Mathematics of Radiation Transport Modelling

through the eyes of a probabilist

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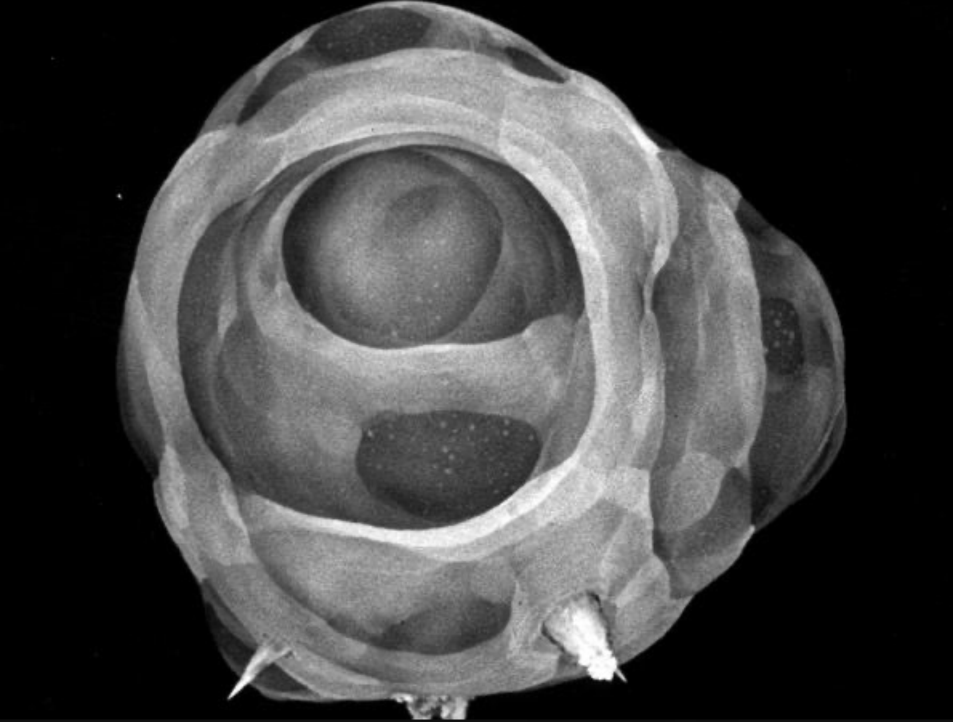
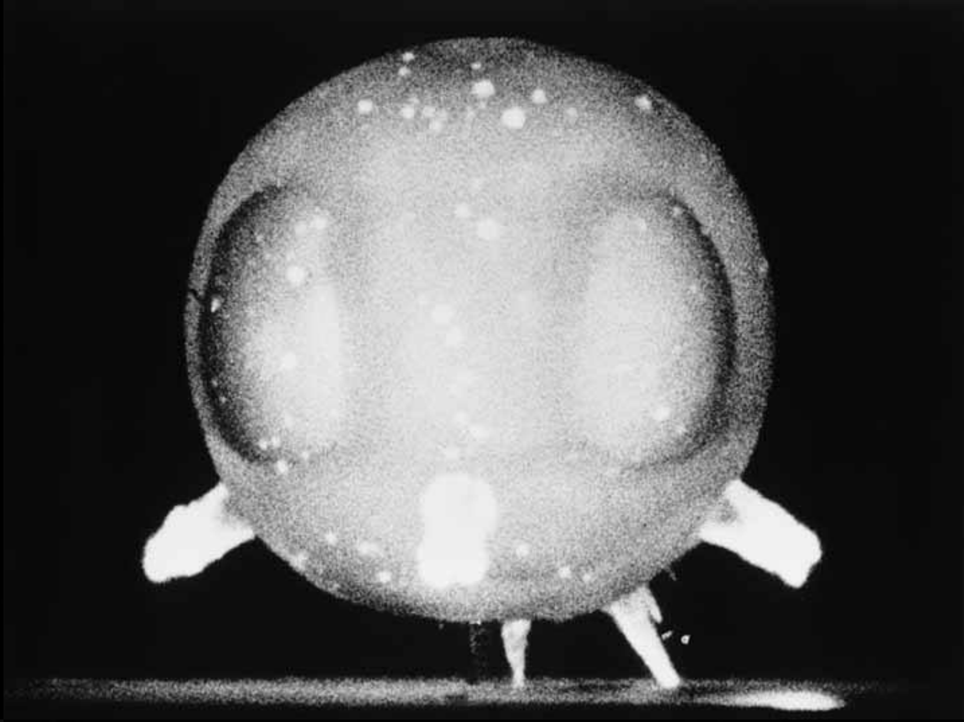
MaThRad

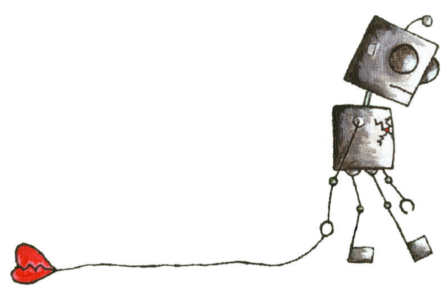
Radiation transport equations

Boltzmann transport equation

Let $\psi = \psi(\boldsymbol{y}) = \psi(t, \boldsymbol{x}, \boldsymbol{\Omega}, e) : \mathbb{R}^7 \to \mathbb{R}$ denote angular flux

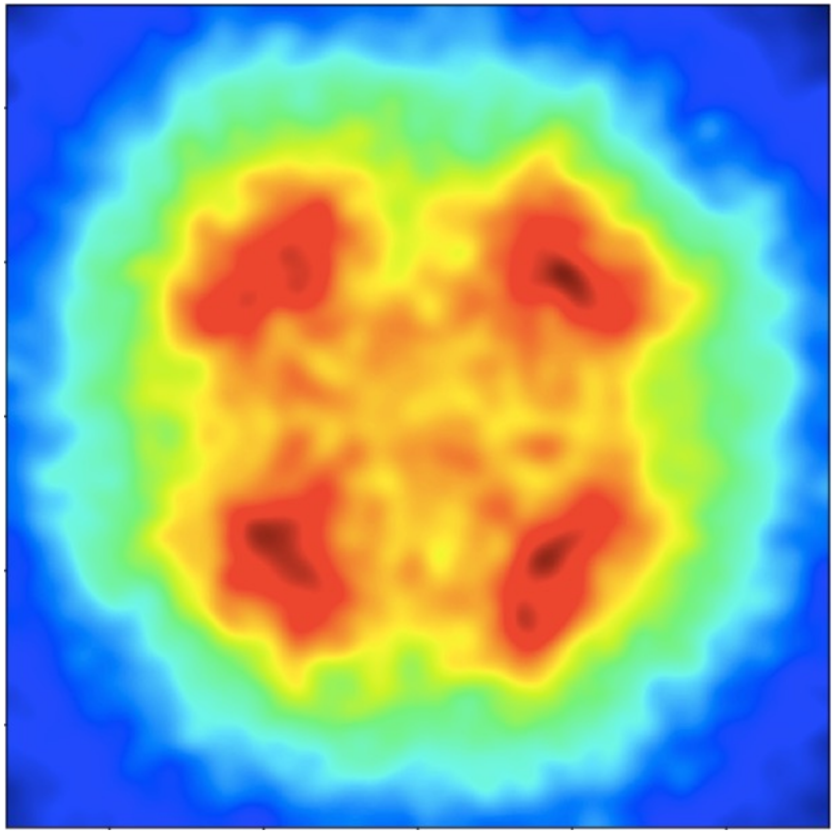
$$\underbrace{\partial_t \psi(\boldsymbol{y}) + \boldsymbol{\Omega} \cdot \nabla_{\boldsymbol{x}} \psi(\boldsymbol{y})}_{\text{Transport}} + \underbrace{\sigma_T(\boldsymbol{x}, e)}_{\text{Total cross section}} \psi(\boldsymbol{y}) = \int_{e'} \int_{\boldsymbol{\Omega}'} \underbrace{\sigma_S(\boldsymbol{x}, \boldsymbol{\Omega}' \to \boldsymbol{\Omega}, e' \to e)}_{\text{Scattering cross section}} \psi(t, \boldsymbol{x}, \boldsymbol{\Omega}', e') \, \mathrm{d}\Omega' \, \mathrm{d}e'$$

$+$ BCs, ICs, source terms



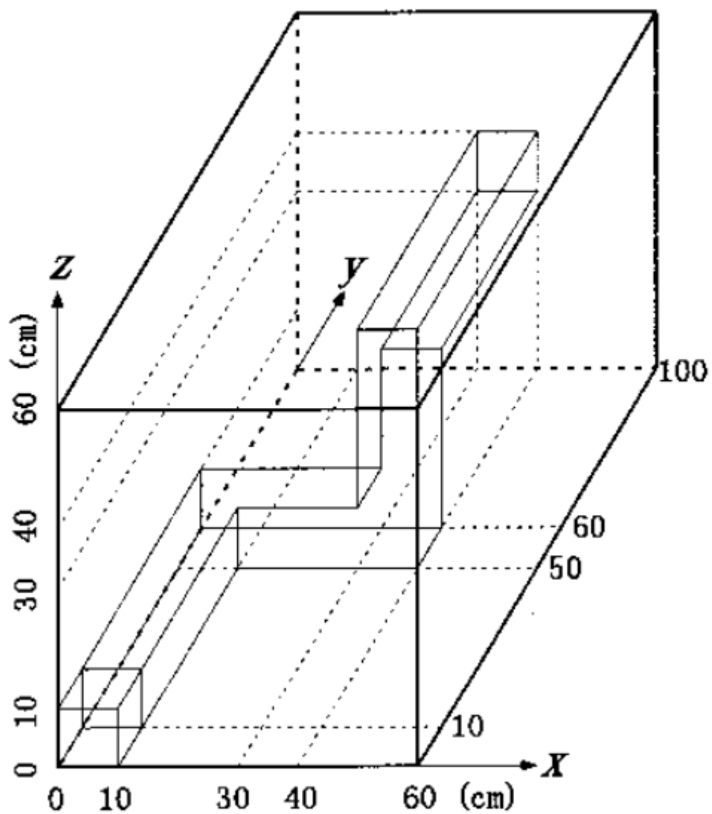
Types of radiation transport problems

- Criticality



Types of radiation transport problems

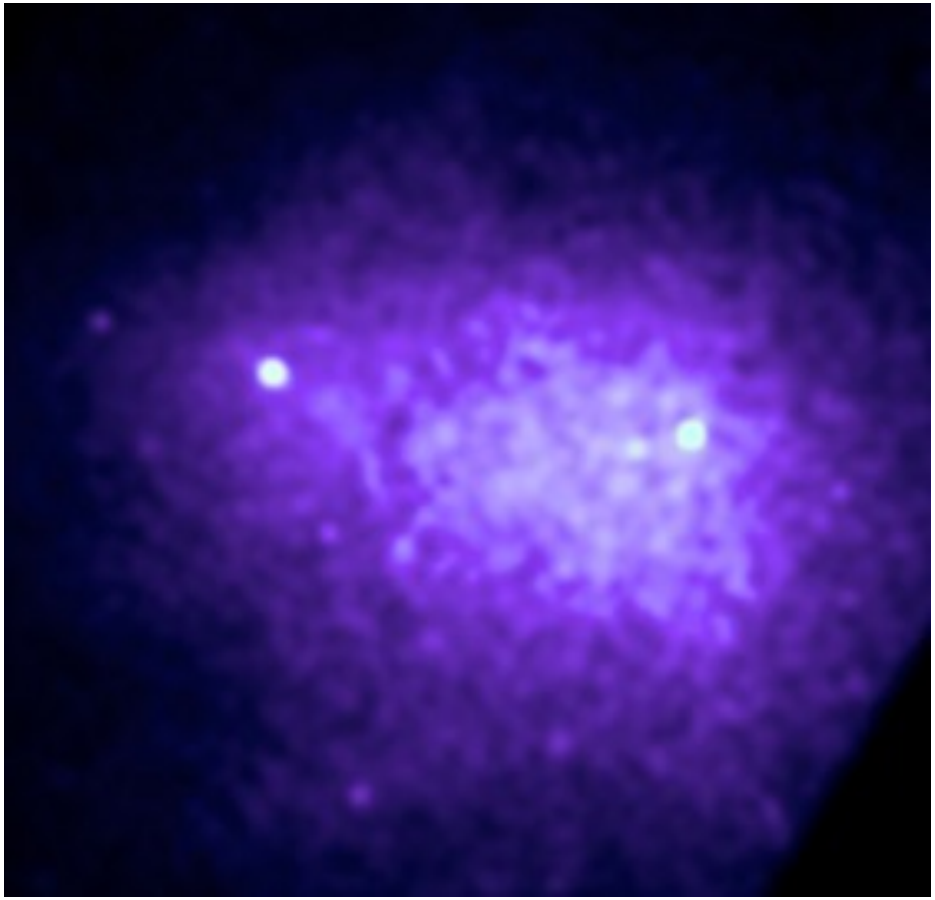
- Shielding



Kobayashi et al. (2000). "3-D Radiation Transport Benchmark Problems and Results for Simple Geometries with Void Regions", NEA-OECD

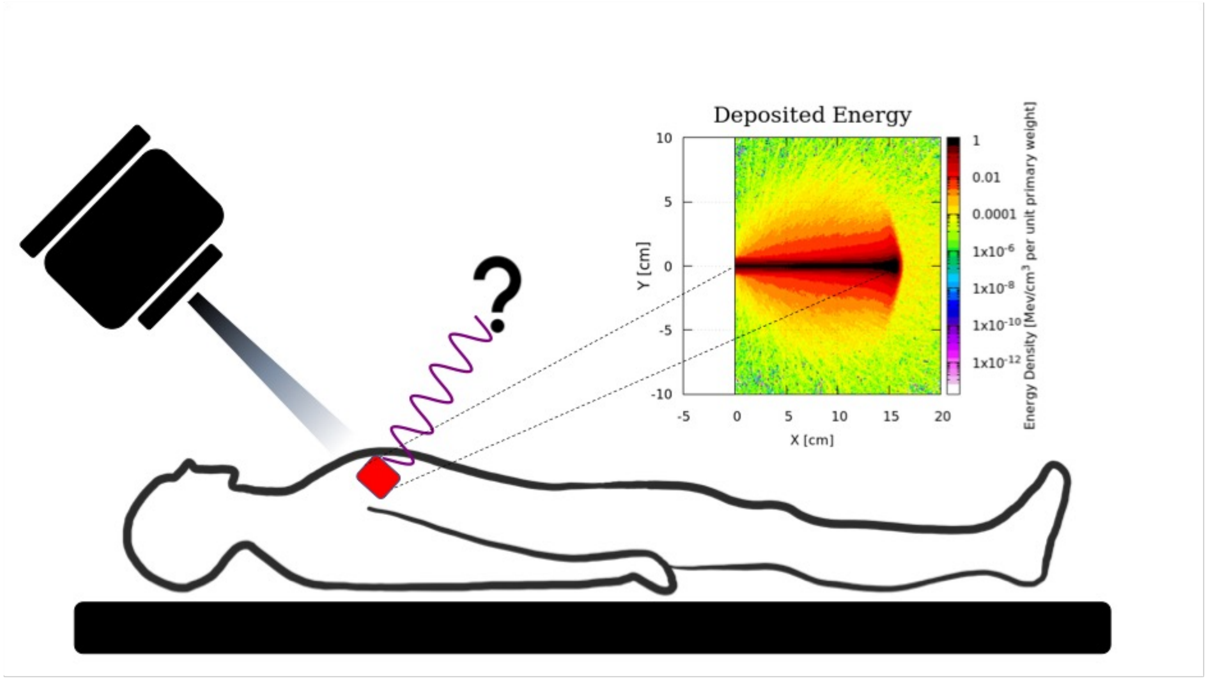
Types of radiation transport problems

- Forward modelling



Types of radiation transport problems

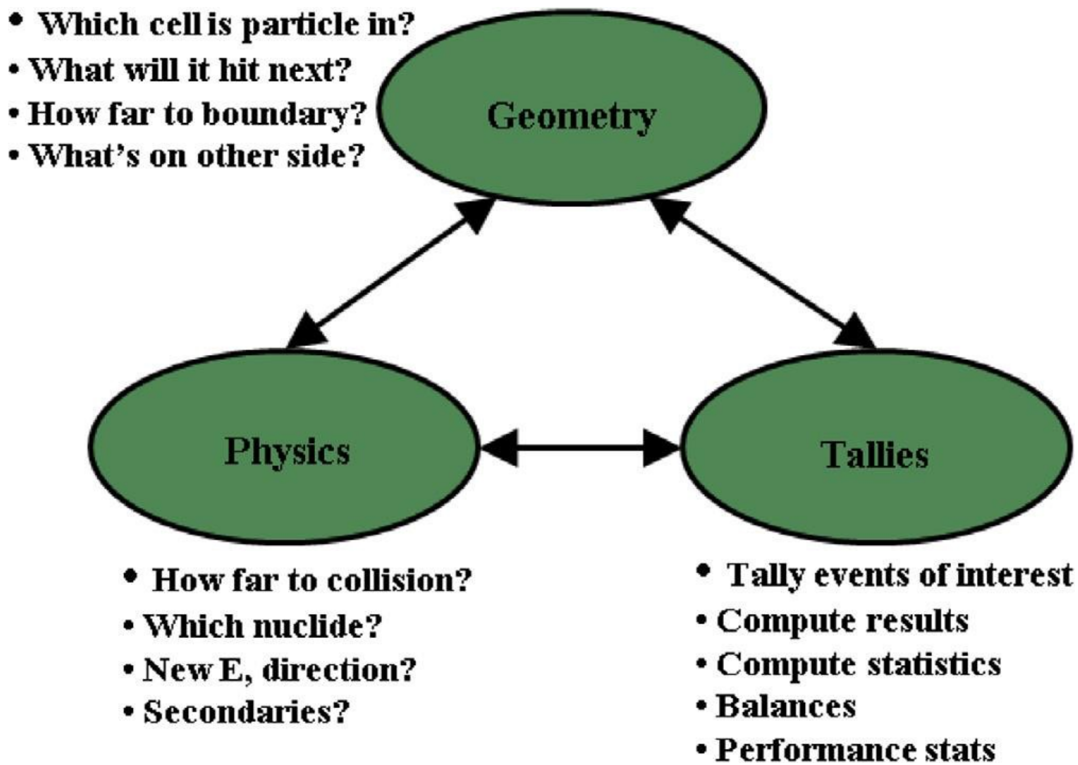
- Inverse modelling



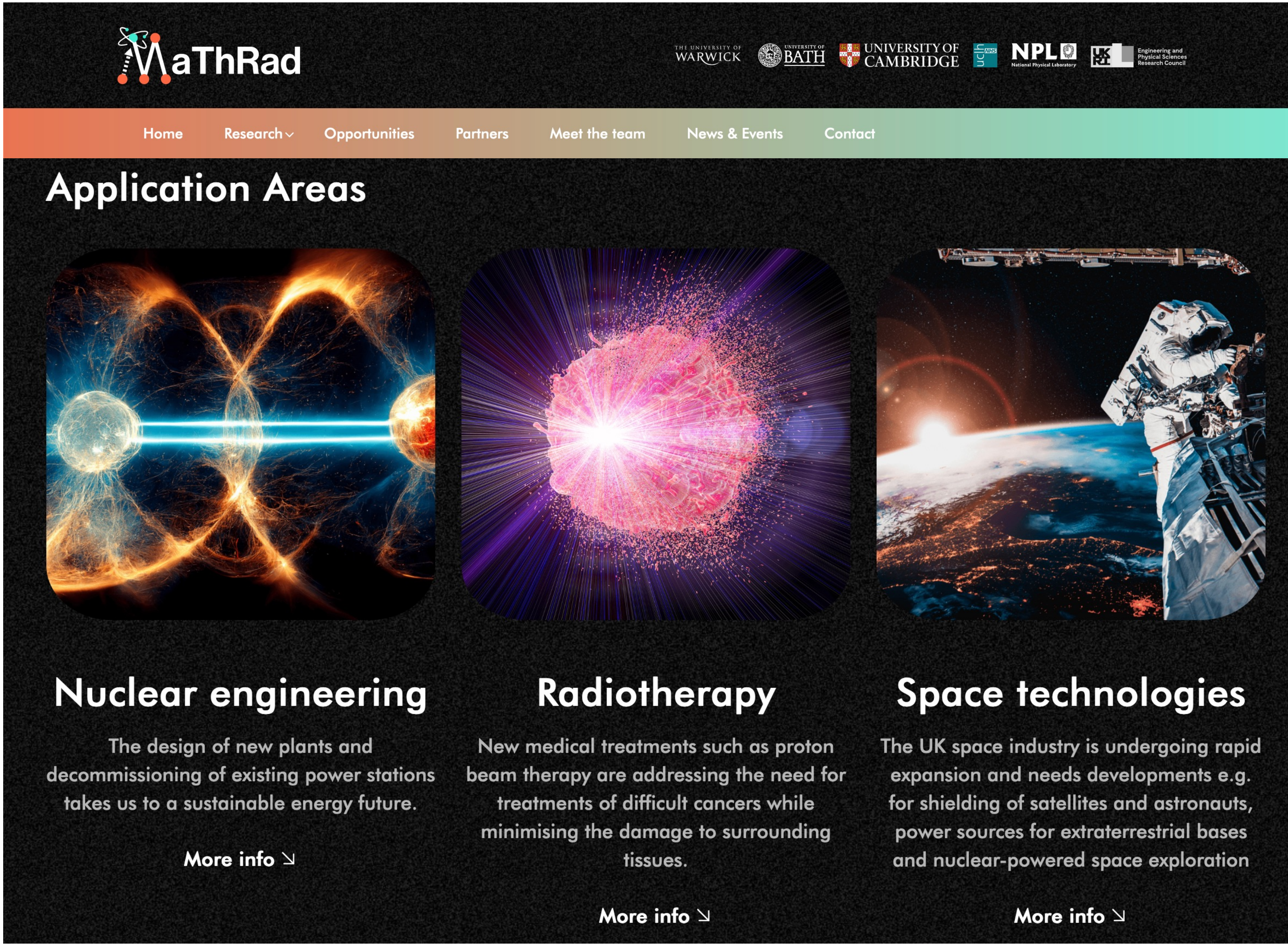
Traditional MC code structure

- Focus on the function of components

- Circular dependence of components

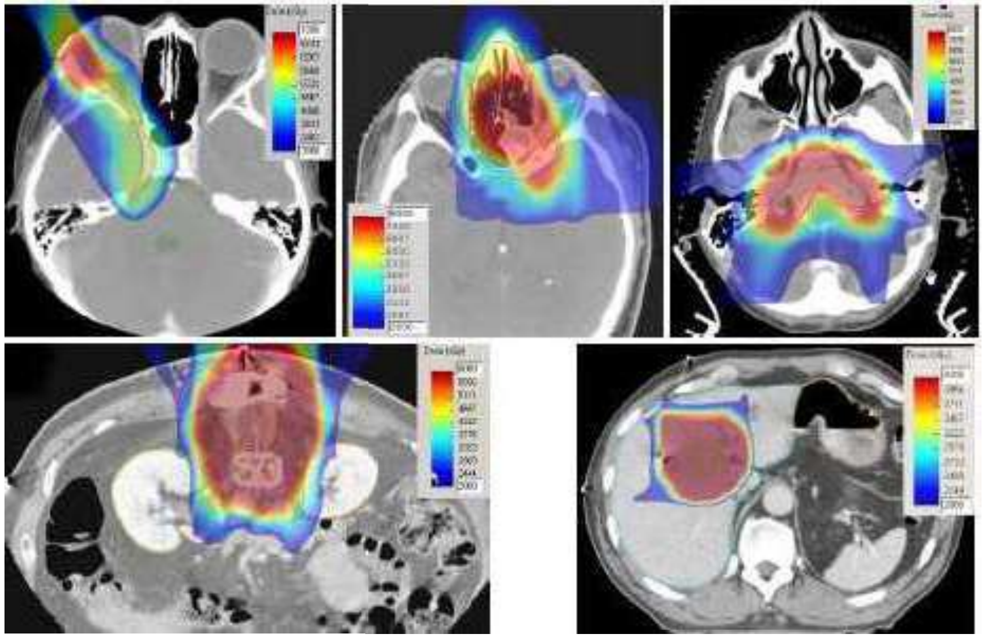


T. Adams, et al., Monte Carlo Application ToolKit (MCATK), Ann. Nucl. En., 82, 41-47, 2015



https://mathrad.ac.uk/

Benefits of PBT

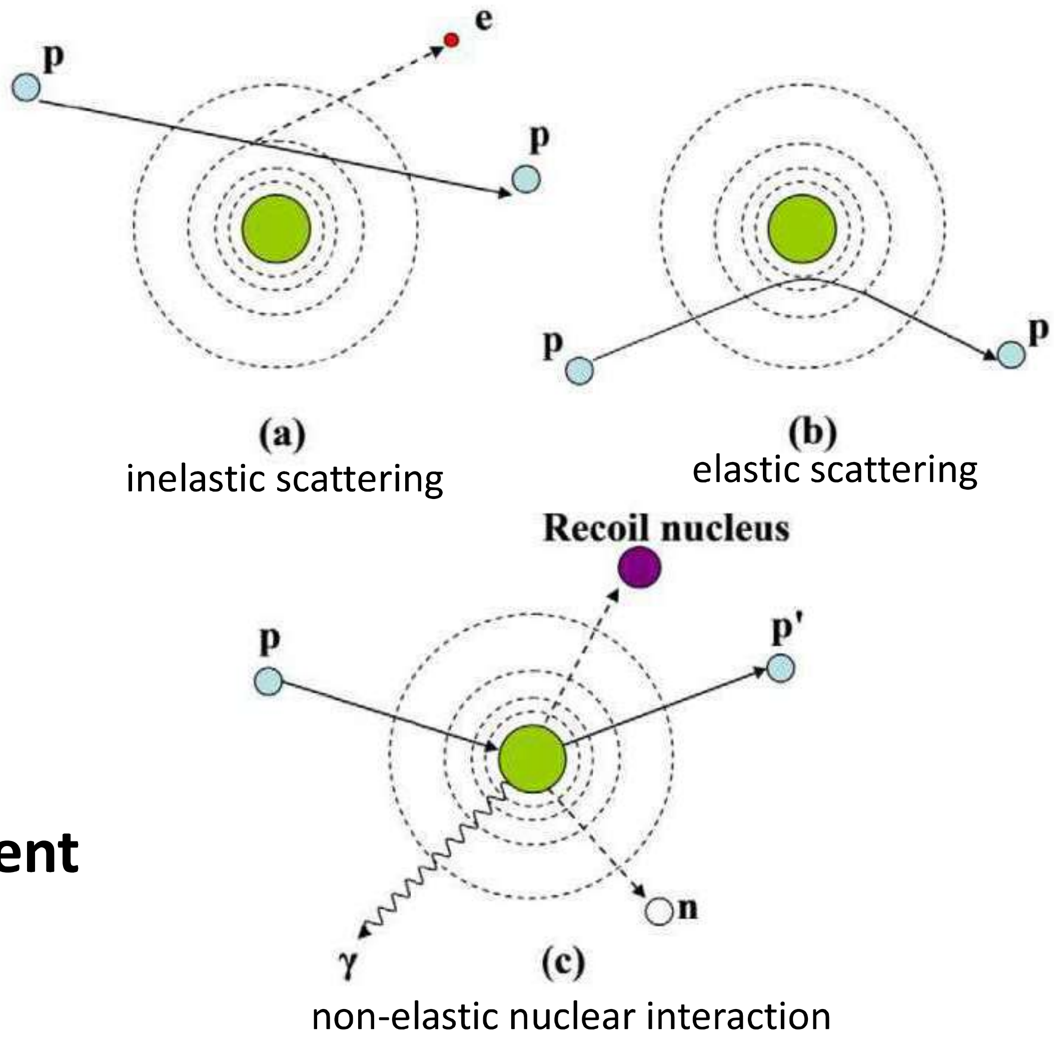


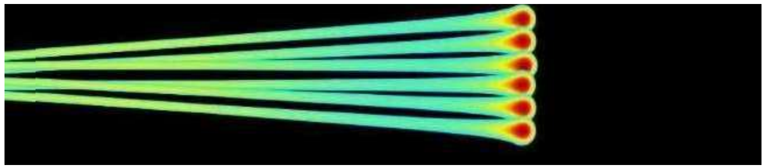
- Spare healthy tissue- reduce risk of secondary malignancies
- Escalate the dose to the target to curative levels
- Re-irradiation settings

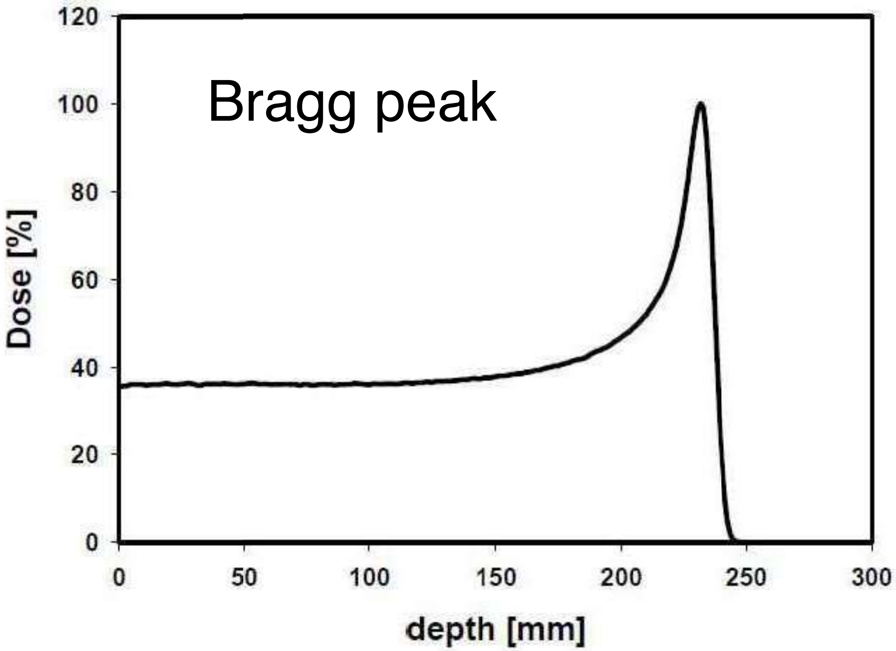
Interactions

- Ionization (Coulomb effect)
- Coulomb interactions with atomic nucleus
- Nuclear interactions with atomic nucleus

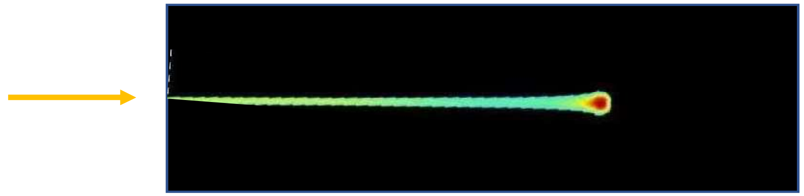
These interactions govern how protons deposit their dose in patient fundamentally







Slow loss of energy due to Coulomb interactions with atomic electrons



$$\frac{dE}{dx} \propto \frac{1}{v^2}\left(\frac{Z}{A}\right)z^2$$

Bethe-Block

Proton beam facility UCLH

Proton beam SDE

A special kind of Stochastic Differential Equation models the energy deposition of individual proton streams: $Y_\ell = (\epsilon_\ell, r_\ell, \Omega_\ell)$

- ϵ_ℓ is the energy of the proton stream after it has traversed a distance ℓ
- r_ℓ is the position of the proton stream after it covers a distance ℓ
- Ω_ℓ is the direction of travel of the proton after it covers a distance ℓ.

$$\begin{aligned}
\epsilon_\ell &= \epsilon_0 - \int_0^\ell \varsigma(Y_{l-})\mathrm{d}l - \int_0^\ell (1-u)\epsilon_{l-} N_{ne}(Y_{l-}; \mathrm{d}l, \mathrm{d}\Omega', \mathrm{d}u) \\
r_\ell &= r_0 + \int_0^\ell \Omega_l \mathrm{d}l \\
\Omega_\ell &= \Omega_0 - \int_0^\ell m(Y_l)^2 \Omega_l \mathrm{d}l + \int_0^\ell m(Y_{l-})\Omega_l \wedge \mathrm{d}B_l \\
&\quad + \int_0^\ell \int_{\mathbb{S}_2} (\Omega' - \Omega_{l-}) N_e(Y_{l-}; \mathrm{d}l, \mathrm{d}\Omega') + \int_0^\ell \int_0^1 \int_{\mathbb{S}_2} (\Omega' - \Omega_{l-}) N_{\boldsymbol{ne}}(Y_{l-}; \mathrm{d}l, \mathrm{d}\Omega', \mathrm{d}u)
\end{aligned}$$

TECHNICALITIES

- Does does law of the solution $(\epsilon_\ell, r_\ell, \Omega_\ell)$ to this SDE have a density with respect to Lebesgue measure on $(0,\infty) \times D \times \mathbb{S}_2$?
- Important because: We can define for a test function f on $(0,\infty) \times D \times \mathbb{S}_2$ (the configuration space of the solution), the 'interrogation' potential of where (and how much) energy is deposited along its stochastic path:

$$U[f] = -\mathbb{E}\left[\int_0^\Lambda f(Y_{\ell-})\mathrm{d}\epsilon_\ell\right],$$

  here Λ is the total distance covered by the proton stream and $Y_\ell = (\epsilon_\ell, r_\ell, \Omega_\ell)$
- If we define

$$\begin{aligned} D[f] &:= -\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\mathbb{E}\left[\int_0^\Lambda \Big(f(r_\ell + \varepsilon\Omega_\ell) - f(r_\ell)\Big)\,\mathrm{d}\,\epsilon_\ell\right] \\ &= \int_\Upsilon \Omega\cdot\nabla_r f(r)\,u(z)\,\mathrm{d}\,z, \end{aligned}$$

  where $u(z)$ is a density associated to $U[f]$.
- Because of the existence of the density, we can appeal to duality to tell us that

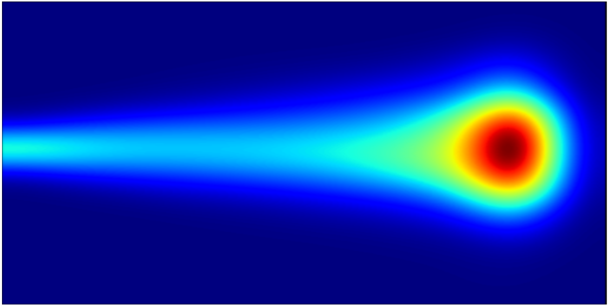
$$D[f] = \langle(\Omega\cdot\nabla_r)[f], u\rangle = -\langle f, (\Omega\cdot\nabla_r)[u]\rangle.$$

Bragg manifold

We defined the *path Bragg manifold* to be the quantity

$$\boxed{b(z) = -\Omega \cdot \nabla_r u(z).}$$

As alluded to above, this is the average rate of directional energy deposition at configuration $z = (\epsilon, r, \Omega) \in \Upsilon$ in the sequential proton track.



Neutron Transport Equation

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

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

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

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

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

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

Underlying stochastics (leading to Monte-Carlo)

- Backwards equation lends itself well to stochastic representation,

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

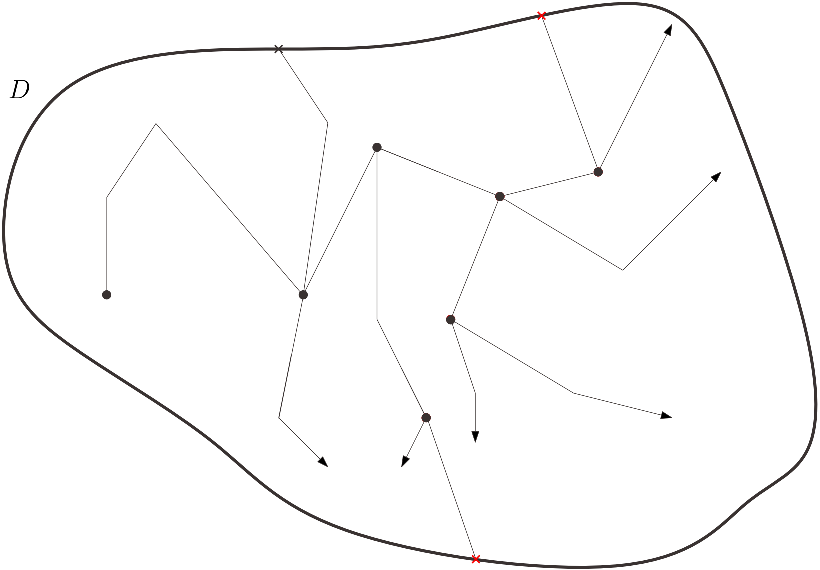
- The physical process of fission is a Markov-additive branching process (*neutron branching process*).
- Represented by a configuration of physical location and velocity of particles in $D \times V$, say $\{(r_i(t), \upsilon_i(t)) : i = 1, \ldots, N_t\}$, where N_t is the number of particles alive at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

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

Neutron branching process



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

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

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 $(\phi_t[g], t \geq 0)$ 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 $\tilde{\varphi} \in L_2^+(D \times V)$

Theorem (Horton, K., Villemonais, 2018)

Suppose that

- *D is non-empty and convex;*
- *Cross-sections $\sigma_{\mathtt{s}}$, $\sigma_{\mathtt{f}}$, $\pi_{\mathtt{s}}$ and $\pi_{\mathtt{f}}$ are uniformly bounded away from infinity;*
- $\inf_{r\in D, \upsilon, \upsilon' \in V} (\sigma_{\mathtt{s}}(r,\upsilon)\pi_{\mathtt{s}}(r,\upsilon,\upsilon') + \sigma_{\mathtt{f}}(r,\upsilon)\pi_{\mathtt{f}}(r,\upsilon,\upsilon')) > 0$

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 $\mathrm{e}^{\lambda_* t}$, 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 $g \in L^+_\infty(D\times V)$,*

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

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

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

---

[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.

λ-eigenvalue and Monte-Carlo logic

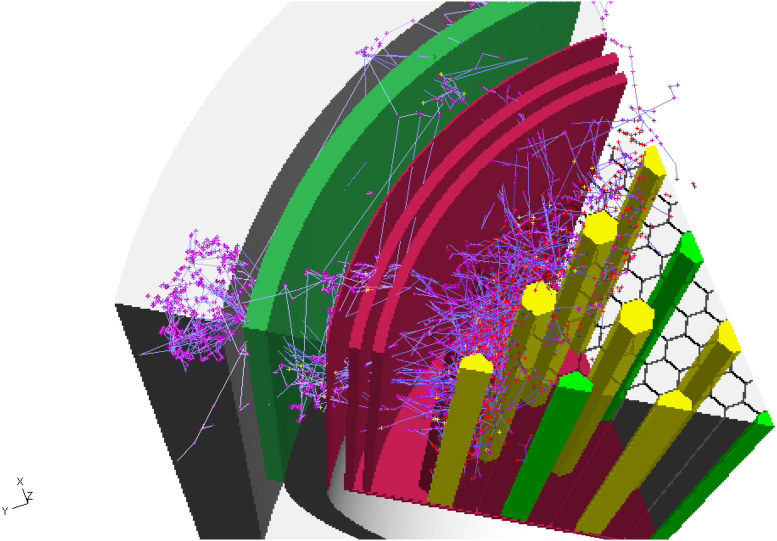
- Suppose now we can efficiently simulate the Neutron branching process, recalling that

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

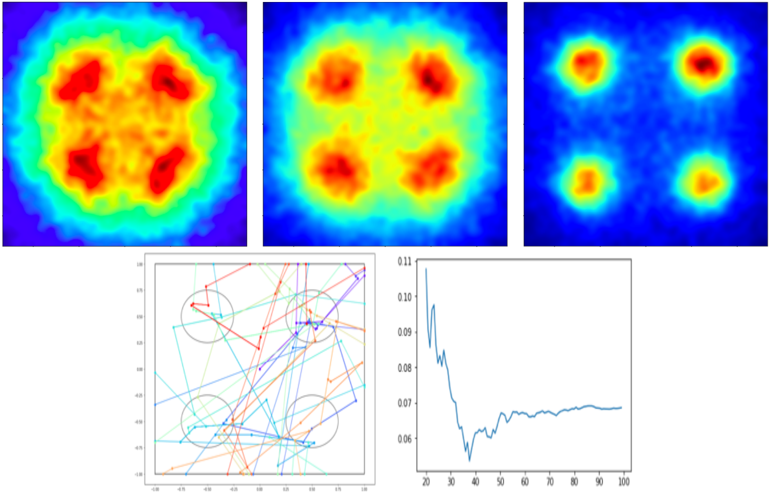
-

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

Monte-Carlo is still difficult



Monte-Carlo, importance map $\tilde{\varphi}$



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

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

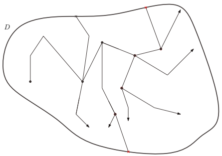
  This is the Markov generator of a neutron random walk (NRW) (R,Υ) (scatters at rate α and chooses new velocity with distribution π) with probabilities $(\mathbf{P}_{(r,\upsilon)},r\in D,\upsilon\in V)$. We have a new representation in terms of (R,Υ),

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

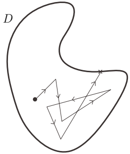
  for $t\geq 0, r\in D,\upsilon\in V$, where

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

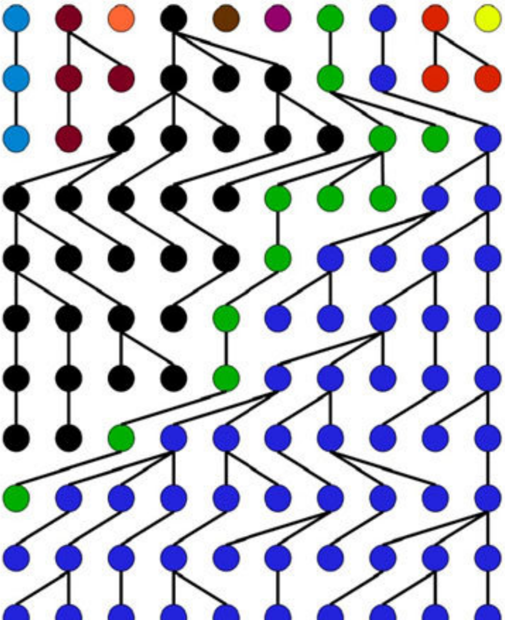
- This affords the opportunity to avoid simulating entire trees:



can be replaced by



Interacting particle Monte-Carlo



Thank you!