Lyapunov exponent of a Lennard-Jones gas: cumulant expansion

Raúl O. Vallejos (CBPF)
Celia Anteneodo (Puc-Rio)
Leonardo Cirto (CBPF, MSc)

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Purpose

- Can the cumulant-expansion approach estimate the Lyapunov exponent of a (dilute) Lennard-Jones gas?

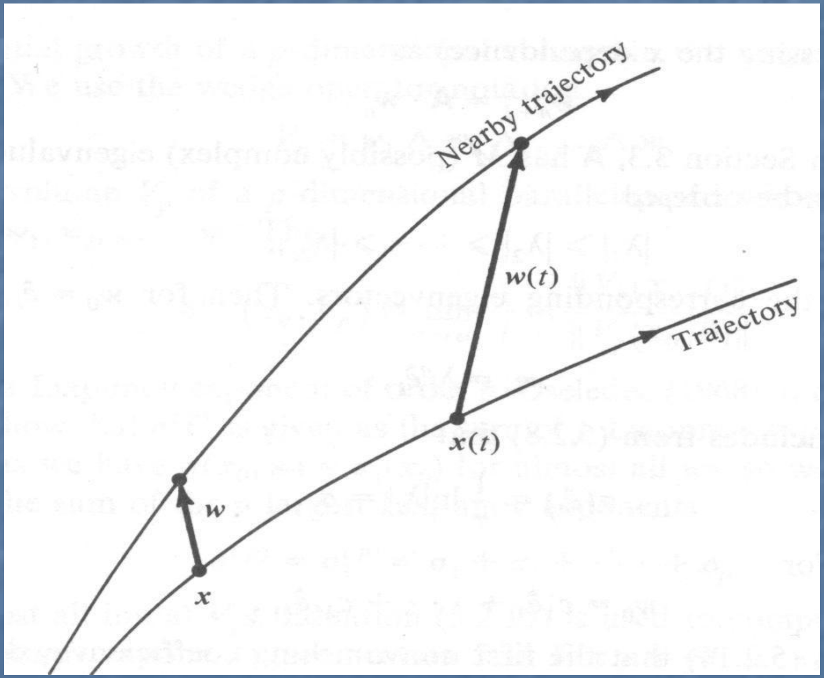
The Lyapunov exponent

Dynamical system

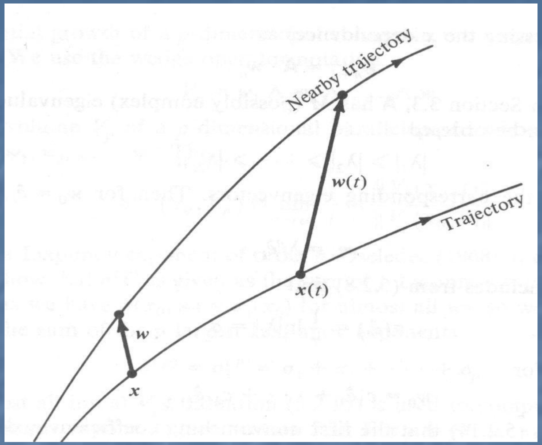
$$\frac{dx}{dt} = f(x), \quad x \in \Re^n$$

Asymptotically

$$|w(t)| \approx |w| e^{\lambda t}$$



Tangent dynamics



In the limit $|w| \to 0,\ w \to \xi$:

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

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

Why λ?

λ quantifies sensitivity to initial conditions, instability, unpredictability, chaos

In classical statistical mechanics:

$\lambda > 0$ necessary for validity of microcanonical formalism

$\lambda \approx 0$ signals thermodynamic anomalies

Theory (Hamiltonian Systems)

$$\frac{d\xi}{dt} = A(t)\,\xi$$

$$\begin{pmatrix} \underline{\underline{0}} & \underline{\underline{1}} \\ -\underline{\underline{\mathrm{V}}}(t) & \underline{\underline{0}} \end{pmatrix}$$

Hessian

Theory (Hamiltonian Systems)

$$1)\quad \lambda = \lim_{t\to\infty} \frac{1}{2t} \ln\left|\xi(t)\right|^2$$

$$\frac{d\xi}{dt} = A(t)\,\xi$$

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Hessian

Theory (Hamiltonian Systems)

$$1)\quad \lambda = \lim_{t\to\infty} \frac{1}{2t} \ln\left|\xi(t)\right|^2$$

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

$$\frac{d\xi}{dt} = A(t)\,\xi$$

$$\begin{pmatrix} \underline{\underline{0}} & \underline{\underline{1}} \\ -\underline{\underline{\mathrm{V}}}(t) & \underline{\underline{0}} \end{pmatrix}$$

Hessian

Theory (Hamiltonian Systems)

$$\frac{d\xi}{dt} = A(t)\,\xi$$

↑

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Hessian

1) $$\lambda = \lim_{t\to\infty} \frac{1}{2t} \ln\left|\xi(t)\right|^2$$

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

3) $$\lambda \approx \lim_{t\to\infty} \frac{1}{2t} \ln\left\langle \left|\xi(t)\right|^2 \right\rangle_{x_0,\xi_0} \equiv \lambda_2$$

↓ if intermittency weak enough

ROV & C. Anteneodo, PRE02
Barnett, Tajima, Nishihara, Ueshima, Furukawa, PRL96

A theory for λ_2

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

Analogous to a Schrödinger equation with a time-dependent nonhermitian Hamiltonian

A theory for λ_2

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Analogous to a Schrödinger equation with a time-dependent nonhermitian Hamiltonian

Solution:

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

time ordering

Second moments

$$\lambda_2 = \lim_{t\to\infty} \frac{1}{2t} \ln \left\langle \left|\xi(t)\right|^2 \right\rangle_{x_0,\xi_0}$$

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

matrix of second moments

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

linear operator

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

Preparatory step

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

"free Hamiltonian" perturbation

$$\hat{A} = \langle \hat{A} \rangle + \delta \hat{A}$$

→ Switch to the interaction representation

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

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

average + integrated autocorrelation function + ...

The cumulant expansion II

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

The generalized Lyapunov exponent is given by

$$\lambda_2 = \frac{1}{2} \max \Re\left(eigenvalues\ of\ \hat{O} \right)$$

Next: calculate and diagonalize Ô. Use symmetries!

Relevant subspace

In some cases → 3D,
ex., dilute gas, Hamiltonian mean field XY model

Other cases → restrict to 3D subspace
(mean field approximation in tangent space)

Final result (second order)

$$\left\| \hat{O} \right\| = \begin{pmatrix} 0 & 0 & 2 \\ 2\sigma^2 \tau_c^{(1)} & -2\sigma^2 \tau_c^{(3)} & -2\mu \\ -\mu + 2\sigma^2 \tau_c^{(2)} & 1 & -2\sigma^2 \tau_c^{(3)} \end{pmatrix}$$

3x3 matrix

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3x3 matrix

$$\mu = \frac{1}{N}\mathrm{Tr}\left\langle \underline{\underline{V}} \right\rangle_\mu$$

average

$$\sigma^2 = \frac{1}{N}\mathrm{Tr}\left\langle \left(\delta\underline{\underline{V}}\right)^2 \right\rangle_\mu$$

variance

$$\tau_c^{(k)} = \int_0^\infty d\tau\, \tau^{k-1} f(\tau)$$

correlation times

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

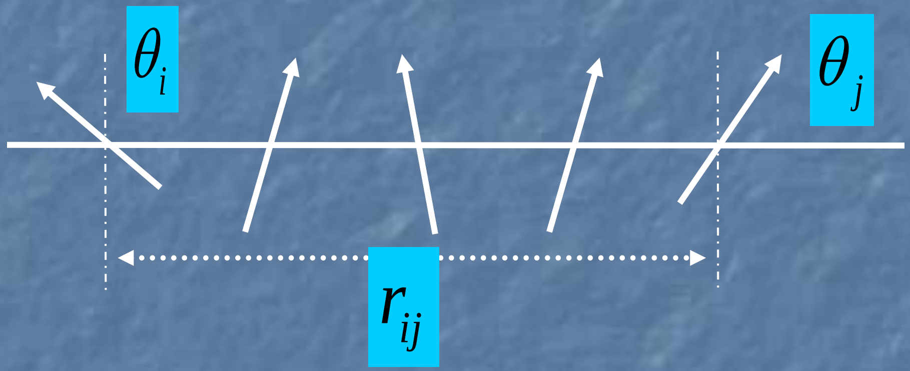
normalized autocorrelation function

Special case

Short correlation time, negligible average fluctuations

$$\lambda_2 \approx \left(\frac{\sigma^2 \tau_c^{(1)}}{2} \right)^{1/3}$$

Testing the theory

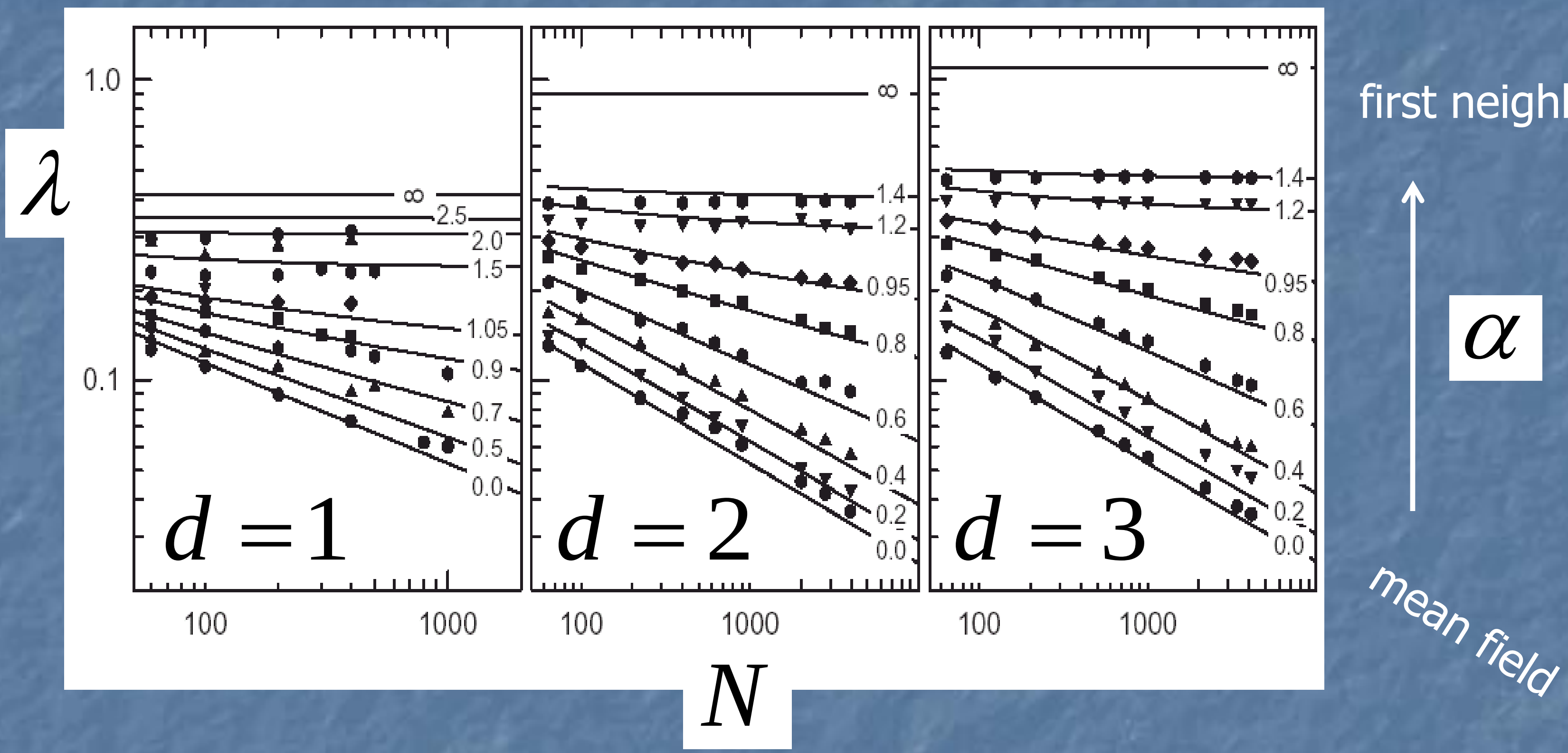


α-XY Hamiltonian model

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

Results λ_{num} *vs* $\lambda_{2\,theo}$

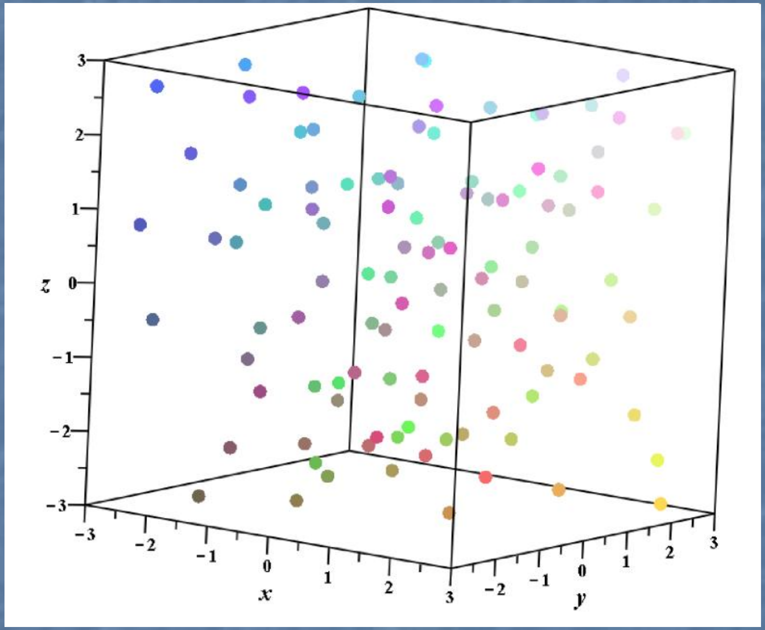
ROV & C. Anteneodo
Physica A (2004)



numerics
- Latora, Rapisarda, Ruffo, PRL (1998)
- Anteneodo & Tsallis, PRL (1998)
- Campa, Giansanti, Moroni, Tsallis, PLA (2001)

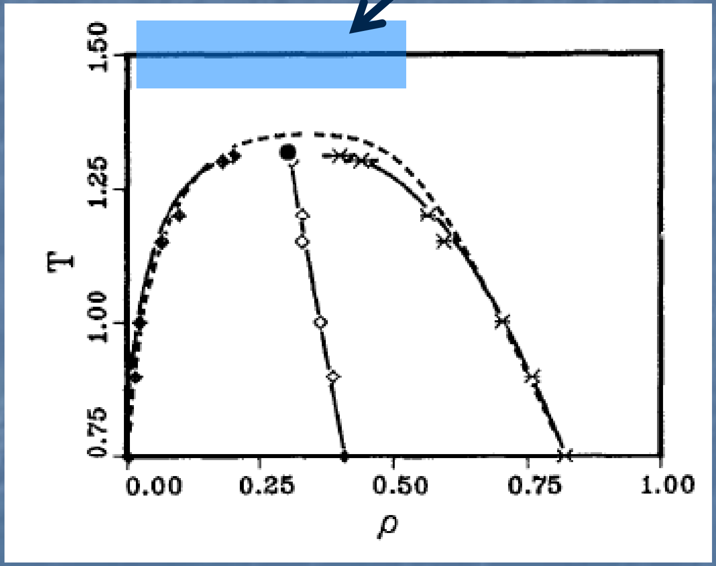
The Lennard-Jones gas

The Lennard-Jones gas



N=108

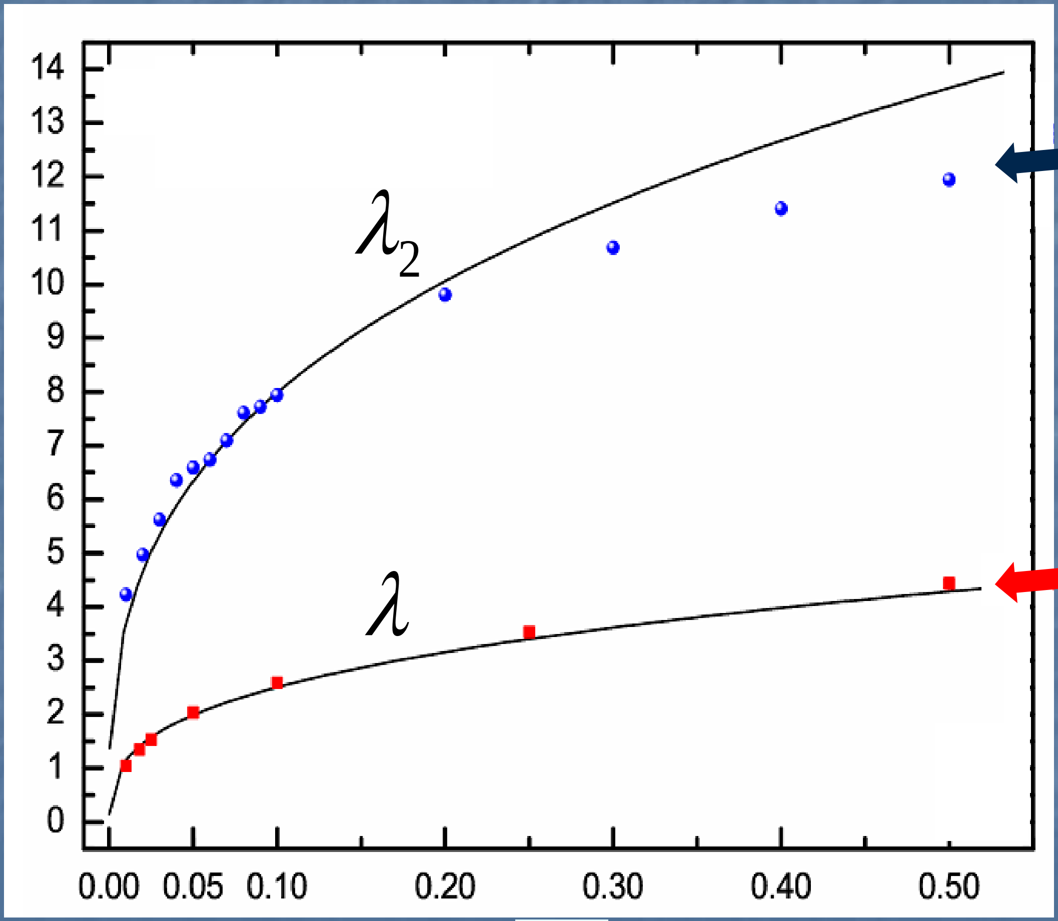
dilute
gas phase



Smit, *JCP* (1992)

L. Cirto, MSc Thesis (2010)

Theory vs numerics



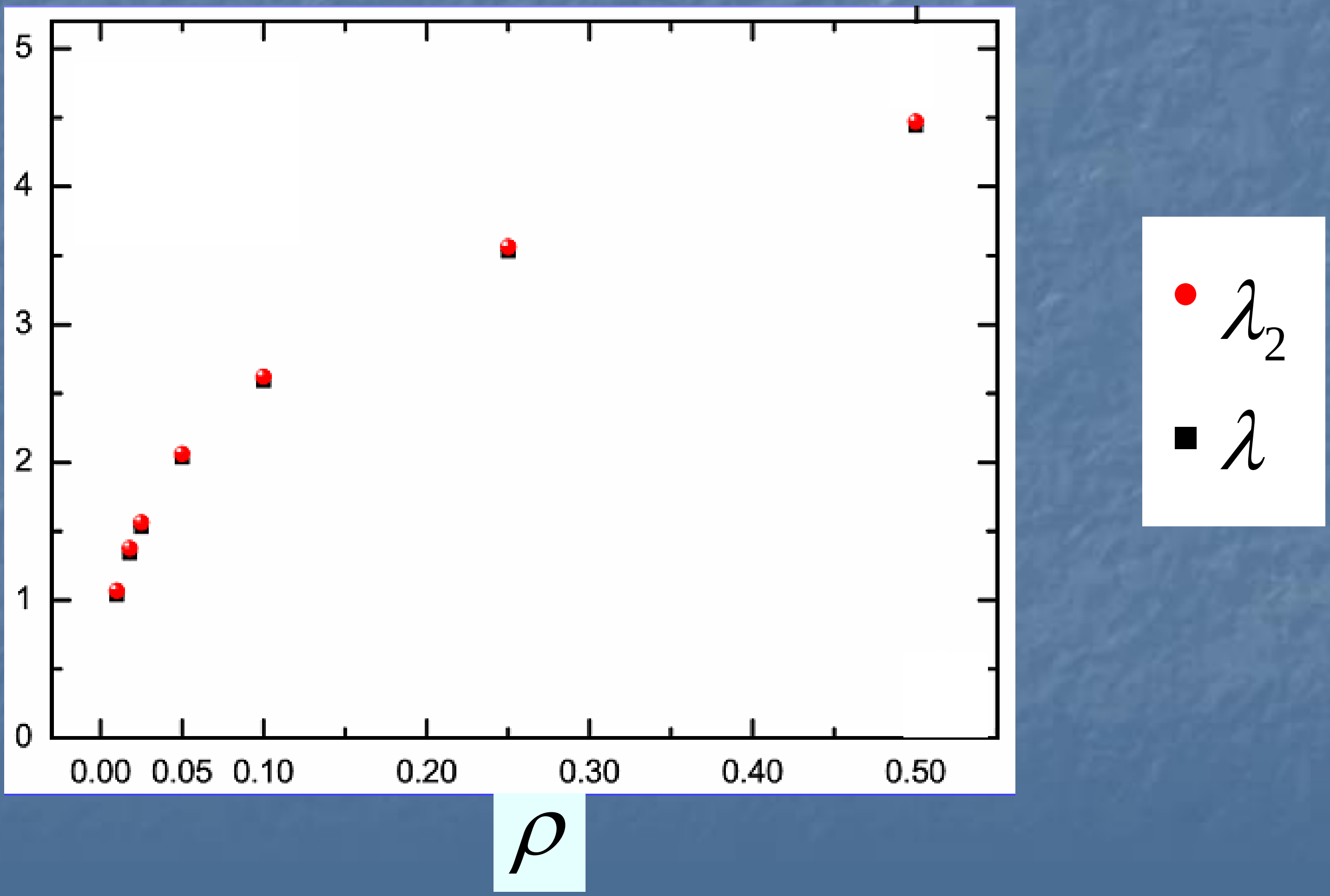
ρ

theory

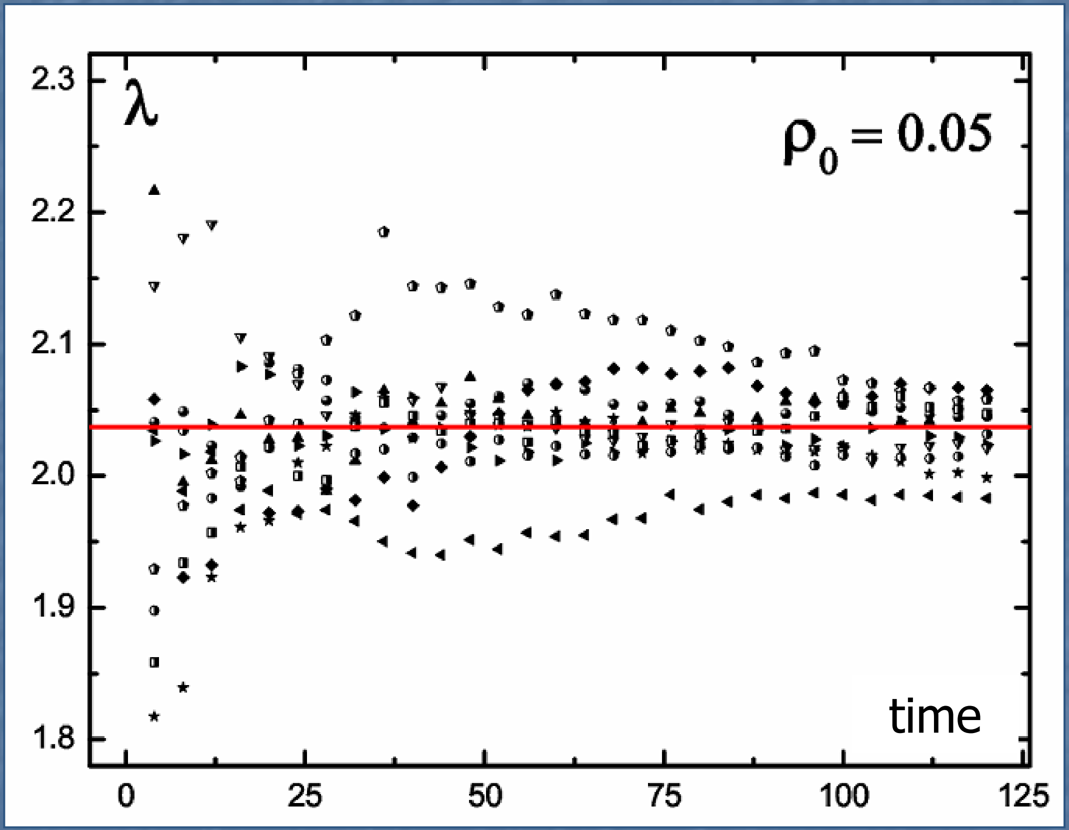
numerical

= Romero Bastida, Braun, JPA08

Generalized vs standard LE (numerical)



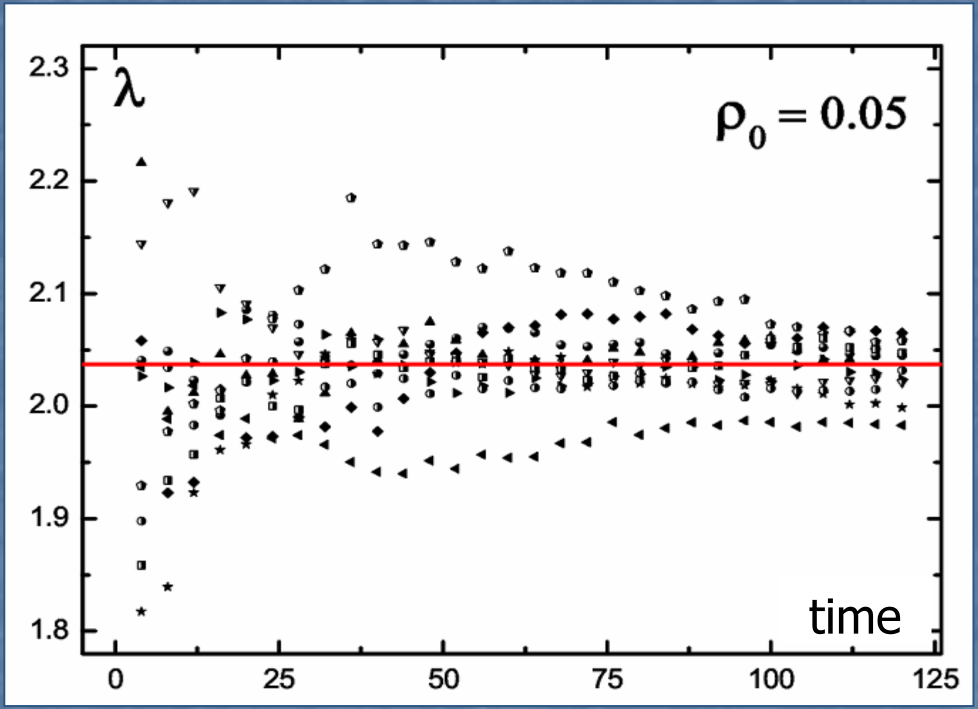
However …



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

average over finite-time Lyapunov exponents

If simple sampling ...

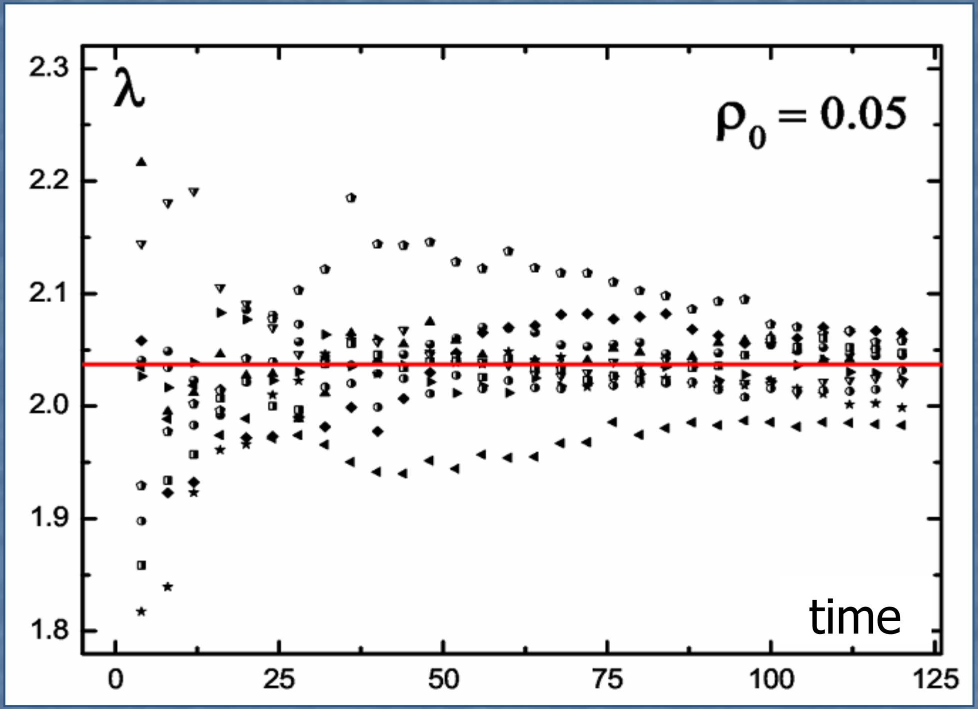


$$\lambda_2 \approx \frac{1}{2t} \ln \left\langle \left| \xi \right|^2 \right\rangle = \frac{1}{2t} \ln \left\langle e^{2t\lambda^{(i)}} \right\rangle$$

dominated by tails

Simple sampling is bound to fail

If simple sampling …



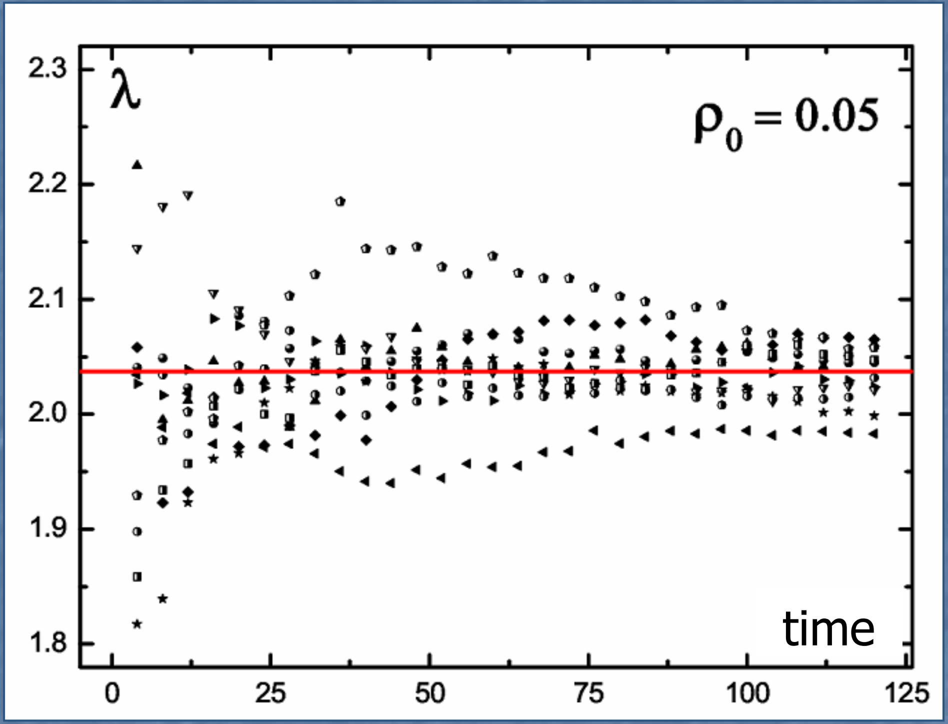
$$\lambda_q \approx \frac{1}{qt} \ln \left\langle \left| \xi \right|^q \right\rangle$$

$$= \frac{1}{qt} \ln \left\langle e^{q t \lambda^{(i)}} \right\rangle$$

dominated by tails

The larger the q, the worse the performance of SS

Simple sampling + Gaussian?



Gaussian approximation

Some improvement but still unsatisfactory

Importance sampling!

stochastic maps

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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
(Received 12 November 2009; published 8 March 2010)

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

cloning and pruning

Test: random frequency oscillator

=1D Anderson localization problem

6N equations (ex., N=108)
for 3D LJ

$$\frac{d\xi}{dt} = A(t)\,\xi$$

↑

Hessian

$$\begin{pmatrix} \underline{\underline{0}} & \underline{\underline{1}} \\ -\underline{\underline{\mathrm{V}}}(t) & \underline{\underline{0}} \end{pmatrix}$$

Test: random frequency oscillator

=1D Anderson localization problem

6N equations (ex., N=108)
for 3D LJ

2 equations

$$\frac{d\xi}{dt} = A(t)\,\xi$$

$$\begin{pmatrix} \dot{\xi}_1 \\ \dot{\xi}_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\nu(t) & 0 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}$$

$$\begin{pmatrix} \underline{\underline{0}} & \underline{\underline{1}} \\ -\underline{\underline{\mathrm{V}}}(t) & \underline{\underline{0}} \end{pmatrix}$$

Hessian

Mimic dilute LJ: white Poisson noise

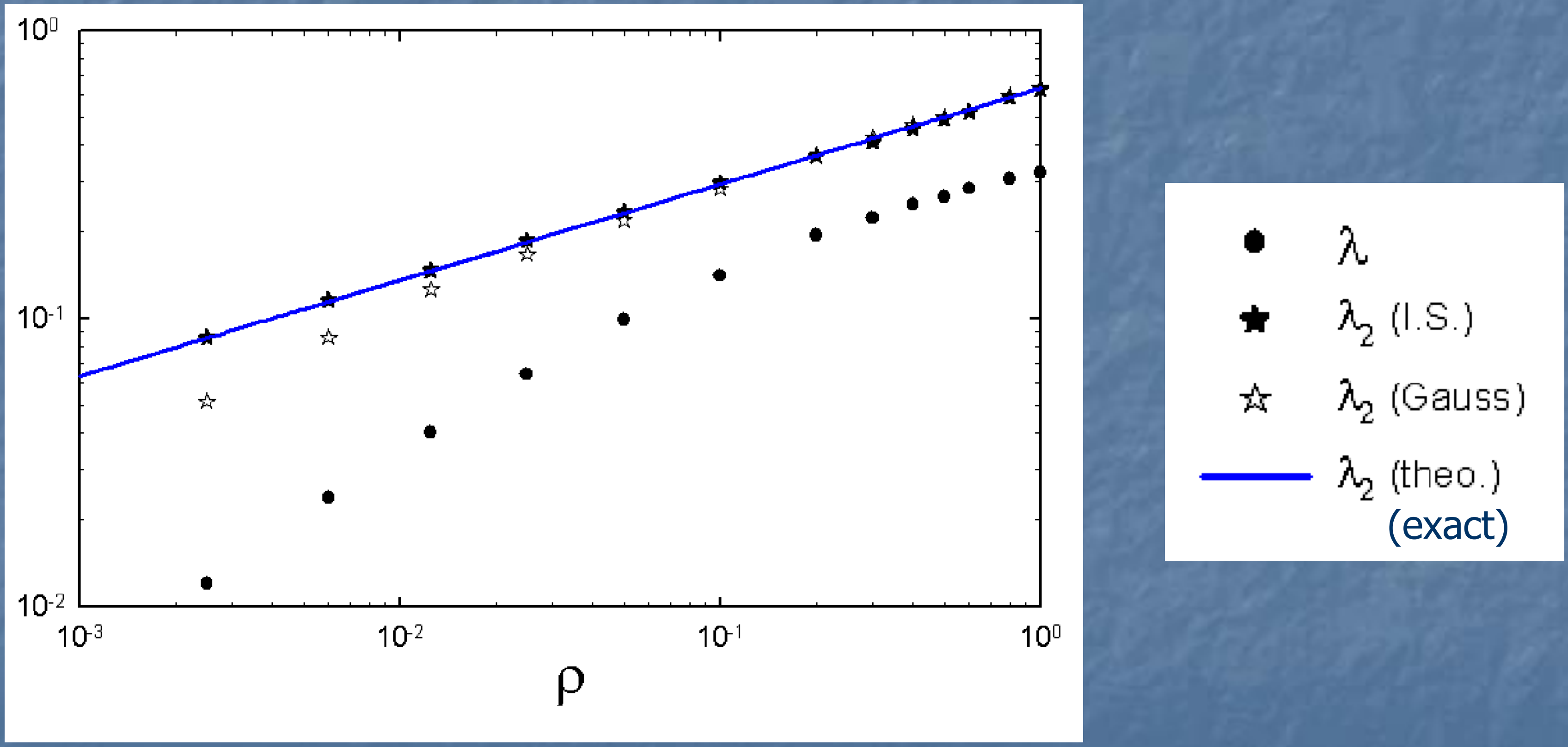
$$\begin{pmatrix} \dot{\xi}_1 \\ \dot{\xi}_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\nu(t) & 0 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix}$$

$$\nu(t) = \sum_k A_k \, \delta(t - \tau_k)$$

ex., i.i. Gaussians

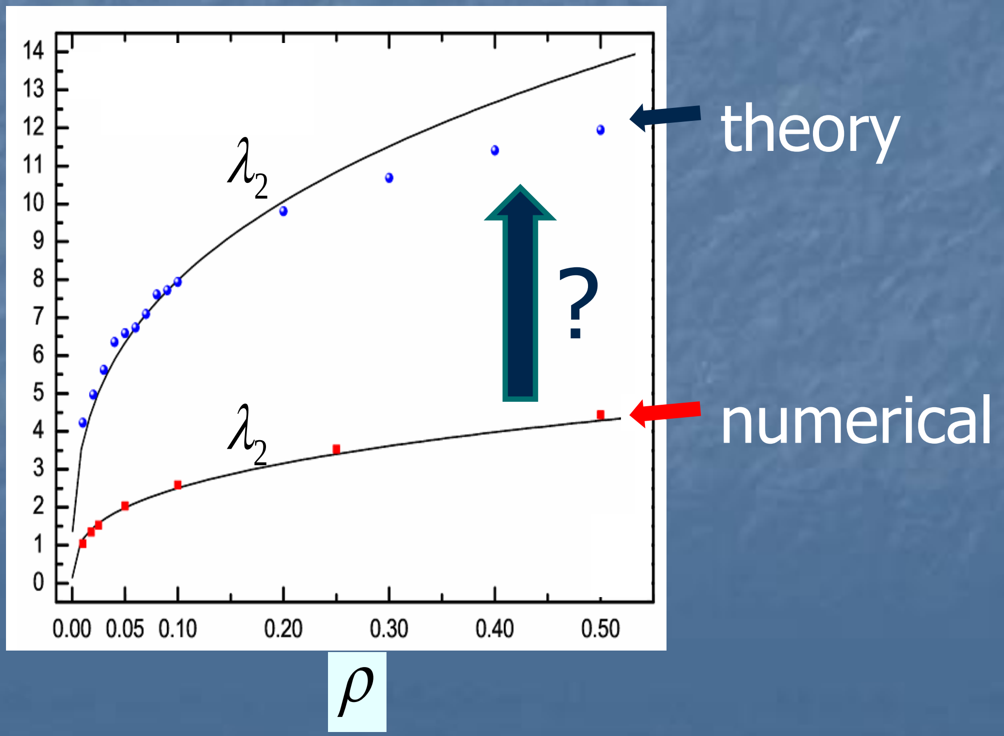
Poisson sequence

Results (preliminary)



Conclusions

- Adapt importance-sampling MC to deterministic LJ dynamics



Thanks!

http://www.cbpf.br/~vallejos/publications

The Kubo number

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