Monte Carlo methods for Neutron Transport

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Outline

– Monte Carlo for the diffusion equation and some relatives (simulating random walks, which obey diffusion-like equations)

– Monte Carlo for the Neutron Transport Equation (simulating the motion of “fictitious” neutrons)

Monte Carlo diffusion

Numerical solution of PDEs…

"Density" $\rho = \rho(x,t), \qquad x \in \mathbb{R}^d, \qquad t \geq 0$

Solve $\partial_t \rho = \triangle \rho$ given $\rho(x,0)$

Or, solve $\partial_t \rho = \nabla \cdot (\nabla \rho - F\rho)$ given $\rho(x,0)$ and $F = F(x)$

[Maybe you know… for a particle obeying a stochastic differential equation

$$\mathrm{d}x = F\mathrm{d}t + \sqrt{2}\,\mathrm{d}B_t$$

… the probability density function ρ for its position solves the PDE above (Fokker-Planck equation)]

Assume normalisation $\int \rho(x,0)\mathrm{d}x = 1$ [equation is linear]

Monte Carlo diffusion

$$\partial_t \rho = \nabla \cdot (\nabla \rho - F\rho) \qquad \mathrm{d}x = F\mathrm{d}t + \sqrt{2}\,\mathrm{d}B_t$$

A possible method for solving this equation:

Initialise a particle at some point x_0, set time $t = 0$

Move it to x_0+Δ with $\Delta = Fh + B$, where B is Gaussian distributed with variance 2h. Increment time by h

Repeat until time reaches end of required interval

Repeat the whole thing many times, with initial x_0 distributed as $\rho(x,0)$

Can prove:

As $h \to 0$, can estimate $\int f(x)\rho(x,t)\mathrm{d}x$ as $\frac{1}{N}\sum_i f(x_i(t))$

(The sum runs over the N simulated particles)

Estimator is unbiased in the limit, variance of estimator ~ $(1\ /\ N)$

Can also show: many similar methods are possible and also work…

Monte Carlo PDEs

General: “guess” a stochastic process which provides estimators of (some aspect of) a solution of a PDE.

How to guess the process?

Physicist approach: Where did the PDE come from?

The neutron transport equation (NTE) arises as a “hydrodynamic” description of the motion of neutrons.

This equation is independent of many details of the neutron motion (cf: diffusion equation applies to very many different physical systems)

We can use a simple stochastic (MC) description of the neutron motion, as long as it gives behaviour consistent with the NTE

Neutron Transport

Suggestion:

Think of the MC method as a *simulation* of a *fictitious process* that obeys the neutron transport equation (NTE)
Proving that the fictitious process obeys the NTE should be the same as the derivation of the NTE…

This means that whatever quantities are relevant for the neutrons can be evaluated directly from the fictitious process,

Neutron Transport

What is different to the diffusing case?

Neutrons have velocities (advective terms in PDE),
and they scatter (scattering terms)

… no more random walks

Neutrons appear from sources and fission (source terms)
disappear (from absorption)

… particles not conserved

We want to solve for a steady state (no explicit time dependence)

… slightly more subtle…

Note, equation is still linear: no interactions between neutrons,
can simulate them “one at a time”

Transport / scattering

$$\frac{1}{v}\partial_t \Psi = (\mathcal{S} - \mathcal{T})\Psi$$

[similar to Scheben thesis, 4.3.2]

Stochastic method:

Choose an initial position and velocity according to $\Psi(t=0)$

Move an exponentially distributed distance x with mean (1/λ) along the velocity direction. Increment time by x/v.

Decide whether to scatter or be absorbed *(see later)*

If absorbed, remove the particle

If scattered, choose a new velocity

Repeat until the particle has disappeared or we reach the end of our time interval

Repeat for many initial positions

(cross section)

$$\lambda = \frac{1}{n_{\mathrm{obstacle}}\sigma_{\mathrm{obstacle}}}$$

λ : mean distance to collision

n_{obstacle} : number density of obstacles

$\sigma_{\mathrm{obstacle}}$: ‘cross section’ of obstacle

(sum σ over different kinds of obstacle)

Transport / scattering

$$\frac{1}{v}\partial_t \Psi = (\mathcal{S} - \mathcal{T})\Psi$$

[similar to Scheben thesis, 4.3.2]

This procedure provides:

The joint velocity/position distribution of surviving neutrons

The time taken for the neutrons to be absorbed

The spatial distribution of absorption/scatter events

… etc…

Proof that this process solves the NTE… non-trivial exercise…

Scatter or absorb?

$$\frac{1}{v}\partial_t \Psi = (\mathcal{S} - \mathcal{T})\Psi$$

[similar to Scheben thesis, 4.3.2]

It is clear that the neutron can either be scattered or absorbed; if it is scattered, it has different probabilities of different final directions etc. Whatever these probabilities are, they set the “kernels” in the NTE

Pick a random number ξ uniformly in (0,1)

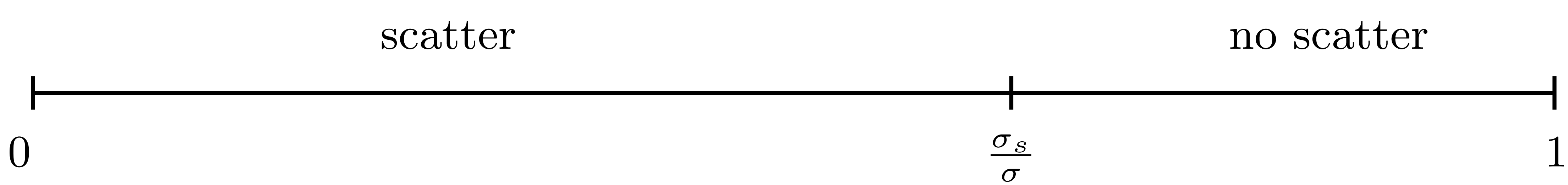

Figure 4.3: *If $\xi \leq \sigma_s/\sigma$ the collision event is a scatter.*

(The distance x that we calculated before is the distance to the first of two independent events… “first scatter” or “first absorption”. more later…)

Inhomogeneous setting

$$\frac{1}{v}\partial_t \Psi = (\mathcal{S} - \mathcal{T})\Psi$$

[similar to Scheben thesis, 4.3.2]

Just one caveat:

We assumed all rates (kernels) constant in space
(when calculating our random distance x)

If the neutron leaves the reactor before any event happens,
we should just remove it from the “simulation”

If the neutron moves into a different kind of material before its next event, we need to stop it at the point where it enters, and recalculate the time to the next event…

Fission and sources

Sources:

Since we treat neutrons one at a time, we can account for sources by simply choosing our insertion points according to the source distribution Q

Fission:

To treat fission, we add in the relevant contribution to the cross section σ, and an extra segment to our "choice of process" line.

If we choose fission, we should use the fission point (and time) as the next starting point for our "loop" over neutrons (or put it into a list of starting points to be considered)

If this list gets out of control, the reactor is supercritical…
need some method to deal with this (reduce fission rate?)

[? talk to Andreas Kyprianou]

MC a la "Gillespie algorithm"

[? talk to Kit Yates]

There are many MC methods similar to the one I have described

The basic idea is that any of several events may happen, all are independent, we need to pick one of them

The method is:

Define $A = \sum_i r_i$ where r_i is the *rate* for event i

Pick an exponentially distributed random number with mean $1/A$, increment the time by this amount

Choose event i to happen with probability r_i/A ("choice of process" line)

To get to the NTE method, we go from a *time between events* to a *distance between events*… this is ok since we know the velocity

Conclusions

The derivation of the NTE is based on *general* features of neutrons' behaviour, independent of microscopic details.

If we can find a "fictitious" stochastic process which obeys the NTE, then simulations of this process can give physical quantities of interest.

We *can* find such a process, it involves independent neutrons that evolve "one at a time" (related to linearity of the equation).

To rationalise the stochastic aspect of the MC process, we can think of a large population of neutrons from which a deterministic PDE appears through a law of large numbers (at each spatial location).