Lyapunov exponent of a Lennard-Jones gas: cumulant expansion

Raúl O. Vallejos, Celia Anteneodo, Leonardo Cirto

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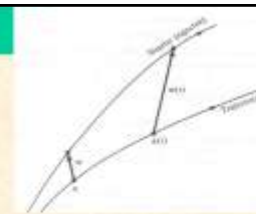
The Lyapunov exponent



Dynamical system:

$$\frac{dx}{dt} = f(x), \quad x \in \Re^n$$

Asymptotically, $|w(t)| = |w| e^{\lambda t}$

In the limit $|w| \to 0,\ w \to \xi,$ we obtain the tangent dynamics

$$\frac{d\xi}{dt} = Df_{x(t)} \cdot \xi$$

Linear system of differential equations with time-dependent coefficients

Operational definition of Lyapunov exponent :

$$\lambda = \lim_{t\to\infty} \frac{1}{t} \ln |\xi(t)|$$

λ does not depend on initial conditions x_0, ξ_0

Lyapunov exponent II

λ indicates *sensitivity to initial conditions, instability, unpredictability* = chaos

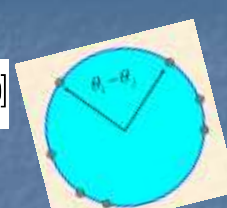
Useful concept in system modeling (economy, biology, meteorology) ; astronomy, etc.

Curiosity : solar system, $1/\lambda$ = 4 million yrs.
A 15 meter error in Earth's position today makes it impossible to predict where the Earth will be in 100 million yrs
(J. Laskar, Nature 1989).

In statistical physics,
$\lambda > 0$ is necessary for the validity of microcanonical formalism
$\lambda = 0$ signals thermodynamic anomalies

HMF

$$H = \sum_{i=1}^{N} \frac{L_i^2}{2I} + \frac{J}{2N} \sum_{i,j=1}^{N} \left[1 - \cos\left(\theta_i - \theta_j\right)\right]$$



Quasi-equilibrium states

Lifetime diverges as **N → ∞, E/N = fixed**

Properties : anomalous diffusion, non Maxwell-Boltzmann velocity distributions, aging, negative specific heat ...

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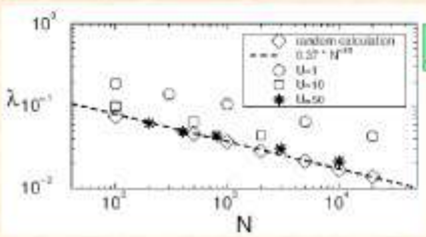
Empirical scaling laws : (1) $\lambda(N)$

Latora, Rapisarda & Ruffo, 1998

High energy and $N \to \infty$



$\lambda \approx N^{-1/3}$

Theoretical explanation ? Yes … (heuristic)

- M.-C. Firpo, PRE98 (geometric method)
- C. Anteneodo & ROV, PRE01 (random matrix theory)

Theories

a) Rigid-sphere systems : well developed theory

Krylov (~1940), Sinai (~1970), Gaspard, Dorfman & van Beijeren (>1990)

b) Smooth Hamiltonians, possibly long-range

geometric method

Casetti, Livi & Pettini, 1995
Casetti, Clementi & Pettini, 1996
Casetti, Pettini, EGD Cohen, 2000

random matrices

Benettin, 1984
Paladin, Vulpiani, Parisi, Ruffo, Crisanti, … >1985

supersymmetric method

Tanase-Nicola & Kurchan, 2003

stochastic approach

Barnett, 1996
Anteneodo & ROV, 2002

A theory for λ -- (I) Introduction

Hamilton equations in compact form

$$\frac{dx}{dt} = J\nabla H(x) \qquad x = (q_1, \ldots, q_N; p_1, \ldots, p_N) \qquad J = \begin{pmatrix} \underline{0} & \underline{1} \\ -\underline{1} & \underline{0} \end{pmatrix}$$

Tangent dynamics

$$\frac{d\xi}{dt} = J\,\underline{\mathrm{H}}[x(t)]\,\xi \equiv A(t)\,\xi$$

linear differential equations

$\underline{\mathrm{H}}$, $\underline{\mathrm{V}}$ Hessian matrices

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + V(q_1, \ldots q_N) \quad \Rightarrow \quad A(t) = \begin{pmatrix} \underline{0} & \underline{1} \\ -\underline{\mathrm{V}}(t) & \underline{0} \end{pmatrix}$$

A theory for λ – Formal solution

$$\frac{d\xi}{dt} = A(t)\xi \quad \Leftrightarrow \quad \frac{d\psi}{dt} = -iH(t)\psi$$

Analogous to a Schrödinger equation with a time-dependent non-hermitian Hamiltonian

Formal solution and starting point :

$$\xi(t; x_0, \xi_0) = T\, e^{\int_0^t A(t_1; x_0)\,dt_1}\, \xi_0$$

A theory for λ --- First steps

Simplification : λ = λ(E), does not depend on initial conditions, we can add an average

$$\lambda = \lim_{t\to\infty} \frac{1}{2t} \left\langle \ln |\xi|^2 \right\rangle_{x_0, \xi_0}$$

$\langle \cdots \rangle_{x_0}$ microcanonical average

Aproximation # 1 : exchange average and logarithm

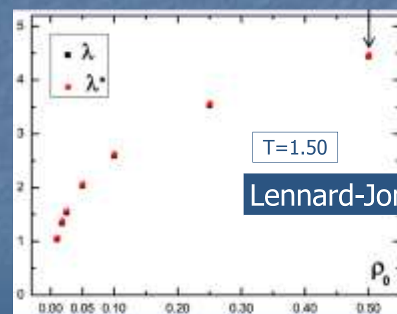
$$\lambda \approx \lim_{t\to\infty} \frac{1}{2t} \ln \left\langle |\xi|^2 \right\rangle_{x_0, \xi_0} \equiv \lambda'$$

may be tested a posteriori

If not : replica trick, supersymmetric approach, ...

Tanase-Nicola & J. Kurchan cond-mat/0210380

Generalized vs standard LE



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A theory for $\left\langle |\xi|^2 \right\rangle = Tr \left\langle \xi \xi^T \right\rangle$

ROV & C. Anteneodo, PRE02
D. M. Barnett et al, PRL96

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + V(q_1, \dots q_N), \quad \dot{\xi} = A(t)\xi, \quad A(t) = \begin{pmatrix} \underline{\underline{0}} & \underline{\underline{1}} \\ -\underline{\underline{V}}(t) & \underline{\underline{0}} \end{pmatrix}$$

Evolution equation for $\langle \xi \xi^T \rangle$

$$\frac{d\xi}{dt} = A\xi \Rightarrow \frac{d}{dt}\xi\xi^T = A\xi\xi^T + \xi\xi^T A^T \equiv \hat{A}\xi\xi^T$$

$\hat{A}$ is a linear operator

Solution :

$$\left\langle \xi\xi^T(t) \right\rangle_{x_0, \xi_0} = \left\langle T\, e^{\int_0^t \hat{A}(t_1; x_0) dt_1} \right\rangle_{x_0} \underbrace{\left\langle \xi_0 \xi_0^T \right\rangle_{\xi_0}}_{\propto \underline{\underline{1}}}$$

Preparing the perturbative expansion :

$$A = \langle A \rangle + \delta A(t) = \begin{pmatrix} \underline{\underline{0}} & \underline{\underline{1}} \\ -\langle \underline{\underline{V}} \rangle & \underline{\underline{0}} \end{pmatrix} + \begin{pmatrix} \underline{\underline{0}} & \underline{\underline{0}} \\ -\delta \underline{\underline{V}}(t) & \underline{\underline{0}} \end{pmatrix} \Rightarrow \hat{A} = \langle \hat{A} \rangle + \delta \hat{A}$$

The cumulant expansion (Kubo, van Kampen, Fox)

Fluctuations of small amplitude and/or short correlation time

$$\left\langle T\, e^{\int_0^t \hat{A}(t_1; x_0) dt_1} \right\rangle = e^{\hat{O}t}$$

$\hat{O}$ is time-independent

$$\hat{O} = \langle \hat{A} \rangle + \int_0^{\infty} d\tau \left\langle \delta\hat{A}(t) e^{\tau \langle \hat{A} \rangle} \delta\hat{A}(t-\tau) e^{-\tau \langle \hat{A} \rangle} \right\rangle + \cdots$$

average + integrated autocorrelation function + ...

Domain of validity (estimate) :

$t >> \tau_c$ — τ_c correlation time

$\sigma \tau_c << 1$ — σ fluctuation amplitude

Cumulant expansion

$$\left\langle e^{ikx}\right\rangle = \sum_{n=0}^{\infty}\frac{(ik)^n}{n!}\boxed{\mu_n} \overset{\text{Gaussian}}{=} e^{-\frac{1}{2}k^2\langle x^2\rangle}$$

$$\mu_n = \left\langle x^n \right\rangle$$

or

cumulants

$$\left\langle e^{ikx}\right\rangle \equiv e^{\sum_{n=1}^{\infty}\frac{(ik)^n}{n!}\boxed{\kappa_n}} \Leftarrow \ln\langle\cdots\rangle = \sum_n a_n \kappa_n$$

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Lyapunov exponent

$$\left\langle |\xi|^2 \right\rangle = Tr\left\langle \xi\xi^T(t)\right\rangle = Tr\, e^{\hat{O}t}\underline{1}$$

The Lyapunov exponent is given by $\lambda = \frac{1}{2}\Re(L_{\max})$

$L_{\max}$ → eigenvalue of Ô with the largest real part

We must calculate and diagonalize Ô (non-hermitean) $6N \times 6N$

It suffices to consider the restriction of Ô to the subspace $\left\{\underline{1}, \hat{O}\underline{1}, \hat{O}^2\underline{1}, \ldots\right\}$

Second-order approximation

$$\hat{O} = \left\langle \hat{A}\right\rangle + \int_0^{\infty} d\tau \left\langle \delta\hat{A}(t) e^{\tau\langle\hat{A}\rangle}\delta\hat{A}(t-\tau)e^{-\tau\langle\hat{A}\rangle}\right\rangle \qquad \sigma\tau_c << 1$$

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Second-order approximation

$$\hat{O} = \left\langle \hat{A}\right\rangle + \int_0^{\infty} d\tau \left\langle \delta\hat{A}(t) e^{\tau\langle\hat{A}\rangle}\delta\hat{A}(t-\tau)e^{-\tau\langle\hat{A}\rangle}\right\rangle \qquad \sigma\tau_c << 1$$

Approximate the free propagator :

$$e^{\tau\langle\hat{A}\rangle} \approx e^{\tau\hat{A}_0} \qquad \langle A\rangle = \begin{pmatrix} \underline{0} & \underline{1} \\ -\langle\underline{V}\rangle & \underline{0}\end{pmatrix} = \begin{pmatrix} \underline{0} & \underline{1} \\ \underline{0} & \underline{0}\end{pmatrix}$$

can be relaxed

Validity : quasi-ballistic regimes,

$$\tau_c < \tau(\underline{V})$$

Diagonalization (HMF)

$$H = \sum_i \frac{L_i^2}{2} + \frac{J}{2N}\sum_{i,j}\left[1-\cos(\theta_i - \theta_j)\right]$$

A basis for HMF :

(i) all particles are statistically equivalent
(ii) all pairs are also equivalent

For HMF one can prove that the subspace $\left\{\underline{1}, \hat{O}\underline{1}, \hat{O}^2\underline{1}, \ldots\right\}$ is six-dimesional

A suitable basis :

$$\begin{pmatrix} \underline{1} & 0 \\ 0 & 0\end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & \underline{1}\end{pmatrix}, \begin{pmatrix} 0 & \underline{1} \\ \underline{1} & 0\end{pmatrix}, \begin{pmatrix} \underline{Z} & 0 \\ 0 & 0\end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & \underline{Z}\end{pmatrix}, \begin{pmatrix} 0 & \underline{Z} \\ \underline{Z} & 0\end{pmatrix}$$

$$\left\langle Z_{ij}\right\rangle = \begin{cases} 1, & i \neq j \\ 0, & i = j\end{cases}$$

Diagonalizing HMF

The contribution of subspace Z is negligible for large N.
It suffices to consider the "isotropic" basis

$$\begin{pmatrix} \underline{1} & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & \underline{1} \end{pmatrix}, \begin{pmatrix} 0 & \underline{1} \\ \underline{1} & 0 \end{pmatrix}$$

The "isotropic" basis amounts to a mean field approximation in tangent space, *i.e.*, one *effective* degree of freedom.

Observation :
The mean field approximation is exact for HMF ;
it is also exact for a homogeneous gas in 3D.

Second-order + mean-field diagonalization

$$\begin{pmatrix} \underline{1} & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & \underline{1} \end{pmatrix}, \begin{pmatrix} 0 & \underline{1} \\ \underline{1} & 0 \end{pmatrix}$$ orthogonal set $\leftarrow \langle A, B \rangle = \mathrm{Tr}\, AB^T$

$$\|\hat{O}\|_{ij} = \frac{\mathrm{Tr}\,(\hat{O} I_j) I_i^T}{\mathrm{Tr}\, I_j I_i^T}$$

$$\|\hat{O}\| = \begin{pmatrix} 0 & 0 & 2 \\ 2\sigma^2\tau_c^{(1)} & -2\sigma^2\tau_c^{(1)} & -2\mu \\ -\mu + 2\sigma^2\tau_c^{(2)} & 1 & -2\sigma^2\tau_c^{(2)} \end{pmatrix}$$

Definitions :

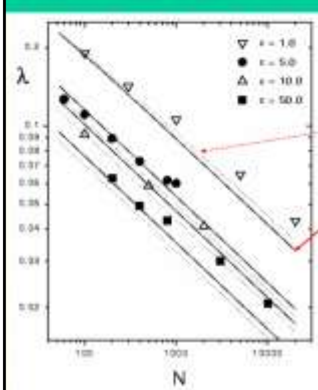
$$\mu = \frac{1}{N}\mathrm{Tr}\langle \underline{\underline{V}} \rangle \qquad \sigma^2 = \frac{1}{N}\mathrm{Tr}\langle (\delta \underline{\underline{V}})^2 \rangle \qquad \tau_c^{(k)} = \int_0^\infty d\tau\, \tau^{k-1} f(\tau)$$

$$f(\tau) = \frac{1}{N\sigma^2}\mathrm{Tr}\langle \delta\underline{\underline{V}}(0)\,\delta\underline{\underline{V}}(\tau) \rangle = \frac{1}{N\sigma^2}\sum_{i,j=1}^{N} \langle \delta V_{ij}(0)\,\delta V_{ij}(\tau) \rangle$$

$\tau_c^{(1)}$ correlation time

normalized autocorrelation function

HXYMF J=1 E>3/4 (II) $\lambda = \lambda(\mu, \sigma; f)$



simulations
Latora, Rapisarda & Ruffo, 1998
Anteneodo & Tsallis, 1998

geometric method
M.-C. Firpo, 1998

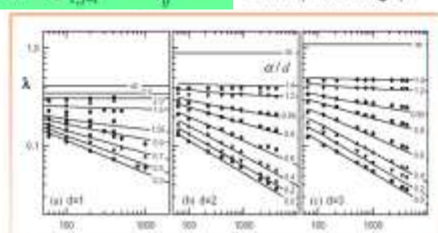
perturbative + mean field,
Anteneodo, Maia & Vallejos

reasonable agreement,
especially for N < 500

correct scaling law $\lambda = N^{-1/3}$

deviations → slow relaxation ?

$$H = \sum_{i=1}^{N} \frac{L_i^2}{2I} + \frac{J'}{2}\sum_{i,j=1}^{N} \frac{1-\cos(\theta_i - \theta_j)}{r_{ij}^{\alpha}}$$ α-XY (finite range)



Vallejos & Anteneodo, Physica A (2004)

numerical results (Benettin's algorithm)

$$\lambda = \left(\frac{\sigma^2 \tau_c^{(1)}}{2}\right)^{1/3}$$

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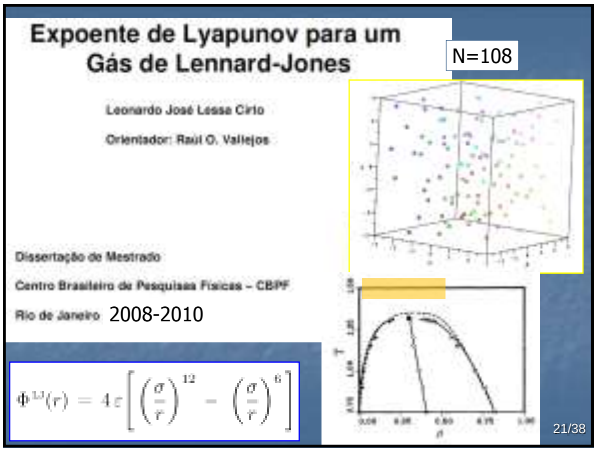
Expoente de Lyapunov para um Gás de Lennard-Jones
N=108
Leonardo José Lessa Cirto
Orientador: Raúl O. Vallejos
Dissertação de Mestrado
Centro Brasileiro de Pesquisas Fisicas – CBPF
Rio de Janeiro 2008-2010
$\Phi^{\text{LJ}}(r) = 4\,\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$
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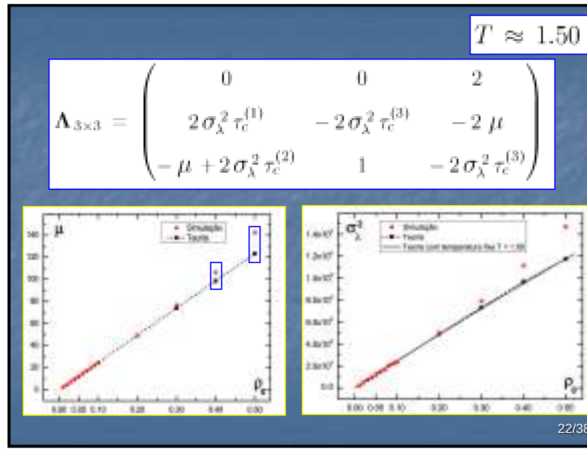
$T \approx 1.50$
$\Lambda_{3\times3} = \begin{pmatrix} 0 & 0 & 2 \\ 2\sigma_\lambda^2\tau_c^{(1)} & -2\sigma_\lambda^2\tau_c^{(3)} & -2\mu \\ -\mu + 2\sigma_\lambda^2\tau_c^{(2)} & 1 & -2\sigma_\lambda^2\tau_c^{(3)} \end{pmatrix}$
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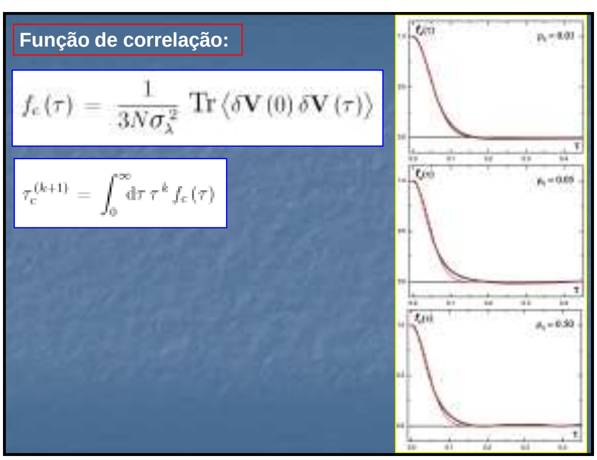
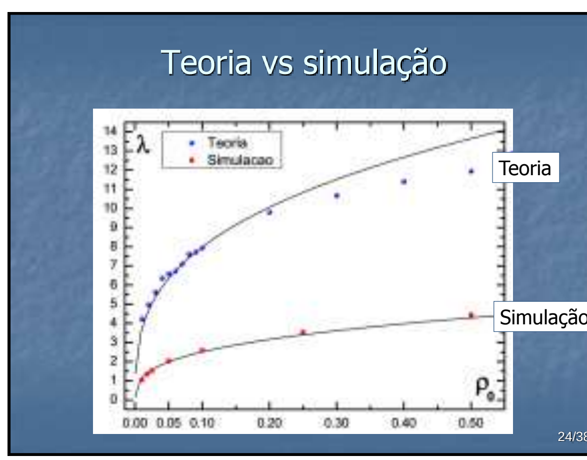

Função de correlação:
$f_c(\tau) = \frac{1}{3N\sigma_\lambda^2}\,\mathrm{Tr}\,\langle \delta\mathbf{V}(0)\,\delta\mathbf{V}(\tau)\rangle$
$\tau_c^{(k+1)} = \int_0^\infty \mathrm{d}\tau\,\tau^k f_c(\tau)$


Teoria vs simulação
Teoria
Simulacao
Teoria
Simulação
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Possible reasons for failure

- Isotropic aproximation?
- Generalized exponent?
- Truncation of the cumulant expansion?

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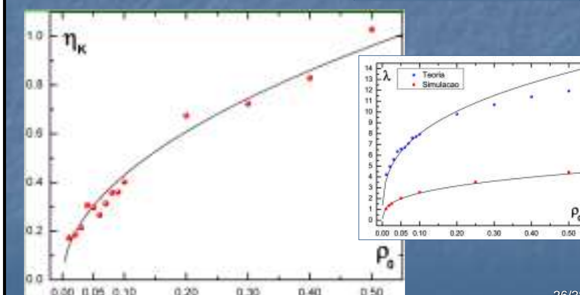
The Kubo number

$$\eta_K = \sigma_\lambda \left(\tau_c^{(1)}\right)^2 \propto \sqrt{\rho_0}$$



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Third, fourth cumulants?

- Study one degree of freedom problem!
- Formally similar to the isotropic N-body
- Much simpler, even exact in some cases

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One-dimensional Kubo oscillator

Anteneodo & Vallejos (2010)

$$\frac{d^2x}{dt^2} + \alpha\frac{dx}{dt} + \left(1+\xi(t)\right)x = 0$$

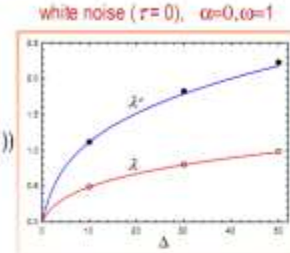
$$\langle \xi(t)\xi(t')\rangle = \frac{\Delta}{2\tau}\exp(-|t-t'|/\tau)$$

white noise ($\tau = 0$), $\alpha=0, \omega=1$

$\hat{\lambda}$: Malick, Peyneau (2006)

$$\hat{\lambda} = \frac{1}{2}\,\text{Max Re}\{\text{Eigenvalues}(K)\}$$

$$K = \begin{pmatrix} 0 & 0 & 2 \\ \Delta & -2\alpha & -2 \\ -1 & 1 & -\alpha \end{pmatrix}$$



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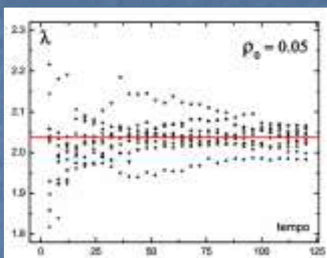
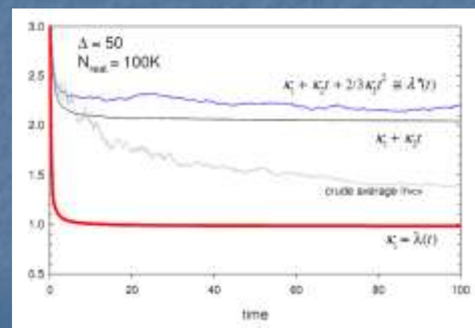
Generalized LE and finite-time LEs



$$\lambda = \lim_{t\to\infty} \frac{1}{2t}\left\langle \ln|\xi|^2 \right\rangle_{x_0,\xi_0}$$

$$\lambda^*(t) = \frac{\ln\left\langle d^2(t)\right\rangle}{2t} = \frac{\ln\left\langle e^{2\tilde{\lambda}(t)t}\right\rangle}{2t} = \sum_{n=1}^{\infty}\frac{(2t)^{n-1}}{n!}\kappa_n(t)$$

Numerical method



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Random damping

$$\frac{d^2x}{dt^2} + (\gamma + \xi(t))\frac{dx}{dt} + x = 0$$

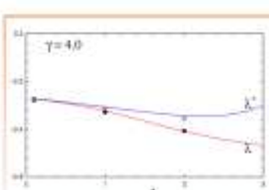
Anteneodo & Vallejos (2010)

$\langle \xi(t)\xi(t')\rangle = \Delta\,\delta(t-t')$

λ Leprevost et al. EPJB (2006)

$\lambda^* = \frac{1}{2}$ Max Re(Eigenvalues(K))

$$K = \begin{pmatrix} 0 & 0 & 2 \\ 0 & -2(\gamma-\Delta) & -2 \\ -1 & 1 & -\gamma+\Delta/2 \end{pmatrix}$$



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Colored noise + fourth cumulant

$$\frac{d^2x}{dt^2} + \alpha\frac{dx}{dt} + (1+\xi(t))x = 0$$

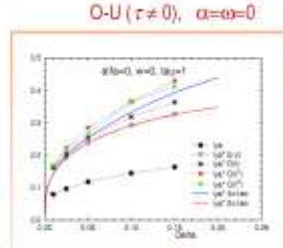
$\langle \xi(t)\xi(t')\rangle = \frac{\Delta}{2\tau}\exp(-|t-t'|/\tau)$

O-U ($\tau \neq 0$), α=ω=0

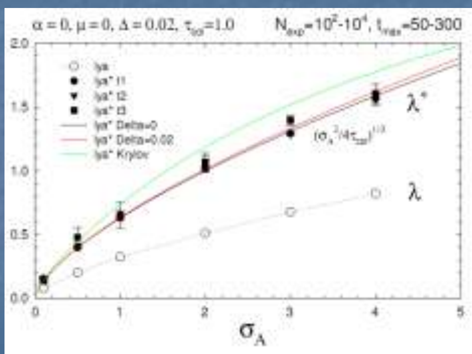
λ: ???

$\lambda^* = \frac{1}{2}$ Max Re(Eigenvalues(K))

$$K = \begin{pmatrix} 0 & 0 & 2 \\ \Delta & -2\alpha-2\Delta\tau^2 & -2 \\ -1+\Delta\tau & 1 & -\alpha-2\Delta\tau^2 \end{pmatrix}$$



Poisson process



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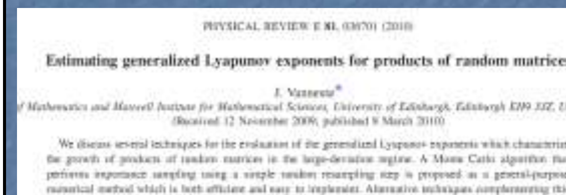
Importance sampling!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Estimating generalized Lyapunov exponents for products of random matrices

J. Vanneste*

of Mathematics and Maxwell Institute for Mathematical Sciences, University of Edinburgh, Edinburgh EH9 3JZ, Uni

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We discuss several techniques for the evaluation of the generalized Lyapunov exponents which characterize the growth of products of random matrices in the large-deviation regime. A Monte Carlo algorithm that performs importance sampling using a simple random resampling step is proposed as a general-purpose numerical method which is both efficient and easy to implement. Alternative techniques complementing this

"Resampling Monte Carlo"

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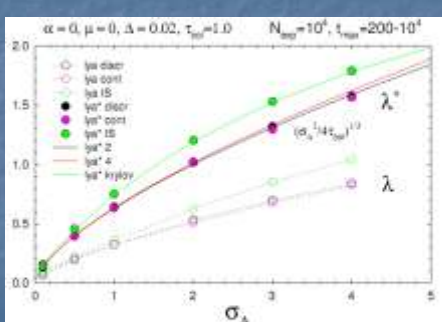
Poisson revisited



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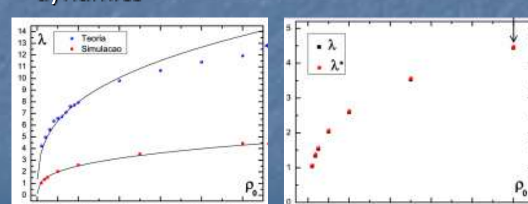
Next steps (Conclusions)

- Adapt resampling MC to deterministic LJ dynamics



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Next steps

- If resampling MC does not eliminate disagreement, then go back to cumulant expansion: Ornstein-Uhlenbeck, Poisson

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Fine

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