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Gaussian approximation to the resolution of master equations

Luis F. Lafuerza, Raúl Toral

IFISC (CSIC-UIB) Palma de Mallorca – Spain.

luis@ifisc.uib-csic.es

Formulation

■ We consider general master equations of the form:

$$\frac{\partial P(n,t)}{\partial t}=\sum_{k=-\infty}^{\infty}(E^k-1)\left[\frac{G_k(n)}{\Omega^{g_k-1}}P(n,t)\right]$$

E: Linear operator such that E[f(n)]=f(n+1)
G_k: Polynomial of degree g_k
Ω: Large parameter of the system (typically the system size)

■ Exact equations for mean value and variance:

$$\frac{d\langle n\rangle}{dt}=\sum_{k=-\infty}^{\infty}\frac{-k}{\Omega^{g_k-1}}\langle G_k(n)\rangle$$

$$\frac{d\langle n^2\rangle}{dt}=\sum_{k=-\infty}^{\infty}\frac{1}{\Omega^{g_k-1}}\langle (k^2-2\mathrm{kn})G_k(n)\rangle$$

We obtain a closed system of equations if we write higher order moments as a function of the two first. We do so as if the probability distribution was Gaussian (non arbitrary assumption since van Kampen's expansion [1] shows that the probability distribution is Gaussian except terms of order $\Omega^{-1/2}$):

Moment	Gaussian approximation
$\langle n^3\rangle$	$\langle n^3\rangle_G=3\langle n^2\rangle\langle n\rangle-2\langle n\rangle^3$
$\langle n^4\rangle$	$\langle n^4\rangle_G=3\langle n^2\rangle^2-2\langle n\rangle^4$
$\langle n^5\rangle$	$\langle n^5\rangle_G=15\langle n^2\rangle^2\langle n\rangle-20\langle n^2\rangle\langle n\rangle^3+6\langle n\rangle^5$
$\langle n^6\rangle$	$\langle n^6\rangle_G=15\langle n^2\rangle^3-30\langle n^2\rangle\langle n\rangle^4+45\langle n\rangle^6$

2 variables

Moment	Gaussian approximation
$\langle n_1^2 n_2\rangle$	$\langle n_1^2\rangle\langle n_2\rangle+2\langle n_1\rangle\langle n_1 n_2\rangle-2\langle n_1\rangle^2\langle n_2\rangle$
$\langle n_1^2 n_2^2\rangle$	$\langle n_1^2\rangle\langle n_2^2\rangle+2\langle n_1 n_2\rangle^2-2\langle n_1\rangle^2\langle n_2\rangle^2$
$\langle n_1^3 n_2\rangle$	$3\langle n_1^2\rangle\langle n_1 n_2\rangle-2\langle n_1\rangle^3\langle n_2\rangle$

Ansatz: $n=\Omega\varphi+\Omega^{1/2}\xi$ $\quad\rightarrow\quad \frac{\langle n^k\rangle_G}{\Omega^k}=\frac{\langle n^k\rangle}{\Omega^k}+O(\Omega^{-1/2})$

	Error in $\langle n\rangle$	Error in σ^2
Gaussian approximation	$O(\Omega^{-1/2})$	$O(\Omega^{1/2})$
1st order van Kampen´s expansion	$O(\Omega^0)$	$O(\Omega^{1/2})$

Examples

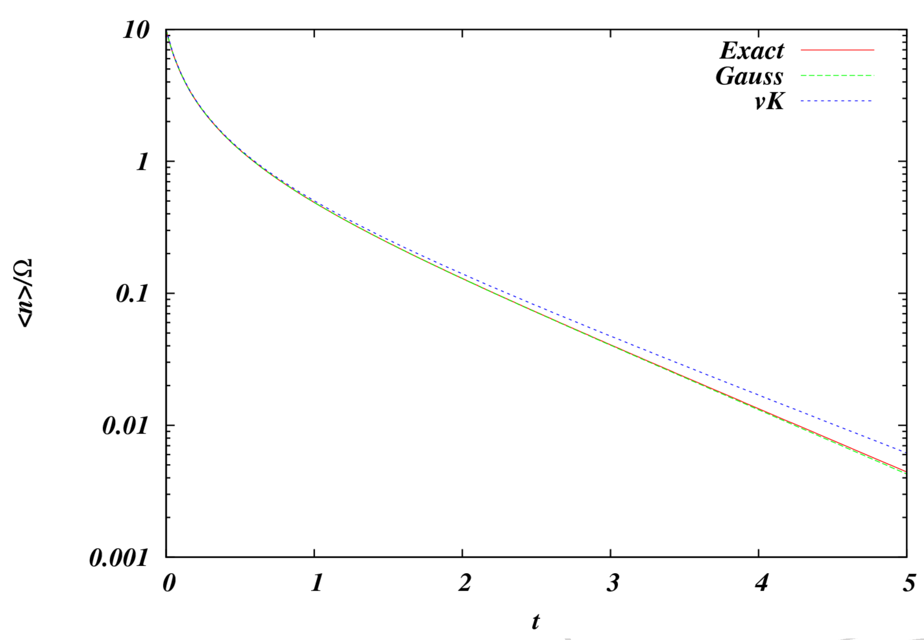
Reaction-limited process: A + B → 0

Master equation: $\frac{\partial P(n,t)}{\partial t}=\frac{\kappa}{\Omega}[(n+1)(\Delta+n+1)P(n+1,t)-n(n+\Delta)P(n,t)]$

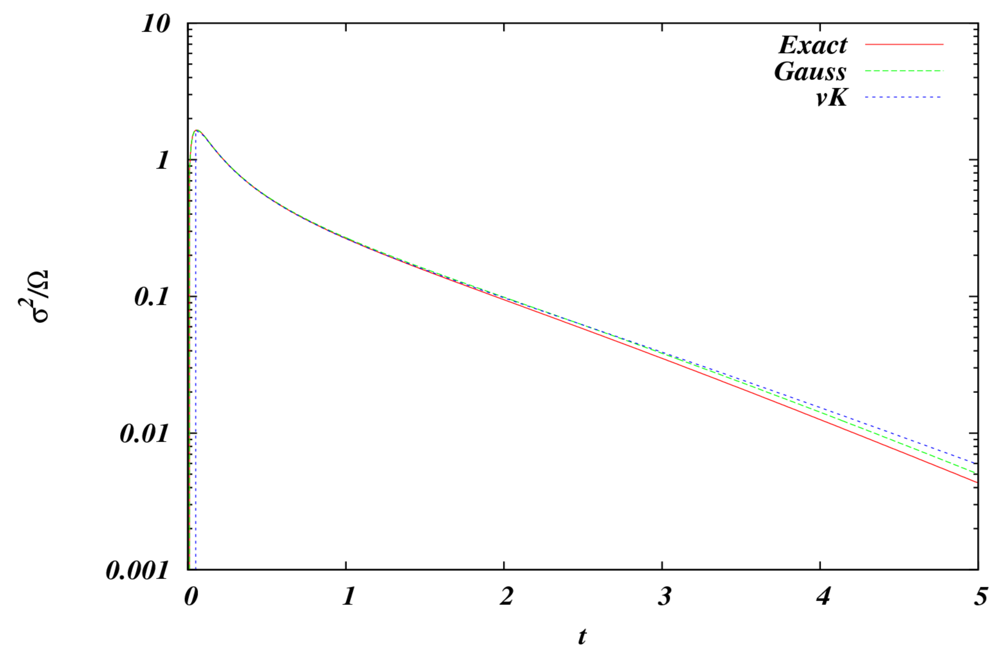
Exact solution: $P(n,t)=\sum^{M} C_k(\Delta,M)B_{n,k}(\Delta)e^{-k(k+\Delta)\kappa t/\Omega}$

M: initial number of particles

n: number of particles of specie A
Δ: difference of the number of A and B particles
Ω: volume of the system



Gaussian approximation (green) is almost indistinguishable from the exact result (red). 1st order van Kampen's expansion gives clearly different result.



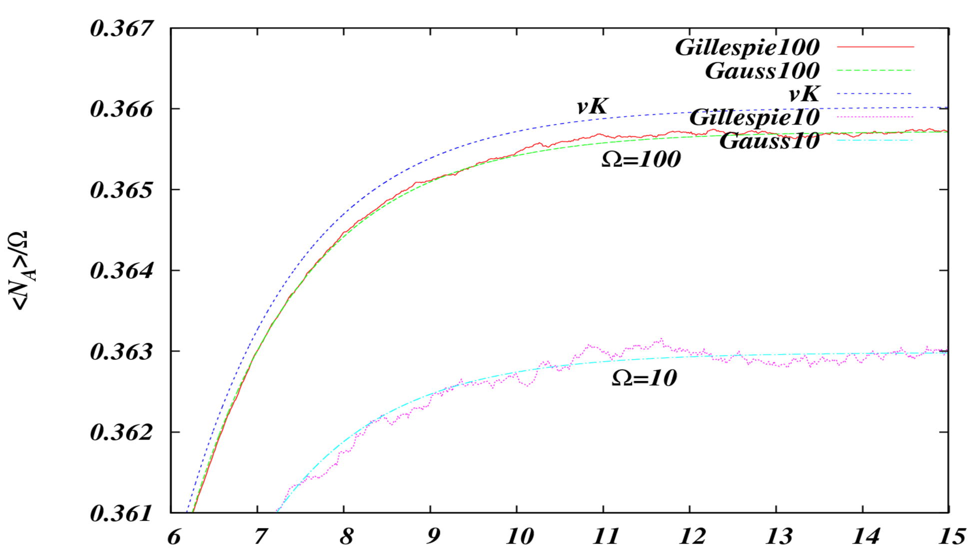
Gaussian approximation (green) is again closer to the exact result (red) than van Kampen's expansion.

Opinion formation

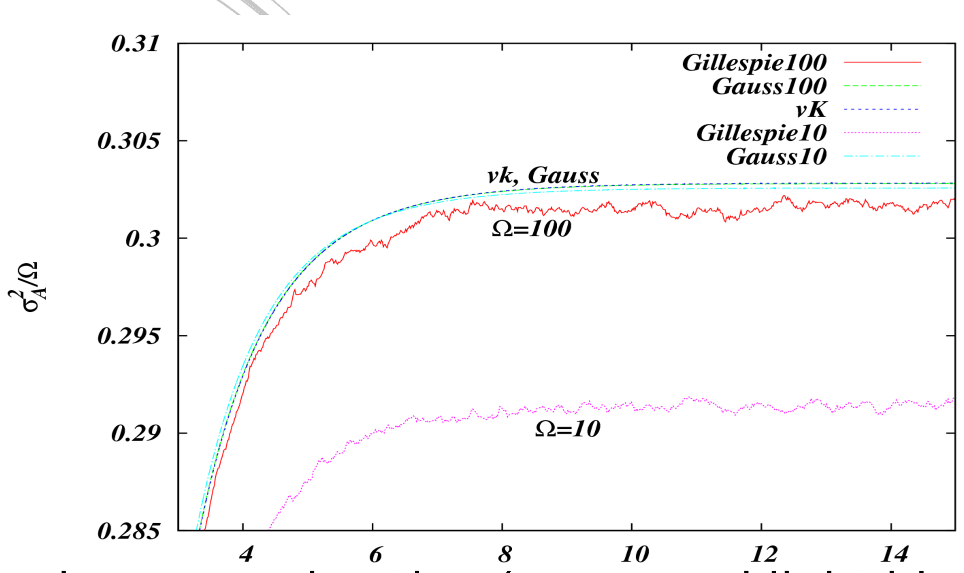
Opinion formation modeled as in [2]:
- 2 parties (A and B) plus a group of undecided agents (I).
- Spontaneous transitions: A → I, I → A, B → I, I → B (rates $\alpha_1,\alpha_2,\alpha_3,\alpha_4$)
- Convincing rules: A + I → 2A, B + I → 2B (rates β_1,β_2)

To compare, we simulate the process with the Gillespie method.

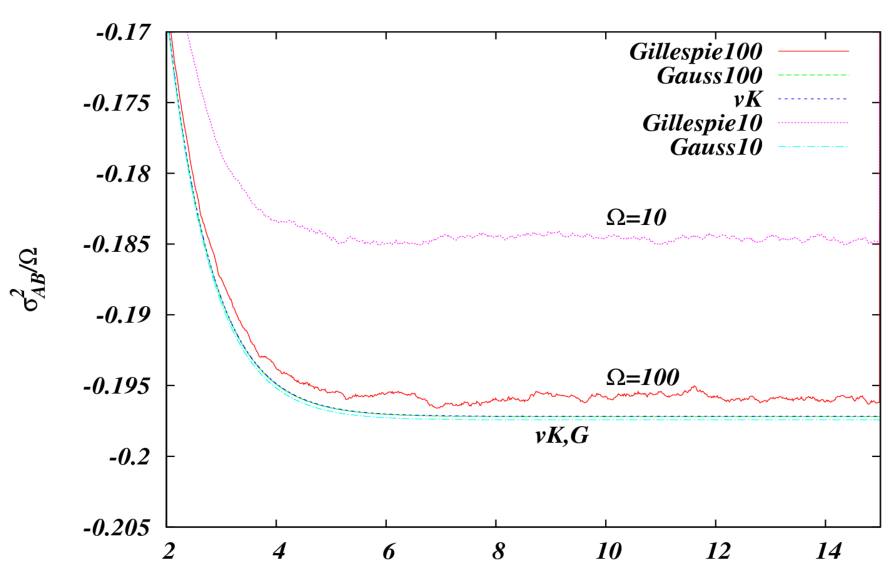
$$\begin{aligned}\frac{\partial P(N_A,N_B,t)}{\partial t}=&\alpha_1(N_A+1)P(N_A+1,N_B,t)+\alpha_3(N_B+1)P(N_A,N_B+1,t)\\&+\alpha_2(\Omega-N_A-N_B+1)P(N_A-1,N_B,t)+\alpha_4(\Omega-N_A-N_B+1)P(N_A,N_B-1,t)\\&+(\Omega-N_A-N_B+1)\left[\frac{\beta_1}{\Omega}(N_A-1)P(N_A-1,N_B,t)+\frac{\beta_2}{\Omega}(N_B-1)P(N_A,N_B-1,t)\right]\\&-\left[\alpha_1N_A+\alpha_3N_B+(\alpha_2+\alpha_4)(\Omega-N_A-N_B)+\frac{\beta_1N_A+\beta_2N_B}{\Omega}(\Omega-N_A-N_B)\right]P(N_A,N_B,t)\end{aligned}$$



Gaussian approximation (green and light blue) follows precisely the Gillespie result whereas van Kampen's expansion (doted blue, independent of Ω) differs clearly, specially for Ω=10.



Gaussian approximation (green and light blue) are almost independent of system size and very close to van Kampen's results (dotted blue). Both are close to Gillespie results for Ω=100, but differ clearly for Ω=10.



Again Gaussian approximation is very close to van Kampen's expansion and both methods fail for small Ω.

References

■ [1] N. G. van Kampen, Stochastic Processes in Physics and Chemistry (North-Holland, Amsterdam, 2004), chap. X.
■ [2] M.S. De la Lama, I.G. Szendro, J.R. Iglesias, H.S. Wio, Eur. Phys. J. B **51**, 435-442 (2006).

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