Derivation of the neutron transport equation from a spatial branching Markov nuclear fission process

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Abstract

We give a stochastic derivation of the neutron transport equation from a stochastic process that resembles the physical process of nuclear fission. Therewith we suggest a new Monte-Carlo simulation technique using spherical time-stepping. None of the arguments are rigorous as they require semi-martingale calculus to firm them up. But they can be made rigorous. Our computations start with a Brownian warm up, but this is more from an exemplary perspective rather than through necessity.

The probabilistic literature on this topic is rather sketchy. I have done some basic googling and found that there seems to be a little probabilistic literature in recent times, however, there has been some older work looking at probabilistic derivations of the neutron transport equation. See for example Pazy and Rabinowitz [**?**], Lewins [2] or Harris [1]. A more recent work is Maire and Talay [3].

Key words: Neutron transport.

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1 Brownian semi-group

To set the scene, let us review some concepts from the theory of Brownian motion which we will appeal to in a conceptual way, but for more general Markov processes, in due course. Suppose that, for some constant $\sigma > 0$, we write $\{\sigma B_t : t \geq 0\}$ with probabilities $\mathbb{P}_x$, $x \in \mathbb{R}^d$ is a d-dimensional Brownian motion with volatility σ. The infinitesimal movements of Brownian motion with volatility σ are intimately associated to the Laplacian operator $\sigma^2\triangle/2$. More formally, the semi-group that describes the innovations of Brownian motion is a solution to the heat equation in the following sense. Suppose that f is a bounded, non-negative measurable function. Define, for $x \in \mathbb{R}^d$ and $t \geq 0$,

$$u_f(x,t) = \mathbb{E}_x[f(\sigma B_t)] = \int_{\mathbb{R}^d} f(y)\Phi_t((y-x)/\sigma)\mathrm{d}y,$$

where we have taken account of the stationary and independent increments of Brownian motion so that

$$\Phi_t(z) = \frac{1}{(2\pi t)^{d/2}}\exp\{-||z||^2/2t\}, \qquad z \in \mathbb{R}^d$$

is the density of B_t under $\mathbb{P}_0$; or said another way, $\mathbb{P}_x(B_t \in \mathrm{d}y) = \Phi_t(y-x)\mathrm{d}y$. Note that a standard computation shows that

$$\frac{\partial}{\partial t}\Phi_t = \frac{\sigma^2}{2}\triangle\Phi_t \qquad \text{on } \mathbb{R}^d,$$

which is to say that Φ_t is the classical solution to the heat equation. Dominated convergence can now be used to confirm that

$$\begin{aligned}
\frac{\partial}{\partial t}u_f(x,t) &= \int_{\mathbb{R}^d} f(y)\frac{\partial}{\partial t}\Phi_t(y-x)\mathrm{d}y \\
&= \int_{\mathbb{R}^d} f(y)\frac{\sigma^2}{2}\triangle_y\Phi_t((y-x)/\sigma)\mathrm{d}y \\
&= \int_{\mathbb{R}^d} f(y)\frac{\sigma^2}{2}\triangle_x\Phi_t((y-x)/\sigma)\mathrm{d}y \\
&= \frac{1}{2}\triangle u_f(x,t).
\end{aligned}$$

In addition to this we also note that there is an initial condition

$$u_f(x,0) = \mathbb{E}_x[f(\sigma B_0)] = f(x).$$

More generally, if we were to replace the Brownian motion by a Brownian motion with directional drift $\boldsymbol{a} \in \mathbb{R}^d$, then we would see that

$$u_f(x,t) = \mathbb{E}_x[f(\sigma B_t + \boldsymbol{a}t)] = \int_{\mathbb{R}^d} f(y)\Phi_t((y-x-\boldsymbol{a}t)/\sigma)\mathrm{d}y.$$

Following the computations through as before, this would result in u solving the PDE

$$\frac{\partial}{\partial t}u_f = \frac{\sigma^2}{2}\triangle u + \boldsymbol{a}\cdot\nabla u_f$$

with initial condition $u_f(x,0) = f(x)$.

2 Markov modulated linear diffusion semi-group

Now let us consider something a little more exotic. We are going to introduce two a new feature to the Brownian model. We are going to modulate the drift of the Brownian motion according to the behaviour of an associated Markov Chain. To this end, let us write $\{J_t : t \geq 0\}$ for the Markov chain with state space $\{1,\cdots,n\}$ intensity matrix $\boldsymbol{Q}$. The Pair $\{(B_t, J_t), t \geq 0\}$ are jointly Markovian and we write its probabilities by $\mathbb{P}_{(x,i)}$, $x \in \mathbb{R}^d$, $i \in \{1,\cdots,n\}$. We are interested in a process $\{X_t : t \geq 0\}$ which is a functional of this pair with dynamics given by

$$\mathrm{d}X_t = \sigma\mathrm{d}B_t + \boldsymbol{a}_{J_t}\mathrm{d}t, \qquad t \geq 0,$$

where $\boldsymbol{a}_i$, $i = 1, \cdots, n$ are the different drifts added to B when J is in each of its states.

Now we need to consider the function $u : \mathbb{R}^d \times \{1, \cdots, n\} \times [0, \infty) \mapsto \mathbb{R}^+$ via

$$u_f(x, i, t) = \mathbb{E}_{(x,i)}[f(X_t)],$$

where f is now a bounded, non-negative measurable function on $\mathbb{R}^d$. In order to write down the dynamics of $u_f(x, i, j, t)$, either a change occurs due to a Brownian movement or due to a change of state in the chain. We thus have the following, (formally, we need semi-martingale calculus to write the following down)

$$\frac{\partial}{\partial t} u_f(x, i, t) \quad = \quad \frac{1}{2} \triangle u_f(x, i, t) + \boldsymbol{a}_i \cdot \nabla u_f(x, i, t) + \sum_k \boldsymbol{Q}_{ik} u_f(x, k, t).$$

Recalling that we can write the rates $\boldsymbol{Q}_{ij}$, for $i \neq j$, in the form $|\boldsymbol{Q}_{ii}| \times \boldsymbol{Q}_{ij} / |\boldsymbol{Q}_{ii}|$, where one understands $|\boldsymbol{Q}_{ii}|$ as the rate at which the chain moves out of state i and $\Theta_S(i, j) := \boldsymbol{Q}_{ij} / |\boldsymbol{Q}_{ii}|$ is the probability that it moves to state j, we have

$$\frac{\partial}{\partial t} u_f(x, i, t) = \frac{\sigma^2}{2} \triangle u_f(x, i, t) + \boldsymbol{a}_i \cdot \nabla u_f(x, i, t) + |\boldsymbol{Q}_{ii}| \int_{\{1, \cdots, n\}} u_f(x, k, t) \Theta_S(i, \mathrm{d}\{k\}). \quad (1)$$

As usual we have that $u_f(x, i, 0) = \mathbb{E}_{(x,i)}[f(X_0)] = f(x)$. We call the kernel $\Theta_S(i, \mathrm{d}\{k\})$ the scattering kernel as it dictates the random change of direction in the drift of the underlying particle.

As a final note in this section, consider what happens as we let $\sigma \to 0$. The process we are considering moves in straight lines in-between the moments that the chain J changes state. Whenever it changes state, say from i to j, the particle that this process models will change from moving in direction $\boldsymbol{a}_i$ to moving in direction $\boldsymbol{a}_j$. The semi-group equation in that case becomes simply

$$\frac{\partial}{\partial t} u_f(x, i, t) = \boldsymbol{a}_i \cdot \nabla u_f(x, i, t) + |\boldsymbol{Q}_{ii}| \int_{\{1, \cdots, n\}} u_f(x, k, t) \Theta_S(i, \mathrm{d}\{k\})$$

with initial condition $u_f(x, i, 0) = f(x)$.

3 Markov modulated branching linear diffusion.

Let us now introduce branching to the Markov modulated Brownian system. At time 0 we issue a Markov modulated linear diffusion, X, from $x \in \mathbb{R}^d$ with modulation i. After an independent and exponentially distributed random time, with rate $q > 0$, a clock rings. At this instance, if the particle has type k, it produces Δ_{kj} offspring of type j where Δ_{kj} is a random variable which is valued in $\{0, 1, 2, 3, \cdots\}$. Each of these individuals move off from their spatial point of birth and execute an **independent** copy of their parent's behaviour albeit that they may now be of a different type. The process thus proceeds to grow. It is important to note that each individual born uses an independent copy of X, an independent clock and independent copies of the variables Δ_{ij}.

Suppose that at time t we have N_t particles, and they are to be found at positions $X_k(t)$ and of type $J_k(t)$, for $k = 1, \cdots, N_t$. We can describe the system at time t by the random measures on $\mathbb{R}^d \times \{1, \cdots, n\}$ by

$$Z_t(\cdot) = \sum_{k=1}^{N_t} \delta_{(X_k(t), J_k(t))}(\cdot), \qquad i = 1, \cdots, n,$$

where $\delta_{(x,i)}(A) = 1$ if $(x, i) \in A$ and zero otherwise. With this notation in mind, we write $\mathbf{P}_{\delta_{(x,i)}}$ for the law of the branching process issued from a single particle of type i at position x. More generally, if we issue the branching process from a configuration $\nu = \sum_\ell \delta_{x_\ell, j_\ell}$ then its law is written $\mathbf{P}_\nu$.

For non-negative, bounded and measurable functions $f : \mathbb{R}^d \times \{1, \cdots, n\} \mapsto \mathbb{R}^+$, we are interested in

$$v_f(x, i, t) = \mathbf{E}_{\delta_{(x,i)}}[\langle f, Z_t \rangle],$$

where

$$\langle f, Z_t \rangle := \int_{\mathbb{R}^d \times \{1, \cdots, n\}} f(y) Z_t(\mathrm{d}y) = \sum_{i=1}^{N_t} f(X_k(t), J_k(t)).$$

Note that, as usual, $v_f(x, i, 0) = f(x, i)$. To write down a PDE for $v_f(x, i, t)$, we can condition on the first birth event, which occurs at time, say, T_1. Specifically, we have

$$\begin{aligned} v_f(x, i, t) &= \mathbb{E}_{(x,i)}[f(X_t)\mathbf{1}_{(T_1 > t)}] + \mathbf{E}_{\delta_{(x,i)}}[\langle f, Z_t \rangle \mathbf{1}_{(T_1 \le t)}] \\ &= \mathrm{e}^{-qt}\mathbb{E}_{(x,i)}[f(X_t)] + \mathbf{E}_{\delta_{(x,i)}}\left[\int_0^t q\mathrm{e}^{-qs} \sum_k m_{J_s k} \mathbb{E}_{(X_s,k)}[\langle f, \tilde{Z}_{t-s} \rangle] \mathrm{d}s\right] \\ &= \mathrm{e}^{-qt} u_f(x, i, t) + \sum_k \int_0^t q\mathrm{e}^{-qs} \mathbb{E}_{(x,i)}\left[m_{J_s k} v_f(X_s, k, t-s)\right] \mathrm{d}s, \end{aligned}$$

where $\tilde{Z}^{(j)}$ is an independent copy of Z and $m_{ij} = \mathbb{E}[\Delta_{ij}]$. Let us assume that everything is smooth enough, especially the initial function f. Differentiating in t and setting t to 0, remembering (1), we get

$$
\begin{aligned}
\frac{\partial}{\partial t} v_f(x,i,0+) &= -q u_f(x,i,0+) + \frac{\partial}{\partial t} u_f(x,i,0+) \\
&\quad + \sum_k q \mathbb{E}_{(x,i)} \left[m_{J_t k} v_f(X_t,k,0) \right] \Big|_{t\downarrow 0} \\
&\quad + \sum_k \int_0^t q \mathrm{e}^{-qs} \mathbb{E}_{(x,i)} \left[m_{J_s k} \frac{\partial}{\partial t} v_f(X_s,k,t-s) \right] \mathrm{d}s \Big|_{t\downarrow 0} \\
&= -q f(x,i) + \frac{\sigma^2}{2} \triangle f(x,i) + \boldsymbol{a}_i \cdot \nabla f(x,i) \\
&\quad + |\boldsymbol{Q}_{ii}| \int_{\{1,\cdots,n\}} f(x,k) \Theta_S(i,\mathrm{d}\{k\}) + \sum_k q m_{ik} f(x,k) \\
&= q \int_{\{1,\cdots,n\}} f(x,k) \Theta_T(i,\mathrm{d}\{k\}) - q f(x,i) + |\boldsymbol{Q}_{ii}| \int_{\{1,\cdots,n\}} f(x,k) \Theta_S(i,\mathrm{d}\{k\}) \\
&\quad + \frac{\sigma^2}{2} \triangle f(x,i) + \boldsymbol{a}_i \cdot \nabla f(x,i). \qquad (2)
\end{aligned}
$$

where the discrete measure $\Theta_T(i,\mathrm{d}\{k\}) = m_{ik}$ is called the **transport kernel**. Now note that

$$
v_f(x,i,t+s) = \mathbf{E}_{\delta_{(x,i)}}[\langle f, Z_{t+s}\rangle] = \mathbf{E}_{\delta_{(x,i)}}[\mathbf{E}_{Z_s}\langle f, \tilde{Z}_t\rangle] = \mathbf{E}_{\delta_{(x,i)}}[\langle v_f(\cdot,t), Z_s\rangle] = v_{v_f(\cdot,\cdot,t)}(x,i,s),
$$

where $\tilde{Z}$ is an independent copy of Z. It follows from (2) that

$$
\frac{\partial}{\partial t} v_f(x,i,t) = \frac{\partial}{\partial s} v_{v_f(\cdot,\cdot,t)}(x,i,s) \Big|_{s\to 0}
$$

and we are left with the **transport equation**

$$
\begin{aligned}
\frac{\partial}{\partial t} v_f(x,i,t) &= q \int_{\{1,\cdots,n\}} v_f(x,k,t) \Theta_T(i,\mathrm{d}\{k\}) - q v_f(x,i,t) \\
&\quad + |\boldsymbol{Q}_{ii}| \int_{\{1,\cdots,n\}} v_f(x,k) \Theta_S(i,\mathrm{d}\{k\}) + \frac{\sigma^2}{2} \triangle v_f(x,i,t) + \boldsymbol{a}_i \cdot \nabla v_f(x,i,t)
\end{aligned}
$$

with initial condition $v_f(x,i,0) = f(x,i)$. Finally, if we 'turn off' the Brownian motion, by taking $\sigma = 0$, then we get a transport equation of the form

$$
\begin{aligned}
\frac{\partial}{\partial t} v_f(x,i,t) &= q \int_{\{1,\cdots,n\}} v_f(x,k,t) \Theta_T(i,\mathrm{d}\{k\}) - q v_f(x,i,t) \\
&\quad + |\boldsymbol{Q}_{ii}| \int_{\{1,\cdots,n\}} v_f(x,k) \Theta_S(i,\mathrm{d}\{k\}) + \boldsymbol{a}_i \cdot \nabla v_f(x,i,t). \qquad (3)
\end{aligned}
$$

This last transport equation corresponds to particles which move in straight lines and, at random times, according to the inter arrival times of their own personal copy of a Markov chain, they change direction. There are only n possible vectorial directions in which to travel however.

4 Nuclear fission and the neutron transport equation: Exercise for students!

In this section, we make the final step to the neutron transport equation as used by Ivan, Paul Smith and others. We need to allow our modulating Markov chain to have an infinite number of states corresponding to the infinite number of possible scattering directions that a particle moving in a straight line will redirect to, as well as the infinite number of possible directions one may send off particles when undergoing fission. Once we enrich he type-space to be infinite (corresponding to all scattering angles) then we also need to be more careful about how we write the measures Θ_S and Θ_T as they now become proper integrals rather than just sums.

In our branching model, particles (neutrons) now move about in $\mathbb{R}^3$. We replace the type space $\{1, \cdots, n\}$ by $\mathbb{S}_2$, meaning the surface of the unit sphere in 3 dimensions. We denote the type by Ω and we think of it as a velocity i.e. particles always move at speed 1 but the direction is determined by the vector $\Omega \in \mathbb{S}_2$. Moreover:

- If a particle is positioned at $x \in \mathbb{R}^3$ and has velocity $\Omega \in \mathbb{S}_2$, then, at rate $\beta_S(x, \Omega)$, it will scatter off another atom and its new velocity is determined by a probabilistic kernel $\Theta_S(x, \Omega, \mathrm{d}\Omega')$, where $\Omega' \in \mathbb{S}_2$ is the new velocity. (By analogy, we are replacing the drift $\boldsymbol{a}_i$, for type $i \in \{1, \cdots, n\}$ by the type Ω itself in $\mathbb{S}_2$, i.e. "$\boldsymbol{a}_\Omega = \Omega$".)

- If a particle is positioned at $x \in \mathbb{R}^3$ and has velocity $\Omega \in \mathbb{S}_2$, then at rate $\beta_T(x, \Omega)$, it will smash an atom releasing further neutrons, i.e. it undergoes fission. The number of neutrons it releases is random, as is their velocities. To describe the neutron release at fission, we suppose that there is a family of random point processes on $\mathbb{S}_2$, say $\Delta_{(x,\Omega)}(\mathrm{d}\Omega')$ whose intensity depends on (r, Ω) and is written $\Theta_T(x, \Omega, \mathrm{d}\Omega')$. To be more precise $\Delta_{(x,\Omega)}(\mathrm{d}\Omega')$ is nothing more than a collection of random points scattered on the sphere $\mathbb{S}_2$ such that for a non-negative, bounded measurable test function $f : \mathbb{S}_2 \mapsto \mathbb{R}^+$,
$$E\left[\int_{\mathbb{S}_2} f(\Omega')\Delta_{(x,\Omega)}(\mathrm{d}\Omega')\right] = \int_{\mathbb{S}_2} f(\Omega')\Theta_T(x, \Omega, \Omega').$$

Following the logic in the preceding sections, can you now derive the full probabilistic transport equation which extends (4)?:

$$\begin{aligned}\frac{\partial}{\partial t}\psi(x, \Omega, t) &= \beta_T(x, \Omega)\int_{\mathbb{S}_2} \psi(x, \Omega', t)\Theta_T(x, \Omega, \Omega') - \beta_T(x, \Omega)\psi(x, \Omega, t)\\ &\quad +\beta_S(x, \Omega)\int_{\mathbb{S}_2} \psi(x, \Omega', t)\Theta_S(x, \Omega, \mathrm{d}\Omega') + \Omega \cdot \nabla\psi(x, \Omega, t),\end{aligned}$$

with boundary condition $\psi(x, \Omega, 0) = f(x, \Omega)$ given.

To be more precise, by describing the configuration of particles at time t by a random counting measure of particle in position and velocity space,

$$Z_t = \sum_{i=1}^{N_t} \delta_{(X_i(t), \Omega_i(t))},$$

where $\{(X_i(t), \Omega_i(t)) : i = 1, \cdots, N_t\}$ are the random positions and velocities of the random number of particles N_t in the system at time t, one should look at the evolution of

$$\psi(x, \Omega, t) = \mathbb{E}_{\delta_{(x,\Omega)}}[\langle f, Z_t \rangle],$$

Up until this point, there have been no boundary restrictions in space. That is to say, particles have been free to roam over the whole of $\mathbb{R}^3$. One may also develop this theory with restrictions on the domain of the particles to e.g. reactor cores or hospital equipment. In that case, more boundary conditions will be needed.

5 Possible PhD directions from the probabilistic side

- Develop the potential analysis of the transport equation i.e. look for positive eigenfunctions and what they and their eigenvalues mean. Martingales will almost certainly come into play. Positive martingales always converge, what does this say about the system? This will be particularly pertinent when looking at branching systems on bounded domains. In diffusion theory there is a concept of the generalised principle eigen value. Here it must also have a meaning and will be related to the growth of particles and the criticality of the system.

- The transport equation is what I would call the linear semigroup equation associated to the branching particle system. There is also a non-linear transport equation, which seems not to have been mentioned by Ivan et al. or indeed any of the literature that I can find. This non-linear equation can be built by considering functionals of the form

  $$\Psi(x, \Omega, t) = \mathbb{E}_{\delta_{(x,\Omega)}}\left[\mathrm{e}^{-\langle f, Z_t \rangle}\right].$$

  This equation will also have positive eigenfunction solutions which will allow one to build positive martingales which will also have limits. What does this say about the system?

- I also have an idea about Monte-Carlo simulation of particles by using a sphere-stepping technique that is common in diffusion theory (apparently). This would require one to be able to characterise the distribution of the collection of particles in the system when they first exit a given spherical domain.

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