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2018 Meeting of the Expert Group on Advanced Monte Carlo Technics

Clustering & spatial correlations in zero power reactors: Preliminary results of the RCF clustering experiment
- Reminder on neutron clustering in Monte Carlo criticality simulations
- Design of a clustering experiment in a zero-power reactor
- Preliminary results of the experiment led at the RCF in August 2017
- Reminder on neutron clustering in Monte Carlo criticality simulations
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Clustering in MC criticality simulations

$\phi(x, n)$ 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
Clustering in diffusion using the BBBM

- **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 $L \gg l$

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 \( D \) [cm\(^2\).s\(^{-1}\)]
- undergoes collision at Poissonian times with rate \( \lambda \) [s\(^{-1}\)]
- at each collision, \( k \) descendants with probability \( p(k) \)
- dimension \( d \)

\[ \begin{align*}
  c_0 &= \text{cte} \\
  <x^2(t)> &= Dt \\
  p(0) &\leftrightarrow \Sigma_c \\
  p(1) &\leftrightarrow \Sigma_s \\
  p(2), p(3), ... &\leftrightarrow \Sigma_f \\
  \nu_1 &= \sum_k kp(k)
\end{align*} \]

this process couples:
\( \Rightarrow \text{Galton-Watson birth-death process} \) to describe fission and absorption
\( \Rightarrow \text{Brownian motion} \) to simulate neutron transport
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:

\[ \frac{\partial}{\partial t} c_t(x) = 0. \]

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

$d$-dimensional Laplacian (diffusion term)

\[ r = |x - y| \]

auto-correlation term leading to $2^{nd}$ moment effects

(2 is the mean number of pairs)

Houchmandzadeh, B., Phys. Rev. E 80, 051920  (2009)
Analytical solution to this equation

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

\[
c_t(x) = c_0 \quad \text{(for all } t)\]

And the solution to the 2-points function is, \textbf{taking dimension } d = 3:\n
\[
g_t(r) = \frac{\lambda v_2}{8Dc_0\pi^{3/2}} \Gamma \left( \frac{1}{2}, \frac{r^2}{8Dt} \right)
\]

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

Amplitude \( \mu \frac{2}{Dc_0} \)

g can be interpreted as the probability to find a neutron next to another
Beyond the Boltzmann equation: Feynman-Kac & Master equations

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

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

- Neutron clustering in MC criticality
- 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

Credits: A. Zoia
- Reminder on neutron clustering in Monte Carlo criticality simulations
- Design of a clustering experiment in a zero-power reactor
- Preliminary results of the experiment led at the RCF in August 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
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)

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

Clustering should be measurable, if certain conditions are gathered:

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

Ideal conditions for an experiment that could characterize clustering?

- Zero power reactor
- Fresh fuel, no burn-up effects
- As big as possible
- Find a way to do spatial measurements

RCF@RPI

MC15 detectors & He3 tubes
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
MORET5 simulations to design the experiment

- MORET 5 code with all Random Noise options activated => kinetic + analog
  - Data library: Endfb71
  - Fission sampling:
    - Freya
    - discrete Zucker and Holden tabulated
    - Pn distributions and corresponding nubars
    - Only Spontaneous fissions

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

Excellent reactivity: Rho = -4 pcm +
Up to 10 mW of simulated power!
Preliminary results of RCF simulation

- Ideal scenario @ RCF => 1\textsuperscript{st} question: are there spatial correlations in the reactor?
  => 2\textsuperscript{nd} 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!

\[
G_P(n, m) = \frac{\langle nm \rangle - \langle n \rangle \langle m \rangle}{\langle n \rangle \langle m \rangle}
\]
- Reminder on neutron clustering in Monte Carlo criticality simulations
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- Preliminary results of the experiment led at the RCF in August 2017
RPI Measurements 2017: Neutron clustering

LANL Advanced Nuclear Technology Group (NEN-2)
IRSN Neutronics Laboratory (PSN-EXP/SNC/LN)
Featuring

IRSN: Eric Dumonteil, Wilfried Monange
LANL: Rian Bahran, Jesson Hutchinson, Geordy McKenzie, Mark Nelson
RPI: Peter Caracappa, Nick Thompson, Glenn Winters
Hudson River picture contest

mine

Rian’s
Hotel View And Rendering
MC 15’s
Are the MC15’s cases waterproof?

Side view of Jesson looking for bubbles!

Top view of Marc making sure that not a single drop of water made it to the inside of the case!
He3 tubes

- He3 tube: 4 inches & 30 atm
- 4 He3 tubes fit in the pin-cell!
Setup Complete
Video of Water Filling Tank
Preliminary analysis & results

- **Preliminary results:**
  - ✓ no systematic error bars
  - ✓ no checks
  - ✓ only sample datas

- **No human intervention** during data acquisition
Preliminary analysis & results

Simulation of in-core flux with He$^3$ tallies

![Graph showing flux vs Z position with clustering indication](image-url)
Preliminary analysis & results

Simulation of in-core flux with He$^3$ tallies

RCF results of in-core flux with He$^3$ tallies

Clustering

Z position
Simulation of spatial correlations vs power

Clustering

\[ g_t(r) = \frac{\lambda v_2}{8 D c_0 \pi^{3/2} r} \Gamma \left( \frac{1}{2}, \frac{r^2}{8 D t} \right) \]

\[ g_t(r) \propto \frac{1}{c_0} = \frac{1}{P} \]
Preliminary analysis & results

Simulation of spatial correlations vs power

RCF results of spatial correlations vs power

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

\[ g_t(r) \propto \frac{1}{P^{1.02 \pm ?}} \]

\[ g_t(r) \propto \frac{1}{c_0} = \frac{1}{P} \]
Preliminary analysis & results

Modelling of spatial correlations vs distance

\[ g_t(r) = \frac{\lambda v_2}{8Dc_0 \pi^{3/2} r} \Gamma \left( \frac{1}{2}, \frac{r^2}{8Dt} \right) \]  
\[ g_t(r) \propto \frac{1}{r} \]
Preliminary analysis & results

Modelling of spatial correlations vs distance

$g(r) = \frac{\lambda v_2}{8 D c_0 \pi^{3/2} r} \Gamma\left(\frac{1}{2}, \frac{r^2}{8Dt}\right)$

$g_t(r) \propto \frac{1}{r}$

RCF results of spatial correlations vs distance

Bin size: 2 ms
HE3
Tube 1 vs tubes 2-4
Power: 1.2 mW
In the close future

- Final analysis currently done by LANL & IRSN & CEA

- This analysis will have to
  - Define appropriate observables
  - Use analog MC simulations (MCNP6 & MORET5) for
    - background noise studies
    - time gate width definition
  - Perform an extensive uncertainty analysis (systematic+statistical) to establish a proof of detection

- Nick Thompson has rejoined LANL & IRSN to help!
Questions ?
**Clustering in mathematics**

**Clustering in biology**

**Clustering in neutronics**
[Dumonteil, E., Courau, T., 2010. Nuclear Technology 172, 120.]
Dumonteil et al, Nuclear Energy Agency of the OECD, Paris (to be published)
Sutton, T., Mittal, A., Proceedings of M&C 2017 (Jeju)

- Observation of clusters in MC criticality simulations
- Theoretical modeling
- Confined geometries
- Population control
- Consequences on MC criticality source convergence (with MIT)
- Effects of delayed neutrons
- OECD/NEA report
- Traveling waves and biases (Jeju best papers)
- cycles/time (Jeju best papers)
Population control

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

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

What equation do MC codes solve?

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

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

Probability that one neutron in x is captured

Large population size

\[ g(x, y, t) \to 0 \]

Flux factorized out of the integral

Small population size

\[ g(x, y, t) \to g_N^\infty(x, y) >> 1 \]

Large population size

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

\[ \frac{\partial_x \phi(x)}{|x = \pm L} \]

Neumann/Reflective bc \[ \nabla^2 \phi = 0 \]

Dirichlet/Absorbing bc \[ \nabla^2 \phi + \frac{\pi^2}{2L^2} \phi = 0 \]

No criticality conditions ;)}
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 nubars
    - Only Spontaneous fissions

- **Highly parallel simulations:**
  - Simulated signal = 1000 s (prompt+delayed)
  - Number of independent simulations = 330
  - Number of neutrons per simulation = $2.4 \times 10^4$

**Excellent reactivity:** Rho = -4 pcm

+ Up to 10 mW of simulated power!
Foreword on the gambler’s ruin

**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?”

---

Blaise Pascal (1623-1662)
mathematician & philosopher

Pierre de Fermat (1605-1665)
mathematician & magistrate

---

$N_0=\$1000$

Almost sure ruin!
Foreword on the gambler’s ruin

Patterns in a bloom of Anabaena flos-aquae.
Courtesy of Pr. Franks
Scripps Institute for Oceanography

Non-linear Wave propagation
Mark J. Ablowitz and Douglas E. Baldwin
Phys. Rev. E 86, 036305

Gambler’s ruin theory

Reactor Critical Facility at the Rensselaer Polytechnic Institute
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
Part 1. Initial motivation: tilts in Monte Carlo criticality simulations

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Broken symmetries

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
- Ad hoc diagnostic tools (ex: entropy of fission sources)

[Martin, Physor 2012] [Lee et al, SNA + MC 2010]

[Gelbard and Prael, 1974] [Brissenden and Garlick, 1986] [Brown, Physor 2006]
Monte-Carlo tallies in criticality (power iteration) mode are affected by cycle-to-cycle correlations

\[ k_{\text{eff}}^{(n+1)} = k_0 \left[ 1 + C_2 \frac{a_1}{a_0} (DR)^n (DR - 1) \right] \]

\[ \phi^{(n+1)} = C_1 \left[ \vec{u}_0 + \frac{a_1}{a_0} (DR)^{n+1} \vec{u}_1 \right] \]

where

\[ DR = \frac{k_1}{k_0} \]

\[ \phi^{(0)} = \sum_{i=0}^{\infty} a_i \vec{u}_i \]

The higher the DR, the stronger those temporal correlations.

What does the DR represent?

1. \( l \) is the typical migration length
   It is a function of \( D \) and \( \Sigma_a \)

2. 1-D 1-group homogeneous pincell of length \( L \)

3. Decoupling between spatial scales: migration length / length of the system

Isn’t it all about spatial correlations?

[Brown, LA-UR-05-4983] [Dumonteil and Courau, NT 2009]
A simple numerical experiment

Variable pin-cell length:
TRIPOLI-4® in criticality mode
UO₂ fuel rod (at 3.25% enrichment)
radius = 0.407 cm
Zr cladding of outer radius = 0.477 cm
H₂O moderator of size = 1.26 cm
T = 300 °K
10³ cycles with 10⁴ neutrons per cycle
Spatially uniform initial guess source
Reflective boundary conditions everywhere
Flux tallies on a 40 bins spatial mesh in x

Flux should be the same
Length = 10 cm or 100 cm or 400 cm
Spatial correlations & clustering

\( \phi(\mathbf{x}, n) \) 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

neutron clustering
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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!)

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

[Young, Nature 2001]
[Houchmandzadeh, PRE 2008]
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 $D$ [cm$^2$.s$^{-1}$]
- undergoes collision at Poissonian times with rate $\lambda$ [s$^{-1}$]
- at each collision, $k$ descendants with probability
- dimension $d$

\[
\begin{align*}
\left\{\begin{array}{l}
c_0 = cte \\
<x^2(t)> = Dt \\
p(0) \leftrightarrow \Sigma_c \\
p(1) \leftrightarrow \Sigma_s \\
p(2), p(3), \ldots \leftrightarrow \Sigma_f \\
\nu_1 = \sum_k k p(k)
\end{array}\right.
\]

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

example with $d=1$
Crash course for clustering in dimension 0

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

- $\text{Proba}(n \rightarrow n+1 \text{ in } dt)$: $W^+(n)dt = \lambda p(2)ndt$
- $\text{Proba}(n \rightarrow n-1 \text{ in } dt)$: $W^-(n)dt = \lambda p(0)ndt$

Forward master equation

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

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

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

Critical:

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

$< n(t) >= n_0$

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

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

$< V(t) >= < n^2(t) > - < n(t) >^2 = \lambda (p(0) + p(2))n_0 t$
From gambler’s ruin to critical catastrophe...

Ultimate fate of this population? 
Controlled by $\nu_1 = \sum_k kp(k)$ (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

\[ < n(t) >= n_0 \]
\[ < V(t) >= \lambda n_0 t \]

Almost sure ruin!

\[ N_0 = $1000 \]

\[ $0 \]
From $d=0$ to $d=2$

$d=0 \Rightarrow \text{Critical castastrophy} \Leftrightarrow \text{Gambler’s ruin}$

$d>0 \Rightarrow \text{Neutron clustering}$

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

We have to take into account the diffusion of neutrons
A little bit of field theory

- fission event
  - proba:
  - action on \( \vec{n} \):
    \[ W^+(\vec{n}, i) dt = \lambda p(2) \eta_i \vec{n} dt \]
    \[ a_i^+ \vec{n} = (\ldots, n_{i-1}, [n_i + 1], n_{i+1}, \ldots) \]
    with \( \eta_i \) the number of neutrons in cell \( i \)
    and \( \lambda p(1) = \frac{D}{2l^2} \)

- capture event
  - proba:
  - action on \( \vec{n} \):
    \[ W^-(\vec{n}, i) dt = \lambda p(0) \eta_i \vec{n} dt \]
    \[ a_i^0 \vec{n} = (\ldots, n_{i-1}, [n_i - 1], n_{i+1}, \ldots) \]

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

Forward master equation

\[
\frac{dP(\vec{n}, t)}{dt} = \sum_i W^+(a_i \vec{n}, i) P(a_i \vec{n}, t) - W^+(\vec{n}, i) P(\vec{n}, t) + \sum_i W^-(a_i^+ \vec{n}, i) P(a_i^+ \vec{n}, t) - W^-(\vec{n}, i) P(\vec{n}, t) + W^m(a_{i-1}^+ a_i \vec{n}, i - 1, i) P(a_{i-1}^+ a_i \vec{n}, t) - W^m(\vec{n}, i, i + 1) P(\vec{n}, t) + W^m(a_{i+1}^+ a_i \vec{n}, i + 1, i) P(a_{i+1}^+ a_i \vec{n}, t) - W^m(\vec{n}, i, i - 1) P(\vec{n}, t)
\]
And a little bit more

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:

\[
\frac{\partial}{\partial t} c_t(x) = 0.
\]

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

with $r = |x - y|$ and $\nu_2 = \sum_k k(k - 1)p(k)$.

The equations obtained stand for any arbitrary dimension $d$ and can be written:

\[
\frac{\partial}{\partial t} c_t(x) = 0.
\]

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

Houchmandzadeh, B., Phys. Rev. E 80, 051920 (2009)
Analytical solution to this equation

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

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

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

$$g_t(r) = \frac{\lambda v_2}{8D c_0 \pi^{3/2}} \Gamma \left( \frac{1}{2}, \frac{r^2}{8Dt} \right)$$

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

Amplitude $\mu \frac{2}{D c_0}$

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 power peaks at arbitrary places!

The typical amplitude of those peaks is controlled by

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

Credits: A. Zoia

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 1: Convergence criteria

Typical separation between particles: \( \ell = \sqrt{\langle r_i^2 \rangle} \)

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

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

| \( L \) (cm) | \( N_0 \) \( \simeq \) | \( N \) \( \gg \) | \( N_0 \) |
|-------------|-----------------|-----------------|
| 10          | 4               | \( N \gg N_0 \) |
| 100         | \( 5 \cdot 10^3 \) | \( N \approx N_0 \) |
| 400         | \( 3 \cdot 10^5 \) | \( N \ll N_0 \) |
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)

\[\Rightarrow\] very good agreement
\[\Rightarrow\] saturation of the 2-points estimator in the MC simulation
Consequence 3:

under-sampling biases

& clustering

& traveling waves
OECD/NEA R1 Benchmark

- Expert Group on Advanced Monte-Carlo Techniques @ OECD/NEA
- R1 Benchmark = ¼ PWR-type reactor core
- Designed to understand biases on local tallies estimates (+uncertainties)

Reflective boundary Conditions (Neumann) vs. Absorbing boundary Conditions (Dirichlet)
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 $D$ [cm$^2$.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

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

$p(0) \propto \gamma$
$p(1) \propto \lambda$
$p(2) \propto \beta$

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

\[
\frac{D N}{\beta L^2} \gg 1
\]

- Poisson statistics
- Cosine shape
- 1-D BBM with population control
- Uniform initial distribution
- 50 neutrons
- \([-L,L]\) Dirichlet

Loosely coupled

\[
\frac{DN}{\beta L^2} << 1
\]

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

- Reproduces the R1 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 $N \sim cte$

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

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

- Fission rate
- Diffusion operator (same demonstration for transport)
- Capture rate
Fission/Capture vs Splitting/Russian Roulette

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

\[ \beta^* N \rightarrow \beta N \]
\[ \gamma^* N \rightarrow \gamma N \]

Renormalization rate depends on N and \( t/g \).

\[ f(N)N \rightarrow \lambda(t)N \]

\[ t \text{ or } g \]
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 \( N \) !

\[
\lambda(t) f(N) N \quad \frac{(N - 1) N}{N^2} \quad \exists \quad N^2
\]

Generalization

\[
\lambda(t) \int dy \ G(x, y, t)
\]

number of pairs


- 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

Rate of renormalization

\[ \partial_t \phi = D \nabla^2 \phi + (\beta - \gamma) \phi + \lambda(t) \int dy \ G(x, y, t) \]

Number of pairs

\[ G(x, y, t) = \left[ 1 + g(x, y, t) \right] \phi(x)\phi(y) \]

Spatial correlation function

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

\[ \partial_t \phi = D \nabla^2 \phi + (\beta - \gamma) \phi + \left( -\beta + \gamma - D \frac{\partial_x \phi(x, t)}{\int_{-L}^{+L} dx \int_{-L}^{+L} dx \, \phi(x, t)^2} \right) \phi(x, t)^2 \]

- Non-linear equation with \( \phi^2 \) term
- Can be simplified under some assumptions


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


- F-KPP equation with traveling waves solutions
- Counter-reaction depending on the sign of \( 1 - \phi \)
Traveling wave & solitons

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

Cluster density profile from the BBM simulation

flux profile obtained by solving the F-KPP equation
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:

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


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