DE LA RECHERCHE À L'INDUSTRIE

REACTOR PHYSICS

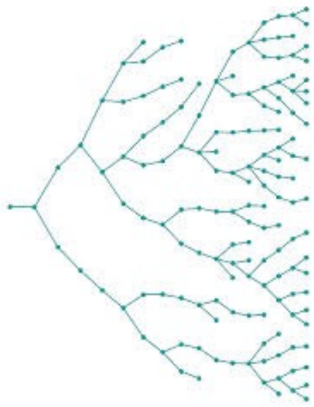
&

BRANCHING BROWNIAN MOTION

ERIC DUMONTEIL

INSTITUT DE RECHERCHE SUR LES LOIS FONDAMENTALES DE L'UNIVERS

CEA SACLAY



www.cea.fr

GDR QCD

June 7th 2022

COLLABORATIONS

- “ I do the talking” but most of theses results were obtained through collaborations…

  - A. Zoia, A. Mazzolo (CEA/DES)
  - A. Rosso (UPS/LPTMS)
  - B. Houchmandzadeh (UJF)
  - H. Louvin (CEA/DRF)
  - B. Dechenaux, K. Fröhlicher (IRSN)
  - T. Lelievre (Ecole des Ponts / Cermics), M. Rousset (INRIA)
  - A. Kyprianou (U. Bath), E. Horton (INRIA)
  - … and others!

⇨ See references for more informations

OUTLINE

- Reactor physics in a nutshell

- Monte Carlo simulation of nuclear reactors
  - Why bother ?
  - What’s the matter ?

- Stochastic modelling of spatial correlations in BBM
  - Branching Brownian Motion
  - Fluctuations & Gambler’s ruin

- Ergodicity breaking
  - Clustering
  - F-KPP traveling waves

- Numerical methods to tackle them
  - From rare events to population control using AMS
  - Results

OUTLINE

- Reactor physics in a nutshell

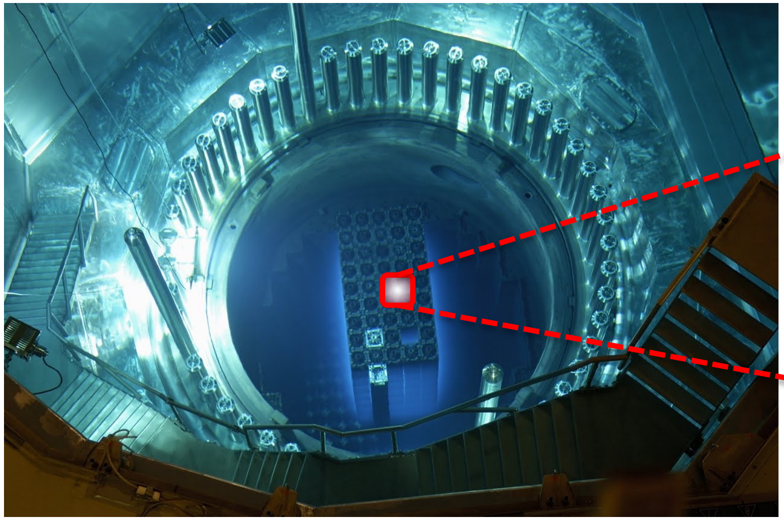
- Monte Carlo simulation of nuclear reactors
  - Why bother ?
  - What’s the matter ?

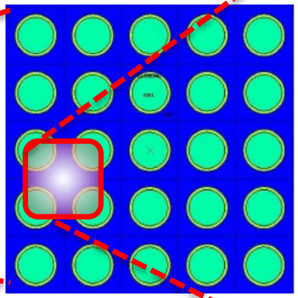
- Stochastic modelling of spatial correlations in BBM
  - Branching Brownian Motion
  - Fluctuations & Gambler’s ruin

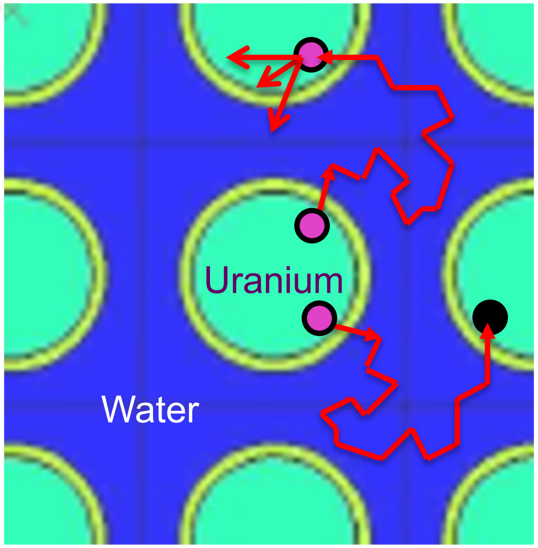
- Ergodicity breaking
  - Clustering
  - F-KPP traveling waves

- Numerical methods to tackle them
  - From rare events to population control using AMS
  - Results

… about **nuclear reactors**, and were afraid to ask







Fission chain: neutron → fission → neutrons + energy → capture or fission → …

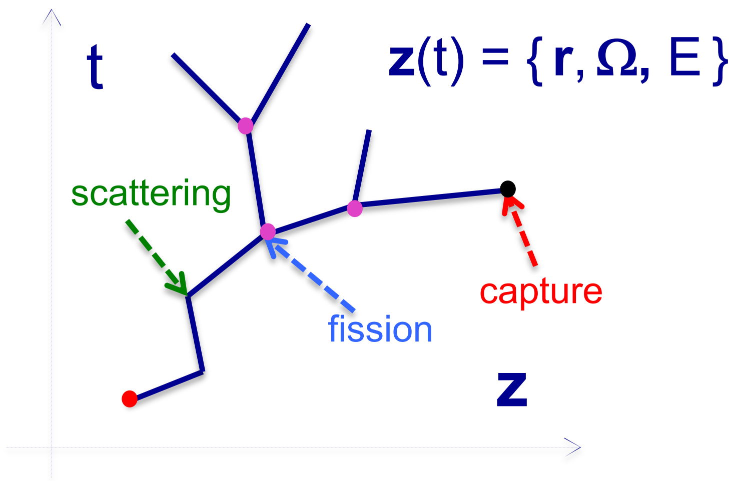
Goal: constant power, i.e., keep the fission chains **stable (critical regime)**

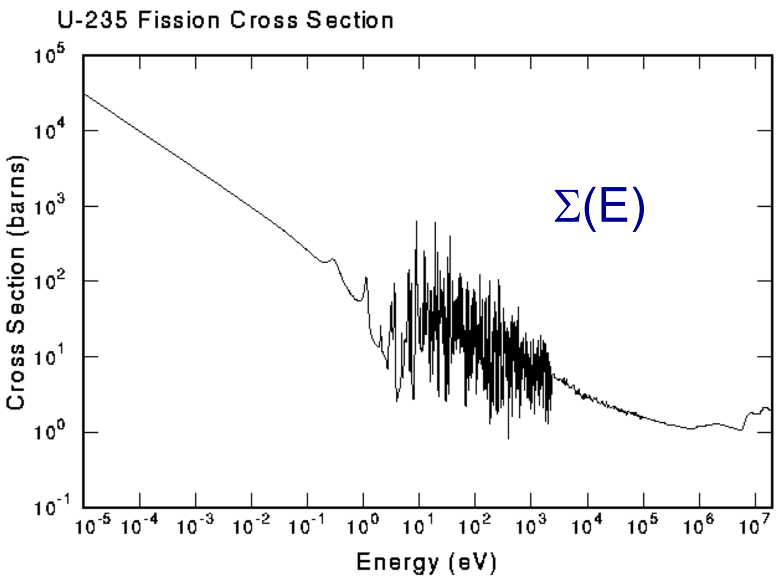
- **Balance** between births and deaths, on **average**

Sources of **fluctuations** in the neutron population: spatial diffusion, fission & capture

Courtesy of A. Zoia

NEUTRON-NUCLEI INTERACTIONS AS A RANDOM WALK





Neutrons as a (*diluted*) **gas** of diffusing particles

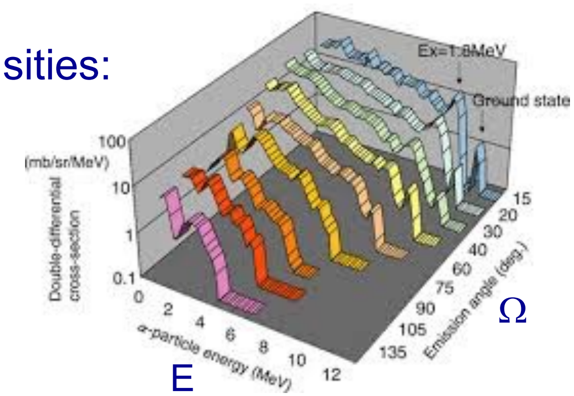
- with birth and death

Stochastic process **z**(t) = { **r**, **Ω**, E }(t):

- **branching** exponential flights

Jump kernel: $T(l) = \Sigma e^{-\Sigma l}$ Σ(E): cross section

Collision densities:



The medium is spatially **heterogeneous**

Courtesy of A. Zoia

OUTLINE

- Reactor physics in a nutshell

- Monte Carlo simulation of nuclear reactors
  - Why bother ?
  - What’s the matter ?

- Stochastic modelling of spatial correlations in BBM
  - Branching Brownian Motion
  - Fluctuations & Gambler’s ruin

- Ergodicity breaking
  - Clustering
  - F-KPP traveling waves

- Numerical methods to tackle them
  - From rare events to population control using AMS
  - Results

MONTE CARLO NEUTRON TRANSPORT CODES & THE NUCLEAR INDUSTRY

- Monte Carlo neutron transport codes :

  - since World War II, close intermixed history between Monte Carlo methods, nuclear applications of fission & supercomputing

- Nuclear energy : MC neutron transport codes are used as reference numerical schemes as

  - no spatial / angular mesh required

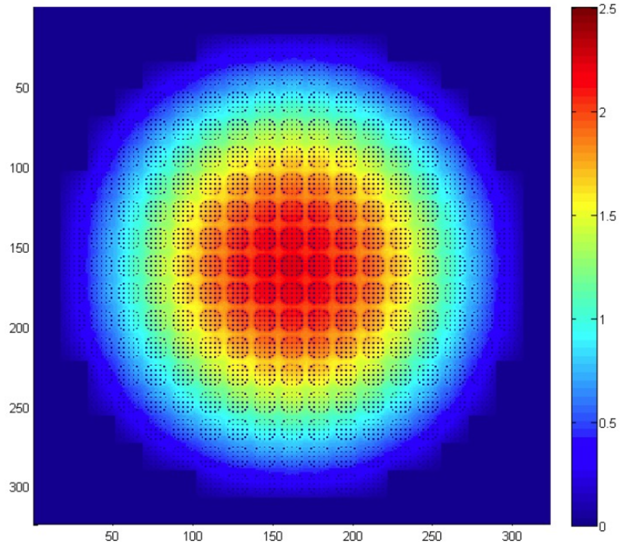
  - no hypotheses on **energy E** (EDF industrial numerical scheme = 2-group diffusion)

- Extremely versatile: Complex geometries without fine tuning of ad hoc schemes

▶ Used for the **design of GenIV** reactors (Fast Reactors, Thorium reactors, …)
▶ Used by **nuclear safety authorities** to validate and qualify all safety procedures

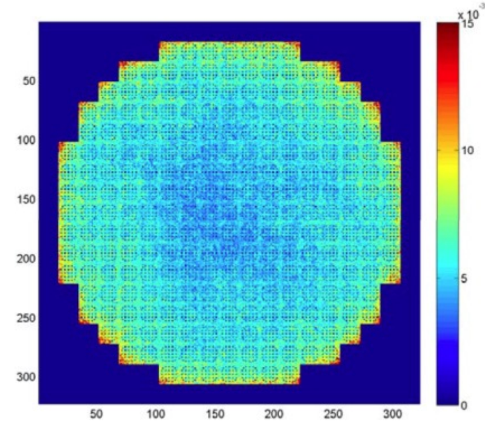
BIAS IN STATISTICAL UNCERTAINTIES ESTIMATIONS

pin power distribution 900 MW PWR

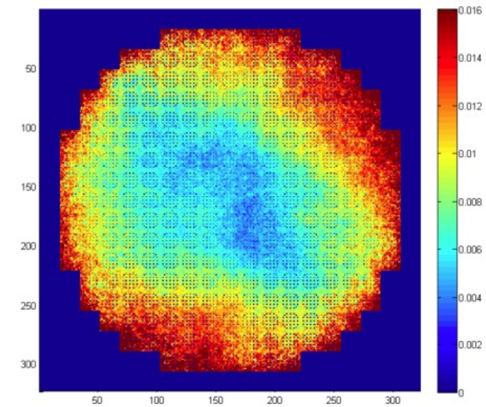


[Martin, Physor2012]

[Lee et al, SNA+MC2010]



apparent std dev



real std dev

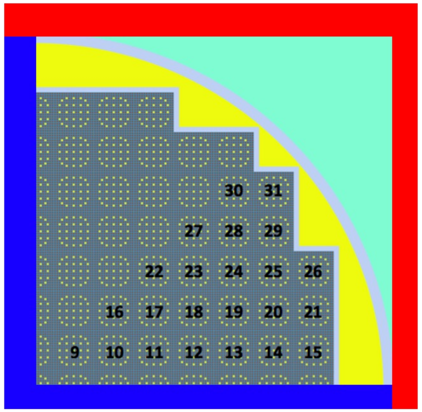
- ❑ Long standing issue (70's)
- ❑ Spatial asymmetries in the flux distribution for symmetric positions
- ❑ Underestimation of statistical uncertainties!

[Gelbard and Prael, 1974] [Brissenden and Garlick, 1986] [Brown, Physor 2006]

BIAS IN AVERAGE QUANTITIES ESTIMATIONS

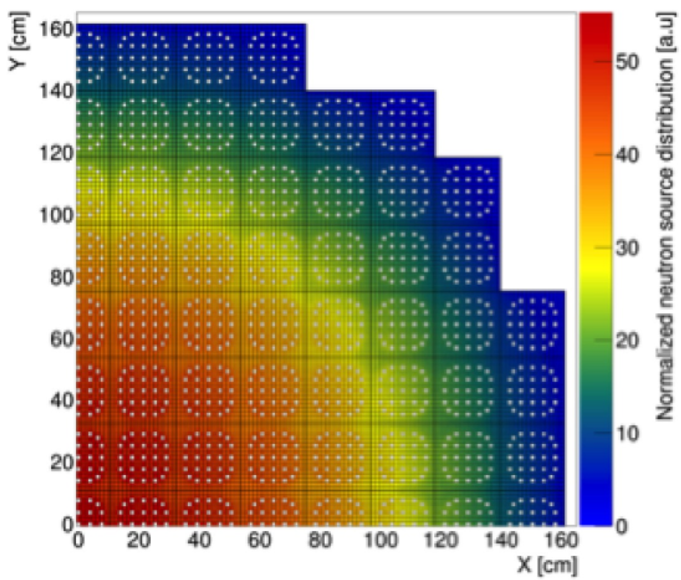
- Benchmark OECD/NEA
- ¼ PWR-type core

Reflective boundary Conditions (Neumann)

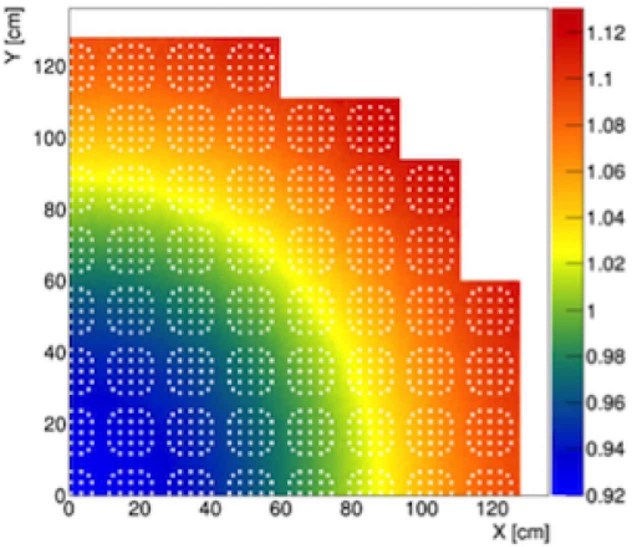


Absorbing boundary Conditions (Dirichlet)

Fluxes (10^4 active cycles of 10^4 neutrons)



$$\frac{\text{Fluxes } (10^6 \text{ active cycles of } 10^2 \text{ neutrons})}{\text{Fluxes } (10^2 \text{ active cycles of } 10^6 \text{ neutrons})}$$



Under-estimation of the flux inside the core, over-estimation for the outer parts

OUTLINE

- Reactor physics in a nutshell
- Monte Carlo simulation of nuclear reactors
  - Why bother ?
  - What's the matter ?
- Stochastic modelling of spatial correlations in BBM
  - Branching Brownian Motion
  - Fluctuations & Gambler's ruin
- Ergodicity breaking
  - Clustering
  - F-KPP traveling waves
- Numerical methods to tackle them
  - From rare events to population control using AMS
  - Results

BRANCHING BROWNIAN MOTION

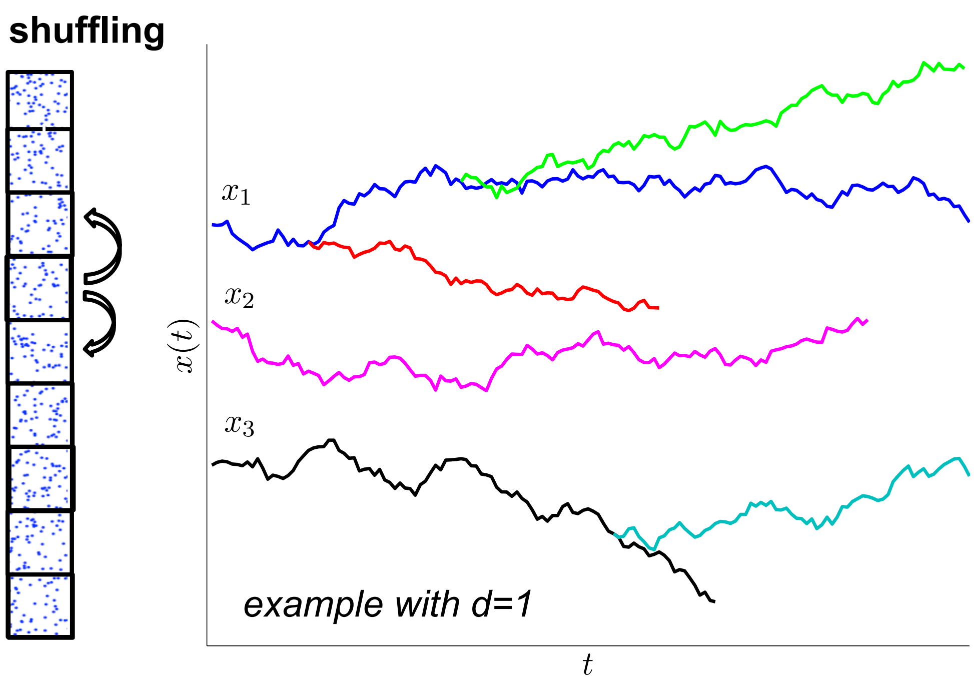
Simplified model for neutron transport in multiplicative media :

- ❑ $N_0 \to \infty$ neutrons, uniformly distributed at t=0
- ❑ Infinite medium ($L \to \infty$)

$\Big\}\ c_0 = cte$

- ❑ No energy dependence
- ❑ Brownian motion with diffusion coefficient *D* [cm2.s-1] $\rightarrow\ < x^2(t) >= Dt$
- ❑ Undergoes collision at Poissonian times with rate λ [s-1]
- ❑ At each collision, k descendants with probability $p(k)$
- ❑ Dimension *d*

$$\left[\begin{array}{l} p(0) \leftrightarrow \Sigma_c \\ p(1) \leftrightarrow \Sigma_s \\ p(2), p(3), \ldots \leftrightarrow \Sigma_f \\ \nu_1 = \sum_k k p(k) \end{array}\right.$$



BBM process couples :

$\Rightarrow$ Galton-Watson birth-death process to describe ***fission*** and ***captures***

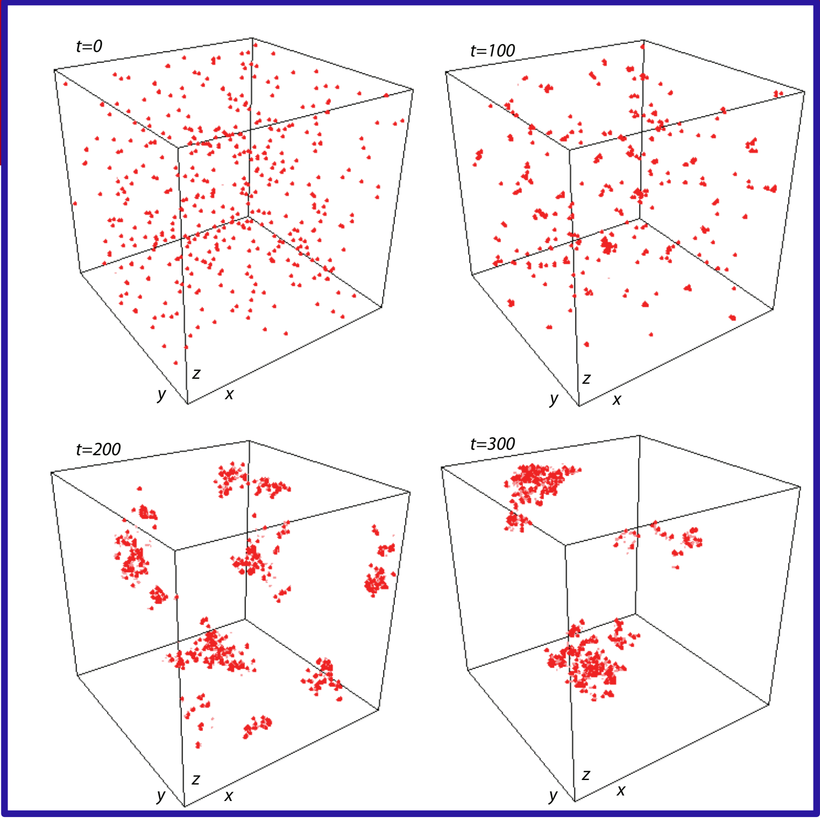
$\Rightarrow$ Brownian motion to simulate ***neutron transport***

NEUTRON CLUSTERING

- Numerical « toy model »
- Exponential flights with typical jump size $1/\Sigma_s \to 0$ to recover the ***diffusion regime***
- Binary branching

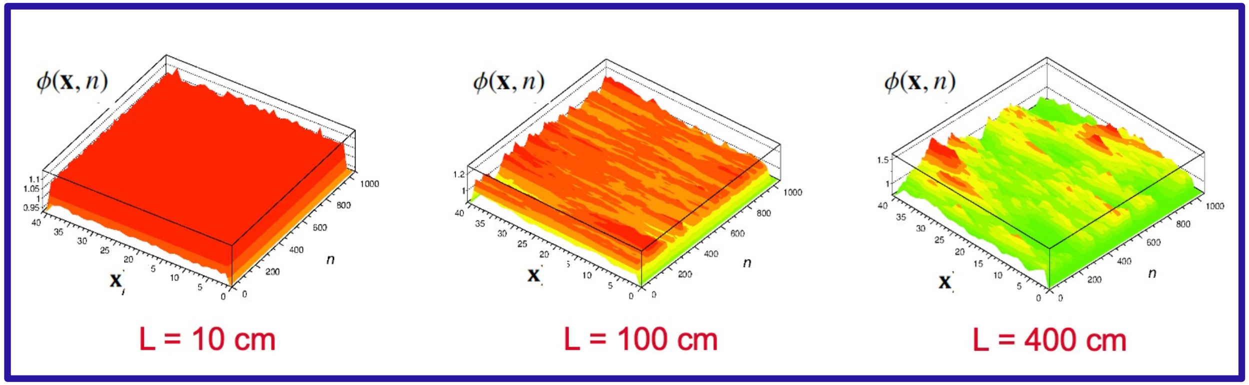
$$p(0) = \frac{1}{2} \qquad p(2) = \frac{1}{2}$$

- Dimension $d = 3$
- Typical length $L >> l$



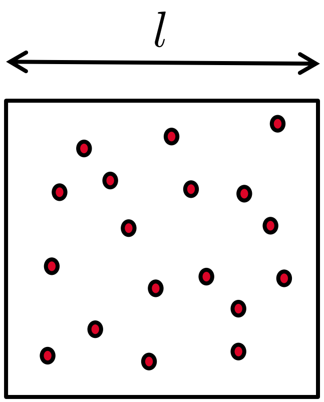
The " 3d " homogeneous cube

The " 1d " rod model



Can we have a quantitative insight into this phenomenon?

FLUCTUATIONS (I.E. CLUSTERING IN DIMENSION 0)



- We consider a "cell" *i* at time *t* with n individuals
- d=0 Branching events with:
  - production rate $\lambda p(2)$
  - capture rate $\lambda p(0)$
- Proba(n➔n+1 in dt): $W^+(n)dt = \lambda p(2) n dt$
- Proba(n➔n-1 in dt): $W^-(n)dt = \lambda p(0) n dt$

$\lambda p(0), \lambda p(2)\ [s^-1]$

$n\ [\#]$

$dt\ [s]$

Forward master equation

$$\boxed{\frac{dP(n,t)}{dt} = W^-(n+1)P(n+1,t) \quad -W^+(n)P(n,t) \\ +W^+(n-1)P(n-1,t) \quad -W^-(n)P(n,t)}$$

Critical :

$$\lambda p(0) = \lambda p(2)$$

$$< n(t) >= n_0$$

$$< V(t) >= \lambda n_0 t$$

$$\left.\begin{aligned} < n(t) > &= \sum_n n P(n,t) \\ < n^2(t) > &= \sum_n n^2 P(n,t) \end{aligned}\right\}$$

$$< n(t) >= n_0 e^{\lambda(p(2)-p(0))t}$$

$$< V(t) >=< n^2(t) > - < n(t) >^2 = \lambda(p(0)+p(2)) n_0 t$$

Blaise Pascal (1623-1662)
mathematician & philosopher

Letter (1656)

" what happens if I have \$1000 at hand
and I play a fair game
(p=0.5 to win, p=0.5 to loose)
betting \$1 at each trial ? "

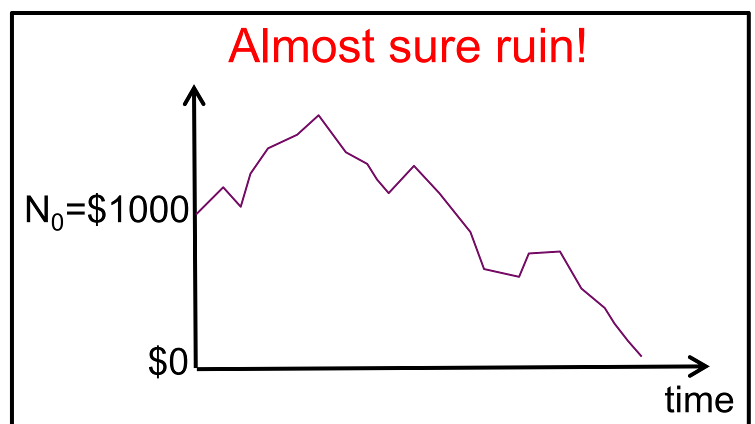
Pierre de Fermat (1605-1665)
mathematician & magistrate

Critical :

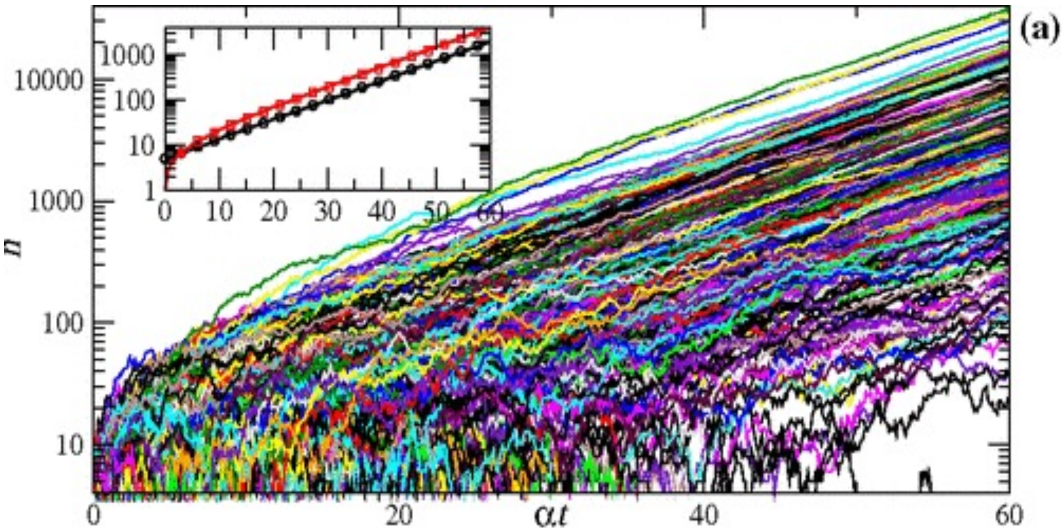
$$\lambda p(0) = \lambda p(2)$$

$$< n(t) >= n_0$$

$$< V(t) >= \lambda n_0 t$$



[Houchmanzadeh, 2008]



as time goes by, less and less "rich" player, getting richer and richer to compensate the ruins

More & more ruins

N $1 coins in a box which are played in a fair game

⇕

N neutrons in a critical spatial cell which undergo fission or capture events

Fair game → criticality in reactor physics

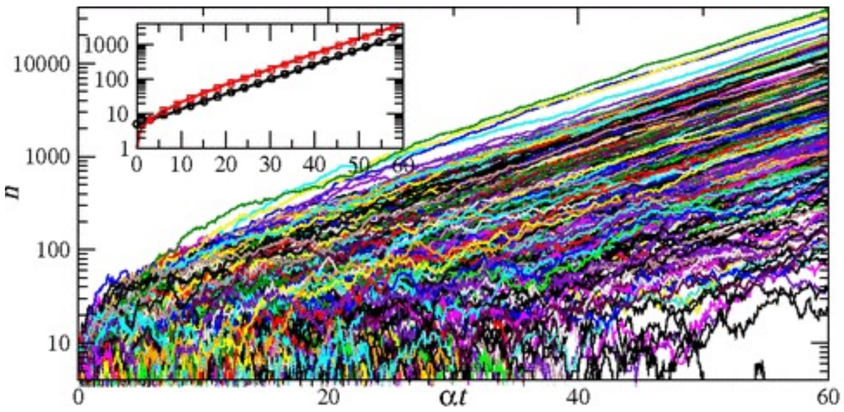
Gambler's ruin → critical catastrophe!

[Williams, 1974]

- ❑ **Could a nuclear reactor shut down alone?**
- ❑ **Possible to conceive such an experiment?**
- ❑ **What about the « proliferating trajectories?**

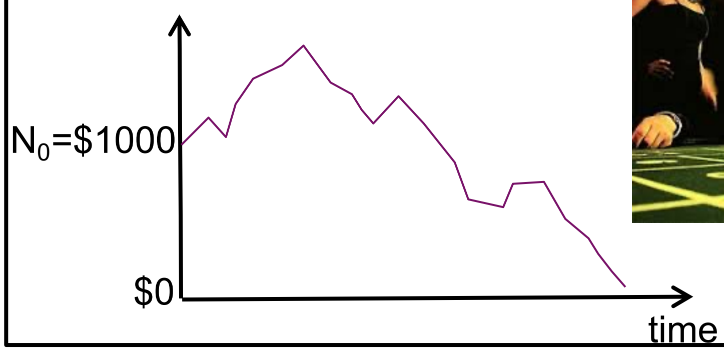
… AND FROM CRITICAL CATASTROPHY TO NEUTRON CLUSTERING

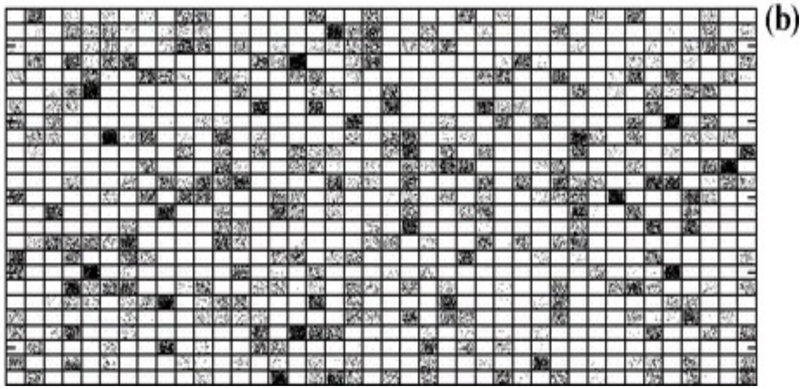
[Houchmandzadeh, PRE 2008]



$$< n(t) >= n_0$$
$$< V(t) >= \lambda n_0 t$$

Almost sure ruin!





OUTLINE

- Reactor physics in a nutshell
- Monte Carlo simulation of nuclear reactors
  - Why bother ?
  - What's the matter ?
- Stochastic modelling of spatial correlations in BBM
  - Fluctuations & Gambler's ruin
  - Spatial correlations & clustering
- Ergodicity breaking
  - Clustering
  - F-KPP traveling waves
- Numerical methods to tackle them
  - From rare events to population control using AMS
  - Results

FROM D=0 TO D=2

d=0 => Critical castastrophy ⇔ Gambler's ruin
d>0 => Neutron clustering

but here the cells were totally decoupled → "fake" d=2

We have to take into account the *diffusion* of neutrons

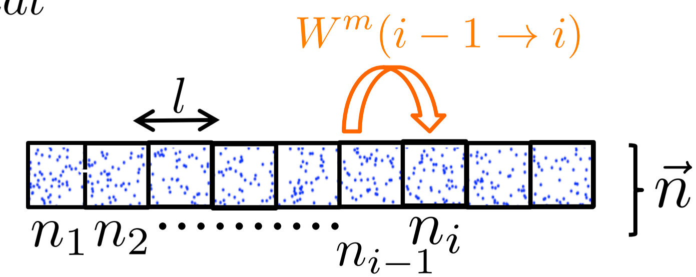
?

A LITTLE BIT OF FIELD THEORY

- ***fission*** event
  - proba: $W^+(\vec{n}, i)dt = \lambda p(2)\eta_i \vec{n} dt$
  - action on $\vec{n}$: $a_i^+ \vec{n} = (\ldots, n_{i-1}, \boxed{n_i + 1}, n_{i+1}, \ldots)$
- ***capture*** event
  - proba: $W^-(\vec{n}, i)dt = \lambda p(0)\eta_i \vec{n} dt$
  - action on $\vec{n}$: $a_i \vec{n} = (\ldots, n_{i-1}, \boxed{n_i - 1}, n_{i+1}, \ldots)$
- ***migration*** event
  - proba: $W^m(\vec{n}, i-1 \to i)dt = \lambda p(1)\eta_i \vec{n} dt$
  - action on $\vec{n}$: $a_i^+ a_{i-1} \vec{n}$

with η_i the number of neutrons in cell i

and $\lambda p(1) = {}^{D}/_{2l^2}$



Forward master equation

$$
\begin{aligned}
\frac{dP(\vec{n},t)}{dt} = \sum_i & W^+(a_i\vec{n}, i)P(a_i\vec{n}, t) && -W^+(\vec{n}, i)P(\vec{n}, t) \\
& +W^-(a_i^+\vec{n}, i)P(a_i^+\vec{n}, t) && -W^-(\vec{n}, i)P(\vec{n}, t) \\
& +W^m(a_{i-1}^+ a_i\vec{n}, i-1, i)P(a_{i-1}^+ a_i\vec{n}, t) && - W^m(\vec{n}, i, i+1)P(\vec{n}, t) \\
& +W^m(a_{i+1}^+ a_i\vec{n}, i+1, i)P(a_{i+1}^+ a_i\vec{n}, t) && - W^m(\vec{n}, i, i-1)P(\vec{n}, t)
\end{aligned}
$$

A LITTLE BIT OF FIELD THEORY

As before one can inject in the Master equation the mean number of neutrons in cell k:

$$< n_k >= \sum_n n_k P(n_k, t)$$

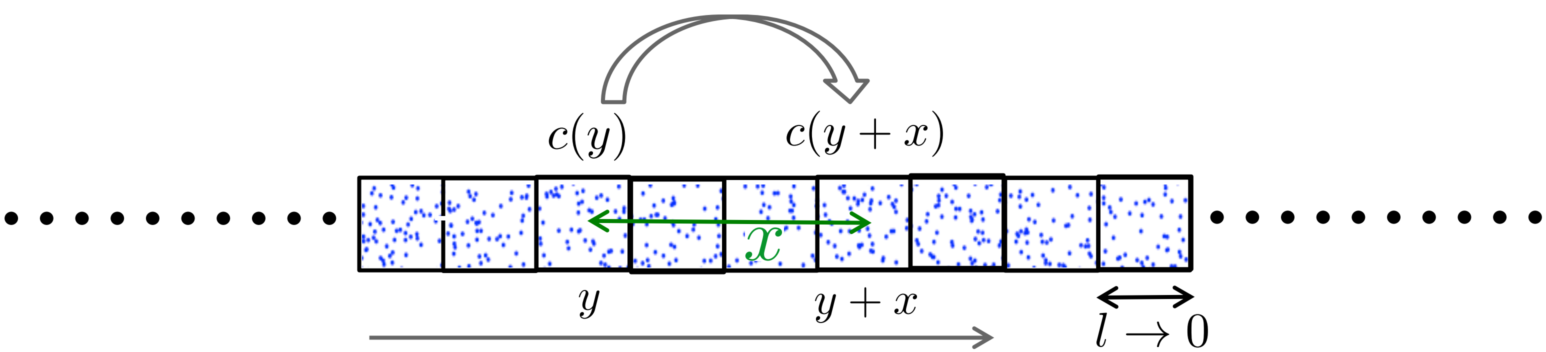
or its continuous version:

$$c(x) = \lim_{l \to 0} \frac{n_k}{l}$$

And define an appropriate tool to study spatial correlations:

the centered correlations without self-contribution

$$g(x,t) = (< c(y)c(y+x) > - c^2 - c\delta(x))/c^2$$



EQUATION FOR THE 2-POINTS CORRELATION FUNCTION

The equations obtained stand for any arbitrary dimension d and in the case $\nu_1 = 1$ can be written :

$$\frac{\partial}{\partial t} c_t(\mathbf{x}) = 0$$

d-dimensional Laplacian (diffusion term)

$$\frac{\partial}{\partial t} g_t(r) = 2D \boxed{\nabla_r^2} g_t(r) + \boxed{\frac{\lambda \nu_2}{c_t} \delta(r)}$$

$$with \quad r = |x - y|$$

$$and \quad \nu_2 = \sum_k k(k-1) p(k)$$

auto-correlation term leading to 2nd moment effects (ν_2 is the mean number of pairs)

Young, W.R., Roberts, A.J., Stuhne, G., Nature 412, 328 (2001)
Houchmandzadeh, B., Phys. Rev. E 66, 052902 (2002)
Houchmandzadeh, B., Phys. Rev. Lett. 101, 078103 (2008)
Houchmandzadeh, B., Phys. Rev. E 80, 051920 (2009)
Dumonteil, E. et al, Annals of Nuclear Energy 63, 612-618 (2014)

ANALYTICAL SOLUTION TO THIS EQUATION

With initial condition $c_0(\mathbf{x}) = c_0$ the solution to the 1st equation is:

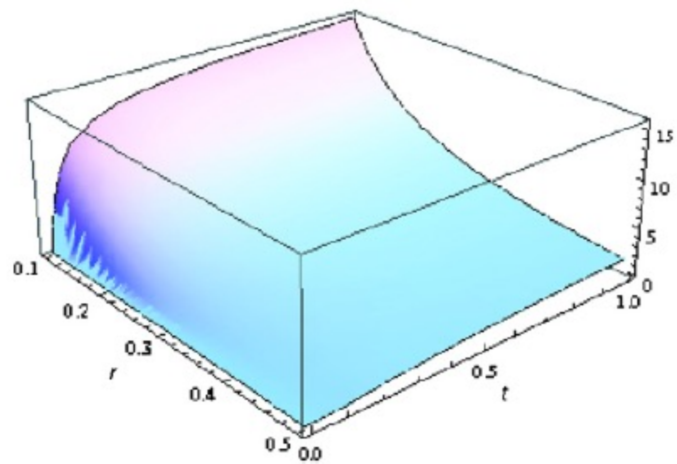
$$c_t(\mathbf{x}) = c_0 \quad \text{(for all t)}$$

And the solution to the 2-points function is, taking dimension d = 3 :

$$g_t(r) = \frac{\lambda \nu_2}{8 D c_0 \pi^{3/2} r} \Gamma\left(\frac{1}{2}, \frac{r^2}{8Dt}\right)$$

where $\Gamma(a, z)$ stands for the incomplete Gamma function

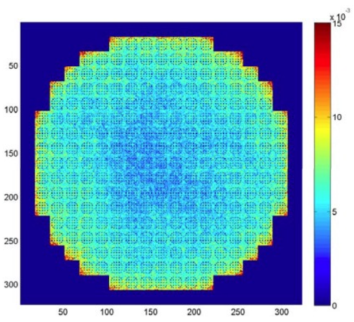
$$\boxed{\text{Amplitude} \propto \frac{\lambda \nu_2}{D c_0}}$$



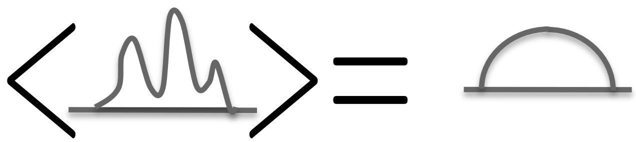
g can be interpreted as the probability to find a neutron next to another

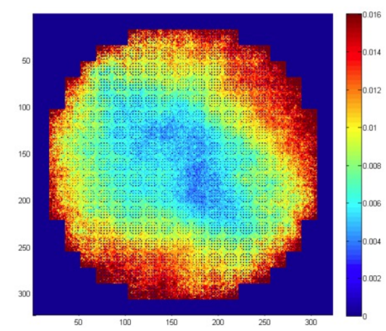
NO 1-DIMENSIONAL NUCLEAR REACTOR

All those equations model the neutron transport in fissile medium
(not only the criticality mode of MC codes)



- The solution to the 2-points function when dimension d = 1 or d = 2 diverges with time…





…a purely 1d infinite system systematically develops <u>power peaks </u>at arbitrary places!

- In 3d the typical amplitude of those peaks is controlled by $\dfrac{\nu_2}{c_0}$

fission process

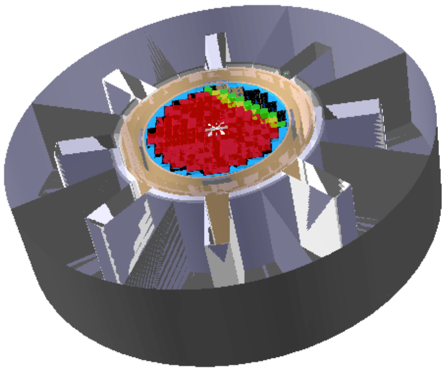
different in reactor physics and MC simu

- Challenge in MC criticality simulations : c_0 << Less than in reality!

POPULATION CONTROL ALGORITHM, KEFF, SPATIAL POWER DISTRIBUTION

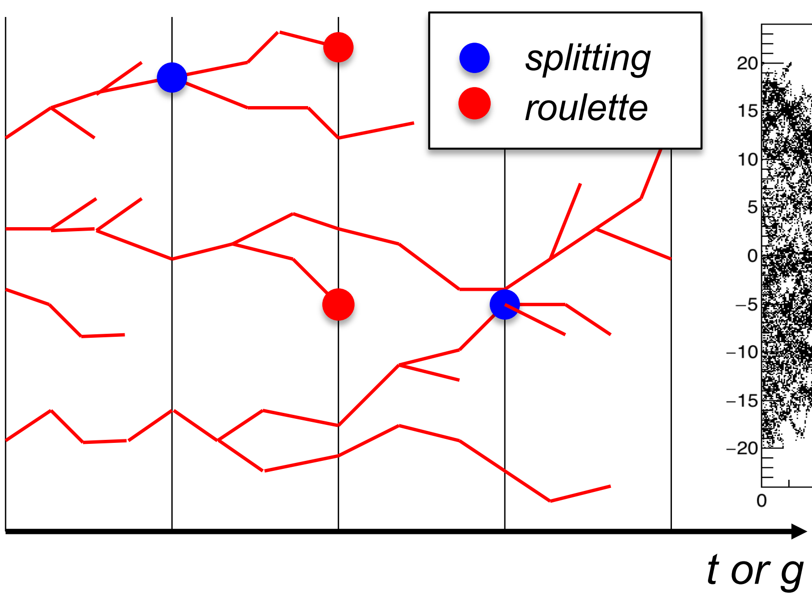
- Neutron transport in fissile media (birth-death process)
- Critical Boltzmann equation
- Population control usually done via 'power iteration'

- Eigenvalue: reproduction factor α (time) or keff (generation)
- Eigenvectors: power distribution

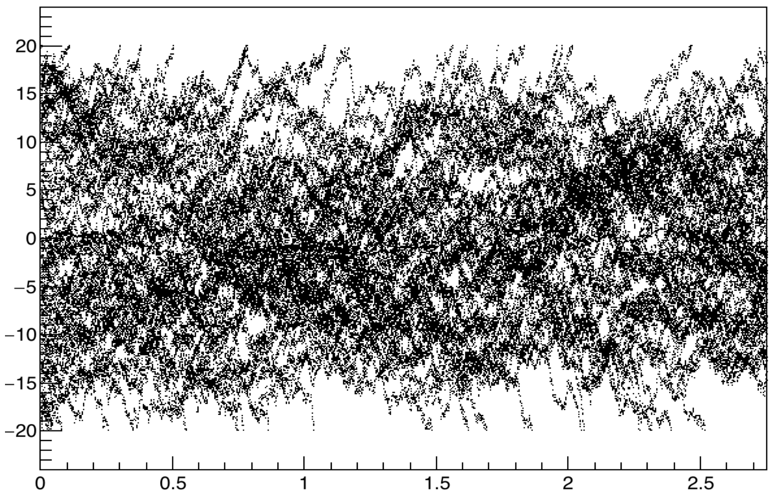


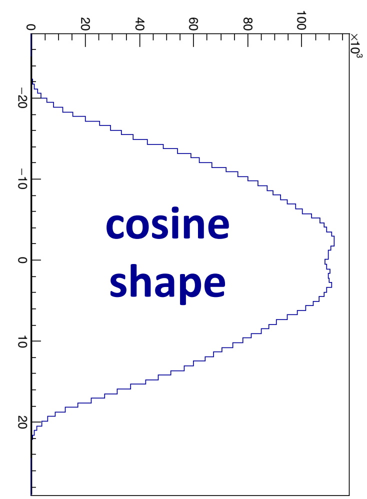
900 MW PWR

Population control algo. to keep N constant



1D mono-E rod



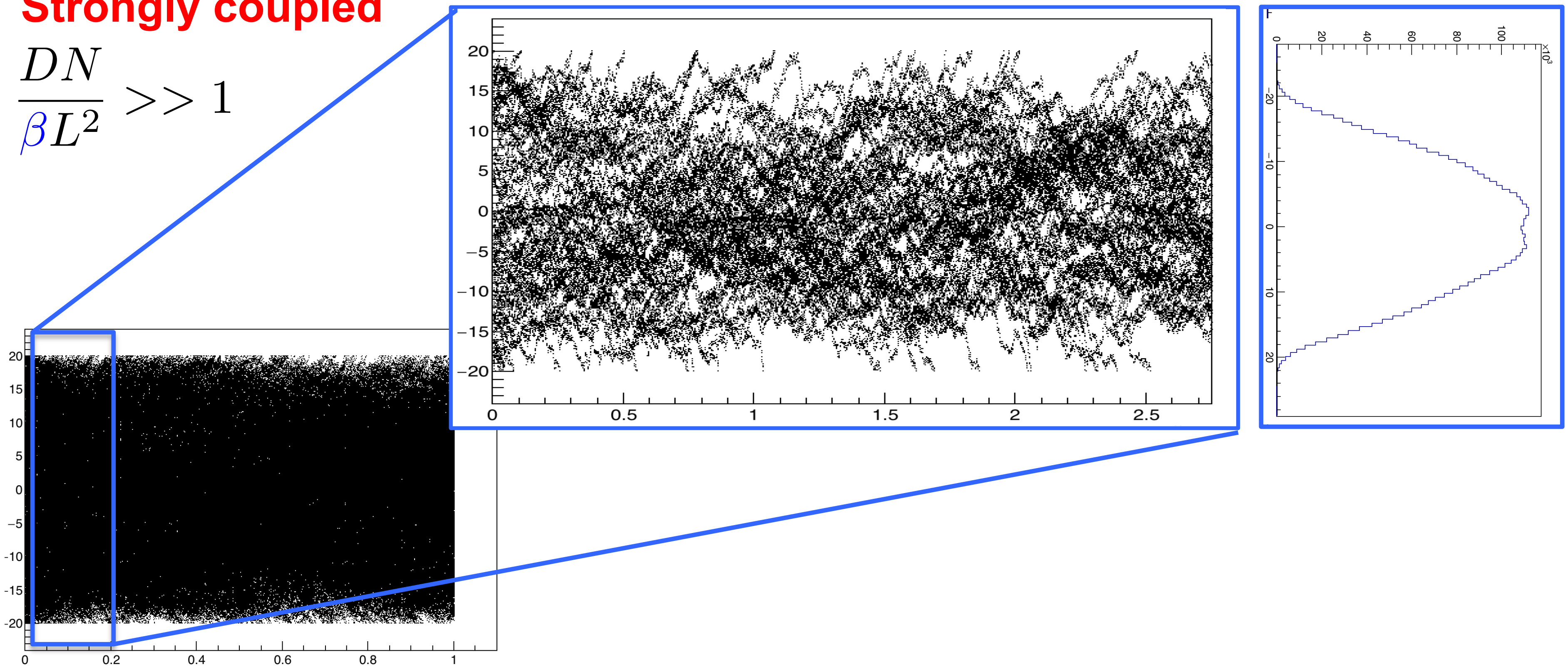


CLUSTERING + POPULATION CONTROL IN STRONGLY COUPLED SYSTEMS

- 1-D BBM **with population control**
- Uniform initial distribution
- 50 neutrons
- **[-L,L] Dirichlet**

Strongly coupled

$$\frac{DN}{\beta L^2} >> 1$$



- Poisson statistics
- Cosine shape

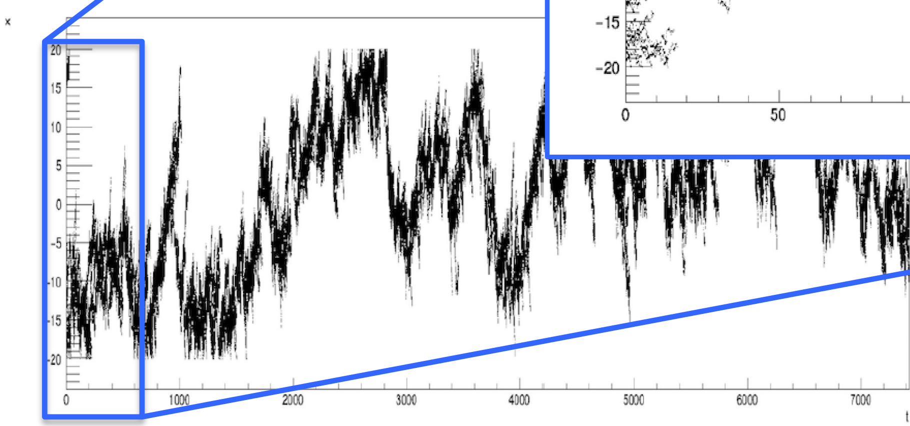
CLUSTERING + POPULATION CONTROL IN DECOUPLED SYSTEMS

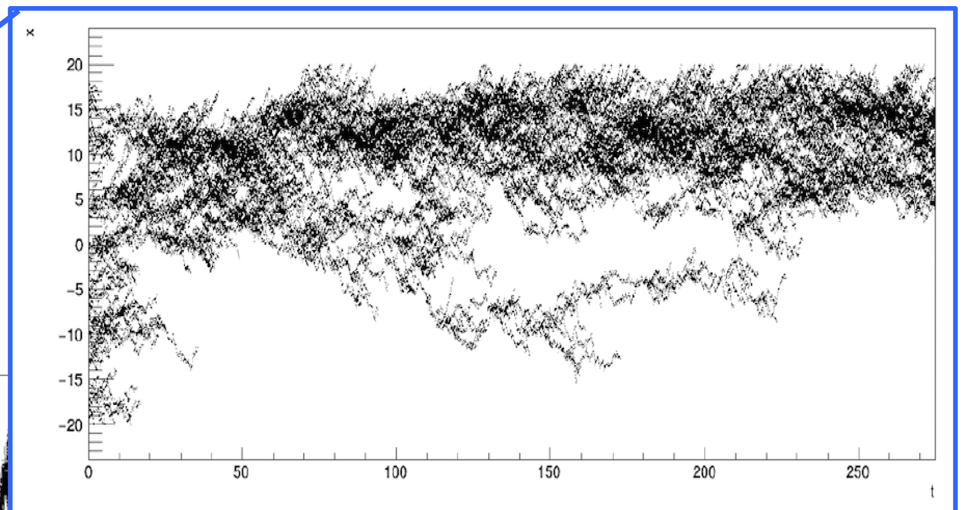
- ❑ 1-D BBM **with population control**
- ❑ Uniform initial distribution
- ❑ 50 neutrons
- ❑ **[-L,L] Dirichlet**

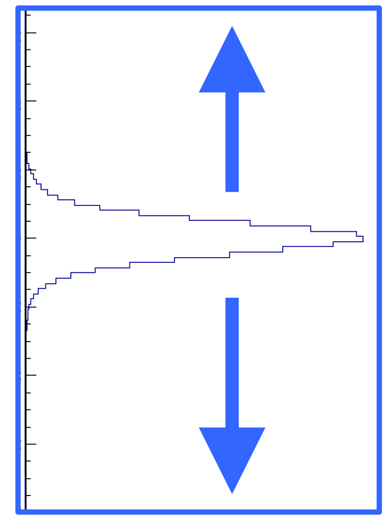
Reflection due to N=constant even if Dirichlet bc !

Loosely coupled

$$\frac{DN}{\beta L^2} << 1$$





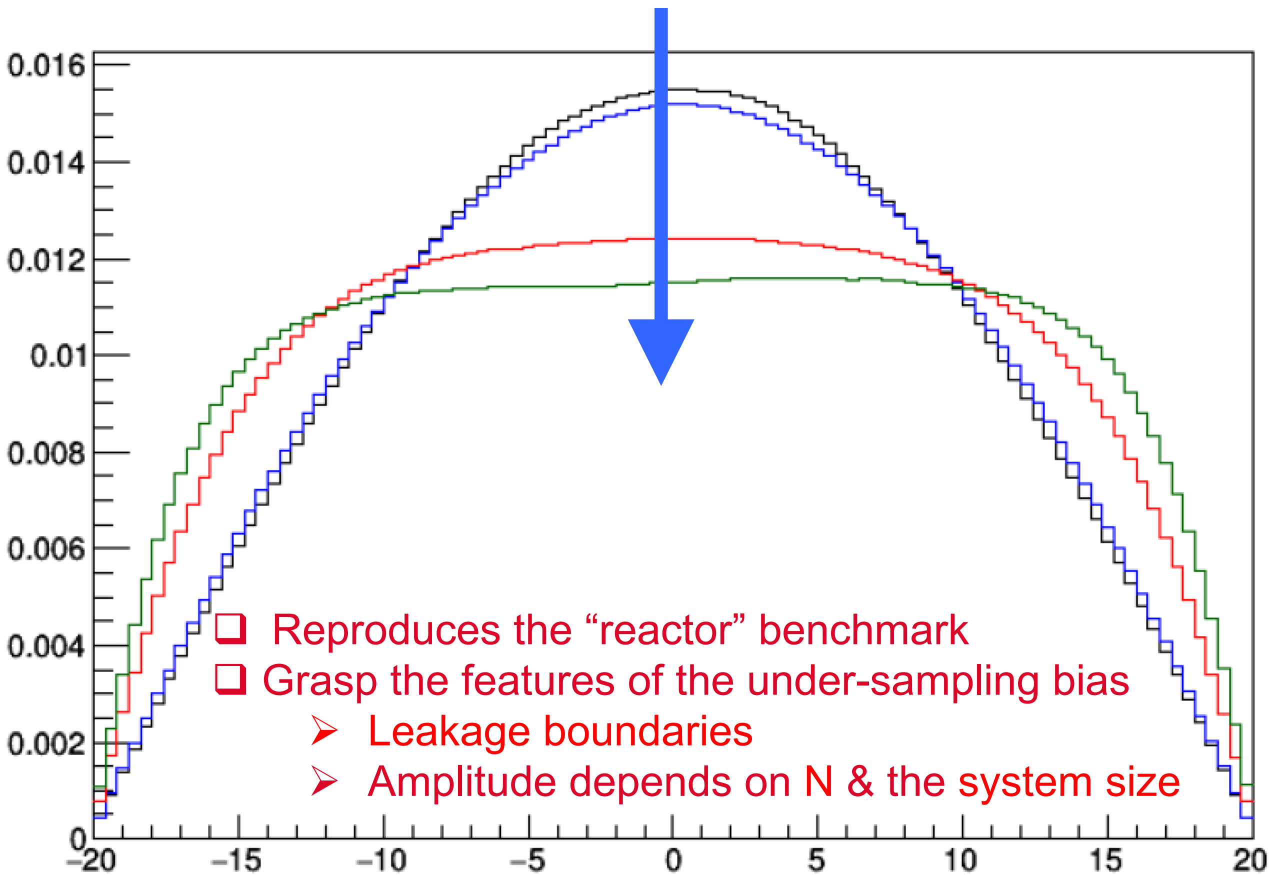


Reflection due to N=constant even if Dirichlet bc !

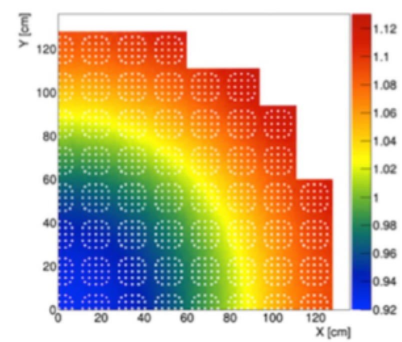
- ❑ Clustering
- ❑ Only one cluster after some time
- ❑ Reflected albeit leaking boundaries !

Splitting = artificial fission ←

From strongest to lousiest coupled systems



- ❑ Reproduces the “reactor” benchmark
- ❑ Grasp the features of the under-sampling bias
  - ➢ Leakage boundaries
  - ➢ Amplitude depends on N & the system size



DIFFUSION EQUATION WITH POPULATION CONTROL

- Monte-Carlo criticality codes = Boltzmann equation **+ population control**
- **Population control** = Weight Watching techniques (i.e. **splitting+roulette**) played at end of cycles to ensure that **N~cte**

Can we build an equation for what MC criticality codes actually solve ?

Fission rate

Splitting = artificial fission

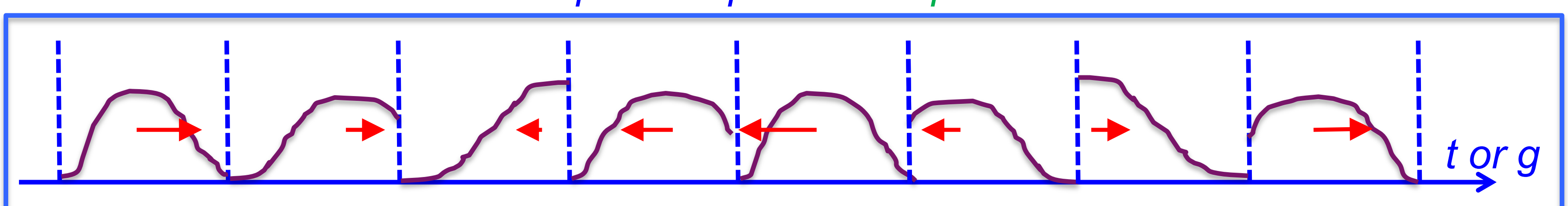
$$\partial_t \phi = D\nabla^2 \phi + (\beta - \gamma)\,\phi \quad + \,?$$

Transport / Diffusion

Capture rate

Roulette = artificial capture

Rate of "artificial" fission/capture depends on spatial correlations and time !

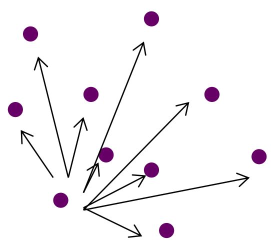


PAIR INTERACTIONS

But how many neutrons do we remove/split at the end of each cycle and how to select them ?

renormalization rate depends on time and N !

$$\lambda(t)\underbrace{f(N)}_{(N-1)N \,\approx\, N^2}N$$



Generalization # neutrons captured in $x \pm dx$ if k>1

$$\lambda(t)\int dy\,\underbrace{G(x,y,t)}_{\text{number of pairs}}$$

Birch et al, Theoretical Population Biology, 70, 26–42 (2006)

- ❑ Combinatorial interactions ! ~ N^2 at first order (# pairs)
- ❑ Depends on the total mass N
- ❑ Depends on the local mass N(x)

DIFFUSION WITH PAIR INTERACTIONS

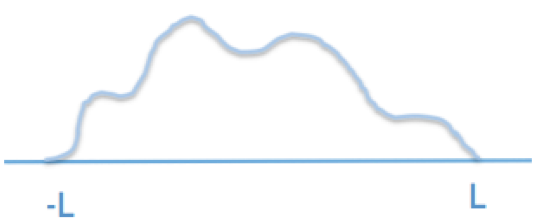
$$\partial_t \phi = D\nabla^2\phi + (\beta - \gamma)\ \phi$$

+ pair interactions

$$\boxed{\partial_t \phi = D\nabla^2\phi + (\beta - \gamma)\ \phi + \overbrace{\lambda(t)}^{\text{rate of renormalization}} \int dy\ \underbrace{G(x,y,t)}_{\text{number of pairs}}}$$

$$G(x,y,t) = \Big[1 + g(x,y,t)\Big]\phi(x)\phi(y)$$

$g(x,y,t)$ spatial correlation function



- ❑ "Hierarchy horror" (2d order moment pops back in the mean field equation!)
- ❑ Clustering = spatial correlations => Bias induced on the flux wrt pure diffusion

POPULATION CONTROL

- N has to be kept constant : $\int_{-L}^{L} dx \; \phi(x,t) = 1$
- λ depends on time!
- Injecting the normalization relation in our equation, we can calculate $\lambda(t)$

$$\lambda(t) = \frac{-\beta + \gamma - D \int_{-L}^{L} dx \; \nabla^2 \phi(x,t)}{\int_{-L}^{L} dx \int_{-L}^{L} dy \; G(x,y,t)}$$

Newman et al, Phys. Rev. Lett., 92, 228103 (2004)

WHAT EQUATION DO MC CODES SOLVE ?

$$\lambda(t) = \frac{-\beta + \gamma - D \int_{-L}^{L} dx \, \nabla^2 \phi(x,t)}{\int_{-L}^{L} dx \int_{-L}^{L} dy \, G(x,y,t)}$$

Probability that one neutron in x is captured

$$\partial_t \phi = D\nabla^2 \phi + (\beta - \gamma)\, \phi + \boxed{\lambda(t)} \boxed{\int_{-L}^{L} dy \, (1 + \boxed{g(x,y,t)})\phi(y,t)} \boxed{\phi(x,t)}$$

Flux factorized out of the integral

Large population size

$$g(x,y,t) \to 0$$

Small population size

$$g(x,y,t) \to g_N^{\infty}(x,y) >> 1$$

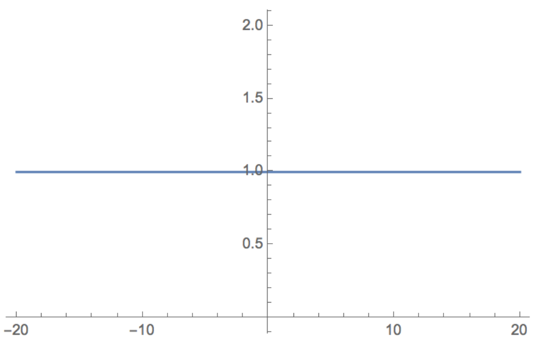
De Mulatier et al, J. Stat. Mech., 15, P08021, 1742–5468 (2015)

$$\nabla^2\phi - \left(\int_{-L}^{L} dx\ \nabla^2\phi(x)\right)\ \phi = 0$$

$$\boxed{\partial_x \phi(x)\Big|_{x=\pm L}}$$

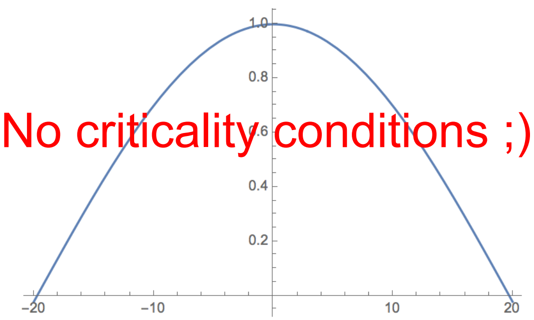
Neumann/Reflective bc

$$\nabla^2\phi = 0$$



Dirichlet/Absorbing bc

$$\nabla^2\phi + \frac{\pi^2}{2L^2}\phi = 0$$



SMALL POPULATION SIZE

$$\partial_t \phi = D\nabla^2\phi + (\beta - \gamma)\ \phi + \left(\frac{-\beta + \gamma - D\ \partial_x \phi(x,t)\big|_{x=\pm L}}{\int_{-L}^{+L} dx \int_{-L}^{+L} dx\ \phi(x,t)^2} \right) \phi(x,t)^2$$

- Non-linear equation with ϕ^2 term
- Can be simplified under some assumptions

Fisher, Ann. Eugenics 7:353-369 (1937)

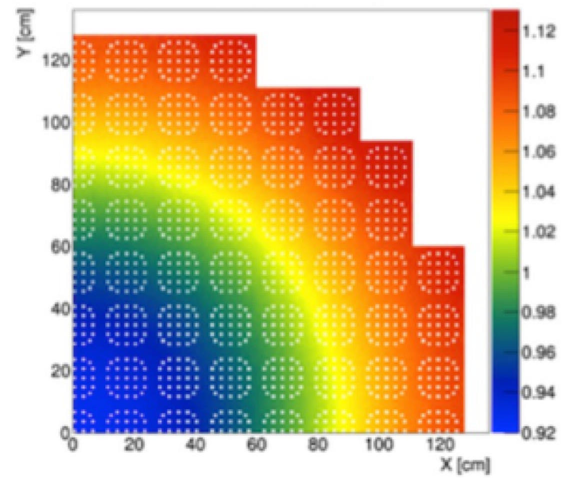
$$\partial_t \phi = D\nabla^2\phi + (\beta - \gamma)\ \phi(1 - \phi)$$

$$\phi(x,t) = \frac{1}{\left(1 + C\exp^{\pm\frac{1}{6}\sqrt{6(\beta-\gamma)}x - \frac{5}{6}(\beta-\gamma)t}\right)^2}$$

- F-KPP equation with traveling waves solutions
- Counter-reaction depending on the sign of $1 - \phi$

TRAVELING WAVE & SOLITONS

- Qualitative & Quantitative scheme to explain under-sampling biases on local MC tallies



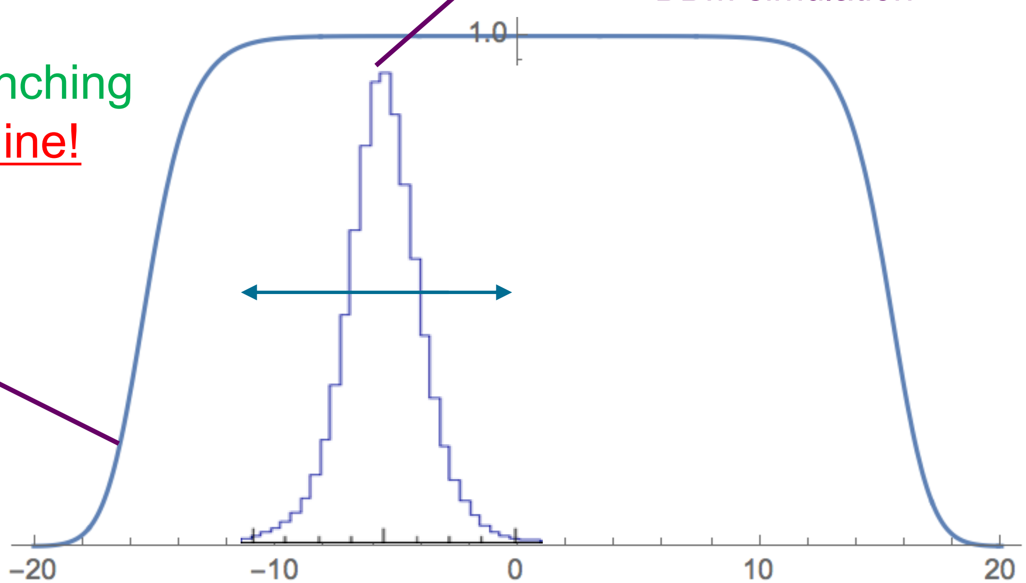
- Fux profile => comes from the averaging through time of the cluster displacement

- Connection between clustering & solitons
  - Clustering typical of branching processes
  - Solitons typical of non-linear equations

- Strong connection with the analysis of QCD semi-classical approximation
  - Neutron branching -> parton branching
  - See Stephane's talk right after mine!

Cluster density profile from the BBM simulation

flux profile obtained by solving the F-KPP equation



OUTLINE

- Reactor physics in a nutshell
- Monte Carlo simulation of nuclear reactors
  - Why bother ?
  - What's the matter ?
- Stochastic modelling of spatial correlations in BBM
  - Branching Brownian Motion
  - Fluctuations & Gambler's ruin
- Ergodicity breaking
  - Clustering
  - F-KPP traveling waves
- Numerical methods to tackle them
  - From rare events to population control using AMS
  - Results

AMS

- 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)

AMS FOR VARIANCE REDUCTION IN PARTICLE TRANSPORT

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

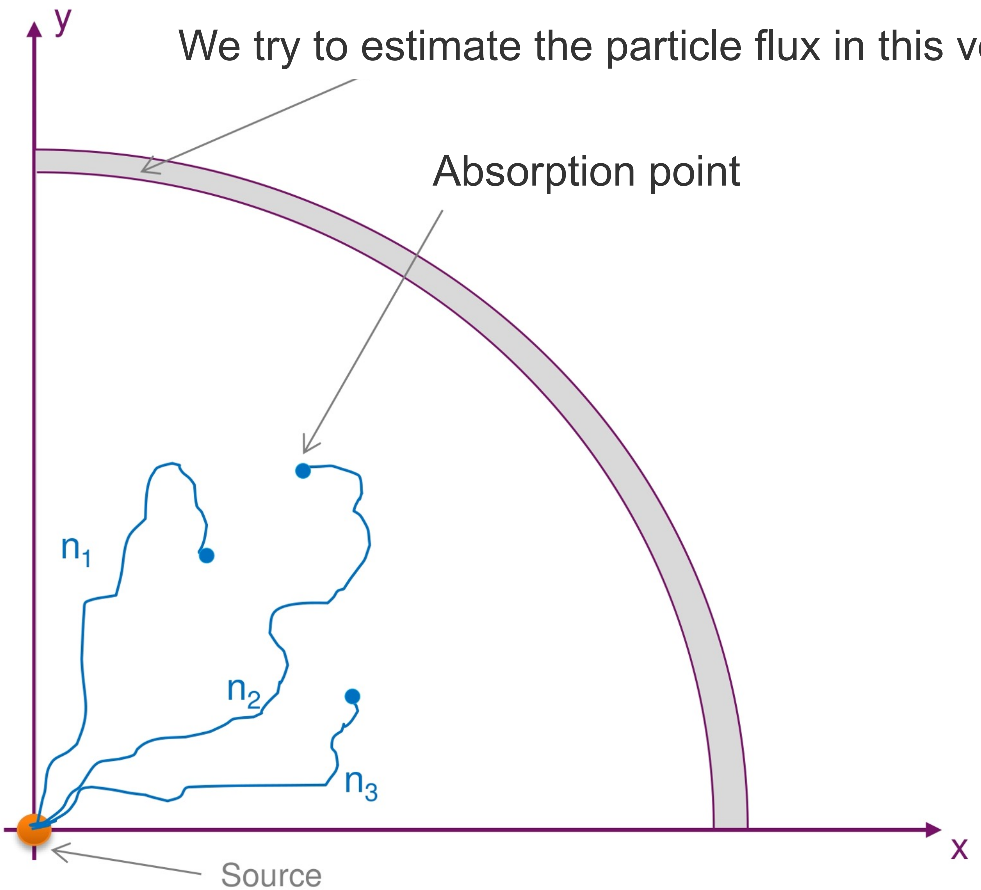
- n particles simulated => tracks are stored
- score is assigned to each neutron track (= Max of ξ over whole trajectory)
- tracks are ranked according to their score
- the k-th "worst" track defines the new splitting level
- the k tracks having scores lesser than this level are deleted
- k tracks are 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:

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

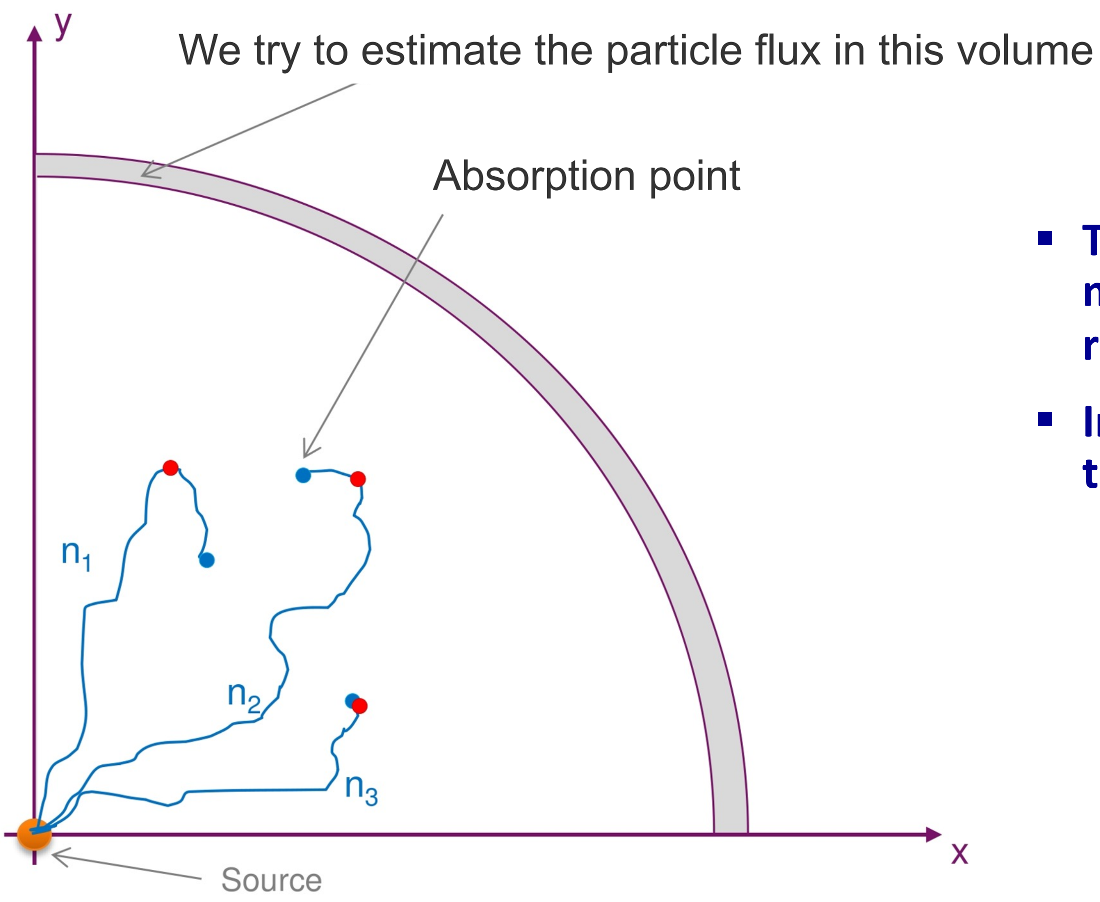
- An unbiased estimator of the flux is calculated "as usual" using the tracks of the last iteration

AMS FOR PARTICLE TRANSPORT : THE ALGORITHM



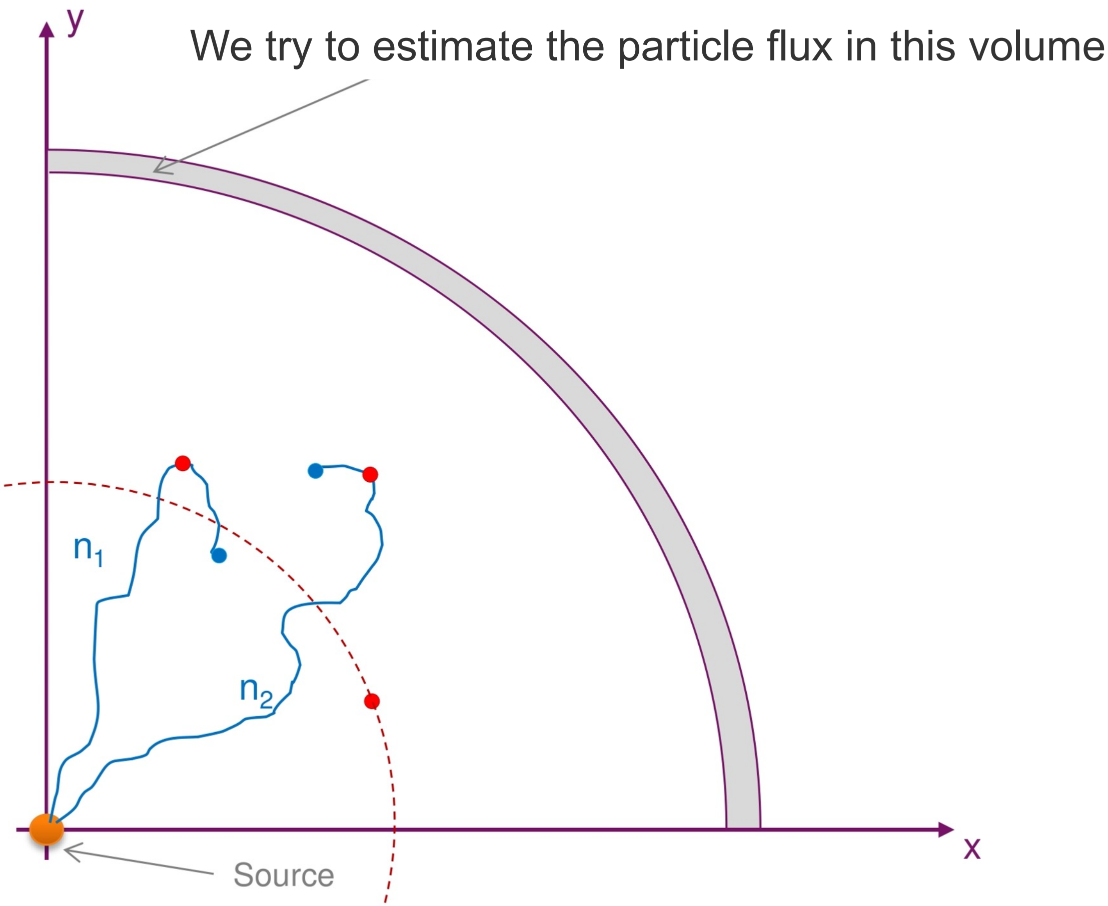
- **n=3**
- **k=1**
- **ξ: distance to the source**
- **Target: spherical shell (purple)**
- **3 particles simulated from the source to their absorption (blue points)**

AMS FOR PARTICLE TRANSPORT : THE ALGORITHM



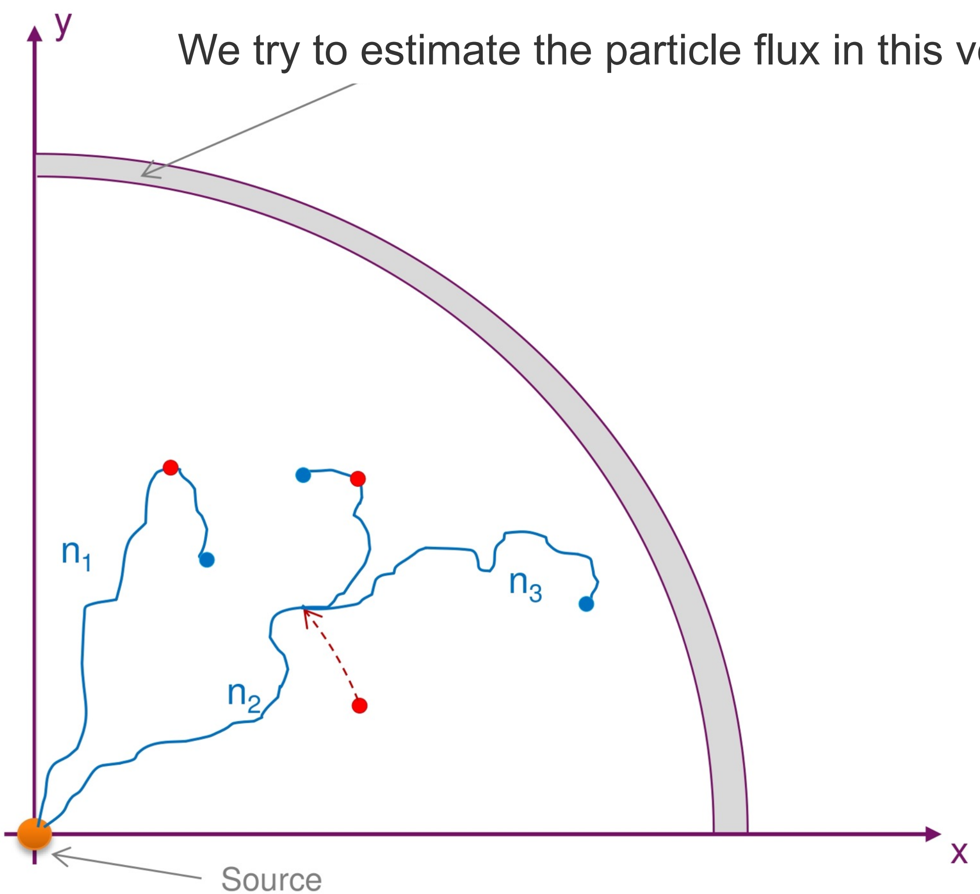
- The importance function is the maximal distance to the source reached by the particle (red points)
- In this case the neutron tracks with the lowest score is n3

AMS FOR PARTICLE TRANSPORT : THE ALGORITHM



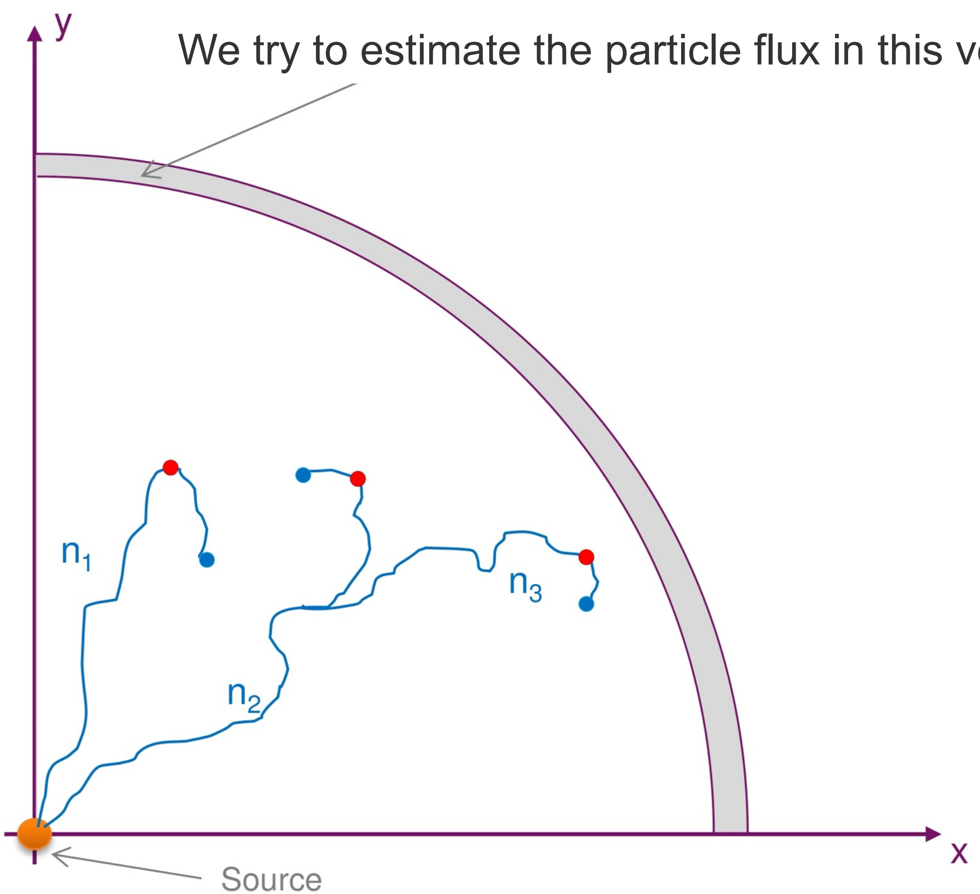
- **The tracks associated to particle 3 is deleted**
- **The maximum score of this track is stored and defines the first splitting level**

AMS FOR PARTICLE TRANSPORT : THE ALGORITHM



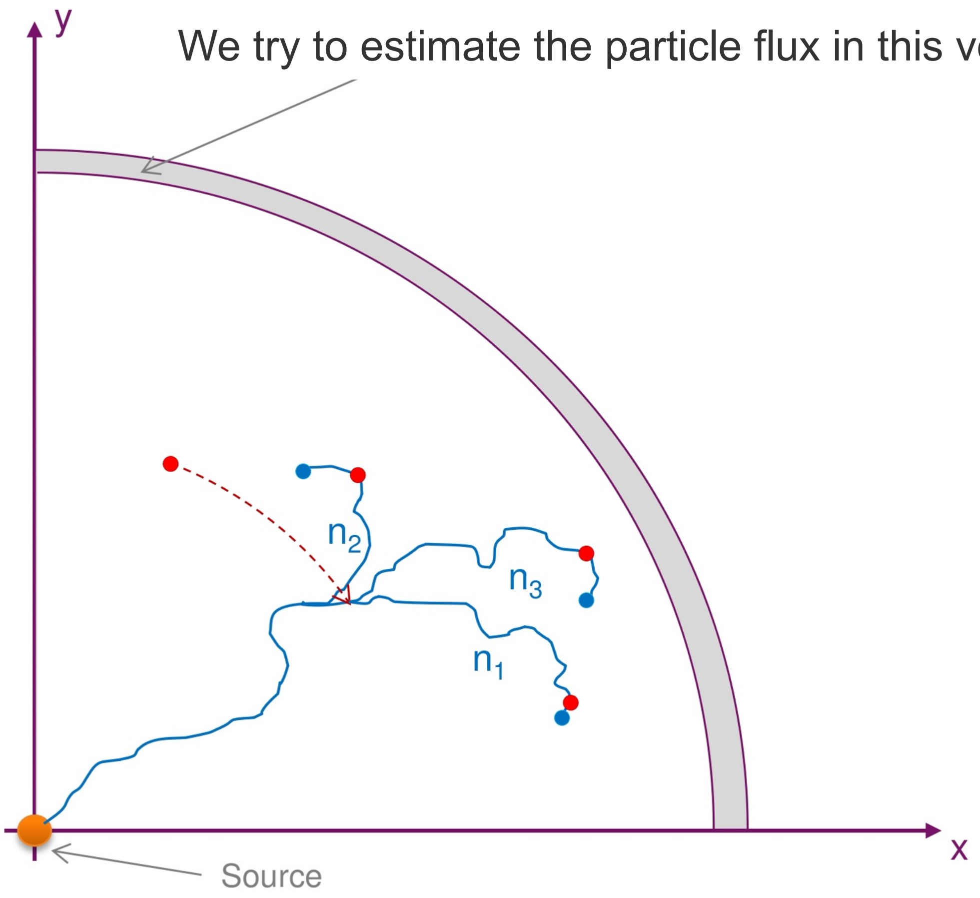
- **Track number 2 is randomly sampled for the splitting**
- **A new particle is simulated from this splitting point until its absorption**

AMS FOR PARTICLE TRANSPORT : THE ALGORITHM



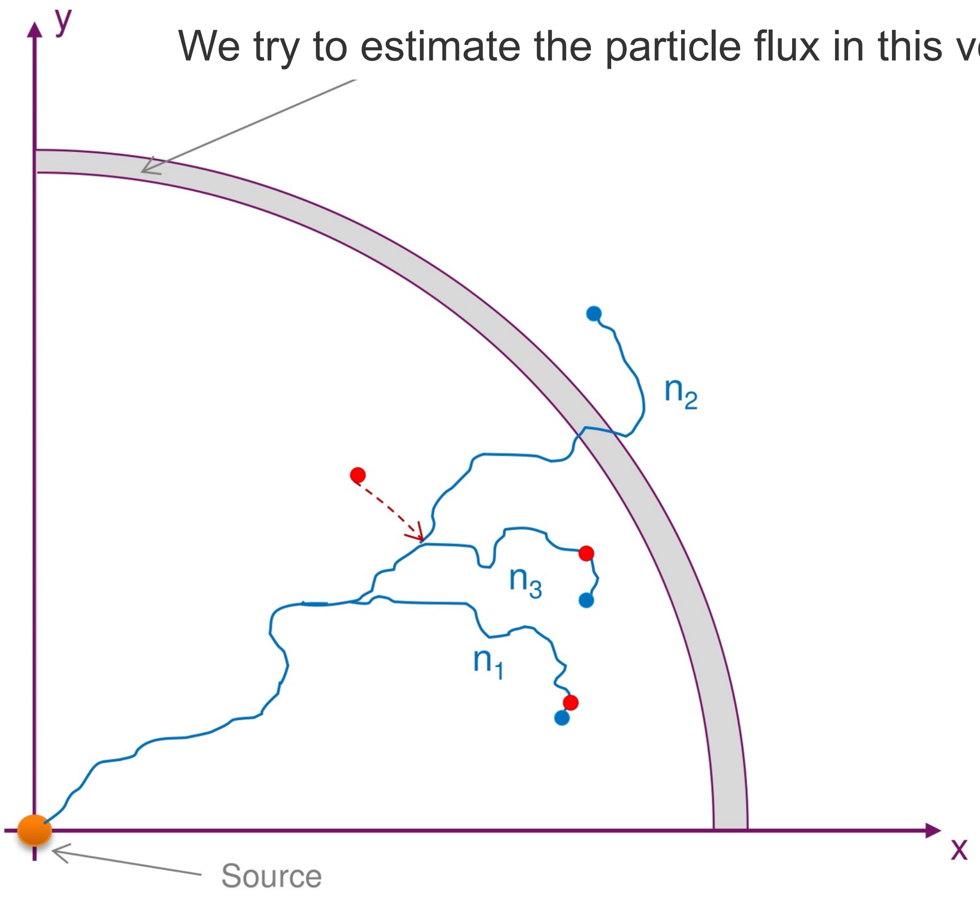
- **The score of this new tracks n3 is calculated**
- **The first iteration is over**
- **The stopping criterium is not meet: the iteration process goes on**

AMS FOR PARTICLE TRANSPORT : THE ALGORITHM



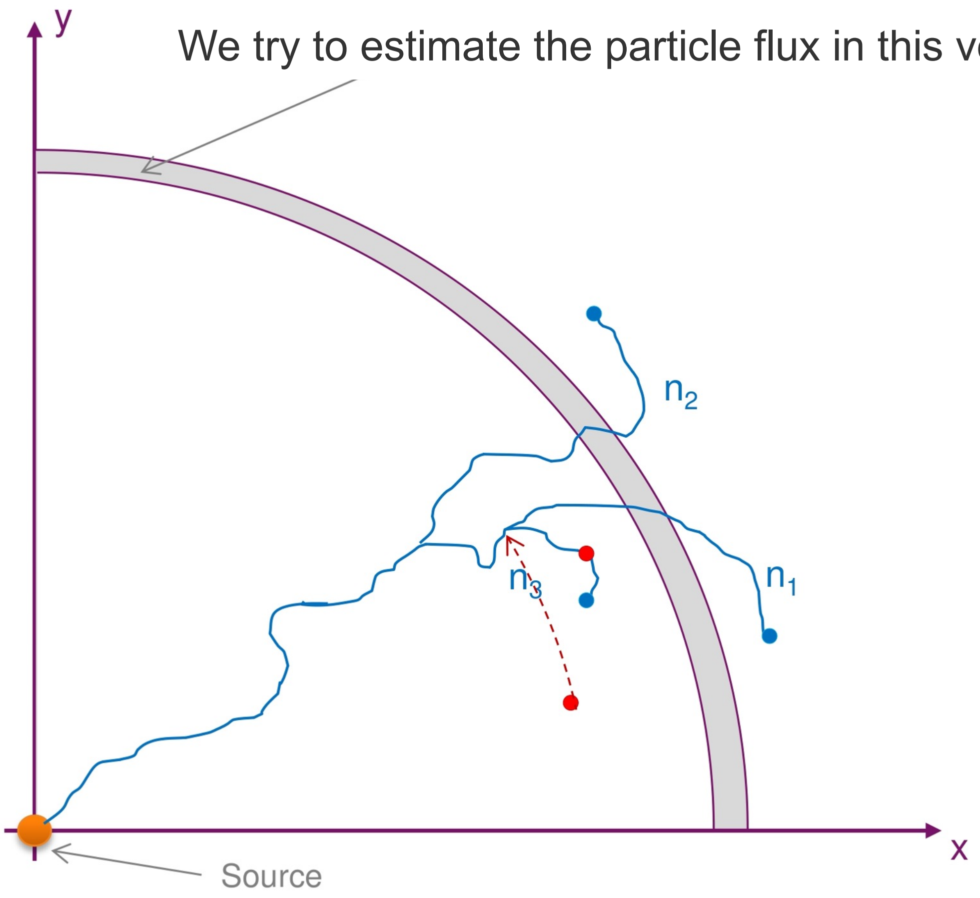
- **Iteration 2**

AMS FOR PARTICLE TRANSPORT : THE ALGORITHM



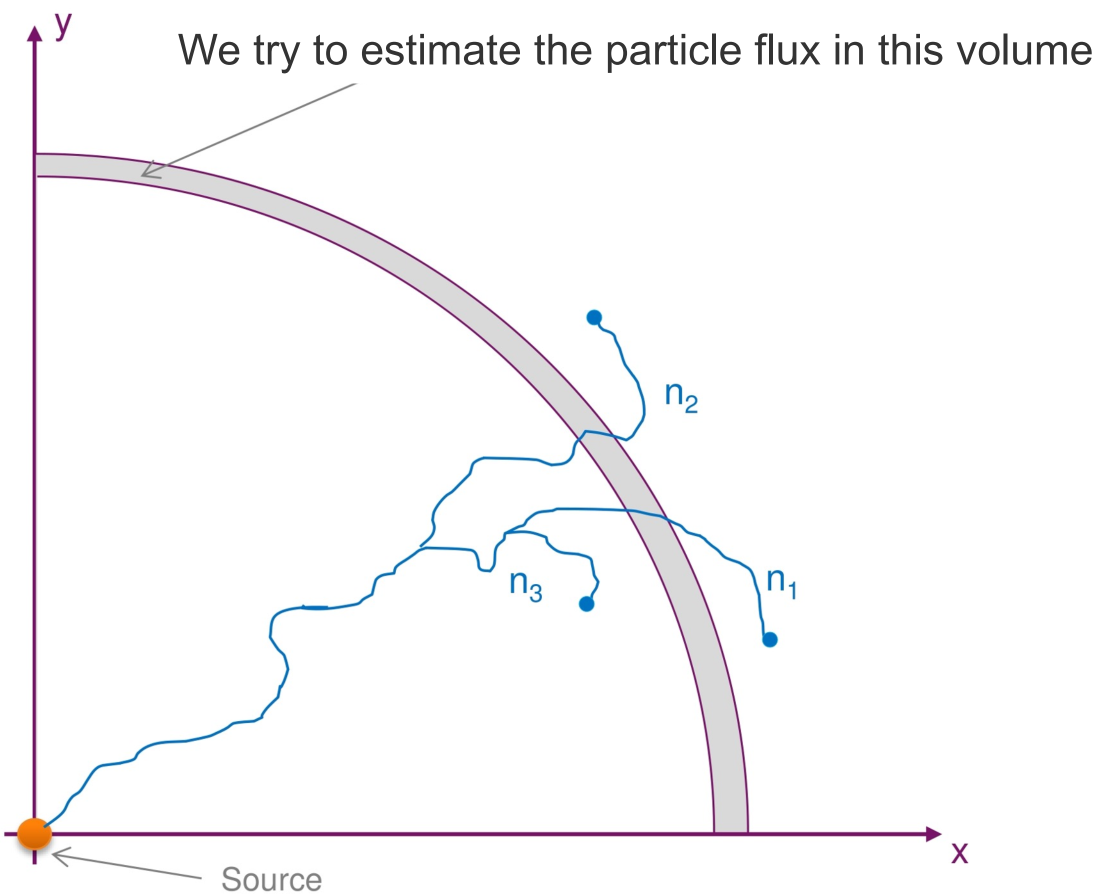
- **Iteration 3**

AMS FOR PARTICLE TRANSPORT : THE ALGORITHM



- **Iteration 4**

AMS FOR PARTICLE TRANSPORT : THE ALGORITHM

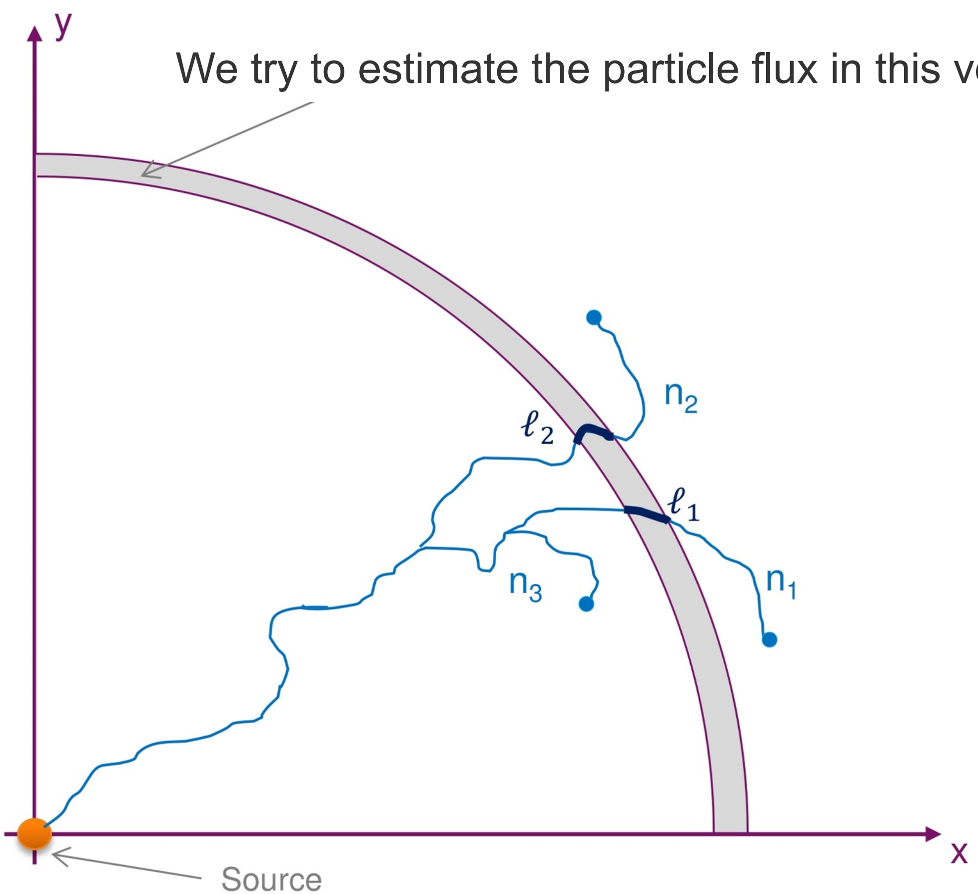


- **Iteration 4**
- **n-k particles have reached the target, the algorithm stops**

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

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

AMS FOR PARTICLE TRANSPORT : THE ALGORITHM



- **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:**

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

REACTOR PHYSICS SEEN AS A VARIANCE REDUCTION PB & USE OF AMS

- **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**

number of neutrons to kill

number of iterations to reach T

target time

$$\underbrace{\left(1-\frac{\pi K_i}{N}\right)^{I} = e^{-\alpha . T}}_{\text{if } \alpha<0 \Rightarrow \text{neutron survival probability at } T}$$

number of initial AMS neutrons

$$\hat{\alpha} = -\frac{I}{T}\ln\left(1-\frac{\pi K_i}{N}\right)$$

number of neutrons to kill

number of iterations to reach g_0

target generation

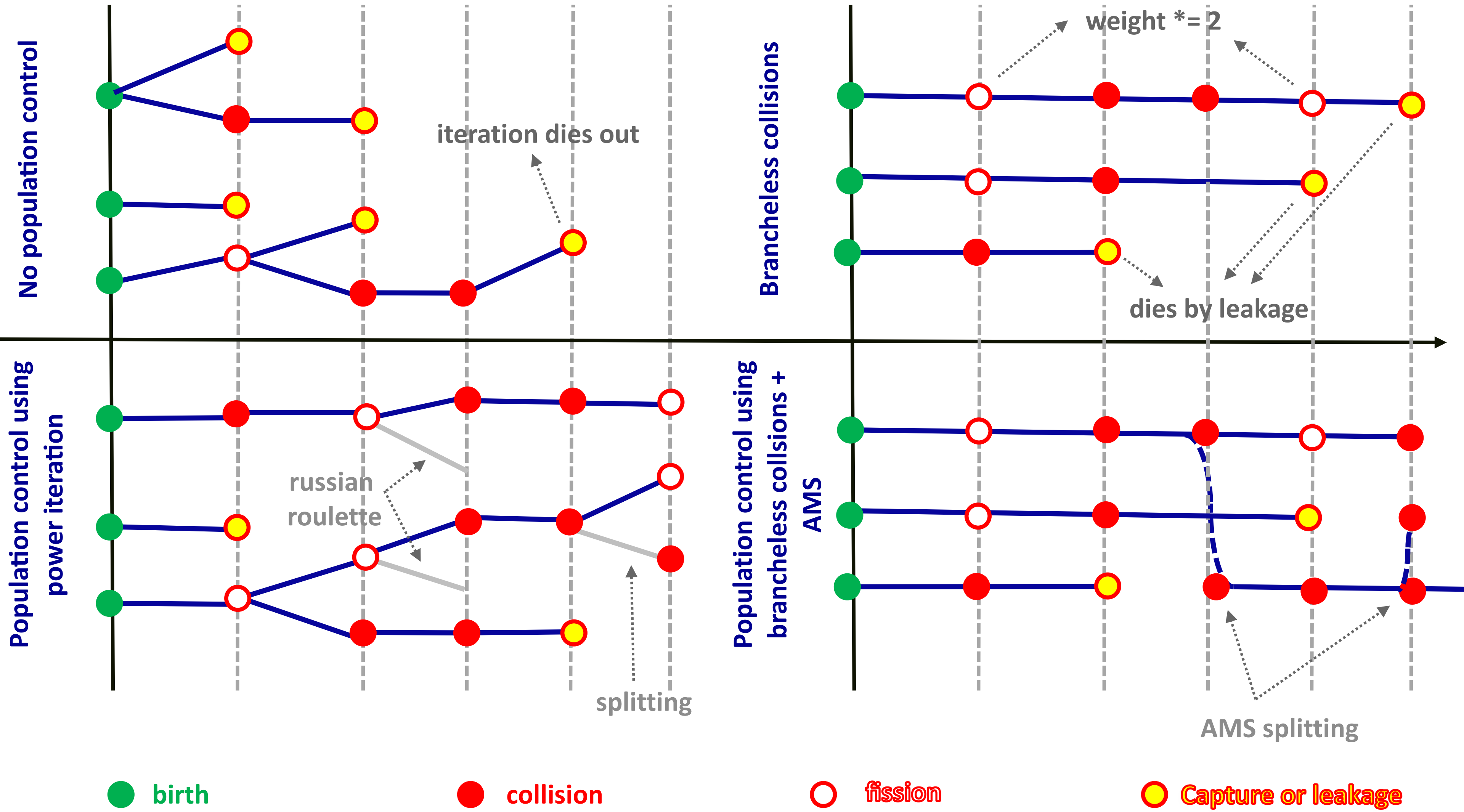
$$\underbrace{\left(1-\frac{\pi K_i}{N}\right)^{I} = k_{eff}^{\,g_0}}_{\text{if } k_{eff}<1 \Rightarrow \text{neutron survival probability at } g_0}$$

number of initial AMS neutrons

$$\hat{k}_{eff} = e^{-\frac{I}{g_0}\frac{\pi K_i}{N}}$$

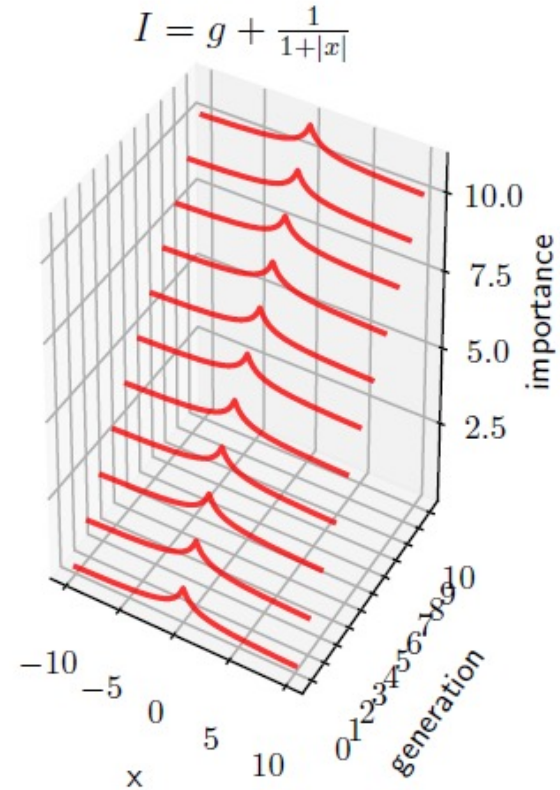
APPLICATION TO REACTOR PHYSICS : POPULATION CONTROL

- AMS used in combination with branchless collisions



APPLICATION TO REACTOR PHYSICS : COST FUNCTION

❑ « 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

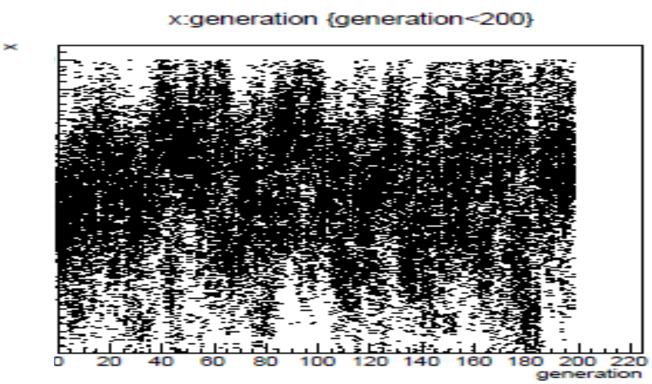
- < 1 : Ensures to rank neutrons inside a generation
- A purely discrete importance can cause the algorithm to prematurely stop

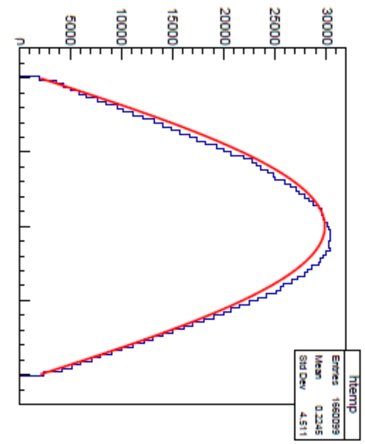
(Phd Kevin Frohlicher, 2022)

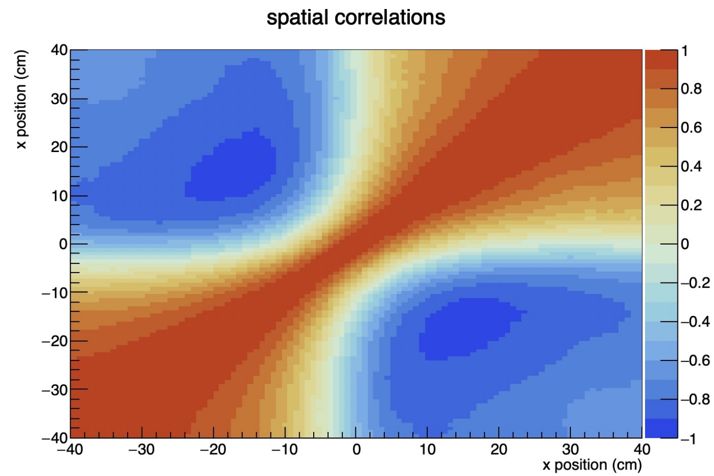
APPLICATION TO REACTOR PHYSICS : SPATIAL CORRELATIONS RESULTS

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

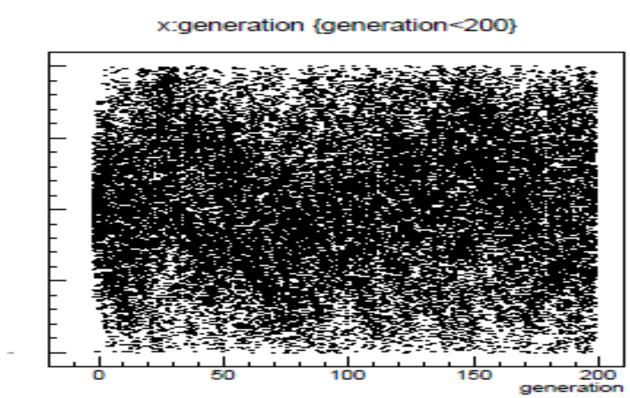
Power iteration analog

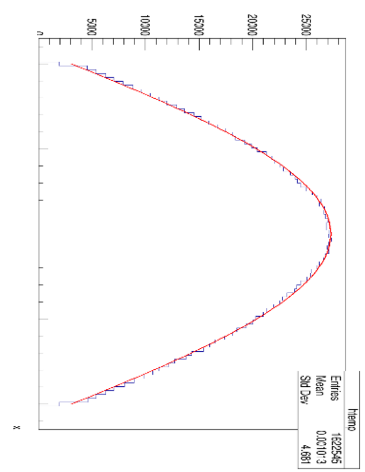


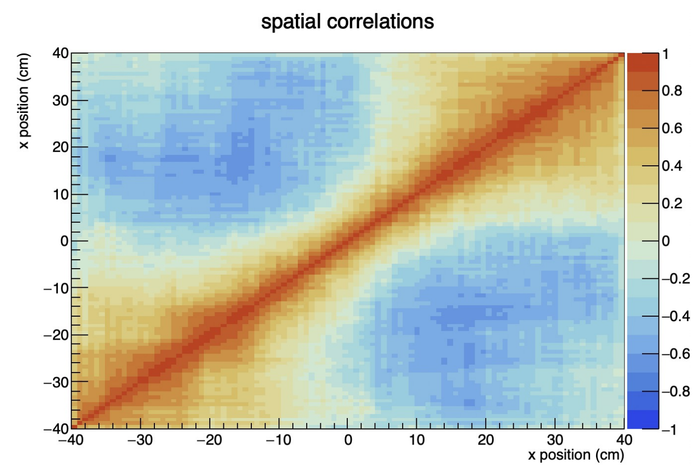




AMS branchless collision







A FEW REFERENCES

CEA *Neutronics*	→	❑ E. Dumonteil et al, Ann. Nucl. Energy **63**, 612-618 (2014).
CEA & UPS/LPTMS *Branching Random Walks*	→	❑ A. Zoia et al, Phys. Rev. E **90**, 042118 (2014). ❑ C. de Mulatier et al, J. Stat. Mech. P08021 (2015).
UJF/Liphy & CEA *Use of QFT*	→	❑ B. Houchmandzadeh et al, Phys. Rev. E **92**, 052114 (2015).
CEA & MIT *Numerics (entropy)*	→	❑ M. Nowak et al, Ann. Nucl. Energy **94** 856-868 (2016).
CEA & CERMICS *Numerics (AMS)*	→	❑ H. Louvin et al, EPJ Nuclear Sci. Technol. 3, 29 (2017).
CEA & IRSN *Traveling waves & FKPP*	→	❑ E. Dumonteil et al, Nuc. Eng. Tech. **49**, 1157-1164 (2017).
IRSN & LANL & CEA *Experiments*	→	❑ E. Dumonteil et al, Nature Comm. Phys. **4**, 151 (2021).
CEA & IRSN *Numerics (AMS)*	→	❑ K. Fröhlicher et al, to be published (2022).
CEA & IRSN *Percolation & renormalization group*	→	❑ B. Dechenaux et al, to be published (2022).

THANKS FOR YOUR ATTENTION…

Commissariat à l'énergie atomique et aux énergies alternatives
Centre de Saclay | 91191 Gif-sur-Yvette Cedex
T. +33 (0)1 69 08 62 75 | Secr :+33 (0)1 69 08 39 61
Etablissement public à caractère industriel et commercial | RCS Paris B 775 685 019

ADVANCED MODELING

- ❑ Dimensionality (3d vs. 1d)
- ❑ Finite-speed effects (transport vs. diffusion)
- ❑ Vacuum boundary conditions (absorbing BC vs. reflecting BC)
- ❑ Delayed neutrons (two time scales vs. single time scale)
- ❑ Population control (N does not depend on time)
- ❑ Clustering and entropy
- ❑ Bias modeling
- ❑ Time => generations

Dumonteil, E. et al, Annals of Nuclear Energy 63, 612-618 (2014)

Zoia, A. et al, Physical Review E, 90, 042118 (2014)

Houchmandzadeh et al, Phys. Rev. E 92 (5), 052114 (2015)

De Mulatier et al, J. Stat. Mech., 15 , P08021, 1742–5468 (2015)

Nowak et al, Ann. Nuc. Ener. 94, 856-868 (2015)

Dumonteil et al, Nuc. Eng. Tech., 10.1016/j.net.2017.07.011 (2017)

Sutton and Mittal, Nuc. Eng. Tech., 10.1016/j.net.2017.07.008 (2017)

Critical fuel rod → Anarchy → Local clustering → Extinction

Critical fuel rod → Control → Local clustering → Stable fluctuations

Credits: A. Zoia

FISSION/CAPTURE VS SPLITTING/RUSSIAN ROULETTE

Probability for a given neutron to be splitted/captured depends on the overall # of neutrons

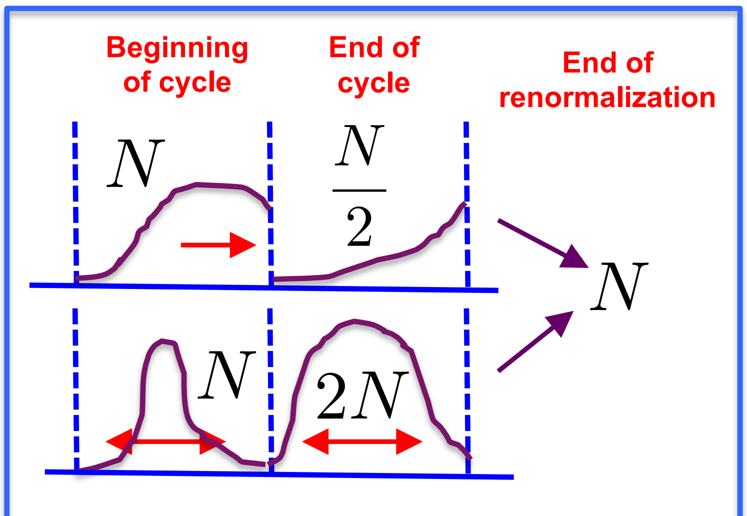
$\beta^* N \longleftarrow \beta N$

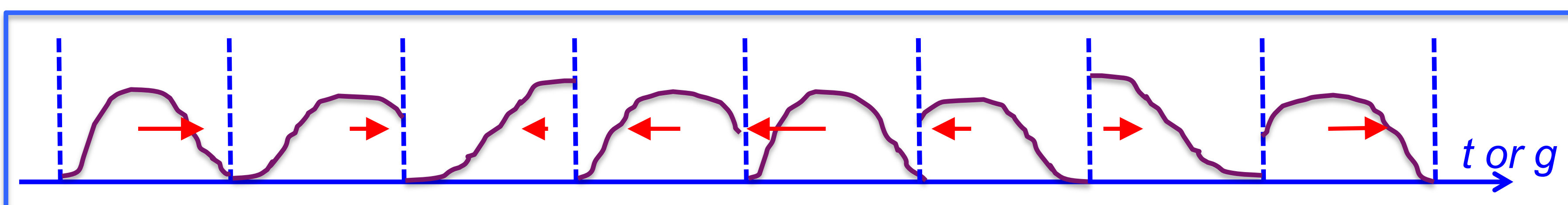
$\gamma^* N \longleftarrow \gamma N$

renormalization rate depends on N and *t/g*

$f(N)N$

$\lambda(t)N$





❑ Blinking & Patchy spatial patterns in nuclear reactors

- 2017 RPI experiments
- Role of spontaneous fission sources

LOOKING FOR THE CRITICAL CATASTROPHE & CLUSTERING @ RCF

- The modeling tells us that both the critical catastrophe & neutron clustering might be observed in a nuclear reactor, if certain conditions are met :

$$\frac{\tau_D}{\tau_E} \simeq \left(\frac{L^2}{D}\right) / \left(\frac{N}{\lambda}\right) = \frac{1}{N}\frac{L^2}{\ell_m^2}$$

$$\boxed{\ell_m^2 = \frac{D}{\lambda}}$$

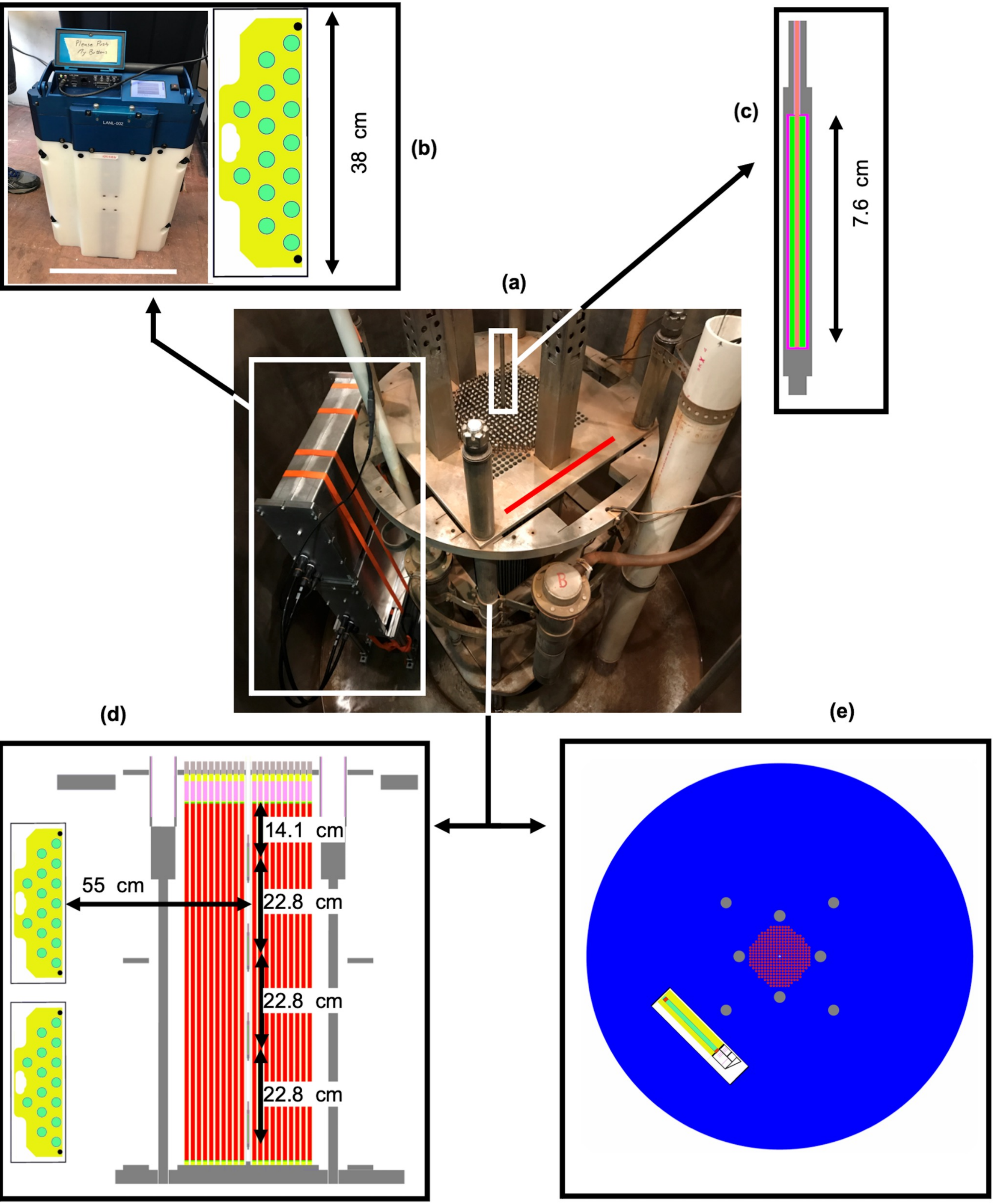
Neutron **migration area**

- Ideal conditions for an experiment that could characterize clustering?
  - ✓ Zero power reactor
  - ✓ Fresh fuel, no burn-up effects
  - ✓ As big as possible

  RCF@RPI

  - ✓ Find a way to do spatial measurements

→ NOMAD detectors & He3 tubes



THE RCF EXPERIMENTS

- Place & date :
  Mid-2017 @ RPI, Troy, USA

- RCF :
  - 4.81% enriched UO2 ceramic fuel
  - 1 mW → 1 W

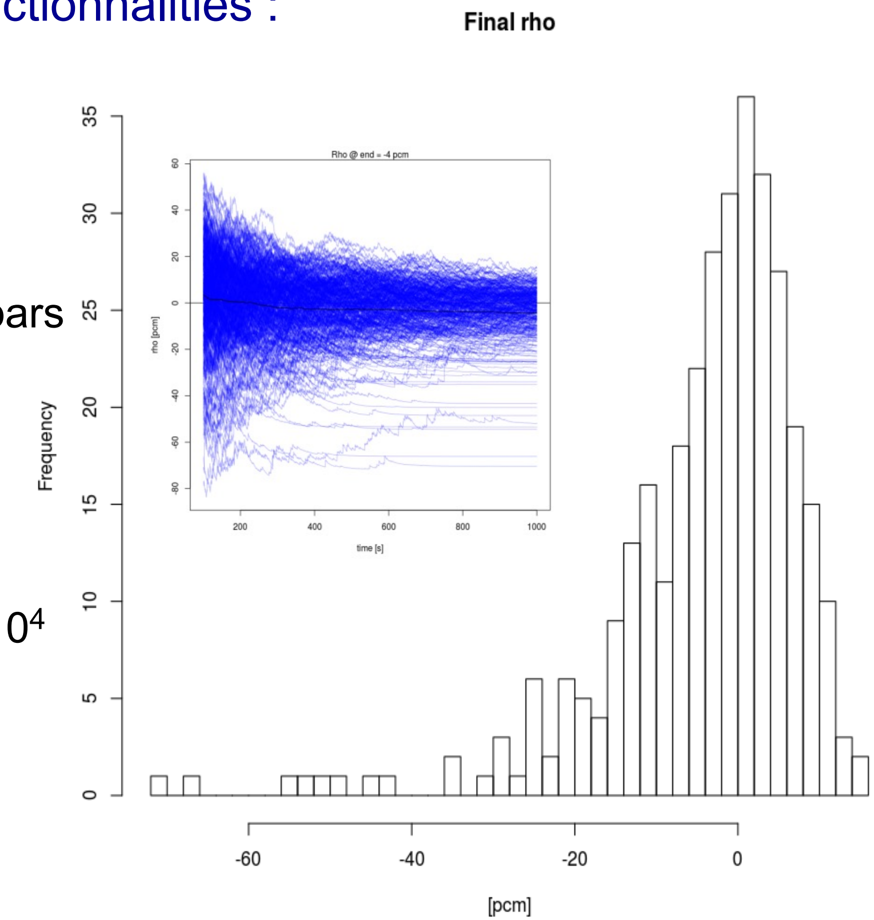
- Experiments :
  - 2.10^3 hours of computing for the design
  - Outer NOMAD detectors provided by LANL
  - Inner detectors: He^3 tubes

Possible to measure :
- time-dependent neutron map within the core
- Fluctuations & correlations

HIGH FIDELITY SIMULATIONS & NUMERICAL TWIN OF THE RCF

Petit & Dumonteil, Nucl. Tech 192, 3 (2015)

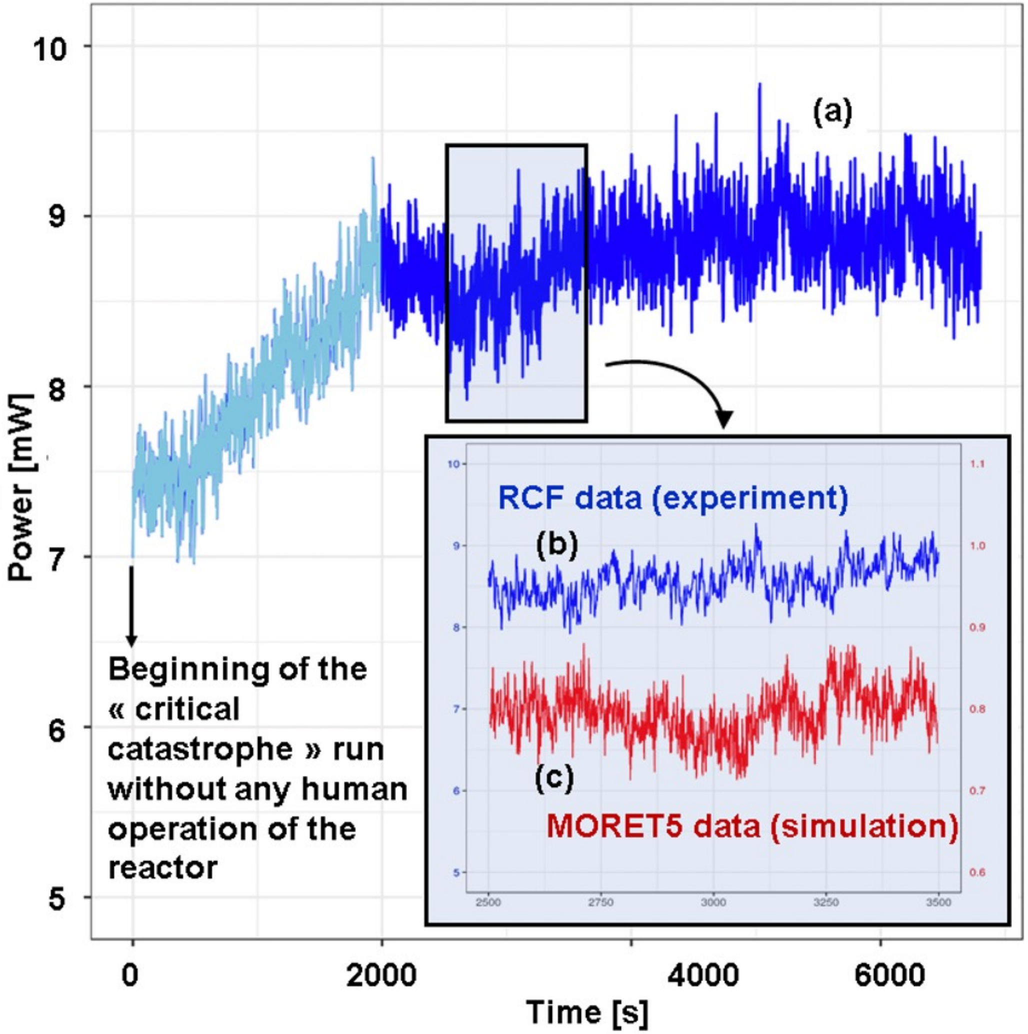
- MORET 6 code using dynamic + analog functionnalities :
  - Data library: Endfb71
  - Fission sampling:
    - ✓ Freya
    - ✓ discrete Zucker and Holden tabulated
    - ✓ Pn distributions and corresponding nubars
    - ✓ Only Spontaneous fissions
- Highly parallel simulations :
  - Simulated signal = 10^3 s (prompt+delayed)
  - Number of initial neutrons per simulation = 10^4
  - Number of independent simulations ~ 10^3



Excellent reactivity: ρ = -4 pcm
+
Up to 10 mW of simulated power!

$$< n(t) >= n_0 e^{\overbrace{\lambda(p(2)-p(0))t}^{=\rho\, t}}$$

THE « CRITICAL CATASTROPHE » RUN



This bounded behavior of fluctuations contradicts the « critical catastrophe »

$$\frac{V_n(t)}{\langle n_t \rangle} = 1 + \frac{\lambda_F \, \overline{\nu_F(\nu_F - 1)}}{n_0} \, t$$

MODELING OF SPONTANEOUS FISSION SOURCES

- Hypothese:

  - spontaneous fissions come from U^{238} (1 n/s/g)
  - spontaneous fissions might prevent the extinction of the neutron population

- capture, inducing transitions $\vec{\mathbf{n}} \to a_k\ \vec{\mathbf{n}}$ at rate λ_{C} per second and per neutron;
- neutron induced fission (with j daughters neutrons), inducing transitions $\vec{\mathbf{n}} \to (a_k^+)^j a_k\ \vec{\mathbf{n}}$ at rate $\lambda_{\mathrm{F}}\, p_j$ per second and per neutron;
- spontaneous fission (with j daughters neutrons), inducing transitions $\vec{\mathbf{n}} \to (a_k^+)^l\ \vec{\mathbf{n}}$ at rate $\lambda_{\mathrm{SF}}\, q_j$ per second and per cell;
- we also allow for migration to occur : neutrons can travel from one cell to adjacent ones. This process induce a transition $\vec{\mathbf{n}} \to (a_{k\pm1}^+)a_k\ \vec{\mathbf{n}}$ and occur at a rate that we define to be γ per second and per neutron.

MODELING OF SPONTANEOUS FISSION SOURCES

$$
\begin{aligned}
\frac{\partial}{\partial t}P(\vec{\mathbf{n}}) = \sum_k \Big\{ & -\lambda_{\mathrm{C}} n_k P(\vec{\mathbf{n}}) + \lambda_{\mathrm{C}}(n_k+1)P(a_k^+\vec{\mathbf{n}}) \\
& -\lambda_{\mathrm{F}}\sum_j p_j n_k P(\vec{\mathbf{n}}) + \lambda_{\mathrm{F}}\sum_j p_j(n_k+1-j)P(a_k^+(a_k)^j\vec{\mathbf{n}}) \\
& -\lambda_{\mathrm{SF}}\sum_j q_j P(\vec{\mathbf{n}}) + \lambda_{\mathrm{SF}}\sum_j q_j P((a_k)^j\vec{\mathbf{n}}) \\
& -2\gamma n_k P(\vec{\mathbf{n}}) + \gamma(n_{k+1}+1)P(a_{k+1}^+a_k\vec{\mathbf{n}}) + \gamma(n_{k-1}+1)P(a_{k-1}^+a_k\vec{\mathbf{n}}) \Big\}
\end{aligned}
$$

$$\langle n\rangle = \sum_n nP(n)$$

$$\langle n^2\rangle = \sum_n n^2P(n)$$

$$\langle n_k\rangle = \sum_{\vec{\mathbf{n}}} n_k P(\vec{\mathbf{n}})$$

$$\langle n_k n_{k+l}\rangle = \sum_{\vec{\mathbf{n}}} n_k n_{k+l} P(\vec{\mathbf{n}})$$

Fluctuations via 0d

$$\frac{V_n(t\to\infty)}{\langle n_\infty\rangle} = 1 + \frac{1}{2}\frac{\overline{\nu_{\mathrm{F}}(\nu_{\mathrm{F}}-1)}}{\overline{\nu_{\mathrm{F}}}}\left(1-\frac{1}{\rho}\right)$$

Clustering via 3d

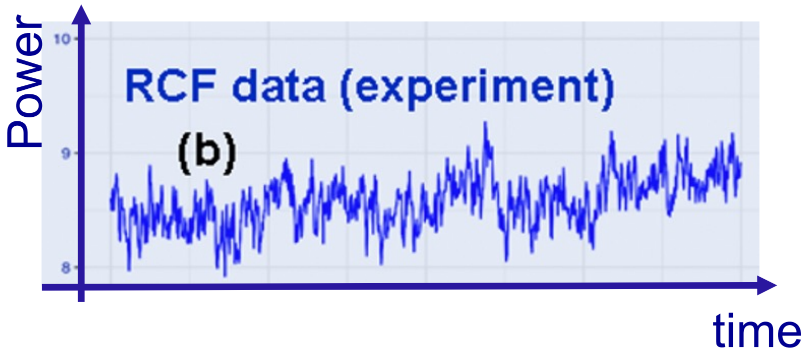
$$g_\infty^{3\mathrm{D}}(z) = \frac{\lambda_{\mathrm{F}}\,\overline{\nu_{\mathrm{F}}(\nu_{\mathrm{F}}-1)}}{8\pi D c_\infty}\left(2L_{\mathrm{T}}\sinh^{-1}(1) - \frac{\pi}{2}z\right)$$

EFFECT OF SPONTANEOUS FISSION SOURCES ON FLUCTUATIONS

$$\frac{V_n(t)}{\langle n_t \rangle} = 1 + \frac{\lambda_F \, \overline{\nu_F(\nu_F - 1)}}{n_0} t \quad \Rightarrow \quad \frac{V_n(t \to \infty)}{\langle n_\infty \rangle} = 1 + \frac{1}{2} \frac{\overline{\nu_F(\nu_F - 1)}}{\overline{\nu_F}} \left(1 - \frac{1}{\rho}\right)$$

- SF explain the bounded behavior of fluctuations that bounce in between
  - Lower bound due to SF themselve
  - Upper bound due to $\rho < 0$

No critical catastrophe



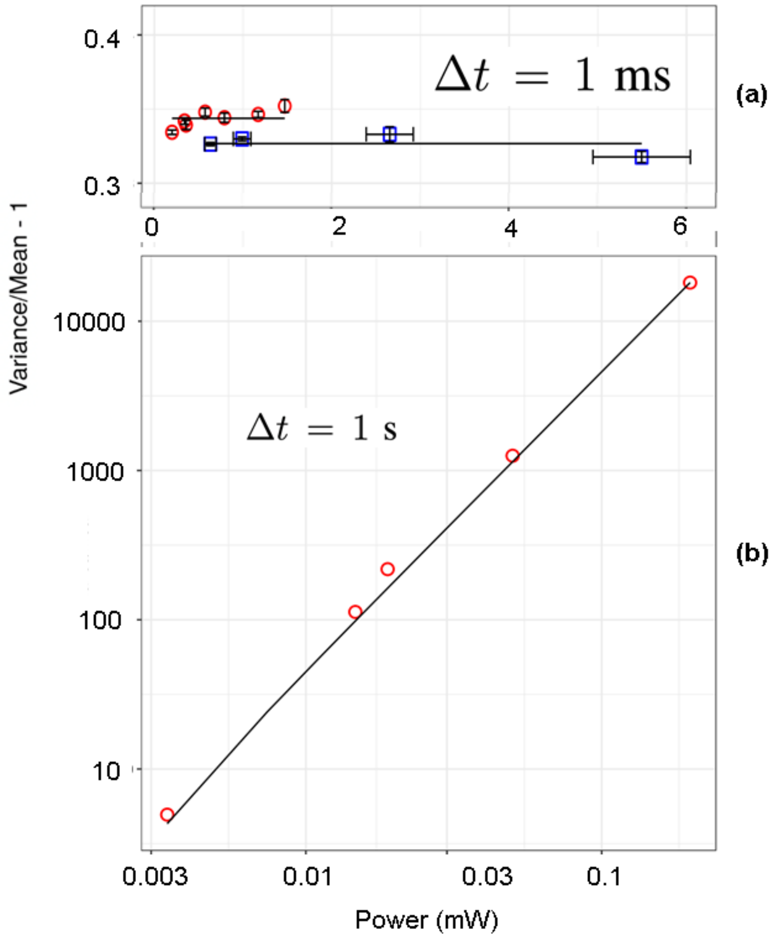
EFFECT OF SPONTANEOUS FISSION SOURCES ON FLUCTUATIONS

$$\frac{V_n(t)}{\langle n_t \rangle} = 1 + \frac{\lambda_F \, \overline{\nu_F(\nu_F - 1)}}{n_0} t \quad \Rightarrow \quad \frac{V_n(t \to \infty)}{\langle n_\infty \rangle} = 1 + \frac{1}{2} \frac{\overline{\nu_F(\nu_F - 1)}}{\overline{\nu_F}} \left(1 - \frac{1}{\rho}\right)$$

- SF explain the bounded behavior of fluctuations that bounce in between
  - Lower bound due to SF themselve
  - Upper bound due to $\rho < 0$

No critical catastrophe

- However, while V/M is bounded, it diverges with $P \propto -1/\rho$!



EFFECT OF SPONTANEOUS FISSION SOURCES ON FLUCTUATIONS

$$\frac{V_n(t)}{\langle n_t\rangle} = 1 + \frac{\lambda_F\,\overline{\nu_F(\nu_F-1)}}{n_0}\,t \quad\Rightarrow\quad \frac{V_n(t\to\infty)}{\langle n_\infty\rangle} = 1 + \frac{1}{2}\frac{\overline{\nu_F(\nu_F-1)}}{\overline{\nu_F}}\left(1-\frac{1}{\rho}\right)$$

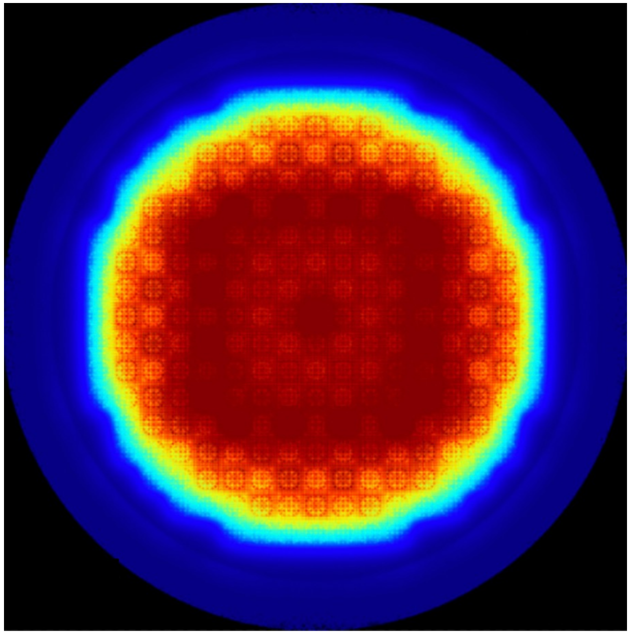
- SF explain the bounded behavior of fluctuations that bounce in between
  - Lower bound due to SF themselve
  - Upper bound due to $\rho < 0$

No critical catastrophe

- However, while V/M is bounded, it diverges with $P \propto 1/\rho$!

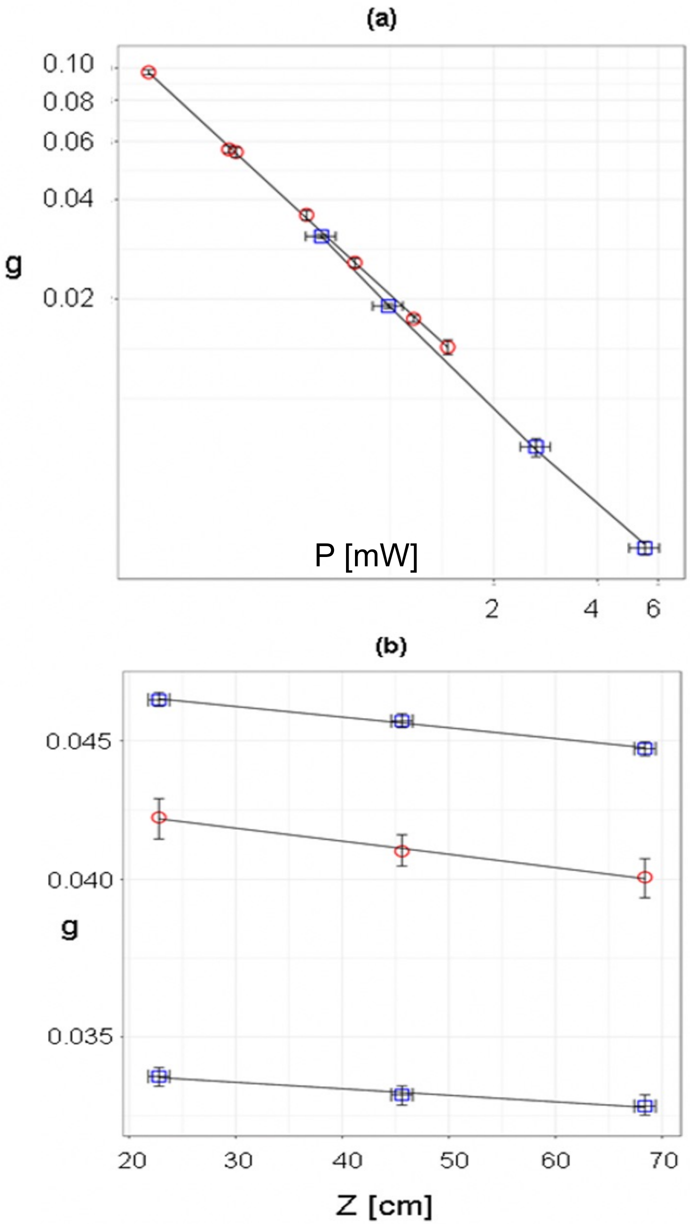
- Thus **fluctuations might develop at high P**

Jinfeng Li, « Monte Carlo Investigation of the UK's First EPR Nuclear Reactor Startup Core Using Serpent », *Energies* 2020, *13*(19), 5168



Safety related questions at low power, as automatic protection systems rely on a time derivative of measured power

EFFECT OF SPONTANEOUS FISSION SOURCES ON CLUSTERING



$$\boxed{g_{\infty}^{3D}(z) = \frac{\lambda_F \overline{\nu_F(\nu_F - 1)}}{8\pi D c_{\infty}} \left(2L_T \sinh^{-1}(1) - \frac{\pi}{2} z\right)}$$

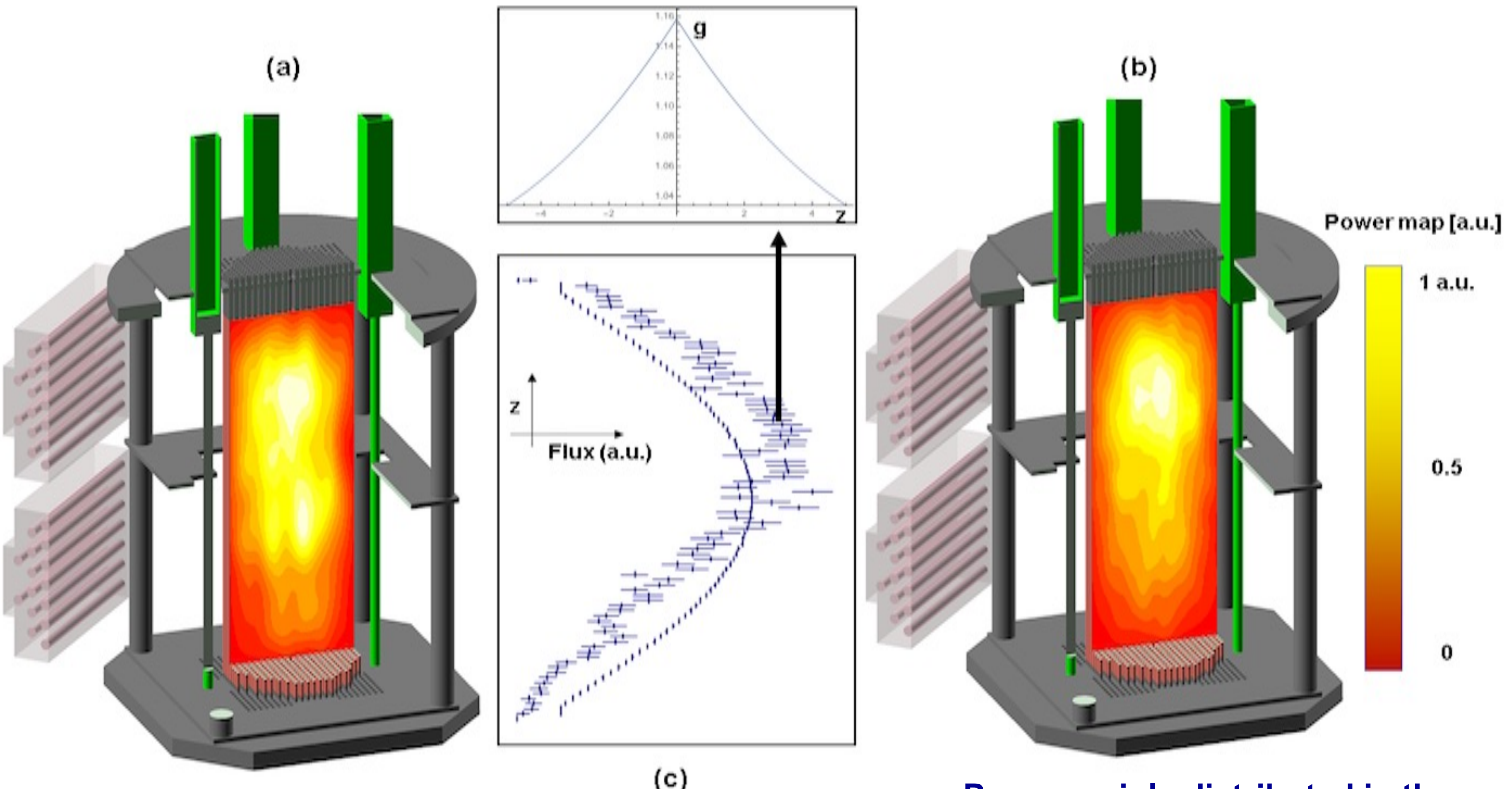
$1/P$ $\quad$ $cte_1 - cte_2.z$

- The spatial correlation function measured at RCF exhibits a 1/P behavior as predicted by the modeling
- Taking into account SF explains the linear decay of spatial correlations (smoother than the Γ function)
- This also might reveal to be a safety concern for decoupled reactors: clustering at the startup of the core might screen over-reactive regions that shall be detected the sooner possible

EFFECT OF SPONTANEOUS FISSION SOURCES ON CLUSTERING

The full neutron statistics has been simulated analogously

- HPC to reproduce 10 mW of signal
- 1 month of simulation time distributed over 10^3 cores
- Overall number of simulated neutrons ~ 10^{12} !



→ **Power smoothely distributed in the core**

→ **Power mainly distributed in the upper region of the reactor**

QUANTUM MECHANICS AS A (BRANCHING) STOCHASTIC PROCESS

- Numerical considerations
  - Quantum mechanics ground state solvers based on DMC (Diffusion Monte Carlo)
  - DMC ~ Branching Brownian Motion with population control => same as NTE

- Theoretical considerations
  - Quantum mechanics seen as a stochastic process [Fenyes, Nelson]
  - Deep connection with (branching) diffusion processes [Nagasawa]
  - Ground state → excited states : still problems (for spin>0)

$$
\begin{aligned}
& i\frac{\partial\psi}{\partial t} + \frac{1}{2}\Delta\psi + i\boldsymbol{b}(t,x)\cdot\nabla\psi - V(t,x)\psi = 0,\\
& -i\frac{\partial\overline{\psi}}{\partial t} + \frac{1}{2}\Delta\overline{\psi} - i\boldsymbol{b}(t,x)\cdot\nabla\overline{\psi} - V(t,x)\overline{\psi} = 0,
\end{aligned}
\quad\Leftrightarrow\quad
\begin{aligned}
& \frac{\partial\phi}{\partial t} + \frac{1}{2}\Delta\phi + \boldsymbol{b}(t,x)\cdot\nabla\phi + c(t,x)\phi = 0,\\
& -\frac{\partial\hat{\phi}}{\partial t} + \frac{1}{2}\Delta\hat{\phi} - \boldsymbol{b}(t,x)\cdot\nabla\hat{\phi} + c(t,x)\hat{\phi} = 0,
\end{aligned}
$$

- Wick rotation : $i\,t \to t$
- Branching process : $-V \to + c$
- Complex conjugate → Adjoint flux

- Neutrons in NTE → "universes/possibilities" in QM ? [Everett]
- Clustering in NTE → decoherence in QM ?