DE LA RECHERCHE À L'INDUSTRIE

www.cea.fr

NEUTRON CLUSTERING DIAGNOSTICS

Eric Dumonteil, Michel Nowak , Andrea Zoia

CEA Saclay, DEN/DM2S/SERMA/LTSD
91191 Gif/Yvette
France

OUTLINE

I. **Theoretical Background on spatial correlations and clustering**

- Context
- Clustering in Physics
- Mathematical modeling of clustering

II. Diagnostics tools

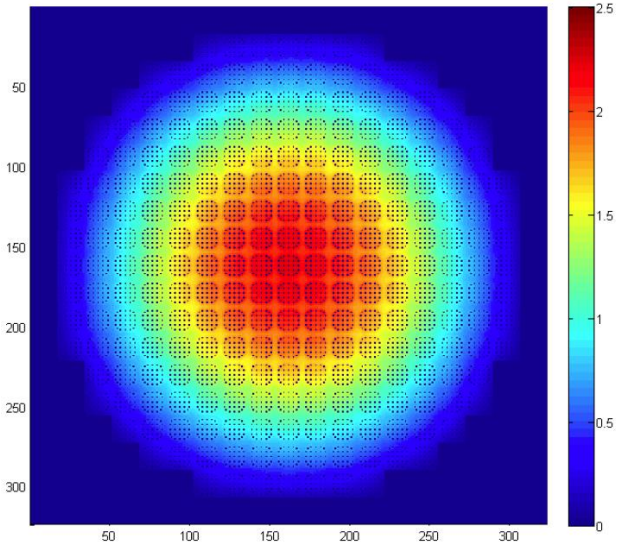
- PWR fuel rod
- Limits of Shannon Entropy
- Pair correlation function
- Center Of mass

III. Simulation Results

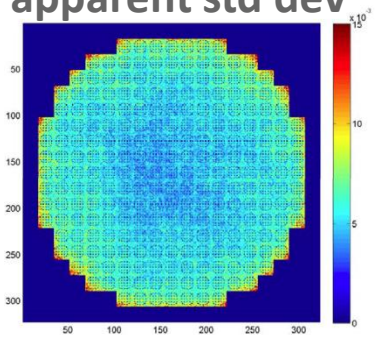
- Burnup
- Checkerboard

INITIAL MOTIVATION: BROKEN SYMMETRIES…

pin power distribution

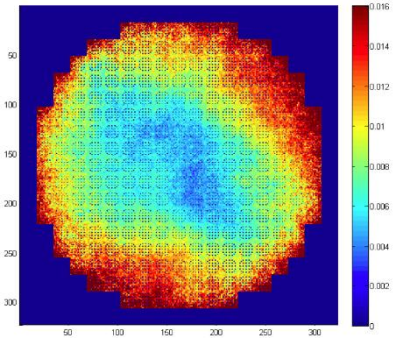


apparent std dev



[Martin, Physor2012]
[Lee et al, SNA+MC2010]

real std dev



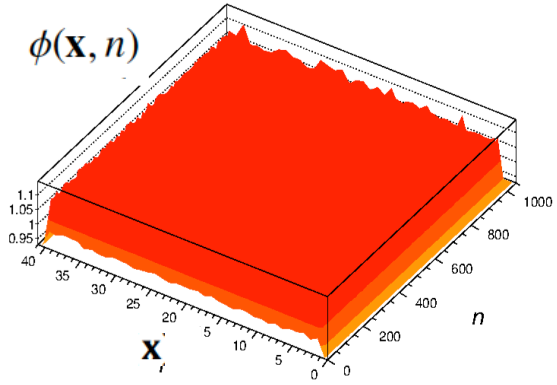
Radial (axial) power tilt in the Monte-Carlo simulation of large reactor cores:

- ❑ long standing issue (70's)
- ❑ spatial asymmetries in the flux distribution for symmetric positions
- ❑ under-estimation of variances?
- ❑ is there some physics hidden behind or is it a simulation artifact?
  - ➢ power iteration and fission source distribution ("temporal" correlations)
  - ➢ renormalization procedure [Gelbard and Prael, 1974] [Brissenden and Garlick, 1986]
- ❑ Many publications and working groups
  (NEA Expert Group on Monte-Carlo source convergence, …)
- ❑ Many diagnostic tools (entropy of fission sources, …) [Brown, Physor 2006]

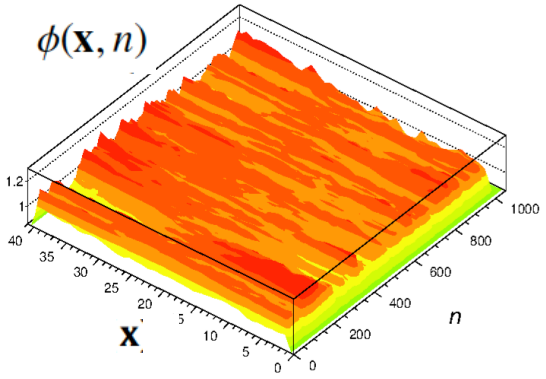
THE PWR PINCELL: INSTANTANEOUS TALLIES

$\phi(\mathbf{x}, n)$ is the "space-time" flux

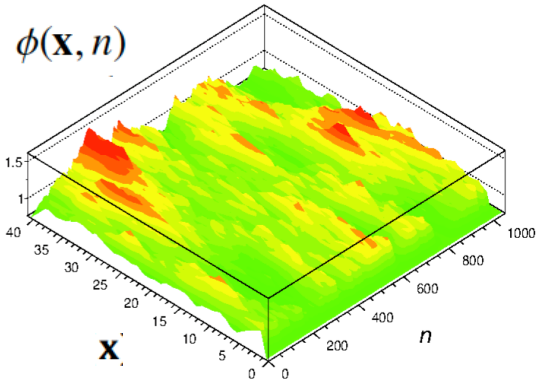
Instead of looking at integrated tallies, can we consider instantaneous tallies?



L = 10 cm



L = 100 cm



L = 400 cm

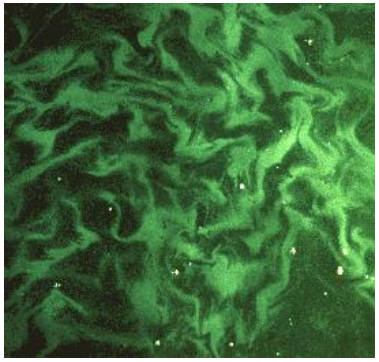
It looks like that cycle-to-cycle correlations are in fact due to spatial correlations:

"neutron clustering"

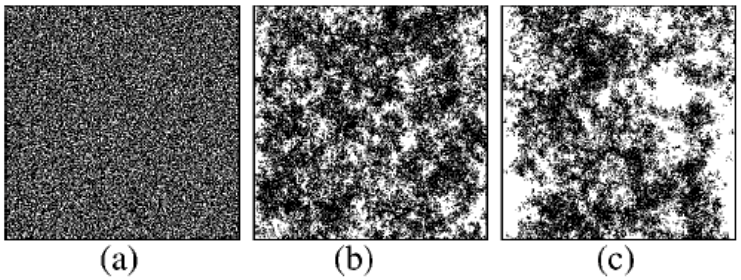
CLUSTERING IN MATHEMATICS AND IN BIOLOGY

- clustering in **theoretical ecology** [Dawson, 1972] [Cox and Griffeath, 1985]

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



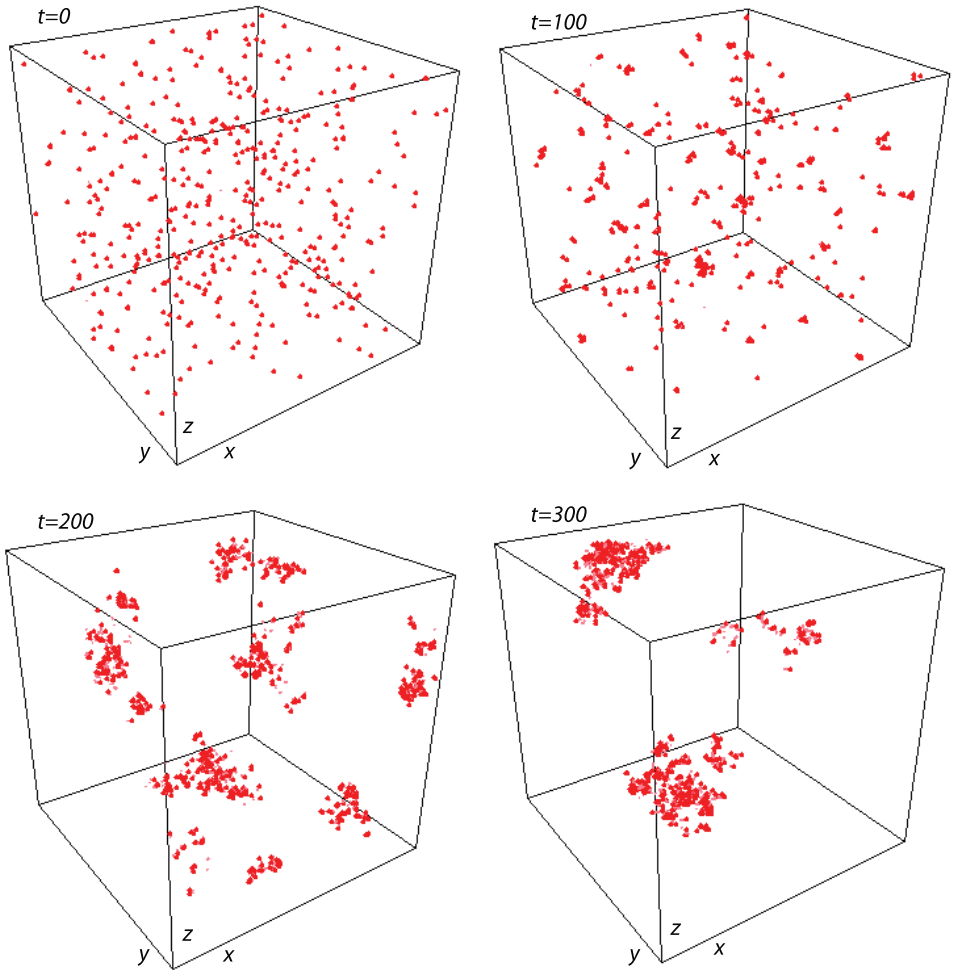
  - plankton are any organisms that live in the water column and are incapable of swimming against a current
  - they **reproduce**, **die** and are **transported** by the water (**like neutrons!**)



[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 $1/\Sigma_s \to 0$ to recover the diffusion regime
- Binary branching

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

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

Can we have a quantitative insight into this phenomenon?

BRANCHING BROWNIAN MOTION

simplified model for neutron transport in multiplicative media:

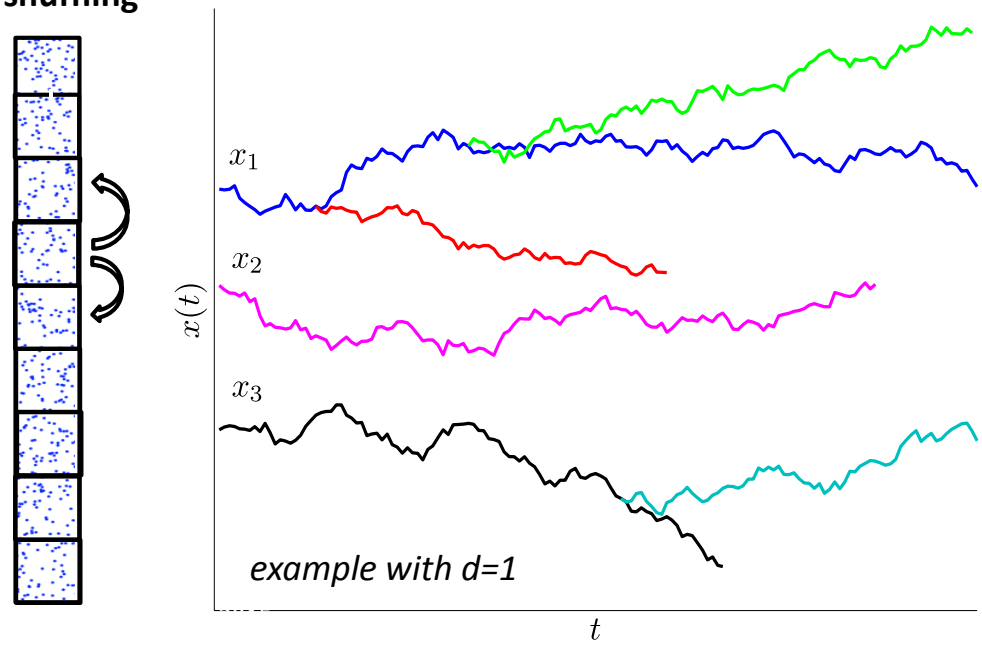
- $N_0 \to \infty$ neutrons, uniformly distributed at t=0
- infinite medium ($L \to \infty$)
- no energy dependence
- Brownian motion with diffusion coefficient D [cm².s⁻¹]
- undergoes collision at Poissonian times with rate λ[s⁻¹]
- at each collision, k descendants with probability $p(k)$
- dimension *d*

$$\left.\begin{array}{l}\\ \\ \end{array}\right\} c_0 = cte$$

$$< x^2(t) >= Dt$$

$$p(0) \leftrightarrow \Sigma_c$$
$$p(1) \leftrightarrow \Sigma_s$$
$$p(2), p(3), \ldots \leftrightarrow \Sigma_f$$
$$\nu_1 = \sum_k k p(k)$$

shuffling

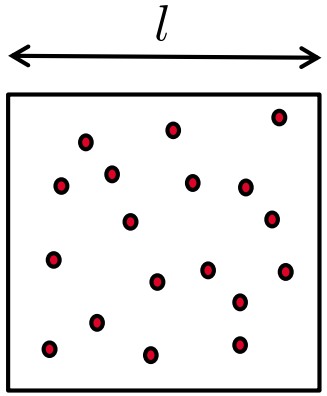


this process couples:

⇒ **Galton-Watson** birth-death process to describe fission and absorption

⇒ **Brownian motion** to simulate neutron transport

CRASH COURSE FOR CLUSTERING IN D=0



- We consider a "cell" *i* at time *t* with n individuals
- d=0 Branching **events** with:
  - production rate $\lambda p(2)$
  - disparition 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

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

$$< n(t) >= \sum_n nP(n,t)$$

$$< n^2(t) >= \sum_n n^2 P(n,t)$$

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

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

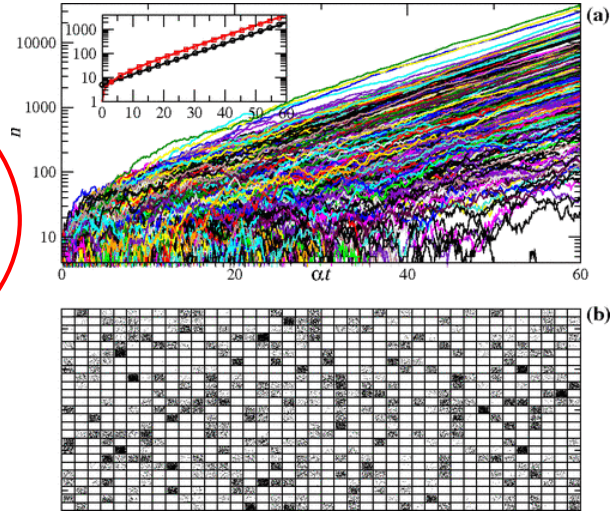
Critical:

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

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

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

[Houchmandzadeh, PRE 2008]



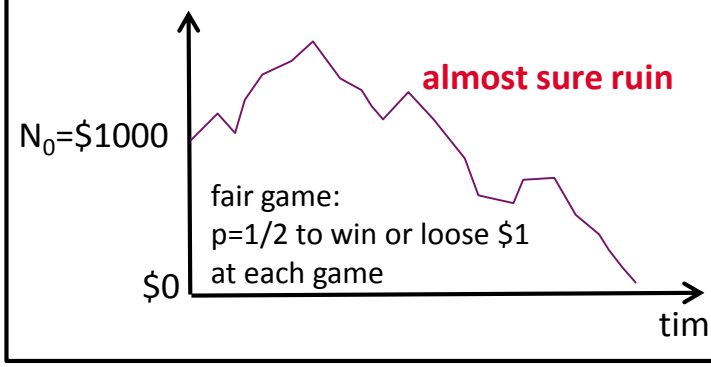
GAMBLER'S RUIN AND CRITICAL CATASTROPHY

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**

[Pascal letter to Fermat, 1656]



Fair game in neutron transport = criticality
Thus $\nu_1 = 1$ is neither representative in:
space because of **clustering**
time because of **critical catastrophe**
[Williams, 1974]

What about
fluctuations in a
given spatial position ?

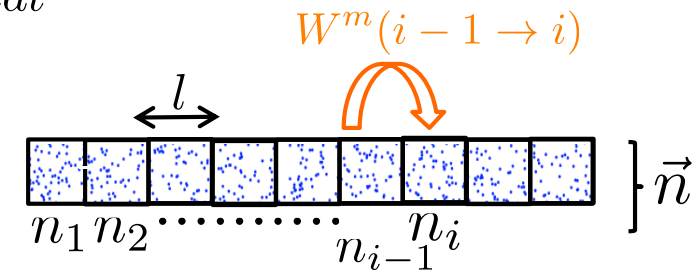
Those are due to **finite** N
(usual Monte-Carlo statistical noise)
+
Competition between neutrons produced by fission in $\mathbf{x}$ and being transported somewhere else (two spatial scales l and $L \to \infty$!)

A LITTLE BIT OF FIELD THEORY

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

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



Forward master equation

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

A LITTLE BIT OF FIELD THEORY (II)

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

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

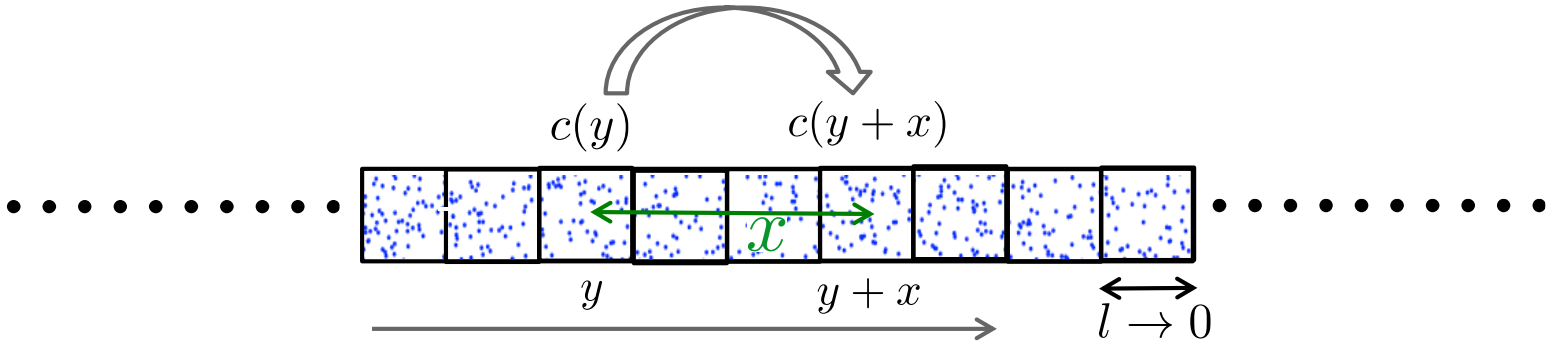
or its continuous version:

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

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:

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

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

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 via η_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.

ANALYTICAL SOLUTION TO THE EQUATION

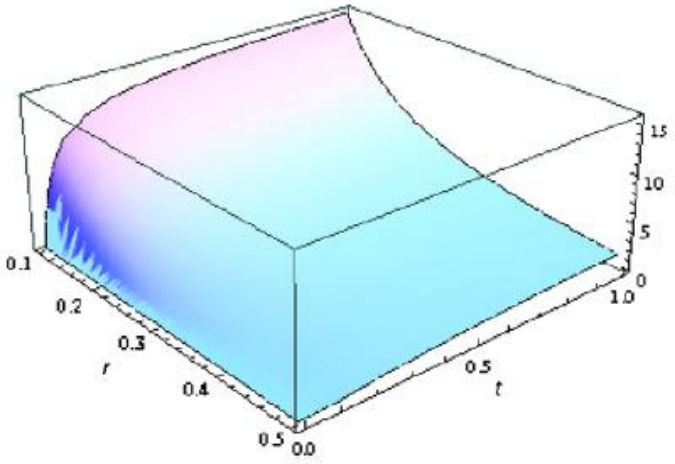
With initial condition $c_0(\mathbf{x}) = c_0$ the solution to the 1st equation is:

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

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

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

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

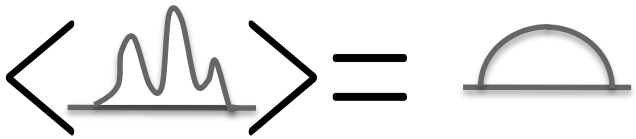


Amplitude $\mu \; I / n_2 Dc_0$

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-system systematically develops power peaks at arbitrary places!

The typical amplitude of those peaks is controlled by $\frac{\nu_2}{c_0}$

- ν_2: fission process
- c_0: different in reactor physics and MC simu

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

OUTLINE

I. Theoretical Background on spatial correlations and clustering

- Context
- Clustering in Physics
- Mathematical modeling of clustering

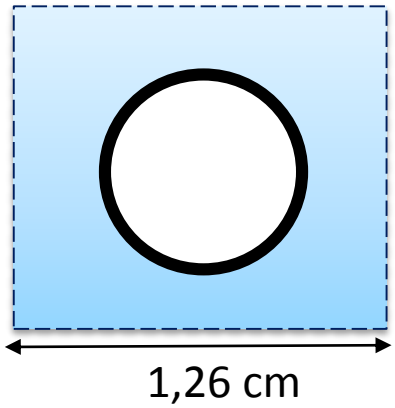
II. Diagnostics tools

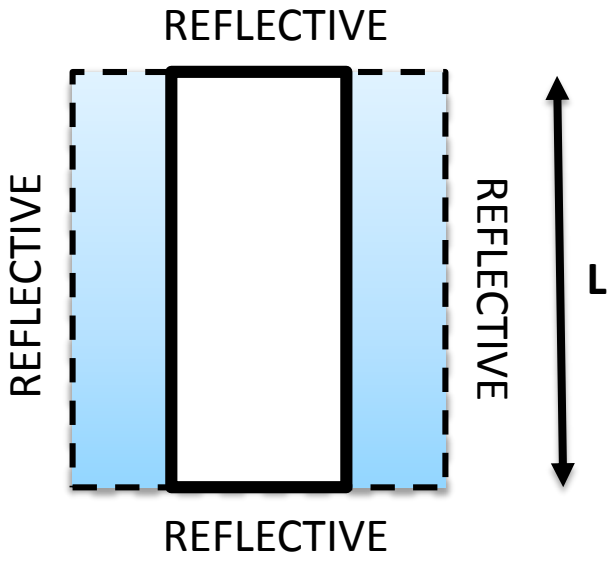
- PWR fuel rod
- Limits of Shannon Entropy
- Pair correlation function
- Center Of mass

III. Simulation Results

- Burnup
- Checkerboard

SIMPLE PWR FUEL PIN





UO_2 fuel rod :

- Enrichment 3,25%
- radius = 0,407 cm

H_20 moderator :

- pitch = 0.477 cm

Libraries : T = 300 K, ENDFB-VII.0
Initial source guess : dirac in the middle
Boundaries : Reflective everywhere
Flux Tallies 18 bins spatial mesh in z

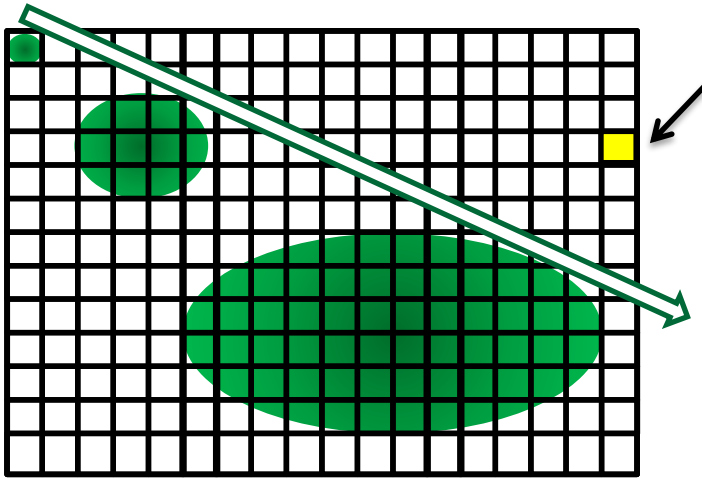
Initial source guess : dirac in the middle
Number of histories per cycle : 10 k
5000 cycles

Length

From : 20cm
To : 400 cm
Step : 20cm

SHANNON ENTROPY FAILURE TO DETECT CLUSTERING

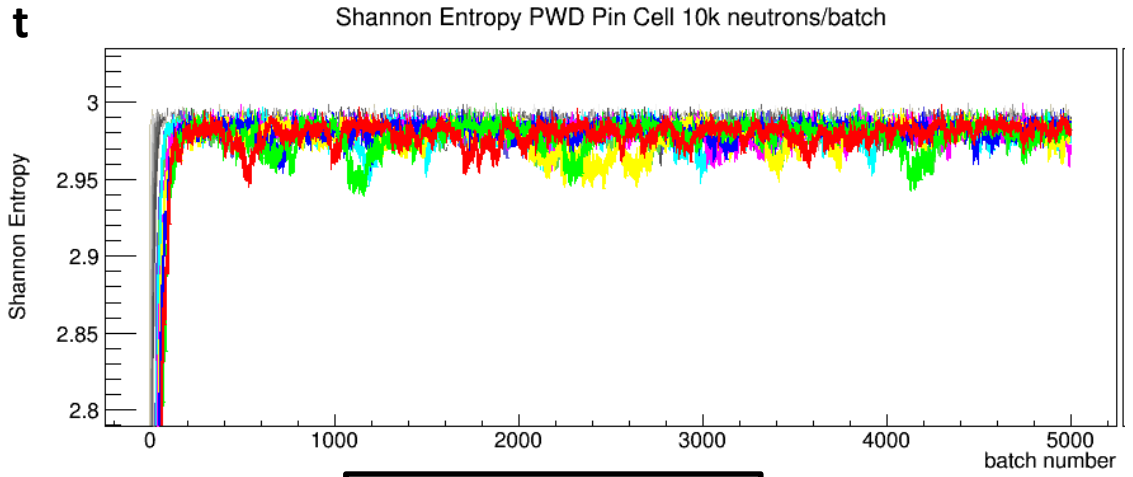
Contractions and dilatations



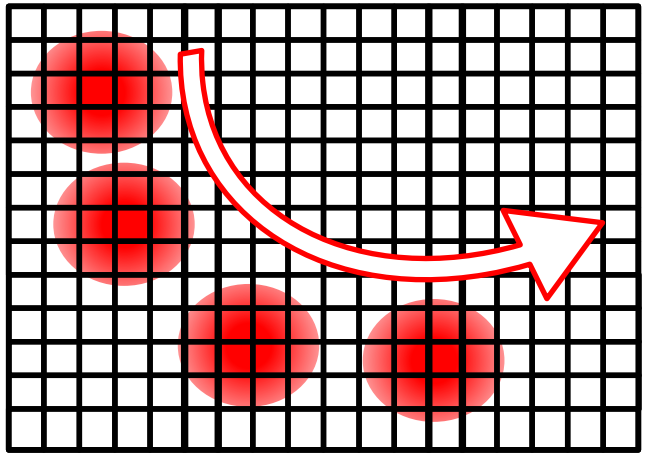
$p_i = probability\ to\ find\ particles\ in\ bin\ i$

Shannon Entropy $S = \sum_{bin\ i} p_i \log(p_i)$

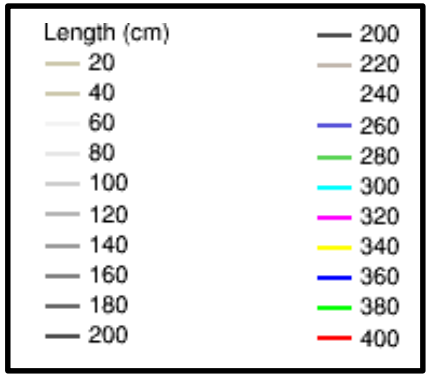
t



Constant entropy for moving cluster



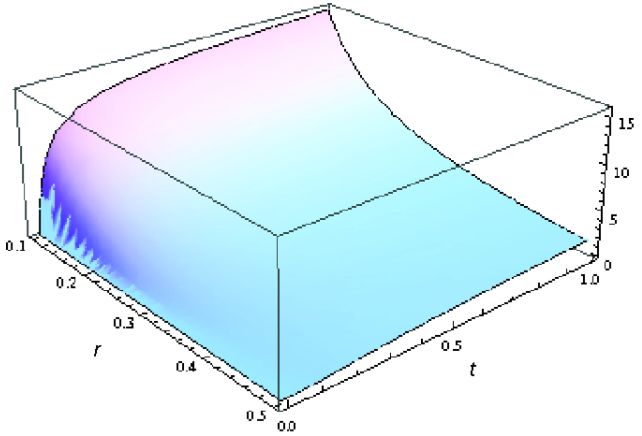
t



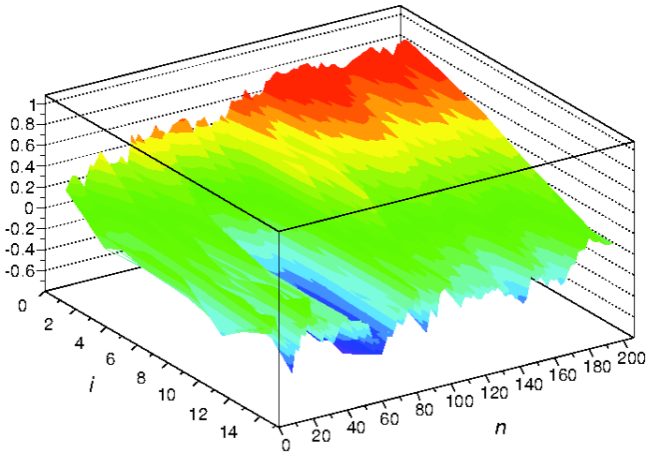
CLUSTERING DIAGNOSTIC WITH THE PAIR CORRELATION FUNCTION

« 3d analytical 2 point correlation function »

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



«Empirical correlation function on a spatial mesh for the TRIPOLI-4® MC criticality simulation of the fuel rod



⇒ very good agreement

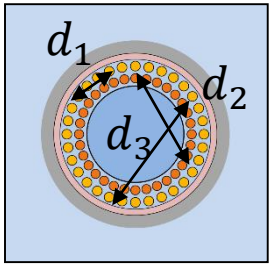
⇒ saturation of the 2-points estimator in the MC simulation

⇒ requires spatial mesh

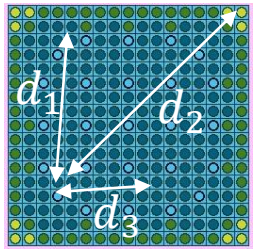
⇒ expensive in computation time

⇒ not appropriate for realistic configurations

Canadian SCWR



PWR Assembly



DISPLACEMENTS OF THE CENTER OF MASS (I)

Mass is kept constant along cycles and
Mean distance travelled by 1 particle = 1

Journal of Statistical Physics, Vol. 58, Nos. 5/6, 1990

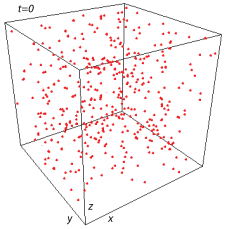
Diffusion Reproduction Processes

Yi-Cheng Zhang,[1] Maurizio Serva,[1] and Mikhail Polikarpov[2]

Received May 12, 1989; revision received September 27, 1989

Interesting physics emerges from studying a population of reproducing individuals. Each can be regarded as a random walker, but it can either duplicate or die. Novel features of the collective behavior are quite surprising: if individuals reproduce or die freely, the life expectation is proportional to the size of the population, and if it is kept constant, the center of mass moves in space as if it were a single walker (i.e., the diffusion constant is independent of population's size). Biology-inspired interactions are also considered.

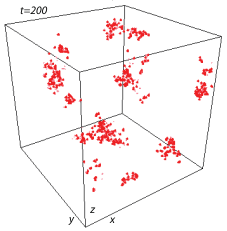
KEY WORDS: Population dynamics; fluctuation; localization.



Free gas

$$x_{MD} = \frac{1}{\sqrt{N}}$$

$$x_{MD} = 1$$

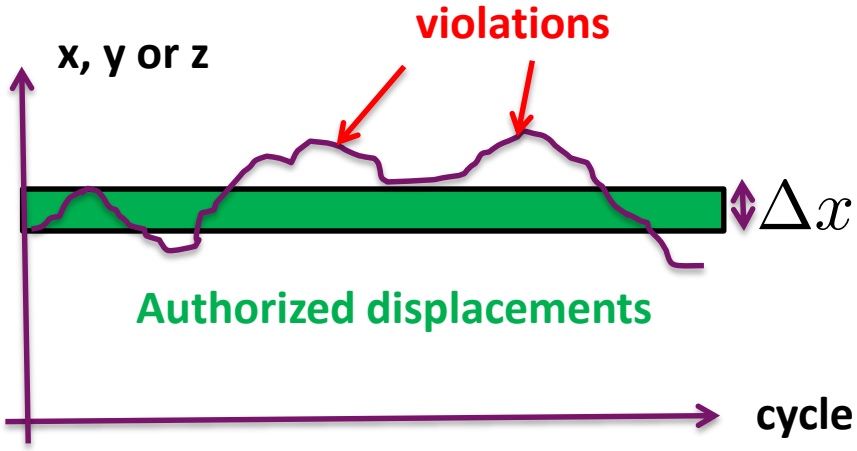


Branching gas

The center of mass of a branching gas undergoes the same diffusion law as a single particle !

DISPLACEMENTS OF THE CENTER OF MASS (II)

Idea : One can use this law to state whether a simulation is prone to develop clustering / spatial correlations



Maximum size of the system

$$x_{MD} = \frac{1}{\sqrt{N}} \Rightarrow \frac{\Delta x}{\sqrt{N}} \leq \frac{\delta l}{\sqrt{N}}$$

Displacement of the center of mass during 1 cycle

SIMPLE PWR FUEL PIN CENTER OF MASS

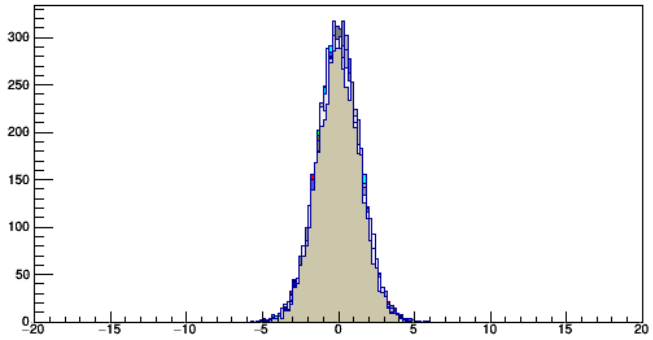
Residuals of the center of mass movements

$$residuals = \sum_{cycles} \frac{x_{com} - \overline{x_{com}}}{\sigma_{cycle}}$$

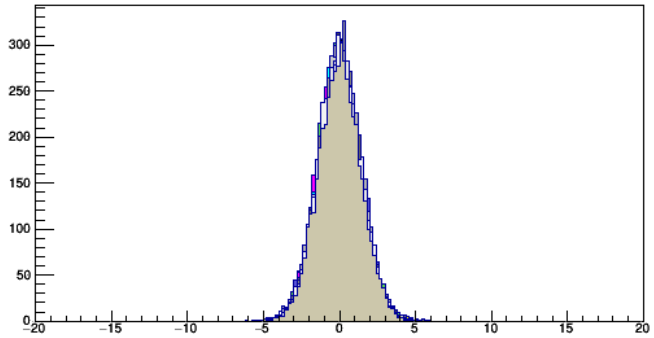
Should follow a normalized gaussian law when :

$$\sigma_{cycle} = \frac{\Delta x}{\sqrt{N}}$$

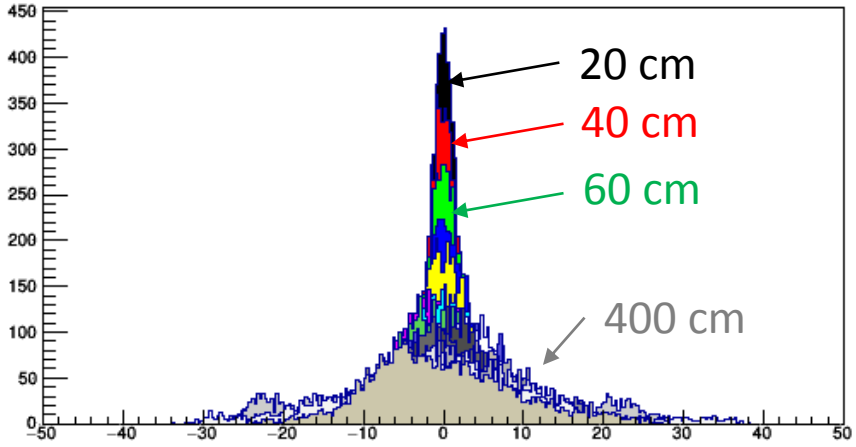
Projected on X



Projected on Y



Projected on Z



⇒ **Axial or radial studies via COM of (X,Y,Z) or (XY,Z) or (XYZ)**

⇒ **Binary answer from a scalar value (std dev of the residuals)**

⇒ **Fits very well to the physics of spatial correlations for a branching gas**

OUTLINE

I. Theoretical Background on spatial correlations and clustering

- Context
- Clustering in Physics
- Mathematical modeling of clustering

II. Diagnostics tools

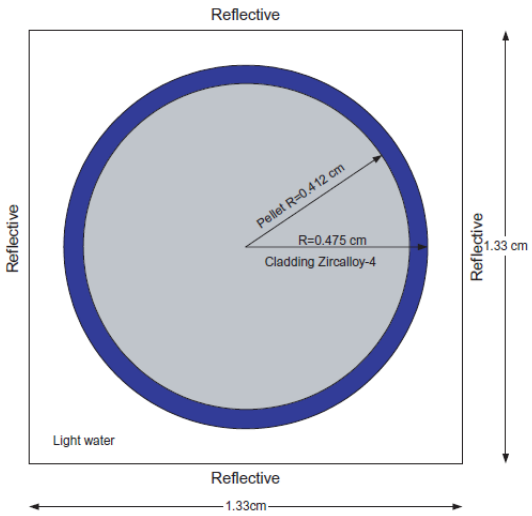
- PWR fuel rod
- Limits of Shannon Entropy
- Pair correlation function
- Center Of mass

III. Simulation Results

- Burnup
- Checkerboard fuel storage

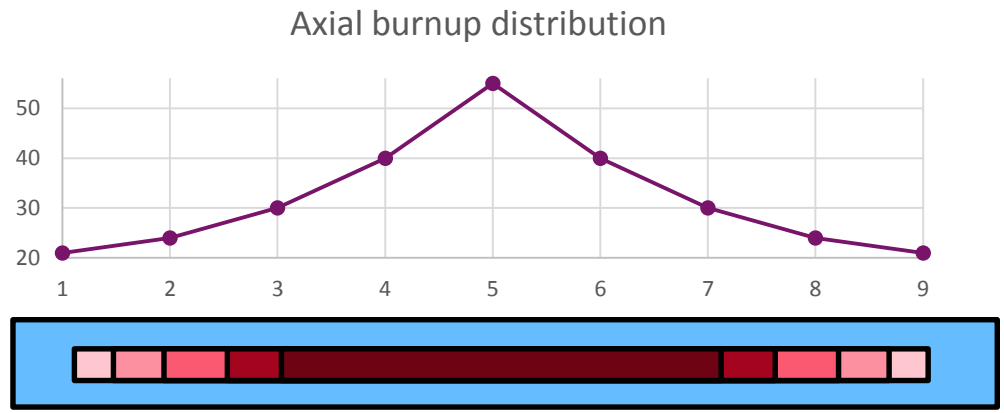
SIMPLE PWR FUEL PIN WITH DIFFERENT BURNUPS CENTER OF MASS

[source convergence benchmark OECD NEA ISBN 92-64-02304-6]

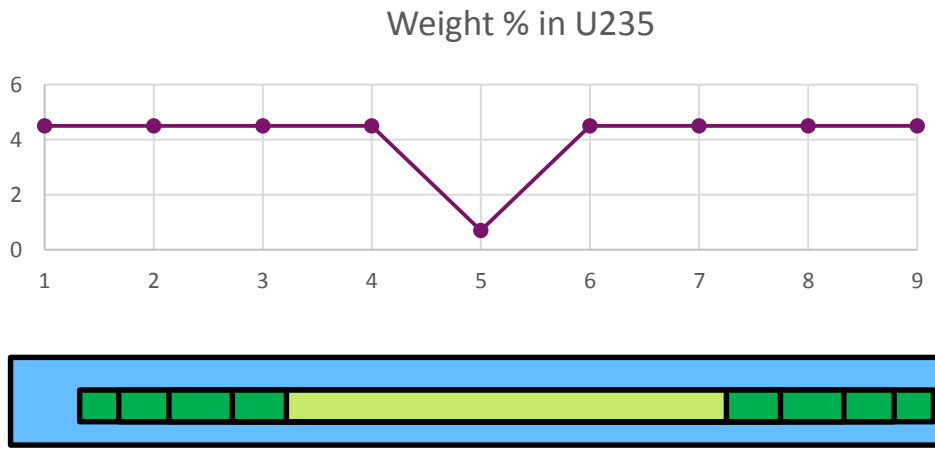


10,000 histories per cycle

Case 1-1

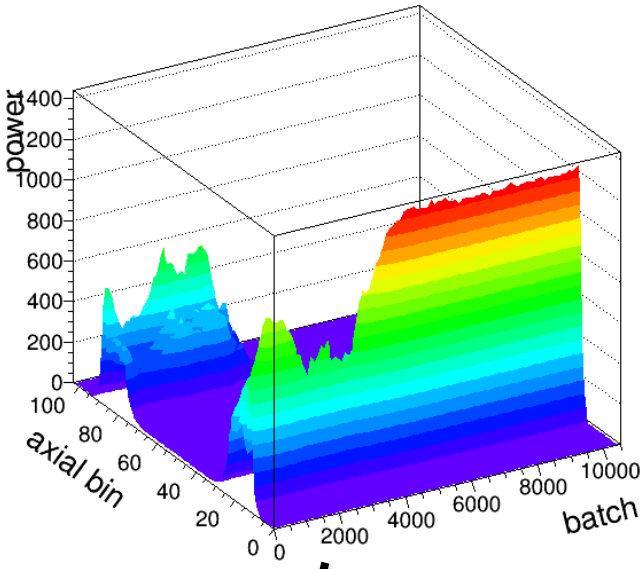


Case 2-1

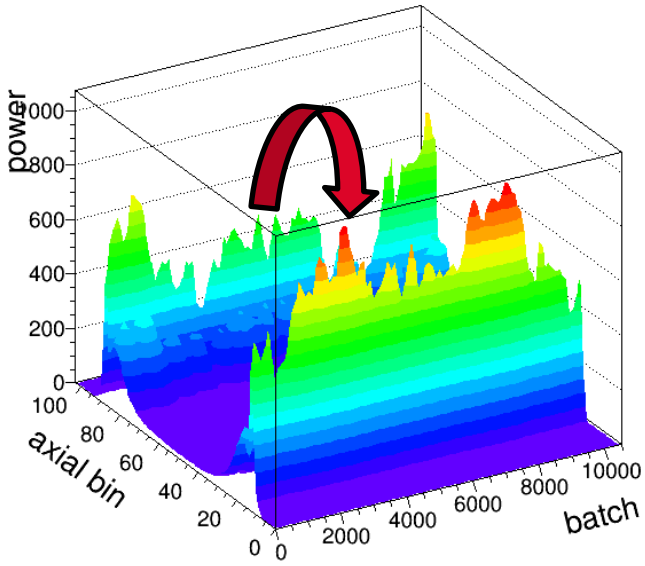


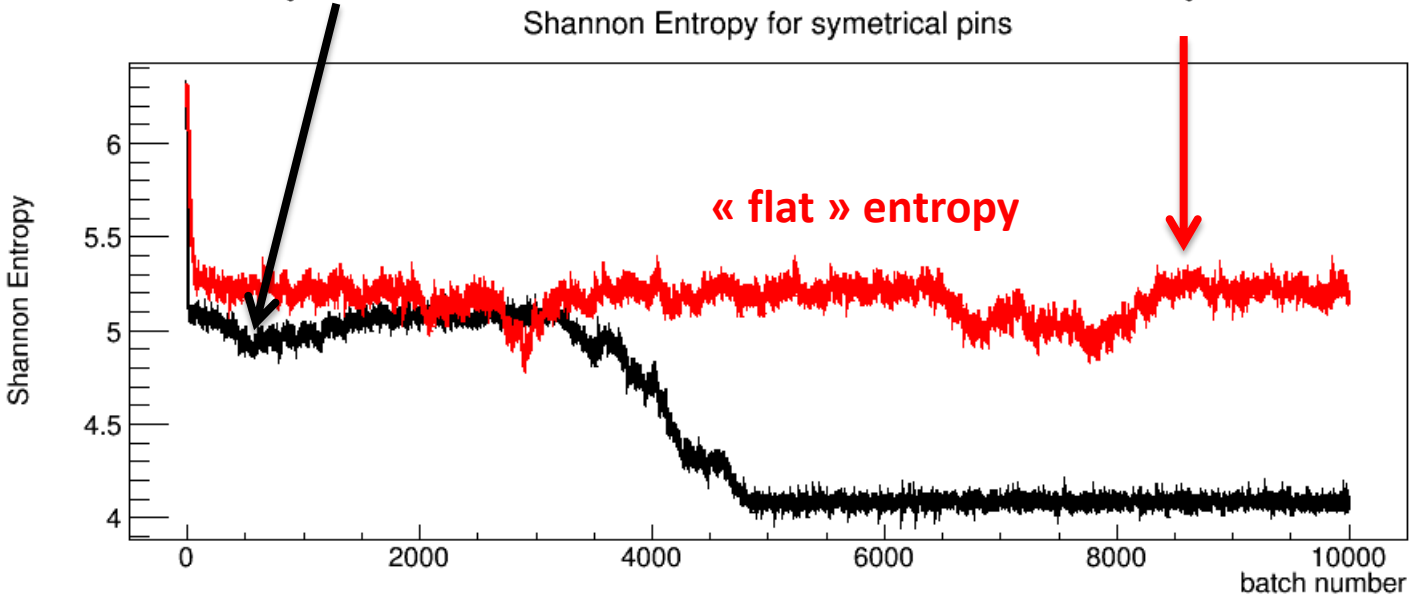
UNCOUPLED FUEL PINS
ENTROPY

Case 1-1



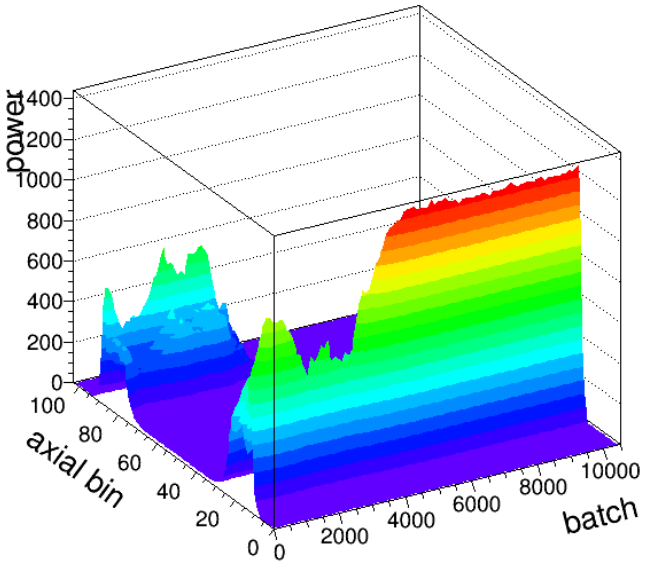
Case 2-1



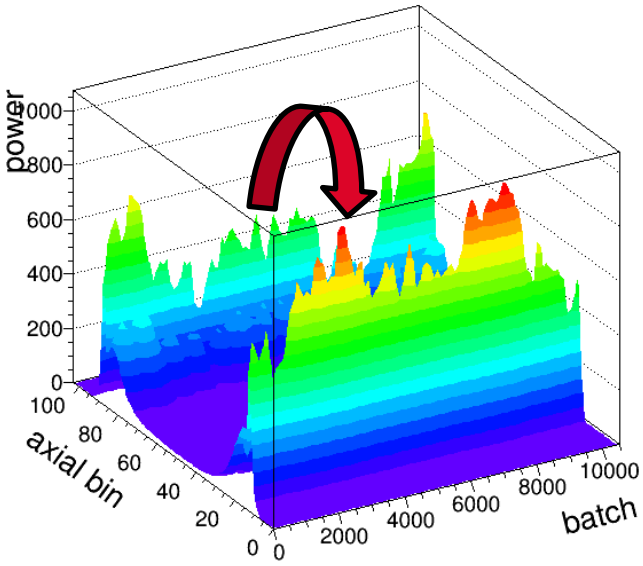


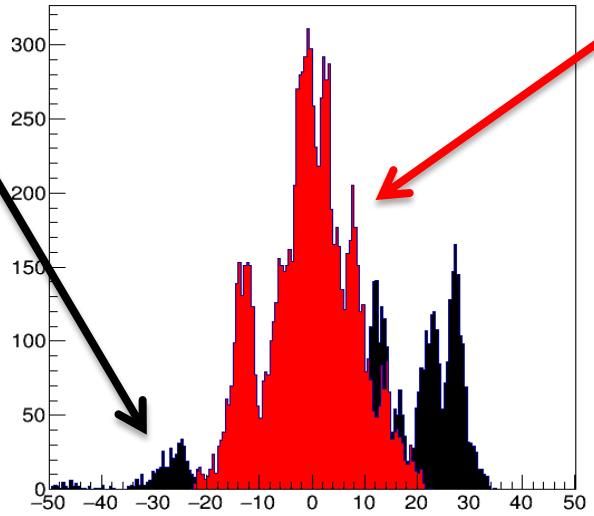
UNCOUPLED FUEL PINS CENTER OF MASS

Case 1-1



Case 2-1



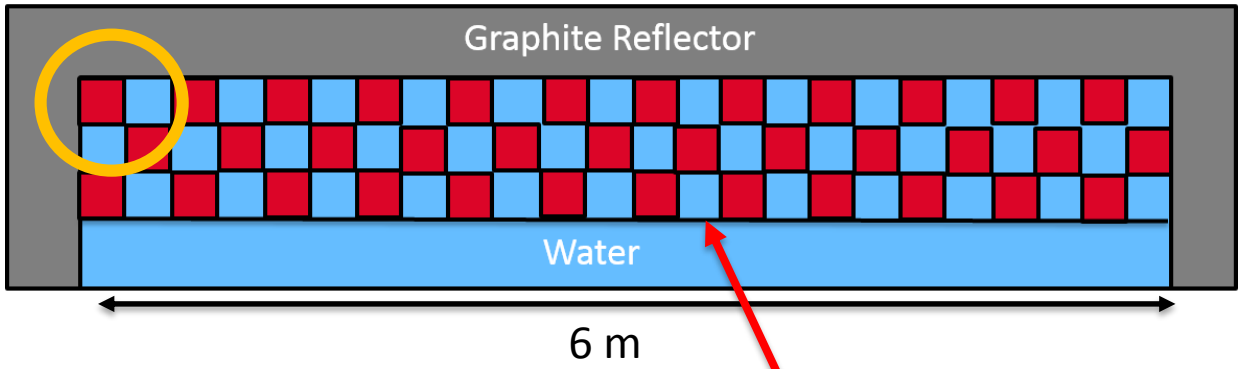


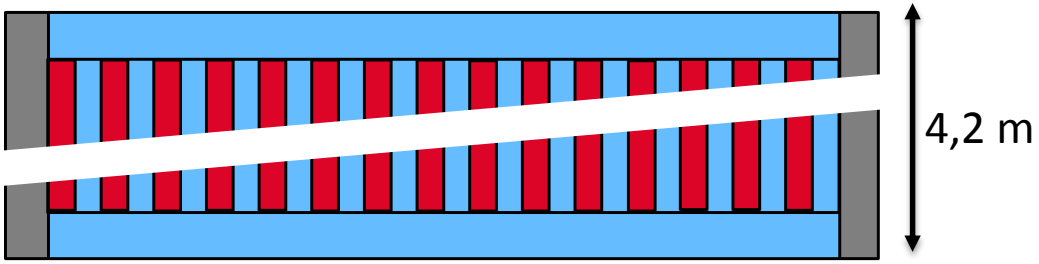
- Mass transfers
- Large deviations from mean
- not a normalized gaussian distribution

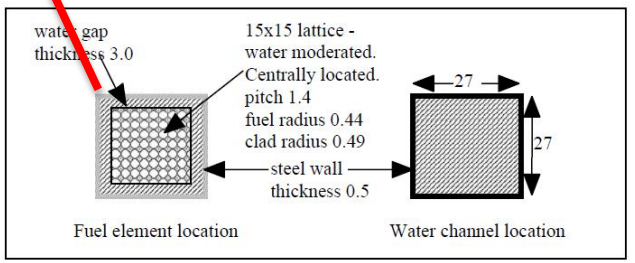
CHECKERBOARD FUEL STORAGE

Most reactive corner

- 2 sides of reflector
- 2 sides of water





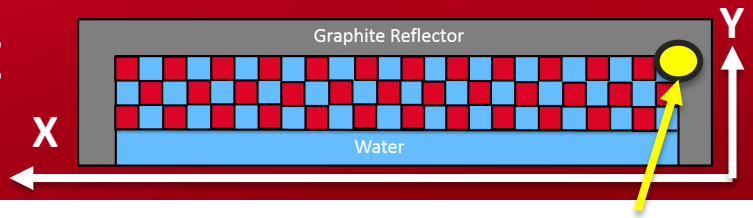


 # histories/c

1000
5000
10,000

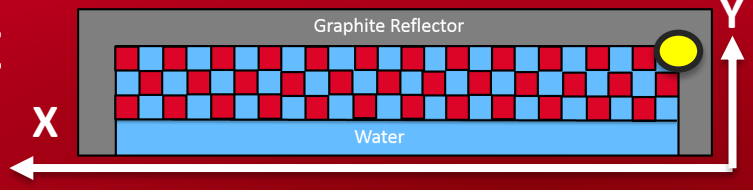
NEA : « observed large variations of the cumulative fission fraction »

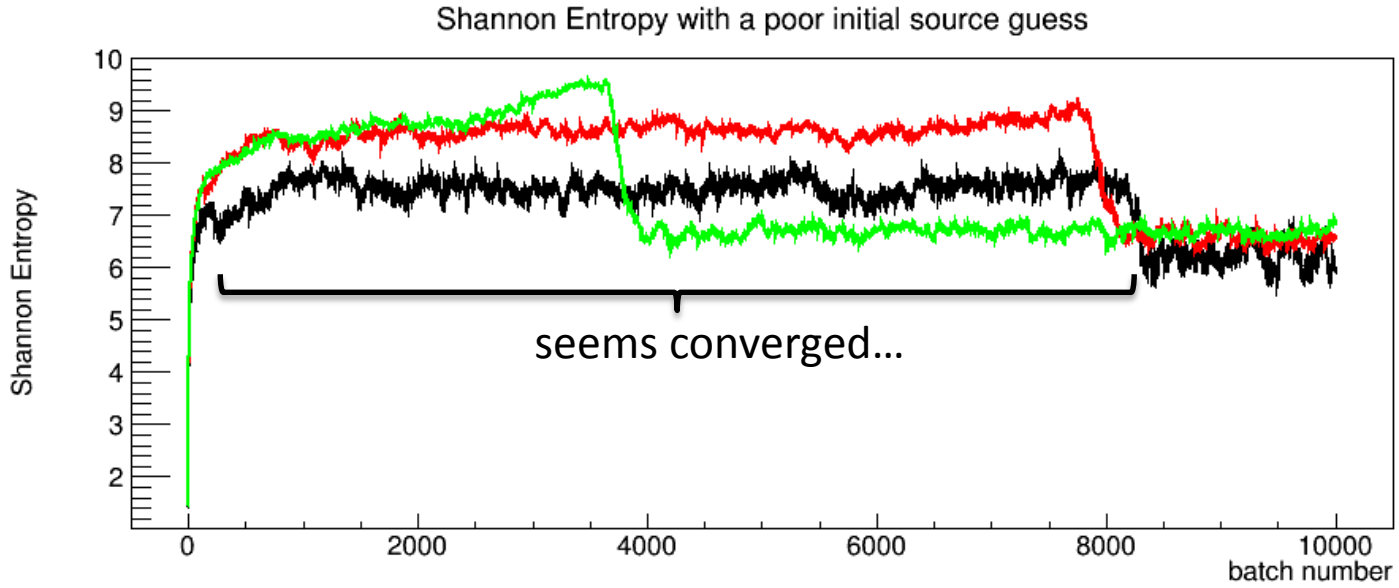
CHECKERBOARD FUEL STORAGE ENTROPY



Initial dirac

CHECKERBOARD FUEL STORAGE ENTROPY

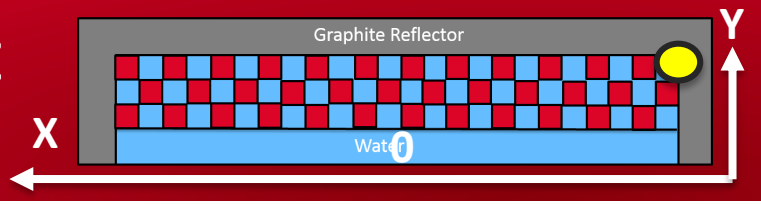


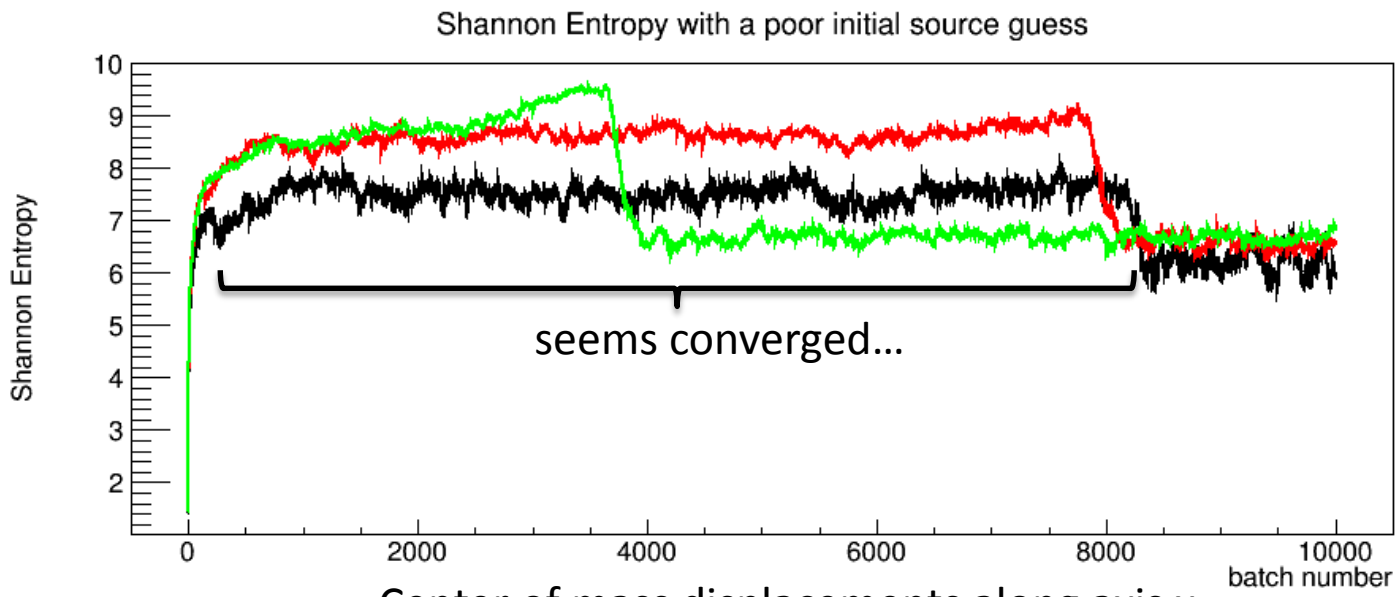


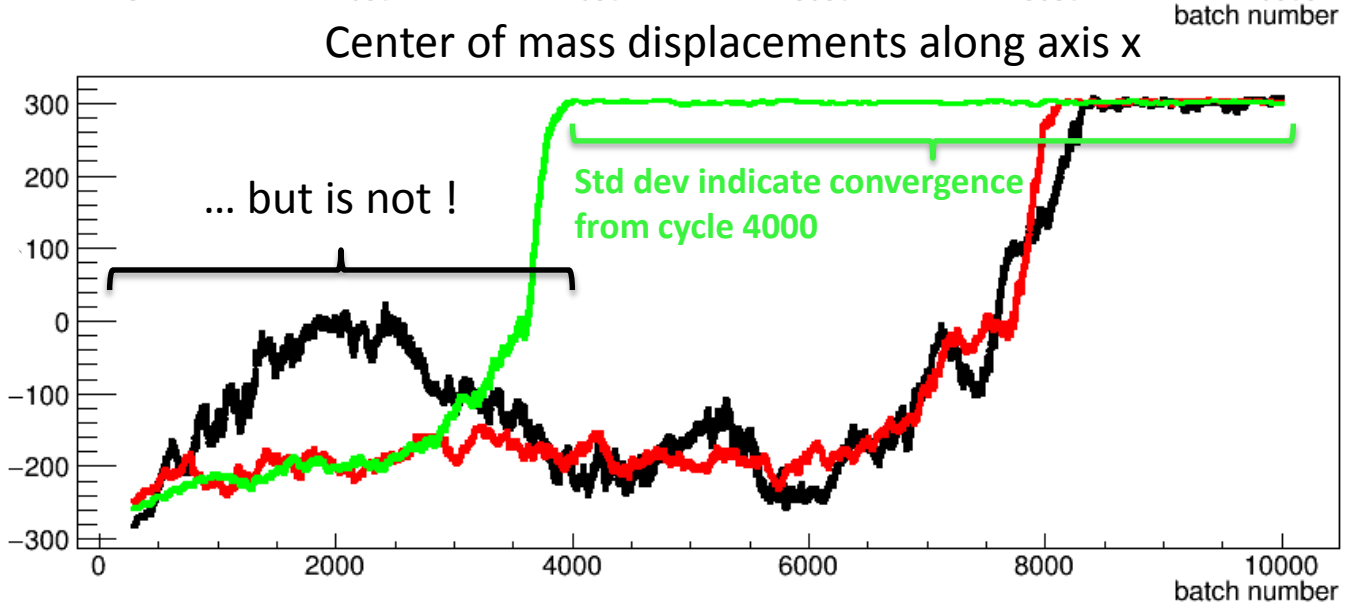
 # histories/c

1000
5000
10,000

CHECKERBOARD FUEL STORAGE ENTROPY



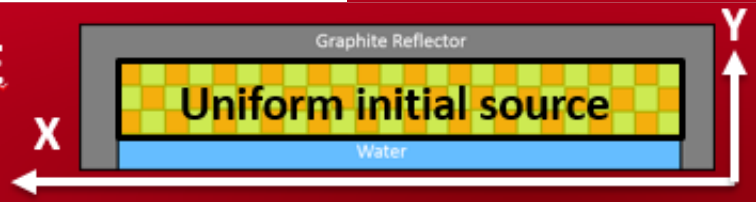


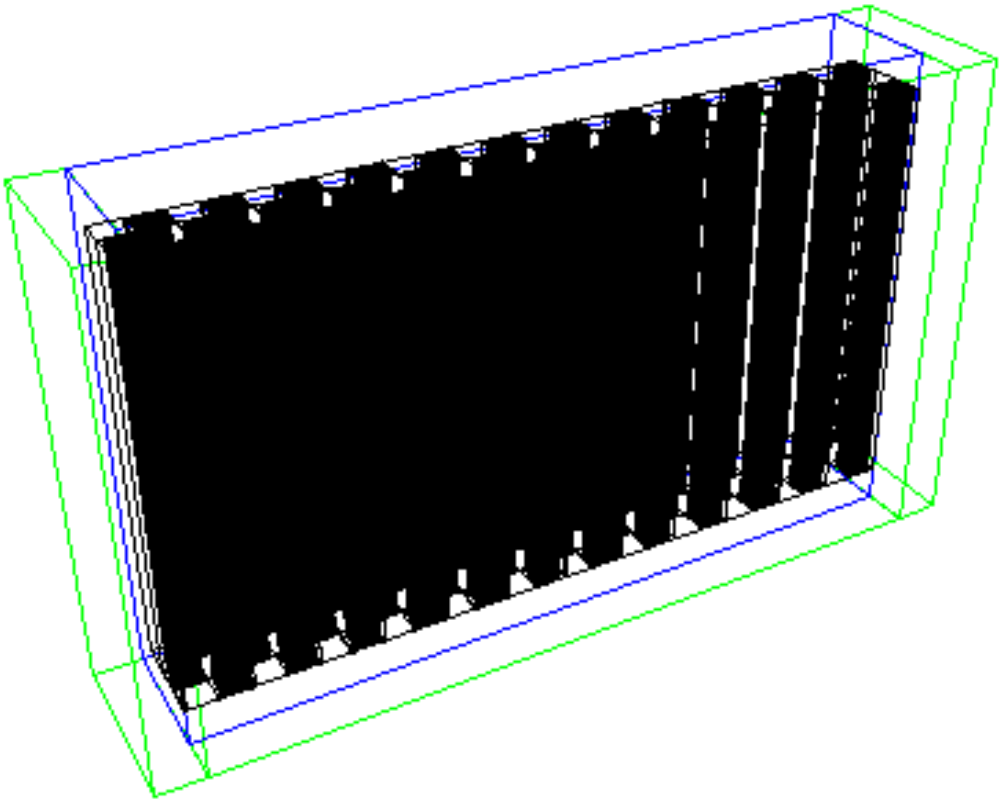


 # histories/c

1000
5000
10,000

CHECKERBOARD FUEL STORAGE ENTROPY





⇒ Clustering effect in the checkerboard fuel storage

⇒ work in progress :

- Other configurations : Hoogenboom-Martin, …
- Publication to follow on clustering diagnostics
- Common work with MIT (OpenMC) and CEA-IRSN (TRIPOLI4)

CONCLUSIONS

Perspective : « theses studies would demonstrate whether the distribution of fission fractions could be used as a measure of convergence »

[source convergence benchmark OECD NEA ISBN 92-64-02304-6]

2 different phases for “source convergence”:

⇒ **phase space exploration**

⇒ **spatial correlations**

⇒ **tallies phase**

REFERENCES

Branching processes in neutronics

Athreya, K.B., Ney, P., 1972. Branching processes. Grundlehren Series, Springer-Verlag, New York.
Bell, G.I., Glasstone, S., 1970. Nuclear reactor theory, Van Nostrand Reinhold Company, New York.
Zoia, A., et al, 2012. J. Phys. A: Math. Theor. 45, 425002.

Clustering in mathematics

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

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.
Dumonteil, E. et al, 2014, Annals of Nuclear Energy 63, 612-618.
Zoia, A. et al, Physical Review E 042118 (2014).

Clustering with mass conservation / center of mass

Yi-Cheng Zhang, Maurizio Serva, Mikhail Polikarpov, Diffusion Reproduction Processes

TRIPOLI-4®

Tripoli-4 Project Team, 2008. Tripoli-4 User guide, Rapport CEA-R-6169.
Brun, E., et al, 2011. Overview of Tripoli-4 version 7 Continuous-energy Monte Carlo Transport Code, Proceedings of ICAPP2011, Nice.