Stochastic Analysis of the Neutron Transport Equation

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Neutron Flux

- **Neutron flux** is a measure of the intensity of neutron radiation, determined by the rate of flow of neutrons.
- The neutron flux value is calculated as:

$$\text{neutron density } (n) \times \text{neutron velocity } (v)$$

  where n is measured in (# neutrons)/cm^3 and v is measured in distance cm/s
- Consequently, neutron flux (nv) is measured in (# neutrons)/cm^2/s.
- We want to describe neutron flux as a function of spatial position and time in complex domains:

$$\psi_g(r, v, t), \qquad r \in D_0 \subseteq \mathbb{R}^d, v \in V := [v_{\mathtt{min}}, v_{\mathtt{max}}] \times \mathbb{S}_2,$$

  for $0 < v_{\mathtt{min}} < v_{\mathtt{max}} < \infty$.
- Sometimes neutron flux is also taken as a function of energy E, but in many settings, this is related to velocity via the relation

$$|v| = \sqrt{\frac{2E}{m}},$$

  where m is neutron.
- More generally the flux of any radioactive particle can be seen in the same way: α, β, γ radiation.

Neutron Transport Equation

Neutron flux is thus identified as $\Psi_g : D \times V \to [0, \infty)$, which solves the integro-differential equation

$$\frac{\partial \Psi_g}{\partial t}(t, r, \upsilon) + \upsilon \cdot \nabla \Psi_g(t, r, \upsilon) + \sigma(r, \upsilon)\Psi_g(t, r, \upsilon)$$
$$= Q(r, \upsilon, t) + \int_V \Psi_g(r, \upsilon', t)\sigma_{\mathtt{s}}(r, \upsilon')\pi_{\mathtt{s}}(r, \upsilon', \upsilon)\mathrm{d}\upsilon' + \int_V \Psi_g(r, \upsilon', t)\sigma_{\mathtt{f}}(r, \upsilon')\pi_{\mathtt{f}}(r, \upsilon', \upsilon)\mathrm{d}\upsilon',$$

where the different components are measurable in their dependency on (r, υ) and are explained as follows:

$\sigma_{\mathtt{s}}(r, \upsilon')$: the rate at which scattering occurs from incoming velocity υ',

$\sigma_{\mathtt{f}}(r, \upsilon')$: the rate at which fission occurs from incoming velocity υ',

$\sigma(r, \upsilon)$: the sum of the rates $\sigma_{\mathtt{f}} + \sigma_{\mathtt{s}}$ and is known as the cross section,

$\pi_{\mathtt{s}}(r, \upsilon', \upsilon)\mathrm{d}\upsilon'$: the scattering yield at velocity υ from incoming velocity υ', satisfying $\pi_{\mathtt{s}}(r, \upsilon, V) = 1$,

$\pi_{\mathtt{f}}(r, \upsilon', \upsilon)\mathrm{d}\upsilon'$: the average neutron yield at velocity υ from fission with incoming velocity υ', satisfying $\pi_{\mathtt{f}}(r, \upsilon, V) < \infty$

$Q(r, \upsilon, t)$: non-negative source term. (Immediately remove the source term $Q = 0$)

We will assume that all quantities are uniformly bounded away from zero and infinity.

Boundary conditions

- Boundary conditions which represent 'fission containment'

$$\begin{cases} \Psi_g(0, r, v) = g(r, v) & \text{for } r \in D, v \in V, \text{ (initial condition)} \\ \Psi_g(t, r, v) = g(r, v) = 0 & \text{for } r \in \partial D \text{ if } v \cdot \mathbf{n}_r < 0, \text{ (neutron annihilation)} \end{cases}$$

- $\mathbf{n}_r$ is the outward facing normal of D at $r \in \partial D$
- $g : D \times V \to [0, \infty)$ is a bounded, measurable function which we will later assume has some additional properties.

(Forward →Backwards) Neutron Transport Equation

- Hence, with similar computations, this tells us that, for $f, g \in L^2(D \times V)$,

$$\langle f, (\mathtt{T} + \mathtt{S} + \mathtt{F})g \rangle = \langle (\mathcal{T} + \mathcal{S} + \mathcal{F})f, g \rangle,$$

where

$$\begin{cases} \mathcal{T}f(r,\upsilon) & := \upsilon \cdot \nabla f(r,\upsilon) & \text{(backwards transport)} \\ \mathcal{S}f(r,\upsilon) & := \sigma_{\mathtt{s}}(r,\upsilon) \int_V f(r,\upsilon')\pi_{\mathtt{s}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon' - \sigma_{\mathtt{s}}(r,\upsilon)f(r,\upsilon) & \text{(backwards scattering)} \\ \mathcal{F}f(r,\upsilon) & := \sigma_{\mathtt{f}}(r,\upsilon) \int_V f(r,\upsilon')\pi_{\mathtt{f}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon' - \sigma_{\mathtt{f}}(r,\upsilon)f(r,\upsilon) & \text{(backwards fission)} \end{cases}$$

- This leads us to the so called *backwards neutron transport equation* (which is also known as the *adjoint neutron transport equation*) given by the Abstract Cauchy Problem on $L^2(D \times V)$,

$$\frac{\partial \psi_g}{\partial t}(t,\cdot,\cdot) = (\mathcal{T} + \mathcal{S} + \mathcal{F})\psi_g(t,\cdot,\cdot)$$

with additional boundary conditions

$$\begin{cases} \psi_g(0,r,\upsilon) = g(r,\upsilon) & \text{for } r \in D, \upsilon \in V, \\ \psi_g(t,r,\upsilon) = 0 & \text{for } r \in \partial D \text{ if } \upsilon \cdot \mathbf{n}_r > 0. \end{cases}$$

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Underlying stochastics (leading to Monte-Carlo)

- Backwards equation lends itself well to stochastic representation in the L_2 sense,

$$\frac{\partial \psi_g}{\partial t}(t,r,\upsilon) = \upsilon \cdot \nabla \psi_g(t,r,\upsilon) - \sigma(r,\upsilon)\psi_g(t,r,\upsilon) + \sigma_{\mathtt{s}}(r,\upsilon)\int_V \psi_g(r,\upsilon',t)\pi_{\mathtt{s}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon' + \sigma_{\mathtt{f}}(r,\upsilon)\int_V \psi_g(r,\upsilon',t)\pi_{\mathtt{f}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon',$$

- The physical process of fission is a Markov-additive branching process (*neutron branching process*).
- Represented by a configuration of physical location and velocity of particles in $D \times V$, say $\{(r_i(t), \upsilon_i(t)) : i = 1, \ldots, N_t\}$, where N_t is the number of particles alive at time $t \geq 0$.
- Represent as a process in the space of the atomic measures

$$X_t(A) = \sum_{i=1}^{N_t} \delta_{(r_i(t),\upsilon_i(t))}(A), \qquad A \in \mathcal{B}(D \times V),\ t \geq 0,$$

where δ is the Dirac measure, define on $\mathcal{B}(D \times V)$, the Borel subsets of D.

- Then the stochastic representation of the backwards NTE is nothing more than

$$\phi_t[g](r,\upsilon) = \mathbb{E}_{\delta_{(r,\upsilon)}}[\langle g, X_t\rangle] = \mathbb{E}_{\delta_{(r,\upsilon)}}\left[\sum_{i=1}^{N_t} g(r_i(t),\upsilon_i(t))\right], \qquad t \geq 0.$$

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Neutron branching process

- A particle position at r with velocity υ (configruration (r, υ)) will continue to move along the trajectory $r + \upsilon t$, until one of the following things happens.
- The particles that leave the physical domain D are killed.
- For a neutron with configuration (r, υ), if $T_{\mathtt{s}}$ is the random time that scattering may occur, then

$$\Pr(T_{\mathtt{s}} > t) = \exp\left\{-\int_0^t \sigma_{\mathtt{s}}(r + \upsilon t, \upsilon))\mathrm{d}s\right\}.$$

- When scattering occurs at space-velocity (r, υ), the new velocity is selected independently with probability $\pi_{\mathtt{s}}(r, \upsilon, \upsilon')\mathrm{d}\upsilon'$.
- For a neutron with configuration (r, υ), if $T_{\mathtt{f}}$ is the random time that scattering may occur, then independently of any other physical event that may affect the neutron,

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- When fission occurs at location $r \in \mathbb{R}^d$ from a particle with incoming velocity $\upsilon \in V$, the quantity $\pi_{\mathtt{f}}(r, \upsilon, \upsilon')\mathrm{d}\upsilon'$ describes the average number of particles released from nuclear fission with outgoing velocity in the infinitesimal neighbourhood of υ'.
- Note, the possibility that $\Pr(N = 0) > 0$ is possible, which will be tantamount to a fission taking place in which no neutrons are released. Experiments show that this is a possible outcome during a fission event.

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Mild equation

- Define for $g \in L^+_\infty(D \times V)$, the (physical process) expectation semigroup

$$\phi_t[g](r, \upsilon) := \mathbb{E}_{\delta_{(r,\upsilon)}}[\langle g, X_t \rangle], \qquad t \geq 0, r \in D, \upsilon \in V,$$

and the advection semigroup

$$\mathtt{U}_t[g](r, \upsilon) = g(r + \upsilon t, \upsilon)\mathbf{1}_{\{t < \kappa^D_{r,\upsilon}\}}, \qquad t \geq 0.$$

where $\kappa^D_{r,\upsilon} := \inf\{t > 0 : r + \upsilon t \notin D\}$.

Lemma

When $g \in L^+_\infty(D \times V)$, the space of non-negative functions in $L^+_\infty(D \times V)$, the expectation semigroup $(\phi_t[g], t \geq 0)$ is the unique bounded solution to the mild equation

$$\phi_t[g] = \mathtt{U}_t[g] + \int_0^t \mathtt{U}_s[(\mathcal{S} + \mathcal{F})\phi_{t-s}[g]]\mathrm{d}s, \qquad t \geq 0.$$

Lemma

The mild solution $(\phi_t, t \geq 0)$, is equal on $L_2(D \times V)$ to $(\psi_g(t, \cdot, \cdot), t \geq 0)$ and dual to $(\Psi_g(t, \cdot, \cdot), t \geq 0)$ on $L_2(D \times V)$, i.e.

$$\langle f, \phi_t[g] \rangle = \langle f, \psi_g(t, \cdot, \cdot) \rangle = \langle \Psi_f(t, \cdot, \cdot), g \rangle$$

for all $f, g \in L_2(D \times V)$.

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Mild equation

- Define for $g \in L^+_\infty(D\times V)$, the (physical process) expectation semigroup

$$\phi_t[g](r,\upsilon) := \mathbb{E}_{\delta_{(r,\upsilon)}}[\langle g, X_t\rangle], \qquad t\geq 0, r\in D, \upsilon\in V,$$

and the advection semigroup

$$\mathtt{U}_t[g](r,\upsilon) = g(r+\upsilon t,\upsilon)\mathbf{1}_{\{t<\kappa^D_{r,\upsilon}\}}, \qquad t\geq 0.$$

where $\kappa^D_{r,\upsilon} := \inf\{t>0 : r+\upsilon t\notin D\}$.

Lemma

When $g\in L^+_\infty(D\times V)$, the space of non-negative functions in $L^+_\infty(D\times V)$, the expectation semigroup $(\phi_t[g], t\geq 0)$ is the unique bounded solution to the mild equation

$$\phi_t[g] = \mathtt{U}_t[g] + \int_0^t \mathtt{U}_s[(\mathcal{S}+\mathcal{F})\phi_{t-s}[g]]\mathrm{d}s, \qquad t\geq 0.$$

Lemma

The mild solution $(\phi_t, t\geq 0)$, is equal on $L_2(D\times V)$ to $(\psi_g(t,\cdot,\cdot), t\geq 0)$ and dual to $(\Psi_g(t,\cdot,\cdot), t\geq 0)$ on $L_2(D\times V)$, i.e.

$$\langle f, \phi_t[g]\rangle = \langle f, \psi_g(t,\cdot,\cdot)\rangle = \langle \Psi_f(t,\cdot,\cdot), g\rangle$$

for all $f, g\in L_2(D\times V)$.

λ-EIGENVALUE PROBLEM

- So far
$$\langle f, \phi_t[g]\rangle = \langle \Psi_f(t,\cdot,\cdot), g\rangle$$
for all $f, g \in L_2(D \times V)$

- We want to play with the eigenfunction $\tilde{\varphi} \in L_2(D \times V)$, e.g.
$$\langle f, \phi_t[\tilde{\varphi}]\rangle = \langle \Psi_f(t,\cdot,\cdot), \tilde{\varphi}\rangle = \mathrm{e}^{\lambda t}\langle f, \tilde{\varphi}\rangle$$
suggesting (at least in the $L_2(D \times V)$ sense)
$$\phi_t[\tilde{\varphi}](r, \upsilon) = \mathbb{E}_{\delta_{(r,\upsilon)}}[\langle \tilde{\varphi}, X_t\rangle] := \mathrm{e}^{\lambda t}\tilde{\varphi}(r, \upsilon)$$
$\Rightarrow$ points us towards Monte-Carlo methods - especially when $\lambda = 0$

- Problem! No good unless $\tilde{\varphi} \in L^+_\infty(D \times V)$, but we only know $\tilde{\varphi} \in L^+_2(D \times V)$

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Theorem (Horton, K., Villemonais, 2018)

Suppose that

- *D is non-empty and convex;*
- *Cross-sections σ_S, σ_F, π_S and π_F are uniformly bounded away from infinity;*
- $\inf_{r\in D,\upsilon,\upsilon'\in V}\left(\sigma_S(r,\upsilon)\pi_S(r,\upsilon,\upsilon') + \sigma_F(r,\upsilon)\pi_F(r,\upsilon,\upsilon')\right) > 0$

Then, for the semigroup $(\phi_t, t \geq 0)$, there exists a $\lambda_* \in \mathbb{R}$, a positive[1] *right eigenfunction $\varphi \in L^+_\infty(D \times V)$ and a left eigenmeasure which is absolutely continuous with respect to Lebesgue measure on $D \times V$ with density $\tilde{\varphi} \in L^+_\infty(D \times V)$, both having associated eigenvalue $e^{\lambda_* t}$, and such that φ (resp. $\tilde{\varphi}$) is uniformly (resp. a.e. uniformly) bounded away from zero on each compactly embedded subset of $D \times V$. In particular, for all $g \in L^+_\infty(D \times V)$,*

$$\langle \tilde{\varphi}, \phi_t[g]\rangle = e^{\lambda_* t}\langle \tilde{\varphi}, g\rangle \quad (\textit{resp. } \phi_t[\varphi] = e^{\lambda_* t}\varphi) \quad t \geq 0.$$

Moreover, there exists $\varepsilon > 0$ such that

$$\sup_{g\in L^+_\infty(D\times V):||g||_\infty\leq 1} \left\| e^{-\lambda_* t}\varphi^{-1}\phi_t[g] - \langle \tilde{\varphi}, g\rangle \right\|_\infty = O(e^{-\varepsilon t}) \textit{ as } t \to \infty.$$

[1] To be precise, by a positive eigenfunction, we mean a mapping from $D \times V \to (0, \infty)$. This does not prevent it being valued zero on ∂D, as D is an open bounded, convex domain.

If the neutron branching process (physical process) begins from a configuration $\mu = \sum_{i=1}^n \delta_{x_i}$, then

$$W_t := e^{-\lambda_* t} \frac{\langle \varphi, X_t \rangle}{\langle \varphi, \mu \rangle}, \qquad t \geq 0,$$

is a martingale.

Theorem (Horton, K. Villemonais)

Suppose that

- *D is non-empty and convex;*
- *Cross-sections σ_s, σ_f, π_s and π_f are uniformly bounded away from infinity;*
- *We have $\sigma_s \pi_s + \sigma_f \pi_f > 0$ on $D \times V \times V$;*
- *There is an open ball B compactly embedded in D such that $\inf_{r \in D, \upsilon, \upsilon' \in V} \sigma_{f(r,\upsilon,\upsilon')} \pi_f(r, \upsilon, \upsilon') > 0$.*

For all $g \in L^+_\infty(D \times V)$ such that, up to a multiplicative constant, $g \leq \varphi$, under the assumptions as the previous Theorem,

$$\lim_{t \to \infty} e^{-\lambda_* t} \langle g, X_t \rangle = \langle g, \tilde{\varphi} \rangle W_\infty.$$

almost surely, where W_∞ is the martingale limit. Moreover, W_∞ is positive with positive probability if and only if $\lambda_* > 0$, otherwise $W_\infty = 0$.

λ-EIGENVALUE AND MC LOGIC

- Suppose now we can efficiently simulate the Neutron branching process, recalling that

$$\phi_t[g](r,\upsilon) := \mathbb{E}_{\delta_{(r,\upsilon)}}[\langle g, X_t\rangle], \qquad t \geq 0, r \in D, \upsilon \in V,$$

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$$\lambda_* = \lim_{t\to\infty} \frac{1}{t} \log \phi_t[g](r,\upsilon) = \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}_{\delta_{(r,\upsilon)}}[\langle g, X_t\rangle], \qquad t \geq 0, r \in D, \upsilon \in V.$$

- and e.g. fix $r \in D, \upsilon \in V$,

$$\frac{\langle \tilde{\varphi}, g\rangle}{\langle \tilde{\varphi}, 1\rangle} = \lim_{t\to\infty} \frac{\phi_t[g](r,\upsilon)}{\phi_t[1](r,\upsilon)} = \lim_{t\to\infty} \frac{\mathbb{E}_{\delta_{(r,\upsilon)}}[\langle g, X_t\rangle]}{\mathbb{E}_{\delta_{(r,\upsilon)}}[\langle 1, X_t\rangle]}$$

where g is a test function in $L^+_\infty(D \times V)$.

λ-eigenvalue and MC logic

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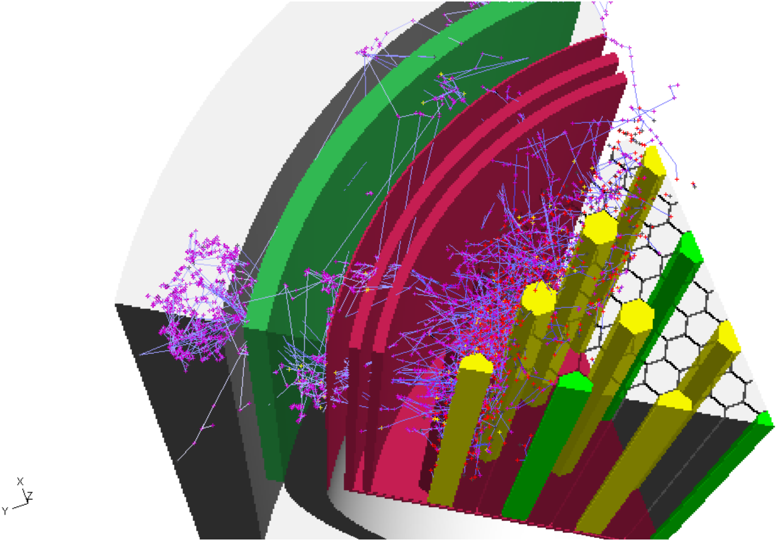
MONTE-CARLO, IMPORTANCE MAP $\tilde{\varphi}$



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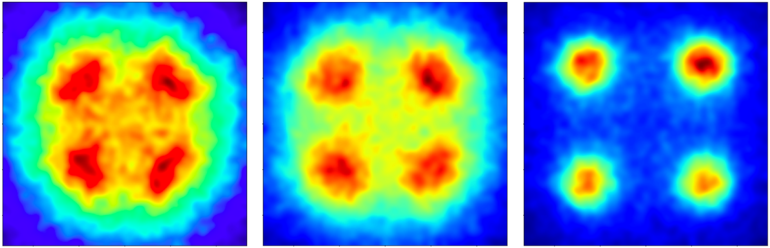

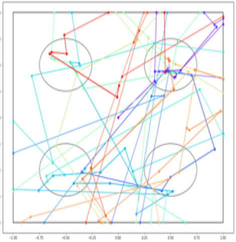

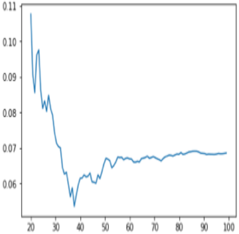

Many-to-one and Monte-Carlo parallelisation

- Recall semigroup operators

$$\mathcal{T}f(r,\upsilon) := \upsilon\cdot\nabla f(r,\upsilon) \quad \text{(backwards transport)}$$

$$\mathcal{S}f(r,\upsilon) := \sigma_{\mathrm{s}}(r,\upsilon)\int_V (f(r,\upsilon')-f(r,\upsilon))\pi_{\mathrm{s}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon' \quad \text{(backwards scattering)}$$

$$\mathcal{F}f(r,\upsilon) := \sigma_{\mathrm{f}}(r,\upsilon)\int_V f(r,\upsilon')\pi_{\mathrm{f}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon' - \sigma_{\mathrm{f}}(r,\upsilon)f(r,\upsilon) \quad \text{(backwards fission)}$$

- Basic algebra gives

$$\mathcal{T}+\mathcal{S}+\mathcal{F} = \upsilon\cdot\nabla f(r,\upsilon,t)+\alpha(r,\upsilon)\int_V (f(r,\upsilon',t)-f(r,\upsilon,t))\pi(r,\upsilon,\upsilon')\mathrm{d}\upsilon'+\beta(r,\upsilon)f(r,\upsilon)$$

where

$$\alpha(r,\upsilon) := \sigma_{\mathrm{s}}(r,\upsilon)+\sigma_{\mathrm{f}}(r,\upsilon)\int_V \pi_{\mathrm{f}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon',$$

$$\pi(r,\upsilon,\upsilon')\mathrm{d}\upsilon' := \alpha(r,\upsilon)^{-1}\left[\sigma_{\mathrm{s}}(r,\upsilon)\pi_{\mathrm{s}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon'+\sigma_{\mathrm{f}}(r,\upsilon)\pi_{\mathrm{f}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon'\right],$$

$$\beta(r,\upsilon) := \alpha(r,\upsilon)-\sigma_{\mathrm{s}}(r,\upsilon)-\sigma_{\mathrm{f}}(r,\upsilon) = \sigma_{\mathrm{f}}(r,\upsilon)\left(\int_V \pi_{\mathrm{f}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon'-1\right).$$

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Many-to-one and Monte-Carlo parallelisation

- The representation $\mathcal{T} + \mathcal{S} + \mathcal{F} = \mathcal{L} + \beta$, where

$$\mathcal{L}f(r,\upsilon) = \upsilon \cdot \nabla f(r,\upsilon,t) + \alpha(r,\upsilon)\int_V \big(f(r,\upsilon',t) - f(r,\upsilon,t)\big)\pi(r,\upsilon,\upsilon')\mathrm{d}\upsilon'.$$

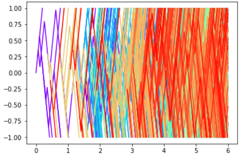
  This is the Markov generator of a neutron random walk (NRW) (R,Υ) (scatters at rate α and chooses new velocity with distribution π) with probabilities $(\mathbf{P}_{(r,\upsilon)}, r \in D, \upsilon \in V)$. We have a new representation in terms of (R,Υ),

$$\phi_t[g](r,\upsilon) = \mathbb{E}_{\delta_{(r,\upsilon)}}[\langle g, X_t\rangle] = \mathbf{E}_{(r,\upsilon)}\left[\mathrm{e}^{\int_0^t \beta(R_u,\Upsilon_u)\mathrm{d}u} g(R_t,\Upsilon_t)\mathbf{1}_{(t<\tau^D)}\right],$$

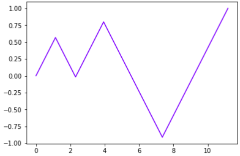
  for $t \geq 0, r \in D, \upsilon \in V$, where

$$\tau^D = \inf\{t > 0 : R_t \notin D\}.$$

- This affords new parallelisable opportunities to Monte-Carlo solve numerically for h:



can be replaced by



GENERATIONAL EVOLUTION AND k_{eff}

- In place of $(X_t, t \geq 0)$, we consider the process $(\mathcal{X}_n, n \geq 0)$, where, for $n \geq 1$, $\mathcal{X}_n$ is $\mathcal{M}(D \times V)$-valued and can be written

$$\mathcal{X}_n = \sum_{i=1}^{\mathcal{N}_n} \delta_{(r_i^{(n)}, \upsilon_i^{(n)})},$$

  where $\{(r_i^{(n)}, \upsilon_i^{(n)}), i = 1, \cdots \mathcal{N}_n\}$ are the position-velocity configurations of the $\mathcal{N}_n$ particles that are n-th in their genealogies to be the result of a fission event.
- $\mathcal{X}_0$ is consistent with X_0 and is the initial configuration of neutron positions and velocities.
- For $n \geq 1$ we can think of $\mathcal{X}_n$ as the n-th generation of the system and we refer to them as the neutron generational process (NGP).

Generational semigroup

- Appealing to the obvious meaning of $\langle g, \mathcal{X}_n \rangle$, define the expectation semigroup $(\Phi_n, n \geq 0)$ by

$$\Phi_n[g](r, \upsilon) = \mathbb{E}_{\delta_{(r,\upsilon)}}\left[\langle g, \mathcal{X}_n \rangle\right], \qquad n \geq 0, r \in D, \upsilon \in V,$$

  with $\Psi_0[g] := g \in L^+_\infty(D \times V)$.

- Associated eigen problem: finding a pair $\kappa > 0$ and $h \in L^+_\infty(D \times V)$ such that, pointwise,

$$\Phi_1[h](r, \upsilon) = \kappa h(r, \upsilon), \qquad r \in D, \upsilon \in V.$$

- By splitting on the first fission event, Φ_n solves the following mild equation

$$\Phi_n[g](r, \upsilon) = \int_0^\infty \mathsf{Q}_s\left[\mathcal{F}\Phi_{n-1}[g]\right](r, \upsilon)\mathrm{d}s, \qquad r \in D, \upsilon \in V, g \in L^+_\infty(D \times V),$$

  where

$$\mathsf{Q}_s[g](r, \upsilon) = \mathbb{E}_{\delta_{(r,\upsilon)}}\left[\mathrm{e}^{-\int_0^s \sigma_{\mathtt{f}}(R_u, \Upsilon_u)\mathrm{d}u} g(R_s, \Upsilon_s)\mathbf{1}_{(s<\tau_D)}\right],$$

  and $(R_s, \Upsilon_s)_{s \geq 0}$ is the $\sigma_{\mathtt{s}}\pi_{\mathtt{s}}$-NRW.

- If the pair (k, h) solves (18), the strong Markov property along with an iteration implies that

$$\kappa^n h(r, \upsilon) = \Phi_n[h](r, \upsilon), \qquad r \in D, \upsilon \in V.$$

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- $\inf_{r\in D,\upsilon,\upsilon'\in V}\sigma_{\mathtt{f}}(r,\upsilon)\pi_{\mathtt{f}}(r,\upsilon,\upsilon')>0$.

Then for the semigroup $(\Phi_n, n\geq 0)$, there exist $k_{\mathit{eff}}\in\mathbb{R}$, a positive right eigenfunction $h\in L^+_\infty(D\times V)$ and a left eigenmeasure, $\tilde{h}$, on $D\times V$, both having associated eigenvalue k^n_{eff}. Moreover, k_{eff} is the leading eigenvalue in the sense that, for all $g\in L^+_\infty(D\times V)$,

$$\langle\tilde{h},\Phi_n[g]\rangle = k^n_{\mathit{eff}}\langle\tilde{h},g\rangle \quad \textit{(resp. } \Phi_n[h]=k^n_{\mathit{eff}}h\textit{)} \quad n\geq 0,$$

and there exists $\gamma>1$ such that, for all $g\in L^+_\infty(D\times V)$,

$$\sup_{g\in L^+_\infty(D\times V):||g||_\infty\leq 1}\left\|k^{-n}_{\mathit{eff}}h^{-1}\Phi_n[g]-\langle\tilde{h},g\rangle\right\|_\infty = O(\gamma^{-n}) \textit{ as } n\to+\infty.$$

GENERATIONAL MAY-TO-ONE

- Let
$$m(r,\upsilon) = \int_V \pi_{\mathtt{f}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon',$$
denote the mean number of offspring generated by a fission event at (r,υ)
- Recall the $\alpha\pi$-neutron random walk (R,Υ) where we define the rate α and the scatter kernel π so that
$$\alpha(r,\upsilon)\pi(r,\upsilon,\upsilon') = \sigma_{\mathtt{s}}(r,\upsilon)\pi_{\mathtt{s}}(r,\upsilon,\upsilon') + \sigma_{\mathtt{f}}(r,\upsilon)\pi_{\mathtt{f}}(r,\upsilon,\upsilon') \qquad r \in D, \upsilon, \upsilon' \in V.$$
i.e.
$$\alpha(r,\upsilon) = \sigma_{\mathtt{s}}(r,\upsilon) + \sigma_{\mathtt{f}}(r,\upsilon)m(r,\upsilon)$$
- Recall that we can build an $\alpha\pi$-NRW (R,Υ) that scatters at rate α and choses its new velocity with π.

GENERATIONAL MAY-TO-ONE

- We can simulate its paths with the following subroutine:
  - (R, Υ) scatters for the k-th time at (r, υ) with rate $\alpha(r, \upsilon)$;
  - A coin is tossed, $\mathtt{I}_k(r, \upsilon) = 1$ with probability $\sigma_{\mathtt{f}}(r, \upsilon)m(r, \upsilon)/\alpha(r, \upsilon)$, a new velocity, $\Theta_k^{\mathtt{f}}(r, \upsilon)$, is chosen with probability $\pi_{\mathtt{f}}(r, \upsilon, \upsilon')/m(r, \upsilon)$;
  - On the other hand, with probability density $\sigma_{\mathtt{s}}(r, \upsilon)/\alpha(r, \upsilon)$ the random variable $\mathtt{I}_k(r, \upsilon) = 0$, a new velocity, $\Theta_k^{\mathtt{s}}(r, \upsilon)$, is chosen with probability density $\pi_{\mathtt{s}}(r, \upsilon, \upsilon')$.
- As such, the velocity immediately after the k-th scatter of the NRW, given that the position-velocity configuration immediately before is (r, υ), is coded by the random variable

$$\mathtt{I}_k(r, \upsilon)\Theta_k^{\mathtt{f}}(r, \upsilon) + (1 - \mathtt{I}_k(r, \upsilon))\Theta_k^{\mathtt{s}}(r, \upsilon).$$

- We thus can identify sequentially, $T_0 = 0$ and, for $n \geq 1$,

$$T_n = \inf\{t > T_{n-1} : \Upsilon_t \neq \Upsilon_{t-} \text{ and } \mathtt{I}_{k_t}(R_t, \Upsilon_{t-}) = 1\},$$

where $(k_t, t \geq 0)$ is the process counting the number of scattering events of the NRW up to time t.

Lemma

Suppose that

- *The cross-sections $\sigma_{\mathtt{S}}$, $\sigma_{\mathtt{f}}$, $\pi_{\mathtt{S}}$ and $\pi_{\mathtt{f}}$ are uniformly bounded away from infinity;*
- *We have $\sigma_{\mathtt{S}}\pi_{\mathtt{S}} + \sigma_{\mathtt{f}}\pi_{\mathtt{f}} > 0$ on $D \times V \times V$;*
- *There is an open ball B compactly embedded in D such that $\sigma_{\mathtt{f}}\pi_{\mathtt{f}} > 0$ on $B \times V \times V$.*

Then the solution to

$$\Phi_n[g](r,\upsilon) = \int_0^\infty \mathcal{Q}_s\left[\mathcal{F}\Phi_{n-1}[g]\right](r,\upsilon)\mathrm{d}s, \qquad r \in D, \upsilon \in V, g \in L^+_\infty(D \times V),$$

among the class of expectation semigroups is unique for $g \in L^+_\infty(D \times V)$ and the semigroup $(\Phi_n, n \geq 0)$ may alternatively be represented as

$$\Phi_n[g](r,\upsilon) = \mathbf{E}_{(r,\upsilon)}\left[\prod_{i=1}^n m(R_{T_i}, \Upsilon_{T_i-}) g(R_{T_n}, \Upsilon_{T_n}) \mathbf{1}_{(T_n < \kappa^D)}\right], \qquad r \in D, \upsilon \in V, n \geq 1,$$

(with $\Phi_0[g] = g$), where $(R_t, \Upsilon_t)_{t\geq 0}$ is the $\alpha\pi$-NRW, and

$$\kappa^D := \inf\{t > 0 : R_t \notin D\}.$$

k_{eff}-EIGENVALUE PROBLEM AND MC LOGIC

- there exists $\gamma > 1$ such that, "uniformly" for all $g \in L^+_\infty(D \times V)$,

$$\Phi_n[g](r,v) \sim k^n_{eff} h(r,v) \langle \tilde{h}, g \rangle + O(\gamma^{-n}) \text{ as } n \to +\infty,$$

  suggesting an estimate over several "generations" of NRW
- But also

$$\frac{\langle \tilde{h}, \Phi_n[g] \rangle}{\langle \tilde{h}, g \rangle} = \frac{1}{\langle \tilde{h}, g \rangle} \int_{D \times V} \Phi_n[g](r,v) \tilde{h}(r,v) \mathrm{d}r \mathrm{d}v = k^n_{eff}$$

- In particular, this suggests an estimate over a single iteration by looking for stability:

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Importance sampling

- Note that we are wasting a lot of simulations to numerically develop the expectation

$$\Phi_1[g](r,\upsilon) = \mathbf{E}_{(r,\upsilon)}\left[m(R_{T_1},\Upsilon_{T_1-})g(R_{T_1},\Upsilon_{T_1})\mathbf{1}_{(T_1<\kappa^D)}\right], \qquad r\in D, \upsilon\in V, n\geq 1,$$

  the indicator means we score zero for many runs of the MC.
- We can use a trick of Doob *h*-transforming (also known as importance sampling), which means we bias the characteristics of the NRW but average a different path function and arrange things so the averaging is still equal to $\Phi_1[g](r,\upsilon)$.

Importance sampling

- Suppose that $H(r, \upsilon)$ is a "good guess" of h. Then there exists a $\Gamma(r, \upsilon)$ such that

$$1 = \mathbf{E}_{(r,\upsilon)}\left[\mathrm{e}^{-\int_0^{T_1} \Gamma(R_s,\Upsilon_s)\mathrm{d}s} \frac{H(R_{T_1}, \Upsilon_{T_1})}{H(r,\upsilon)} \right], \qquad r \in D, \upsilon \in V,$$

In fact, $\Gamma(r, \upsilon) = H^{-1}(r, \upsilon)\mathcal{L}H(r, \upsilon)$, where

$$\mathcal{L}f(r,\upsilon) = \upsilon \cdot \nabla f(r,\upsilon,t) + \alpha(r,\upsilon)\int_V \big(f(r,\upsilon',t) - f(r,\upsilon,t)\big)\pi(r,\upsilon,\upsilon')\mathrm{d}\upsilon'.$$

- We "change measure"

$$\frac{\mathrm{d}\mathbf{P}^H_{(r,\upsilon)}}{\mathrm{d}\mathbf{P}_{(r,\upsilon)}} = \mathrm{e}^{-\int_0^{T_1} \Gamma(R_s,\Upsilon_s)\mathrm{d}s} \frac{H(R_{T_1}, \Upsilon_{T_1})}{H(r,\upsilon)}$$

- Then write Φ_1 in terms of $\mathbf{P}^H$,

$$\Phi_1[g](r,\upsilon) = H(r,\upsilon)\mathbf{E}^H_{(r,\upsilon)}\left[\mathrm{e}^{\int_0^{T_1} \Gamma(R_s,\Upsilon_s)\mathrm{d}s} m(R_{T_1}, \Upsilon_{T_1-}) \frac{g(R_{T_1}, \Upsilon_{T_1})}{H(R_{T_1}, \Upsilon_{T_1})} \right]$$

- Under $\mathbf{P}^H$ the characteristics of the NRW can be described via the generator

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- We can now build our MC sampling around a NRW (R, Υ) under $\mathbf{P}^H$.
- That is

$$\Phi_1[g](r,\upsilon) = \mathbf{E}_{(r,\upsilon)}\left[m(R_{T_1}, \Upsilon_{T_1-})g(R_{T_1}, \Upsilon_{T_1})\mathbf{1}_{(T_1<\kappa^D)}\right],$$

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- Hence
  - no simulating trees
  - no simulating NRW paths that leave the domain of the reactor (i.e. every NRW path counts).
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Thank you!