MONTE CARLO POWER ITERATION:
ENTROPY AND SPATIAL CORRELATIONS

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Power iteration with Monte Carlo

The impact of correlations in criticality simulations

- Entropy and convergence
- Spatial moments and correlations
- Relation to neutron clustering theory

Perspectives
We would like to determine

- the **fundamental mode** \( \varphi_1 \)
- and the associated **fundamental eigenvalue** \( k_1 \) of

\[
L \varphi(r, v) = \frac{1}{k} \mathcal{F} \varphi(r, v)
\]

Critical Boltzmann equation for the **neutron flux** \( \varphi \)

**Net disappearance operator** \( L \)

\[
L f = \Omega \cdot \nabla f + \Sigma_t f - \int \Sigma_s(r, v' \rightarrow v) f(r, v') \, dv'
\]

**Creation (fission) operator** \( \mathcal{F} \)

\[
\mathcal{F} f = \chi(r, v) \int \nu(v') \Sigma_f(r, v') f(r, v') \, dv'
\]
A generalized eigenvalue equation

\[ L \varphi = \frac{1}{k} F \varphi \]

**Power iteration algorithm:**

- **Guess solution**
  \[ \hat{\varphi}^{(0)} = \sum_i c_i \varphi_i \]

- **Iterate**
  \[ \text{for } m = 1, 2, \ldots, G - 1 \]
  \[ \hat{\varphi}^{(m+1)} = L^{-1} F \hat{\varphi}^{(m)} \]

**Hypothesis**
\[ |k_1| > |k_2| \geq |k_3| \geq \cdots |k_i| \geq \cdots \]

**Convergence**
\[ \hat{\varphi}^{(G)} \simeq \varphi_1 + \sum_i c_i \left( \frac{k_i}{k_1} \right)^G \varphi_i \]
MONTE CARLO APPROACH: CRITICALITY SIMULATION

Fission chain

Source

1st gen. 2nd gen. 3rd gen. 4th gen. 5th gen.

Source

1st gen. 2nd gen. 3rd gen.

N₀ particles

Fission generations
POWER ITERATION: THE STANDARD (?) TOOL

Source 1\textsuperscript{st} gen. ... G\textsuperscript{th} gen. (G+1)\textsuperscript{th} gen. ... M\textsuperscript{th} gen.

N\textsubscript{0} particles

Convergence to the fundamental mode $\varphi_1$ (statistical equilibrium)

Stationarity: sample $\varphi_1 = \langle \varphi_1(g) \rangle$

Hypothesis: (I)ID replicas

What about correlations?
A TOY MODEL OF A NUCLEAR REACTOR

Assumption: the reactor is **critical**

\[ k_{\text{eff}} = \frac{\bar{\nu} \Sigma_f}{\Sigma_c + \Sigma_f} = 1 \]

Expected fundamental mode \( \phi_1 \): **spatially uniform** over the box

Neutrons in a box

Scattering \( \Sigma_s = 0.27 \), Capture \( \Sigma_c = 0.02 \), Fission \( \Sigma_f = \frac{\Sigma_c}{\bar{\nu} - 1.0} \)

Descendants per fission \( \bar{\nu} = 2.5 \)

Reflecting boundary conditions
Delta-like source at the center of the box

Initial number of neutrons per generation $N = 10^4$
IMPACT OF SYSTEM SIZE L ON POWER ITERATION

Neutrons per generation $N = 10^4$

- $L = 100\text{ cm}$
- $L = 200\text{ cm}$
- $L = 400\text{ cm}$

Neutron clustering
IMPACT OF POPULATION SIZE N ON POWER ITERATION

Delta-like source at the center of the box

System size $L = 400 \text{ cm}$
IMPACT OF POPULATION SIZE N ON POWER ITERATION

System size $L = 400$ cm

Neutron clustering
Shannon entropy: 

\[ S(g) = - \sum_{i,j,k} p_{i,j,k}(g) \log_2[p_{i,j,k}(g)] \]

Generations to convergence: 

\[ m \approx \frac{L^2}{\ell^2} \]
THE EFFECTS OF CLUSTERING ON THE ENTROPY FUNCTION

Shannon entropy:

\[ S(g) = - \sum_{i,j,k} p_{i,j,k}(g) \log_2[p_{i,j,k}(g)] \]

Theoretical expected value for independent replicas

Measured value

Impact of correlations between generations
ANALYSIS OF SPATIAL MOMENTS: THE CENTER OF MASS

\[ \mathbf{r}_{\text{com}}(g) = \frac{\sum_i w_i \mathbf{r}_i}{\sum_i w_i} \]

\[ x_{\text{com}}(\text{cm}) \]

\[ L = 400 \text{ cm} \]
\[ L = 200 \text{ cm} \]
\[ L = 100 \text{ cm} \]

\[ N = 10^3 \]
\[ N = 10^4 \]
\[ N = 10^5 \]
A STATISTICAL MECHANICS DESCRIPTION

Neutrons as a collection of N stochastic particles: \( \{x_1, x_2, \ldots x_i, \ldots x_N\} \)

A remarkable **identity** for the spatial moments:

Square COM

Mean square displacement: \( \langle r^2 \rangle (g) \)

\[
\langle r_{\text{com}}^2 \rangle (g) + \frac{1}{2} \frac{N - 1}{N} \langle r_p^2 \rangle (g) = \langle r^2 \rangle (g)
\]

Mean square pair distance: \( \langle r_p^2 \rangle (g) \)
Neutrons as a collection of N stochastic particles: \( \{x_1, x_2, \ldots x_i, \ldots x_N\} \)

A remarkable **identity** for the spatial moments:

\[
\langle r^2 \rangle (g) = \int x^2 \psi(x, g) \, dx
\]

Square COM

Mean square displacement:

\[
\langle r_{\text{com}}^2 \rangle (g) + \frac{1}{2} \frac{N - 1}{N} \langle r_p^2 \rangle (g) = \langle r^2 \rangle (g)
\]

Mean square pair distance:

\[
\langle r_p^2 \rangle (g) = \frac{\int dx \int dy |x - y|^2 h(x, y, g)}{\int dx \int dy h(x, y, g)}
\]

Average particle density \( \psi \)

Pair correlation function \( h \)
**Forward** time flow

Measure in $z$

\[ \mathcal{L}_z \]

Source $Q$

\[ \rho (\{\text{measure}\}|\{\text{source}\}) \]

\[ \frac{\partial}{\partial t} \psi(z, t) = \mathcal{L}_z \psi(z, t) \]

\[ \psi(z, 0) = Q(z) \]

**Backward** time flow

Measure in $z$

\[ \mathcal{L}_{z_0}^* \]

Source $z_0$

\[ \rho (\{\text{source}\}|\{\text{measure}\}) \]

\[ \frac{\partial}{\partial t} G_t(z, z_0) = \mathcal{L}_{z_0}^* G_t(z, z_0) \]

\[ G_0(z, z_0) = \delta(z - z_0) \]

\[ \langle \mathcal{L} f, g \rangle = \langle f, \mathcal{L}^* g \rangle \]
\[ \psi(z, t) = \int dz_0 Q(z_0) G_t(z, z_0) \]
THE PAIR CORRELATION FUNCTION

\[ h(z_1, z_2, t) = \psi(z_1, t)\psi(z_2, t)U(t) \]

\[ + \int_0^t dt' \int dz' G_{t-t'}(z_1, z')G_{t-t'}(z_2, z') \rho_t(t')\psi(z', t') \]

Correlated measurements

\( z_1 \rightarrow z' \quad z_2 \rightarrow z' \quad z' \rightarrow z_0 \)

Source

\( U(t) = 1 - \int_0^t \rho_t(t')dt' \)
Average neutron density: 

$$\psi(x, t) \rightarrow \psi(x) = \frac{N}{L^3}$$

Pair correlation function: 

$$h(x, y, t) \rightarrow h(x, y) = \frac{N(N-1)}{L^6} + F(x, y; \chi)$$

Single dimensionless parameter

$$\chi = \frac{1}{N} \frac{L^2}{M^2}$$

System size $L$

Population size $N$

Migration area $M^2$
POWER ITERATION AS A FUNCTION OF $\chi$

\[ \| \frac{h(x, y)}{\psi(x) \psi(y)} \| \leq \chi = \frac{1}{N} \frac{L^2}{M^2} \]

\(\chi \approx 0.7\)

\(\chi \approx 0.07\)

Uniform initial condition
POWER ITERATION AS A FUNCTION OF $\chi$

\(\chi \approx 0.7\)

Uniform initial condition
Mean square displacement

\[ \langle r^2 \rangle = \int x^2 \psi(x) dx = \frac{L^2}{4} \]

Mean square pair distance

\[ \langle r_{p}^2 \rangle = \frac{\int dx \int dy |x - y|^2 h(x, y)}{\int dx \int dy h(x, y)} \]

\[ = 12 \frac{L^2}{\chi} \left[ 1 - \sqrt{\frac{8}{\chi}} \tanh \left( \sqrt{\frac{\chi}{8}} \right) \right] \]

\[ \langle r_{p}^2 \rangle_{\text{id}} = \frac{L^2}{2} \]

\[ \chi = \frac{1}{N} \frac{L^2}{\mathcal{M}^2} \]
Mean square displacement
\[ \langle r^2 \rangle = \int x^2 \psi(x) dx = \frac{L^2}{4} \]

Mean square pair distance
\[
\langle r_p^2 \rangle = \frac{\int dx \int dy |x - y|^2 h(x, y)}{\int dx \int dy h(x, y)} = 12 \frac{L^2}{\chi} \left[ 1 - \sqrt{\frac{8}{\chi}} \tanh \left( \sqrt{\frac{\chi}{8}} \right) \right]
\]

Square COM
\[
\langle r_{com}^2 \rangle + \frac{1}{2} \frac{N - 1}{N} \langle r_p^2 \rangle = \langle r^2 \rangle
\]

Fluctuations of COM
\[ \sigma_{com} = \sqrt{\langle r_{com}^2 \rangle} \]
SPATIAL MOMENTS: STATISTICAL ANALYSIS

**Theory** | **MC**
---|---
| L [cm] | $\sigma_{com}^x$ [cm] | $\hat{\sigma}_{com}^x$ [cm] |
| 100 | 1.2 | 1.5 |
| 200 | 4.7 | 5.9 |
| 400 | 18.3 | 19.9 |

**Theory** | **MC**
---|---
| N | $\sigma_{com}^x$ [cm] | $\hat{\sigma}_{com}^x$ [cm] |
| $10^5$ | 5.8 | 7.3 |
| $10^4$ | 18.3 | 19.9 |
| $10^3$ | 57.8 | 64.4 |

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Spatial moments

Power iteration
CONCLUSIONS

- Statistical mechanics approach to power iteration
- Neutron clustering can be suppressed by acting on $\chi$
- Applicability to real-world (heterogeneous) systems?
Thanks for your attention

SPATIAL BEHAVIOUR OF THE NEUTRON DENSITY

Pure diffusion (ideal gas)

Initial condition: $N_0$ particles with uniform density
SPATIAL BEHAVIOUR OF THE NEUTRON DENSITY

Initial condition:
\( N_0 \) particles with uniform density

Fluctuations:
\[ \langle n \rangle \pm \sqrt{\langle n \rangle} \]
SPATIAL BEHAVIOUR OF THE NEUTRON DENSITY

Initial condition: \( N_0 \) particles with uniform density

Fluctuations:
\[ \langle n \rangle \pm \sqrt{\langle n \rangle} \]
SPATIAL BEHAVIOUR OF THE NEUTRON DENSITY

Initial condition:

\( N_0 \) particles with uniform density

Diffusion + branching + capture

(critical gas)
SPATIAL BEHAVIOUR OF THE NEUTRON DENSITY

Initial condition: \( N_0 \) particles with uniform density

Fluctuations:
\[
\langle n \rangle \pm \sqrt{\langle n \rangle}
\]
SPATIAL BEHAVIOUR OF THE NEUTRON DENSITY

Initial condition: \( N_0 \) particles with uniform density

Mixing time

\[ \tau_D \approx \frac{L^2}{D} \]

Capture

Fission

Diffusion

Clustering
SPATIAL BEHAVIOUR OF THE NEUTRON DENSITY

Initial condition: $N_0$ particles with uniform density

Mixing time

$\tau_D \simeq \frac{L^2}{D}$

Renewal time

$\tau_E \simeq \frac{N_0}{\lambda}$

Clustering

Capture

Fission

Diffusion
Neutrons as a collection of N particles

Spatial moments:

- Mean square displacement: \[ \langle r^2 \rangle (g) \equiv \frac{1}{N} \sum_i \langle r_i^2 (g) \rangle \]

- Mean square pair distance: \[ \langle r_p^2 \rangle (g) \equiv \frac{1}{N(N-1)} \sum_{i,j} \langle |r_i (g) - r_j (g)|^2 \rangle \]

- Center of mass: \[ \langle r_{com}^2 \rangle (g) \equiv \left\langle \left( \frac{1}{N} \sum_i r_i (g) \right)^2 \right\rangle \]