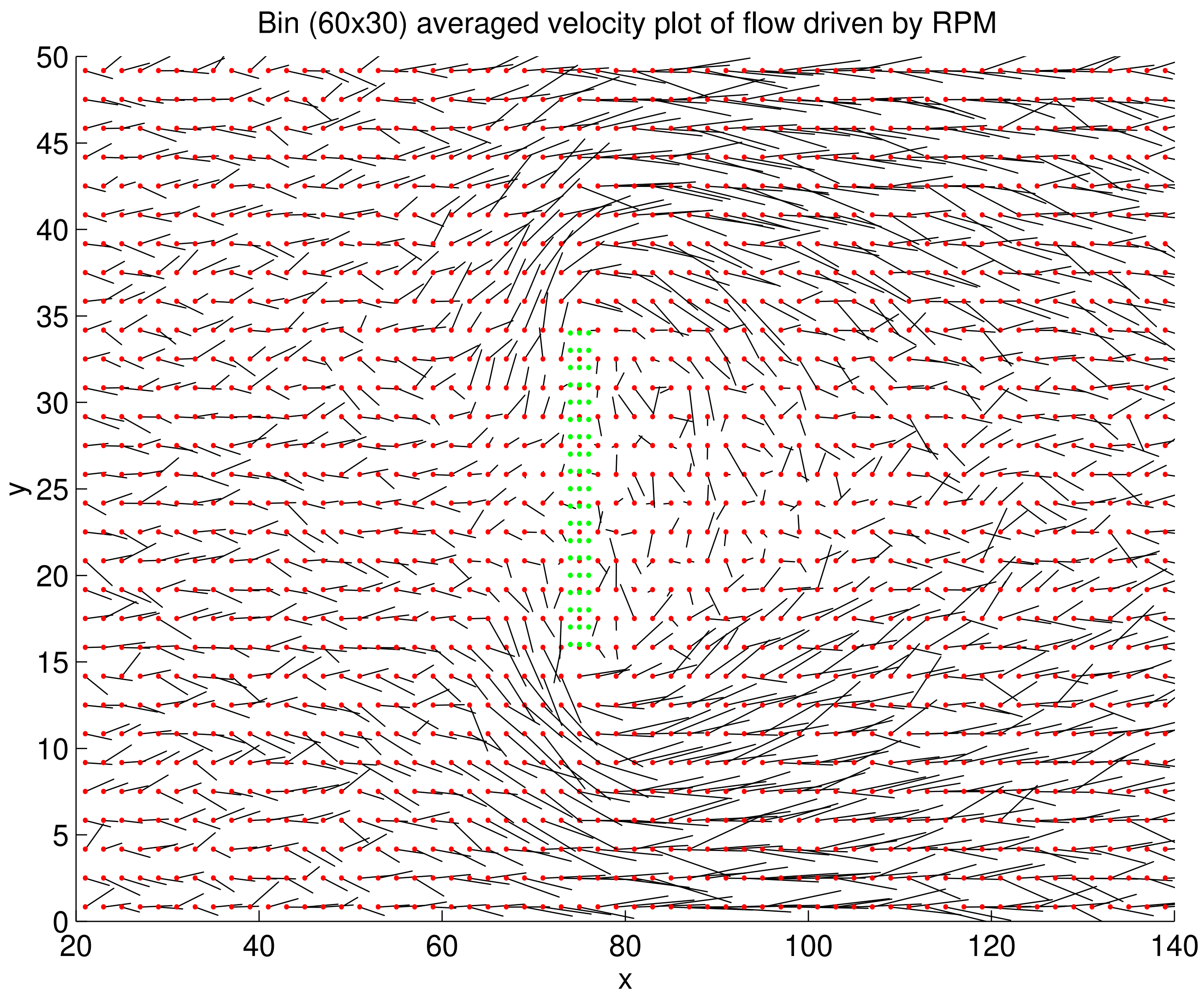


Snapshot of a 2D liquid system with 500 atoms which is heated on one side ($x = 1$) and cooled on the other ($x = 0$). Dots represent particle positions (x) and kinetic energies (y). A sliding bin average (size=0.12) is taken to give the zig-zag curve, representing an instantaneous temperature profile; our method (4 bases) gives the smooth curve, which laces through the bin-averaged results. The physical origin of this method gives us confidence in the quality of the estimation, which is of great value in the general coupling formalism.

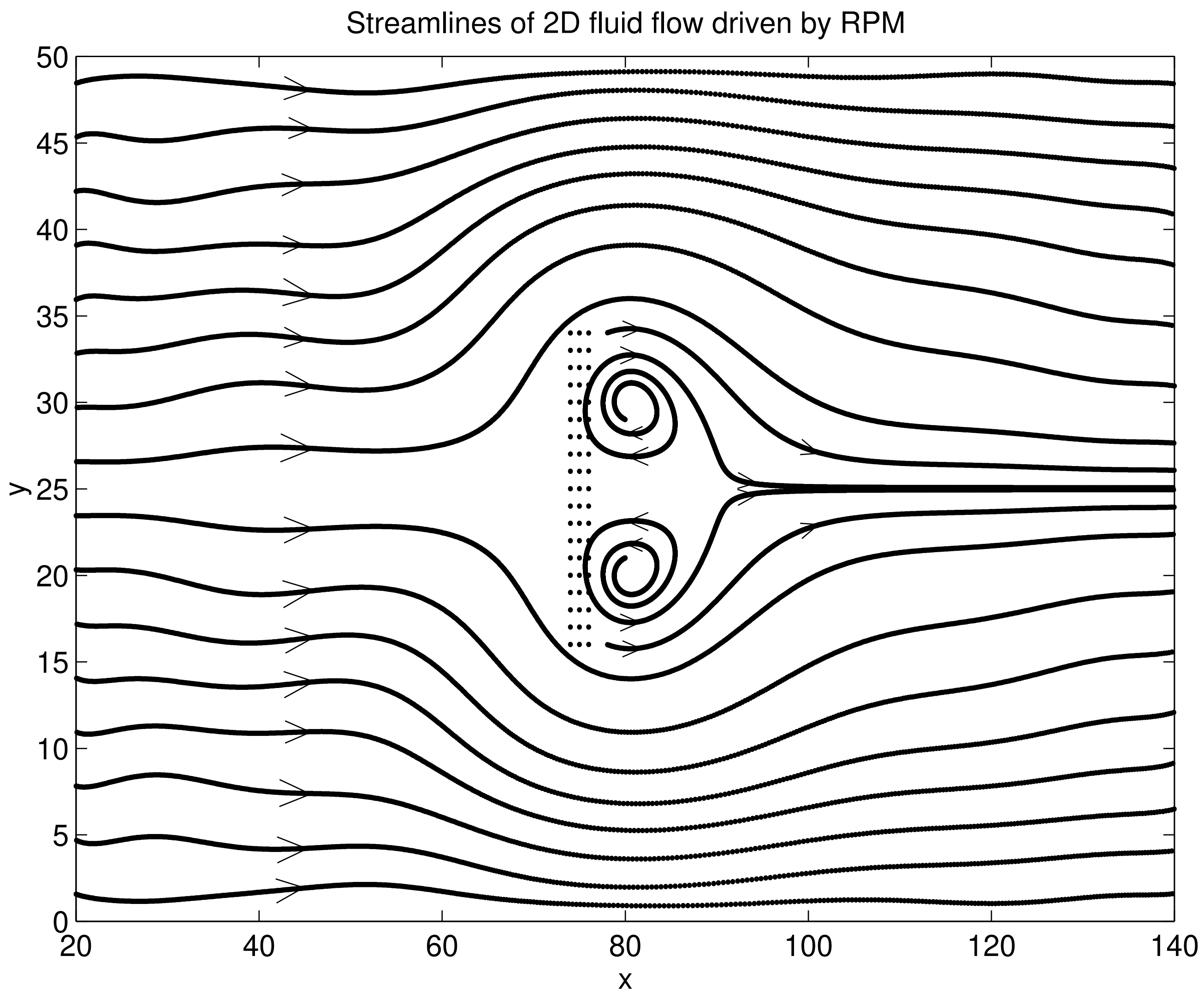
Applying Field Estimator to Fluid Flow:

The Results:

Following two graphs are bin-averaged (60×30) plot of the fluid velocity and corresponding streamline plot based on fields given by the estimator. The flow (2D LJ6-12 system, 150×50, 2000 atoms, $T \approx 1.50$) is driven by RPM ($p = 1$, two membranes), with a vertical wall barrier (fixed atoms) in midstream. 200,000 particle data (collected in 50,000 time steps) are fed into the field estimator (same data are used in the bin-average), which employs 4 basis functions for the T field and 121 basis functions for v_x, v_y fields inside domain $(20, 0) - (140, 50)$. The geometrical singularity (the barrier) inside the domain may influence the accuracy but not the qualitative features of the estimation, especially, the vortices are believed to be real. From the continuum perspective, the Reynolds number $\mathrm{Re} = \rho v L/\mu$ is around 10^1, which corresponds to vortex generation in similar fluid mechanical situations. But the high flow speed and significant temperature and density variations ($\sim 20\%$) along the flow deem it difficult to be fully treated by any continuum descriptions.



Bin (60x30) averaged velocity plot of flow driven by RPM
y
x
50
45
40
35
30
25
20
15
10
5
0
20
40
60
80
100
120
140



Streamlines of 2D fluid flow driven by RPM
y
x
0
5
10
15
20
25
30
35
40
45
50
20
40
60
80
100
120
140

Optimal Particle Controller – Prelude

- **A Case of Failure:**

Consider a simple fluid system for which we want to have high temperature T_h at $x = 0$ boundary and low temperature T_l at $x = 1$ boundary, to study convectionless heat conduction. One immediate idea is that when a particle crosses either boundary, give it a random velocity drawn from distribution $f_{\mathrm{M}}(\mathbf{v})$ with parameters $\bar{\mathbf{v}} = 0$, $T = T_h$ (or T_l) and put the particle back.

This method **fails**. For simplicity let us take $T_l = T_h$, i.e., *homogeneous heating*. We have implemented the scheme on both 1D fluid with soft-core interactions, and on 2D LJ6-12 fluid where we only re-sample the normal velocities v_x, when particles cross the boundaries. Both simulations end up with the bulk temperatures dropping to approximately $T_h/2$!

- **Reason:**

We are dealing with a **conditional probability** problem: the speed distribution of atoms which cross the boundary (say, from left to right) is *different* from that of atoms in the bulk

$$dP = \frac{1}{\sqrt{2\pi T}} \exp\left(-\frac{{v_x}^2}{2T}\right) dv_x, \qquad -\infty < v_x < +\infty, \tag{0.1}$$

but weighted by the normal velocity $v_x > 0$

$$dP = \frac{v_x \exp\left(-\frac{{v_x}^2}{2T}\right) dv_x}{\int_0^{+\infty} v_x \exp\left(-\frac{{v_x}^2}{2T}\right) dv_x} = \frac{v_x}{T} \exp\left(-\frac{{v_x}^2}{2T}\right) dv_x, \qquad 0 < v_x < +\infty. \tag{0.2}$$

Optimal Particle Controller – Prelude

It can be checked that $\langle {v_x}^2 \rangle$ from distribution (2) is $2T$, not T. Thus, if we rescale the *boundary crossing atoms* using bulk distribution (1) with parameter $T = T_h$, the energy can only be balanced when the bulk temperature reaches $T_h/2$.

Insight:

A more obscure defect of the scheme is that, for whatever the incoming velocity $\mathbf{v}_{\mathrm{in}}$ of the particle before hitting the boundary, a new velocity $\mathbf{v}_{\mathrm{out}}$ is drawn from a given distribution, say $g(\mathbf{v})$, entirely *independent* of $\mathbf{v}_{\mathrm{in}}$. Thus if we evaluate the disturbance to particle dynamics using $B = \langle |\mathbf{v}_{\mathrm{out}} - \mathbf{v}_{\mathrm{in}}|^2 \rangle$ for the scheme, it is going to be big. Take the example of homogeneous heating, where we shall use the correct distribution (2) as $g(\mathbf{v})$ in drawing $\mathbf{v}_{\mathrm{out}}$'s: even when the system *reaches* T_h, the desired temperature, the scheme still disturbs particle dynamics by giving each boundary crossing atom a new $\mathbf{v}_{\mathrm{out}}$; on the other hand, if we just let $\mathbf{v}_{\mathrm{out}} = \mathbf{v}_{\mathrm{in}}$, i.e., do nothing, the system temperature stays at T_h! In fact, a "smart" method should be able to automatically tune down its influence when the system approaches the desired state – and just do nothing if the actual distribution *is* the desired distribution. We shall call this the *coalescence* property.

Optimal Particle Controller:

Objective:

We want to achieve certain macroscopic field boundary conditions on $\partial\mathcal{D}$, on the cost of **least** disturbing the particle dynamics inside $\mathcal{D}$. Any artificial interference besides the natural course of evolution for the particles, such as temperature rescaling, acceleration, or RPM, constitute disturbances to the local dynamics. Very often acting on $\partial\mathcal{D}$ (or beyond) is desirable because the deeper in $\mathcal{D}$, the less the effect. A reasonable quantification for such "boundary disturbance" is

$$B = \langle |\Delta \mathbf{v}_n|^2 \rangle = \langle |\mathbf{v}_n^{\text{out}} - \mathbf{v}_n^{\text{in}}|^2 \rangle$$

where $\Delta \mathbf{v}_n$ is the change in particle velocity before and after the nth particle crosses the boundary. Field "boundary conditions" on $\partial\mathcal{D}$ are satisfied if outgoing particles conform to $f_{\text{M}}(\mathbf{x}, \mathbf{v})$ distribution with the desired on-site parameters $\{\rho(\mathbf{x}), T(\mathbf{x}), \mathbf{v}(\mathbf{x})\}$.

Let us formulate these ideas mathematically. Suppose we have incoming random number series $\{X_n\}$, conforming to distribution function $f(X) : dP(\eta < X < \eta + d\eta) = f(X)d\eta$, but we would like the series to conform to distribution $g(X)$. We believe that by replacing X with another random number Y which has distribution $g(Y)$, we will be able to gradually achieve that purpose (let us first not consider the **overshooting** approach). Thus our goal is to find a transformation $\mathcal{T} : X_n \to Y_n$, with the requirement that if $\{X_n\}$ conforms to distribution $f(X)$, $\{Y_n\}$ will conform to distribution $g(Y)$.

There exist many possible $\mathcal{T}$'s:

- $\mathcal{T}_1 \Rightarrow$ Draw Y randomly from $g(Y)$ without referencing X.
- $\mathcal{T}_2 \Rightarrow$ Take $Y = X$ if $p \leq \frac{g(X)}{Kf(X)}$, but randomly draw Y from $g(Y)$ if otherwise. Here p is a random number uniformly distributed over $[0, 1]$, and K is a constant such that $Kf(X) \geq g(X)$ for all X. $\mathcal{T}_2$ satisfy the coalescence property[a]. *But is it the best?*
- $\mathcal{T}_3 \Rightarrow$ Solve Y from X by the implicit equation: $\int_{-\infty}^{X} f(\xi)d\xi = \int_{-\infty}^{Y} g(\eta)d\eta$.

[a] If $\mathcal{T}$ satisfy the requirement that *when* $f \equiv g$, $Y_n = X_n$, it is said to have the coalescence property.

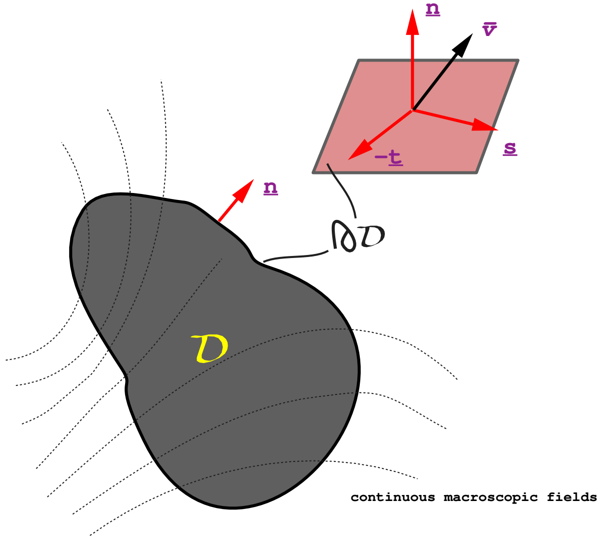
If we come back to our previous idea about **minimally influencing the dynamics**, let us adopt the reasonable criterion that $B[\mathcal{T}] = \langle (Y - X)^2 \rangle$ *be* **minimized** *among all possible $\mathcal{T}$'s.* That is, we want a series $\{Y_n\}$ which is **least** altered from $\{X_n\}$, yet representing a desired distribution $g(Y)$. We believe that $\mathcal{T}_3$ is the mathematically **optimal** transformation which minimizes B. A tentative proof is given at the end. $\mathcal{T}_3$ works rather well in our applications, but it is an implicit algorithm and could be computationally demanding.

- **How can we know $f(X)$ at $\partial\mathcal{D}$, in order to use $\mathcal{T}$?**

A straight forward answer would be to collect incoming data $\{X_n\}$ of the past for a certain period of time, to compile a histograph. For fields with spatial and temporal variations this turns out to be not a very good idea, because boundary-hitting is rare compared to bulk data. If we believe that the actual fields have small spatial variations, then particle data inside the bulk carry useful information about the system and should *not* be discarded: this is where the **thermodynamic field estimator** comes into use, because the continuous function we get for the field using Maximum Likelihood Inference is based on **all** particle data. Especially, field values at the boundary can be thought of as **extrapolations** from the bulk, where each particle data makes a contribution. This is of course based on the assumption that quasi-equilibrium distribution $f_{\mathrm{M}}(\mathbf{x}, \mathbf{v}|\{\rho(\mathbf{x}), T(\mathbf{x}), \bar{\mathbf{v}}(\mathbf{x}\})$ holds, which is the bridge between macroscopic fields (continuum) and microscopic statistical mechanics (MD).

General 3D Boundary Particle Controller

$\mathcal{D}$ is our domain of interest, $\partial\mathcal{D}$ is its boundary upon which the particle controller acts on in order to achieve the desired macroscopic fields. For any small piece of the boundary, we can always choose the local coordinate frame to express the desired (g) macroscopic velocity field as $\bar{\mathbf{v}} = (v_n, v_s, 0)$. In the same frame the actual (f) velocity field is $\bar{\mathbf{v}}' = (v'_n, v'_s, v'_t)$.



We found that (v_n, v_s, v_t) distributions for boundary hitting ($-\mathbf{n} \to \mathbf{n}$) atoms are decoupled. And they are, respectively,

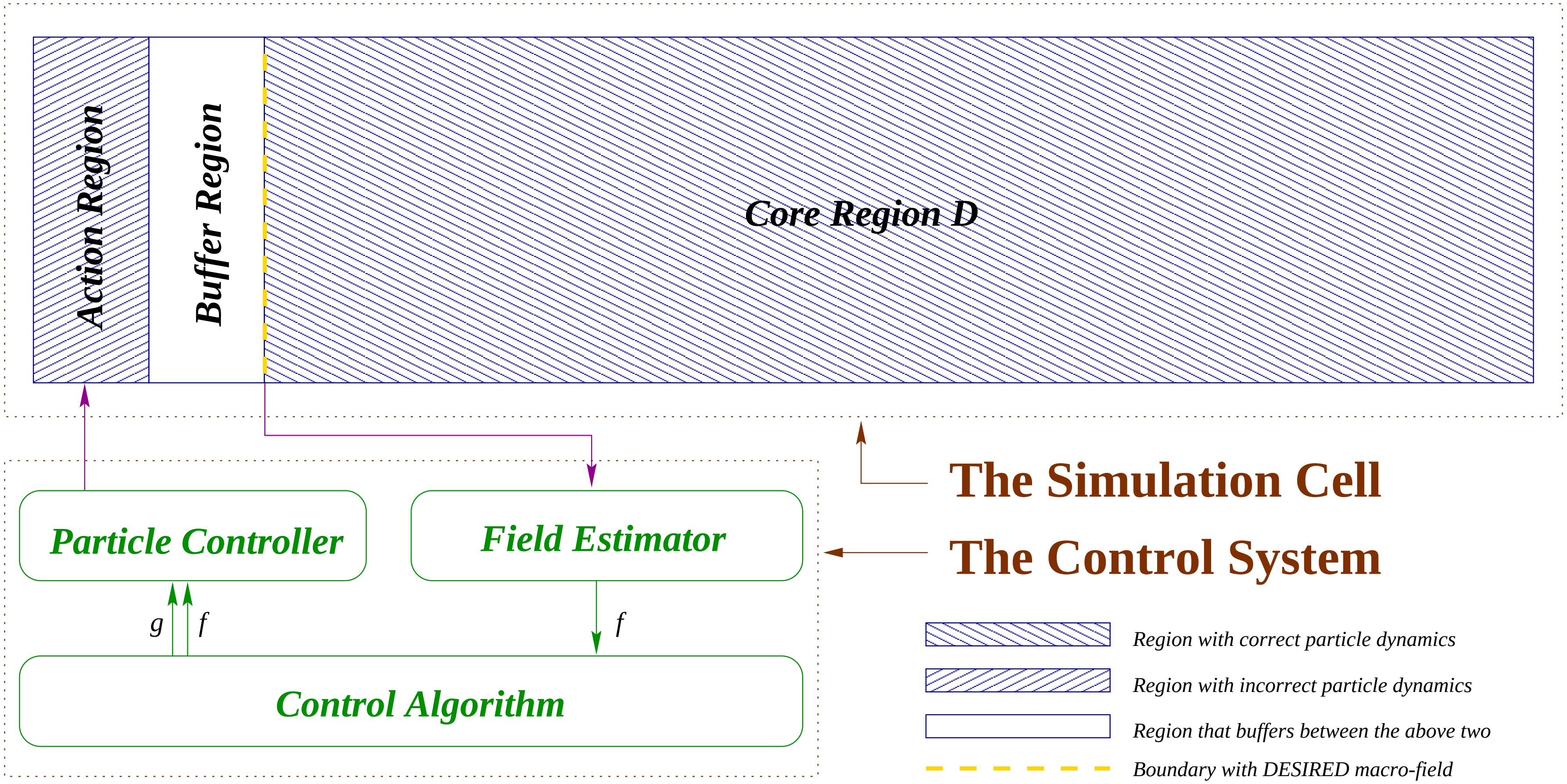
$$g_n(v_n) = \frac{(2\pi T)^{-1/2} v_n \exp(-(v_n - \bar{v}_n)^2/2T)}{\frac{1}{2}\bar{v}_n(1 + \mathrm{erf}(\frac{\bar{v}_n}{\sqrt{2T}})) + \sqrt{\frac{T}{2\pi}}\exp(-\frac{\bar{v}_n^2}{2T})} \qquad v_n \in (0, +\infty)$$

$$g_s(v_s) = \frac{1}{\sqrt{2\pi T}} \exp(-(v_s - \bar{v}_s)^2/2T) \qquad v_s \in (-\infty, +\infty)$$

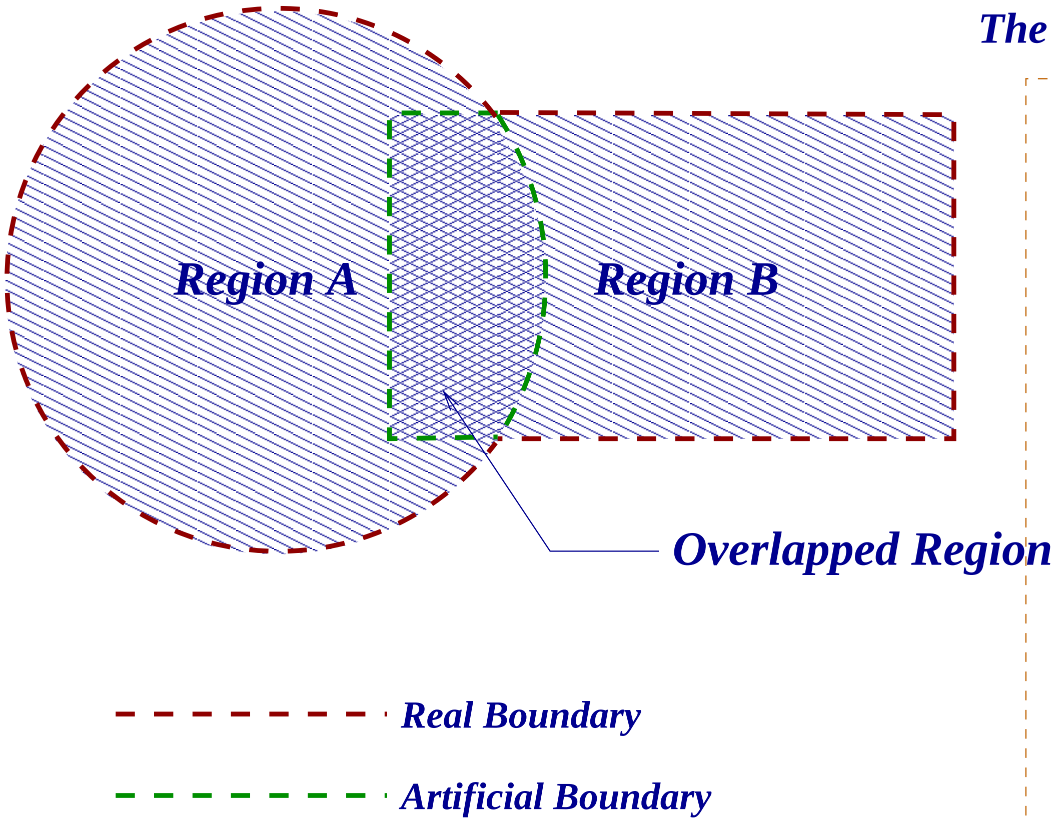
$$g_t(v_t) = \frac{1}{\sqrt{2\pi T}} \exp(-v_t^2/2T) \qquad v_t \in (-\infty, +\infty)$$

$\{f_n(v'_n), f_s(v'_s), f_t(v'_t)\}$ have similar expressions. We only need to plug each (f, g) pair into $\mathcal{T}_3$ to calculate the ($v'_n \to v_n$, $v'_s \to v_s$, $v'_t \to v_t$) action for each boundary hitting atom, and it is believed to be *optimal*.

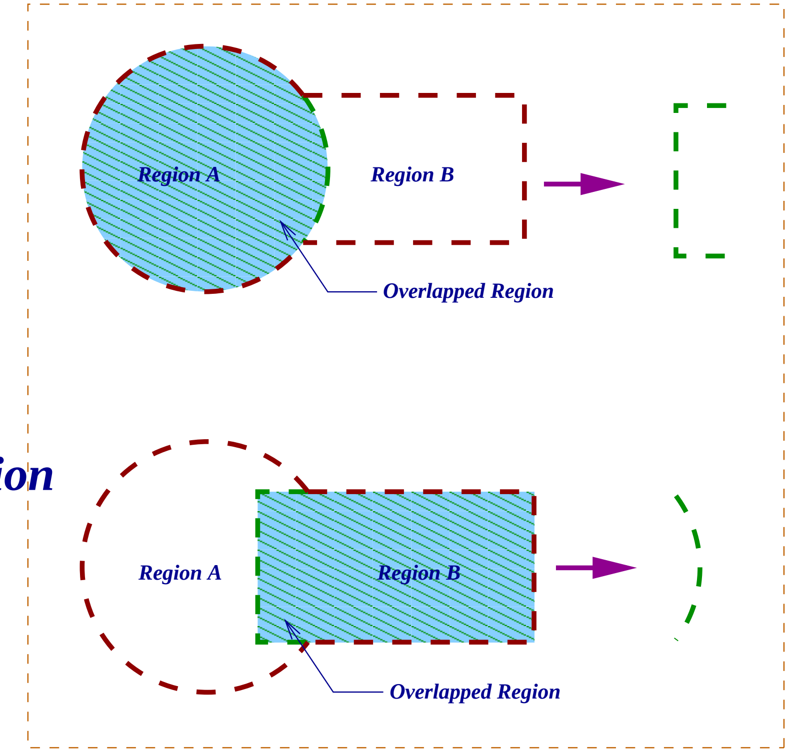
General Feedback Control Formalism:



Schwarz Coupling:



The two alternitive steps of schwarz coupling:



Appendix. The proof that $\mathcal{T}_3$ is optimal:

In our definition, a transformation is an operation which gives an output Y from an input X, but not necessarily in a deterministic manner, which differs from the concept of a function. $\mathcal{T}_1, \mathcal{T}_2$ and $\mathcal{T}_3$ are all examples of such transformations. Mathematically it is equivalent to a mapping from a real number $x = X$ to a real *function* in y, which is just the conditional probability distribution $W(y|x)$, from which Y is drawn. The joint probability distribution function is simply

$$W(x, y) = W(y|x)f(x) \tag{.3}$$

for the two random variables on xy plane.

$W(x, y)$ has the properties of:

1. Non-negativeness:
$$\forall x, y \in (-\infty, +\infty) \quad W(x, y) \geq 0 \tag{.4}$$

2. Normalization:
$$\int_{-\infty}^{+\infty} W(x, y)dy = f(x) \tag{.5}$$
$$\int_{-\infty}^{+\infty} W(x, y)dxdy = 1 \tag{.6}$$

3. Basic requirement:
$$\int_{-\infty}^{+\infty} W(x, y)dx = g(y) \tag{.7}$$

Now, we want to find the $W_{\min}(x, y)$ which minimizes "disturbances" to the sequence, quantified as

$$B[W] = \int_{-\infty}^{+\infty} (x - y)^2 W(x, y)dxdy$$

We want to show that the distribution $W_{\min}$ **must be zero almost everywhere** on the xy plane. Suppose we have found

$W_{\min}$, and $W_{\min}(x,y) > 0$ everywhere in a small region $\mathcal{A}$. We can always find some function $S_{\mathcal{A}}(x,y)$ which is nonzero only inside $\mathcal{A}$, satisfying

$$\int_{\mathcal{A}} S_{\mathcal{A}}(x,y)dx = 0 \tag{.8}$$

$$\int_{\mathcal{A}} S_{\mathcal{A}}(x,y)dy = 0 \tag{.9}$$

and zero elsewhere[3].

Since the expression for $B[W]$ contains $(x-y)^2$, it can not be that $B[S_{\mathcal{A}}] = 0$ for all valid $S_{\mathcal{A}}$'s, and we can always choose a small enough λ to ensure that $|\lambda S_{\mathcal{A}}(x,y)| \leq W(x,y)$ everywhere. Let $W_{\text{new}} = W_{\min} + \lambda S_{\mathcal{A}}$: W_{new} will also satisfy the constraints (4) to (7). Lastly let us pick the sign of λ to make $\lambda B[S_{\mathcal{A}}] < 0$, so

$$B[W_{\text{new}}] = B[W_{\min}] + \lambda B[S_{\mathcal{A}}] < B[W_{\min}] \tag{.10}$$

which is a contradiction. So, a finite area $\mathcal{A}$ where $W_{\min}(x,y) > 0$ does not exist, which can only be explained if $W_{\min}(x,y)$ are combinations of δ-functions; that is, the optimal transformation $\mathcal{T}$ is function-like mapping from X to Y where (almost all) the extra randomness are gone.

Now, assuming $W_{\min}$ takes the form $W_{\min} = \delta(y - H(x))$, which is equivalent to saying that the transformation is a function $y = H(x)$. Then the problem simplifies to finding a function $H_{\min}$ which minimizes the sum (for illustrative purposes we use summation here instead of integration)

$$B[H] = \lim_{N\to\infty} \sum_i (x_i - H(x_i))^2/N, \tag{.11}$$

with the requirement that x_i's are from distribution f and $H(x_i)$'s will conform to distribution g.

We want to show that $H_{\min}(x)$ must be a **monotonicly non-decreasing** function: because if there exists a pair

$$x_1 > x_2 \;\; \text{but} \;\; H(x_1) < H(x_2)$$

[3] For instance in a rectangular area $(x1,y1)-(x2,y2)$, we can pick $S_{\mathcal{A}}(x,y) = \sin(2\pi n_x \frac{x-x_1}{x_2-x_1})\sin(2\pi n_y \frac{y-y_1}{y_2-y_1})$ where n_x, n_y are non-zero integers.

we can construct an $\tilde{H}(x)$ with x_1, x_2 exchanged

$$\tilde{H}(x) = \begin{cases} H(x) & (x \neq x_1, x \neq x_2) \\ H(x_2) & (x = x_1) \\ H(x_1) & (x = x_2) \end{cases} \tag{.12}$$

without influencing g, however

$$\begin{aligned} & (x_1 - \tilde{H}(x_1))^2 + (x_2 - \tilde{H}(x_2))^2 \\ = & (x_1 - H(x_2))^2 + (x_2 - H(x_1))^2 \\ = & (x_1 - H(x_1))^2 + (x_2 - H(x_2))^2 - (x_1 - x_2)(H(x_2) - H(x_1)) \\ < & (x_1 - H(x_1))^2 + (x_2 - H(x_2))^2 \end{aligned}$$

so $B[\tilde{H}] < B[H]$, which is a contradiction.

Thus there must be a unique, one-to-one relationship between x and y. And because of the basic requirement,

$$dP = f(x)dx = g(y)dy \tag{.13}$$

since any small interval $(x, x + dx)$ is uniquely and deterministicly mapped into $(y, y + dy)$ by the optimal transformation. So if we integrate from $x, y \to -\infty$ where $P = 0$, there must be

$$\int_{-\infty}^{x} f(\xi)d\xi = \int_{-\infty}^{y} g(\xi)d\xi$$

which is the $\mathcal{T}_3$ transformation.

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