# Neutron Transport Monte-Carlo and the Many-to-one Short-cut

Andreas Kyprianou
Alex Cox, Simon Harris, Emma Horton, Minmin Wang

University of Bath, U.K.

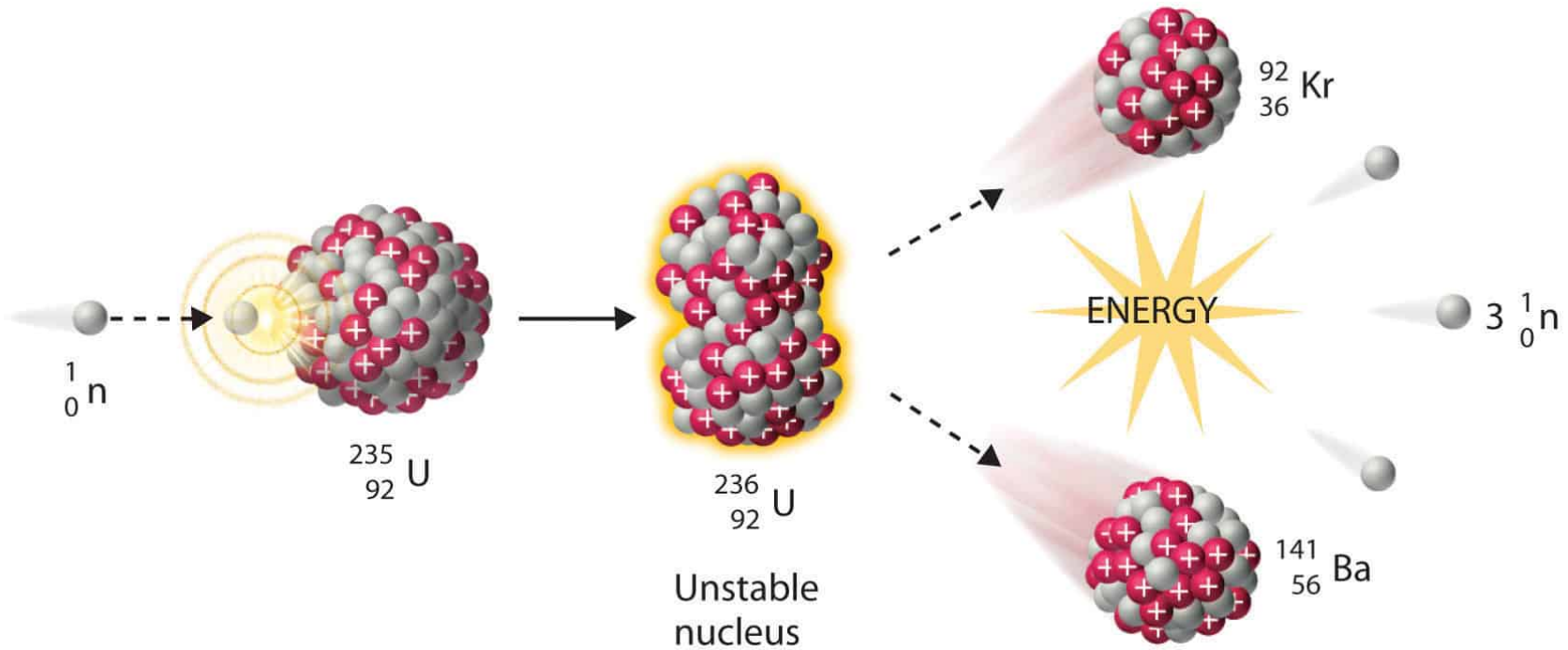
# Neutron Flux

- We want to describe neutron flux as a function of spatial position and time in complex domains:

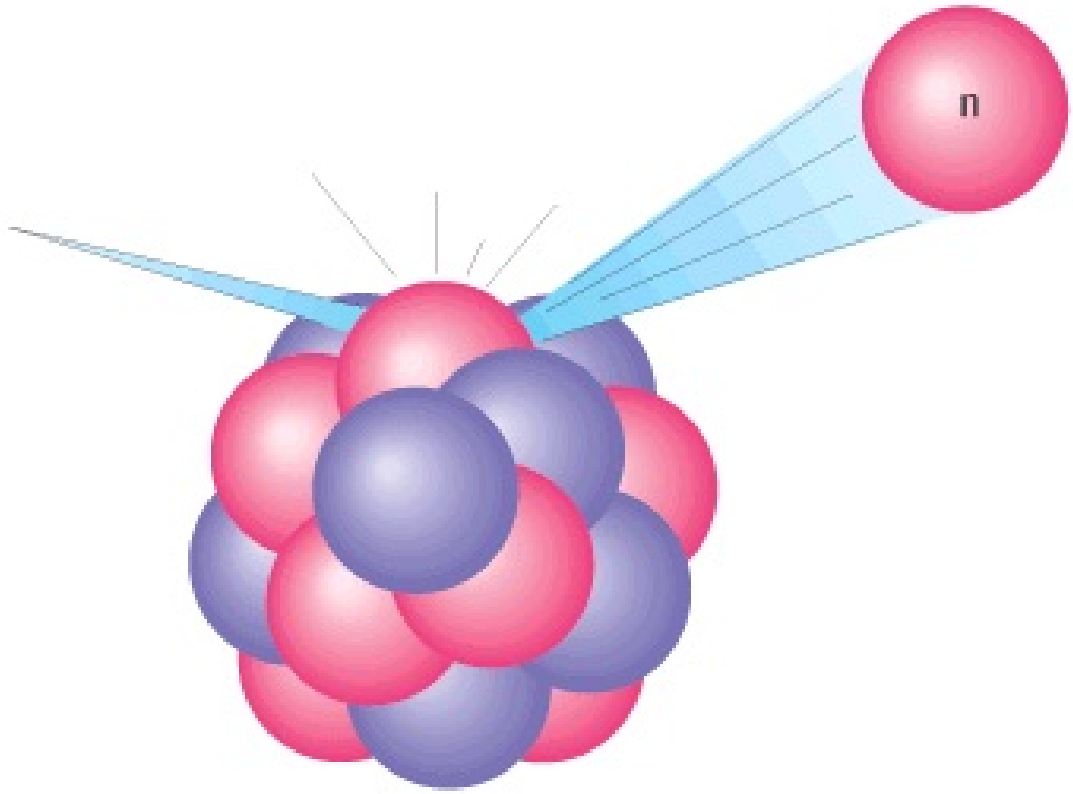
$$\Psi(r, \upsilon, t), \qquad r \in D \subseteq \mathbb{R}^d, \upsilon \in V := [\upsilon_{\mathtt{min}}, \upsilon_{\mathtt{max}}] \times \mathbb{S}_2,$$

for $0 < \upsilon_{\mathtt{min}} < \upsilon_{\mathtt{max}} < \infty$.

# Neutron Fission



# Neutron Scattering



# (Forward) Neutron Transport Equation

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

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

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

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

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

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

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

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

$Q(r, v, t)$ : non-negative source term.

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

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# Boundary conditions

- Boundary conditions which represent 'fission containment'

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

- $\mathbf{n}_r$ 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 $\to$Backwards) Neutron Transport Equation

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

- Remove the source term $Q = 0$
- The notion of a solution of the form NTE turns out to be too strong to expect a natural solution (continuity and regularity become problematic with the advection term).
- With some rearrangements, the components of NTE separate into transport, scattering and fission. Specifically,

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

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

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

# (Forward $\to$Backwards) Neutron Transport Equation

- Adjoint operators in $f, g \in L^2(D \times V)$:

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

where

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

- This leads us to the so called *backwards neutron transport equation* (which is also known as the *adjoint neutron transport equation*) given by

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

with additional boundary conditions

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

# UNDERLYING STOCHASTICS

- Backwards equation lends itself well to stochastic representation,

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

- 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 $\delta$ 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

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

# Neutron branching process

- A particle position at $r$ with velocity $v$ (configruration $(r, v)$) 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

$$\Pr(T_s > t) = \exp\left\{-\int_0^t \sigma_s(r + vt, v))\mathrm{d}s\right\}.$$

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

$$\Pr(T_f > t) = \exp\left\{-\int_0^t \sigma_f(r + vt, v))\mathrm{d}s\right\}.$$

- When fission occurs at location $r \in \mathbb{R}^d$ from a particle with incoming velocity $v \in V$, the quantity $\pi_f(r, v, v')\mathrm{d}v'$ describes the average number of particles released from nuclear fission with outgoing velocity in the infinitesimal neighbourhood of $v'$.
- 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.

# STEADY-STATE REACTORS

- What constitutes a nuclear reactor?
- Look for an associated triple of eigenvalue $\lambda \in \mathbb{R}$, positive eigenfunction pair $\varphi : \bar{D} \times V \to [0, \infty)$ and $\tilde{\varphi}$ on $\bar{D} \times V$ in $L^2(D \times V)$ satisfying boundary conditions

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

  so that that with $\lambda = 0$

  $$\text{“}(\mathtt{T} + \mathtt{S} + \mathtt{F})\tilde{\varphi} = 0\text{”}$$

  Backwards : $\lambda\langle f, \varphi\rangle = \langle(\mathcal{T} + \mathcal{S} + \mathcal{F})\varphi, f\rangle$ and $\lambda\langle\tilde{\varphi}, f\rangle = \langle(\mathcal{T} + \mathcal{S} + \mathcal{F})f, \tilde{\varphi}\rangle$.

  so that that with $\lambda = 0$

  $$\text{“}(\mathcal{T} + \mathcal{S} + \mathcal{F})\varphi = 0\text{”}$$

- $\varphi$ is the importance map giving a radiation profile in steady state ($\lambda = 0$).

# QUASI-STATIONARITY AND MARTINGALES

- The eigen function $\tilde{\varphi}$ is a quasi-stationary distribution for the neutron branching process

$$\int_{D\times V} \tilde{\varphi}(r,v)\mathbb{E}_{\delta_{(r,v)}}[\langle g, X_t\rangle] = \langle \tilde{\varphi}, g\rangle$$

- The importance map makes

$$\langle \varphi, X_t\rangle, \qquad t \geq 0.$$

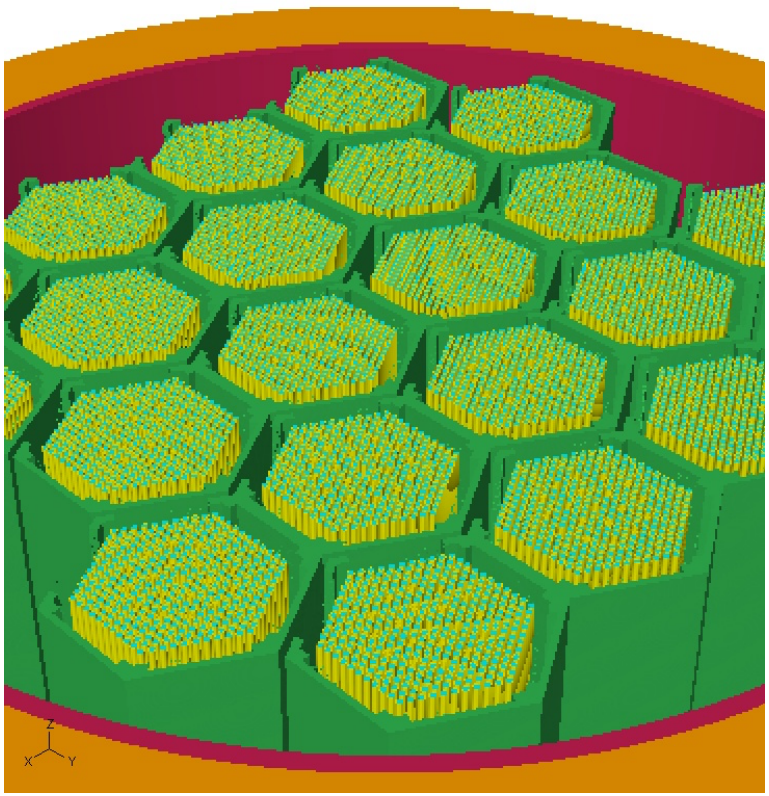
  a martingale. Which means

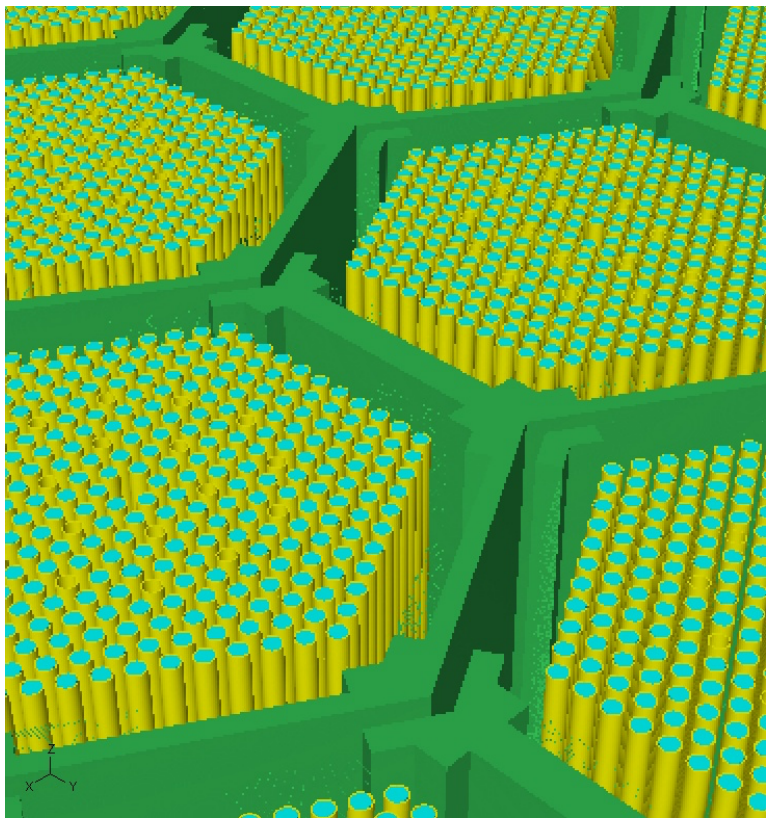
$$\mathbb{E}_{\delta_{(r,v)}}[\langle \varphi, X_t\rangle] = \varphi(r,v)$$

- We also know that by projecting onto the lead eigenvalue

$$\mathbb{E}_{\delta_{(r,v)}}[\langle g, X_t\rangle] = \psi_g(t,r,v) \sim \varphi(r,v)\langle \tilde{\varphi}, g\rangle + O(\mathrm{e}^{-\varepsilon t})$$

# Monte-Carlo complexity





# Many-to-one and Monte-Carlo parallelisation

- Recall semigroup operators

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

- Write $\mathcal{L} = \mathcal{T} + \mathcal{S} + \mathcal{F}$. Basic algebra gives

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

where

$$\begin{aligned}
\alpha(r,v) &:= \sigma_{\mathtt{s}}(r,v) + \sigma_{\mathtt{f}}(r,v)\int_V \pi_{\mathtt{f}}(r,v,v')\mathrm{d}v',\\
\pi(r,v,v')\mathrm{d}v' &:= \alpha^{-1}(r,v)\left[\sigma_{\mathtt{s}}(r,v)\pi_{\mathtt{s}}(r,v,v')\mathrm{d}v' + \sigma_{\mathtt{f}}(r,v)\pi_{\mathtt{f}}(r,v,v')\mathrm{d}v'\right],\\
\beta(r,v) &:= \alpha(r,v) - \sigma_{\mathtt{s}}(r,v) - \sigma_{\mathtt{f}}(r,v).
\end{aligned}$$

# MANY-TO-ONE

- Recall that,

$$\frac{\partial \psi_g}{\partial t} = (\mathcal{T} + \mathcal{S} + \mathcal{F})\psi_g, \qquad \psi_g = g \text{ at } t = 0 \text{ and } \psi_g = 0 \text{ for } r \in \partial D, v \cdot \mathbf{n}_r < 0$$

has stochastic representation

$$\psi_g(t, r, v) = \mathbb{E}_{\delta_{(r,v)}}[\langle g, X_t \rangle]$$

for neutron branching process $(X_t, t \geq 0)$.

- The representation

$$(\mathcal{T} + \mathcal{S} + \mathcal{F})f(r, v)$$
$$= \underbrace{v \cdot \nabla f(r, v, t) + \alpha(r, v) \int_V \big(f(r, v', t) - f(r, v, t)\big)\pi(r, v, v')\mathrm{d}v'}_{=:\mathcal{L}f} + \beta(r, v)f(r, v)$$

implies

$$\psi_g(t, r, v) = \mathbf{E}_{(r,v)}\left[\mathrm{e}^{\int_0^t \beta(R_u, \Upsilon_u)\mathrm{d}u} g(R_t, \Upsilon_t)\mathbf{1}_{(t<\tau^D)}\right], \qquad t \geq 0, r \in \bar{D}, v \in V.$$

where $((R_t, \Upsilon_t), t \geq 0)$ is the *neutron random walk* associated to $\mathcal{L}$ and

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

# Many-to-one

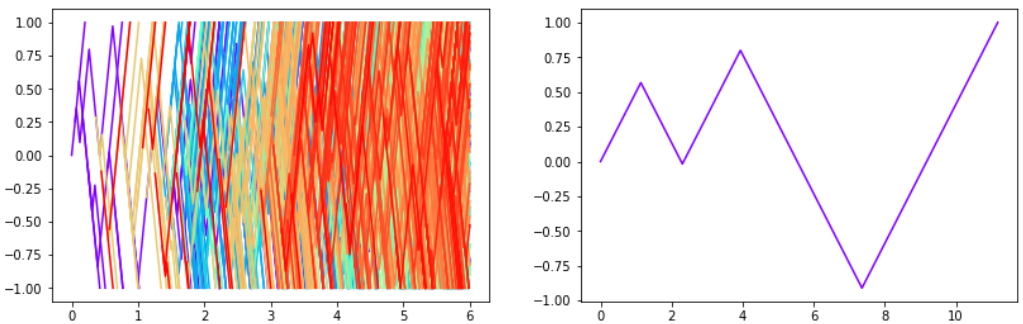
- Solving "$(\mathcal{T}+\mathcal{S}+\mathcal{F})\varphi = \mathcal{L}\varphi = 0$" now means

$$\mathrm{e}^{\int_0^t \beta(R_u,\Upsilon_u)\mathrm{d}u}\varphi(R_t,\Upsilon_t)\mathbf{1}_{(t<\tau^D)}, t \geq 0$$

  is a martingale.
- Which means

$$\mathbf{E}_{(r,v)}\left[\mathrm{e}^{\int_0^t \beta(R_u,\Upsilon_u)\mathrm{d}u}\varphi(R_t,\Upsilon_t)\mathbf{1}_{(t<\tau^D)}\right] = \varphi(r,v)$$

  Here the process
- This affords new parallelisable opportunities to Monte-Carlo solve numerically for the importance map:



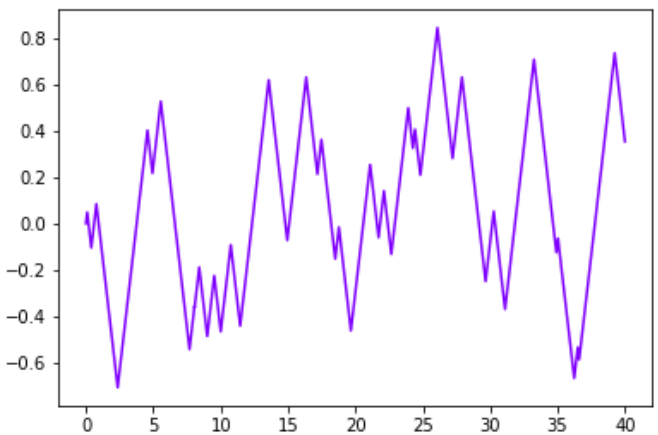
# IMPORTANCE SAMPLING

- Importance sampling and MC efficiencies: Pick a 'first guess' of $\varphi$ (lets call it $h$) and "change the statistics of the neutron random walk"
- Gives new neutron random walk characterised by

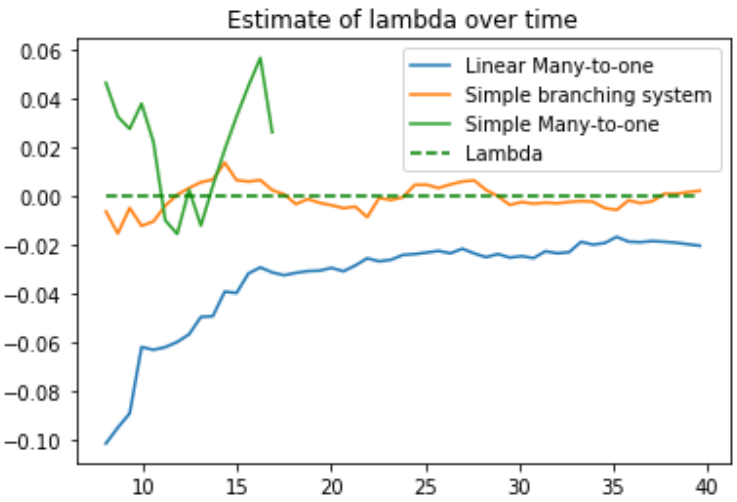
$$\mathcal{L}_h f(r,v) = v \cdot \nabla f(r,v) + \int_V \left(g(r,v') - g(r,v)\right) \frac{h(r,v')}{h(r,v)} \pi(r,v,v') \mathrm{d}v'.$$

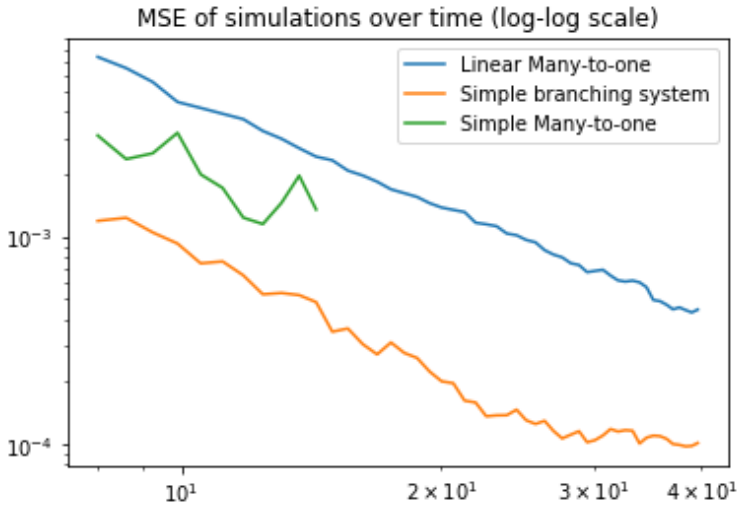
Moreover,

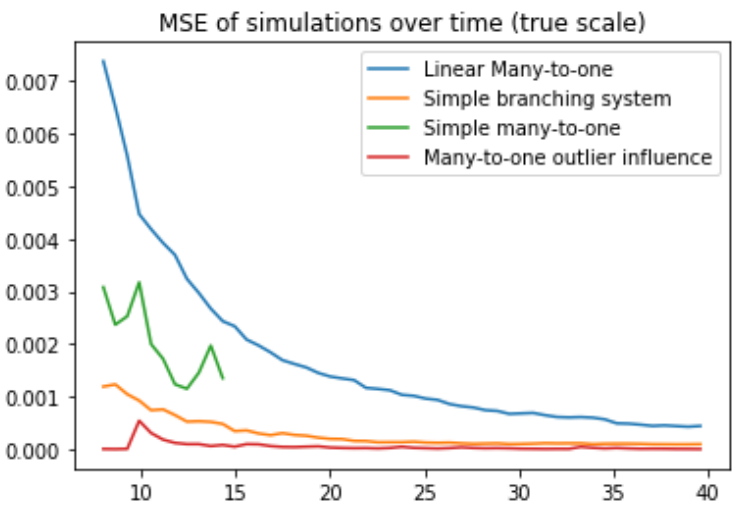
$$\psi_g(t,r,v) = \mathbf{E}^h_{(r,v)} \left[ \exp\left( \int_0^t \frac{(\mathcal{L}+\beta)h(R_s,\Upsilon_s)}{h(R_s,\Upsilon_s)} \mathrm{d}s \right) \frac{h(R_t,\Upsilon_t)^{-1}}{h(r,v)^{-1}} g(R_t,\Upsilon_t) \right]$$

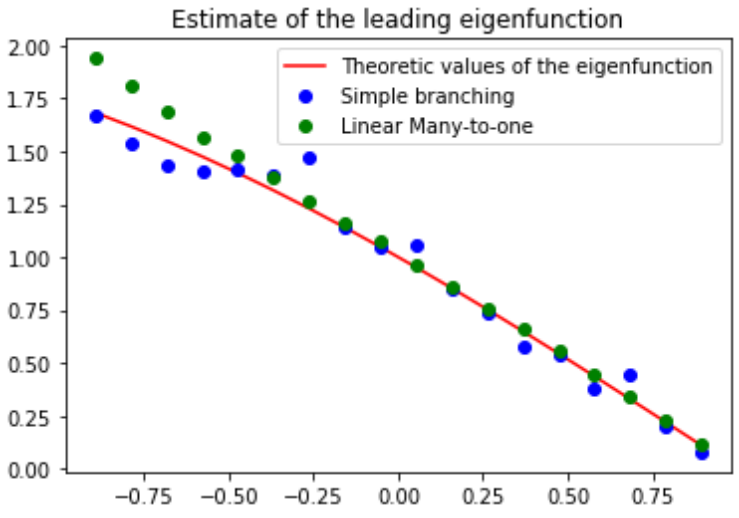


# Importance sampling



Thank You!