Stochastic analysis of the neutron transport equation

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Based on joint work with Alex Cox (University of Bath), Simon Harris (University of Auckland), Andreas Kyprianou (University of Bath), Denis Villemonais (Université de Lorraine) and Minmin Wang (University of Sussex). Funded by Jacobs.

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Overview

- Interested in modelling neutrons in fissile environments and their long-term behaviour.

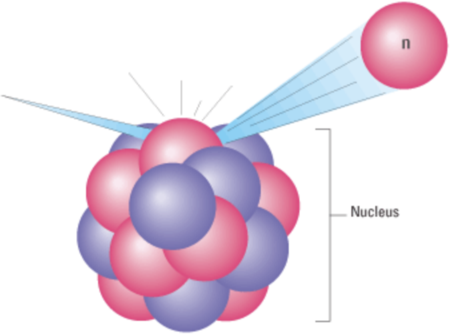
- One quantity of interest is the neutron flux, which is a function of
  - time, $t \geq 0$,
  - neutron positionm $r \in D \subset \mathbb{R}^3$,
  - neutron direction $\Omega \in \mathbb{S}^2$
  - neutron energy, $E \in (0, \infty)$.

- However, often neutron energy and direction are combined into velocity, $\upsilon \in V$.

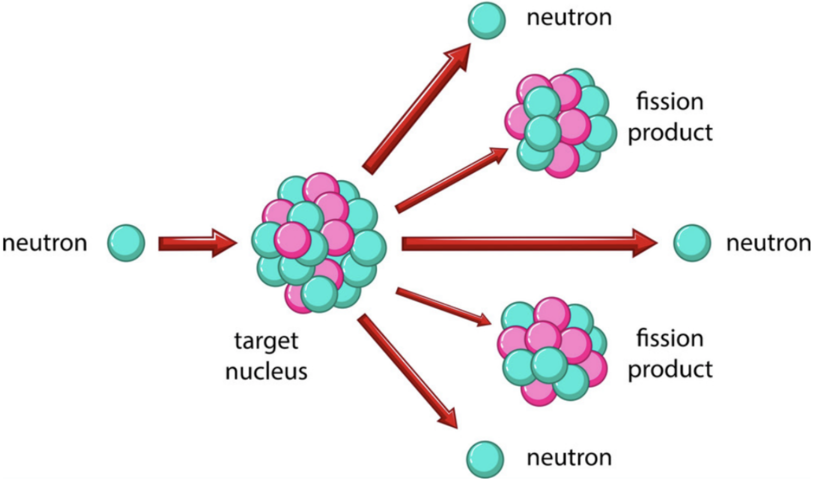
- Represent the neutron flux at time t as

$$\Psi_t(r, \upsilon), \qquad r \in D, \, \upsilon \in V.$$

Scattering



Fission



neutron
fission
product
neutron
neutron
target
nucleus
fission
product
neutron

Neutron transport equation (forwards equation)

$$
\begin{aligned}
\frac{\partial \Psi_t}{\partial t}(r,\upsilon) = Q(r,\upsilon,t) - \Omega\cdot\nabla_r \Psi_t(r,\upsilon) - (\sigma_{\mathtt{s}}(r,\upsilon)+\sigma_{\mathtt{f}}(r,\upsilon))\Psi_t(r,\upsilon) \\
+ \int_V \sigma_{\mathtt{s}}(r,\upsilon')\pi_{\mathtt{s}}(r,\upsilon',\upsilon)\Psi_t(r,\upsilon')\mathrm{d}\upsilon' \\
+ \int_V \sigma_{\mathtt{f}}(r,\upsilon')\pi_{\mathtt{f}}(r,\upsilon',\upsilon)\Psi_t(r,\upsilon')\mathrm{d}\upsilon'
\end{aligned} \tag{1}
$$

$$
= Q(r,\upsilon,t) + \overrightarrow{T}\Psi_t(r,\upsilon) + \overrightarrow{S}\Psi_t(r,\upsilon) + \overrightarrow{F}\Psi_t(r,\upsilon), \tag{2}
$$

where

$Q(r,\upsilon,t)$: neutron source,

$\sigma_{\mathtt{s}}(r,\upsilon)$: is the rate at which a neutron scatters,

$\sigma_{\mathtt{f}}(r,\upsilon)$: is the rate at which a fission event occurs,

$\pi_{\mathtt{s}}(r,\upsilon',\upsilon)$: is the probability a neutron with incoming velocity υ' scatters with new velocity υ,

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Initial and boundary conditions

- Initial conditions:

$$\Psi_0(r, \upsilon) = g(r, \upsilon), \qquad (r, \upsilon) \in D \times V.$$

- Boundary conditions:

$$\Psi_t(r, \upsilon) = 0, \qquad r \in \partial D, \, \mathbf{n}_r \cdot \upsilon < 0,$$

where $\mathbf{n}_r$ is the outward unit normal at $r \in \partial D$.

Neutron transport equation (backwards equation)

Set $Q = 0$. For $f, g \in L^2(D \times V)$, we have

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

where

$$\begin{aligned}
\overleftarrow{T}g &= \Omega \cdot \nabla_r g(r, \upsilon) - (\sigma_{\mathtt{s}}(r, \upsilon) + \sigma_{\mathtt{f}}(r, \upsilon))g(r, \upsilon) \\
\overleftarrow{S}g &= \sigma_{\mathtt{s}}(r, \upsilon) \int_V \pi_{\mathtt{s}}(r, \upsilon, \upsilon')g(r, \upsilon')\mathrm{d}\upsilon' \\
\overleftarrow{F}g &= \sigma_{\mathtt{f}}(r, \upsilon) \int_V \pi_{\mathtt{f}}(r, \upsilon, \upsilon')g(r, \upsilon')\mathrm{d}\upsilon'.
\end{aligned}$$

This leads to the backwards NTE given by the abstract Cauchy problem

$$\frac{\partial \Phi_t}{\partial t}(r, \upsilon) = (\overleftarrow{T} + \overleftarrow{S} + \overleftarrow{F})\Phi_t(r, \upsilon), \tag{3}$$

with

- Initial conditions:

$$\Phi_0(r, \upsilon) = g(r, \upsilon), \qquad (r, \upsilon) \in D \times V.$$

- Boundary conditions:

$$\Phi_t(r, \upsilon) = 0, \qquad r \in \partial D,\ \mathbf{n}_r \cdot \upsilon > 0,$$

where $\mathbf{n}_r$ is the outward unit normal at $r \in \partial D$.

Find $(\alpha, \varphi, \tilde{\varphi})$ such that

$$(\overleftarrow{T} + \overleftarrow{S} + \overleftarrow{F})\varphi(r, \upsilon) = \alpha\varphi(r, \upsilon),$$

$$\langle \tilde{\varphi}, (\overleftarrow{T} + \overleftarrow{S} + \overleftarrow{F})f \rangle = \alpha \langle \tilde{\varphi}, f \rangle,$$

where we have the following classifications

$$\alpha \begin{cases} < 0, & \text{system is subcritical} \\ = 0, & \text{system is critical} \\ > 0, & \text{system is supercritical.} \end{cases}$$

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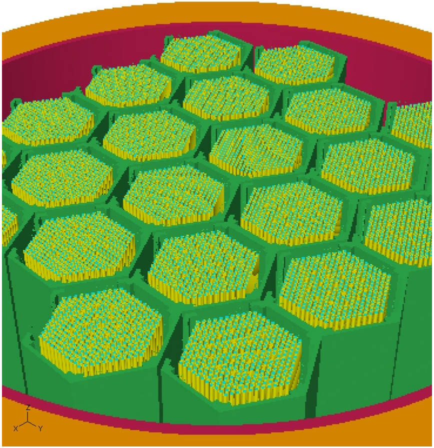
Problems...



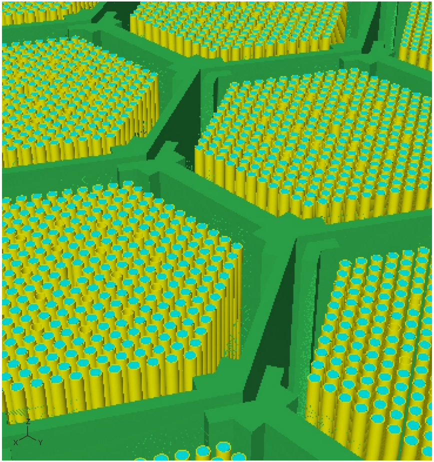


Figure: Model of a pressurised water reactor. Images provided by ANSWERS.

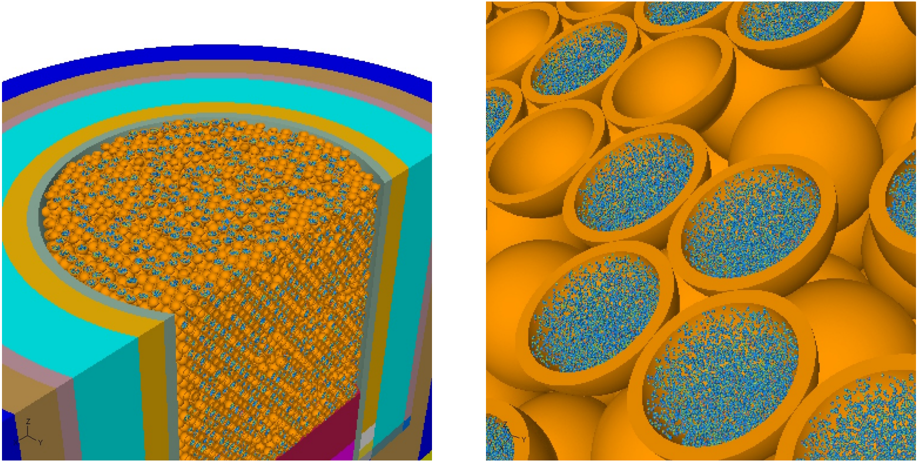


Figure: Model of a pebble bed modular reactor. Images provided by ANSWERS.

Cross-sections

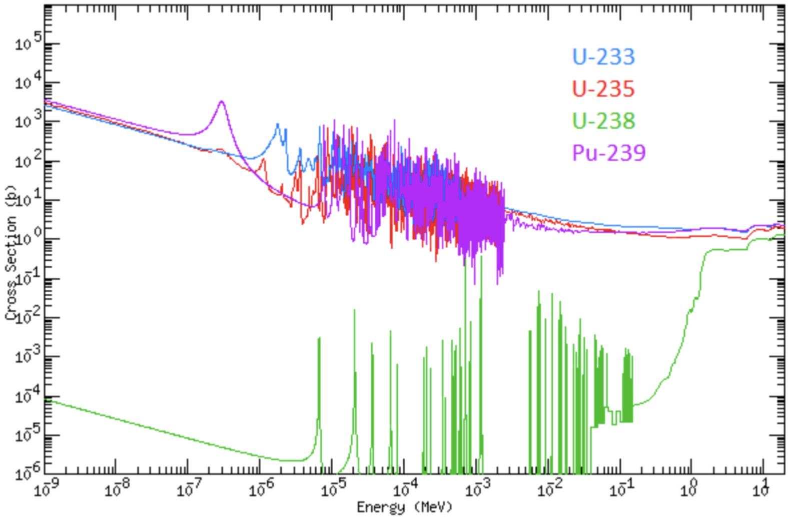


Figure: Example of fission cross-sections. Image provided by Wikipedia.

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Neutron branching process

- Let D be a non-empty, bounded, open subset of $\mathbb{R}^3$.
- We take the velocity space to be $V := (\upsilon_{\mathtt{min}}, \upsilon_{\mathtt{max}}) \times \mathbb{S}_2$.
- Let N_t be the number of particles alive at time t.
- Let $\{(r_i(t), \upsilon_i(t)) : i = 1, \ldots, N_t\}$ denote their configurations in $D \times V$.

- A neutron with configuration (r, υ) moves along the trajectory $r + \upsilon s$, $s \geq 0$ until one of three things occur.
  - the neutron hits the boundary of the domain, at which point it is killed.
  - at a random time $T_{\mathtt{s}}$, which is distributed as

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

    the neutron scatters. It's new velocity is chosen according to $\pi_{\mathtt{s}}(r + \upsilon s, \upsilon, \cdot)$.
  - at a random time $T_{\mathtt{f}}$, which is distributed as

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

    a fission occurs. A random number, N, of neutrons with velocities $\{\upsilon_i, i = 1, \ldots, N\}$ are produced according to $(\mathcal{Z}, \mathcal{P})$, which satisfies

$$\int_V g(\upsilon')\pi_{\mathtt{f}}(r, \upsilon, \upsilon')\mathrm{d}\upsilon' = \mathcal{E}_{(r,\upsilon)}[\langle g, \mathcal{Z}\rangle].$$

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  $$\int_V g(\upsilon')\pi_{\mathtt{f}}(r, \upsilon, \upsilon')\mathrm{d}\upsilon' = \mathcal{E}_{(r,\upsilon)}[\langle g, \mathcal{Z}\rangle].$$

- We can represent the branching process via the atomic measures

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

- Define the expectation semigroup

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

- Note that

$$\psi_0[g](r,\upsilon) = g(r,\upsilon) \quad \text{and} \quad \psi_t[g](r,\upsilon) = 0 \text{ for } r \in \partial D, \mathbf{n}_r \cdot \upsilon > 0. \tag{4}$$

(H1) Cross-sections $\sigma_{\mathtt{s}}$, $\sigma_{\mathtt{f}}$, $\pi_{\mathtt{s}}$ and $\pi_{\mathtt{f}}$ are uniformly bounded away from infinity.

(H2) We have $\inf_{r\in D,\upsilon,\upsilon'\in V}(\sigma_{\mathtt{s}}\pi_{\mathtt{s}}+\sigma_{\mathtt{f}}\pi_{\mathtt{f}})>0$.

Lemma (Cox, Harris, H., Kyprianou)

Under (H1) and (H2), for $r\in D$, $\upsilon\in V$, $t\geq 0$ and $g\in L^\infty_+(D\times V)$, $\psi_t[g](r,\upsilon)$ is the unique solution to

$$
\begin{aligned}
\psi_t[g](r,\upsilon) &= g(r+\upsilon t,\upsilon)\mathbf{1}_{\{t<\kappa_{r,\upsilon}\}} - \int_0^t (\sigma_{\mathtt{s}}(r+\upsilon s,\upsilon)+\sigma_{\mathtt{f}}(r+\upsilon s,\upsilon))\psi_{t-s}[g](r+\upsilon s,\upsilon)\mathrm{d}s \\
&\quad + \int_0^t \sigma_{\mathtt{s}}(r+\upsilon s,\upsilon)\int_V \psi_{t-s}[g](r+\upsilon s,\upsilon')\pi_{\mathtt{s}}(r+\upsilon s,\upsilon,\upsilon')\mathrm{d}s \\
&\quad + \int_0^t \sigma_{\mathtt{f}}(r+\upsilon s,\upsilon)\int_V \psi_{t-s}[g](r+\upsilon s,\upsilon')\pi_{\mathtt{f}}(r+\upsilon s,\upsilon,\upsilon')\mathrm{d}s,
\end{aligned}
$$

where $\kappa_{r,\upsilon}=\inf\{t>0 : r+\upsilon t\notin D\}$ and with boundary and initial conditions given by (4).

Lemma (Cox, Harris, H., Kyprianou)

Under (H1) and (H2), the mild solution $\psi_t[g]$, is equal on $L_2(D \times V)$ to $(\Phi_t, t \geq 0)$ and dual to $(\Psi_t, t \geq 0)$ on $L_2(D \times V)$, i.e.

$$\langle f, \psi_t[g] \rangle = \langle f, \Phi_t^g \rangle = \langle \Psi_t^f, g \rangle$$

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

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Theorem (H., Kyprianou and Villemonais)

Under the assumptions (H1) and (H2), there exist

- $\lambda_* \in \mathbb{R}$, and
- positive, bounded functions $\varphi, \tilde{\varphi}$ on $D \times V$,

such that for all bounded, measurable functions $g : D \times V \to [0, \infty)$,

$$\langle \tilde{\varphi}, \psi_t[g] \rangle = \mathrm{e}^{\lambda_* t} \langle \tilde{\varphi}, g \rangle \quad \textit{and} \quad \psi_t[\varphi] = \mathrm{e}^{\lambda_* t} \varphi, \quad t \geq 0. \tag{5}$$

Moreover, there exist $C, \varepsilon > 0$ such that, for all $g \in L_\infty^+(D \times V)$,

$$\sup_{\|g\| \leq 1} \left\| \varphi^{-1} \mathrm{e}^{-\lambda_* t} \psi_t[g] - \langle \tilde{\varphi}, g \rangle \right\|_\infty \leq C \mathrm{e}^{-\varepsilon t}, \qquad \text{for all } t \geq 0. \tag{6}$$

Implications of PF decomposition

From the PF decomposition, we have

$$\psi_t[g] \sim \mathrm{e}^{\lambda_* t}\langle\tilde{\varphi}, g\rangle\varphi, \quad t \to \infty.$$

Manipulation of this asymptotic allows us to simulate the eigen-elements:

- $\lambda_* = \lim_{t\to\infty} \frac{1}{t} \log \psi_t[\mathbf{1}](r, v) = \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}_{\delta_{(r,v)}}[N_t]$.
- $\langle\tilde{\varphi}, g\rangle\varphi(r, v) = \lim_{t\to\infty} \frac{1}{t} \int_0^t \mathrm{e}^{-\lambda_* s}\psi_s[g](r, v)\mathrm{d}s$.

Toy model

Toy model

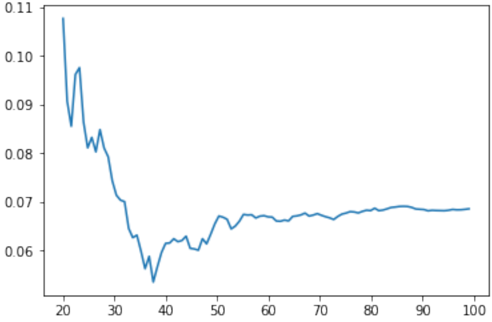


Figure: Estimate of λ_*

Toy model

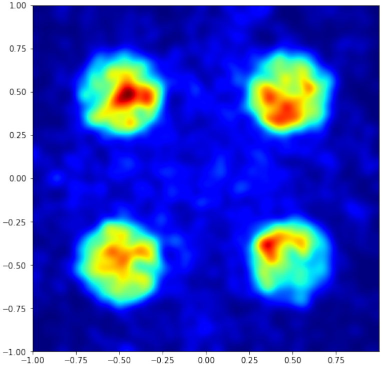


Figure: Estimate of $\tilde{\varphi}$

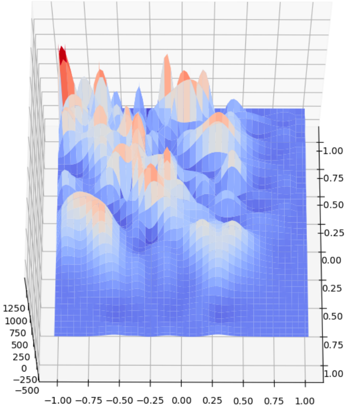
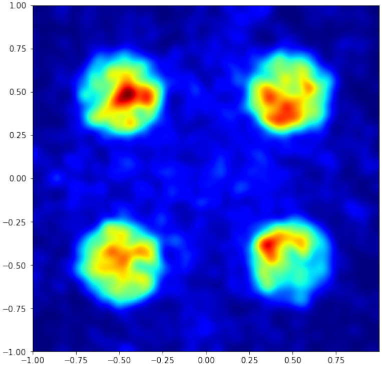


Figure: Estimate of φ



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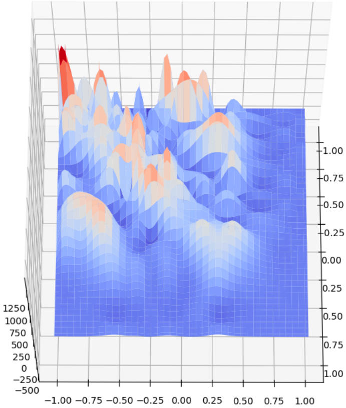

Figure: Estimate of φ

BUT...

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- Let $(R,\Upsilon) = ((R_t,\Upsilon_t)_{t\geq 0})$ denote the process in $D\times V$ that, from an initial configuration (r,υ), moves along the trajectory $r+\upsilon s$, $s\geq 0$ until it either exits the domain or, at rate $\alpha(r+\upsilon s,\upsilon)$, the process scatters and chooses a new velocity according to $\pi(r+\upsilon s,\upsilon,\cdot)$.
- Define the semigroup associated with the NRW via

$$\phi_t[g](r,\upsilon) := \mathbf{E}_{(r,\upsilon)}\left[\mathrm{e}^{\int_0^t \beta(R_s,\Upsilon_s)\mathrm{d}s} g(R_t,\Upsilon_t)\mathbf{1}_{(t<\tau_D)}\right],$$

for some bounded function $\beta : D\times V \to \mathbb{R}$.

Then

$$\phi_t[g](r,\upsilon) = g(r+\upsilon t,\upsilon)\mathbf{1}_{\{t<\kappa_{r,\upsilon}\}} - \int_0^t \left(\alpha(r+\upsilon s,\upsilon) - \beta(r+\upsilon s,\upsilon)\right)\phi_{t-s}[g](r+\upsilon s,\upsilon)\mathrm{d}s$$
$$+ \int_0^t \alpha(r+\upsilon s,\upsilon)\int_V \phi_{t-s}[g](r+\upsilon s,\upsilon')\pi(r+\upsilon s,\upsilon,\upsilon')\mathrm{d}\upsilon'\mathrm{d}s$$

Neutron random walk

- Let $(R, \Upsilon) = ((R_t, \Upsilon_t)_{t\geq 0})$ denote the process in $D \times V$ that, from an initial configuration (r, υ), moves along the trajectory $r + \upsilon s, s \geq 0$ until it either exits the domain or, at rate $\alpha(r + \upsilon s, \upsilon)$, the process scatters and chooses a new velocity according to $\pi(r + \upsilon s, \upsilon, \cdot)$.
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for some bounded function $\beta : D \times V \to \mathbb{R}$.

Then

$$\phi_t[g](r,\upsilon) = g(r+\upsilon t,\upsilon)\mathbf{1}_{\{t<\kappa_{r,\upsilon}\}} - \int_0^t \left(\alpha(r+\upsilon s,\upsilon) - \beta(r+\upsilon s,\upsilon)\right)\phi_{t-s}[g](r+\upsilon s,\upsilon)\mathrm{d}s$$

$$+ \int_0^t \alpha(r+\upsilon s,\upsilon)\int_V \phi_{t-s}[g](r+\upsilon s,\upsilon')\pi(r+\upsilon s,\upsilon,\upsilon')\mathrm{d}\upsilon'\mathrm{d}s$$

- Let $(R, \Upsilon) = ((R_t, \Upsilon_t)_{t\geq 0})$ denote the process in $D \times V$ that, from an initial configuration (r, υ), moves along the trajectory $r + \upsilon s$, $s \geq 0$ until it either exits the domain or, at rate $\alpha(r + \upsilon s, \upsilon)$, the process scatters and chooses a new velocity according to $\pi(r + \upsilon s, \upsilon, \cdot)$.

- Define the semigroup associated with the NRW via

$$\phi_t[g](r,\upsilon) := \mathbf{E}_{(r,\upsilon)}\left[\mathrm{e}^{\int_0^t \beta(R_s,\Upsilon_s)\mathrm{d}s} g(R_t,\Upsilon_t)\mathbf{1}_{(t<\tau_D)}\right],$$

  for some bounded function $\beta : D \times V \to \mathbb{R}$.

Then

$$\phi_t[g](r,\upsilon) = g(r+\upsilon t,\upsilon)\mathbf{1}_{\{t<\kappa_{r,\upsilon}\}} - \int_0^t \left(\alpha(r+\upsilon s,\upsilon) - \beta(r+\upsilon s,\upsilon)\right)\phi_{t-s}[g](r+\upsilon s,\upsilon)\mathrm{d}s$$
$$+ \int_0^t \alpha(r+\upsilon s,\upsilon)\int_V \phi_{t-s}[g](r+\upsilon s,\upsilon')\pi(r+\upsilon s,\upsilon,\upsilon')\mathrm{d}\upsilon'\mathrm{d}s$$

Neutron random walk

For $(r, \upsilon) \in D \times V$ and $\upsilon' \in V$, define

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

$$\pi(r,\upsilon,\upsilon') = \frac{\sigma_{\mathtt{s}}(r,\upsilon)\pi_{\mathtt{s}}(r,\upsilon,\upsilon') + \sigma_{\mathtt{f}}(r,\upsilon)\pi_{\mathtt{f}}(r,\upsilon,\upsilon')}{\alpha(r,\upsilon)},$$

$$\beta(r,\upsilon) = \alpha(r,\upsilon) - \sigma_{\mathtt{s}}(r,\upsilon) - \sigma_{\mathtt{f}}(r,\upsilon) = \sigma_{\mathtt{f}}(r,\upsilon)\left(m(r,\upsilon) - 1\right).$$

Lemma (Many-to-one)

Under the assumptions (H1) and (H2), for $(r,\upsilon) \in D \times V$, $g \in L^\infty_+(D \times V)$ and $t \geq 0$, the semigroup

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is also a solution to the NTE, and hence $\psi_t = \phi_t$.

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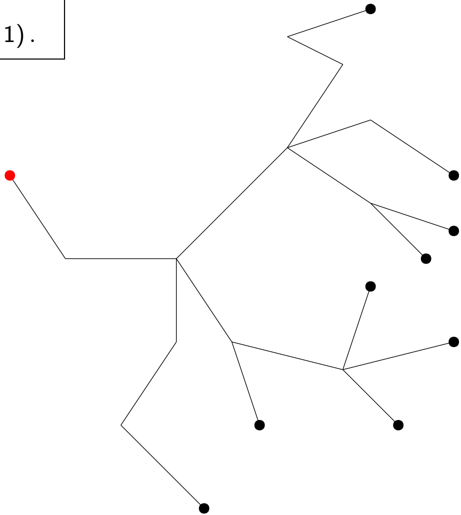
Neutron random walk

$$\alpha = \sigma_{\mathtt{s}} + \sigma_{\mathtt{f}}\, m,$$
$$\pi(r, \upsilon, \upsilon') = \frac{\sigma_{\mathtt{s}}\pi_{\mathtt{s}} + \sigma_{\mathtt{f}}\pi_{\mathtt{f}}}{\alpha},$$
$$\beta(r, \upsilon) = \sigma_{\mathtt{f}}\,(m - 1)\,.$$



Monte Carlo implications

From the Perron Frobenius result, we have

$$\phi_t[g] \sim \mathrm{e}^{\lambda_* t}\langle\tilde{\varphi}, g\rangle\varphi, \quad t \to \infty.$$

Using instead the NRW, we have

- $\lambda_* = \lim_{t\to\infty} \frac{1}{t}\log \phi_t[\mathbf{1}](r, v) = \lim_{t\to\infty} \frac{1}{t}\log \mathbf{E}_{(r,v)}\left[\mathrm{e}^{\int_0^t \beta(R_s,\Upsilon_s)\mathrm{d}s}\mathbf{1}_{t<\tau_D}\right].$
- $\langle\tilde{\varphi}, g\rangle\varphi(r, v) = \lim_{t\to\infty} \frac{1}{t}\int_0^t \mathrm{e}^{-\lambda_* s}\phi_s[g](r, v)\mathrm{d}s.$

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- $\langle\tilde{\varphi}, g\rangle\varphi(r, v) = \lim_{t\to\infty} \frac{1}{t} \int_0^t \mathrm{e}^{-\lambda_* s}\phi_s[g](r, v)\mathrm{d}s.$

BUT...

- Due to the Perron Frobenius theorem and the many-to-one representation,

$$\mathbb{E}_{\delta_{(r,\upsilon)}}[\langle\varphi, X_t\rangle] = \mathrm{e}^{\lambda_* t}\varphi(r,\upsilon) = \mathbf{E}_{(r,\upsilon)}\left[\mathrm{e}^{\int_0^t \beta(R_s,\Upsilon_s)\mathrm{d}s}\varphi(R_t,\Upsilon_t)\right].$$

- Thus,

$$W_t^1 := \mathrm{e}^{-\lambda_* t}\frac{\langle\varphi, X_t\rangle}{\varphi(r,\upsilon)} \quad \text{and} \quad W_t^2 := \mathrm{e}^{-\lambda_* t+\int_0^t \beta(R_s,\Upsilon_s)\mathrm{d}s}\frac{\varphi(R_t,\Upsilon_t)}{\varphi(r,\upsilon)}$$

are unit mean martingales under $\mathbb{P}_{\delta_{(r,\upsilon)}}$ and $\mathbf{P}_{(r,\upsilon)}$, respectively.

- We will study W_t^1 later. For now, we consider W_t^2. Define the change of measure

$$\left.\frac{\mathrm{d}\mathbf{P}^{\varphi}_{(r,\upsilon)}}{\mathrm{d}\mathbf{P}_{(r,\upsilon)}}\right|_{\mathcal{F}_t} = W_t^2.$$

- We would like to understand the processes $((R,\Upsilon),\mathbf{P}^{\varphi})$.

(H3) Fission offspring are bounded in number by the constant $n_{\max} > 1$.

Theorem (H., Kyprianou, Villemonais)

Under the assumptions (H1), (H2) and (H3) the process $((R, \Upsilon), \mathbf{P}^{\varphi})$ is a NRW, characterised by the scattering rate and kernel

$$K_{\varphi,r,\upsilon}\alpha(r,\upsilon) \quad \text{and} \quad K^{-1}_{\varphi,r,\upsilon}\frac{\varphi(r,\upsilon')}{\varphi(r,\upsilon)}\pi(r,\upsilon,\upsilon').$$

Moreover, it is conservative with stationary distribution $\varphi\tilde{\varphi}$.

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Moreover, it is conservative with stationary distribution $\varphi\tilde{\varphi}$.

BUT...

Some open questions/future research directions

- Monte Carlo techniques and complexity analysis
  - Biasing techniques/h-transform/twisted particle filters
  - Feynman-Kac models/population control/sequential Monte Carlo
  - Optimal number of particles/run time
  - Stability analysis
- Multitype processes:

$$
\begin{aligned}
\frac{\partial}{\partial t}\psi_t(i,r,\upsilon) = \upsilon\cdot\nabla\psi_t(i,r,\upsilon) - (\sigma^i_{\mathtt{s}}(r,\upsilon)+\sigma^i_{\mathtt{f}}(r,\upsilon))\psi_t(i,r,\upsilon) \\
+ \sigma^i_{\mathtt{s}}(r,\upsilon)\int_V \psi_t(i,r,\upsilon)\pi^i_{\mathtt{s}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon' \\
+ \sigma^i_{\mathtt{f}}(r,\upsilon)\sum_{j=1}^{\ell}\int_V \psi_t(j,r,\upsilon)\pi^{i,j}_{\mathtt{f}}(r,\upsilon,\upsilon')\mathrm{d}\upsilon'.
\end{aligned}
$$

To be continued...