DE LA RECHERCHE À L'INDUSTRIE

STATISTICS OF FAMILY TREES IN KINETIC MONTE CARLO SIMULATIONS

Mercredi 7 décembre 2022

T. Bonnet D. Mancusi A. Zoia
CEA-SACLAY DES/ISAS/DM2S/SERMA/LTSD

PLAN

Context

A model of prompt neutron kinetics

A model of neutrons and precursors

Conclusions

Outline

Context

A model of prompt neutron kinetics

A model of neutrons and precursors

Conclusions

Reactor Physics

- The goal of reactor physics is to model the dynamics of a nuclear reactor. A simplified reactor model can be defined as follows:
  - Neutrons can induce scattering, sterile capture, or fission
  - Between events, they undergo exponential flights.
  - Fission produces (prompt) neutrons and fission fragments (heavy nuclei).
  - Some fission fragments (called “precursors”) are unstable and decay emitting “delayed” neutrons
- Several challenges: spatial heterogeneity, uncertainties on cross-sections, fuel burn-up, coupling with thermal-hydraulics through feedback effects. . .
- No analytical solutions: simulation codes are used, and there is a need for experimental validation. However, some experiments are hard to perform: operational or accidental transients. (cf. préconisations du Guide 28 ASN)

Monte Carlo (MC) Simulations

- Monte-Carlo Simulations (MC) give information on statistical moments of physical observables
  - Probabilistic approach emulating “real” physics: no *a priori* approximation, unlike deterministic solvers
  - Gives estimates of the statistical moments of interest, up to quantifiable uncertainties
  - Can be “analog”: simulates physics exactly; or “non-analog”: samples "modified" physics preserving 1st moments and modifies higher-order moments.
- Exact but slow: mostly used for validation of faster, albeit approximate, deterministic solvers in lieu of experiments.
- Stationary MC has been extensively studied over the year, while time-dependent (kinetic) MC was mostly unattainable, although needed for validation of deterministic transient simulations.

Kinetic MC

- Recent algorithmic breakthroughs by E. Hoogenboom & al [1], combined with computer's improvements allowed for time-dependent MC simulation.
- Challenge: existence of two time-scales:
  - Long timescale for precursors, up to several order of magnitude longer than for neutrons
  - Very costly: simulation of a single transient in a small research reactor can easily take thousands of hours of computing time [2]
- Need for efficient variance reduction methods (non-analog methods), and we need to understand their impact on simulations

Correlations and Fluctuations

- Previous works exhibited several issues in kinetic MC simulations:
  - “critical catastrophe": when the reactor is critical (i.e. parameters are tuned so that the population is constant on average), the variance diverges and after some time one fluctuation can kill the entire population.
  - “clustering": when critical, the distribution of neutrons can exhibit strong spatial heterogeneity with non-Poisson fluctuations [3, 4, 5].
- In real reactors, these phenomena are for the most part prevented because of feedback effects (and the large number of particles) that keep the variance finite
- Clustering has been shown to be directly related to the reproduction of neutrons; when a neutron undergoes fission, its children are correlated.
- The "fixation time" needed for all surviving neutrons to become correlated allows characterizing time-correlations in the system.

In This Work

- In what follows, we aim at characterizing the so-called **fixation time**, if possible analytically.
- The complexity of full-fledged reactor physics make it hard to understand precisely the working of some phenomena
- We will consider a simplified point-kinetics model retaining the key ingredients; neutron reproduction and death will be represented as a modified Galton-Watson process; feedback will be represented as population control mechanisms

Outline

Context

A model of prompt neutron kinetics

A model of neutrons and precursors

Conclusions

A model of prompt neutron kinetics

- Before diving in the full model of neutrons and precursors, one can consider the simpler case where only prompt neutrons are considered.
- Let N neutrons evolve in time following a spatially homogeneous Galton-Watson birth-death process. Each neutron can either induce fission with rate β (the neutron dies and yields on average ν_p children), or sterile capture with rate γ (the neutron dies without descendants).
  - We assume a critical system, which is embodied in the condition $\beta(\nu_p - 1) = \gamma$.
  - To simplify further, we consider binary fission: $\nu_p = 2$.
- Without population control, this system undergoes clustering and eventually leads to the critical catastrophe [6]
- An idealized feedback is introduced conditioning capture on fission: each excess neutron produced by fission is compensated by killing another randomly chosen neutron (the population is kept exactly constant).

Family trees and surnames

- The fixation time is closely related to the problem of the extinction of 'family names' in the Galton-Watson process. [7, 8]
- Recently, it has been revisited in the context of discrete-time [9] and continuous-time fission chain analysis [10].
- Let each source neutron be assigned an identifier in $\{1, \ldots, F\}$.
  - Neutrons sharing the same identifier form a family.
  - When a neutron induces fission, it transmits its identifier to its descendants; a family is extinct when the last of its member dies.
  - The number of existing families is thus a decreasing function of time.
- The population has reached **fixation** when there is only one surviving family left.

Fixation time and total expectation law

- Let a random variable τ_p be the fixation time for one MC replica. Insights on the statistics of τ_p can be obtained by restricting ourselves to the study of the fixation time for a family A of n initial individuals.
- Let $\mathbb{E}[\tau_p^k|A](n)$ be the k-th moment of τ_p *conditioned to the event of the fixation of family A*.
- Let $f_p(n)$ be the probability that fixation happens on family A. In our case, homogeneity allows for $f_p(n) = n/N$.
- The law of total expectation states that, if $\{A_i\}_i$ is a finite set of events and X is a random variable, then

$$\mathbb{E}[X] = \sum_i \mathbb{E}[X|A_i]P(A_i), \tag{1}$$

where $P(A_i)$ is the probability that event A_i happens.

Moment equations for the fixation time (1)

Eq.(1) translates to

$$f_p(n)\mathbb{E}\left[\tau_p^k|A\right](n) = \quad p_+ f_p(n+1)\mathbb{E}\left[(\tau_p+\delta(n))^k|A\right](n+1) \\ +p_- f_p(n-1)\mathbb{E}\left[(\tau_p+\delta(n))^k|A\right](n-1), \tag{2}$$

where $p_\pm$ is the probability that a transition from n to $n \pm 1$ happens.
$\delta(n) = (N-1)/[\beta n(N-n)]$ is the inverse of the rate of 'useful transitions'.

Moment equations for the fixation time (2)

Eq. (2) can be rewritten in the form of a simple difference equation:

$$\Delta g_k(n) = Q_k(n), \tag{3}$$

where $g_k(n) = n\mathbb{E}[\tau_p^k|A](n)$, Δ is the discrete Laplacian and $Q_k(n)$ is a source term depending on the order of the moment of interest.

Analytical solutions

Analytical solutions for the first two moments:

$$\mathbb{E}[\tau_p|A](n) = \frac{N-1}{\beta n}[1 - n + (N-n)(H_{N-1} - H_{N-n})] + (N-1)\tau_c, \tag{4}$$

with H_n the n-th harmonic number, and

$$\mathbb{E}[\tau^2|A](n) = \tau_2^S(n) - \mathbb{E}[\tau|A](n) + C_N, \tag{5}$$

where

$$\tau_2^S(n) = 2N\tau_c^2 \left(\frac{N}{n} \sum_{j=1}^{n-1} \frac{H_{N-j}(n-j)}{j} - [1 + NH_{N-1}]\,(H_n - 1) \right)$$

$$C_N = \tau_c^2 \left\{ 2N \left[(H_N - 1)(1 + NH_{N-1}) - \sum_{j=1}^{N-1} \frac{H_{N-j}(N-j)}{j} \right] - 1 \right\}.$$

Comparison with MC

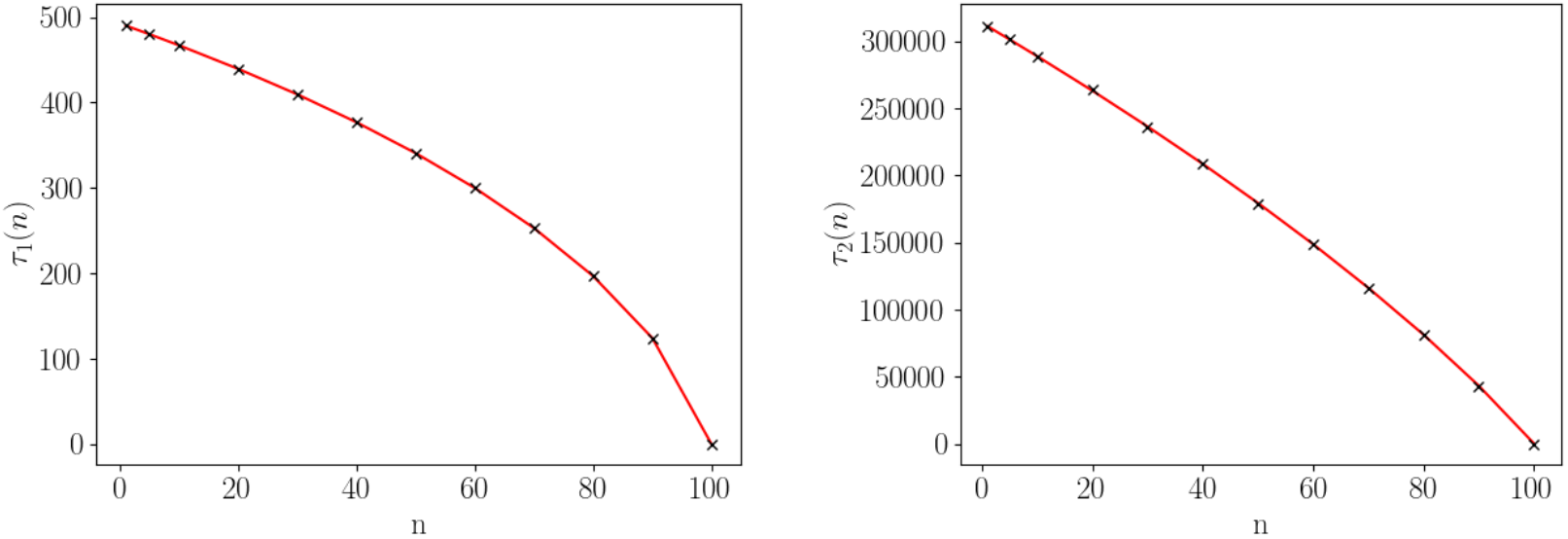


Figure 1: Fixation time $\tau_1(n)$ (left) and 2nd order statistical moment $\tau_2(n)$ (right) for $N = 100$. The fission rate is given by $\beta = 0.2$ with a yield of 2. Red: analytical solution; black: Monte Carlo solution with 10^6 replicas (error-bars are barely visible).

Outline

Context

A model of prompt neutron kinetics

A model of neutrons and precursors

Conclusions

Galton-Watson model with neutrons and precursors

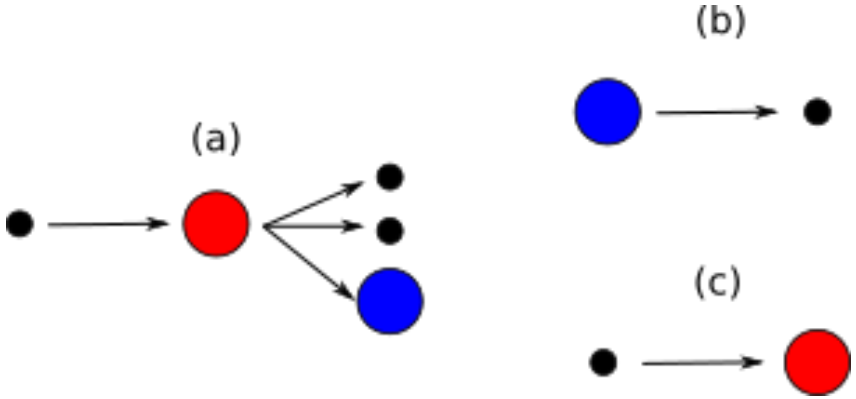


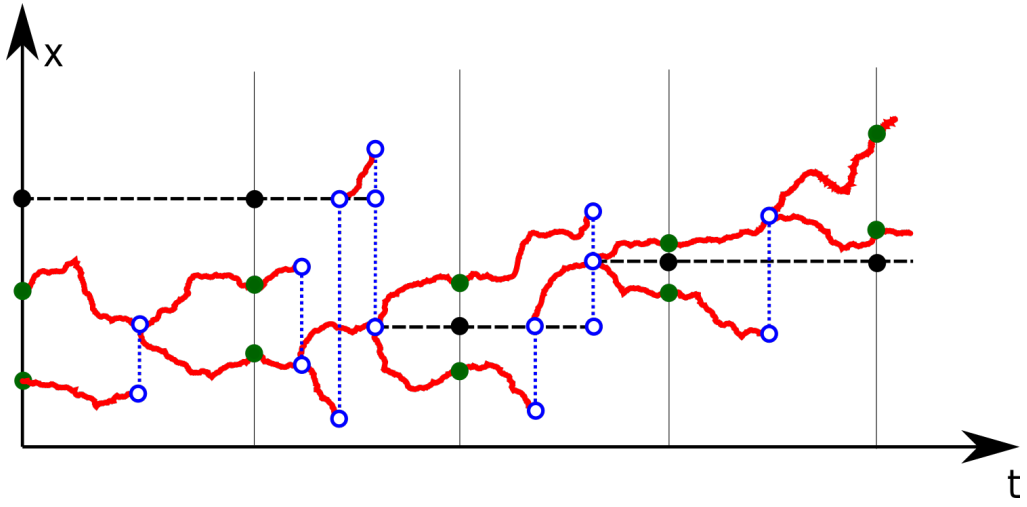
Figure 2: Stochastic events : (a) a neutron induces fission with rate β, on average yields ν_p prompt neutrons and ν_d precursors; (b) exponential decay of a precursor with rate λ; (c) sterile capture of a neutron with rate γ

- Time-scale separation driven by $\theta = \lambda/\beta\nu_d \ll 1$.
- Critical reactor: the average number of prompt neutrons (N) and precursors (M) is constant.
- Equilibrium source distribution : $M = N/\theta$

Adding population control to the previous model

- Mimic an ideal feedback effect on neutrons and precursors by enforcing strict population size conservation.
- The moment equations for space correlations yield an infinite hierarchy when enforcing population control only on N [10].
- In the following, we apply population control on N and M.
- $\theta \to 1$ implies both control schemes to have very similar behaviour when $M = N/\theta$.

Population control on N and M



- Capture is conditioned on fission events and decay event: whenever an excess neutron is produced, another randomly chosen neutron is killed.
- Precursor destruction is conditioned on fission events where a precursor is produced: precursors do not disappear when they decay.
- N and M are thus kept exactly constant.

Family trees and surnames

- Let each source particle be assigned an identifier in $\{1, \ldots, F\}$.
  - Particles sharing the same identifier form a family. Each family can be made of n neutrons and m precursors
  - When a neutron induces fission, it transmits its identifier to its descendants, and so does a precursor when it decays.
  - A family is extinct when the last of its member dies.
  - The number of families is thus a decreasing function of time.
- We restrict ourselves to the study of $\mathbb{E}[\tau^k|A](n)$, the k-th moment of the fixation time *conditioned to the event of the fixation of family A*

Fixation probability

- Useful transitions are $(n, m) \to (n + v_1, m + v_2)$ where $\mathbf{v} \in \{(\pm 1, 0), (0, \pm 1), \pm(1, 1)\}$. Let $p_{\mathbf{v}}$ be the probability that transition with rate $\beta_{\mathbf{v}}$ happens.
- Let $f_\tau(n, m)$ be the fixation probability for a family starting with n neutrons and m precursors. Relying again on the law of total expectation, an equation for $f_\tau(n, m)$ is

$$f_\tau(n, m) = \sum_{\mathbf{v} \in T} p_{\mathbf{v}} f_\tau(n + v_1, m + v_2) \tag{6}$$

- Its solution is

$$f_\tau(n, m) = \frac{Nn + M\theta m}{N^2 + \theta M^2}. \tag{7}$$

Moments of the fixation time

We can now write the general equation for the moments of the fixation time

$$f_\tau(n,m)\mathbb{E}[\tau^k|A](n,m) = \sum_{\mathbf{v}\in T} p_{\mathbf{v}} f_\tau(n+v_1, m+v_2)\left(\mathbb{E}[(\tau+\delta(n,m))^k|A](n+v_1, m+v_2)\right), \tag{8}$$

whose analytical solution we could not attain. However, Eq. (8) is a difference equation that can be straightforwardly solved numerically, without approximations

Comparison of first moment with MC

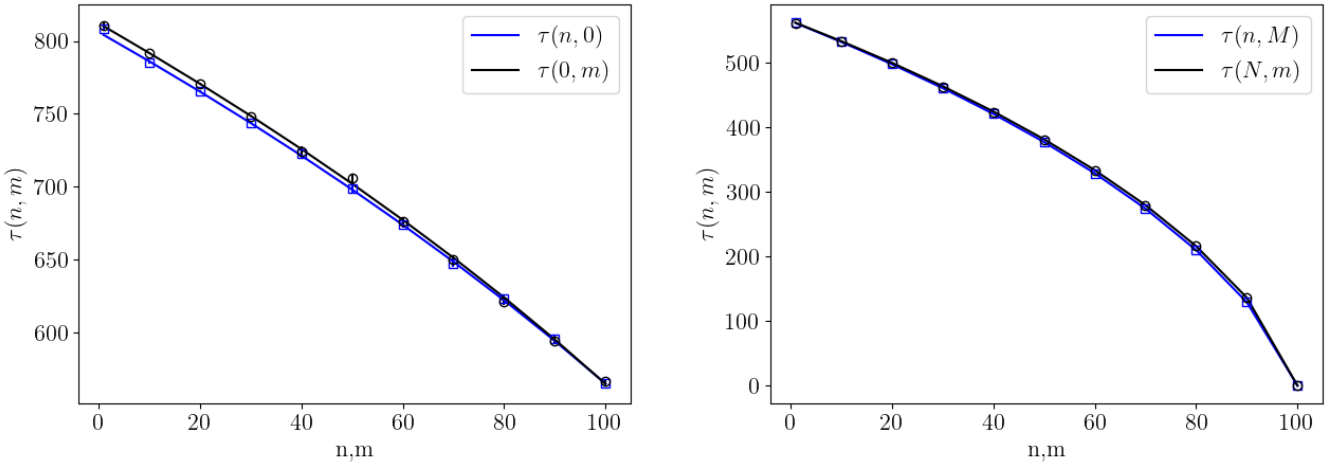


Figure 3: Cuts of the average fixation time $\tau(n, m)$ for $N = 100$, $M = 100$, $\beta = 0.2$, $\nu_d = 0.5$, and $\lambda = 0.1$, so that $\theta = 1$, showing Monte-Carlo simulations (with markers) and the numerical results (in solid lines).

- Left side: almost linear, and not a big difference between the influence of precursors and that of neutrons.
- Right side: the difference is even more subtle.

Comparison of second moment with MC

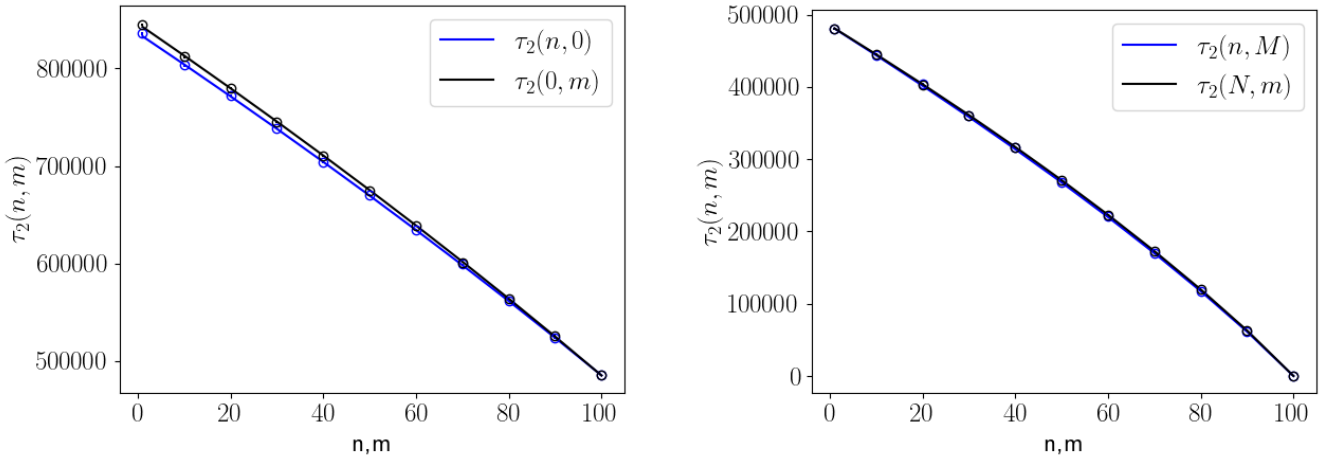
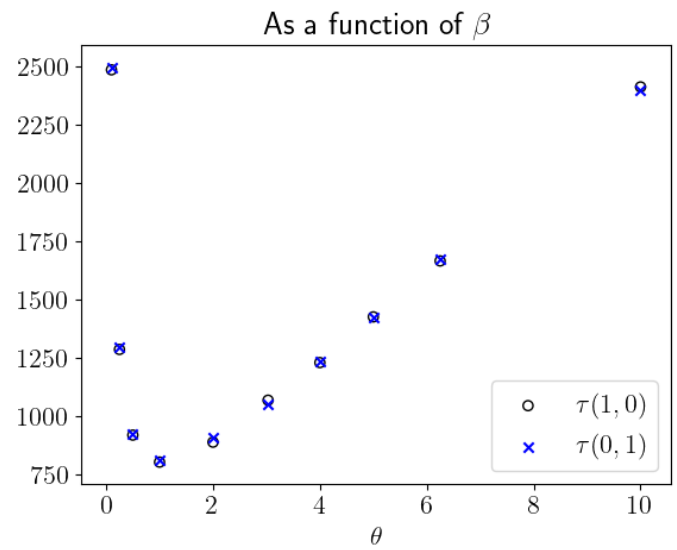
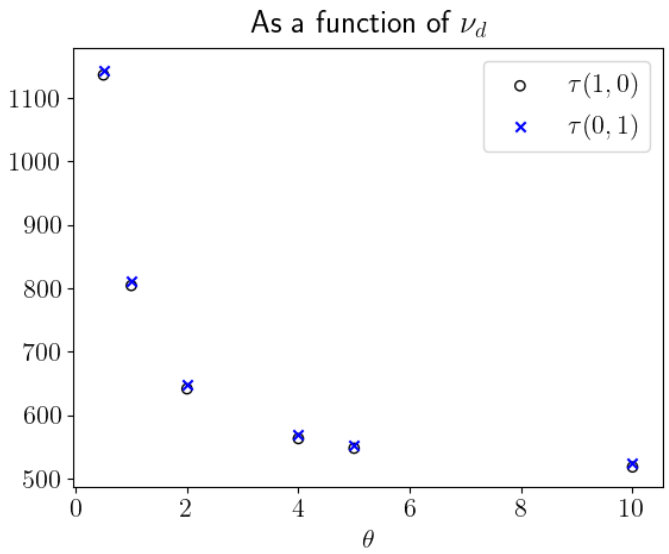


Figure 4: Cuts of the 2nd moment of the fixation time $\tau_2(n,m)$ for $N = 100$, $M = 100$, $\beta = 0.2$, $\nu_d = 0.5$, and $\lambda = 0.1$, so that $\theta = 1$, showing Monte-Carlo simulations (with markers) and the numerical results (in solid lines).

- The 2nd moment behaves as the 1st moment.

Parametric study





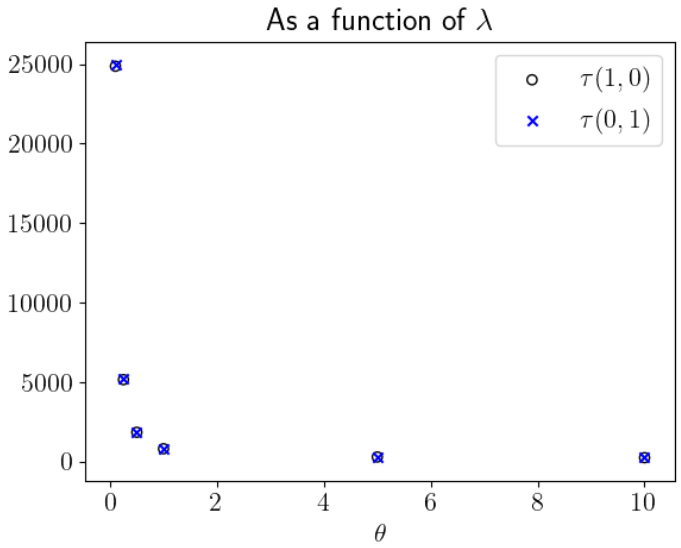


Figure 6: Dependence of the average fixation time with respect to different parameters. The equilibrium condition $N = \theta M$ is respected.

- $\theta \ll 1$ implies that τ increases.
- Also the case in a milder way when θ increases as β decreases.

Outline

Context

A model of prompt neutron kinetics

A model of neutrons and precursors

Conclusions

Conclusions

- In kinetic Monte Carlo simulation of nuclear reactors, fission-induced correlations strongly affect the statistics of the neutron and precursor populations.
- To improve our understanding of this behaviour, we have investigated a the ‘fixation time’ of particles within a modified Galton-Watson process with population control
- Particles sharing the same common ancestor in the source belong to families. The fixation time is the time for which only one family remains, i.e. all particles are correlated.
- We derived an exact equation for the fixation time of a population of neutrons and precursors under strict population control, and showed that the introduction of precursors considerably increases this time when $\theta \ll 1$.
- The prompt fixation time is the subject of a submission to M&C23.

References I

[1] B. L. Sjenitzer and J. E. Hoogenboom, “Dynamic Monte Carlo Method for Nuclear Reactor Kinetics Calculations,” *Nuclear Science and Engineering*, vol. 175, pp. 94–107, Sept. 2013.

[2] D. Mancusi, M. Faucher, and A. Zoia, “Monte Carlo simulations of the SPERT III E-core transient experiments,” *The European Physical Journal Plus*, vol. 137, p. 127, Jan. 2022.

[3] A. Zoia, E. Dumonteil, A. Mazzolo, C. de Mulatier, and A. Rosso, “Clustering of branching Brownian motions in confined geometries,” *Physical Review E*, vol. 90, p. 042118, Oct. 2014.

[4] P. Cosgrove, E. Shwageraus, and G. Parks, “Neutron clustering as a driver of Monte Carlo burn-up instability,” *Annals of Nuclear Energy*, vol. 137, p. 106991, Mar. 2020.

References II

[5] E. Dumonteil, R. Bahran, T. Cutler, B. Dechenaux, T. Grove, J. Hutchinson, G. McKenzie, A. McSpaden, W. Monange, M. Nelson, N. Thompson, and A. Zoia, "Patchy nuclear chain reactions," *Communications Physics*, vol. 4, pp. 1–10, July 2021.

[6] M. Meyer, S. Havlin, and A. Bunde, "Clustering of independently diffusing individuals by birth and death processes," *Physical Review E*, vol. 54, pp. 5567–5570, Nov. 1996.

[7] Y. C. Zhang, M. Serva, and M. Polikarpov, "Diffusion reproduction processes," *Journal of Statistical Physics*, vol. 58, pp. 849–861, Mar. 1990.

[8] M. Serva, "On the genealogy of populations: Trees, branches and offspring," *Journal of Statistical Mechanics: Theory and Experiment*, vol. 2005, pp. P07011–P07011, July 2005.

References III

[9] T. M. Sutton, “Toward a More Realistic Analysis of Neutron Clustering,” *Nuclear Science and Engineering*, pp. 1–12, May 2022.

[10] T. Bonnet, D. Mancusi, and A. Zoia, “Space and time correlations for diffusion models with prompt and delayed birth-and-death events,” *Physical Review E*, vol. 105, p. 064105, June 2022.

Thanks! Any questions?