

IRSN

INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Faire avancer la sûreté nucléaire



Neutron clustering: from Blaise Pascal's ruin theory to the Reactor Critical Facility at RPI

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on behalf of the LANL-IRSN collaboration

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Foreword on the gambler's ruin



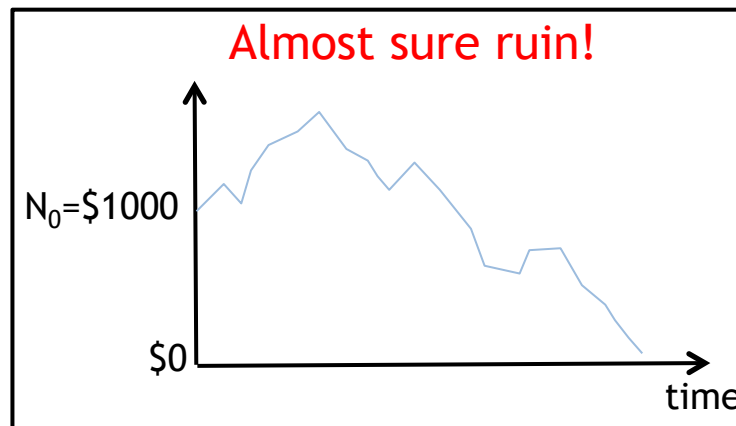
Blaise Pascal (1623-1662)
mathematician & philosopher

Letter (1656) →

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



Pierre de Fermat (1605-1665)
mathematician & magistrate



Outline

Part 1. Initial motivation:
tilts in Monte Carlo criticality simulations

Part 2. Beyond the Boltzmann critical equation:
stochastic modeling of spatial correlations

Part 3. Consequences on eigenvalue calculations:
traveling waves & clustering

Part 4. Consequences on experimental reactor physics:
measuring spatial correlations at RCF

Outline

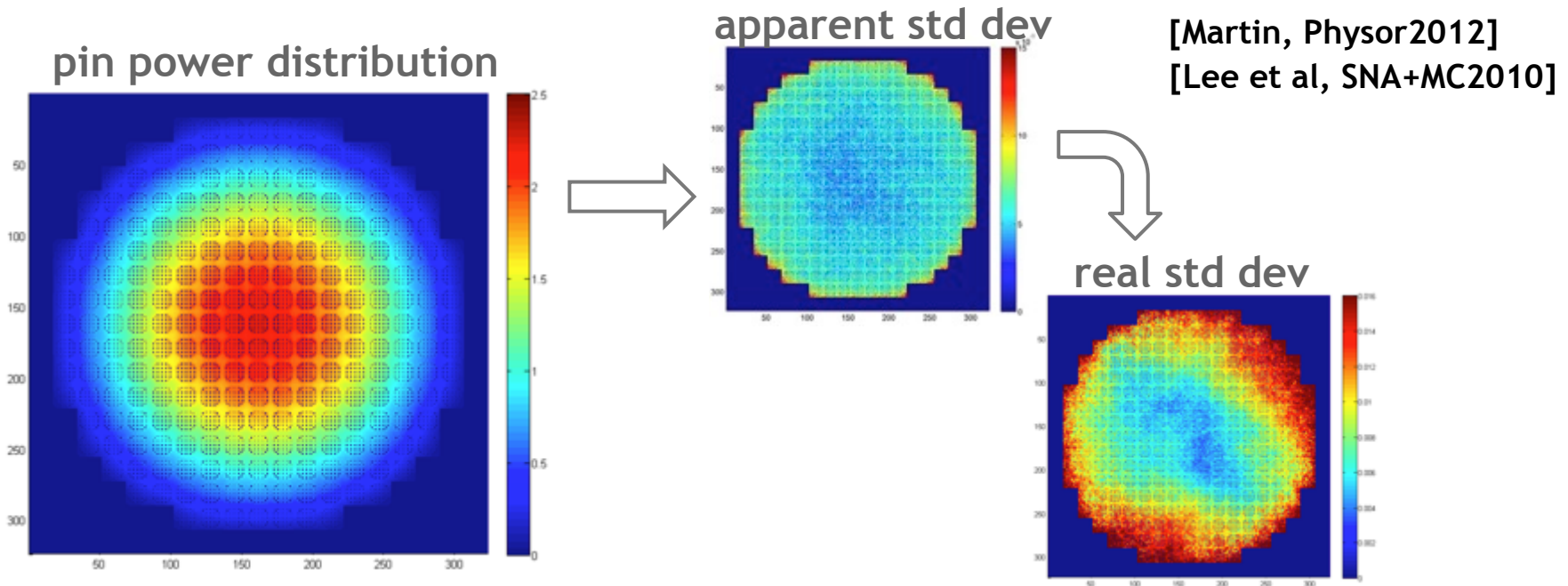
Part 1. Initial motivation:
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Initial motivation: numerical tilts?



Power tilt in the Monte-Carlo simulation of large reactor cores:

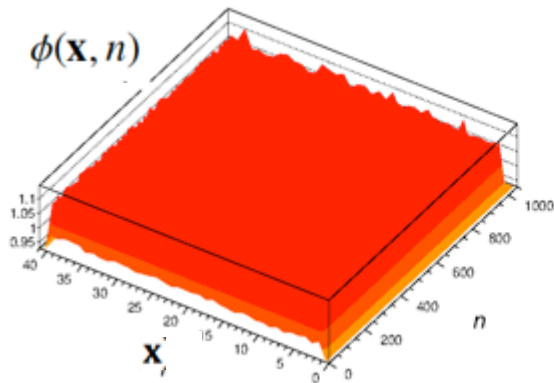
Long standing issue (70's): dedicated publications, expert groups, ...
Strong under-estimation of error bars develop

=> problem for criticality-safety assessment !

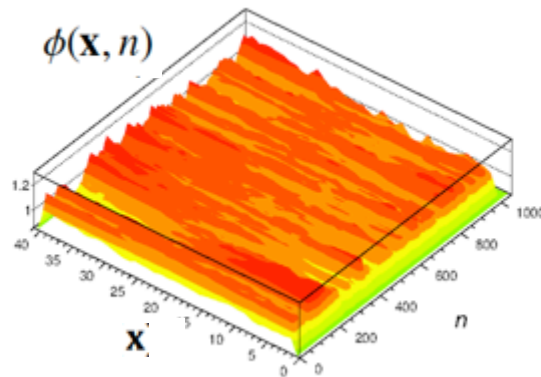
If we look closer ...

$\phi(\mathbf{x}, n)$ is the “space-time” flux in a pincell

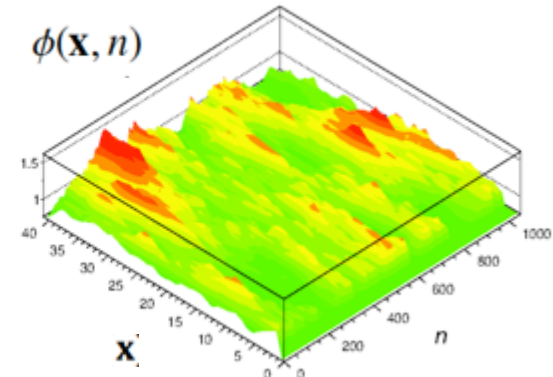
Instead of looking at integrated tallies, can we consider instantaneous tallies?



$L = 10$ cm



$L = 100$ cm



$L = 400$ cm

Strong spatial correlations develop for loosely coupled systems

“neutron clustering”

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Clustering in mathematics and in biology

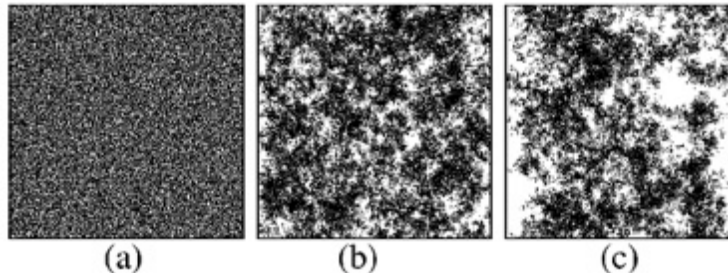
- clustering in theoretical ecology

[Dawson, 1972]

[Cox and Griffeth, 1985]

- clustering in biology (where it is aka brownian bugs):

- plankton are any organisms that live in the water column and are incapable of swimming against a current
- they **reproduce**, **die** and are **transported** by the water (like neutrons!)

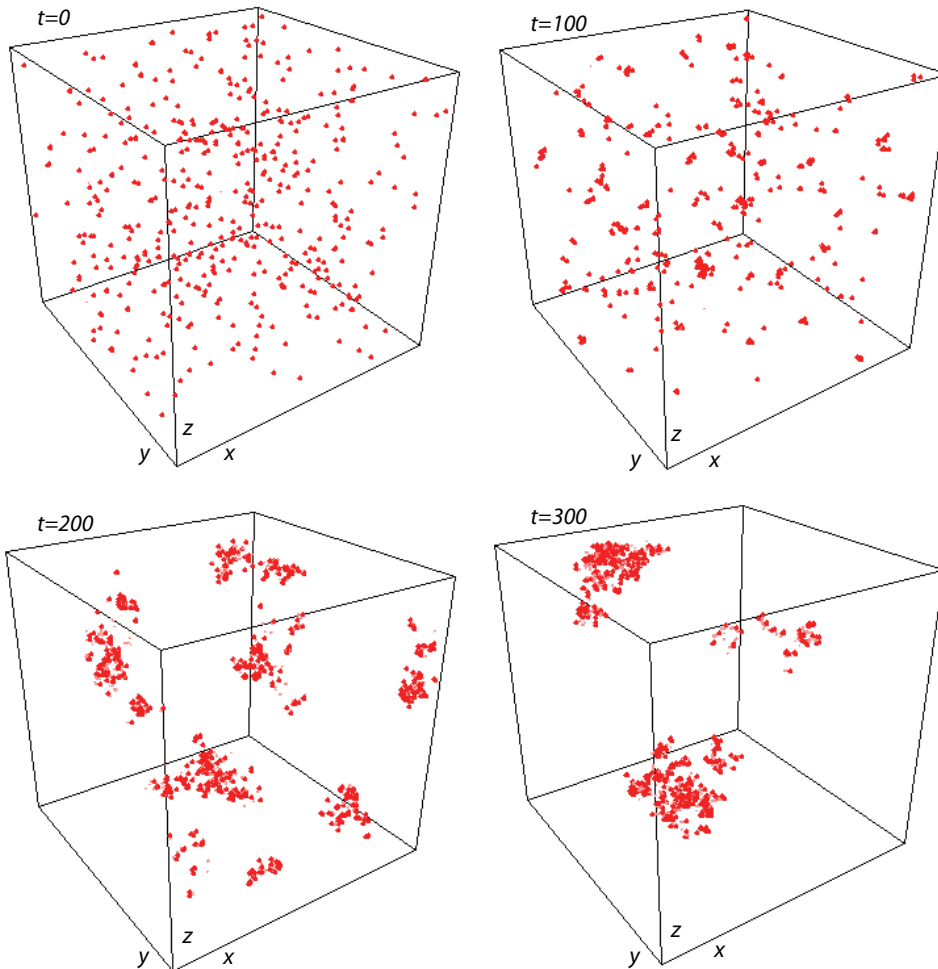


[Young, Nature 2001]

[Houchmandzadeh, PRE 2008]

- tools to describe clustering in physics: statistical mechanics, in particular *Branching Brownian Motion (BBM)*

Neutron clustering



❑ TRIPOLI-4®

❑ Exponential flights with

❑ typical jump size $1/\Sigma_s \rightarrow 0$

❑ to recover the diffusion regime

❑ Binary branching

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

❑ Dimension $d = 3$

❑ Typical length $L \gg l$

Can we have a quantitative insight into this phenomenon?

Branching Brownian motion

simplified model for neutron transport in multiplicative media:

- $N_0 \rightarrow \infty$ neutrons, uniformly distributed at $t=0$
- infinite medium ($L \rightarrow \infty$)
- no energy dependence
- Brownian motion with diffusion coefficient D [$\text{cm}^2 \cdot \text{s}^{-1}$]
- undergoes collision at Poissonian times with rate λ [s^{-1}]
- at each collision, k descendants with probability $p(k)$
- dimension d

$$\left. \begin{array}{l} \square N_0 \rightarrow \infty \text{ neutrons, uniformly distributed at } t=0 \\ \square \text{ infinite medium } (L \rightarrow \infty) \end{array} \right\} c_0 = cte$$

$$\langle x^2(t) \rangle = Dt$$

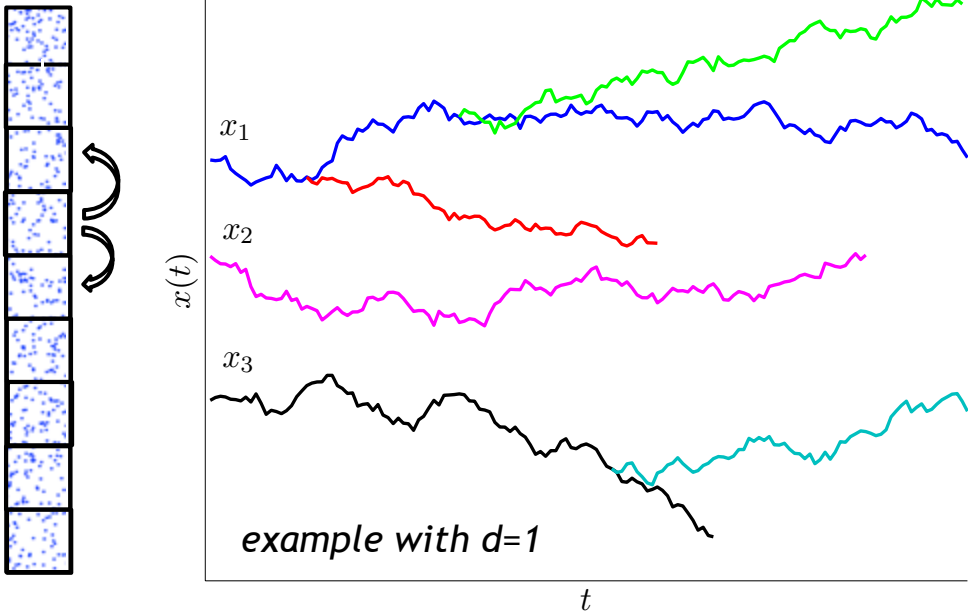
$$p(0) \leftrightarrow \Sigma_c$$

$$p(1) \leftrightarrow \Sigma_s$$

$$p(2), p(3), \dots \leftrightarrow \Sigma_f$$

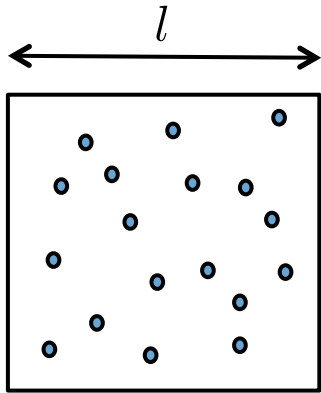
$$\nu_1 = \sum_k kp(k)$$

shuffling



this process couples:
 ⇒ Galton-Watson birth-death process to describe fission and absorption
 ⇒ Brownian motion to simulate neutron transport

Crash course for clustering in dimension 0



□ We consider a “cell” i at time t with n individuals

□ $d=0$ Branching events with:

➤ production rate $\lambda p(2)$

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

➤ disparition rate $\lambda p(0)$

$n [\#]$

□ Proba($n \rightarrow n+1$ in dt): $W^+(n)dt = \lambda p(2)ndt$

$dt [s]$

□ Proba($n \rightarrow n-1$ in dt): $W^-(n)dt = \lambda p(0)ndt$

Forward master equation

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

Critical:

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

$$\langle n(t) \rangle = n_0$$

$$\langle V(t) \rangle = \lambda n_0 t$$

$$\langle n(t) \rangle = \sum_n n P(n, t)$$

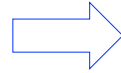
$$\langle n^2(t) \rangle = \sum_n n^2 P(n, t)$$

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

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

From gambler's ruin to critical catastrophe...

Ultimate fate of this population?
Controlled by $\nu_1 = \sum_k k p(k)$
(mean number of part/collision)

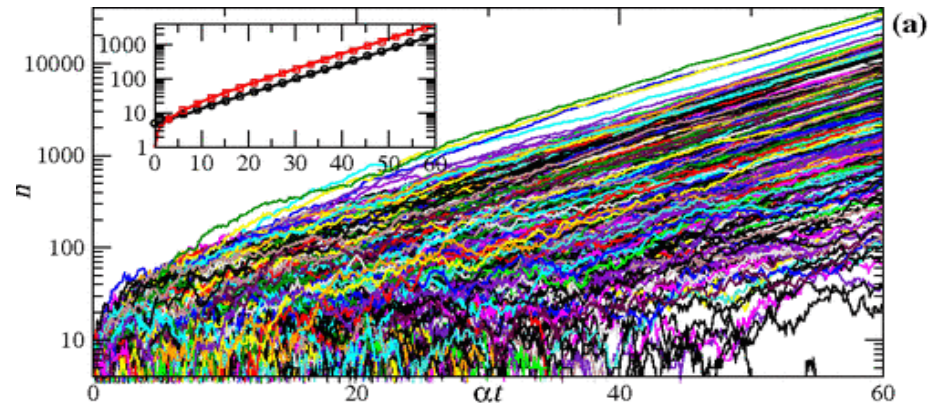
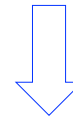


$\nu_1 > 1$	population grows unbounded
$\nu_1 < 1$	population becomes extinct
$\nu_1 = 1$	population constant on average: critical condition

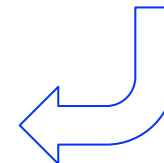
**N neutrons in a critical spatial cell
which undergo fission or capture
events**



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



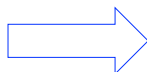
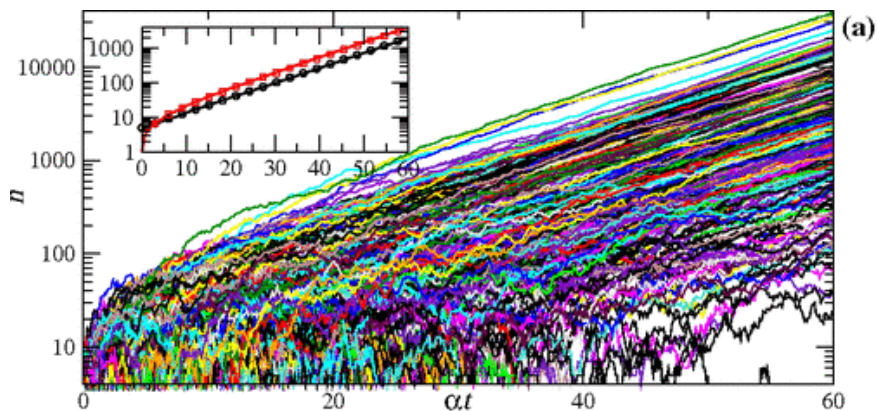
Fair game in neutron transport = criticality
Gambler's ruin = critical catastrophe!



[Williams, 1974]

... and from critical catastrophe to neutron clustering

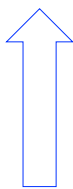
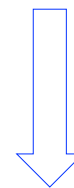
[Houchmandzadeh, PRE 2008]



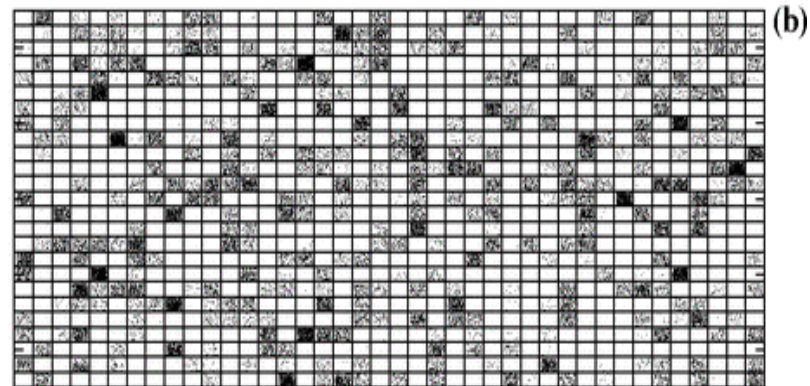
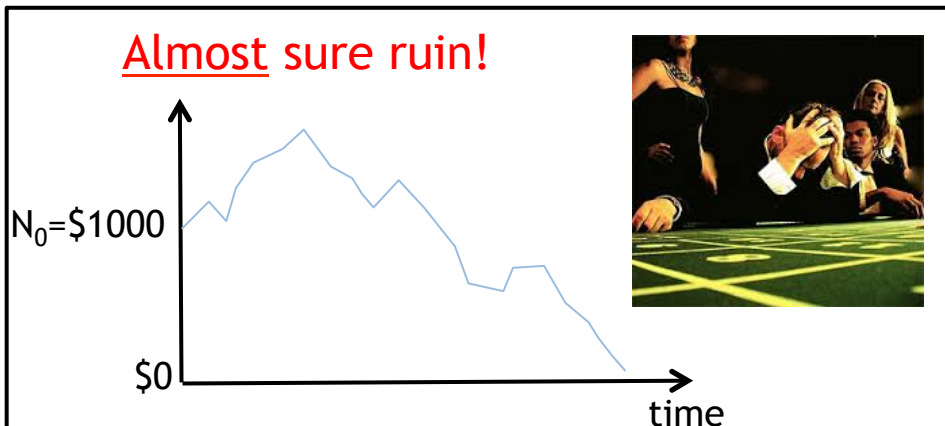
(b)

$$\langle n(t) \rangle = n_0$$

$$\langle V(t) \rangle = \lambda n_0 t$$



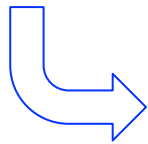
Almost sure ruin!



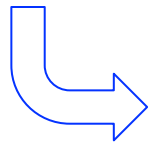
From $d=0$ to $d=2$

$d=0 \Rightarrow$ **Critical castastrophe** \Leftrightarrow **Gambler's ruin**

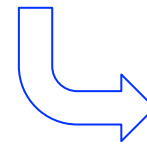
$d>0 \Rightarrow$ **Neutron clustering**



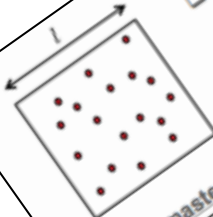
but here the cells where totally decoupled
“fake” $d=2$



We have to take into account the
diffusion of neutrons



STOCHASTIC MODELING & THEORY



We consider a "cell" l at time t with n individuals
 $d=0$ Branching events with:
 > production rate $\lambda p(2)$
 > dispartition rate $\lambda p(0)$
 Probab($n \rightarrow n+1$ in dt): $W^+(n)dt = \lambda p(2)ndt$
 Probab($n \rightarrow n-1$ in dt): $W^-(n)dt = \lambda p(0)ndt$

$\lambda p(0), \lambda p(2) [s^{-1}]$
 n [#]
 dt [s]

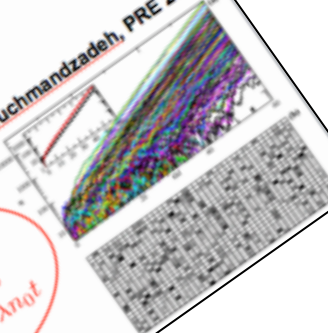
Forward master equation
 $\frac{dP(n,t)}{dt} = W^-(n+1)P(n+1,t) - W^-(n)P(n,t) + W^+(n-1)P(n-1,t) - W^+(n)P(n,t)$

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

$\langle n(t) \rangle = n_0 e^{\lambda(p(2) - p(0))t}$
 $\langle n(t) \rangle^2 = \lambda p(0) + p(2) n_0 t$

Critical:
 $\lambda p(0) = \lambda p(2)$
 $\langle n(t) \rangle = n_0$
 $\langle V(t) \rangle = \lambda n_0 t$

[Houchmandzadeh, PRE 2008]



STOCHASTIC MODELING & THEORY

□ We consider a "cell" l at time t with n individuals

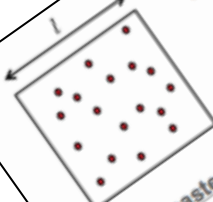
□ $d=0$ Branching events with:

- production rate $\lambda p(2)$
- disappearance rate $\lambda p(0)$

□ Probab($n \rightarrow n+1$ in dt): $W^+(n)dt = \lambda p(2)ndt$

□ Probab($n \rightarrow n-1$ in dt): $W^-(n)dt = \lambda p(0)ndt$

$\lambda p(0), \lambda p(2) [s^{-1}]$
 n [#]
 dt [s]



Forward master equation

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

$\langle n(t) \rangle = \sum n P(n,t)$

$\langle n^2(t) \rangle = \sum n^2 P(n,t)$

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

$\langle V(t) \rangle = \langle n^2(t) \rangle - \langle n(t) \rangle^2$

Criticality

□ fission event

- proba: $W^+(\vec{n}, i)dt = \lambda p(2)\eta_i \vec{n} dt$
- action on \vec{n} : $a_i^+ \vec{n} = (\dots, n_{i-1}, n_i + 1, n_{i+1}, \dots)$

□ capture event

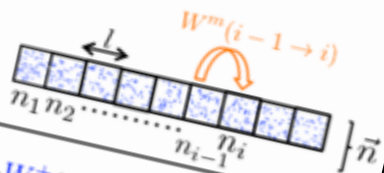
- proba: $W^-(\vec{n}, i)dt = \lambda p(0)\eta_i \vec{n} dt$
- action on \vec{n} : $a_i^- \vec{n} = (\dots, n_{i-1}, n_i - 1, n_{i+1}, \dots)$

□ migration event

- proba: $W^m(\vec{n}, i-1 \rightarrow i)dt = \lambda p(1)\eta_i \vec{n} dt$
- action on \vec{n} : $a_i^+ a_{i-1}^- \vec{n}$

with η_i the number of neutrons in cell l
 and $\lambda p(1) = D/2l^2$

Forward master equation

$$\frac{dP(\vec{n}, t)}{dt} = \sum_i \left[W^+(a_i \vec{n}, i)P(a_i \vec{n}, t) + W^-(a_i^+ \vec{n}, i)P(a_i^+ \vec{n}, t) + W^m(a_{i-1}^+ a_i \vec{n}, i-1, i)P(a_{i-1}^+ a_i \vec{n}, t) + W^m(a_{i+1}^+ a_i \vec{n}, i+1, i)P(a_{i+1}^+ a_i \vec{n}, t) - W^+(\vec{n}, i)P(\vec{n}, t) - W^-(\vec{n}, i)P(\vec{n}, t) - W^m(\vec{n}, i, i+1)P(\vec{n}, t) - W^m(\vec{n}, i, i-1)P(\vec{n}, t) \right]$$


STOCHASTIC MODELING & THEORY

□ We consider a "cell" l at time t with n individuals

□ $d=0$ Branching events with:

- production rate $\lambda p(2)$
- disappearance rate $\lambda p(0)$

□ Probab($n \rightarrow n+1$ in dt): $W^+(n)dt = \lambda p(2)ndt$

□ Probab($n \rightarrow n-1$ in dt): $W^-(n)dt = \lambda p(0)ndt$

□ fission event

- proba: $\lambda p(2)$
- action on \vec{n} : $W^+(\vec{n}, i)dt = \lambda p(2)\eta_i \vec{n} dt$

□ capture event

- proba: $\lambda p(0)$
- action on \vec{n} : $W^-(\vec{n}, i)dt = \lambda p(0)\eta_i \vec{n} dt$

□ migration event

- proba: $\lambda p(1)$
- action on \vec{n} : $W^m(\vec{n}, i-1, i)dt = \lambda p(1)\eta_i \vec{n} dt$

Forward master equation

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

with η_i the number of neutrons in cell l

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

The equations obtained stand for any arbitrary dimension d and in the case $v_1 = 1$ can be written:

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

$$\frac{\partial}{\partial t} g_i(r) = 2D \nabla_r^2 g_i(r) + \frac{\lambda v_2}{c_i} \delta(r)$$

d-dimensional Laplacian
(diffusion term)

with $r = |\mathbf{x} - \mathbf{y}|$

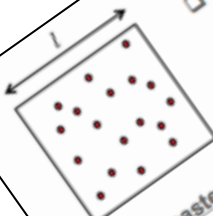
$$\text{and } v_2 = \sum_k k(k-1)p(k)$$

auto-correlation term leading to 2nd moment effects via v_2 (the second factorial moment of the number of particles)

Young, W.R., Roberts, A.J., Stuhne, G., 2001. Nature 412, 328.
 Houchmandzadeh, B., 2002. Phys. Rev. E 66, 052902.
 Houchmandzadeh, B., 2008. Phys. Rev. Lett. 101, 078103.
 Houchmandzadeh, B., 2009. Phys. Rev. E 80, 051920.

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Forward master equation

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

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

$$\langle n(t) \rangle = n_0 e^{\lambda p(2)t}$$

$$\langle V(t) \rangle = \langle n^2(t) \rangle$$

The equations obtained $v_1 = 1$ can be written:

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

$$\frac{\partial}{\partial t} g_i(r) = 2D \nabla_r^2 g_i(r) + \frac{\lambda v_2}{c_i} g_i(r)$$

auto-correlation term leading to 2nd moment effects via v_2 (the second factorial moment of the number of particles)

- fission event
 - proba: $W^+(\bar{n})$
 - action on \bar{n} : $a_i^+ \bar{n}$
- capture event
 - proba: $W^-(\bar{n})$
 - action on \bar{n} : $a_i^- \bar{n}$
- migration event
 - proba: $W^m(\bar{n})$
 - action on \bar{n} : $a_i^m \bar{n}$

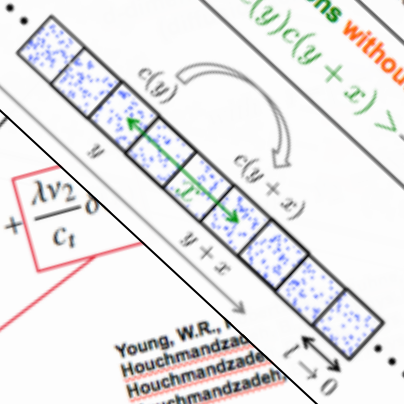
Forward

As before one can inject in the **Master equation** the mean number of neutrons in cell k : or its continuous version:

$$\langle n_k \rangle = \sum_n n_k P(n_k, t)$$

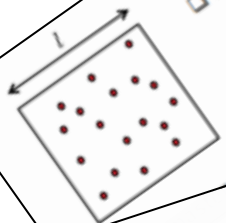
$$c(x) = \lim_{l \rightarrow 0} \frac{n_k}{l}$$

And define an appropriate tool to study spatial correlations: the **centered correlations without self-contribution**

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


Young, W.R., Houchmandzadeh, Houchmandzadeh, Houchmandzadeh

STOCHASTIC MODELING & THEORY



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- Probab($n \rightarrow n-1$ in dt): $W^-(n) dt = \lambda p(0) n dt$

- fission event
 - proba: $W^+(n)$
 - action on \vec{n} : $a_i^+ \vec{n}$
- capture event
 - proba: $W^-(n)$
 - action: $a_i^- \vec{n}$
- migration

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

$$W_t(u_i, u_j | x_0) = \mathbb{E}[u_i^{n_{v_i}(x_0, t)} u_j^{n_{v_j}(x_0, t)} | x_0] = \sum_{n_{v_i}} \sum_{n_{v_j}} u_i^{n_{v_i}(x_0, t)} u_j^{n_{v_j}(x_0, t)} P_t(n_{v_i}, n_{v_j} | x_0)$$

The moments of the observables can be obtained by derivation:

Average occupation at a detector

$$\mathbb{E}_t[n_{v_i} | x_0] = \frac{\partial}{\partial u_i} W_t(u_i, u_j | x_0) |_{u_i=1, u_j=1}$$

Correlations between detectors

$$\mathbb{E}_t[n_{v_i} n_{v_j} | x_0] = \frac{\partial^2}{\partial u_i \partial u_j} W_t(u_i, u_j | x_0) |_{u_i=1, u_j=1}$$

auto-correlation term leading to 2nd moment effects via v_2 (the second factorial moment of the number of particles)

previous version: $\langle n_k \rangle = \sum_n n_k P(n_k, t)$

to study spatial correlations: the

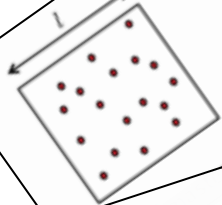
$$c(x) = \lim_{l \rightarrow 0} \frac{n_k}{l}$$

self-contribution $2 - c\delta(x) / c^2$



Young, W.R., Houchmandzadeh, Houchmandzadeh, Houchmandzadeh

STOCHASTIC MODELING & T...



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 - ▷ production rate $\lambda p(2)$
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- Probab($n \rightarrow n-1$ in dt): $W^-(n) dt = \lambda p(0) n dt$

$$\lambda p(0), \lambda p(2) \left[\frac{n-1}{n} \right] \frac{dn}{dt} [s]$$

- fission
- ▷ pro...
- ▷ action
- capture event
- ▷ proba:
- ▷ action
- migration

$$W_t(u_i, u_j | x_0) = \mathbb{E}[u_i^{n_{v_i}(x_0, t)} u_j^{n_{v_j}(x_0, t)}] = \sum_{n_{v_i}} \sum_{n_{v_j}} u_i^{n_{v_i}(x_0, t)} u_j^{n_{v_j}(x_0, t)} P(n, t)$$

The moments of the observables can be obtained by derivation:

Average occupation at a detector

$$\mathbb{E}_t[n_{v_i} | x_0] = \frac{\partial}{\partial u_i} W_t(u_i, u_j | x_0) |_{u_i=1, u_j=1}$$

Correlations between detectors

$$\mathbb{E}_t[n_{v_i} n_{v_j} | x_0] = \frac{\partial^2}{\partial u_i \partial u_j} W_t(u_i, u_j | x_0) |_{u_i=1, u_j=1}$$

auto-correlation term leading to 2nd moment effects via v_2 (the second factorial moment of the number of particles)

And with initial condition

$$W_0(u_i, u_j | x_0) = u_i^{n_{v_i}(x_0, 0)} u_j^{n_{v_j}(x_0, 0)}$$

Where

$$G[z] = \sum_k g_{k-z-k}$$

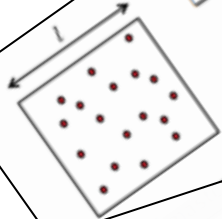
$$\frac{\partial}{\partial t} W_t = D \nabla_{x_0}^2 W_t - \lambda W_t + \lambda G[W_t]$$

It can be shown that W satisfies the backward equation

Young, W.R., Houchmandzadeh, Houchmandzadeh, Houchmandzadeh

STOCHASTIC MO

- We consider a "cell" of size l at time t with n individuals
- $d=0$ Branching events with:
 - > production rate $\lambda p(2)$
 - > disappearance rate $\lambda p(0)$
- Probab($n \rightarrow n+1$ in dt): $W^+(n) dt = \lambda p(2) n dt$
- Probab($n \rightarrow n-1$ in dt): $W^-(n) dt = \lambda p(0) n dt$



$$W_t(u_i, u_j | x_0) = \mathbb{E}[u_i^{n_{v_i}(x_0, t)} u_j^{n_{v_j}(x_0, t)} | x_0]$$

The moments of the observables can be obtained from the generating function

Average occupation at a detector

$$\mathbb{E}_t[n_{v_i} | x_0] = \frac{\partial}{\partial u_i} W_t(u_i, u_j | x_0) |_{u_i=1, u_j=1}$$

Correlations between detectors

$$\mathbb{E}_t[n_{v_i} n_{v_j} | x_0] = \frac{\partial^2}{\partial u_i \partial u_j} W_t(u_i, u_j | x_0) |_{u_i=1, u_j=1}$$

auto-correlation term leading to 2nd moment effects via v_2 (the second factorial moment of the number of particles)

Green function for the critical fuel rod:

$$G_t(x, x_0) = \frac{1}{2L} + \frac{1}{L} \sum_{k=1}^{\infty} e^{-k^2 \frac{t}{\tau_D}} \varphi_k(x) \varphi_k(x_0)$$

"Mixing time":

$$\tau_D = \left(\frac{2}{\pi}\right)^2 \frac{L^2}{D}$$

Average density: $\psi(x, t) = \frac{N}{2L}$

Correlation function:

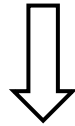
$$h(x_i, x_j, t) = \underbrace{\left(\frac{N}{2L}\right)^2}_{\text{Divergence in time}} \left[\frac{t}{\tau_E} + \underbrace{\frac{\tau_D}{\tau_E} \sum_{k=1}^{\infty} \frac{1 - e^{-2k^2 \frac{t}{\tau_D}}}{k^2}}_{\text{Bounded}} \varphi_k(x_i) \varphi_k(x_j) \right]$$

$$\tau_D < \tau_E$$

Where $\frac{\partial}{\partial t} W_t = D \nabla_{x_0}^2 W_t$
It can be shown that W satisfies the boundary conditions

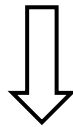
Young, W.R., Houchmandzadeh, Houchmandzadeh, Houchmandzadeh

Master equation
for branching processes



Solving of the 1st moment
of that equation

=> flux



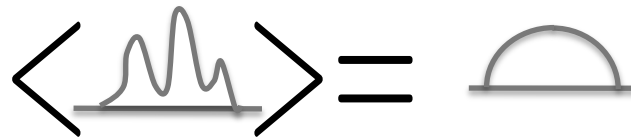
Solving of the 2^d moment
of that equation

=> spatial correlations

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 power peaks at arbitrary places!

●
The **typical amplitude** of those peaks is controlled by

$\frac{\nu_2}{C_0}$ → fission process
different in reactor physics and MC simu

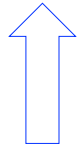
●
Challenge in **MC criticality simulations**: $C_0 \ll$ Less than in reality!

Beyond the Boltzmann equation: Feynman-Kac & Master equations

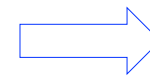
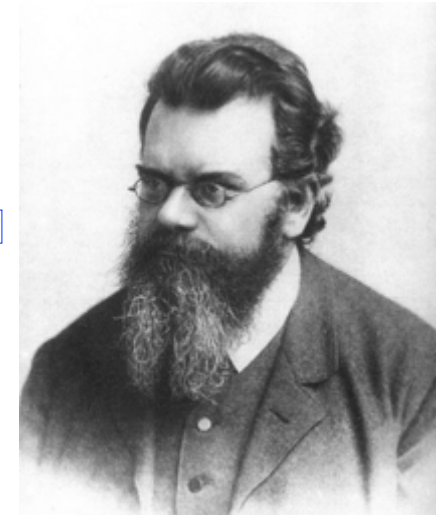
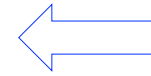
Feynman
1918-1988



Kac
1914-1984



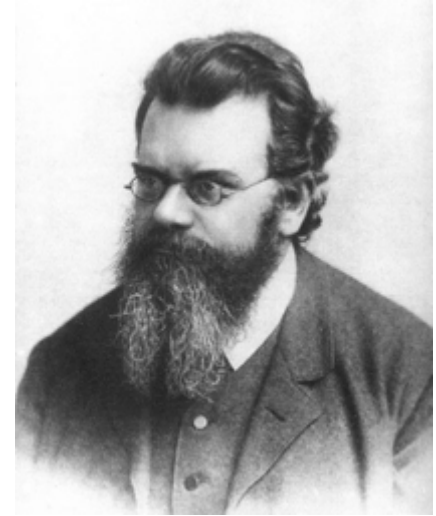
Boltzmann
1844-1906



Ulam
1909-1984

Beyond the Boltzmann equation: Feynman-Kac & Master equations

- ❑ The Boltzmann critical equation calculates **mean quantities**
- ❑ The Feynman-Kac path integral approach (backward equations) or Fokker-Planck type equations are equations for the **probability => mean + variance/correlations + ...**



**And surprisingly
variance & correlations
take the lead over
mean statistics !**

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)

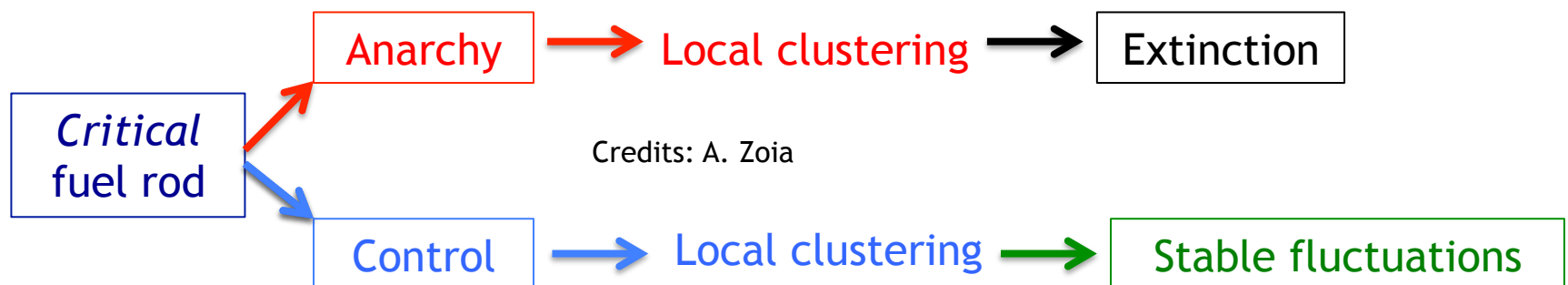
Houchmandzadeh et al, Phys. Rev. E 92 (5), 052114 (2015)

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)



Outline

Part 1. Initial motivation:
tilts in Monte Carlo criticality simulations

Part 2. Beyond the Boltzmann critical equation:
stochastic modeling of spatial correlations

Part 3. Consequences on eigenvalue calculations:
traveling waves & clustering

Part 4. Consequences on experimental reactor physics:
measuring spatial correlations at RCF

Consequence 3:

under-sampling biases

& clustering

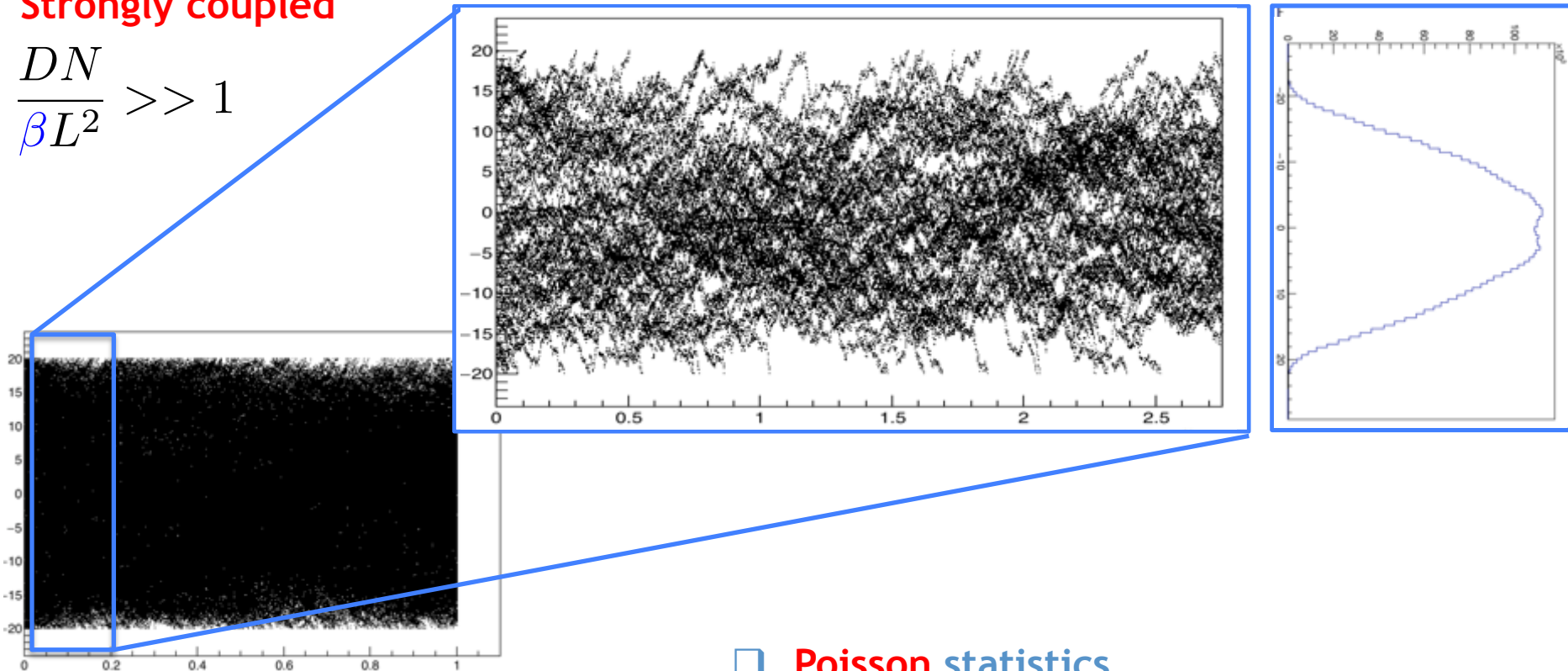
& traveling waves

- ❑ 1-D BBM with population control
- ❑ Uniform initial distribution

- ❑ 50 neutrons
- ❑ $[-L, L]$ Dirichlet

Strongly coupled

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



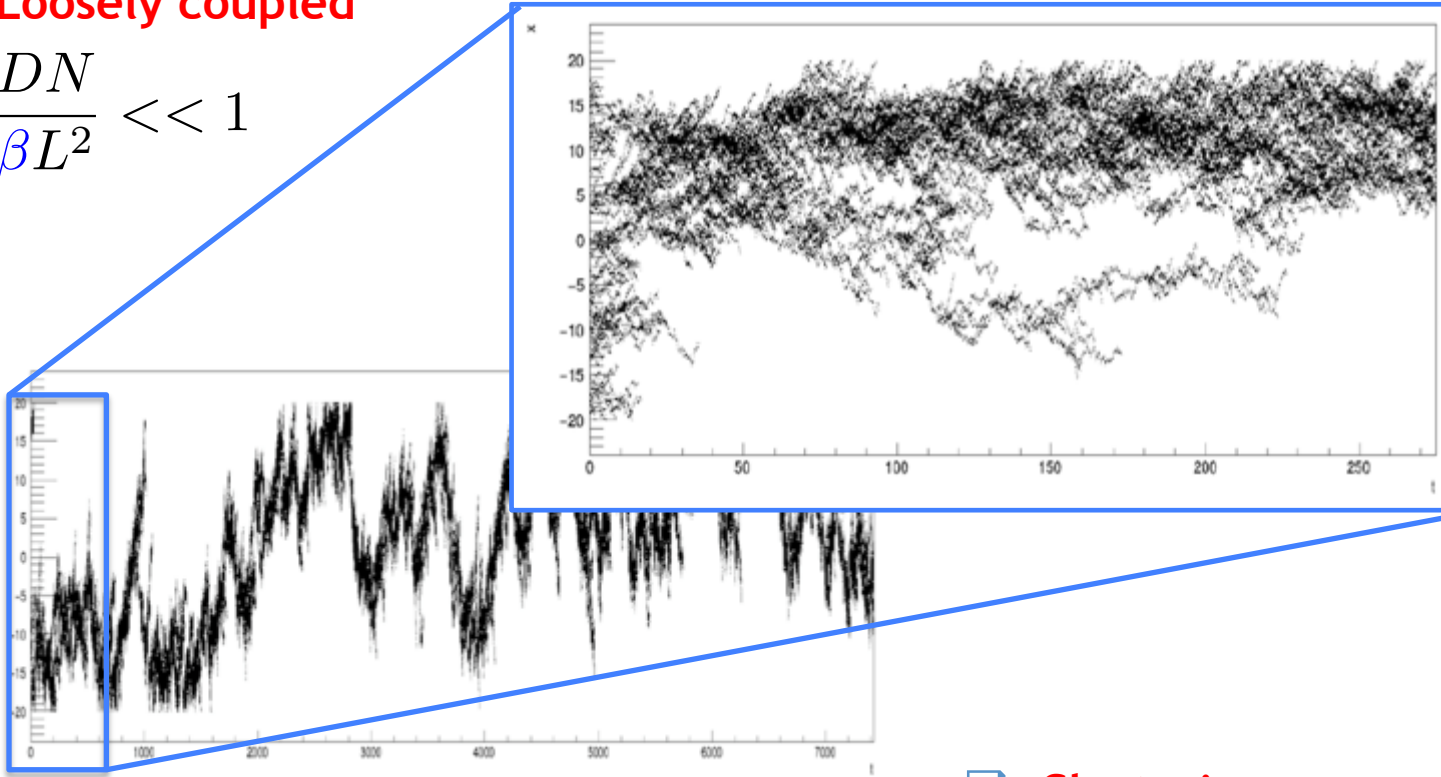
- ❑ Poisson statistics
- ❑ Cosine shape

- ❑ 1-D BBM with population control
- ❑ Uniform initial distribution

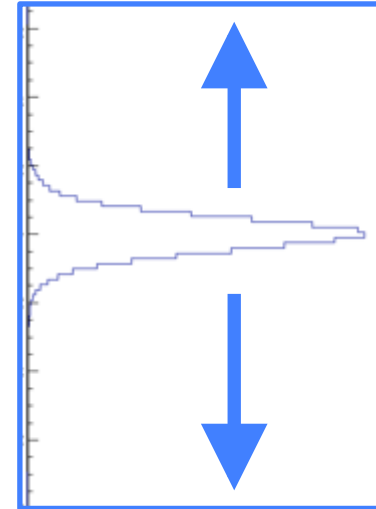
- ❑ 50 neutrons
- ❑ $[-L, L]$ Dirichlet

Loosely coupled

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



Reflection due to $N=\text{constant}$!



Reflection due to $N=\text{constant}$!

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

Population control & traveling waves

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

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

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

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

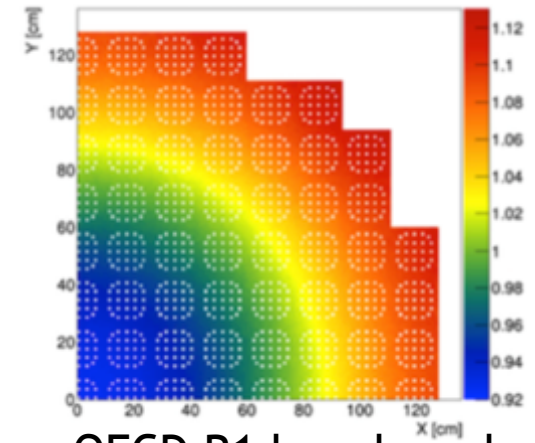
$$\phi(x, t) = \frac{1}{\left(1 + C \exp^{\pm \frac{1}{6} \sqrt{6(\beta - \gamma)} x - \frac{5}{6} (\beta - \gamma) t} \right)^2}$$

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

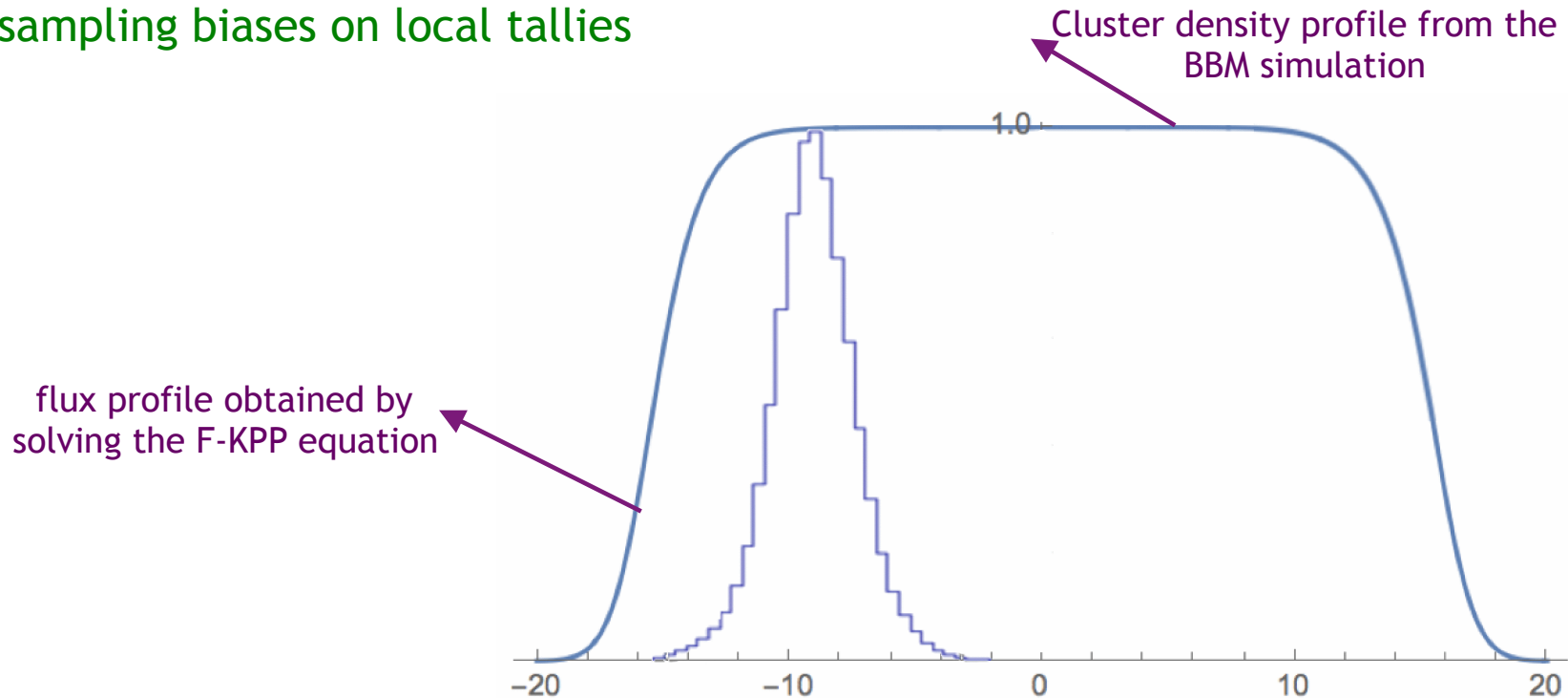
- ❑ F-KPP equation with traveling waves solutions
- ❑ Counter-reaction depending on the sign of $1 - \phi$

Traveling wave & solitons

- ❑ Flux 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
- ❑ Qualitative & Quantitative scheme to explain **under-sampling biases on local tallies**



OECD R1 benchmark



Outline

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traveling waves & clustering

Part 4. Consequences on experimental reactor physics:
measuring spatial correlations at RCF

Is it possible to observe/characterize clustering effects through experiments?

- Clustering **should be measurable**, if certain conditions are gathered:

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

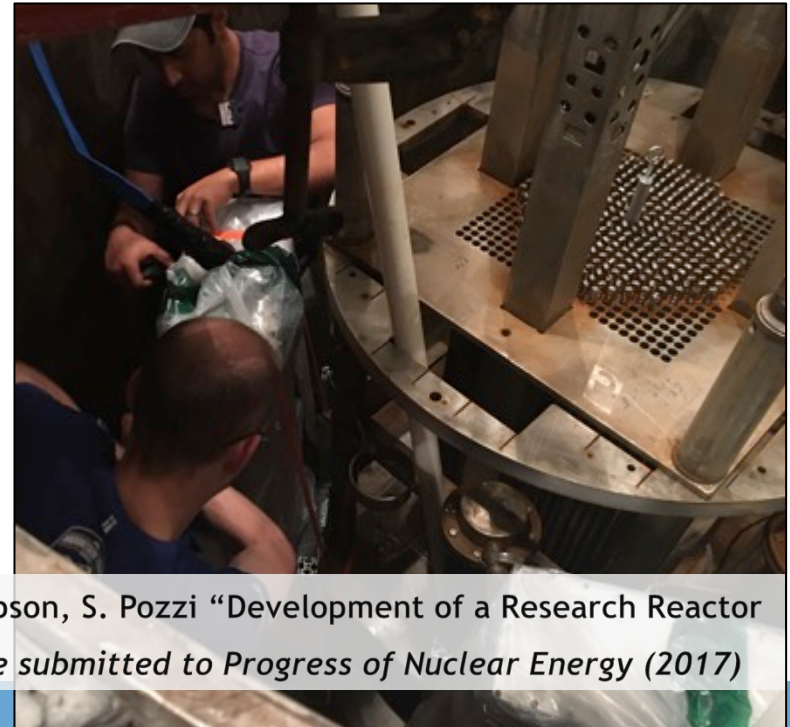
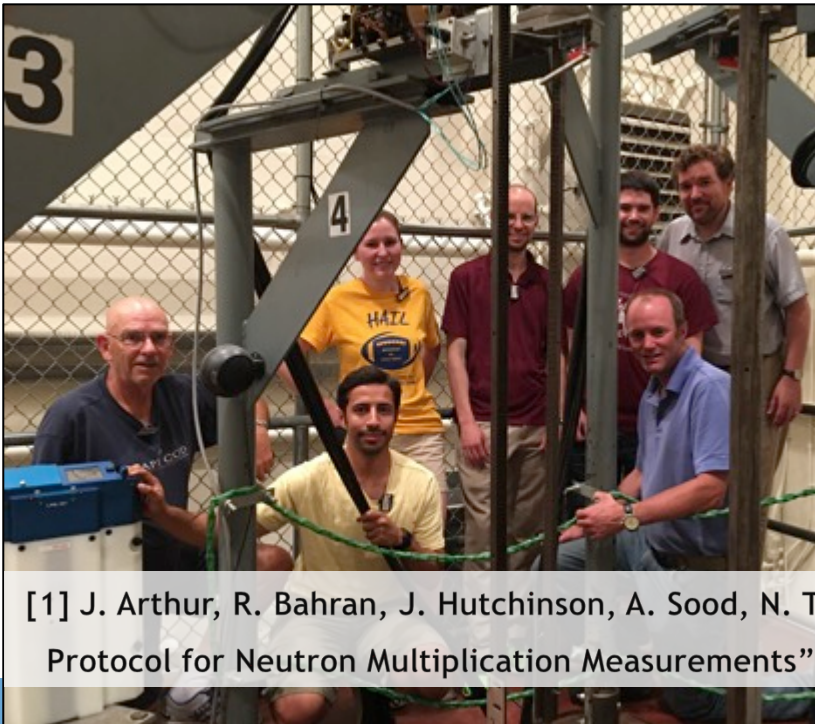
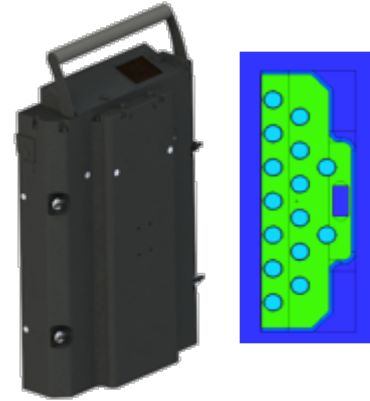
$$\ell_m^2 = \frac{D}{\lambda}$$

Neutron
migration area

In 2016, LANL/UMich Performed Subcritical Measurements at the RPI-RCF with LANL Neutron Multiplicity Detectors

□ Two important goals achieved:

- ✓ established a protocol for subcritical neutron multiplication measurements at a research reactor [1]
- ✓ did not drown very expensive state-of-the-art LANL multiplicity detectors aka MC-15 detectors (15 He-3 tubes encased in poly)



[1] J. Arthur, R. Bahrn, J. Hutchinson, A. Sood, N. Thompson, S. Pozzi “Development of a Research Reactor Protocol for Neutron Multiplication Measurements” *to be submitted to Progress of Nuclear Energy* (2017)

Is it possible to observe/characterize clustering effects through experiments?

- ❑ Clustering **should be measurable**, if certain conditions are gathered:

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

$\ell_m^2 = \frac{D}{\lambda}$ 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 **MC15 detectors & He3 tubes**

MORET 5 simulations to design the experiment

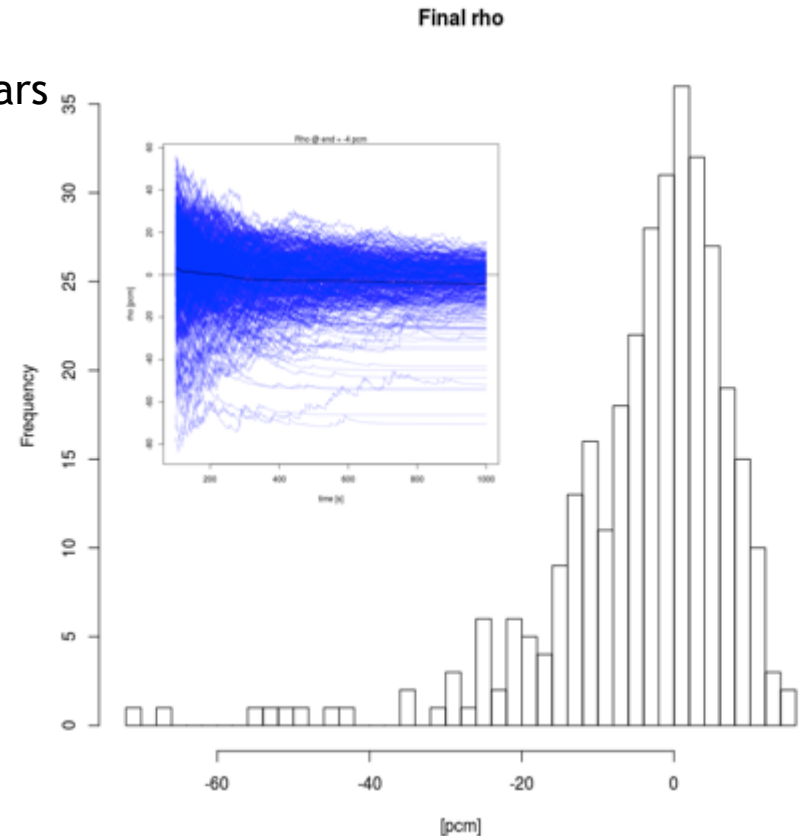
❑ MORET 5 code with all Random Noise options activated => **dynamic + analog**

- ❑ Data library: Endfb71
- ❑ Fission sampling:
 - ✓ Freya
 - ✓ discrete Zucker and Holden tabulated
 - ✓ Pn distributions and corresponding nubar
 - ✓ Only Spontaneous fissions

❑ **Highly parallel simulations:**

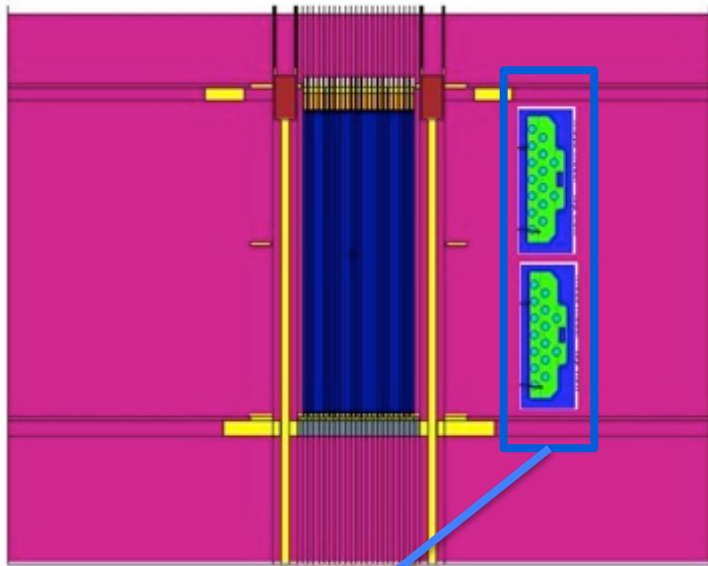
- ❑ Simulated signal = 1000 s (prompt+delayed)
- ❑ Number of independent simulations = 330
- ❑ Number of neutrons per simulation = $2.4 \cdot 10^4$

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

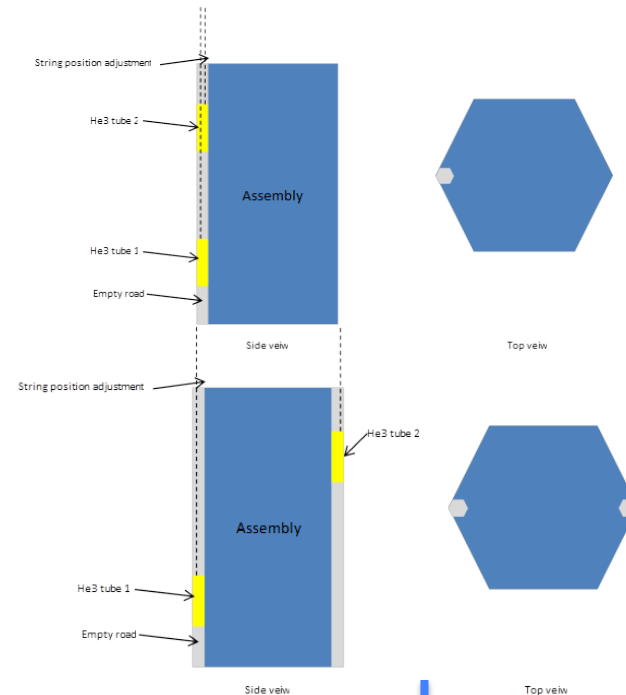


Preliminary results of RCF simulation

- Ideal scenario@RCF => 1st question: are there spatial correlations in the reactor ?
=> 2nd question: if yes, are there measurable?



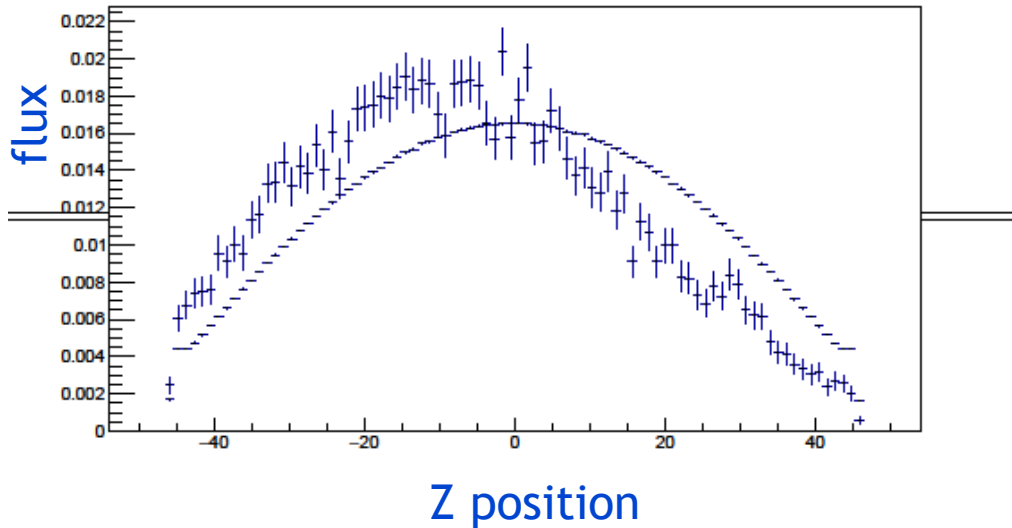
Simulation of expected signal in the MC15 detectors



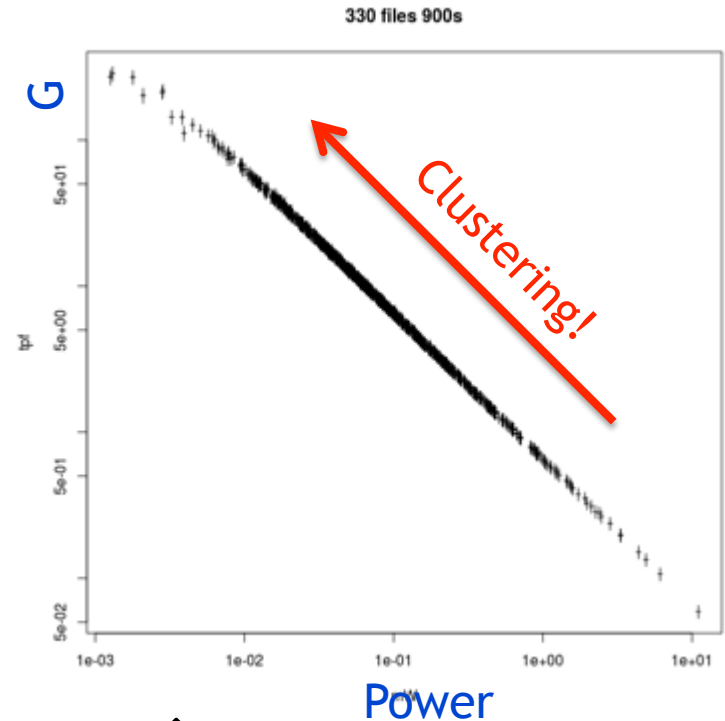
Simulation of in-core effects with tallies defined over He3 tubes

Simulation of RCF in-core effects

Simulation of in-core effects
with He³ tallies



Simulation of expected signal
in the MC15 detectors



❑ Experimental program should include:

- ✓ Power scan
- ✓ PuBe source effects

❑ RCF has the potential to be conclusive
regarding the neutron clustering theory!

$$G_P(n, m) = \frac{\langle nm \rangle - \langle n \rangle \langle m \rangle}{\langle n \rangle \langle m \rangle} \Big|_P$$

Partial conclusions (see N. Thompson's talk!)

- ❑ Stochastic modelling is used to characterize the behavior of loosely coupled systems and predicts a:
 - ❑ clustering phenomenon...
 - ❑ ...obeying traveling waves equations
- ❑ Analog Monte Carlo simulations (with MCNP and/or MORET) were used to design such an experiment, using LANL MC15 detectors and the RCF@RPI reactor
- ❑ This experiment happened in August 2017 and showed that...
 - [see Nick Thompson's talk!](#)
- ❑ Nick Thompson is currently working @ LANL and will rejoin IRSN in June to improve the analyses of the data

Thank you !

Clustering theory

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} : $a_i^+ \vec{n} = (\dots, n_{i-1}, \boxed{n_i + 1}, n_{i+1}, \dots)$

with η_i the number of neutrons in cell i

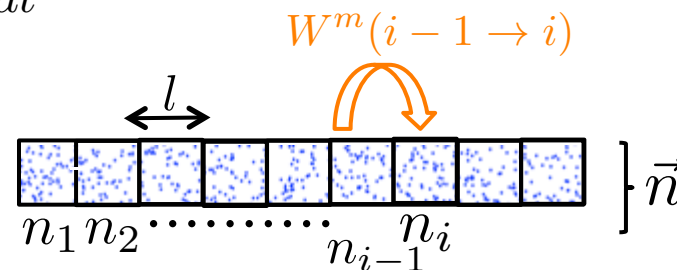
□ capture event

- proba: $W^-(\vec{n}, i)dt = \lambda p(0)\eta_i \vec{n} dt$
- action on \vec{n} : $a_i^- \vec{n} = (\dots, n_{i-1}, \boxed{n_i - 1}, n_{i+1}, \dots)$

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

□ migration event

- proba: $W^m(\vec{n}, i-1 \rightarrow i)dt = \lambda p(1)\eta_i \vec{n} dt$
- action on \vec{n} : $a_i^+ a_{i-1}^- \vec{n}$



Forward master equation

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

And a little bit more

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

$$\langle n_k \rangle = \sum_n n_k P(n_k, t)$$

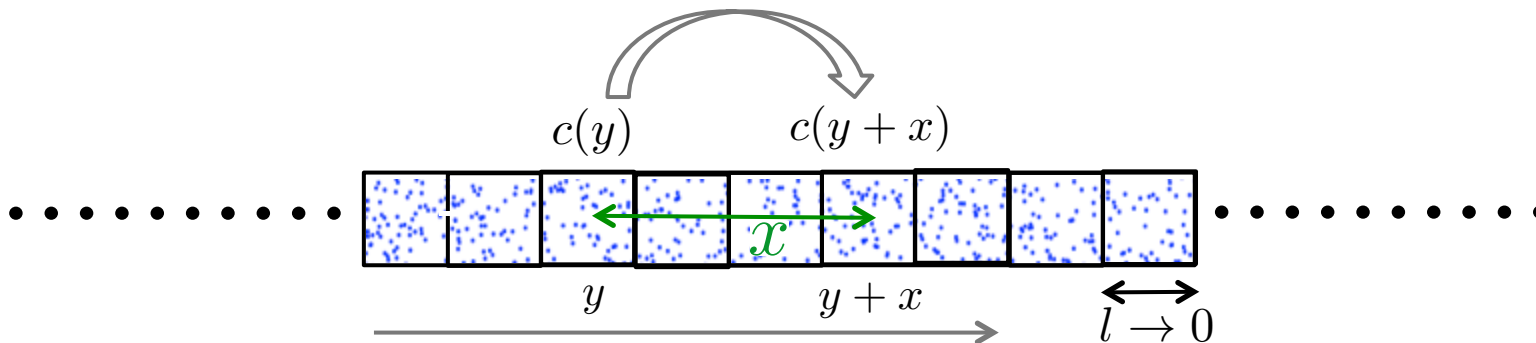
or its continuous version:

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

And define an appropriate tool to study spatial correlations:

the centered correlations without self-contribution

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



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:

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

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

**d-dimensional Laplacian
(diffusion term)**

with $r = |x - y|$

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

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:

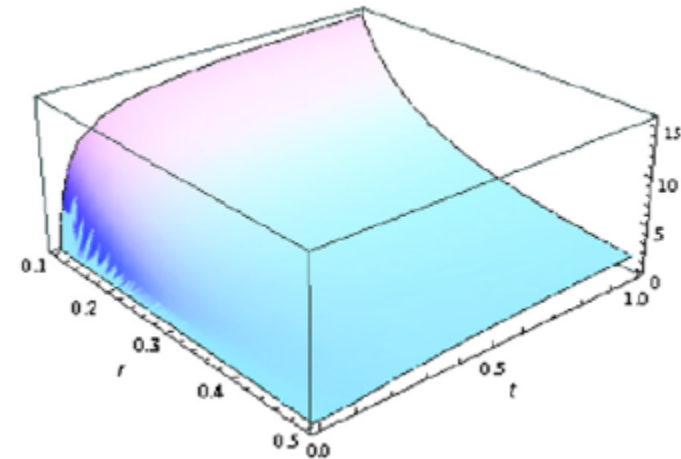
$$c_t(\mathbf{X}) = c_0 \quad (\text{for all } t)$$

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

$$g_t(r) = \frac{\lambda v_2}{8Dc_0\pi^{3/2}r} \Gamma\left(\frac{1}{2}, \frac{r^2}{8Dt}\right)$$

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

Amplitude $\propto \frac{\lambda v_2}{Dc_0}$



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

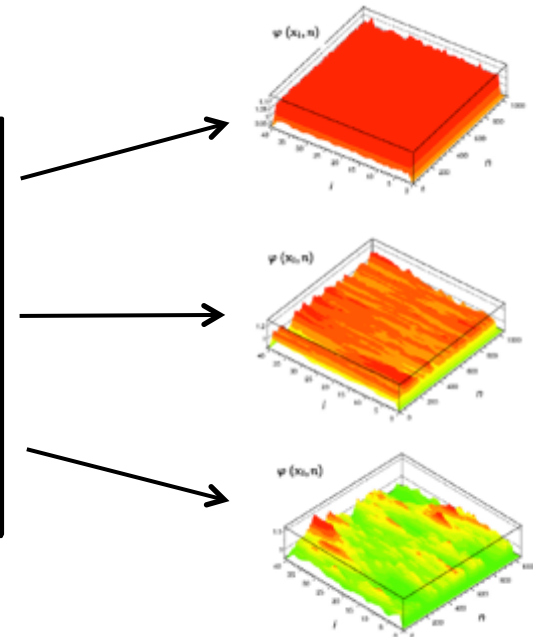
Consequence 1: Convergence criteria

Typical separation between particles: $\ell = \sqrt{\langle r_a^2 \rangle}$

Number of particles to suppress clustering: $N_0 \Rightarrow N_0 \gg (L/\ell)^3$

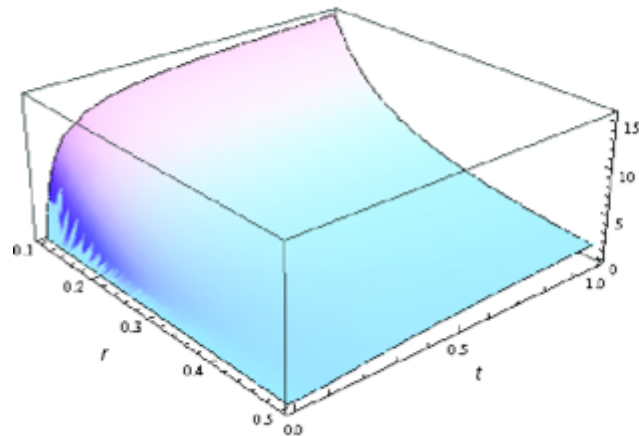
Let's go back to the pincell test-case: $\ell \simeq 6 \text{ cm}$ and $N = 10^4$ (# particles simulated)

$L = 10 \text{ cm}$	$N_0 \simeq 4$	$N \gg N_0$
$L = 100 \text{ cm}$	$N_0 \simeq 5 \cdot 10^3$	$N \simeq N_0$
$L = 400 \text{ cm}$	$N_0 \simeq 3 \cdot 10^5$	$N \ll N_0$

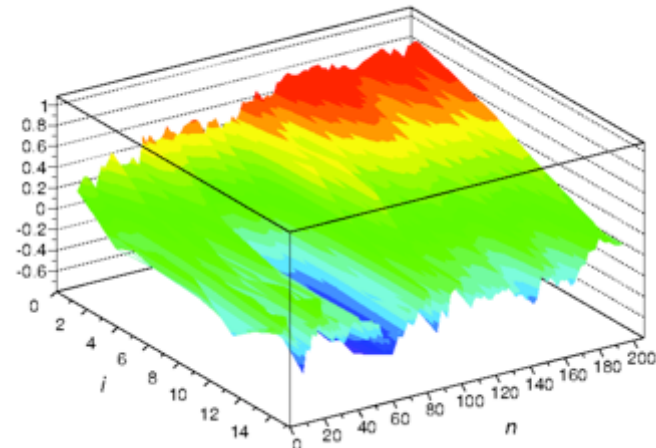


Consequence 2: Diagnostic tool

2-points correlation function versus (r,t) for the 3-d analytical function (i,n) for the TRIPOLI-4® simulation of the pincell (i is the bin number)



« theory »



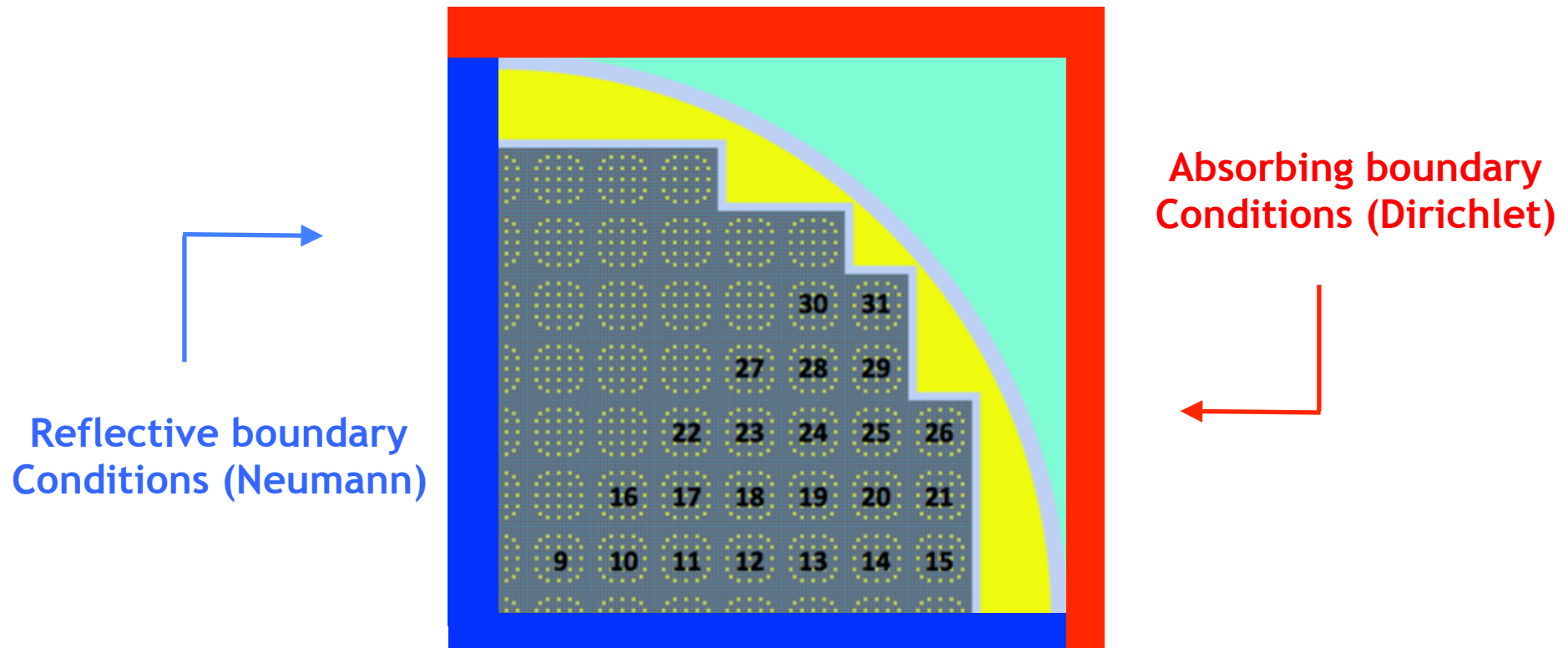
« MC criticality simulation »
clustering diagnostic tool in TRIPOLI-4®:
histogram of inter-collisions distances

- ⇒ very good agreement
- ⇒ **saturation** of the 2-points estimator
in the MC simulation

Traveling waves

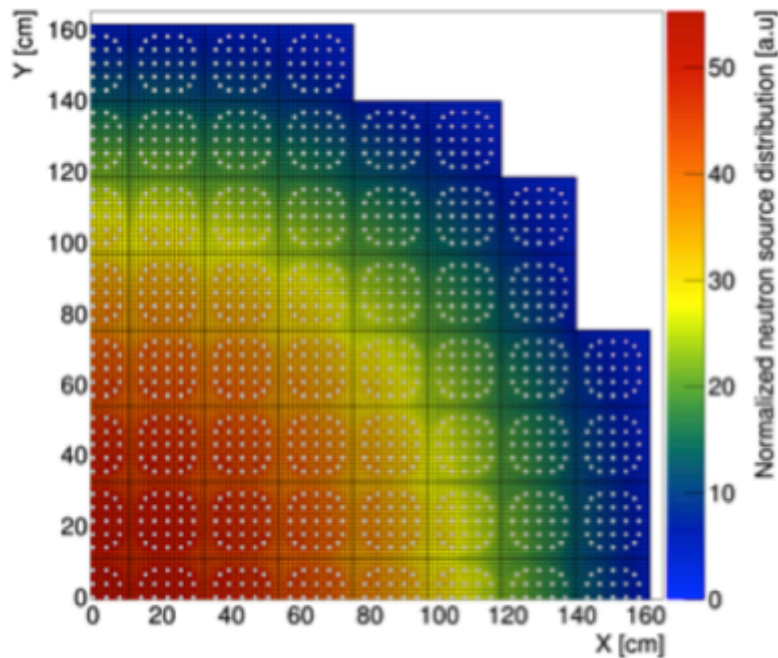
OECD/NEA R1 Benchmark

- ❑ Expert Group on Advanced Monte-Carlo Techniques @ OECD/NEA
- ❑ R1 **Benchmark** = 1/4 PWR-type reactor core
- ❑ Designed to understand **biases on local tallies** estimates (+uncertainties)



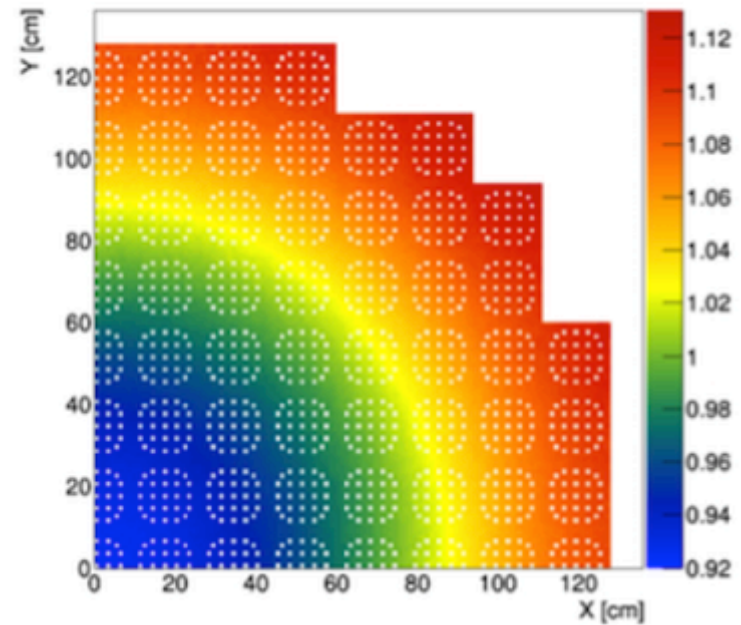
MORET Simulation of the R1 benchmark

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



Fluxes (10^6 active cycles of 10^2 neutrons)

Fluxes (10^2 active cycles of 10^6 neutrons)



Under-estimation inside the core, over-estimation for the outer assemblies

1-D binary branching Brownian motion

- Uniform material, mono-energy, leakage bc
- Brownian motion with diffusion coefficient D [$\text{cm}^2.\text{s}^{-1}$]
- undergoes collision at Poissonian times with rate $\beta + \gamma + \lambda$ [s^{-1}]
- at each collision, k descendants with probability $p(k)$
- total number of particles N kept constant

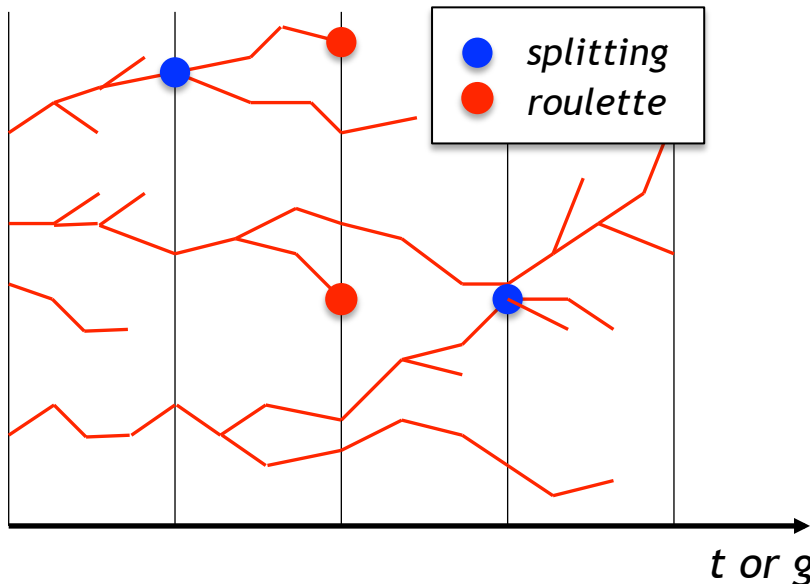
$$\langle x^2(t) \rangle = Dt$$

$$p(0) \propto \gamma$$

$$p(1) \propto \lambda$$

$$p(2) \propto \beta$$

Population control algo. to keep N constant



Branching Brownian motion with population control couples:

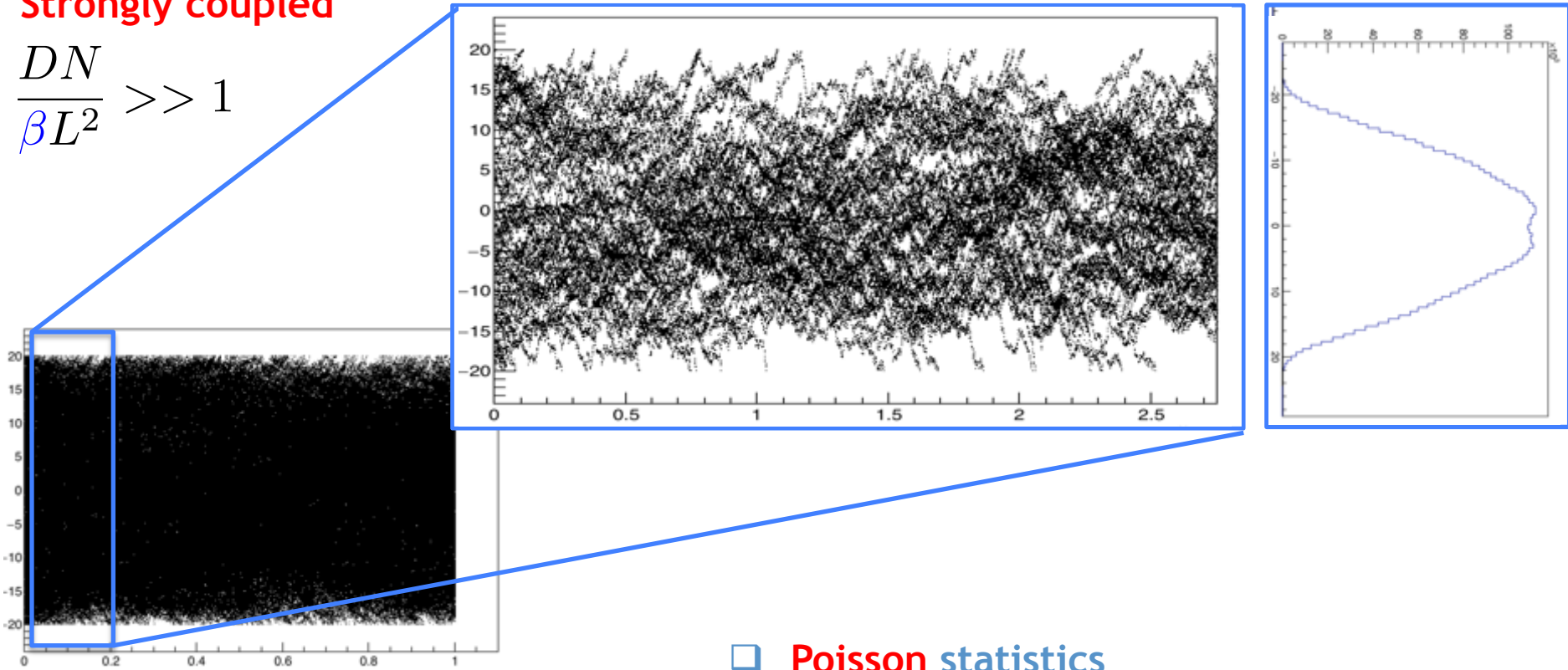
- ⇒ Galton-Watson birth-death process to describe fission and absorption
- ⇒ Brownian motion to simulate neutron transport
- ⇒ Population control that reproduces the end of cycle renormalization of MC criticality codes

- ❑ 1-D BBM with population control
- ❑ Uniform initial distribution

- ❑ 50 neutrons
- ❑ $[-L, L]$ Dirichlet

Strongly coupled

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



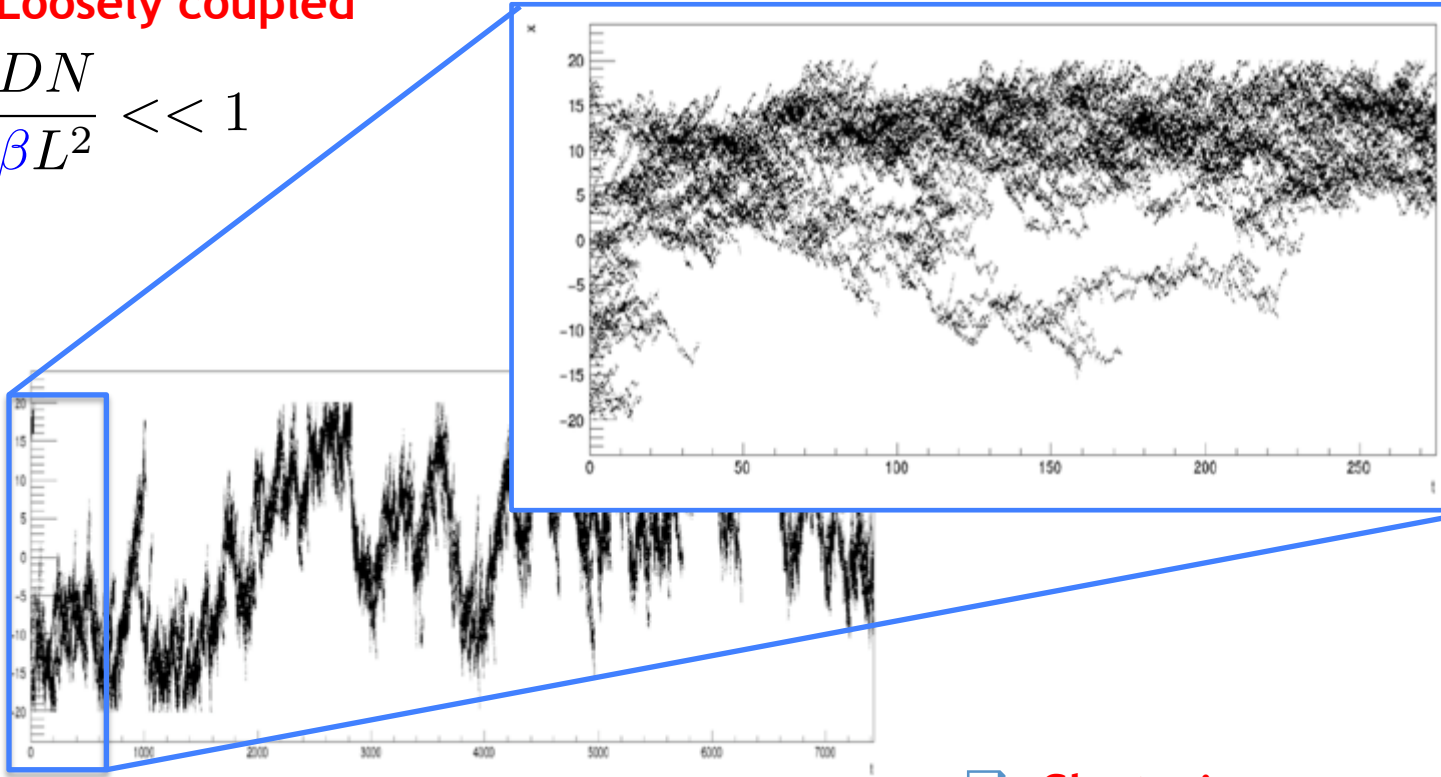
- ❑ Poisson statistics
- ❑ Cosine shape

- ❑ 1-D BBM with population control
- ❑ Uniform initial distribution

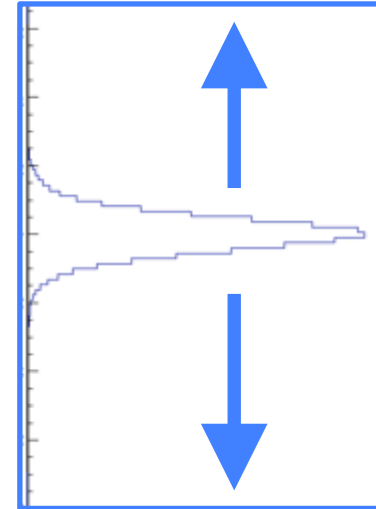
- ❑ 50 neutrons
- ❑ $[-L, L]$ Dirichlet

Loosely coupled

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



Reflection due to $N=\text{constant}$!

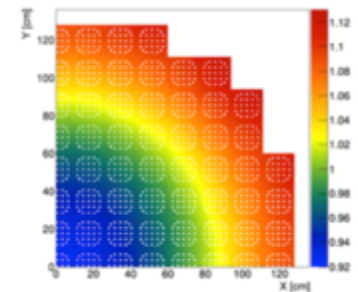
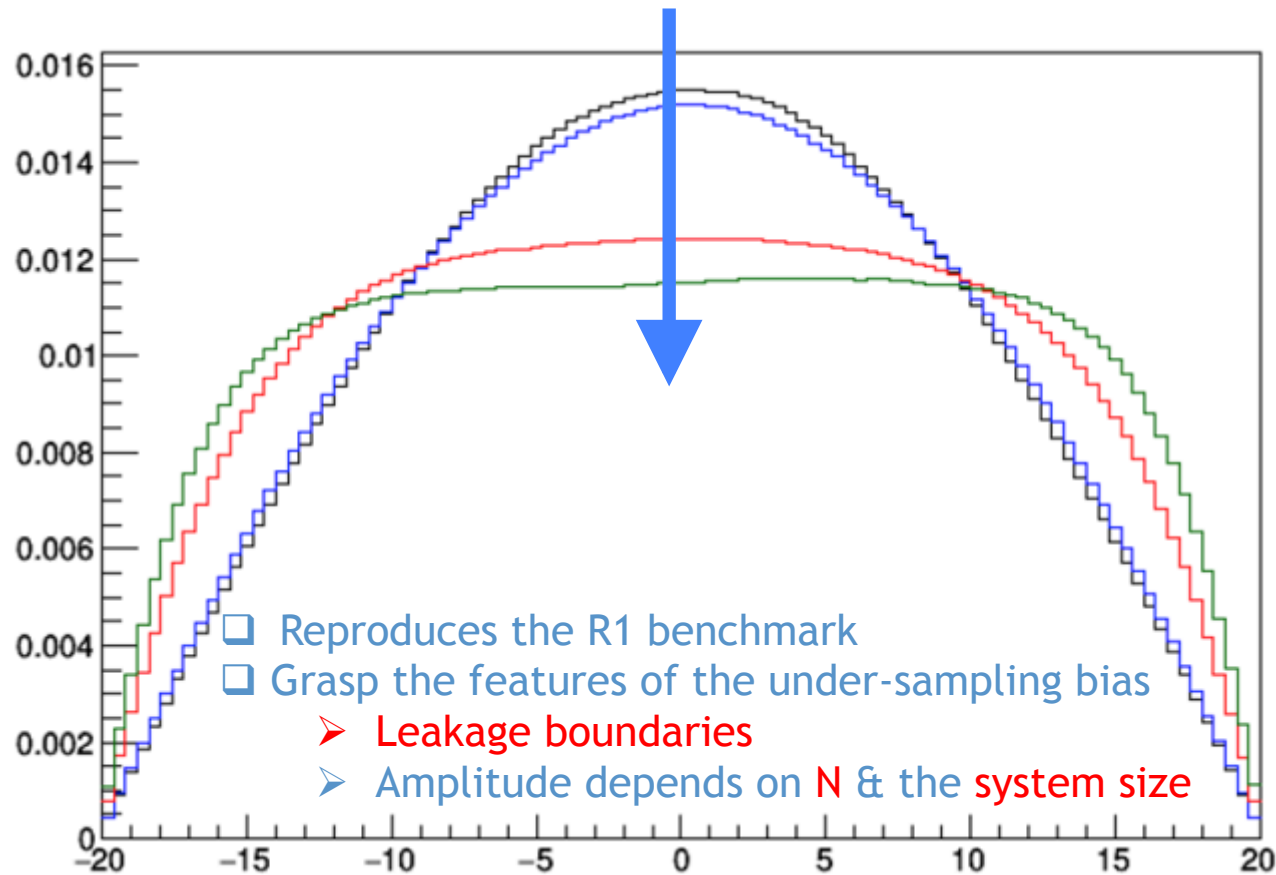


Reflection due to $N=\text{constant}$!

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

How do these processes average through time ?

From strongest to lousiest coupled systems



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 ?

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

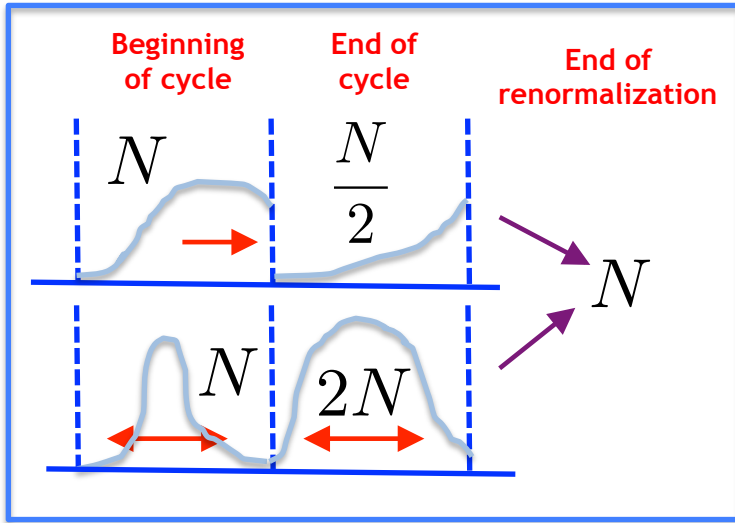
Diffusion operator
(same demonstration for transport)

Fission rate

Capture rate

Fission/Capture vs Splitting/Russian Roulette

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



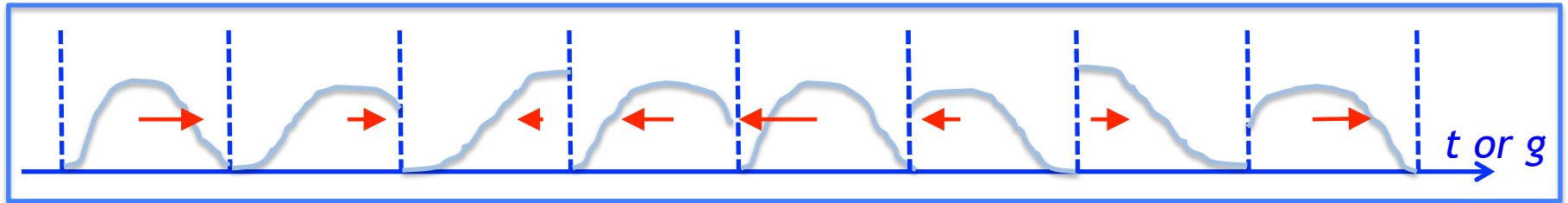
$$f(N)N$$

$$\beta^* N \leftarrow \beta N$$

$$\gamma^* N \leftarrow \gamma N$$

renormalization rate depends on N and t/g

$$\lambda(t)N$$



Pair interactions

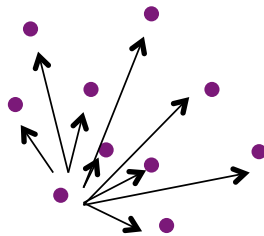
But how many neutrons do we remove/split at the end of each cycle and how to select them ?

renormalization rate depends on time and N !

$$\lambda(t) \underbrace{f(N) N}$$

$$(N - 1) N$$

$$\rightsquigarrow N^2$$



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

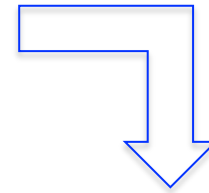
$$\lambda(t) \int dy \underbrace{G(x, y, t)}_{\text{number of pairs}}$$

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 $N(x)$

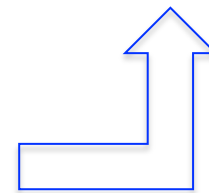
Diffusion with pair interactions

$$\partial_t \phi = D \nabla^2 \phi + (\beta - \gamma) \phi \left. \vphantom{\partial_t \phi} \right\} \begin{array}{l} \\ + \text{pair interactions} \end{array}$$



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

$$G(x, y, t) = \left[1 + g(x, y, t) \right] \phi(x) \phi(y) \left. \vphantom{G(x, y, t)} \right\} \begin{array}{l} \\ g(x, y, t) \text{ spatial correlation function} \end{array}$$



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

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)

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

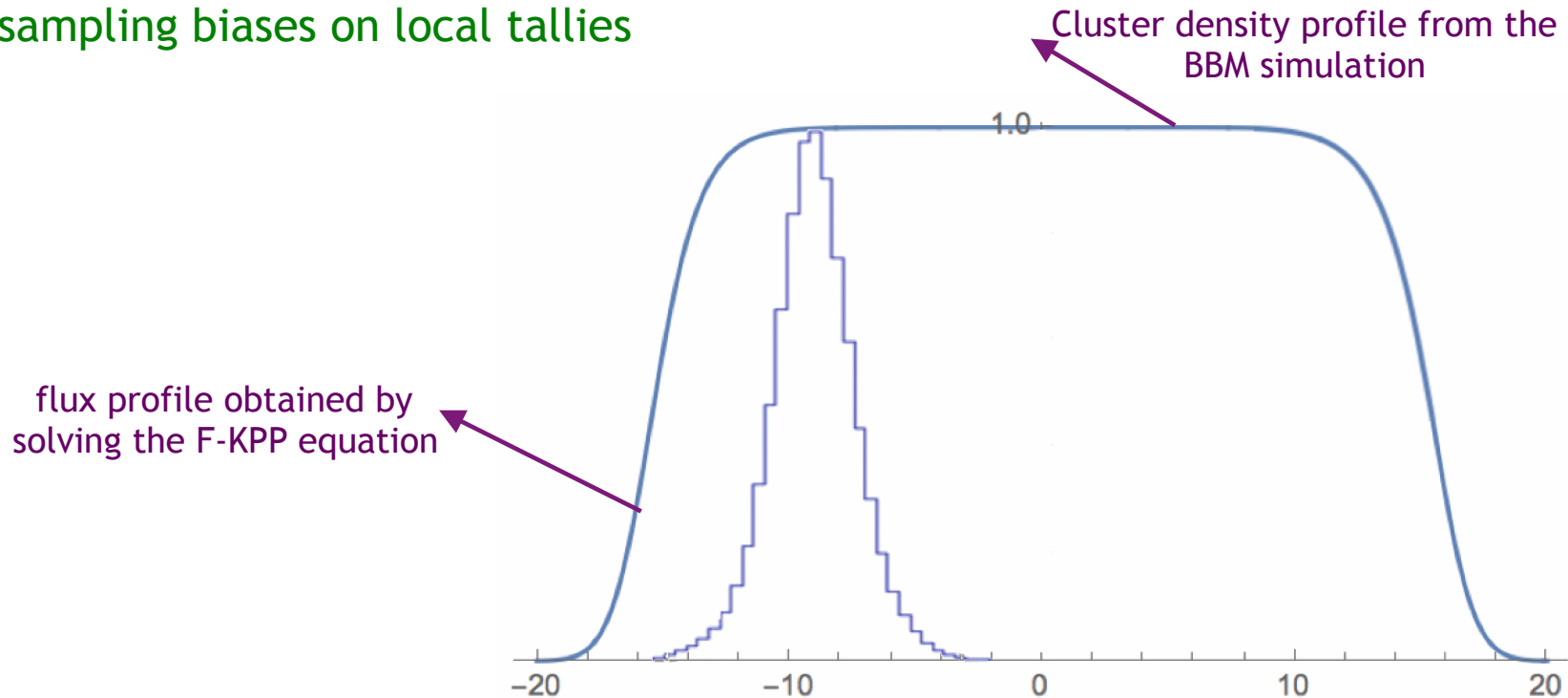
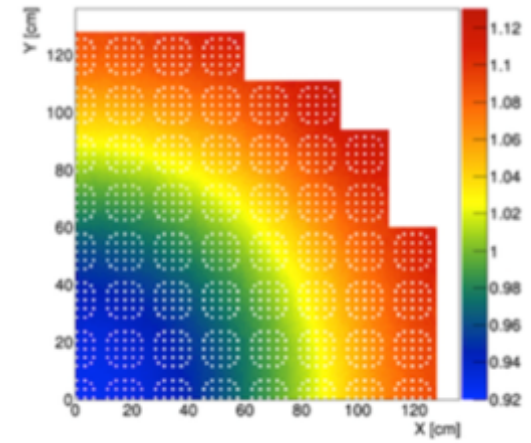
$$\phi(x, t) = \frac{1}{\left(1 + C \exp^{\pm \frac{1}{6} \sqrt{6(\beta - \gamma)} x - \frac{5}{6} (\beta - \gamma) t} \right)^2}$$

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

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

Traveling wave & solitons

- ❑ Flux 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
- ❑ Qualitative & Quantitative scheme to explain **under-sampling biases on local tallies**

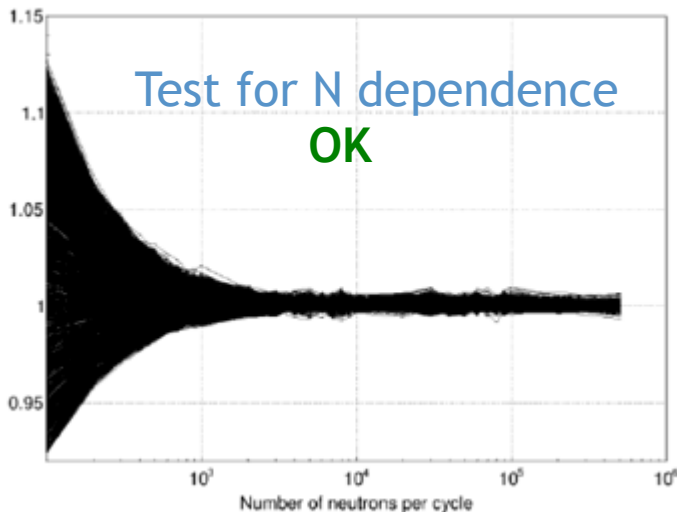
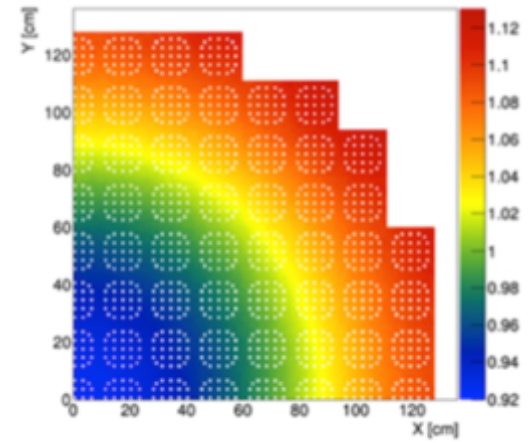


Back to the under-sampling bias

- Under-sampling bias due to combination between **clustering + population control + bc**
- Parameters controlling the amplitude of the under-sampling bias are linked to the spatial correlation function:

$$|g_c(x_i, x_j, t)| \leq \frac{\lambda \nu_2}{N} \frac{2}{3} \frac{L^2}{D}$$

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



- N
- Total reaction rate
- Typical size of the system
- Diffusion coefficient
- Second moment of the descending factorial of $p(z)$

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

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

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

Large population size

Flux factorized out of the integral

$$g(x, y, t) \rightarrow g_N^\infty(x, y) \gg 1$$

Small population size

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

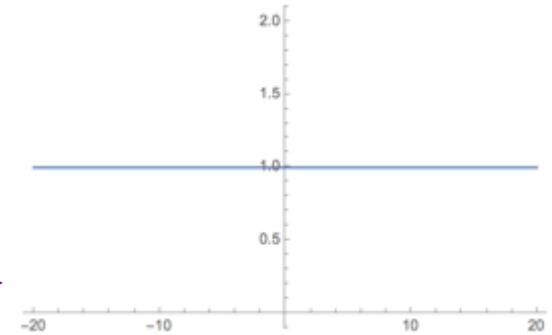
Large population size

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

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

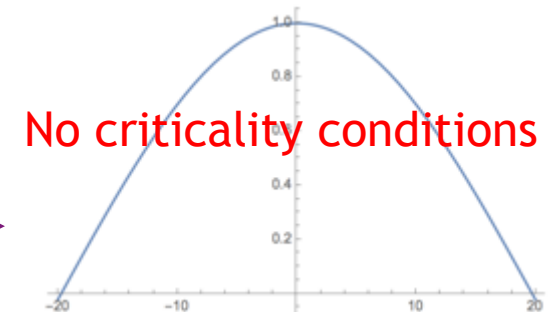
Neumann/Reflective bc

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



Dirichlet/Absorbing bc

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



No criticality conditions ;)

Experimental design

In more details

- **Size** of the reactor (the bigger, the better) => control rod insertion matters
- **Power** of the reactor (the lower, the better) => ideally different run at different power. Ability to differentiate the power “signal” (fission chains) and the following “noise” sources:
 - (alpha,n) reactions have to be simulated
 - Spontaneous fission level has to be simulated
 - Inhibition of triggering sources as much as possible (PuBe)
- Define the **time** gate width (analysis) to reveal the non-Poissonian effects
- **Spatial extension** of the measurement => detector with a spatial resolution over more than few 10 cm, or at least being able to move the detector

MORET Simulations to design the experiment

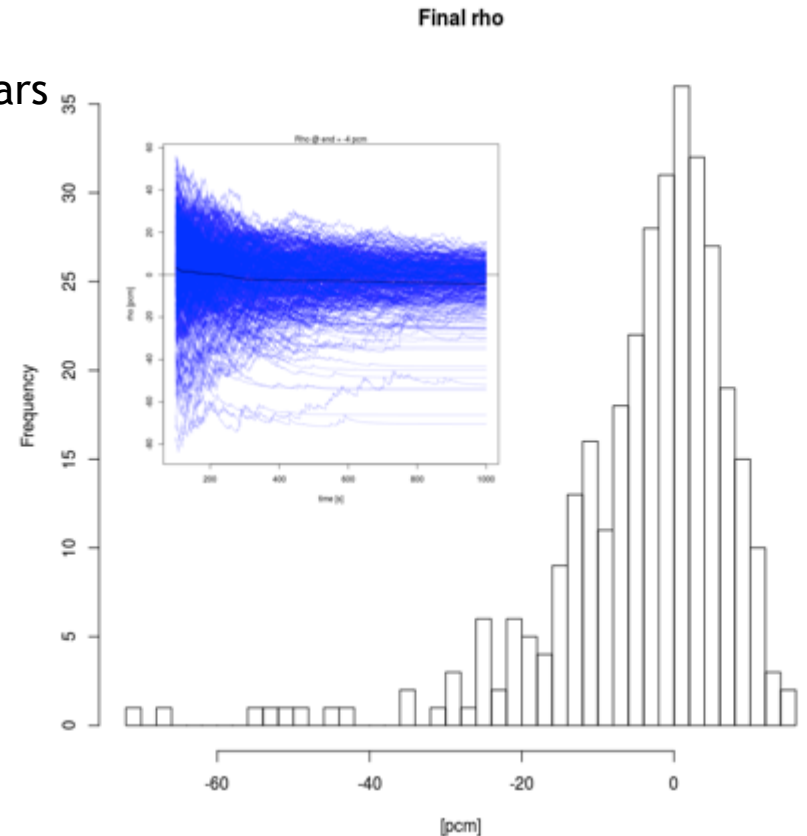
❑ MORET5 code with all Random Noise options activated:

- ❑ Data library: Endfb71
- ❑ Fission sampling:
 - ✓ Freya
 - ✓ discrete Zucker and Holden tabulated
 - ✓ Pn distributions and corresponding nubar
 - ✓ Only Spontaneous fissions

❑ Highly parallel simulations:

- ❑ Simulated signal = 1000 s (prompt+delayed)
- ❑ Number of independent simulations = 330
- ❑ Number of neutrons per simulation = $2.4 \cdot 10^4$

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



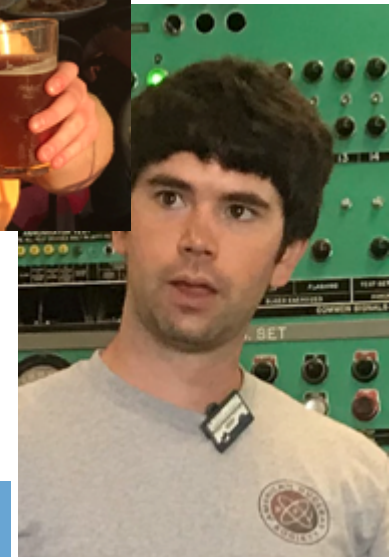
RPI Measurements 2017: Neutron clustering

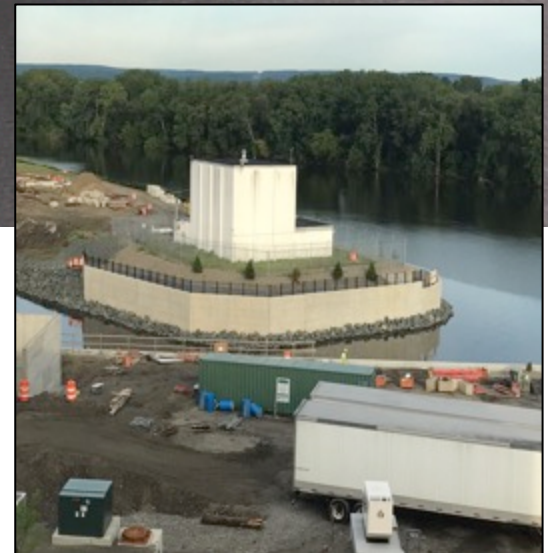


Featuring



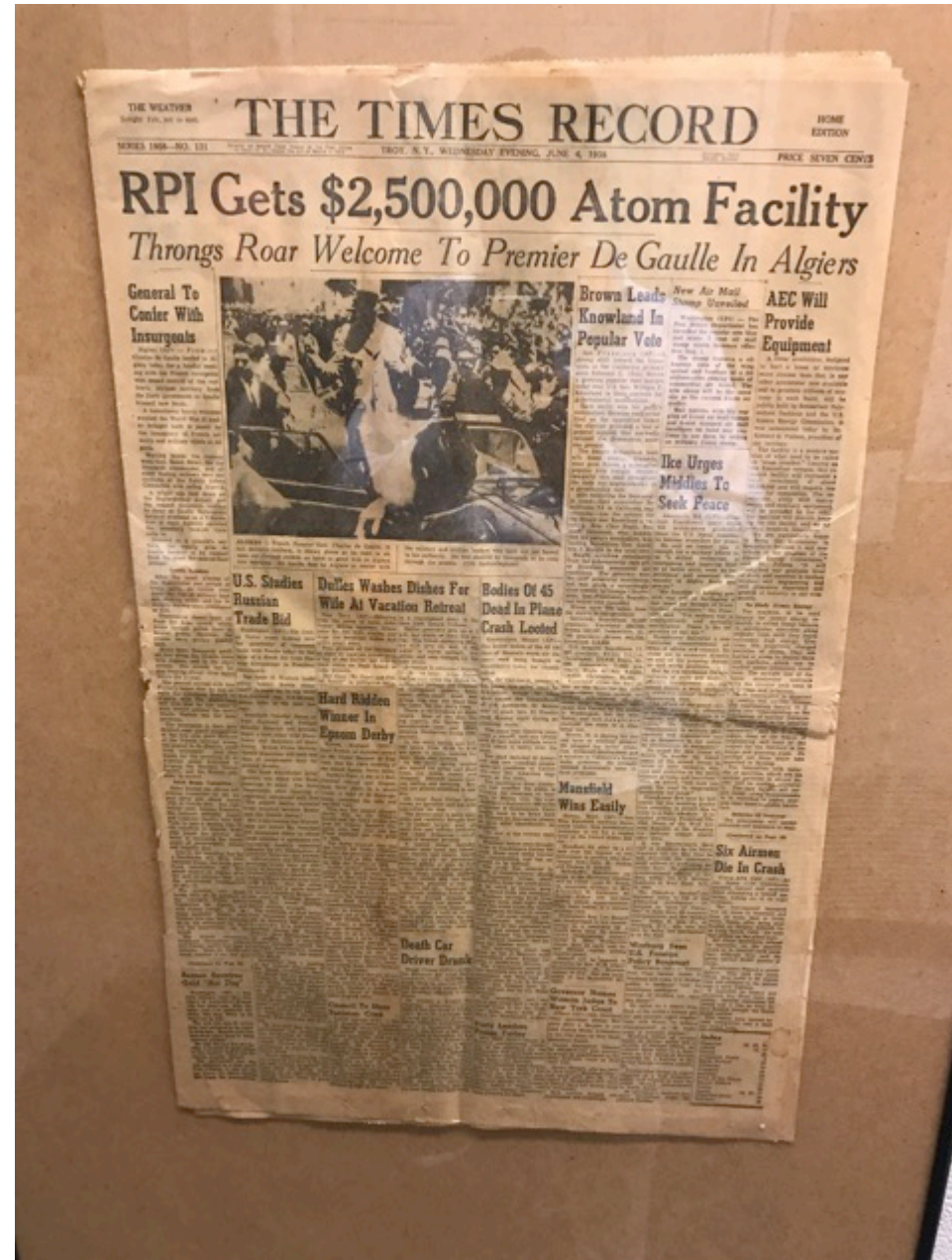
IRSN : Eric Dumonteil, Wilfried Monange
LANL: Rian Bahrn, Jesson Hutchinson,
Geordy McKenzie, Mark Nelson
RPI: Peter Caracappa, Nick Thompson,
Glenn Winters





Surprise #1 Hotel View And Rendering

Surprise #2 De Gaulle





IRSN LANL & RPI



Good moments

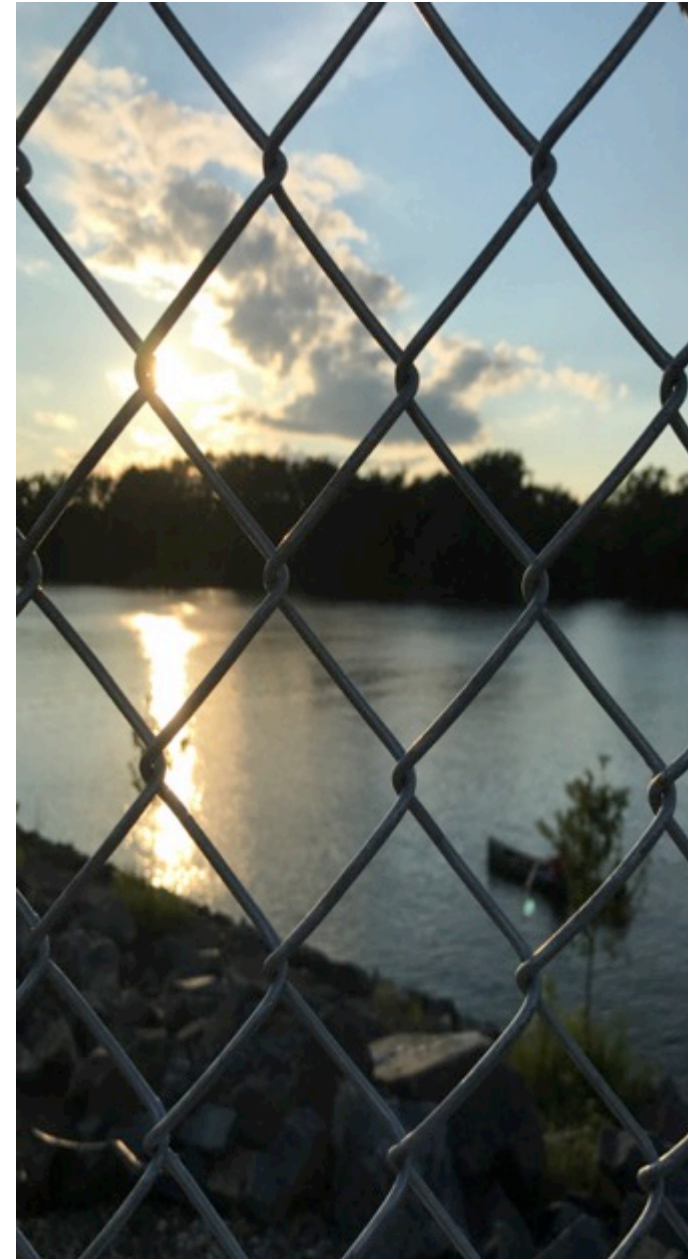


Beautiful RCF outside views

mine

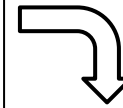


Rian's



Clustering in mathematics

Dawson, D.A., 1972. Z. Wahrsch. Verw. Gebiete 40, 125.
Cox, J.T., Griffeath, D., 1985. Annals Prob. 13, 1108.



Clustering in biology

Young, W.R., et al, 2001. Nature, 412, 328.
Houchmandzadeh, B., 2002. Phys. Rev. E 66, 052902.
Houchmandzadeh, B., 2008. Phys. Rev. Lett. 101, 078103.
Houchmandzadeh, B., 2009. Phys. Rev. E 80, 051920.



Clustering in neutronics

[Dumonteil, E., Courau, T., 2010. Nuclear Technology 172, 120.] → Observation of clusters in MC criticality simulations

Dumonteil, E. et al, 2014, Annals of Nuclear Energy 63, 612-618. → Theoretical modeling

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

De Mulatier et al, J. Stat. Mech., 15, P08021, 1742-5468 (2015) → Population control

Nowak et al, Ann. Nuc. Ener. 94, 856-868 (2015) → Consequences on MC criticality source convergence (with MIT)

Houchmandzadeh et al, Phys. Rev. E 92 (5), 052114 (2015) → Effects of delayed neutrons

Dumonteil et al, Nuclear Energy Agency of the OECD, Paris (to be published) → OECD/NEA report

Dumonteil et al, Nuc. Eng. Tech., 10.1016/j.net.2017.07.011 (2017) → Traveling waves and biases (Jeju best papers)

Sutton, T., Mittal, A., Proceedings of M&C 2017 (Jeju) → cycles/time (Jeju best papers)