DE LA RECHERCHE À L'INDUSTRIE

Adaptive Multilevel Splitting for Particle Transport

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CONTEXT

- **Collaborative** work between :

  - E. Dumonteil (CEA/DRF/IRFU/DPhN)
  - K. Frohlicher (IRSN/PSN-RES/SNC) → PhD 2022
  - T. Lelievre (Ecole des Ponts/CERMICS)
  - H. Louvin (CEA/DRF/IRFU/DEDIP) → PhD 2017
  - D. Mancusi (CEA/DES/ISAS/DM2S)
  - M. Nowak (Previsions.io) → PhD 2018
  - M. Rousset (INRIA Rennes)
  - L. Thulliez (CEA/DRF/IRFU/DPhN)

Past & undergoing publications:

- **Louvin et al, EPJ Nuclear Sci. Technol. Vol 3 (2017)**
- **Nowak et al, Nuc. Sci. Eng., Vol 193 (2019)**
- **Mancusi et al, Trans. Am. Nuc. Soc., Vol. 120 (2019)**
- **Frohlicher et al, undergoing work (2021)**
- **Thulliez et al, undergoing work (2021)**

OUTLINE

- **Context**
  - Motivations
  - AMS for MC particle transport codes: basic ideas
  - Implementation & validation
- **Adaptation of AMS for particle transport**
  - On-the-fly scoring
  - Branching tracks
  - Multi-particles/particles cascades
  - Towards self-learning of the cost function
- **Use of AMS in reactor physics**
  - Chain reaction & population control
  - Spatial correlations
  - AMS & branchless collisions
  - Results

❑ Context

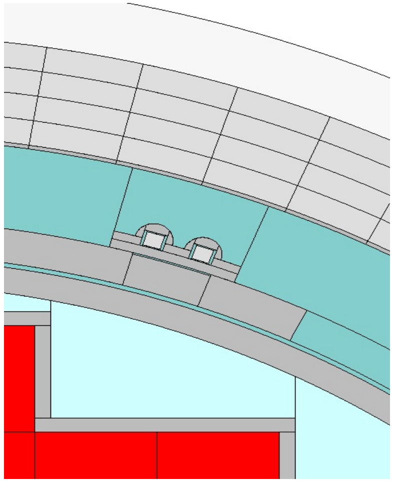
- Motivations
- AMS for MC particle transport codes: basic ideas
- Implementation & validation

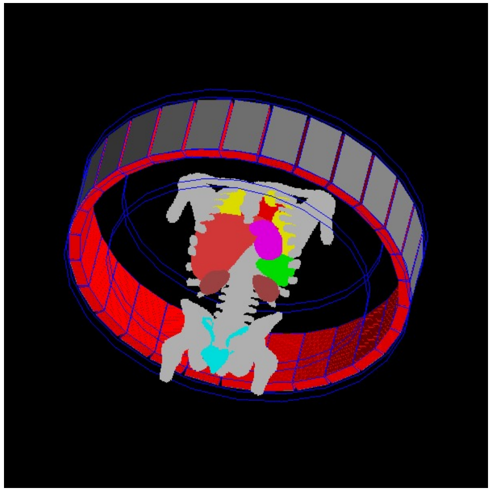
MONTE-CARLO FOR SHIELDING & MEDICAL APPLICATIONS

- Particle physics in its large sense: radiation protection, medical, fundamental, etc.
- Boltzmann equation in non-reproductive media and fixed sources
- Neutrons, photons, électrons, muons, etc. at all energies
- Main challenge: variance reduction w.r.t. x and E parameters

Radioactive waste management

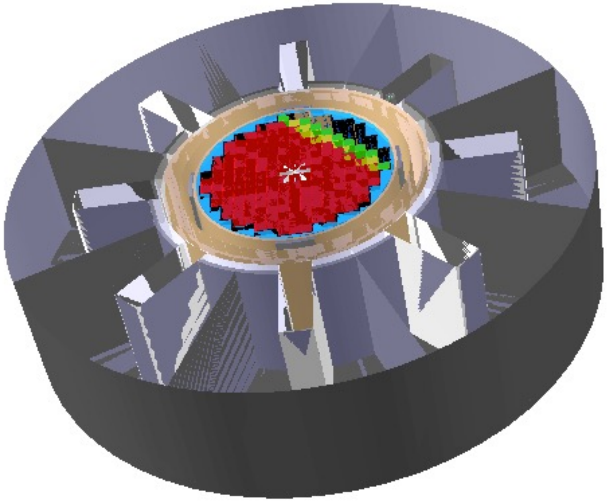
Ex-core dosimetry & PWR vessel fluence

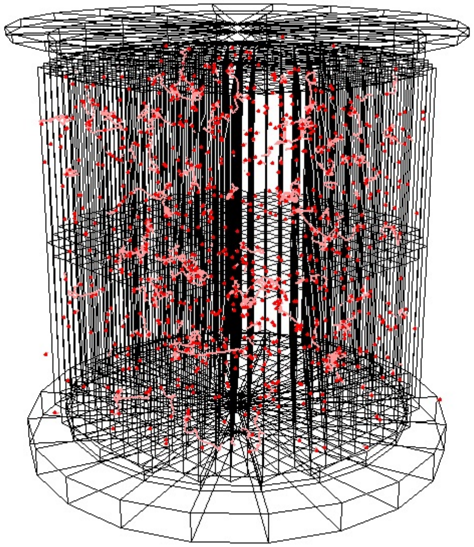




Radiotherapy (opengatecollaboration.org)

- Static linear Boltzmann equation in fissile media (no fixed sources)
- Neutrons between 0 and 20 MeV
- Main challenge: finding eigenvalues and eigenvectors while tackling with correlations





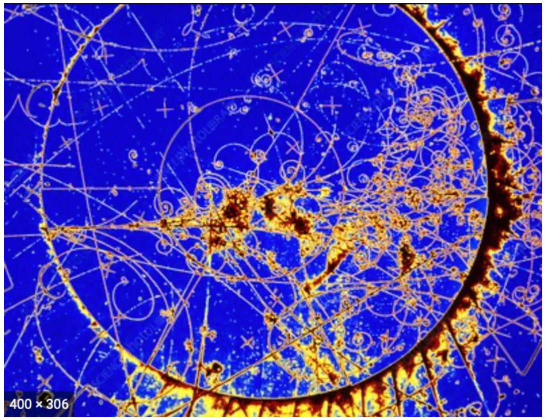
AMS FOR PARTICLE TRANSPORT

- **Originates from applied mathematics applied to molecular dynamic**
  - **(Cerou et al, 2007)**
  - **(Cerou et al, 2011)**
  - **(Aristoff et al, 2015)**

- **Adaptation to particle transport**
  - **CEMRACS@CIRM 2013 (Lelievre & Dumonteil)**
  - **(Louvin, Dumonteil, Lelievre, Rousset 2017)**
  - **(Louvin, Mancusi & Dumonteil 2019)**

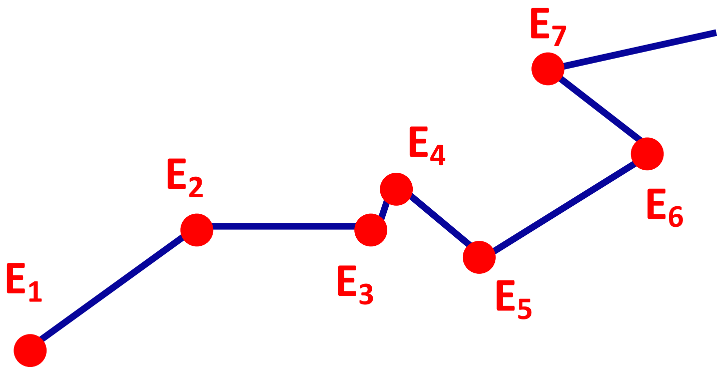
- **Objective of the different developments presented is to fit in the framework of AMS for discrete Markov chains detailed in (Brehier et al, 2016)**

- Term ”tracks” originates from first bubble chambers
- Parameter space (position, direction, energy, time, particle type)
- Non-charged particle tracks are
  - Markovian everywhere in (position, direction, energy)
  - Markovian at collision points i {(position, energy)}$_i$
  - Markovian at collision points i {(position, direction, energy)}$_i$
  - …

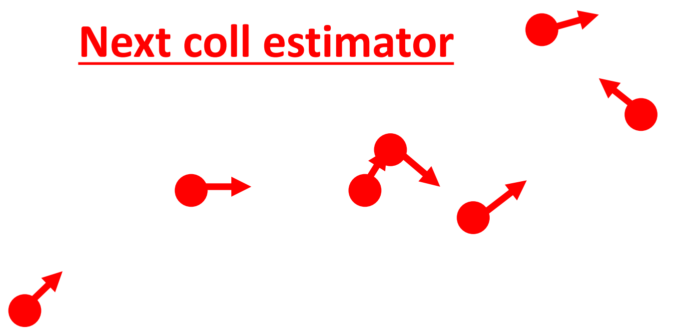


Tracks left by a neutrino interacting with a neutron

- AMS for discrete Markov chains is the most suitable AMS « flavor »



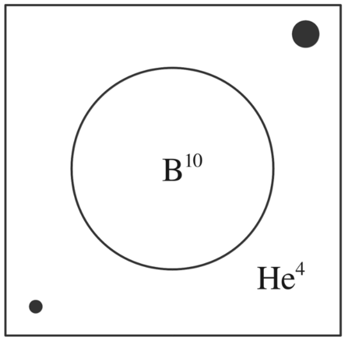
Typical exponential flight undergone by a neutron with anisotropic collision kernel C(E)

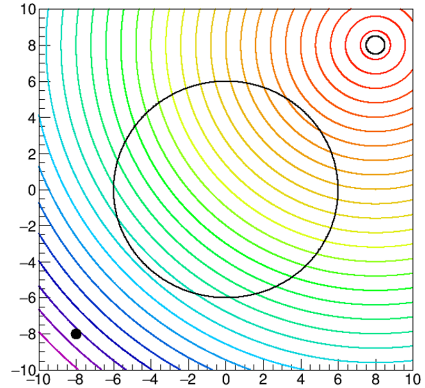


Flight seen at the collision points i {(position, direction, energy)}$_i$

AMS FOR PARTICLE TRANSPORT : ALGORITHM

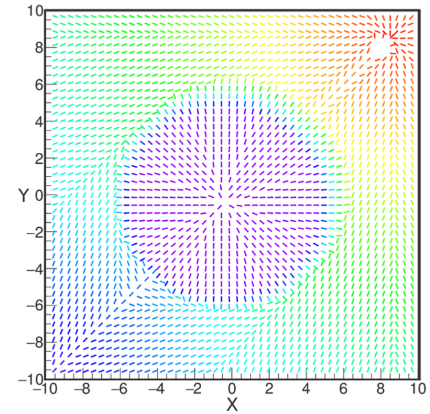
Example of cost functions:





Simple only-spatial
ξ =1/(1+d)

Material+energy taken into account in ξ



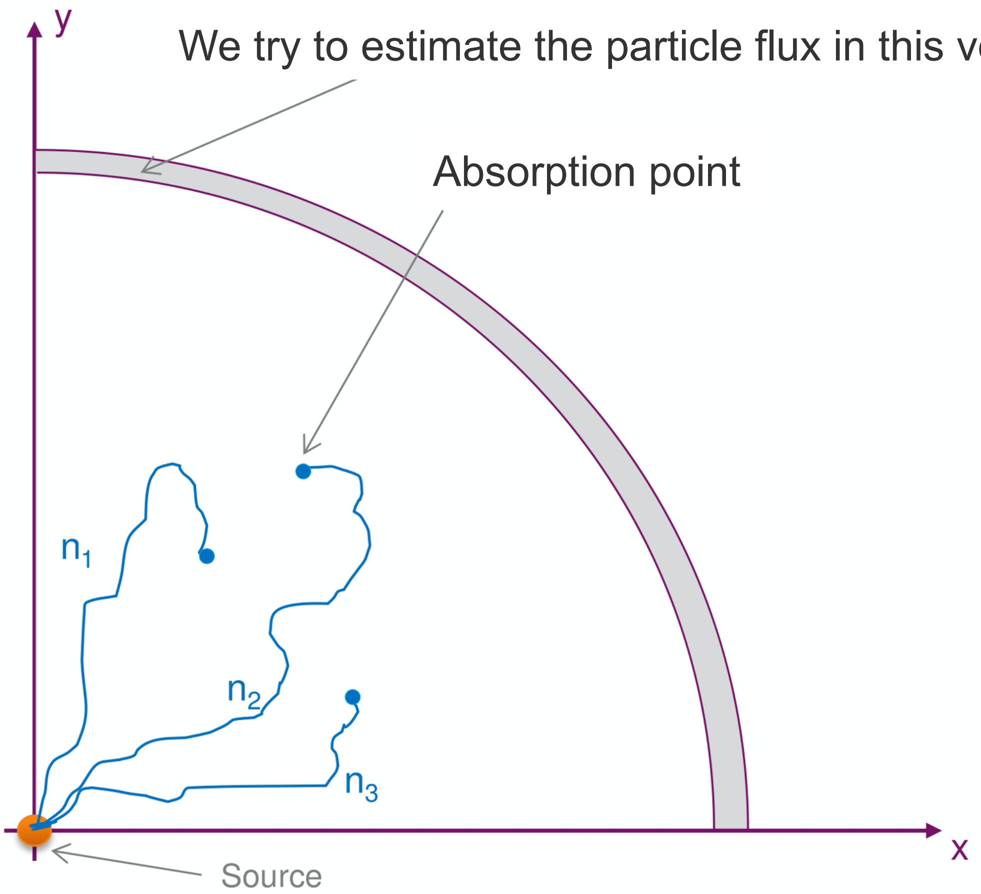
Algorithm with parameters
- n (# of particles)
- k (# of particles duplicated/iteration)
- ξ (cost function)

- n particles simulated => tracks are stored
- score is assigned to each neutron track (= Max of ξ over whole trajectory)
- tracks are ranked according to their score
- the k-th "worst" track defines the new splitting level
- the k tracks having scores lesser than this level are deleted
- k tracks are randomly selected and duplicated at the splitting level
- a new set of n particles is obtained, and we start the whole process again

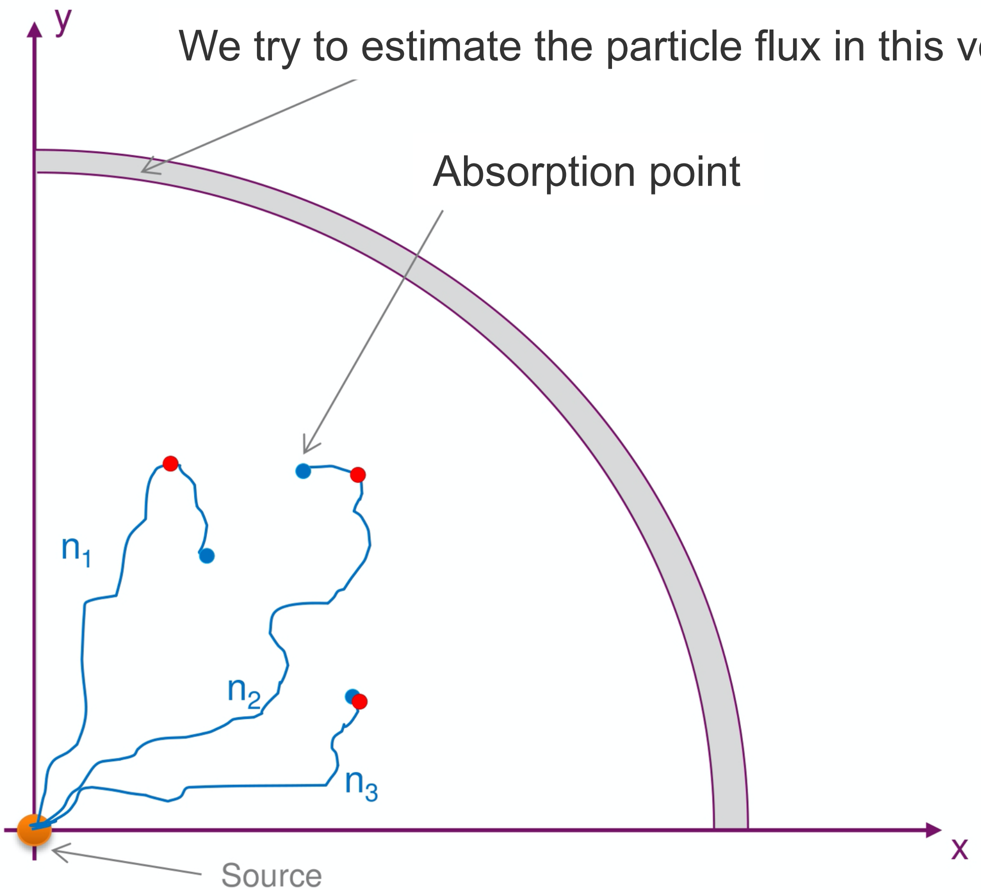
- **Stopping criterium:**
  - **When n-k tracks have reached the "detector", the algorithm stops**
  - **The number of iteration corresponding to reach that criterium is N**
  - **Each neutron is assigned a statistical weight α being:**

$$\alpha = \left(1 - \frac{k}{n}\right)^N$$

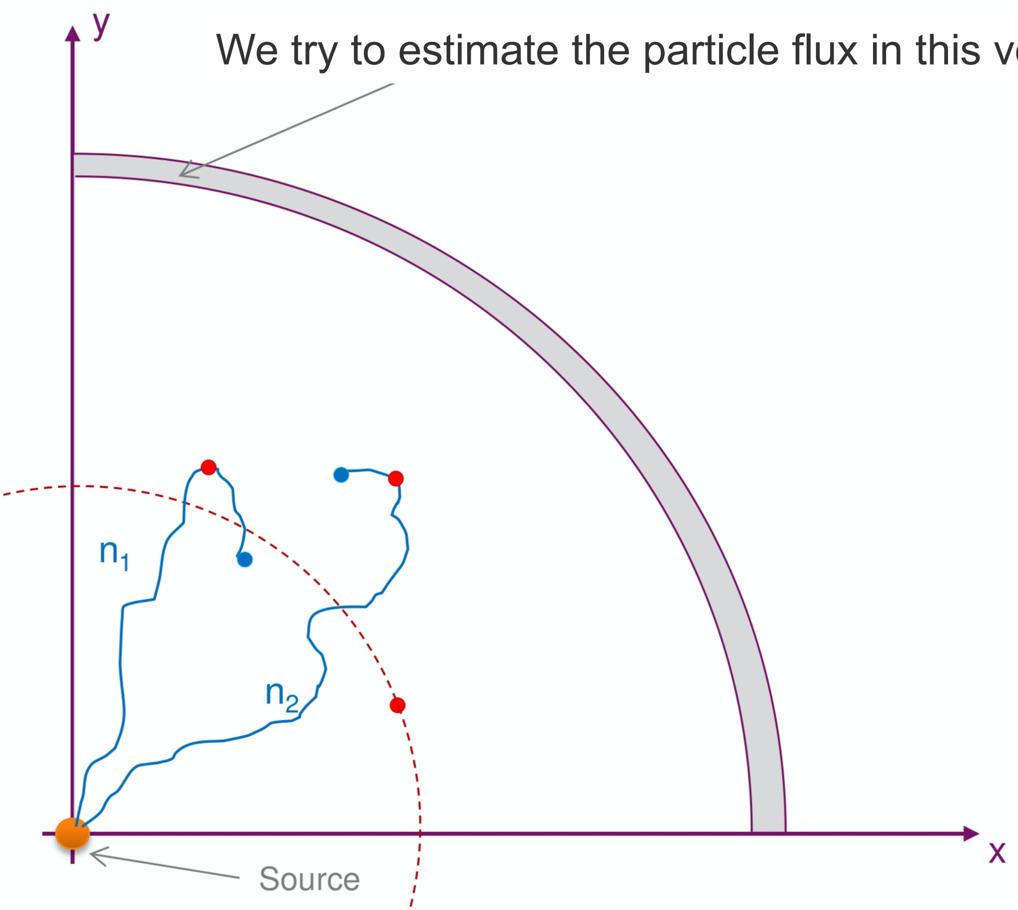
- **An unbiased estimator of the flux is calculated "as usual" using the tracks of the last iteration**



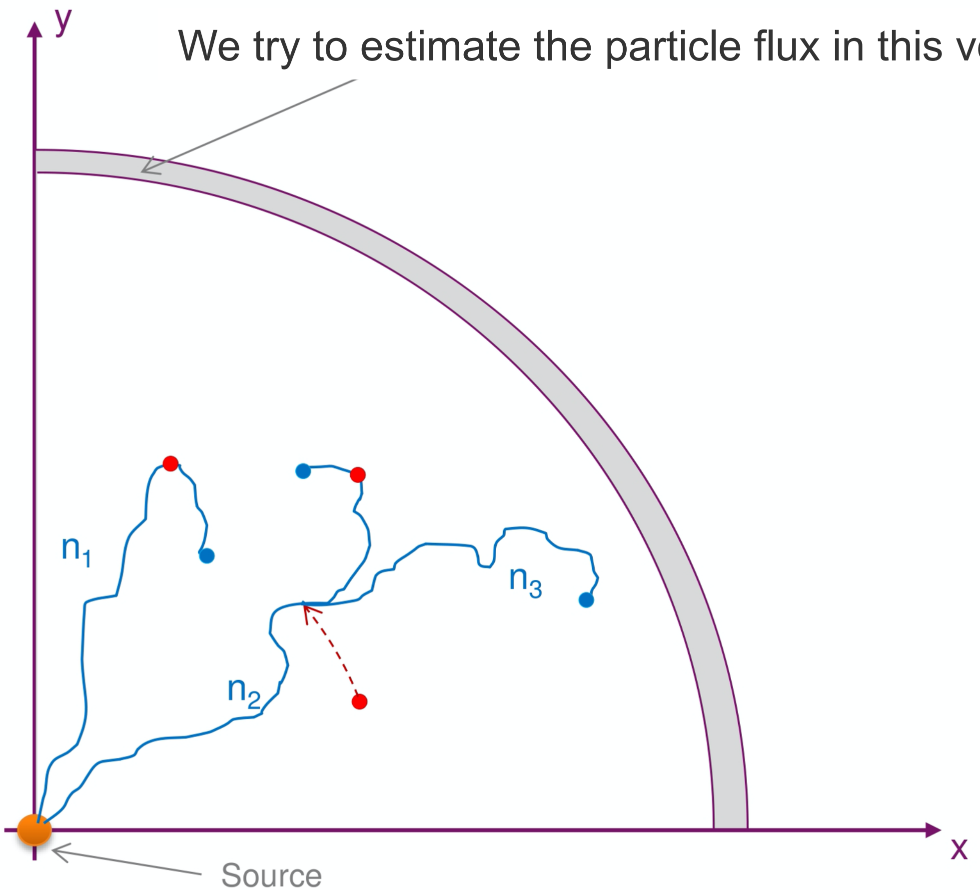
- **n=3**
- **k=1**
- **ξ: distance to the source**
- **Target: spherical shell (purple)**
- **3 particles simulated from the source to their absorption (blue points)**



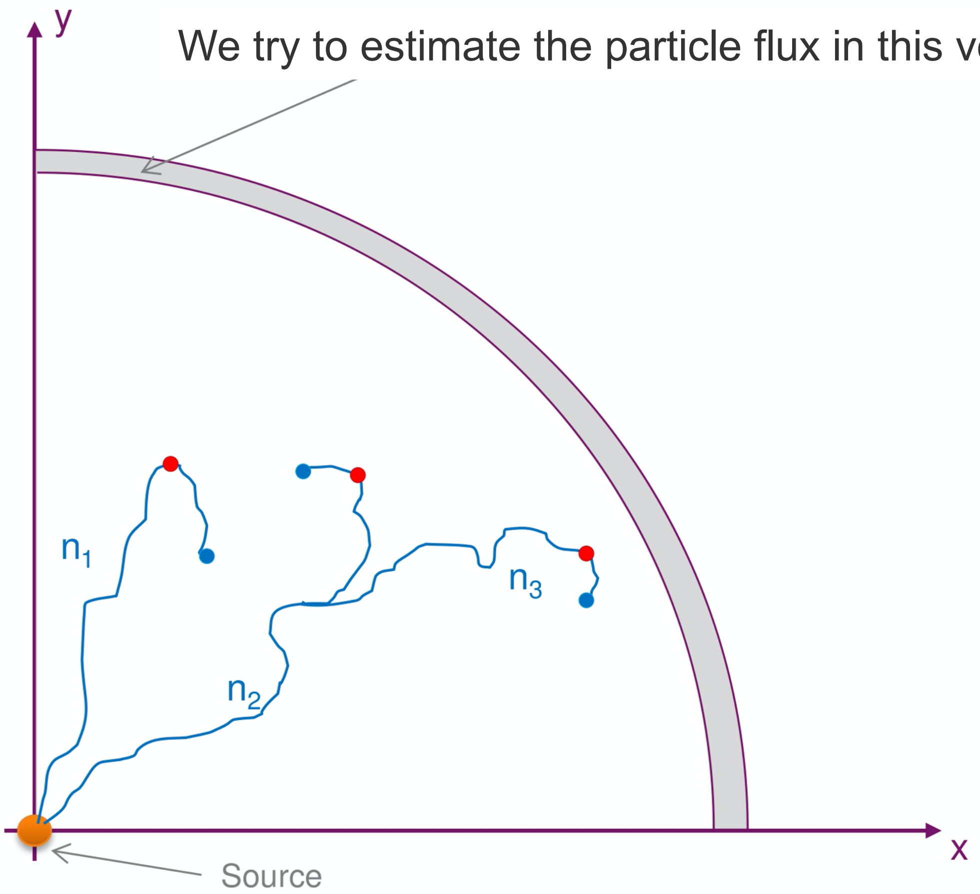
- **The importance function is the maximal distance to the source reached by the particle (red points)**
- **In this case the neutron tracks with the lowest score is n3**



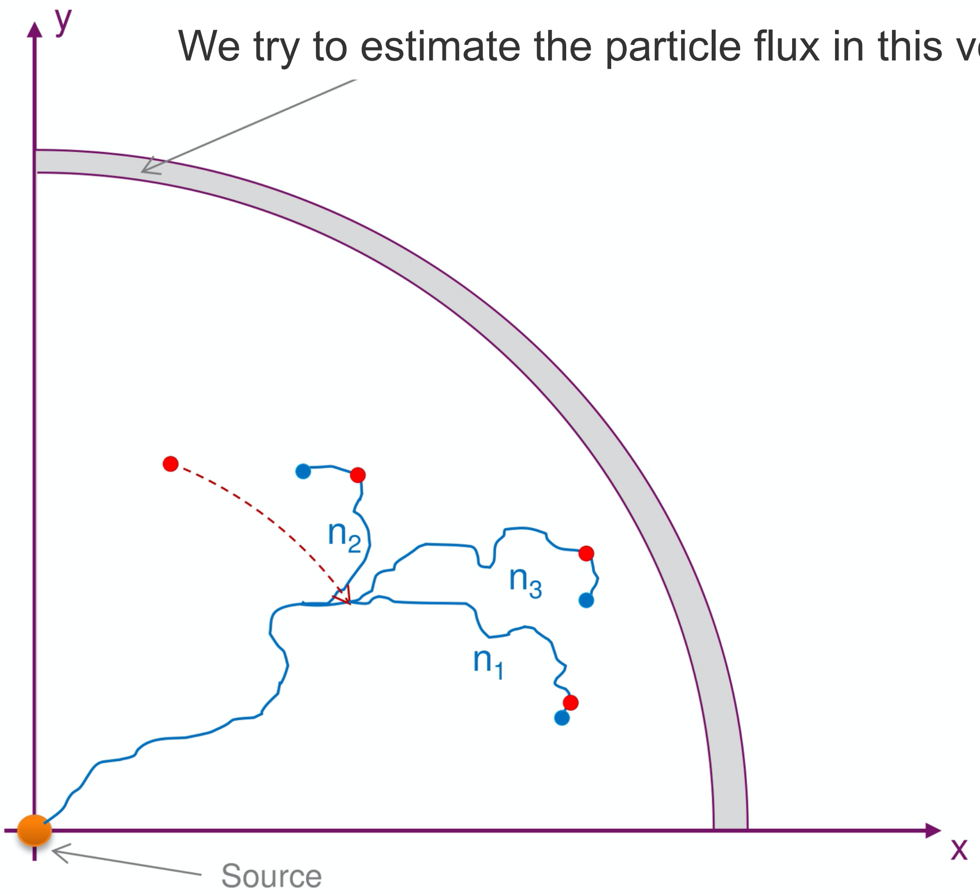
- **The tracks associated to particle 3 is deleted**
- **The maximum score of this track is stored and defines the first splitting level**



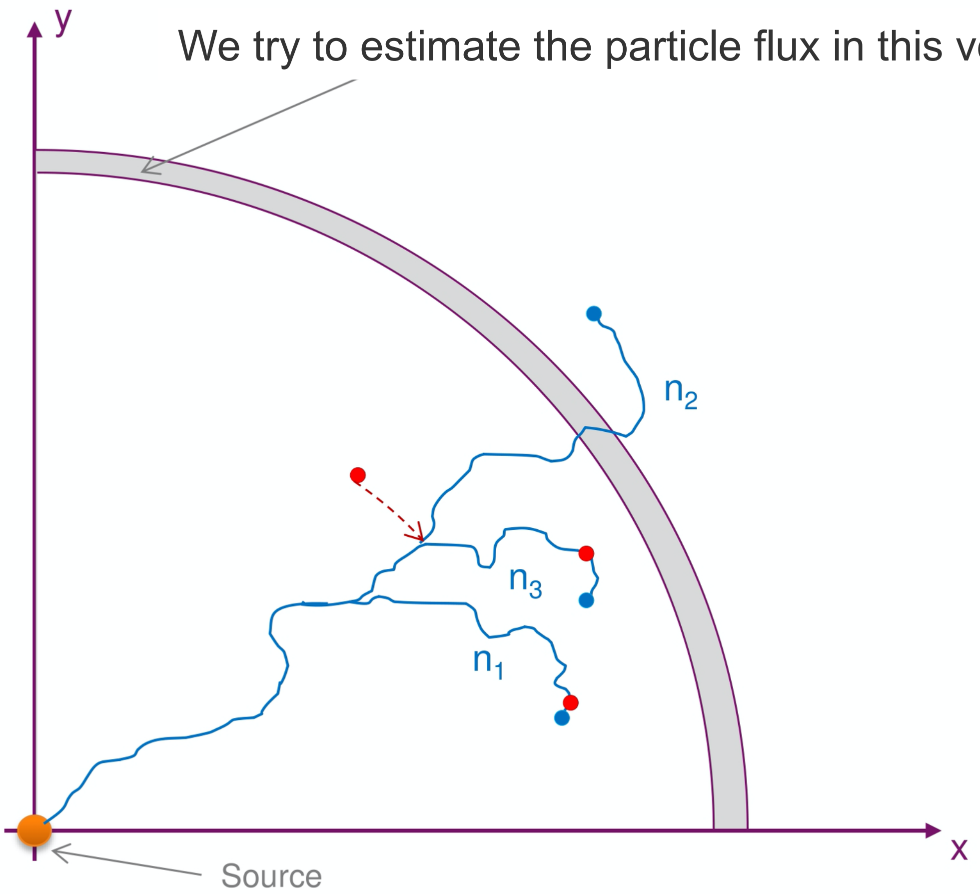
- **Track number 2 is randomly sampled for the splitting**
- **A new particle is simulated from this splitting point until its absorption**



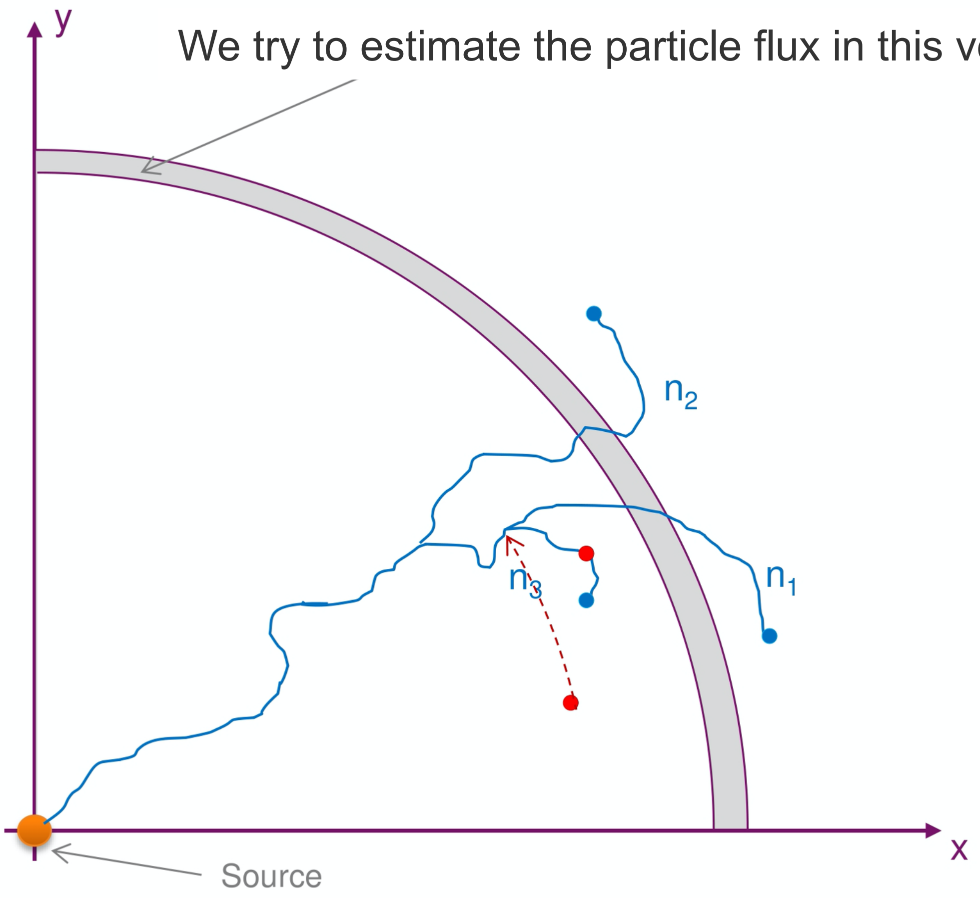
- **The score of this new tracks n3 is calculated**
- **The first iteration is over**
- **The stopping criterium is not meet: the iteration process goes on**


y
We try to estimate the particle flux in this volume
n2
n3
n1
x
Source

- **Iteration 2**

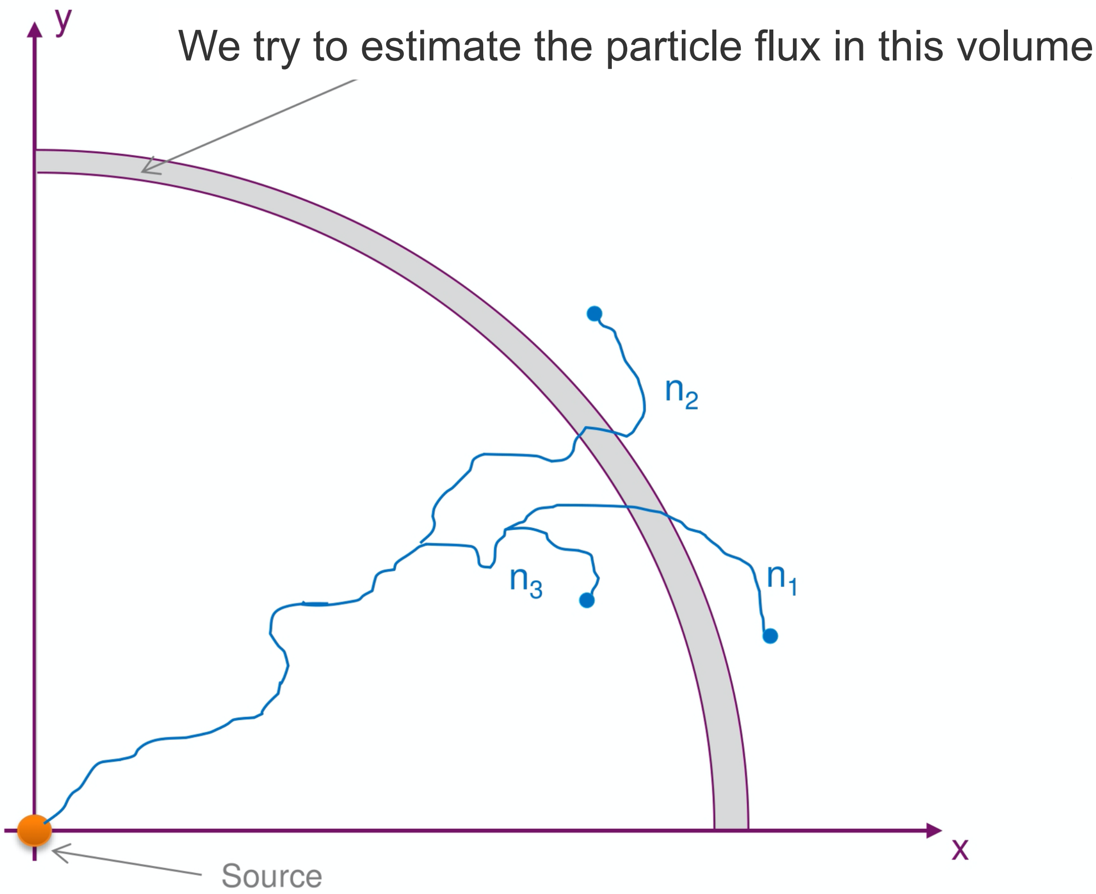

y
We try to estimate the particle flux in this volume
n2
n3
n1
x
Source

- **Iteration 3**



y
We try to estimate the particle flux in this volume
n2
n1
n3
x
Source

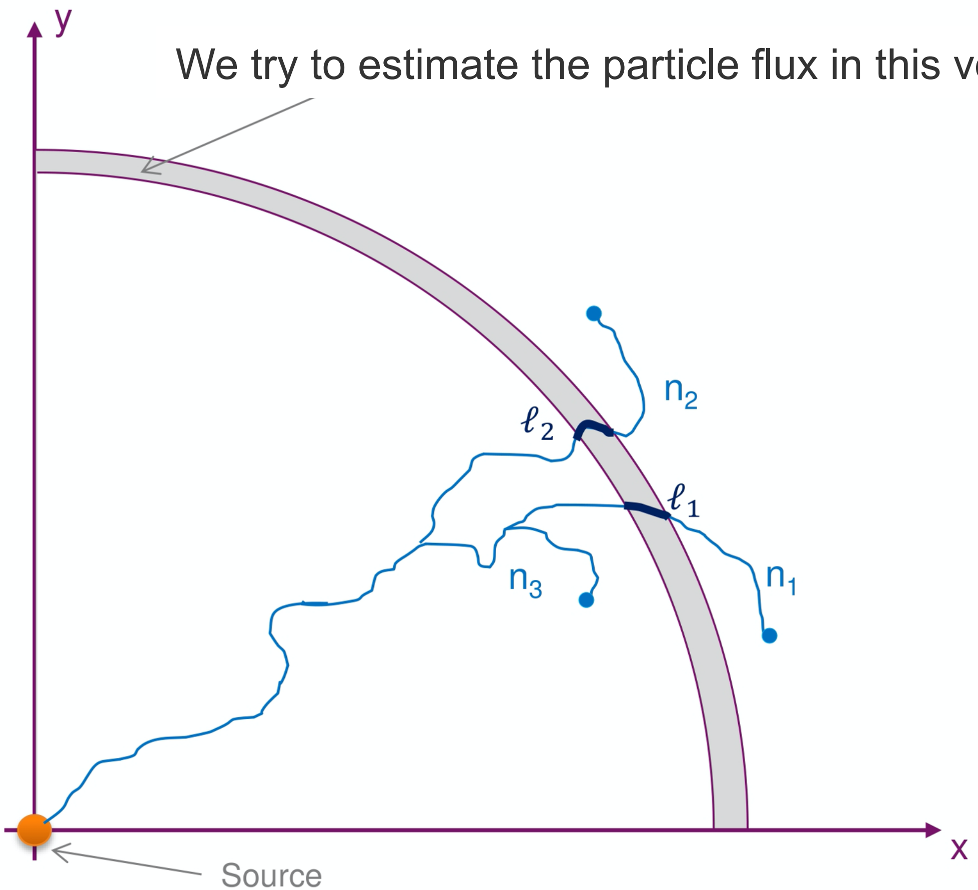
- **Iteration 4**



- **Iteration 4**
- **n-k particles have reached the target, the algorithm stops**

- **The statistical weight of the particles is :**

$$\alpha = \left(1 - \frac{1}{3}\right)^4$$



- **The flux is calculated according to standard MC flux estimators. For example the travelled length in the spherical shell can be used to tally the flux:**

$$\varphi = \frac{1}{3}\alpha(l_1 + l_2)$$

CODE DEVELOPMENT

TRIPOLI 4®

- TRIPOLI-4 @ CEA
- Distributed by OECD/NEA
- Neutron, gamma, e+, e-
- E < 20 MeV
- Evaluated cross-sections
- (Brun et al, 2015)
- www.cea.fr/energies/tripoli-4
- Nuclear industry

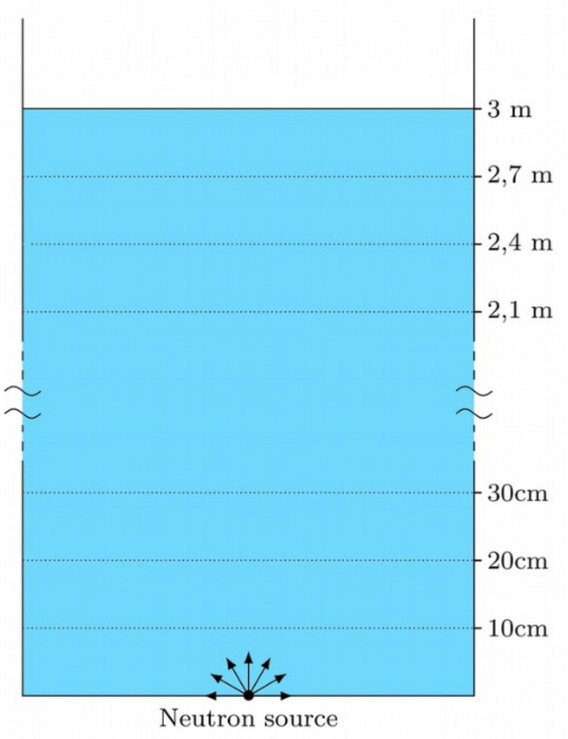
- Geant4 @ CERN
- Open-source
- All particles
- All energies
- Both evaluated cross-sections & models
- (Agostinelli et al, 2003)
- geant4.web.cern.ch
- Fundamental / medical / spatial

AMS has been implemented in a light (few classes) C++ framework
Will be released and distributed as open-source package in 2021
Small 'user guide' to link it to other transport codes
Provided with basic cost functions (distance to spatial detector, radial, …)
Verified through analytical benchmarks

❑ ADAPTATION OF AMS FOR PARTICLE TRANSPORT

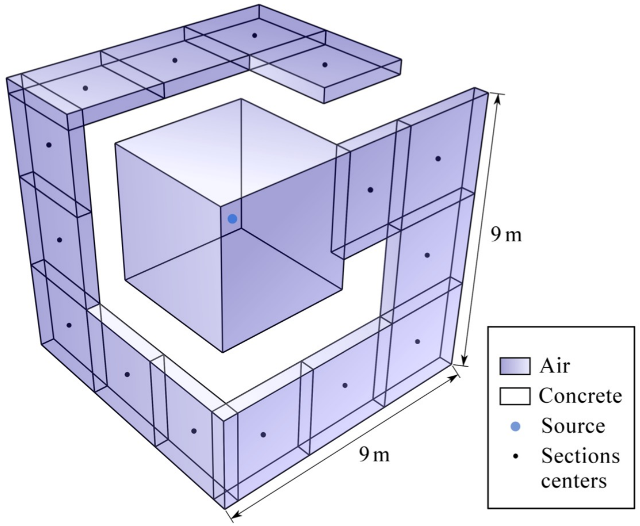
- On-the-fly scoring
- Branching tracks
- Multi-particles/particles cascades
- Towards self-learning of the cost function

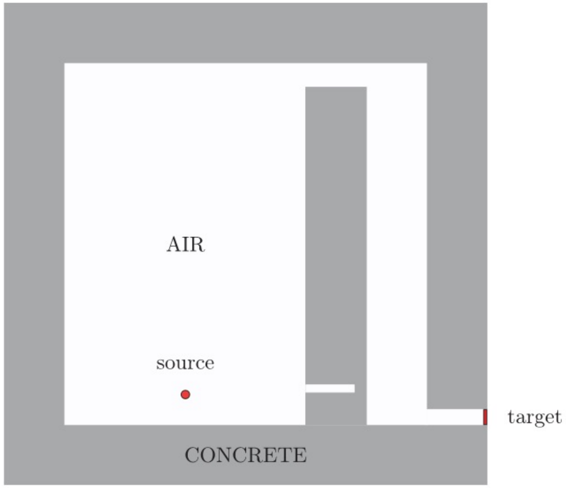
- Many radiation protection problems require to score quantities "everywhere"



Flux calculation in the cooling pool of a reactor

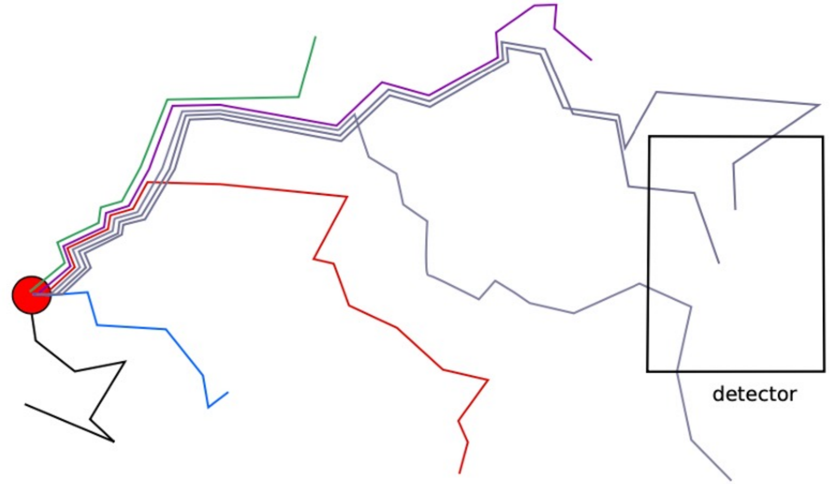
Streaming problems as can be met in nuclear marine propulsion





Dose calculations while dimensioning shielding rooms

- Following (Brehier, 2016), the idea consists inbuilding a particle genealogy
  - Old tracks are kept in memory
  - New tracks = copy of the track selected for duplication from 1st point up to splitting point



We consider the analog Monte Carlo unbiased estimate $\hat{\psi}_{MC} = \frac{1}{n}\sum_{i=1}^{n}\psi(X_i),$

of a score ψ, where $(X_i)_{i\in[1,n]}$ is a set of analog tracks

For any iteration q of the scoring process we define the following unbiased estimate:

$$\hat{\psi}_q = w_q\hat{\psi}_q^{\text{on}} + \sum_{j=0}^{q} w_j\hat{\psi}_j^{\text{off}},$$

with

$$w_j = \begin{cases} \frac{1}{n} & \text{if } j = 0 \\ \frac{1}{n}\prod_{i=0}^{j-1}\left(1 - \frac{K_i}{n}\right) & \text{if } j > 0 \end{cases}$$

$$\hat{\psi}_q^{\text{on}} = \sum_{X\in T_q^{\text{on}}}\psi(X) \quad \text{and} \quad \hat{\psi}_q^{\text{off}} = \sum_{X\in T_q^{\text{off}}}\psi(X).$$

T_q^{on} → T / $\xi > Z_q$

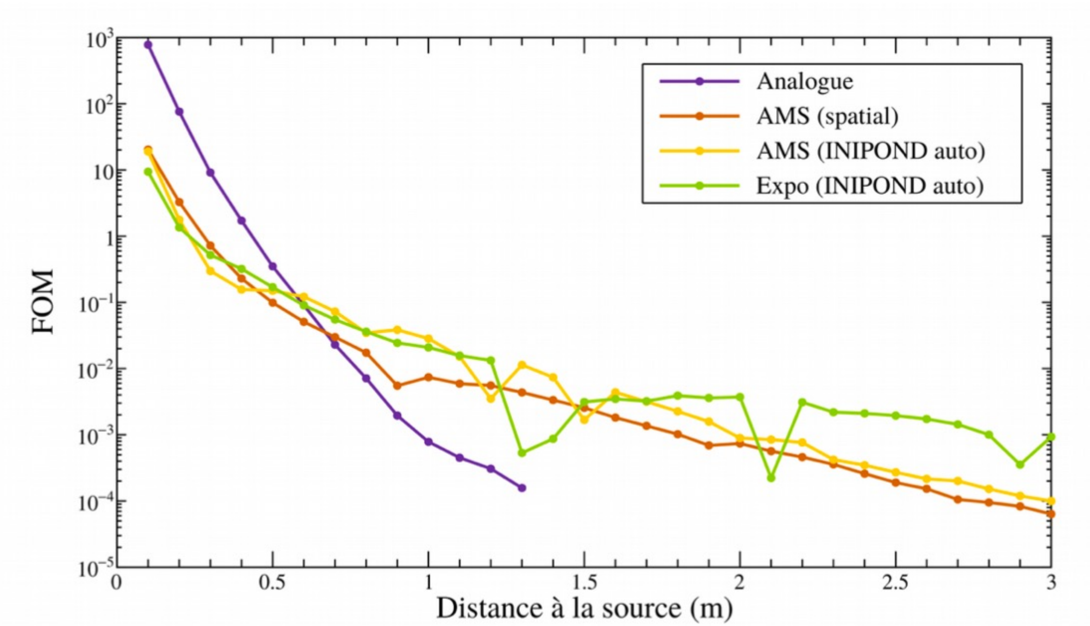
T_q^{off} → T / $\xi < Z_q$

K_q = # tracks / $\xi < Z_q$

z_q = splitting level

ON-THE-FLIGHT SCORING

❑ Cooling water pool



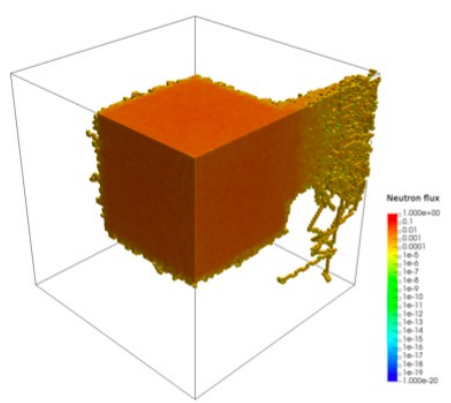
TRIPOLI-4 embedded deterministic solver for ~adjoint flux calculation

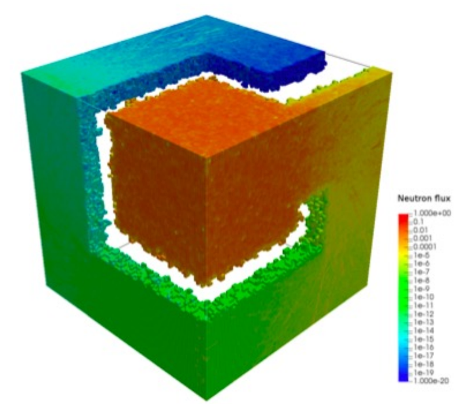
↑

- ξ either spatial or INIPOND
- AMS FOM close to ET …
- … even with naïve ξ !

❑ Labyrinth

- 2 MeV isotropic neutron source
- Air surrounded by concrete
- ET fails due to air concentration
- AMS ξ = 0 in concrete, growing following path to exit





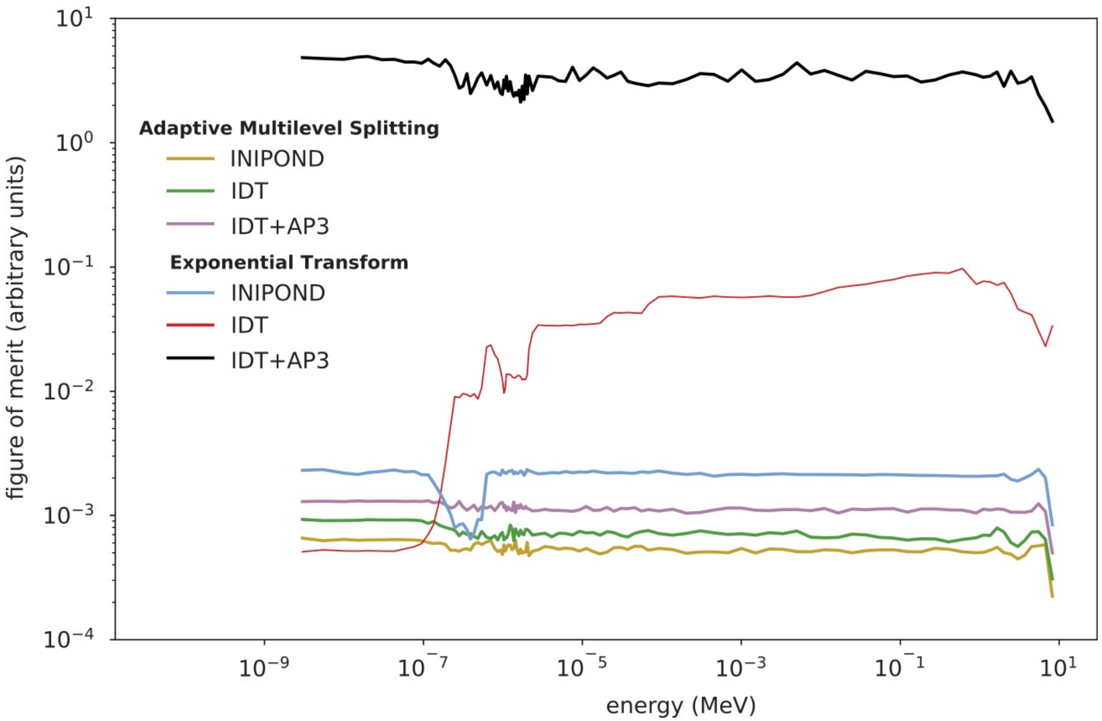
(a) Analog neutron flux

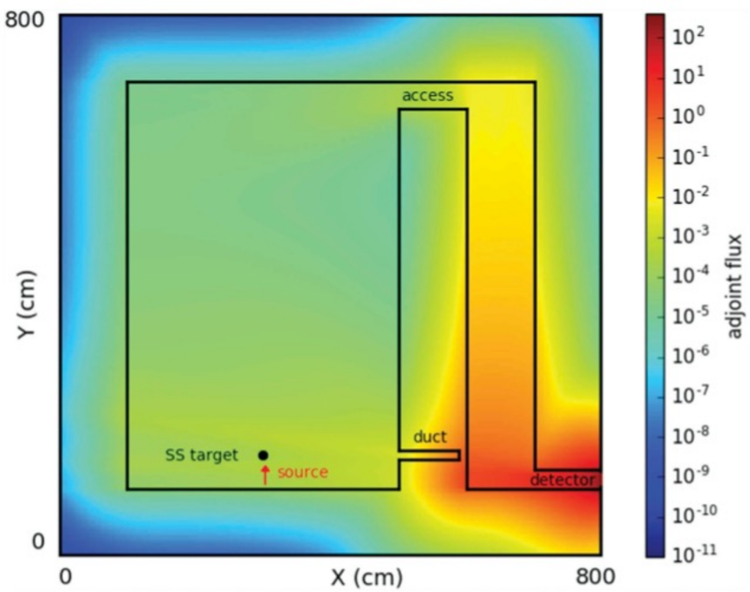
(b) AMS neutron flux

ON-THE-FLIGHT SCORING + CADIS

- Bunker benchmark
- (Mancusi et al, 2018)
- First coupling between CADIS* & AMS
- Comparison coarsest->finest: INIPOND/IDT/IDT+AP3

ξ = adjoint flux from IDT deterministic solver





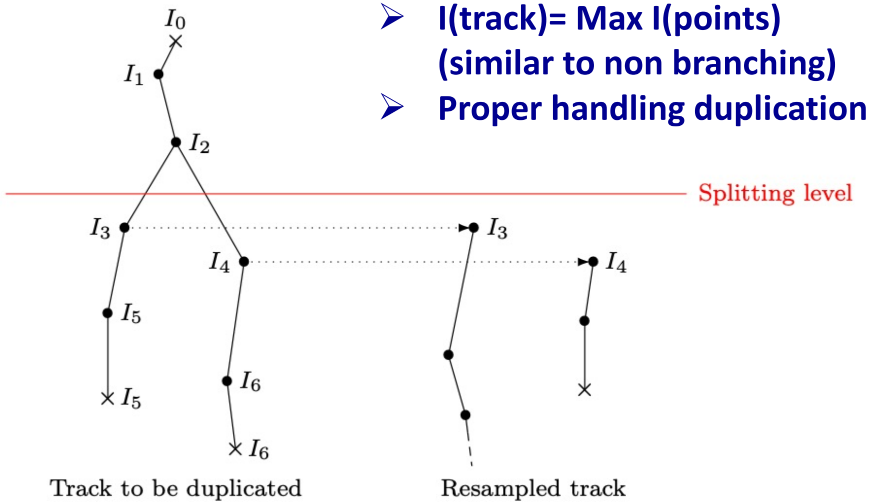
- ET : larger FOM if ξ well-known
- AMS & ET exhibit similar FOM for 'intermediate' ξ

CADIS* = Consistent Adjoint Driven Importance Sampling (Haghighat, 2003)
IDT = 3D Cartesian deterministic solver for the multigroup time-independent transport equation (Zmijarevic, 2001)
AP3 = improved adjoint flux wrt anisotropy, upscattering, and energy during cross section condensation (Schneider, 2016)

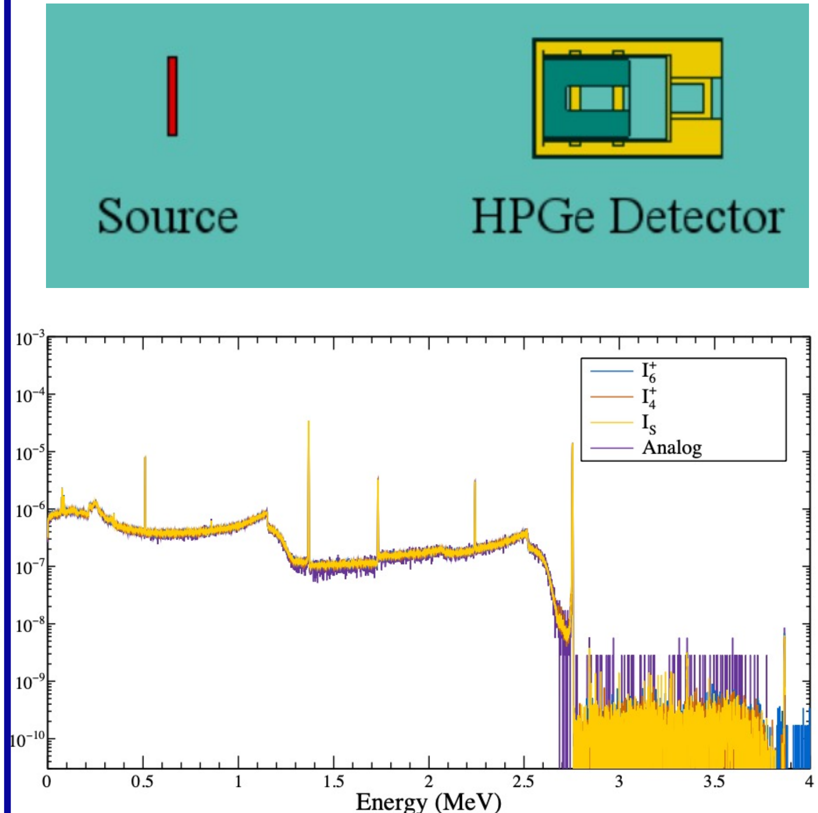
BRANCHING TRACKS

- **Many examples of branching structures in particle transport:**
  - **(n,2n)**
  - **electromagnetic cascade**
  - **fissions**
  - **Intranuclear cascade**
- **Weights/particles could be introduced but correlations would be lost**
- **Handled by an appropriate algorithm within AMS so as to preserve correlations**

- **I(track)= Max I(points) (similar to non branching)**
- **Proper handling duplication**

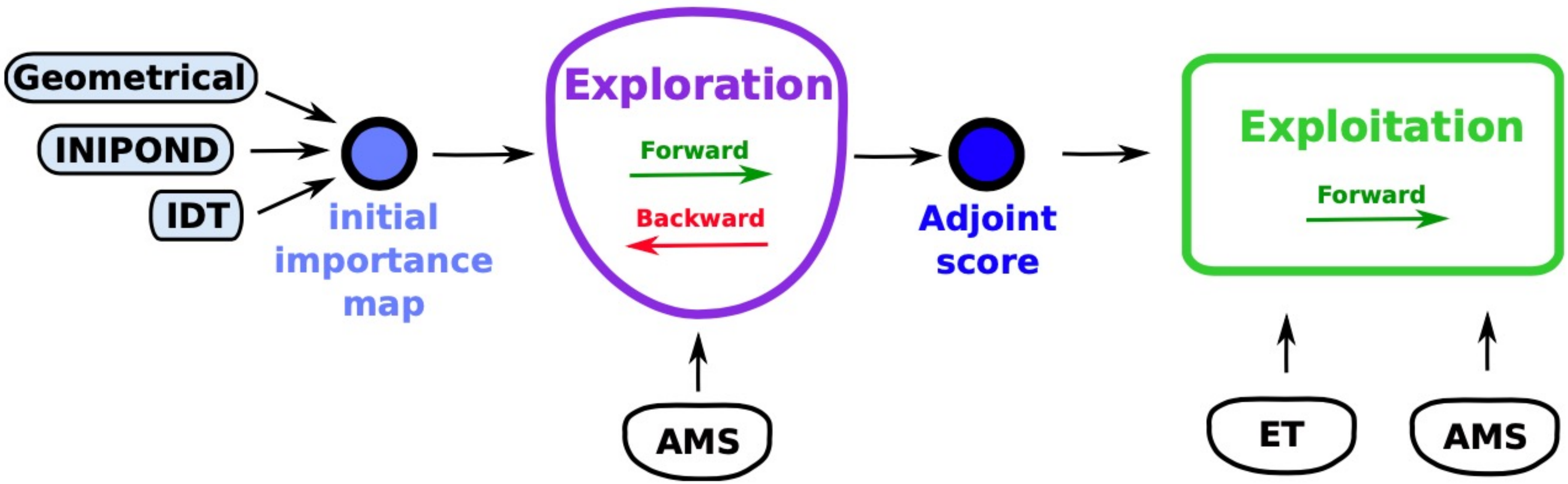


HPGe detector: g, e^+, e^-



- **FOM_{AMS}/FOM_{analog} ~ 10^2**

- Investigating the use of machine learning to improve the estimation of the adjoint flux
- (Nowak et al, 2018)
- Numerical 2-step scheme using AMS to adaptively improve the cost function / adjoint flux :



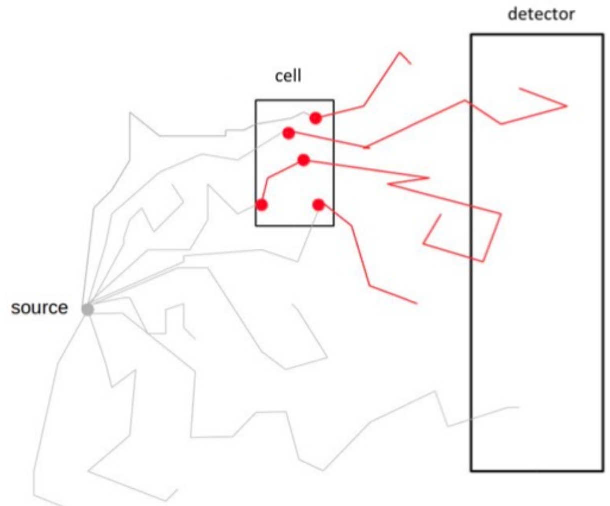
❑ Standard MC estimator of the adjoint flux

Expected contribution c of a point in the phase space

$$x = (\vec{\mathbf{r}}, \vec{\boldsymbol{\Omega}}, E)$$

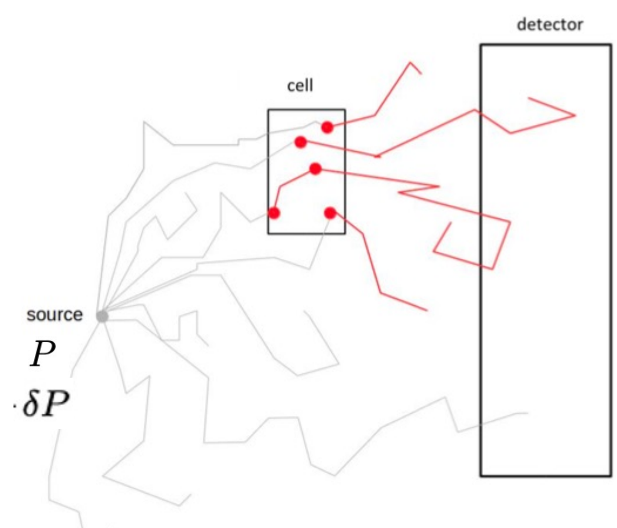
to a response (flux in a detector).

$$\psi^\dagger(P) = \mathbb{E}(c|P)$$



- N histories $\{T_0, \ldots, T_N\}$
- N_i points $\{P_0^{(i)}, \ldots, P_{N_i}^{(i)}\}$

$$\psi^\dagger(P) = \frac{\sum_{P_i \in \mathcal{T}} c_i \, \mathbb{1}_{\delta P}(\boldsymbol{r}_i, E_i, \boldsymbol{\Omega}_i)}{\sum_{P_i \in \mathcal{T}} \mathbb{1}_{\delta P}(\boldsymbol{r}_i, E_i, \boldsymbol{\Omega}_i)}$$



- **AMS estimator of the adjoint flux => the same with weights given by**

$$\psi^{\dagger}(P) = \frac{\sum_{P_i \in \mathcal{T}} c_i \, \mathbb{1}_{\delta P}(\boldsymbol{r}_i, E_i, \boldsymbol{\Omega}_i)}{\sum_{P_i \in \mathcal{T}} \mathbb{1}_{\delta P}(\boldsymbol{r}_i, E_i, \boldsymbol{\Omega}_i)}$$

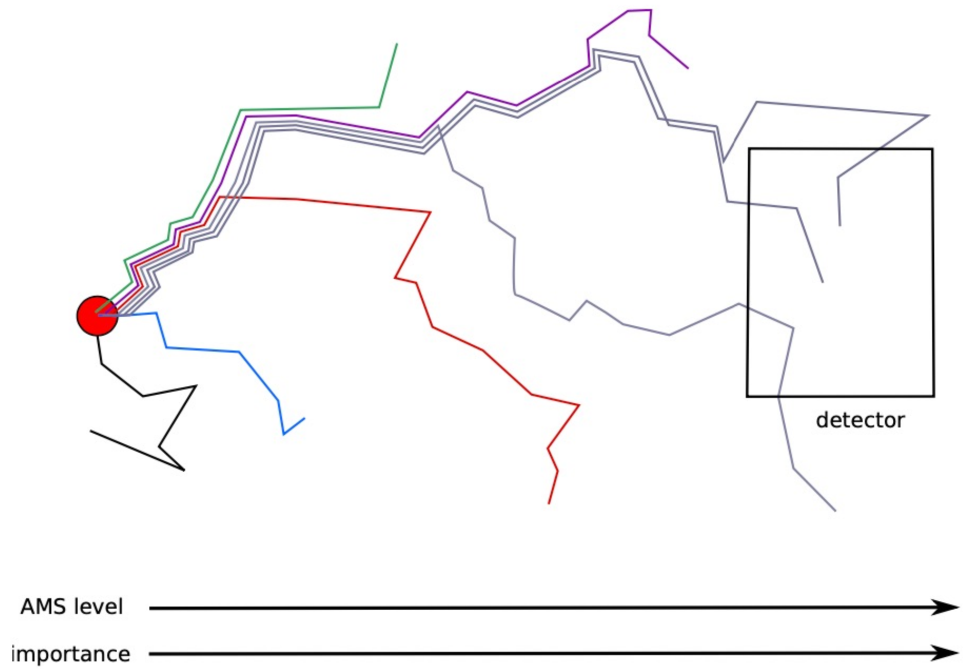
becomes

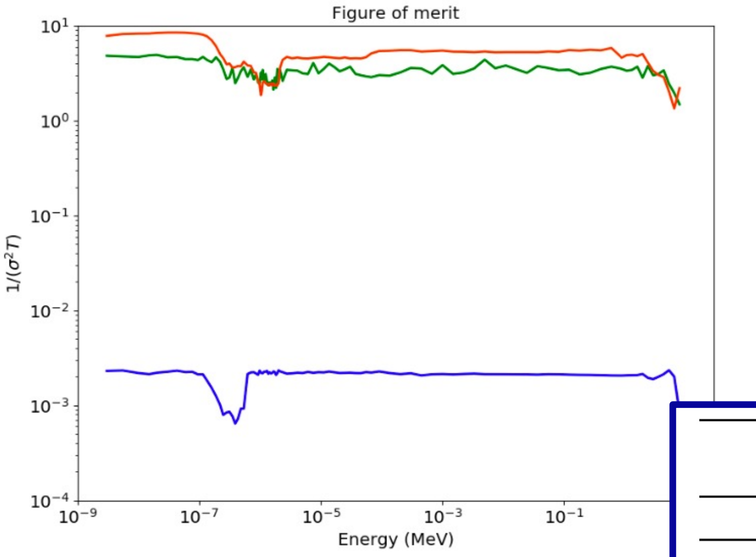
$$\frac{\sum_{\mathcal{T} \in T^{\mathrm{AMS}}} w_{\mathrm{AMS}}(\mathcal{T}) \sum_{P_i \in \mathcal{T}} c_i \, \mathbb{1}_{\delta P}(\boldsymbol{r}_i, E_i, \boldsymbol{\Omega}_i)}{\sum_{\mathcal{T} \in T^{\mathrm{AMS}}} w_{\mathrm{AMS}}(\mathcal{T}) \sum_{P_i \in \mathcal{T}} \mathbb{1}_{\delta P}(\boldsymbol{r}_i, E_i, \boldsymbol{\Omega}_i)}$$

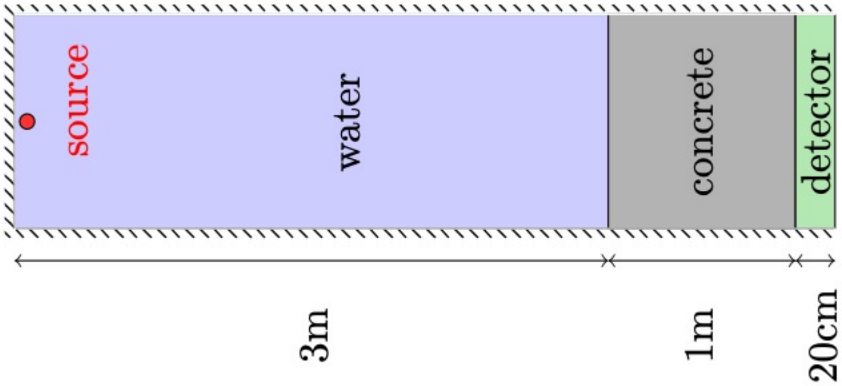
with AMS weights given by the genealogy formula

$$w_{\mathrm{AMS}}(\mathcal{T}) = \frac{1}{N} \prod_{i=0}^{j} \left(1 - \frac{K_i}{N}\right)$$

$$\text{for } \mathcal{T} \in T^{\mathrm{AMS}} = \left(\bigcup_{q=0}^{Q} S_q^{\mathrm{off}}\right) \bigcup S_Q^{\mathrm{on}}$$







Importance map (properties)	Mean$(n/cm^3/s)$	error(%)	time(s)	FOM (arbitrary units)
Adaptive Multilevel Splitting				
INIPOND (Manual mode)	2.58×10^{-15}	9.90	1.67×10^5	9
IDT (cross sections from TRIPOLI4)	2.61×10^{-15}	9.83	1.20×10^5	13
IDT (cross sections from APOLLO3)	2.78×10^{-15}	7.11	1.59×10^5	16
Adjoint score (scored with AMS)	2.66×10^{-15}	9.98	1.08×10^5	13
Exponential Transform				
INIPOND (Manual mode)	2.55×10^{-15}	6.51	9.41×10^4	39
IDT (cross sections from TRIPOLI4)	2.04×10^{-15}	6.60	2.39×10^5	23
IDT (cross sections from APOLLO3)	2.81×10^{-15}	0.82	3.27×10^3	576
Adjoint score (scored with AMS)	2.77×10^{-15}	0.52	4.33×10^3	1313

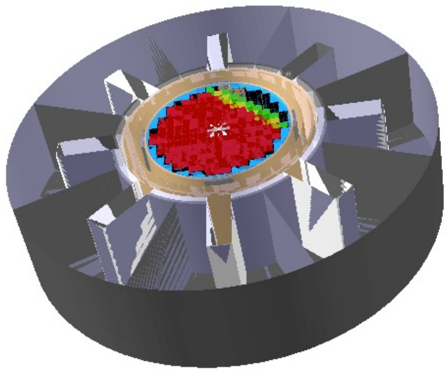
- **AMS with AMS ξ has a FOM equivalent to AMS with deterministic ξ**
- **ET with AMS ξ has FOM 2 times than ET with deterministic ξ**

❑ Use of AMS in reactor physics

- Chain reaction & population control
- Spatial correlations
- AMS & branchless collisions
- Results

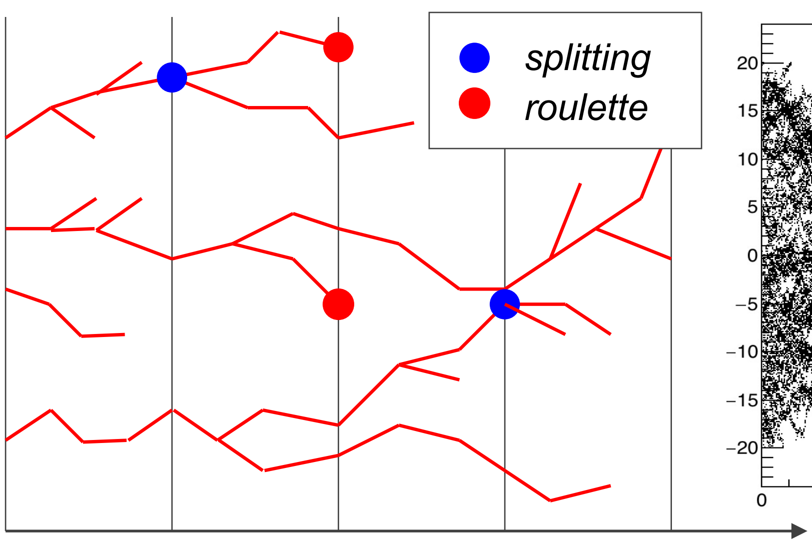
- Neutron transport in fissile media (birth/death-killing process)
- Critical Boltzmann equation
- Simplified mono-E model : BBBM with population control
- Population control usually done via 'power iteration'

- Eigenvalue: reproduction factor α (t) or keff (g)
- Eigenvectors: power distribution

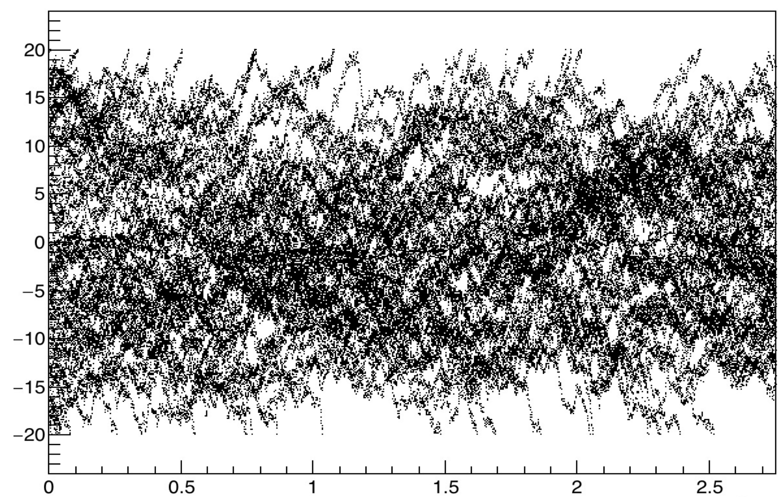


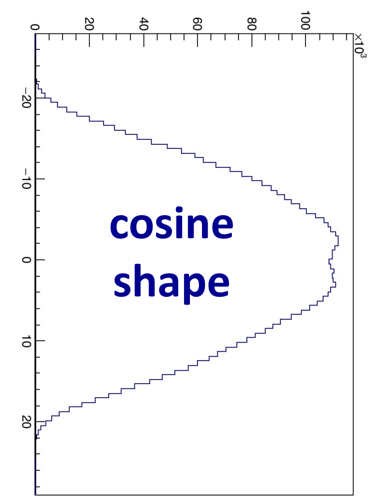
900 MW PWR

Population control algo. to keep N constant

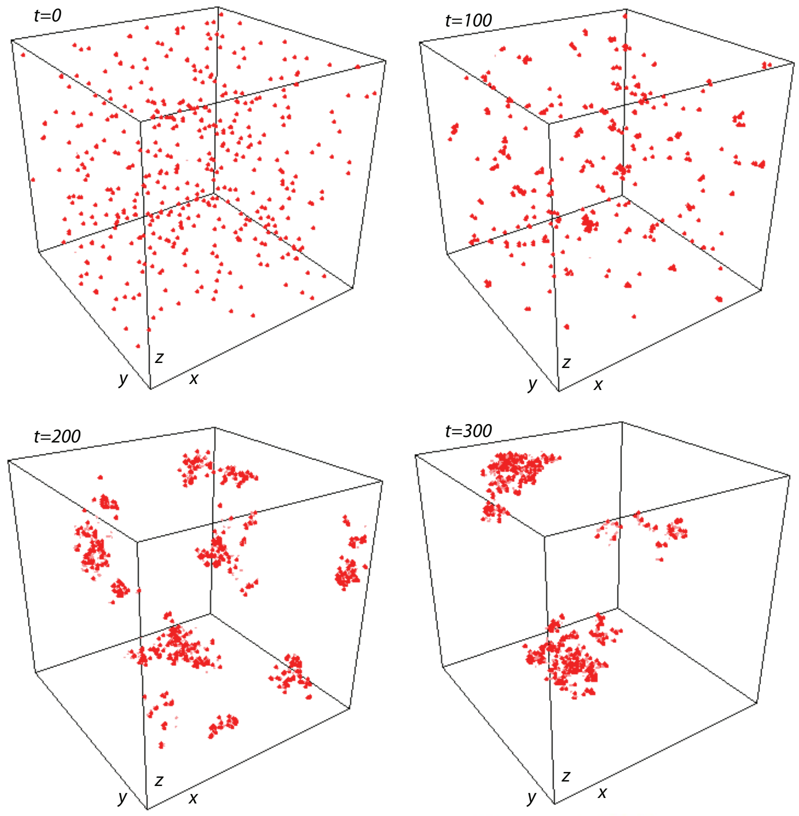


1D mono-E rod



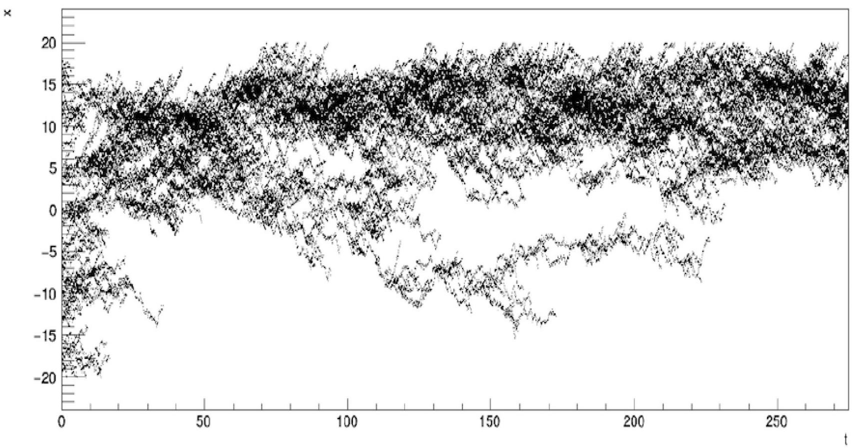


- **Branching nature of the fission process induces spatial correlations & clustering**

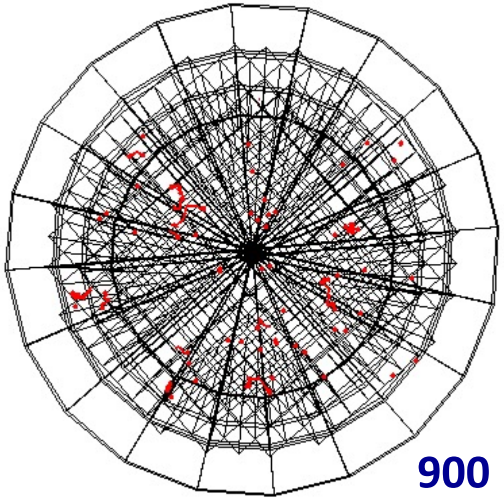


$$g_t(r) = \frac{\lambda \nu_2}{8Dc_0\pi^{3/2}r}\Gamma\left(\frac{1}{2}, \frac{r^2}{8Dt}\right)$$

(Dumonteil, 2014)



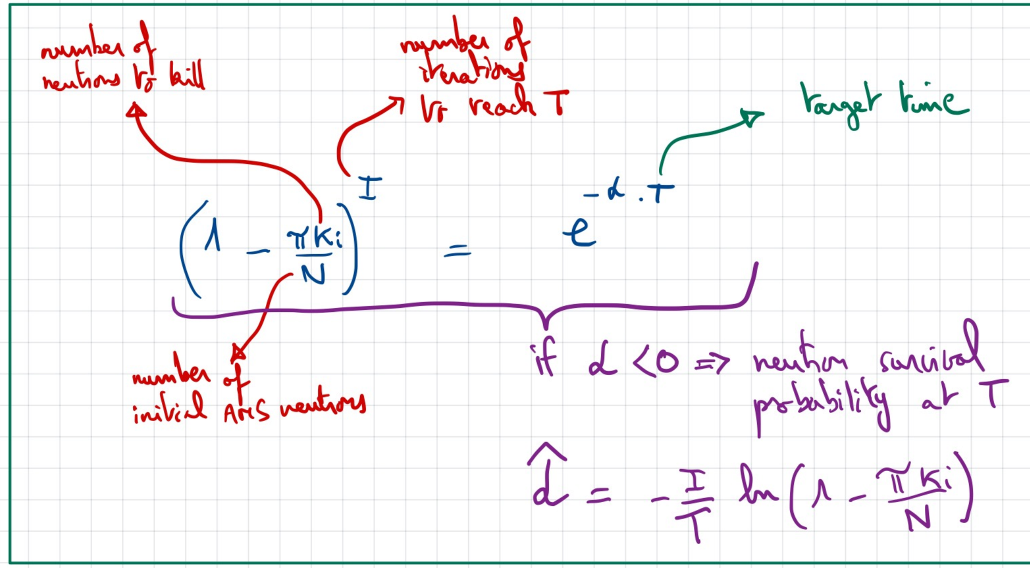
decoupled 1D mono-E rod

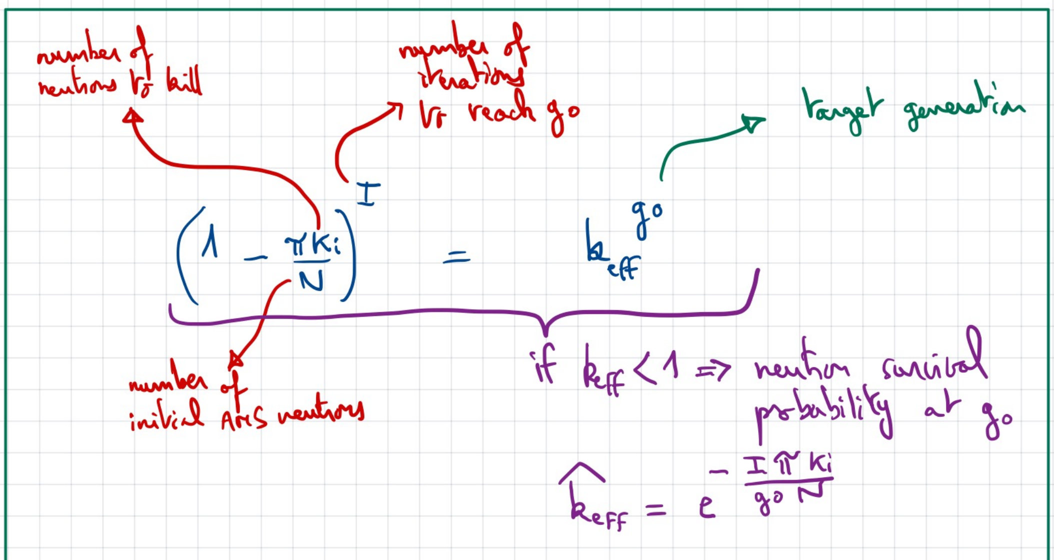


900 MW PWR

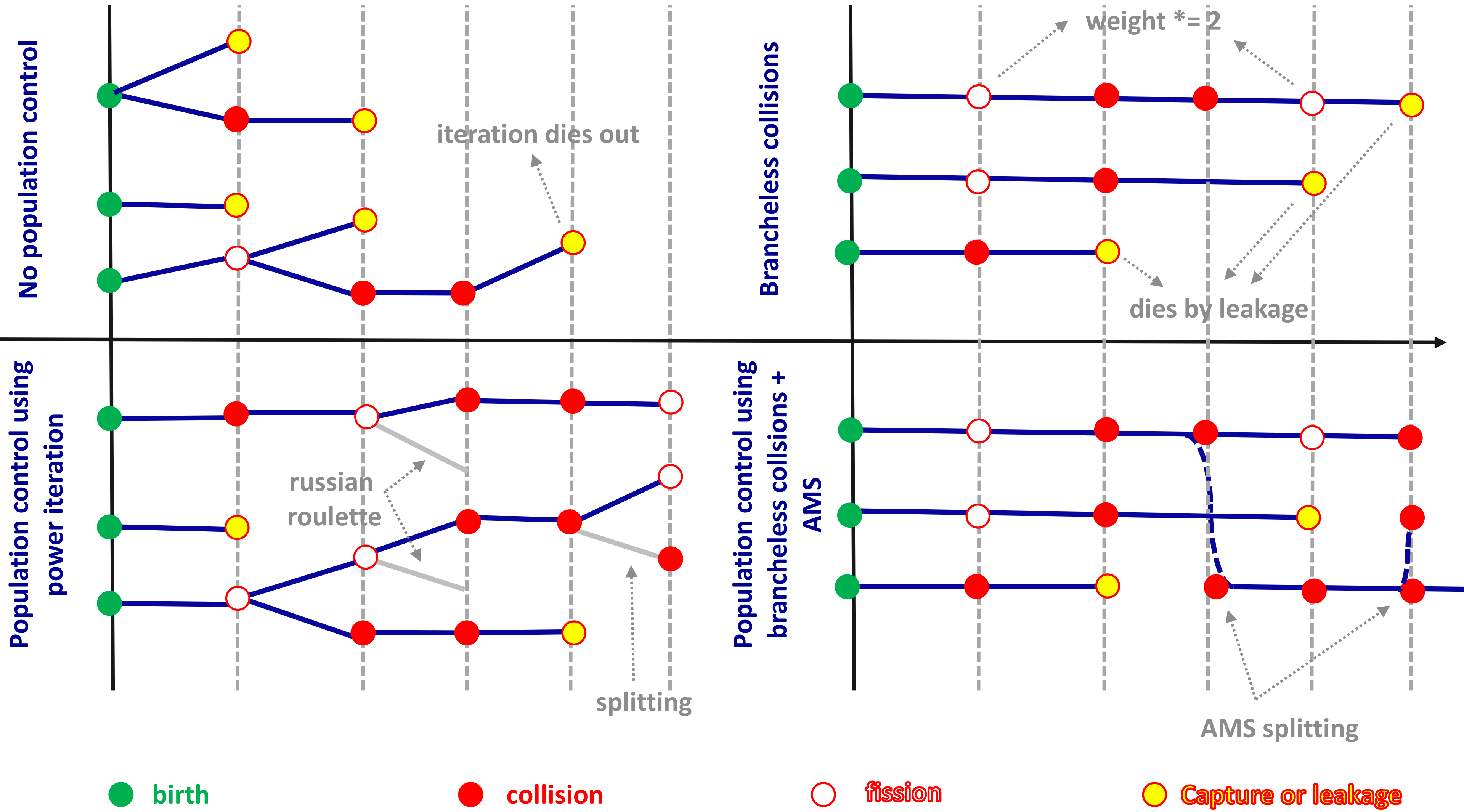
- **Power iteration induces a saturation of spatial correlations while preserving them**

- **AMS can be seen as a tool for both**
  - population control
  - variance reduction
- **Example:**
  - keff<1
  - detector = time/generation
  - rare event = surviving population
- **Similarity with a Fleming-Viot particle system**

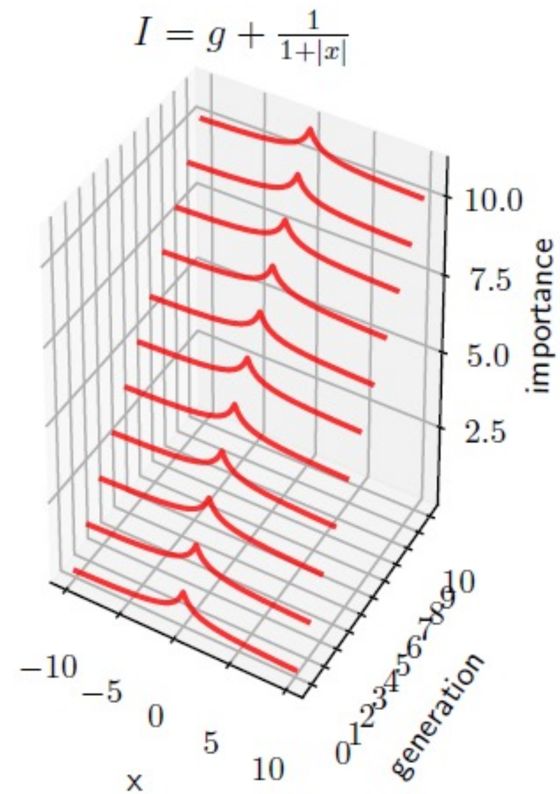




❑ AMS used in combination with branchless collisions



- « Robustness » of AMS : tracks only need to be ranked (absolute value of importance has no physical meaning)



$$\Longrightarrow Importance = g + \frac{1}{1+|x|}$$

Dominant term to rank tracks by generations & push neutrons through generations

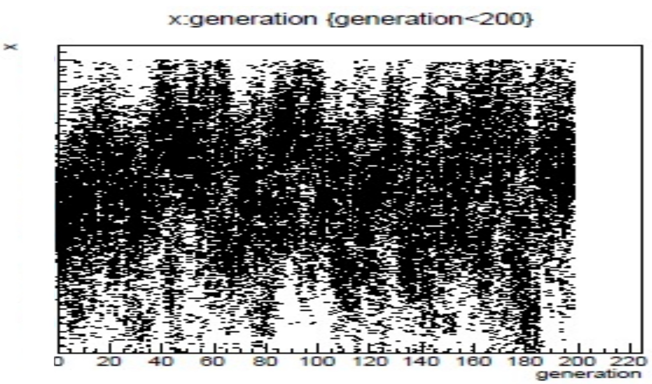
- **< 1 : Ensures to rank neutrons inside a generation**
- **A purely discrete importance can cause the algorithm to prematurely stop**

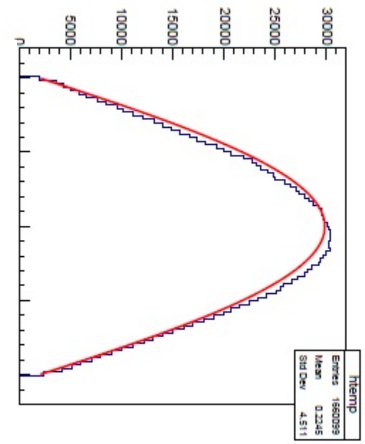
(Phd Kevin Frohlicher, 2022)

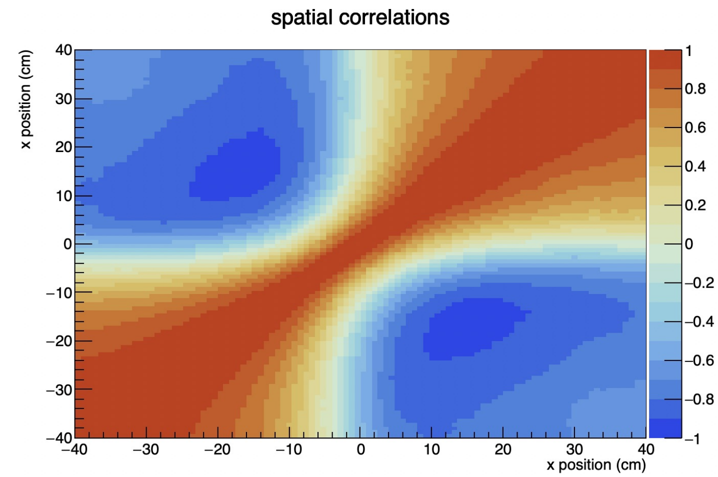
APPLICATION TO REACTOR PHYSICS : SPATIAL CORRELATIONS RESULTS

- 80 cm slab / binary branching ‘almost’-Brownian motion
- 100 independent simulations / 1000 neutrons per generation / 1000 generations
- Spatial correlations are strongly attenuated (less clustering)

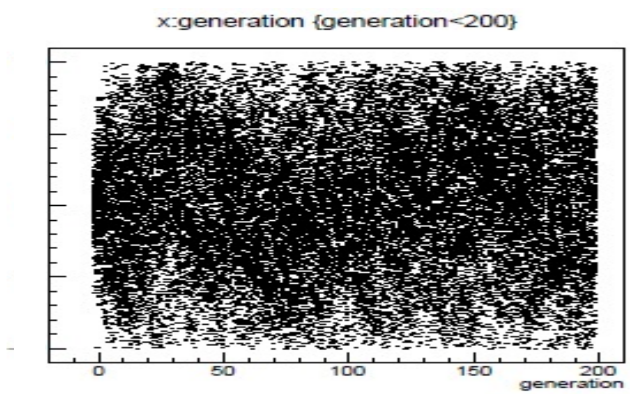
Power iteration analog

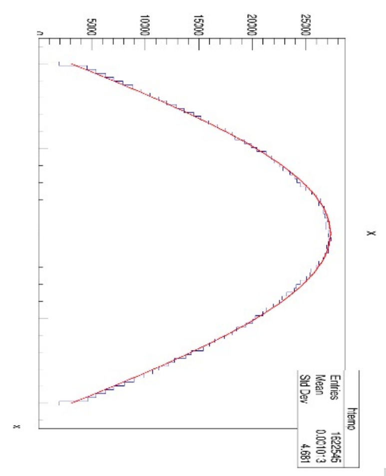


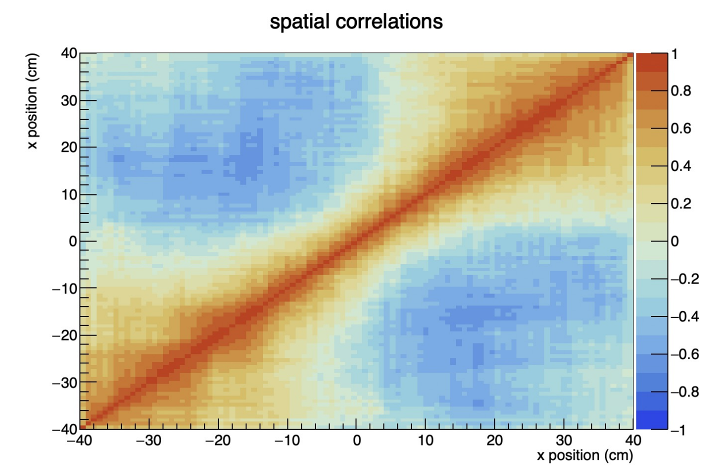




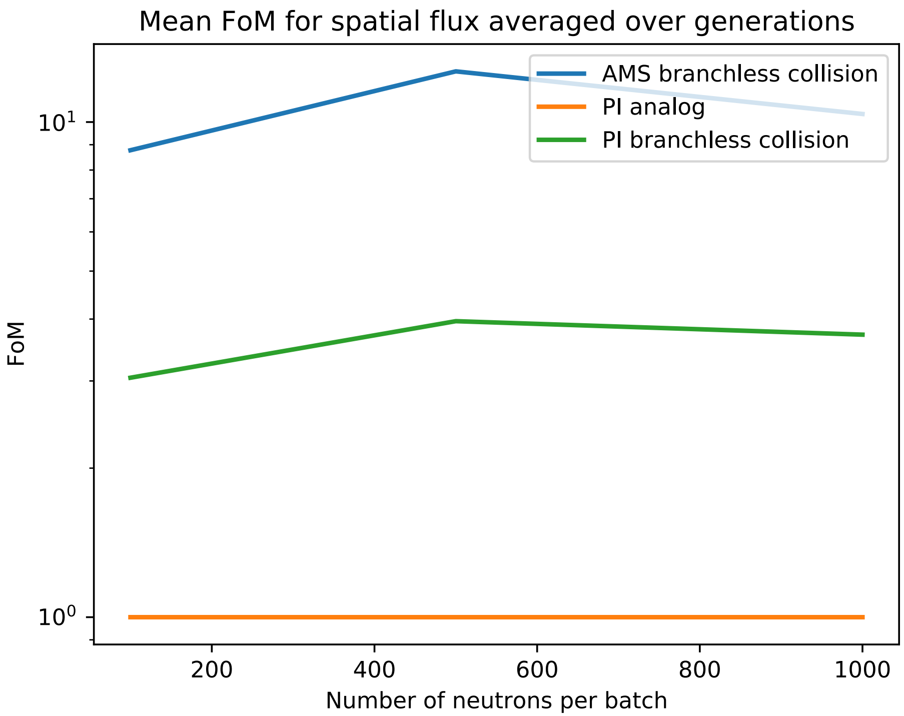
AMS branchless collision

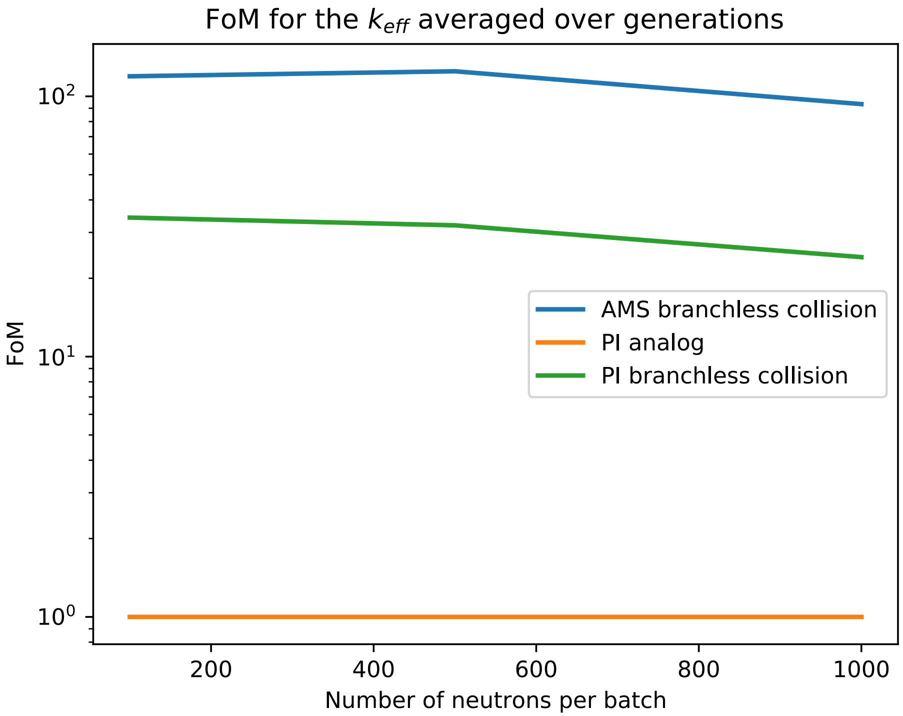






APPLICATION TO REACTOR PHYSICS : FOM





- **FOMs are sensitively improved**
- **And spatial correlations are tempered**
- **Leaves room for (spatial,directional,energetic,generational/time) variance reduction !**

CONCLUSIONS

- **AMS vs exponential transform :**
  - If exponential transform uses 0-variance schemes, AMS exhibits lower FOM
  - Way more robust (the cost function is only sensitive to ranking)
  - Requires less specific user skills (0-variance schemes of ET can take weeks to be tuned)
  - Only viable option to preserve correlations

- **Already used in "production code" by the nuclear industry** (TRIPOLI-4®) in radiation protection contexts

- **Developments on their way to popularize the method in (astro-)particle physics** (Geant4)
  - Physics beyond standard model. Ex: background calculation of elastic neutrino-nucleus scattering experiments
  - Dark matter experiments where both signal&background look for rare events

- **Openings towards quantum mechanics codes (diffusion Monte Carlo)** following the developments of AMS for eigenvalue/eigenvectors problems

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Thank you for your attention