



DE LA RECHERCHE À L'INDUSTRIE

SPACE AND TIME CORRELATIONS FOR DIFFUSION MODELS WITH PROMPT AND DELAYED BIRTH-AND-DEATH EVENTS

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Théophile Bonnet (theophile.bonnet@cea.fr)

CEA-SACLAY DES/ISAS/DM2S/SERMA/LTSD

Context: kinetic Monte Carlo simulations

Free population of neutrons and precursors

Population control

Conclusion and perspectives

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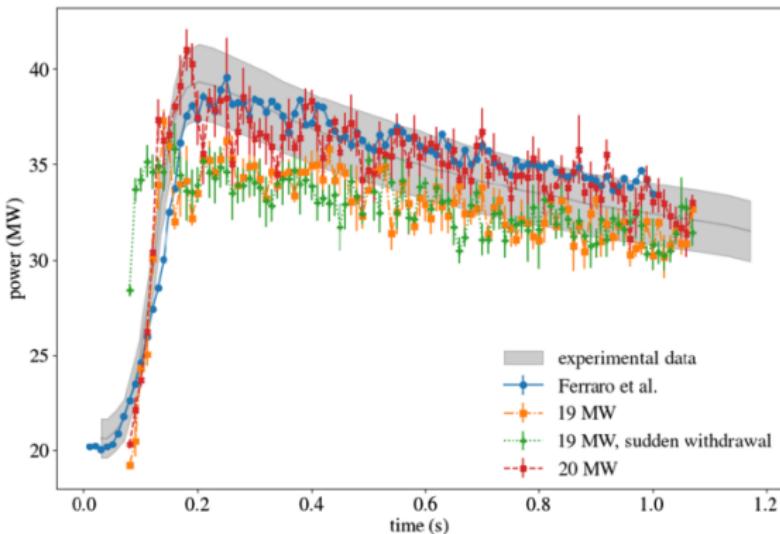
Conclusion and perspectives

- ▶ Reactor physics is concerned with the behaviour of neutrons in reactor cores, as they undergo scattering, induce fission and die by sterile capture (birth-and-death process).
- ▶ Analytical solutions are hardly attainable in most cases, hence numerical simulations are used in order to estimate the physical observables.
- ▶ Probabilistic Monte-Carlo simulations, being ‘exact’, are customarily used to obtain reference results (at CEA: TRIPOLI-4).
- ▶ Due to the involved requirements in computer time, until recently Monte Carlo simulations in reactor physics were limited to stationary regimes.
- ▶ Recent advances in available computer power and efficient variance reduction methods have paved the way to the simulation of the time-dependent (‘kinetic’) regime, which is required in order to take into account transient and accidental reactor behaviour.

Kinetic Monte Carlo simulations: state of the art

- ▶ Kinetic Monte Carlo methods in TRIPOLI-4 can simulate the kinetics of a reactor, including neutrons, precursors and thermal-hydraulics feedback but are extremely expensive in computer time [1].

Fig. 18 Total reactor power as a function of time during the T-84 transient experiment. We report the results of the TRIPOLI-4/SUBCHANFLOW calculations for an initial reactor power of 19 MW (orange) or 20 MW (red). The green line corresponds to a 19 MW calculation with sudden withdrawal of the transient rod. The result of the Serpent 2/SUBCHANFLOW calculation by Ferraro et al. [24] is also shown (blue). All the TRIPOLI-4/SUBCHANFLOW calculation results have been shifted forward in time by 70 ms. Statistical error bars (one standard error) are shown



- ▶ Understanding fluctuations and correlations in kinetic Monte Carlo simulations is a complex problem.

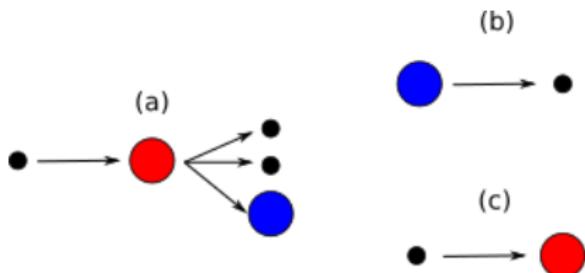


Figure 1: Main stochastic events: (a) a neutron induces fission with rate β , creating ν_p prompt neutrons and ν_d precursors on average; (b) a precursor produces one (delayed) neutron by exponential decay, with rate λ ; (c) a neutron is captured without subsequent production, with rate γ .

- ▶ Separation of time scales (neutrons and precursors):
 $\theta = \lambda/\beta\nu_d \ll 1$. Moreover, in a reactor we have
 $\nu_d/(\nu_p + \nu_d) \ll 1$.
- ▶ Parameters are tuned so that the reactor is **critical**, i.e the average numbers of neutrons and precursors are constant.
- ▶ Equilibrium initial distribution of neutrons (N) and precursors (M): $M = N/\theta \gg N$.

The concept of clustering

- ▶ Births-and-deaths induce spatial correlations. The competition between this mechanism and diffusion leads to *neutron clusters* (with strong non-Poisson fluctuations), whereas the population is expected to be uniformly distributed

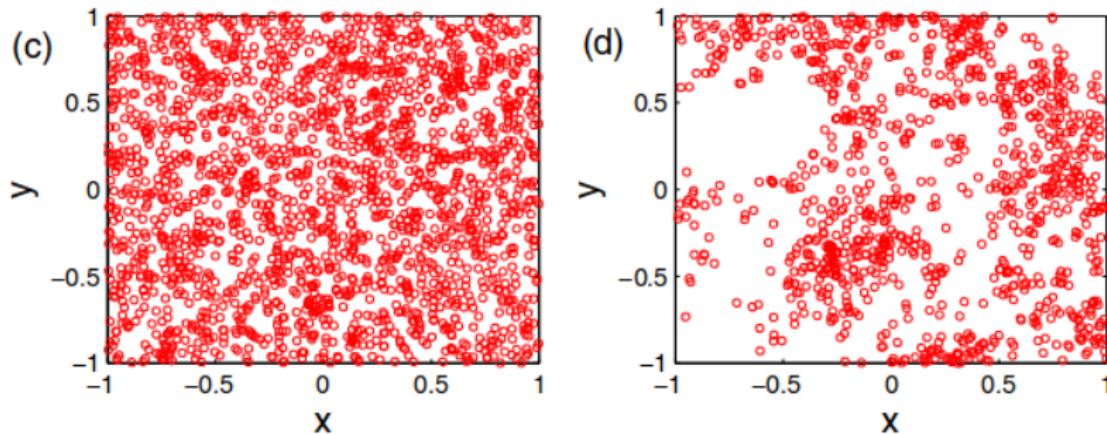


Figure 2: Typical distribution of neutrons for a binary branching process, left when $t = 0$, right when $t = 100$. Picture taken from A. Zoia & al. [2]

- ▶ Investigate an analog Monte Carlo game for time-dependent problems, including population control mechanisms
- ▶ Using the theory of stochastic processes [3, 4, 5, 6]
 - Partition the phase space into cells $1, 2, \dots, k$ ('detectors')
 - Write the master equation for $P(\{n_1, m_1, \dots, n_k, m_k\}, \{t_1, \dots, t_k\})$: too much information, hence we derive *moment equations* instead.
 - We are especially interested in the average density $n(x, t) = \langle n(x_1, t_1) \rangle$ and in the pair correlation function $u(x_1, t_1, x_2, t_2) = \langle n(x_1, t_1) n(x_2, t_2) \rangle$.
- ▶ We conceived a test-bed incrementally-developed Monte Carlo code
- ▶ When possible, we compare simulations with analytical solutions
 - 1D with spatially uniform parameters
 - Reflection boundary conditions
 - Between collision events: diffusion with coefficient \mathcal{D}

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Pair correlation function

- ▶ Pair correlation function (linearly) diverges in time: *critical catastrophe*
- ▶ Tent-like asymptotic spatial shape: spatial clustering

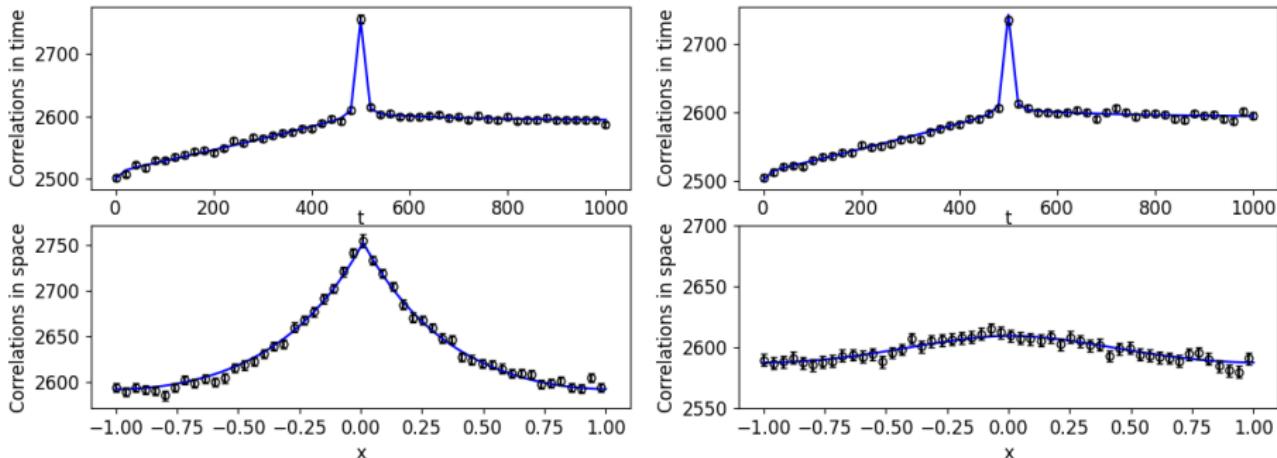


Figure 3: Left: top is time correlations for $x_1 = x_2 = 0$ and $t_1 = 500$, bottom is space correlations for $t_1 = t_2 = 1000$ and $x_1 = 0$. Right: top is time correlations for $x_1 = 0$, $x_2 = -0.1$ and $t_1 = 500$, bottom is space correlations for $t_1 = 990$, $t_2 = 1000$ and $x_1 = 0$. Blue solid lines: analytical solutions; black circles: Monte-Carlo with 10^6 replicas.

- ▶ From the pair correlation function we can derive the (square) pair distance $\langle r^2(t) \rangle = \frac{\iint (x-y)^2 \tilde{u}_t(x,y) dx dy}{\iint \tilde{u}_t(x,y) dx dy}$
- ▶ Two regimes:
 - Short times: wild fluctuations and spatial clustering
 - Long times: global fluctuations at the scale of the box and extinction

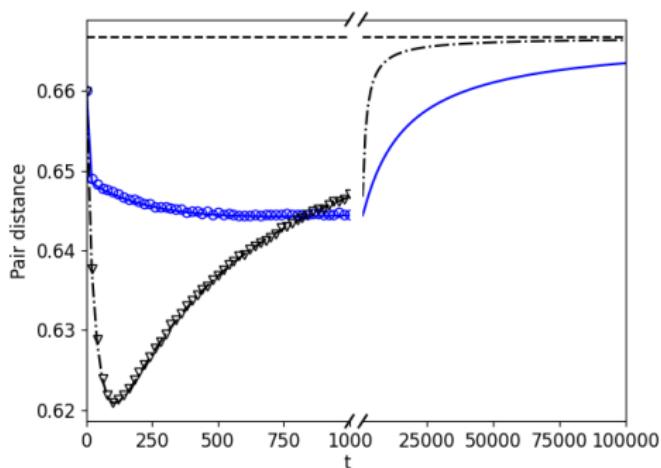


Figure 4: Circles are for Monte-Carlo results and full lines for analytical results. Blue lines: $\theta = 0.1$. Black lines: $\theta = 1$.

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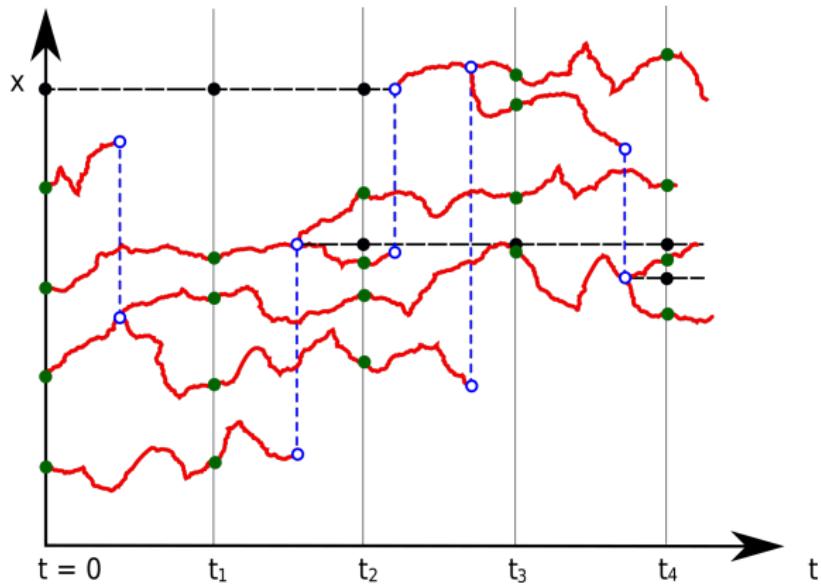
In an attempt to model *idealized feedback effect*, we will consider two different models of population control applied to a population of neutrons and precursors

- ▶ N -control model
 - neutron number kept constant
- ▶ NM -control model
 - neutron and precursor numbers kept constant

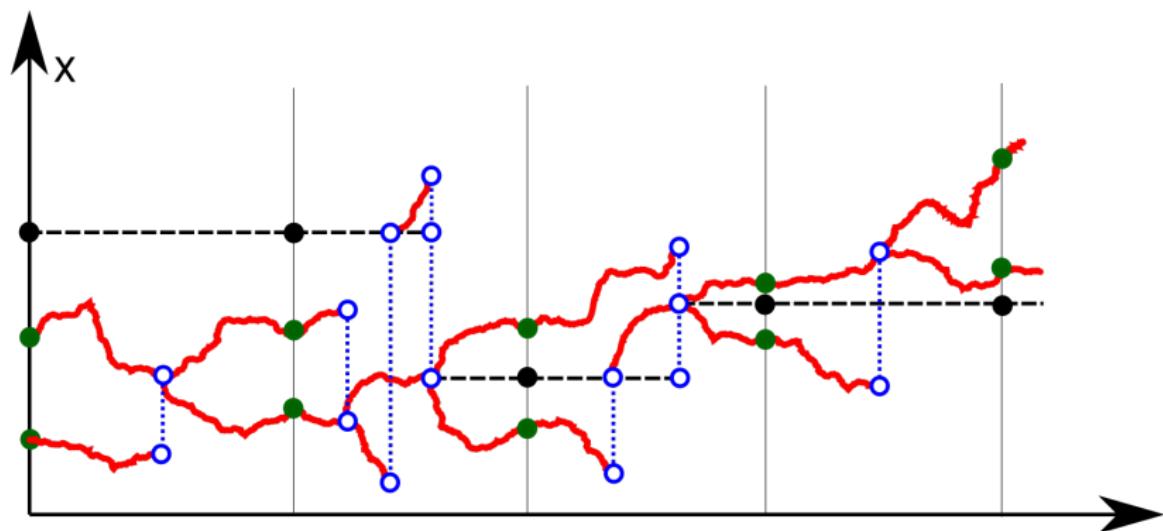


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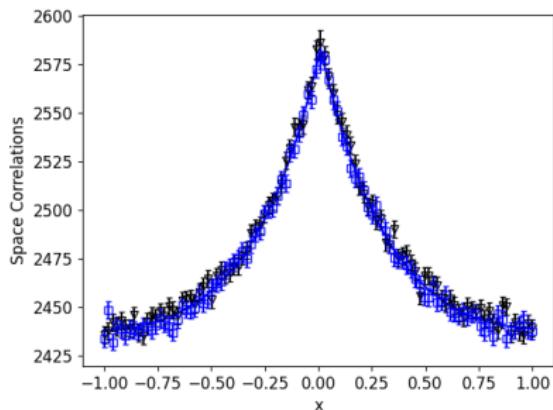
- ▶ Population control enforced on neutrons: whenever a neutron is produced, by fission or following the decay of a precursor, we kill another randomly chosen neutron
- ▶ We obtain non-closed moment equations from the master equation



- ▶ Closure issue solved by enforcing population control on neutrons and precursors
- ▶ Unchanged dynamics for neutrons, but a precursor may only be killed when another is produced by fission

- ▶ Asymptotic solutions are obtained in the form of Fourier series
- ▶ Good approximation of the N -control model for $\theta \ll 1$

$$\theta = 10^{-3}$$



$$\theta = 1$$

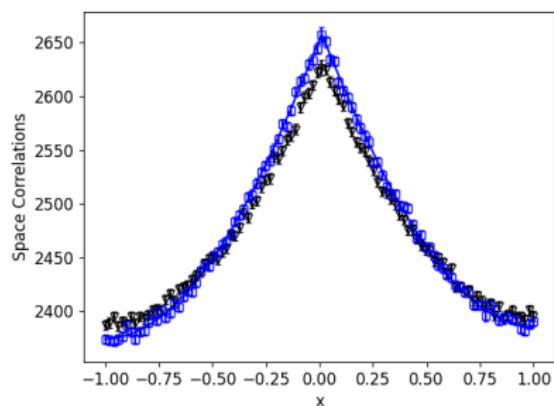
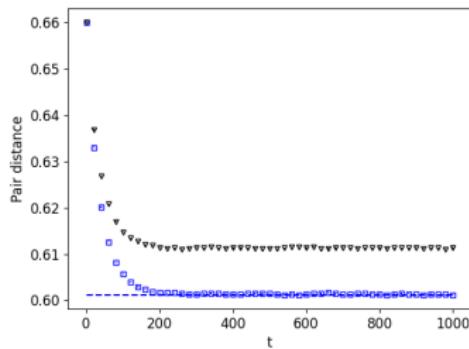


Figure 5: Black triangles: Monte Carlo results of N -control model. Blue solid line: analytical results of NM -control model. Blue squares: Monte Carlo simulation of NM -control model. All Monte-Carlo simulations are obtained with 10^6 replicas.

- ▶ Clustering regime is enforced by population control.

$$\theta = 1$$



$$\theta = 10^{-3}$$

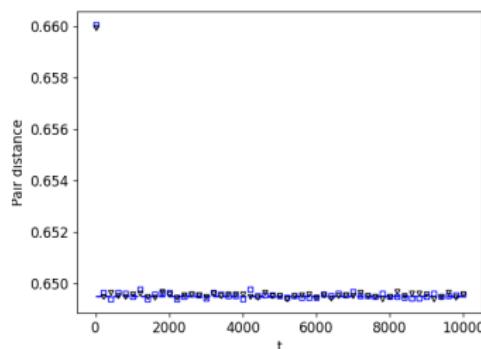


Figure 6: Blue square: N -control model Monte-Carlo results; Black triangles: NM -control model Monte-Carlo results; blue dashed-line: N -control model analytical result.

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Conclusions:

- ▶ Formal framework for treating correlations and fluctuations in a simplified model for kinetic Monte Carlo simulations
- ▶ Characterizing the effects of ideal population control on correlations and spatial fluctuations

Perspectives:

- ▶ Ongoing: more realistic transport models, and focus on the effects of variance reduction methods on correlations
- ▶ Investigating neutron branching trees and their impact on correlations
- ▶ Analysis of feedback effects on spatial correlations (MSc internship)
- ▶ Towards zero-variance time-dependent Monte Carlo games [7]

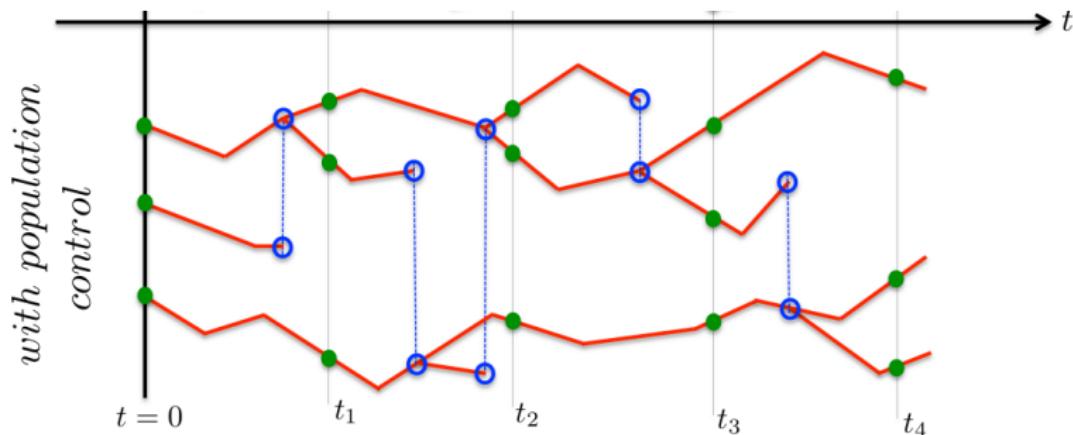
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Thanks! Any questions?



- ▶ Mass conservation: each extra neutron produced by fission is compensated by a captured neutron. Generalizing previous works [8].
- ▶ Fission chains are not independent anymore
- ▶ Failure of backward formalism \implies forward formalism
- ▶ We still get exact solutions in forward formalism, see next slide

Population of neutrons alone II

- ▶ Defining $\tilde{u}_t(x, y) = u_t(x, y) - \delta(x - y)n_t(x)$, we get the equation for the pair correlations from the forward master equation instead of using a heuristic argument as in [9, 10]

$$\partial_t \tilde{u}_t(x, y) = \mathcal{D} \left(\nabla_x^2 + \nabla_y^2 \right) \tilde{u}_t(x, y) - \tau_0^{-1} \tilde{u}_t(x, y) + 2\beta \delta(x - y) n_t(x)$$

- ▶ Exponential relaxation with renewal time $\tau_0 = \frac{N-1}{2\beta}$.

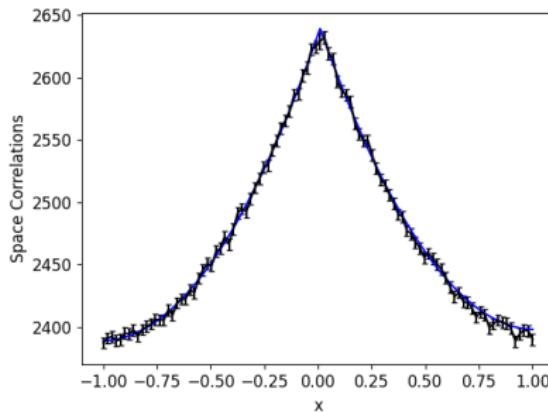


Figure 7: Blue: analytical result. Black: Monte Carlo result with 10^6 replicas.

- ▶ Pair distance always saturates at $\langle r_\infty^2(t) \rangle < \frac{2L^2}{3}$

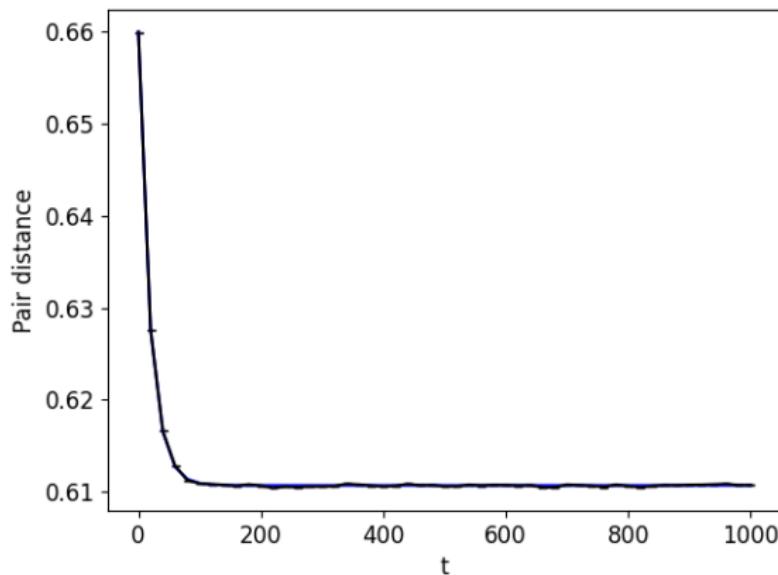


Figure 8: Blue: analytical result. Black: Monte Carlo result with 10^6 replicas.

Indeed, the equations for the averages read

$$\partial_t n_t(x) = \mathcal{D} \Delta n_t(x) + \lambda \left(m_t(x) - \frac{\langle n_t(x) M(t) \rangle}{N} \right) \quad (1)$$

$$\partial_t m_t(x) = \beta \nu_d n_t(x) - \lambda m_t(x) \quad (2)$$

- ▶ In Eq. (1) the last term is a statistical moment of order 2 coupling local neutron density with the fluctuating, total number of precursors
- ▶ Thus, although we still have Monte Carlo simulation, exact analytical solutions are unattainable in this case

$$\begin{aligned}\partial_t \tilde{u}_t(x, y) &= \mathcal{D} \left(\nabla_x^2 + \nabla_y^2 \right) \tilde{u}_t(x, y) - \tau_0^{-1} \tilde{u}_t(x, y) \\ &\quad + \lambda C_N (v_t(x, y) + v_t(y, x)) - \frac{2\lambda}{N} \langle M n_t(x) n_t(y) \rangle \\ &\quad + \delta(x - y) \left(2\beta n_t(x) + \frac{2\lambda}{N} \langle M n_t(x) \rangle \right)\end{aligned}$$

$$\begin{aligned}\partial_t v_t(x, y) &= \mathcal{D} \nabla_x^2 v_t(x, y) - \lambda C_N v_t(x, y) - \frac{\lambda}{N} \langle M n(x) m(y) \rangle \\ &\quad + \beta \eta C_{N-1} \tilde{u}_t(x, y) + \lambda \tilde{w}_t(x, y) + \delta(x - y) \frac{\beta \eta N}{N-1} n_t(x)\end{aligned}$$

$$\partial_t \tilde{w}_t(x, y) = \beta \eta (v_t(x, y) + v_t(y, x)) - 2\lambda \tilde{w}_t(x, y)$$

$$\begin{aligned}\partial_t \tilde{u}_t(x, y) = & \mathcal{D} \left(\nabla_x^2 + \nabla_y^2 \right) \tilde{u}_t(x, y) - \left(\tau_0^{-1} + \frac{2\lambda M}{N} \right) \tilde{u}_t(x, y) \\ & + \lambda C_N (v_t(x, y) + v_t(y, x)) + 2\beta\delta(x - y)n_t(x)\end{aligned}$$

$$\begin{aligned}\partial_t v_t(x, y) = & \mathcal{D} \nabla_x^2 v_t(x, y) - \left(\frac{\beta\eta N}{M} + \lambda \frac{M}{N} \right) v_t(x, y) \\ & + \beta\eta C_{N-1} \tilde{u}_t(x, y) + \lambda \tilde{w}_t(x, y) \\ & + \delta(x - y) (2\beta\eta n_t(x) + \lambda m_t(x))\end{aligned}$$

$$\partial_t \tilde{w}_t(x, y) = \beta\eta C_M (v_t(x, y) + v_t(y, x)) - \frac{2\beta\eta N}{M} \tilde{w}_t(x, y)$$

The equation for the average is simply

$$\partial_t n_t(x) = \mathcal{D} \nabla_x^2 n_t(x) - \frac{\lambda M}{N} n(x, t) + \lambda M Q(x),$$

and for the pair correlation function we have

$$\begin{aligned}\partial_t \tilde{u}_t(x, y) &= \mathcal{D} \left(\nabla_x^2 + \nabla_y^2 \right) \tilde{u}_t(x, y) - \tau_1^{-1} \tilde{u}_t(x, y) \\ &\quad + \lambda M C_N (n_t(x) Q(y) + n_t(y) Q(x)) + 2\beta \delta(x - y) n_t(x)\end{aligned}$$

where $\tau_1 = \left(\frac{2\beta}{N-1} + \frac{2\lambda M}{N} \right)^{-1}$ is the renewal time for neutrons and $\tilde{u}_t(x, y) = u_t(x, y) - \delta(x - y) n_t(x)$ the modified pair correlation function.



Thanks! Any questions?