Large-Scale Numerical Investigations into the Dynamics of Nonlinear Classical Systems

SIAM Conference on Applications of Dynamical Systems

Sebastian Micluța-Câmpeanu

Snowbird, 22 May 2019

University of Bucharest

Outline

Acknowledgements

- I would like to thank A.I. Nicolin, and V. Băran for helping and motivating me.
- The author has been supported by the research project PN-III-P4-ID-PCE-2016-0792 funded by the Romanian Minisrty of Research and Inovation.
- All numerical simulations were performed on the computing cluster of Department of Computational Physics and Information Technologies, “Horia Hulubei” National Institute for Physics and Nuclear Engineering.

Introduction

The model

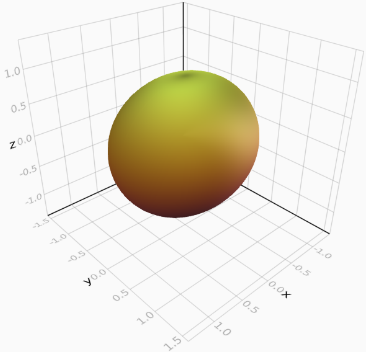
- The physical system that we model is the surface of heavy nuclei.
- We use a Hamiltonian that describes the constrained motion of the vibrational quadrupole degrees of freedom of the nuclear surface.

The model

The Hamiltonian of the system

$$H = \frac{A}{2}\left(p_0^2 + p_2^2\right) + \frac{A}{2}\left(q_0^2 + q_2^2\right) + \frac{B}{\sqrt{2}} q_0 \left(3q_2^2 - q_0^2\right) + \frac{D}{4}\left(q_0^2 + q_2^2\right)^2$$

- Harmonic oscillator part
- Integrable part
- Non-integrable term

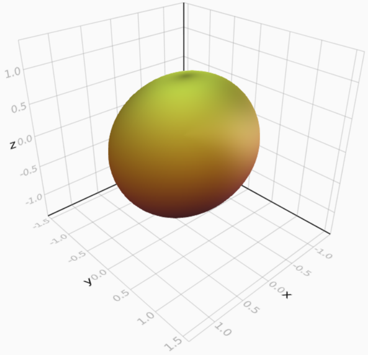


The model

The Hamiltonian of the system

$$H = \frac{A}{2}\left(p_0^2 + p_2^2\right) + \frac{A}{2}\left(q_0^2 + q_2^2\right) + \frac{B}{\sqrt{2}} q_0 \left(3q_2^2 - q_0^2\right) + \frac{D}{4}\left(q_0^2 + q_2^2\right)^2$$

- Harmonic oscillator part
- Integrable part
- Non-integrable term

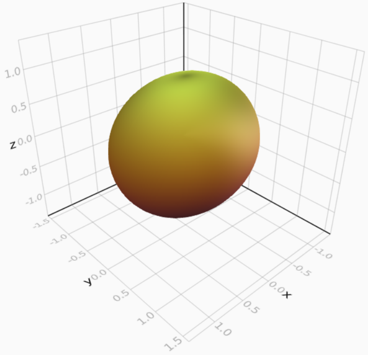


The model

The Hamiltonian of the system

$$H = \frac{A}{2}\left(p_0^2 + p_2^2\right) + \frac{A}{2}\left(q_0^2 + q_2^2\right) + \frac{B}{\sqrt{2}} q_0 \left(3q_2^2 - q_0^2\right) + \frac{D}{4}\left(q_0^2 + q_2^2\right)^2$$

- Harmonic oscillator part
- Integrable part
- Non-integrable term



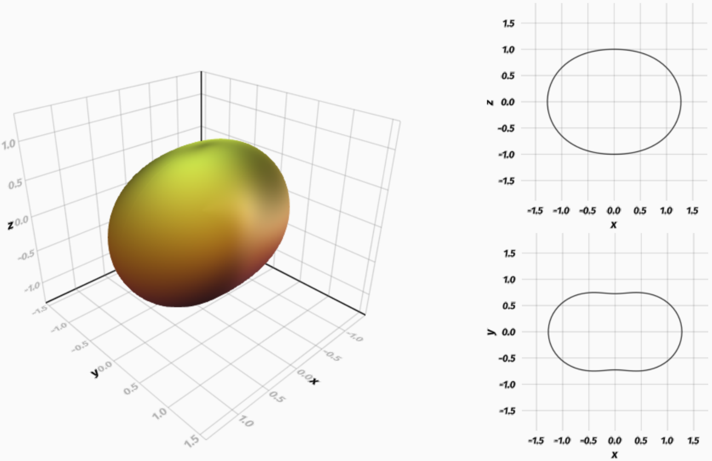


Figure 1: The nuclear surface and its sections

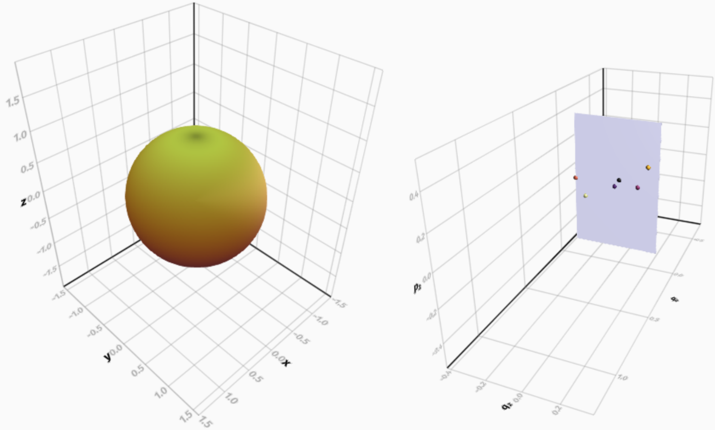


Figure 2: The nucleus and the corresponding trajectory in the phase space for a chaotic trajectory with $B = 0.5, E = 0.3$

Numerical simulations

Julia

- Numerical simulations and the visualizations of the results was done in `Julia` [1] (`DifferentialEquations.jl` [4] and `DynamicalSystems.jl` [2] for simulations and respectively `Plots.jl` and `Makie.jl` for visualizations).
- Having access to the implementations of a large number of integrators helps us taking an informed decision for the choiche of the integration algorithm.

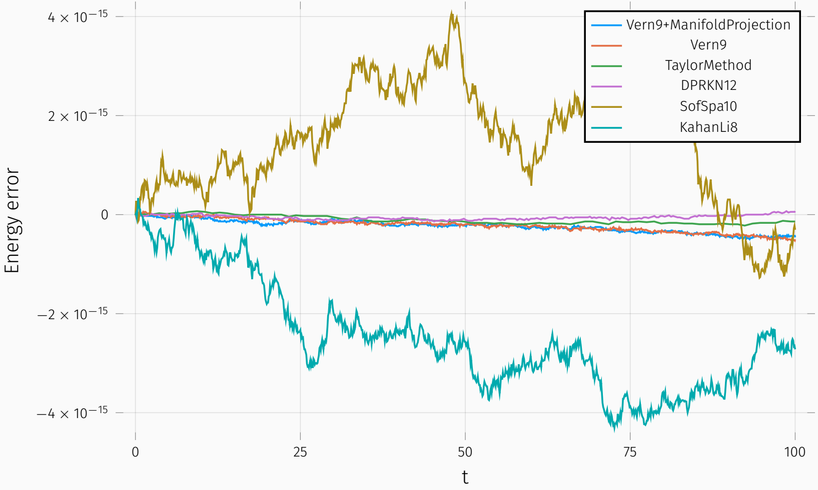


Figure 3: Energy error benchmark for short integration time

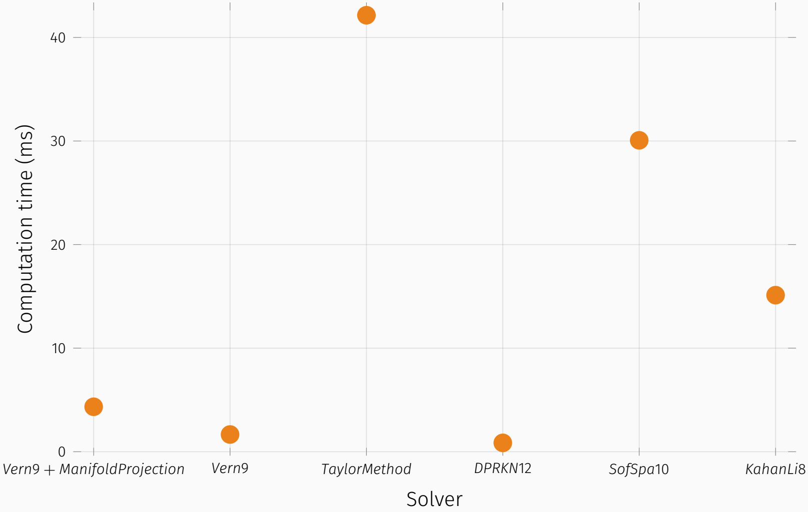


Figure 4: Computational time benchmark for short integration time

Figure 5: Energy error benchmark for long integration time

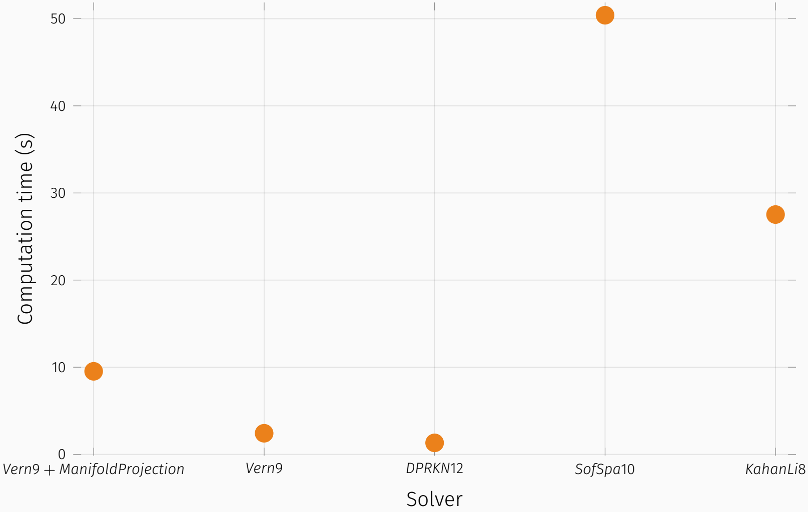


Figure 6: Computational time benchmark for long integration time

Quantifying chaoticity

- The maximal Lyapunov exponent is defined as

$$\lambda = \lim_{t \to \infty} \frac{1}{t} \ln \frac{\mathrm{d}x\,(t)}{\mathrm{d}x\,(0)}$$

- One of the signature characteristics of chaos is the sensitivity to the initial conditions ($\lambda > 0$).
- We can get some intuitive insight for the sensitivity to the initial conditions by following the evolution of two nearby initial conditions.

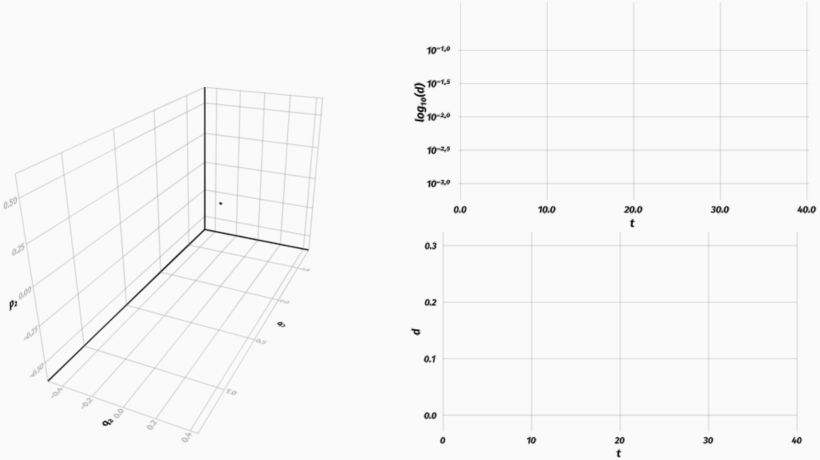


Figure 7: The distance between nearby trajectories for $B = 0.5$ and $E = 0.3$.

Interactive exploratinos

- For a given set of parameters (B and E) we have a set of compatible initial conditions.
- Poincaré sections give us a global picture of the dynamics.
- For a better (visual) understanding of the dynamics we can show the Lyapunov exponents on the Poincaré map.

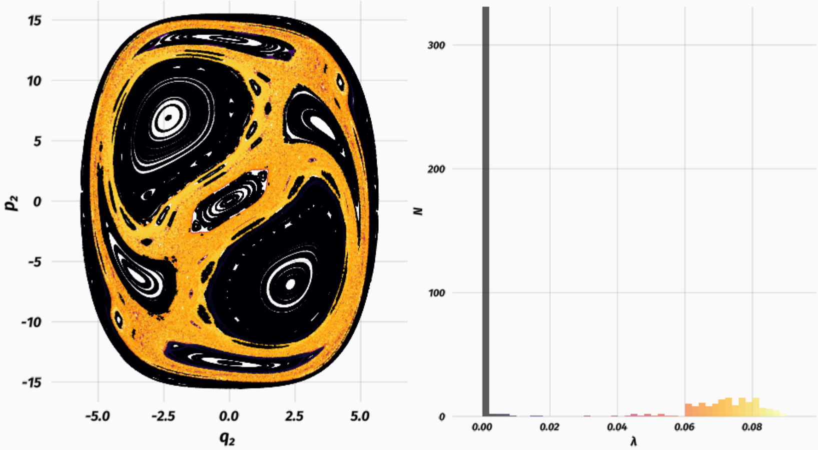


Figure 8: A Poincaré section at $B = 0.5, E = 120$

A note regarding the λ histogram

- Theoretically the Lyapunov exponent histogram should have two sharp peaks: one for the regular part and one for the chaotic one.
- The spread in the chaotic part is given by finite time effects.
- To better understand this we will take a look at how the integration time affects the results.

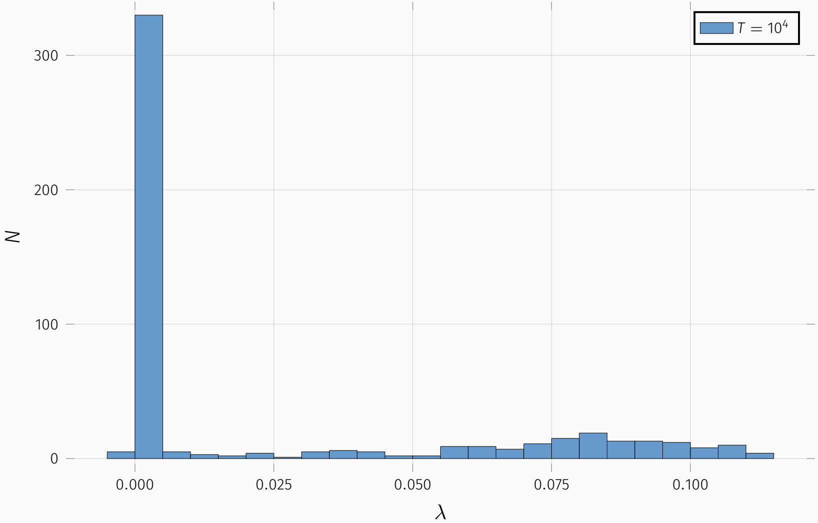


Figure 9: Maximal Lyapunov coefficient histogram for $B = 0.5$ and $E = 120$.

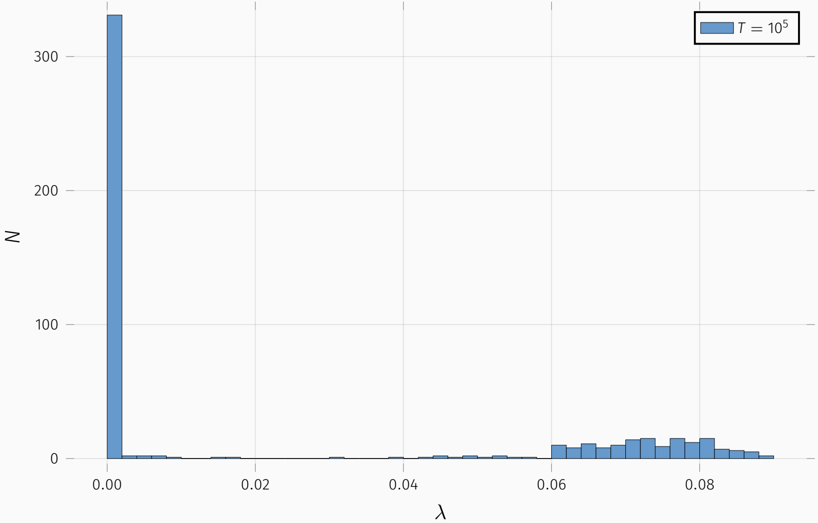


Figure 10: Maximal Lyapunov coefficient histogram for $B = 0.5$ and $E = 120$.

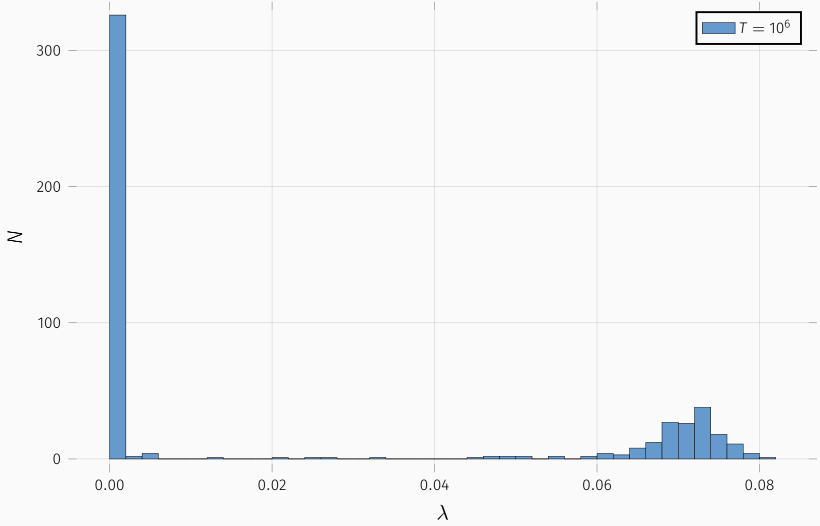


Figure 11: Maximal Lyapunov coefficient histogram for $B = 0.5$ and $E = 120$.

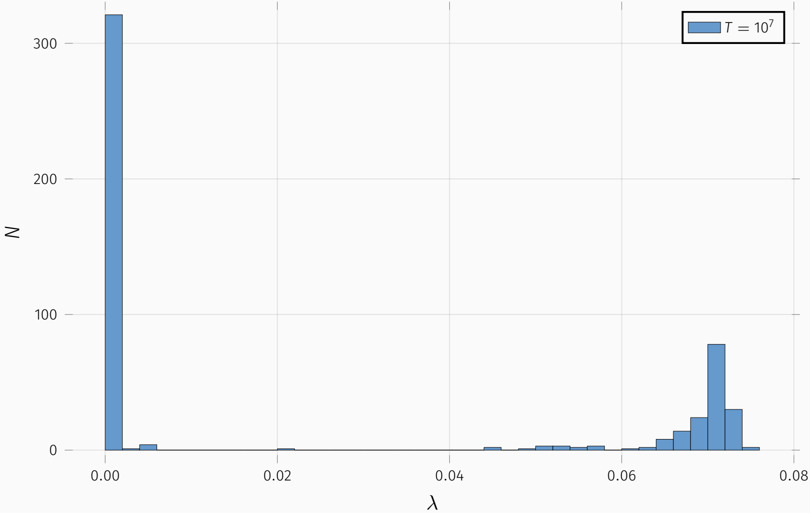


Figure 12: Maximal Lyapunov coefficient histogram for $B = 0.5$ and $E = 120$.

Averaging λ over the initial conditions

- We define the averaged Lyapunov coefficient as the mean of the maximal Lyapunov exponents in the chaotic region.
- We need a sufficiently robust method of selecting the λs in the chaotic region.
- We consider as chaotic everything after the first local maxima in the histogram.

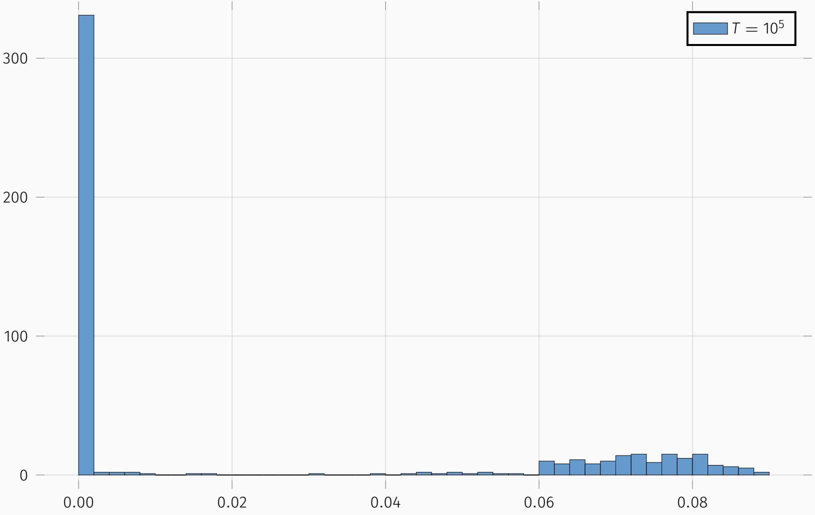


Figure 13: Selecting the chaotic trajectories for $B = 0.5$ and $E = 120$.

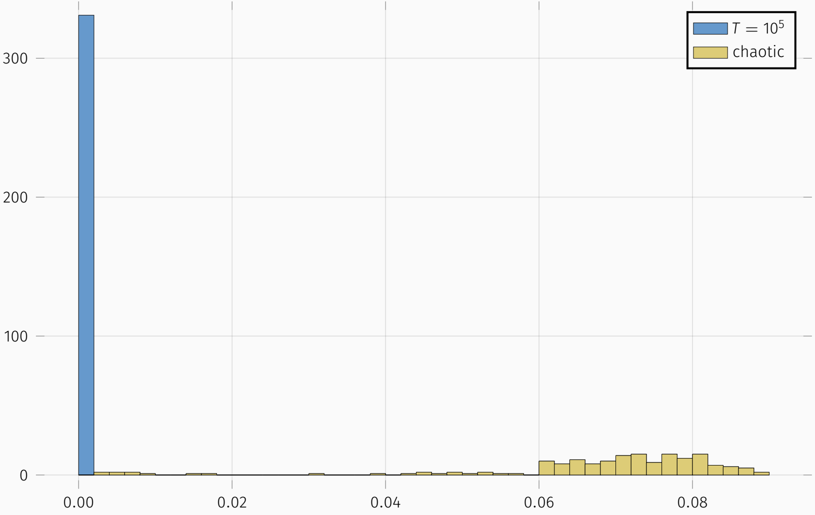


Figure 14: Selecting the chaotic trajectories for $B = 0.5$ and $E = 120$.

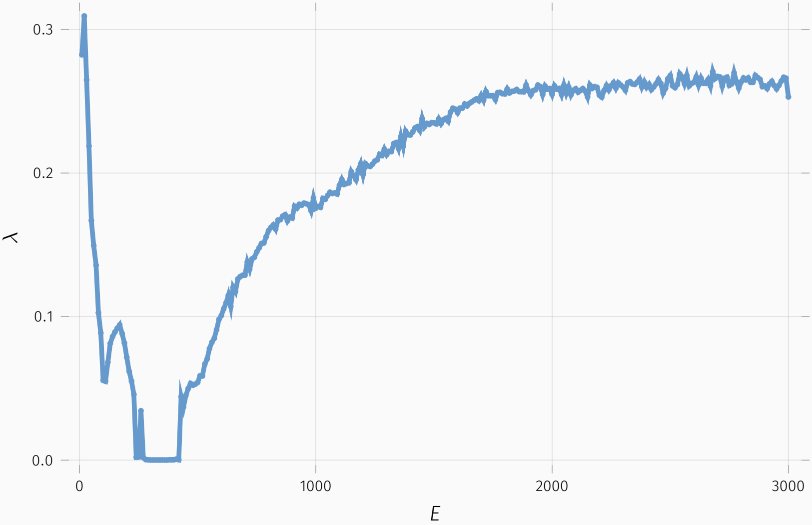


Figure 15: Averaged λ for $B = 0.5$ and $E \in (10, 3000)$.

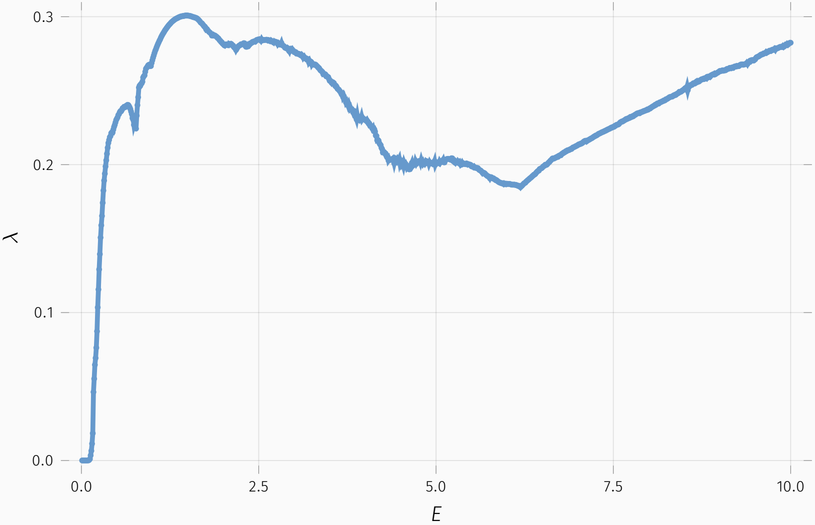


Figure 16: Averaged λ for $B = 0.5$ and $E \in (0.01, 10)$.

Other indicators

- We can look at the distance between two nearby trajectories in the limit of $T \to \infty$ in order to get an estimate of the phase space volume.
- In a finite phase space volume we cannot have only an exponential divergence of trajectories, so there must be some something that folds the trajectories back after the initial divergence.
- We define Γ as a measure of folding

$$\Gamma = \frac{\mathrm{e}^{\lambda} - 1}{d_\infty}$$

- We can apply similar averaging techniques as for λ.

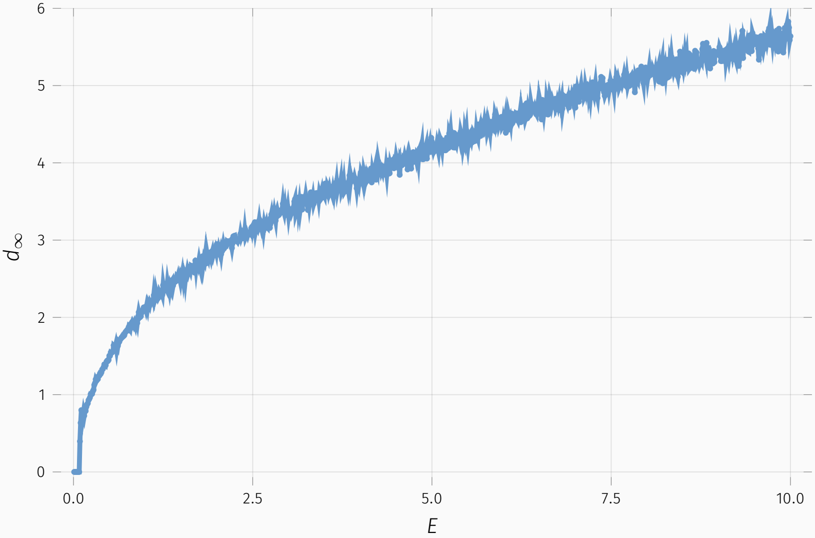


Figure 17: Averaged d_∞ for $B = 0.5$ and $E \in (0.01, 10)$.

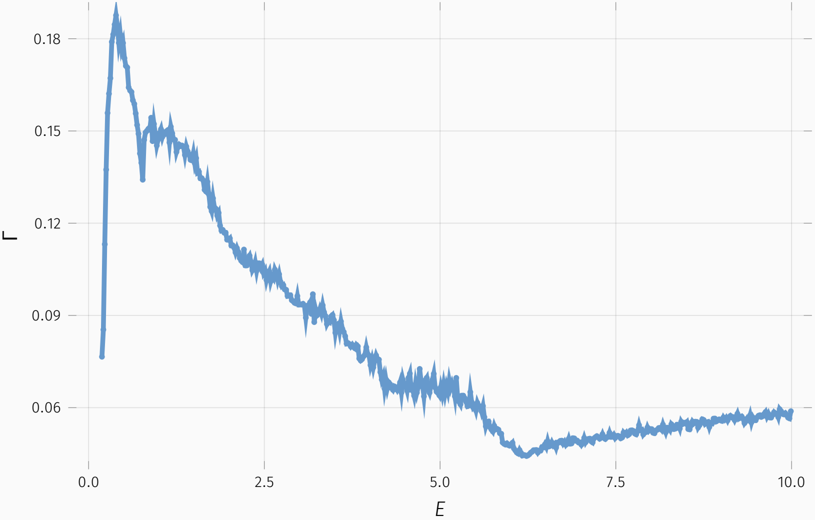


Figure 18: Averaged Γ for $B = 0.5$ and $E \in (0.01, 10)$.

Averaging λ over the energy

- We can get a global picture of the sistem by integrating the averaged Lyapunov coefficient over an energy interval.
- For a small energy interval in the low energy limit we get a monotonusly increasing dependence.
- For a large energy interval we have a non-trivial dependence of the averaged Lyapunov exponent with respect to the non-integrability parameter B.

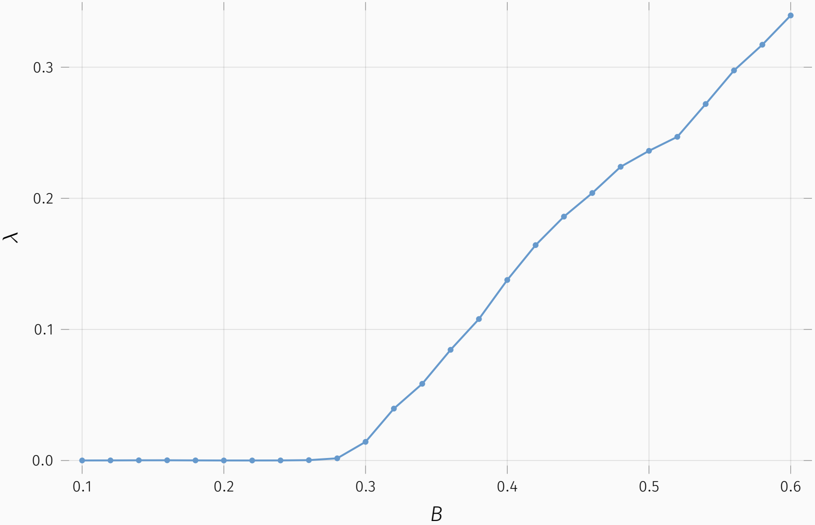


Figure 19: Averaged λ for $B = 0.5, E \in (10, 3000)$ and $B \in (0.1, 0.6)$.

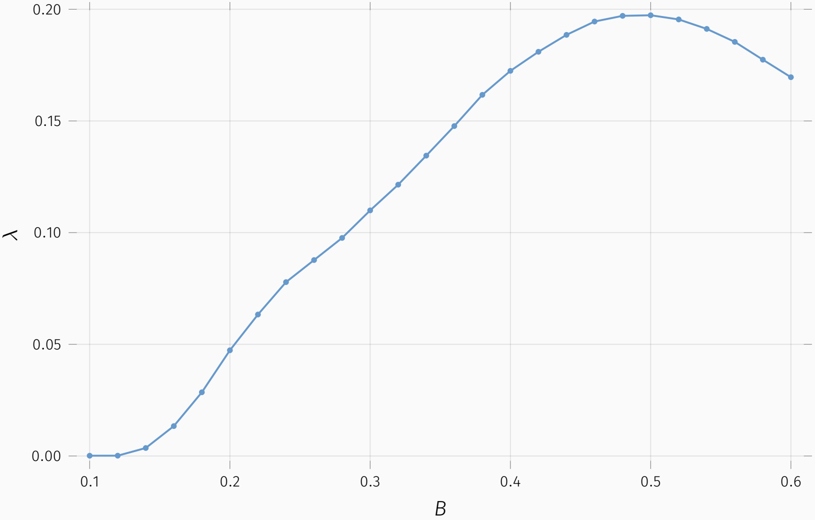


Figure 20: Averaged λ for $B = 0.5$, $E \in (0.01, 10)$ and $B \in (0.1, 0.6)$.

Conclusions

Conclusions

- The `Julia` ecosystem provides performant and flexible tools for exploring dynamical systems.
- We investigated in detail the classical dynamics of a non-integrable system and found a series of interesting phenomena with respect to its phase-space structure as function of energy and the non-integrability parameter.
- In order to propote open and reproducible[3, 5] science the presentation and the dataset needed for the visualizations are freely available online at `https://github.com/SebastianM-C/DS19Presentation`.

References i

J. Bezanson, A. Edelman, S. Karpinski, and V. B. Shah.
Julia: A fresh approach to numerical computing.
SIAM Review, 59(1):65–98, 2017.

G. Datseris.
Dynamicalsystems.jl: A julia software library for chaos and nonlinear dynamics.
Journal of Open Source Software, 3(23):598, mar 2018.

G. M. Kurtzer, V. Sochat, and M. W. Bauer.
Singularity: Scientific containers for mobility of compute.
PLOS ONE, 12(5):1–20, 05 2017.

C. Rackauckas and Q. Nie.
Differentialequations.jl – a performant and feature-rich ecosystem for solving differential equations in julia.
Journal of Open Research Software, 5(1):15, 2017.

L. White, R. Togneri, W. Liu, and M. Bennamoun.
Datadeps.jl: Repeatable data setup for replicable data science, 2018.

Thank you!

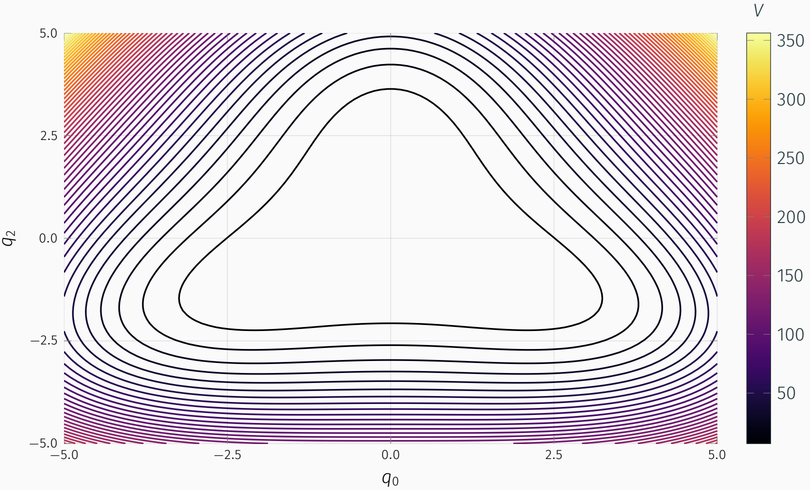


Figure 21: The equipotential lines for V at $B = 0.5$.

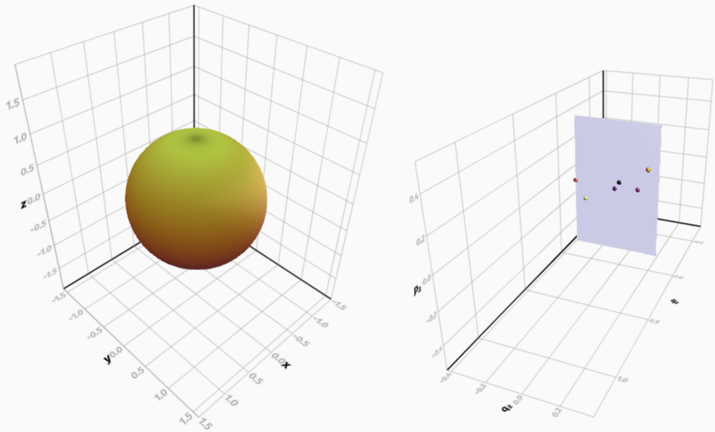


Figure 22: The nucleus and the corresponding trajectory in the phase space for a regular trajectory with $B = 0.5, E = 0.3$

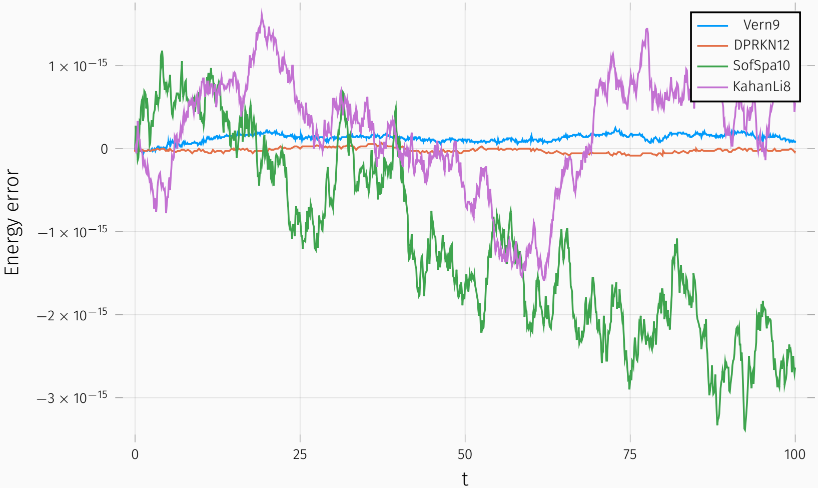


Figure 23: Energy error benchmark for short integration time with rescaling

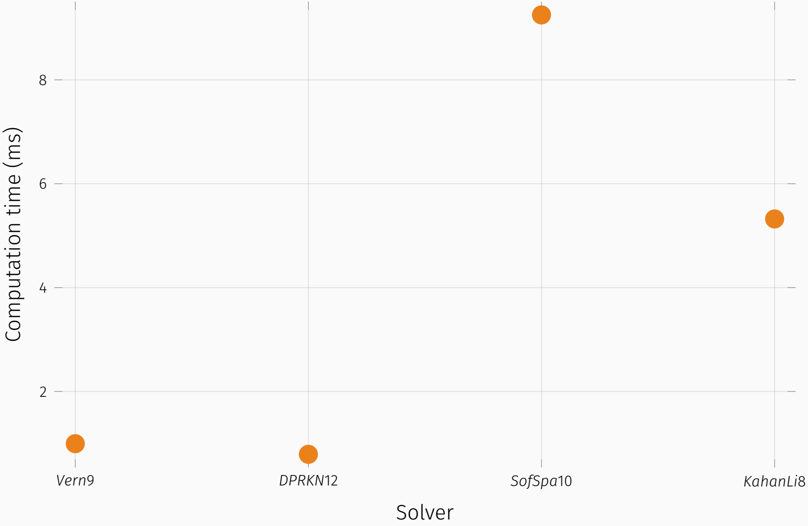


Figure 24: Computational time benchmark for short integration time with rescaling

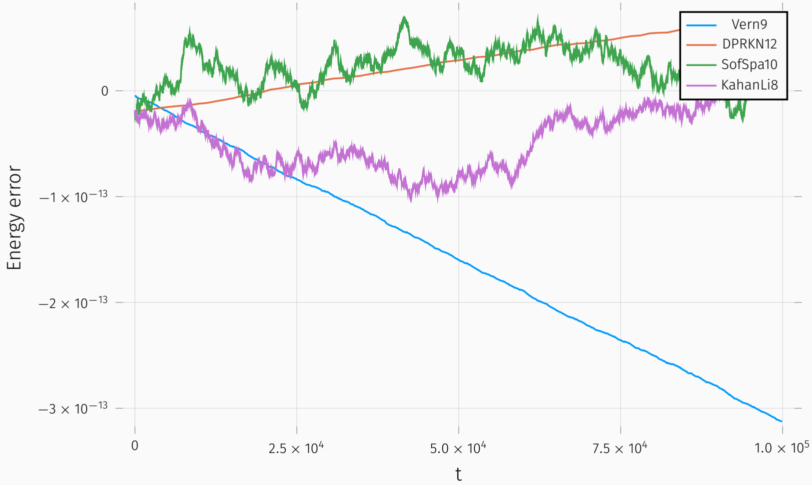


Figure 25: Energy error benchmark for long integration time with rescaling

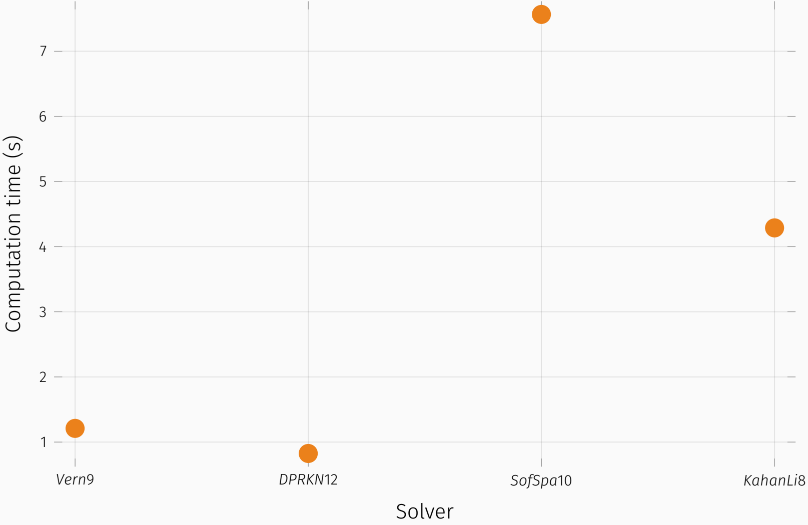


Figure 26: Computational time benchmark for long integration time with rescaling

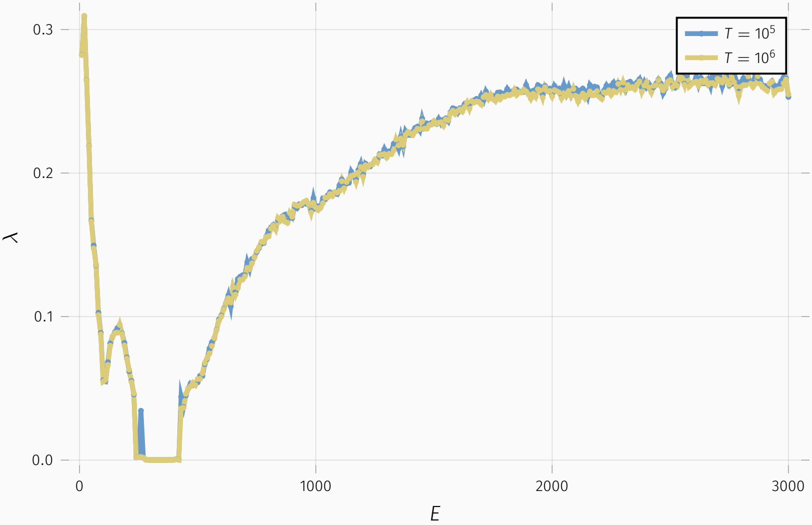


Figure 27: Averaged λ for $B = 0.5$ and $E \in (10, 3000)$.

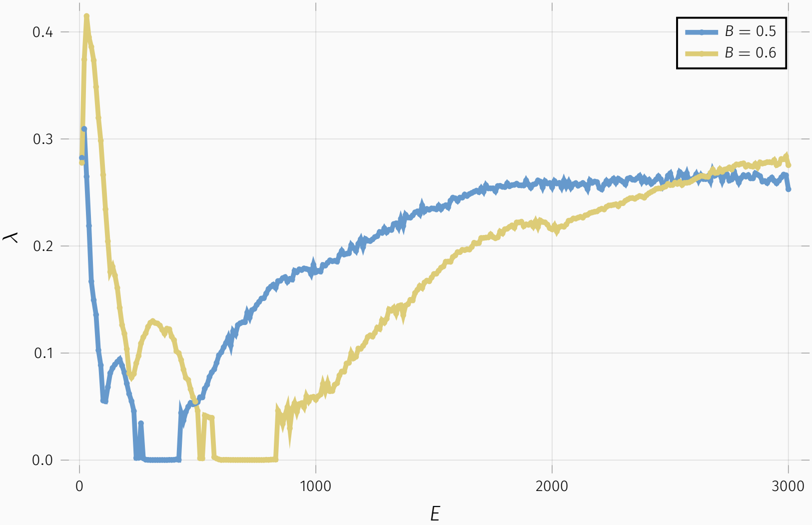


Figure 28: Averaged λ for $B \in 0.5, 0.6$ and $E \in (10, 3000)$.