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; measured in (# neutrons)/cm²/s.
- We want to describe neutron flux as a function of spatial position and time in complex domains:

$$\begin{split} \Psi(r,v,t), & r\in D\subseteq \mathbb{R}^d, v\in V:=\{v\in \mathbb{R}^d: v_{\min}\leq |v|\leq v_{\max}\},\\ \text{for } 0< v_{\min}< v_{\max}<\infty. \end{split}$$

NEUTRON FISSION



NEUTRON SCATTERING





NEUTRON TRANSPORT EQUATION

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

$$\begin{split} &\frac{\partial \Psi_g}{\partial t}(t,r,\upsilon) + \upsilon \cdot \nabla \Psi_g(t,r,\upsilon) + \sigma(r,\upsilon)\Psi_g(t,r,\upsilon) \\ &= Q(r,\upsilon,t) + \int_V \Psi_g(r,\upsilon',t)\sigma_s(r,\upsilon')\pi_s(r,\upsilon',\upsilon)d\upsilon' + \int_V \Psi_g(r,\upsilon',t)\sigma_f(r,\upsilon')\pi_f(r,\upsilon',\upsilon)d\upsilon', \end{split}$$

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

- $\sigma_{s}(r, v'): \text{ the rate at which scattering occurs from incoming velocity } v',$ $\sigma_{f}(r, v'): \text{ the rate at which fission occurs from incoming velocity } v',$ $\sigma(r, v): \text{ the sum of the rates } \sigma_{f} + \sigma_{s} \text{ and is known as the cross section,}$ $\pi_{s}(r, v', v) dv': \text{ the scattering yield at velocity } v \text{ from incoming velocity } v',$ $\text{ satisfying } \pi_{s}(r, v, V) = 1, \text{ and}$
- $\begin{aligned} \pi_{\rm f}(r,\upsilon',\upsilon){\rm d}\upsilon': \mbox{ the neutron yield at velocity }\upsilon \mbox{ from fission with incoming velocity }\upsilon', \\ \mbox{ satisfying } \pi_{\rm f}(r,\upsilon,V) < \infty \mbox{ and } \end{aligned}$

Q(r, v, 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 which represent 'fission containment'

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

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

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NEUTRON TRANSPORT EQUATION

$$\begin{split} &\frac{\partial \Psi_g}{\partial t}(t,r,\upsilon) + \upsilon \cdot \nabla \Psi_g(t,r,\upsilon) + \sigma(r,\upsilon)\Psi_g(t,r,\upsilon) \\ &= \int_V \Psi_g(r,\upsilon',t)\sigma_{\scriptscriptstyle \rm S}(r,\upsilon')\pi_{\scriptscriptstyle \rm S}(r,\upsilon',\upsilon)\mathrm{d}\upsilon' + \int_V \Psi_g(r,\upsilon',t)\sigma_{\scriptscriptstyle \rm T}(r,\upsilon')\pi_{\scriptscriptstyle \rm T}(r,\upsilon',\upsilon)\mathrm{d}\upsilon', \end{split}$$

 With some rearrangements, the components of NTE separate into transport, scattering and fission. Specifically,

$$\begin{cases} \mathbb{T}g(r,v) &:= -v \cdot \nabla g(r,v) - \sigma(r,v)g(r,v) & \text{(forwards transport)} \\ Sg(r,v) &:= \int_V g(r,v')\sigma_s(r,v')\pi_s(r,v',v)dv' & \text{(forwards scattering)} \\ \mathbb{F}g(r,v) &:= \int_V g(r,v')\sigma_g(r,v')\pi_g(r,v',v)dv' & \text{(forwards fission)} \end{cases}$$

More natural to look for solutions as time-varying in $L^2(D \times V)$ so that, for $f \in L^2(D \times V)$,

$$\frac{\partial}{\partial t} \langle f, \Psi_g(t, \cdot, \cdot) \rangle = \langle f, (\mathbb{T} + \mathbb{S} + \mathbb{F}) \Psi_g(t, \cdot, \cdot) \rangle$$

Abstract Cauchy problem - taking the problem into the domain of c₀-semigroups

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Abstract Cauchy problem - taking the problem into the domain of c_0 -semigroups

• Written more simply with everything in understood in the $L^2(D \times V)$ space

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

 \triangleright c₀-semigroup allows us to see the solution to this problem as the orbit in L^2 space:

$$\Psi_g(t,r,\upsilon) = \mathrm{e}^{(\mathrm{T}+\mathrm{S}+\mathrm{F})t}g(r,\upsilon), \qquad t \ge 0,$$

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where $e^{(T+S+F)t} = \sum_{k=0}^{\infty} (T+S+F)^k t^k / k!$

- More generally can replace $L^2(D \times V)$ by $L^p(D \times V)$ for $p \in (1, \infty)$.
- Problems occur for the transport operator if one is to look at $L^1(D \times V)$ or $L^{\infty}(D \times V)$: A shame as this is normally where we do probability theory!

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What constitutes a nuclear reactor?



Heuristically we want to find an eigenvalue $\lambda \in \mathbb{R}$, positive eigenfunction pair $h: D \times V \to [0, \infty)$ and \tilde{h} on $D \times V$ such that, ideally with $\lambda = 0$

Forwards: $\lambda \langle h, f \rangle = \langle h, (T + S + F)f \rangle$ and $\lambda \langle g, \tilde{h} \rangle = \langle g, (T + S + F)\tilde{h} \rangle$

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The eigenfunction h is called an *importance map* and gives the first order neutron flux (radioactivity) profile

Roughly speaking, now as an Abstract Cauchy Problem on $L^2(D \times V)$,

 $\frac{\partial \psi_h}{\partial t} = (\mathbb{T} + \mathbb{S} + \mathbb{F})\psi_h, \qquad \psi_h = h \text{ at } t = 0 \text{ and } \psi_h = 0 \text{ for } r \in \partial D, v \cdot \mathbf{n}_r > 0$

the solution can be thought of as

$$\psi_{h}(t,r,\upsilon) = \mathrm{e}^{(\mathrm{T}+\mathrm{S}+\mathrm{F})t}h(r,\upsilon) := \sum_{k\geq 0} \frac{t^{k}}{k!}(\mathrm{T}+\mathrm{S}+\mathrm{F})^{k}h(r,\upsilon)$$

• Hence for $f \in L^2(D \times V)$,

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Said another way

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- T is a nasty (unbounded) operator making it harder than usual to find eigenfunctions, S and F are nice (bounded) operators whose spectral analysis is easier to handle.
- In looking for λ, h as a lead eigen pair we need

$$(\mathbf{T} + \mathbf{S} + \mathbf{F})h = \lambda h \implies (\mathbf{T} - \lambda I)^{-1}(\mathbf{S} + \mathbf{F})h = h$$

Fix μ, use either operator perturbation methods or Krein-Rutman Theorem to deduce that (as a linear operator on an L² space),

$$(\mathbf{T} - \mu I)^{-1}(\mathbf{S} + \mathbf{F})$$

has a spectral radius r_{μ} and positive eigenfunction h_{μ}

- Verify that r_{μ} varies continuously with μ on a range $(0, r^*)$, where $r^* > 1$.
- Now vary μ and find λ_* such that $r_{\lambda_*} = 1$. The accompanying eigenfunction is h and together they solve

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Projecting onto the lead eigenvalue, $\exists \varepsilon > 0$:

 $\mathrm{e}^{-\lambda_* t} \psi_g(t,r,\upsilon) \sim h(r,\upsilon) \langle \tilde{h},g \rangle + O(\mathrm{e}^{-\varepsilon t})$

Theorem

Let D be convex. Assume that $\sigma_{\mathcal{E}}(r, \upsilon) \pi_{\mathcal{E}}(r, \upsilon, \upsilon')$ and $\sigma_{\mathcal{S}}(r, \upsilon) \pi_{\mathcal{S}}(r, \upsilon, \upsilon')$ are piece-wise continuous and uniformly bounded from above and below on $D \times V \times V$. Then,

 (i) the neutron transport operator (T + S + F) has a leading eigenvalue λ_{*} ∈ ℝ, which is simple and isolated and which has a corresponding positive right and left eigenfunctions in L₂(D × V), h and h
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(ii) there exists an $\varepsilon > 0$ such that, as $t \to \infty$,

$$||e^{-\lambda_* t}\psi_g(t,\cdot,\cdot) - \langle \tilde{h}, g \rangle h||_2 = O(e^{-\varepsilon t}),$$
(1)

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

The sign of λ_* dictates the criticality of the system:

- ▶ $\lambda_* < 0$: subcritical and fission dies out
- $\lambda_* = 0$: critical, i.e. a nuclear reactor
- ▶ $\lambda_* > 0$: supercritical (not quite a bomb, that would be non-existence of λ_*)

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OVER WHAT DOMAINS DO WE NEED EIGENFUNCTIONS OF THE NTE?



▶ Note that, for $f, g \in L^2(D \times V)$, with f respecting the boundary condition g(r, v) = 0 for $r \in \partial D$ if $v \cdot \mathbf{n}_r < 0$, we can verify with a simple integration by parts that

$$\langle f, \upsilon \cdot \nabla g \rangle = \int_{\partial D \times V} (\upsilon \cdot \upsilon') f(r, \upsilon') g(r, \upsilon') dr d\upsilon' - \langle \upsilon \cdot \nabla f, g \rangle = -\langle \upsilon \cdot \nabla f, g \rangle$$

providing we insist that *f* respects the boundary f(r, v) = 0 for $r \in \partial D$ if $v \cdot \mathbf{n}_r > 0$. Moreover, Fubini's theorem also tells us that, for example, with $f, g \in L^2(D \times V)$,

$$\langle f, \int_V g(\cdot, \upsilon') \sigma_{\mathfrak{s}}(\cdot, \upsilon') \pi_{\mathfrak{s}}(\cdot, \upsilon', \cdot) \mathrm{d}\upsilon' \rangle = \langle \sigma_{\mathfrak{s}}(\cdot, \cdot) \int_V f(\cdot, \upsilon) \pi_{\mathfrak{s}}(\cdot, \cdot, \upsilon) \mathrm{d}\upsilon, g \rangle.$$

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

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

where

$$\begin{cases} \mathcal{T}f(r,v) &:= v \cdot \nabla f(r,v) & \text{(backwards transport)} \\ \mathcal{S}f(r,v) &:= \sigma_{s}(r,v) \int_{V} f(r,v') \pi_{s}(r,v,v') dv' - \sigma_{s}(r,v) f(r,v) & \text{(backwards scattering)} \\ \mathcal{F}f(r,v) &:= \sigma_{f}(r,v) \int_{V} f(r,v') \pi_{f}(r,v,v') dv' - \sigma_{f}(r,v) f(r,v) & \text{(backwards fission)} \end{cases}$$

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 $L^2(D \times V)$,

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

with additional boundary conditions

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

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UNDERLYING STOCHASTICS (LEADING TO MONTE-CARLO)

▶ Backwards equation lends itself well to stochastic representation in the *L*₂ sense,

$$\begin{split} \frac{\partial \psi}{\partial t}(t,r,\upsilon) &= \upsilon \cdot \nabla \psi(t,r,\upsilon) - \sigma(r,\upsilon)\psi(t,r,\upsilon) \\ &+ \sigma_{s}(r,\upsilon) \int_{V} \psi(r,\upsilon',t)\pi_{s}(r,\upsilon,\upsilon') d\upsilon' + \sigma_{f}(r,\upsilon) \int_{V} \psi(r,\upsilon',t)\pi_{f}(r,\upsilon,\upsilon') d\upsilon', \end{split}$$

- 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 $\{(r_i(t), v_i(t)) : i = 1, ..., N_t\}$, where N_t is the number of particles alive at time $t \ge 0$.
- Represent as a process in the space of the atomic measures

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

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

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

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- A particle position at *r* with velocity v (configuration (r, v)) will continue to move along the trajectory r + vt, until one of the following things happens.
- ▶ The particles that leave the physical domain *D* are killed.
- For a neutron with configuration (r, v), if T_s is the random time that scattering may occur, then

$$\Pr(T_{s} > t) = \exp\left\{-\int_{0}^{t} \sigma_{s}(r + \upsilon t, \upsilon)) \mathrm{d}s\right\}.$$

- ▶ When scattering occurs at space-velocity (r, v), the new velocity is selected independently with probability π_s(r, v, v')dv'.
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MILD EQUATION

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

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

and the advection semigroup

$$U_t[g](r,\upsilon) = g(r+\upsilon t,\upsilon)\mathbf{1}_{\{t < \kappa_{r,\upsilon}^D\}}, \qquad t \ge 0.$$

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

Lemma

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

$$\phi_t[g] = U_t[g] + \int_0^t U_s[(\mathcal{S} + \mathcal{F})\phi_{t-s}[g]] \mathrm{d}s, \qquad t \ge 0.$$

Lemma

The mild solution $(\phi_t, t \ge 0)$, is dual to $(\psi(t, \cdot, \cdot), t \ge 0)$ on $L_2(D \times V)$, i.e.

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EIGENFUNCTIONS OF THE EXPECTATION SEMI-GROUP?

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 $\tilde{h} \in L_2(D \times V)$, e.g.

$$\langle f, \phi_t[\tilde{h}] \rangle = \langle \psi_f(t, \cdot, \cdot), \tilde{h} \rangle = \mathrm{e}^{\lambda t} \langle f, \tilde{h} \rangle$$

suggesting (at least in the $L_2(D imes V)$ sense)

$$\phi_t[\tilde{h}](r,\upsilon) = \mathbb{E}_{\delta_{(r,\upsilon)}}[\langle \tilde{h}, X_t \rangle] := \mathrm{e}^{\lambda t} \tilde{h}(r,\upsilon)$$

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 \Rightarrow points us towards Monte-Carlo methods - especially when $\lambda = 0$

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

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$$\langle f, \phi_t[\tilde{h}] \rangle = \langle \psi_f(t, \cdot, \cdot), \tilde{h} \rangle = \mathrm{e}^{\lambda t} \langle f, \tilde{h} \rangle$$

suggesting (at least in the $L_2(D \times V)$ sense)

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 \Rightarrow points us towards Monte-Carlo methods - especially when $\lambda = 0$

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EIGENFUNCTIONS OF THE EXPECTATION SEMI-GROUP?

So far

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

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PERRON-FROBENIUS AGAIN

Recent work of Champagnat and Villemonais on quasi-stationary distributions for Markov semigroups (in the spirit of Tweedie's *R*-theory) allows us to conclude the following

Theorem

Suppose that D is non-empty and convex,

$$\underline{\beta} := \inf_{r \in D, v \in V} \sigma_{f}(r, v) \left(\int_{V} \pi_{f}(r, v, v') \mathrm{d}v' - 1 \right) > 0.$$

Then there exists a $\lambda_* \in \mathbb{R}$, a positive 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 $e^{\lambda_c t}$, 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 $g \in L^+_{\infty}(D \times V)$

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

Moreover, there exists $\varepsilon > 0$ *such that, for all* $g \in L^+_{\infty}(D \times V)$ *,*

$$\left\| \mathrm{e}^{-\lambda_* t} \varphi^{-1} \phi_t[g] - \langle \tilde{\varphi}, g \rangle \right\|_{\infty} = O(\mathrm{e}^{-\varepsilon t}) \text{ as } t \to +\infty.$$

STOCHASTIC PERRON-FROBENIUS

Theorem

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,

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

almost surely, where W_{∞} is a special random variable (in fact a martingale limit). Moreover, W_{∞} is positive with positive probability if and only if $\lambda_* > 0$, otherwise $W_{\infty} = 0$.

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We are now Monte-Carlo-Ready

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

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

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

and e.g.

$$\frac{\varphi(r,v)}{\varphi(r_0,v_0)} = \lim_{t \to \infty} \frac{\phi_t[g](r,v)}{\phi_t[g](r_0,v_0)} = \lim_{t \to \infty} \frac{\mathbb{E}_{\delta(r,v)}[\langle g, X_t \rangle]}{\mathbb{E}_{\delta_{(r_0,v_0)}}[\langle g, X_t \rangle]}$$

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MONTE-CARLO, IMPORTANCE MAP AND SUPERCOMPUTERS

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MONTE-CARLO, IMPORTANCE MAP AND SUPERCOMPUTERS







OOPS...



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PROBLEM!

Needs a massive supercomputer to deal with an industrial scale simulation

Simulating (inhomogeneous) branching trees is no joke: cannot be parallelised.

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$Many\mbox{-}to\mbox{-}one \mbox{ and } Monte\mbox{-}Carlo\mbox{ parallelisation}$

Recall semigroup operators

$$\mathcal{T}f(r,v) := v \cdot \nabla f(r,v) \qquad (backwards transport)$$

$$\mathcal{S}f(r,v) := \sigma_{s}(r,v) \int_{V} (f(r,v') - f(r,v)) \pi_{s}(r,v,v') dv' \qquad (backwards scattering)$$

$$\mathcal{F}f(r,v) := \sigma_{f}(r,v) \int_{V} f(r,v') \pi_{f}(r,v,v') dv' - \sigma_{f}(r,v) f(r,v) \qquad (backwards fission)$$

$$P Basic algebra gives$$

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

where

$$\begin{split} \alpha(r,\upsilon) &:= \sigma_{\mathfrak{s}}(r,\upsilon) + \sigma_{\mathfrak{f}}(r,\upsilon) \int_{V} \pi_{\mathfrak{f}}(r,\upsilon,\upsilon') \mathrm{d}\upsilon', \\ \pi(r,\upsilon,\upsilon') \mathrm{d}\upsilon' &:= \alpha^{-1}(r,\upsilon) \left[\sigma_{\mathfrak{s}}(r,\upsilon) \pi_{\mathfrak{s}}(r,\upsilon,\upsilon') \mathrm{d}\upsilon' + \sigma_{\mathfrak{f}}(r,\upsilon) \pi_{\mathfrak{f}}(r,\upsilon,\upsilon') \mathrm{d}\upsilon' \right], \\ \beta(r,\upsilon) &:= \alpha(r,\upsilon) - \sigma_{\mathfrak{s}}(r,\upsilon) - \sigma_{\mathfrak{f}}(r,\upsilon). \end{split}$$

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MANY-TO-ONE AND MONTE-CARLO PARALLELISATION

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

$$\mathcal{L}f(r,\upsilon) = \upsilon \cdot \nabla f(r,\upsilon,t) + \alpha(r,\upsilon) \int_{V} (f(r,\upsilon',t) - f(r,\upsilon,t)) \pi(r,\upsilon,\upsilon') d\upsilon'$$

implies

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

for $t \ge 0, r \in D, v \in V$, where

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

and $((R_t, \Upsilon_t), t \ge 0)$ with probabilities $\mathbf{P}_{(r,\upsilon)}, r \in V, \upsilon \in D$, is the \mathcal{L} -neutron random walk.

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



IMPORTANCE SAMPLING

- Pick a 'first guess' of φ , denoted here by η , that satisfies $\eta(r, v) = 0$ for $r \in \partial D$ if $v \cdot \mathbf{n}_r > 0$.
- Perform the Doob η-transform

$$\frac{\mathrm{d}\mathbf{P}^{\eta}_{(r,\upsilon)}}{\mathrm{d}\mathbf{P}_{(r,\upsilon)}}\bigg|_{\sigma\left((R_{s},\Upsilon_{s}),s\leq t\right)} := \exp\left(-\int_{0}^{t}\frac{\mathcal{L}\eta(R_{s},\Upsilon_{s})}{\eta(R_{s},\Upsilon_{s})}\mathrm{d}s\right)\frac{\eta(R_{t},\Upsilon_{t})}{\eta(r,\upsilon)}\mathbf{1}_{(t<\tau^{D})}$$

Gives new neutron random walk characterised by

$$\mathcal{L}_{\eta}f(r,\upsilon) = \upsilon \cdot \nabla f(r,\upsilon) + \alpha(r,\upsilon) \int_{V} \left(g(r,\upsilon') - g(r,\upsilon) \right) \frac{\eta(r,\upsilon')}{\eta(r,\upsilon)} \pi(r,\upsilon,\upsilon') d\upsilon'.$$

Lemma

Moreover,

$$\begin{split} \psi_t[g](r,\upsilon) &= \mathsf{E}_{(r,\upsilon)}^{\eta} \Bigg[\exp\left\{ \int_0^t \left(\frac{\overleftarrow{k} \eta(R_s,\Upsilon_s)}{\eta(R_s,\Upsilon_s)} + \beta(R_s,\Upsilon_s) - \alpha(R_s,\Upsilon_s) \right) \, \mathrm{d}s \right\} \\ &\qquad \times \prod_{i=1}^{N_t} \frac{\eta(R_{T_i},\Upsilon_{T_{i-1}})}{\eta(R_{T_i},\Upsilon_{T_i})} g(R_t,\Upsilon_t) \mathbf{1}_{(t<\tau^D)} \Bigg] \end{split}$$

where

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Moreover,

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Want to choose η so that the Neutron Random Walk \mathcal{L}_{η} remains trapped in *D*

Theorem *A sufficient condition on* η *for* (R, Υ) *under* \mathbf{P}^{η} *to be conservative is that*

 $\inf_{r \in \partial D, v \cdot \mathbf{n}_r > 0} |v \cdot \nabla \eta(r, v)| > 0$



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Theorem

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IMPORTANCE SAMPLING: INTERVAL REACTOR


Complexity analysis of rates of convergence of Monte-Carlo schemes

- Hybrid constrained neutron branching / random walk methods
- Stochastic growth methods at criticality e.g. conditionally on survival,

$$\lim_{t\to\infty} \operatorname{Law}\left(\left.\frac{1}{t}\langle f, X_t\rangle\right|\langle 1, X_t\rangle\right) \sim^d \mathbf{e}$$

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- Fleming-Viot methods (resampling / bootstrapping)
- Scalable for industry?

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where **e** is an exponential distribution.

Fleming-Viot methods (resampling / bootstrapping)

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- Fleming-Viot methods (resampling / bootstrapping)
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Thank you!

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