The background of the slide features a dark blue space-themed illustration. It is filled with numerous concentric, glowing golden-yellow circles of varying sizes, resembling planetary orbits or ripples in space-time. Interspersed among these circles are several stylized celestial bodies: small white and gold spheres of different sizes, larger blue and brown spheres, and a few larger red spheres. The overall effect is a complex, multi-layered representation of a gravitational system.

Solving the Gravitational N-body problem with Machine Learning

Verónica Saz Ulibarrena

Contents

Introduction

PART 1: Physics-aware neural networks

Chapter 2: A hybrid approach for solving the gravitational N -body problem with Artificial Neural Networks

Chapter 3: A Generalized Framework of Neural Networks for Hamiltonian Systems

Contents

Introduction

PART 1: Physics-aware neural networks

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Chapter 3: A Generalized Framework of Neural Networks for Hamiltonian Systems

PART 2: Reinforcement Learning for time-step estimation

Chapter 4: Reinforcement Learning for Adaptive Time-Stepping in the Chaotic Gravitational Three-Body Problem

Chapter 5: Reinforcement Learning for the determination of the bridge time step in cluster dynamics simulations

Contents

Introduction

PART 1: Physics-aware neural networks

Planetary Systems

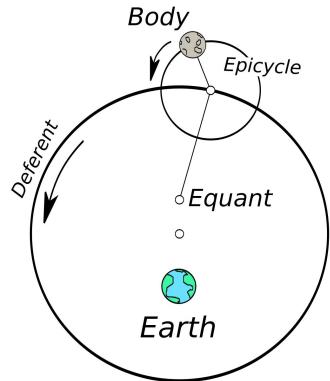
A bit of 3-Body problem

PART 2: Reinforcement Learning for time-step estimation

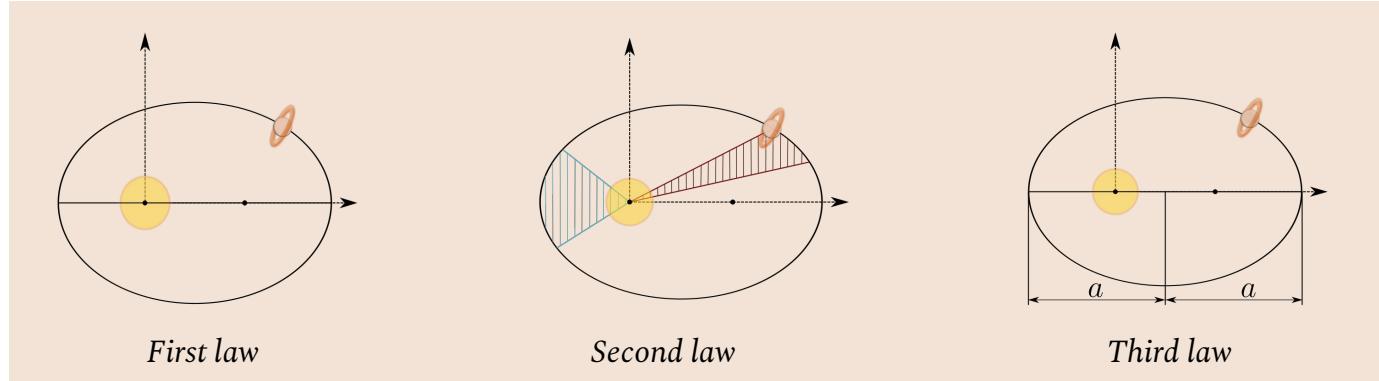
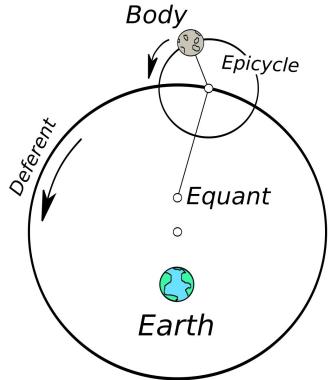
A lot of 3-Body problem

Star cluster + planetary systems

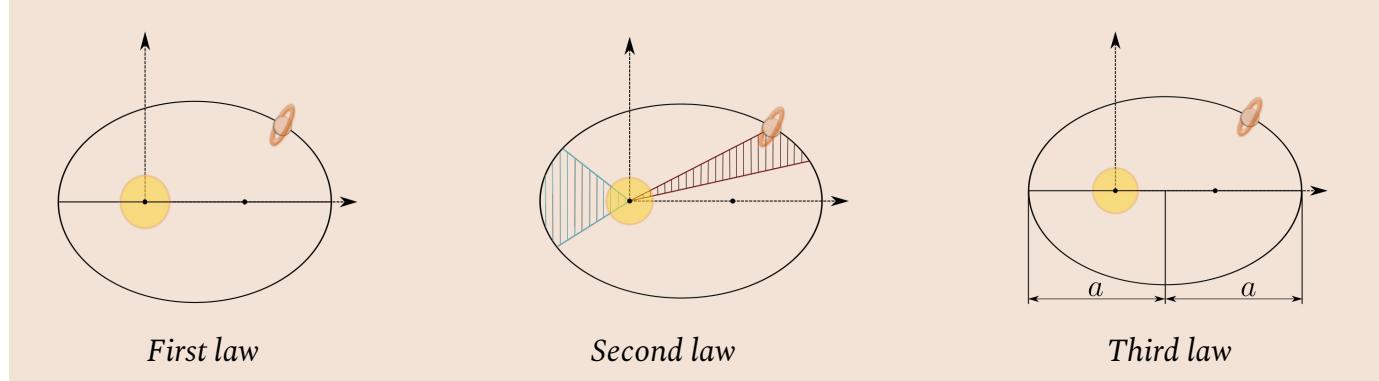
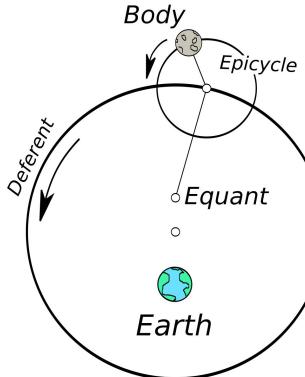
The beginning of the N -body problem



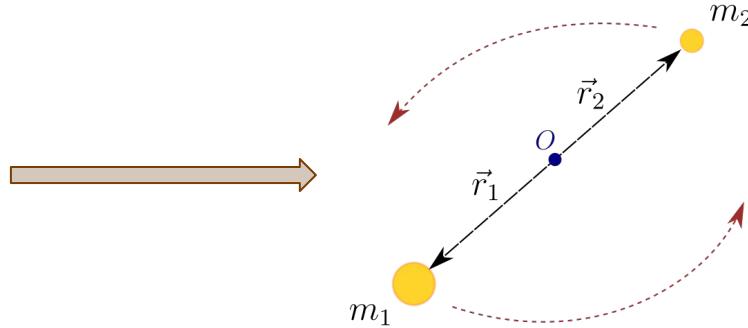
The beginning of the N -body problem



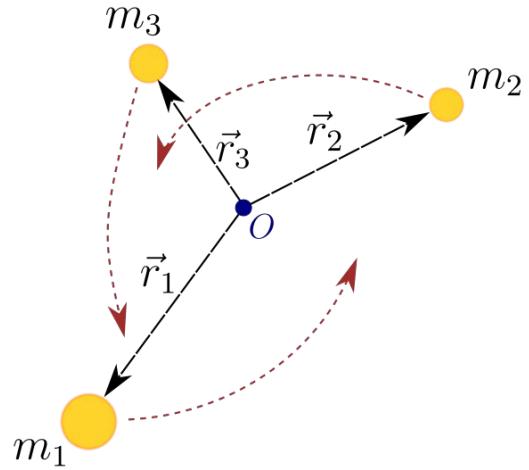
The beginning of the N -body problem



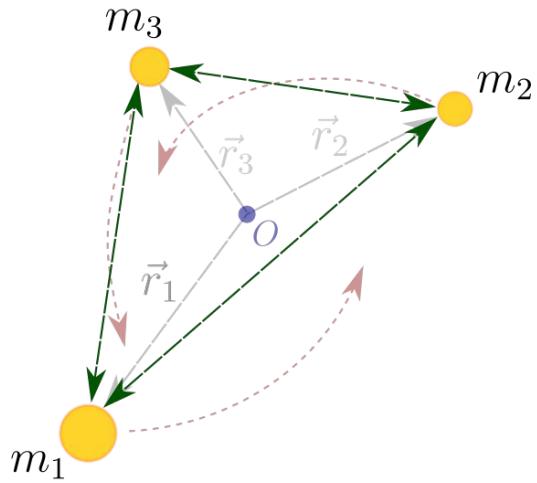
$$\vec{F} = G \frac{m_1 m_2}{|\vec{r}_{12}|^3} \vec{r}_{12}$$



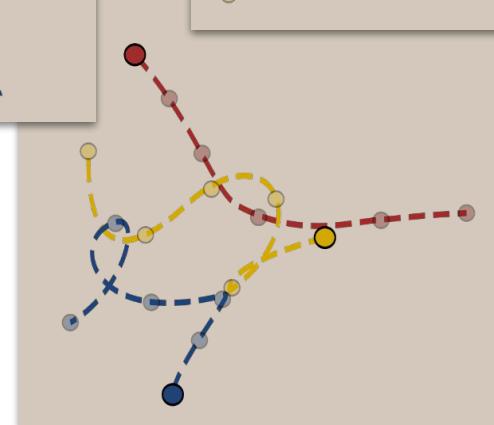
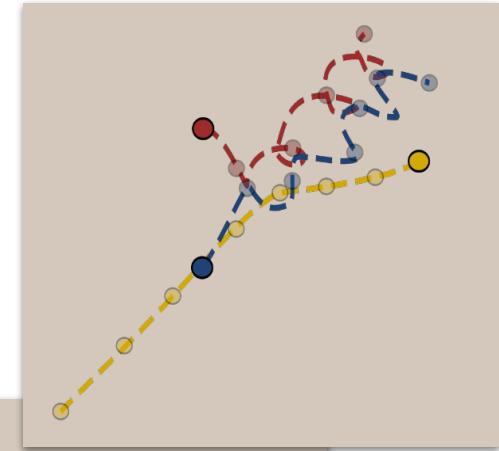
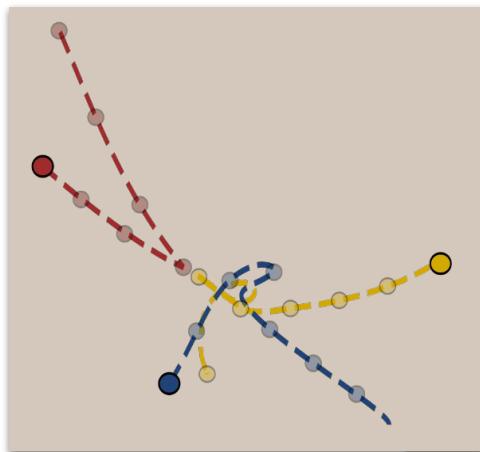
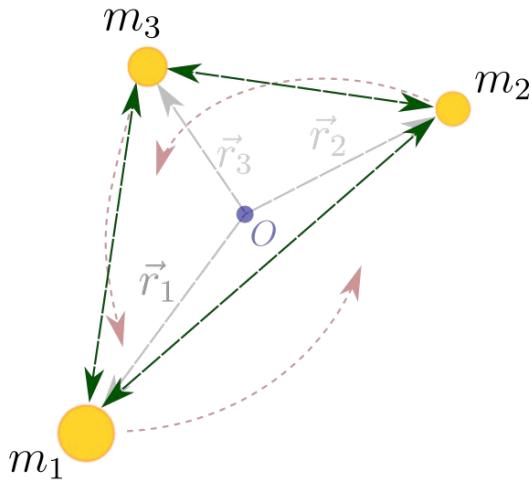
The three-body problem



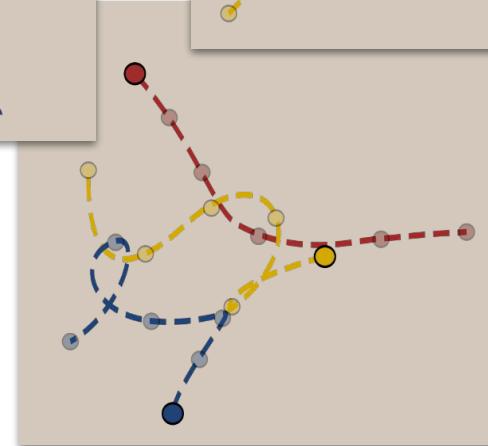
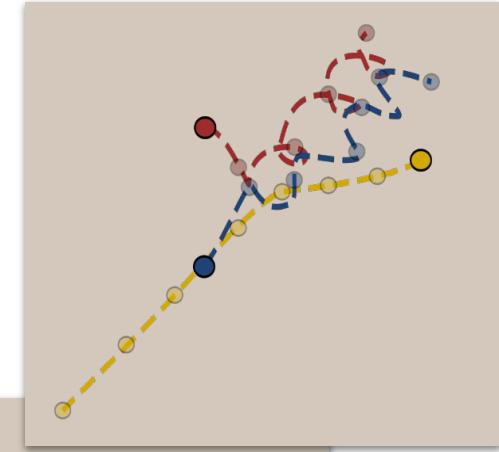
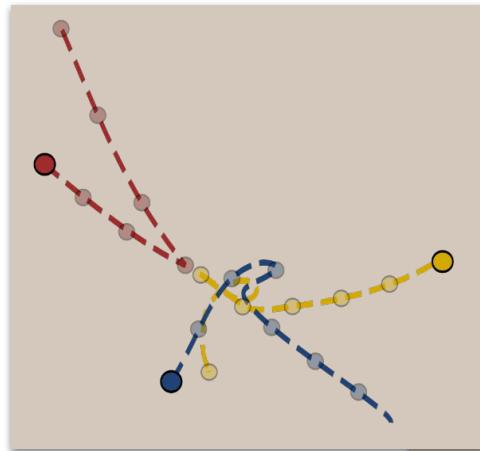
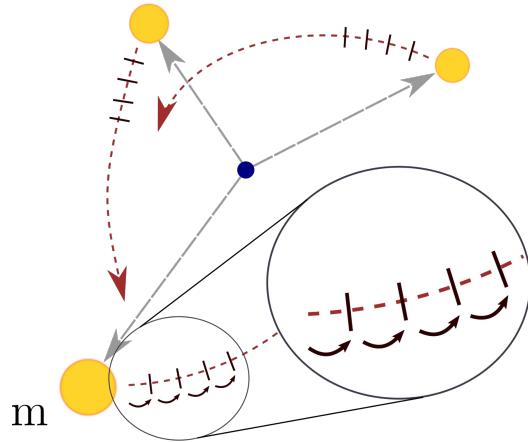
The three-body problem



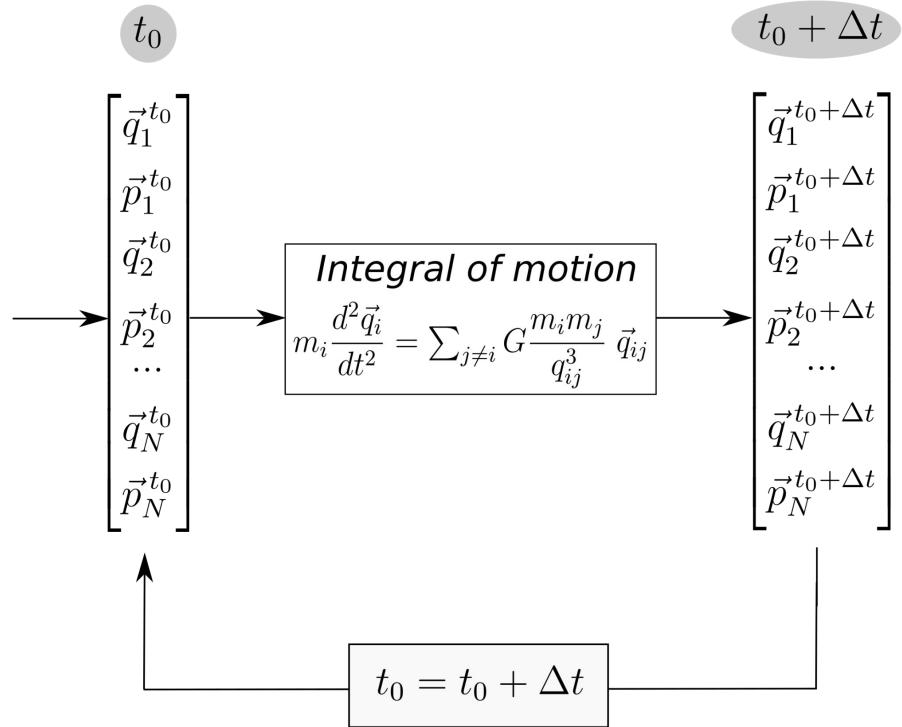
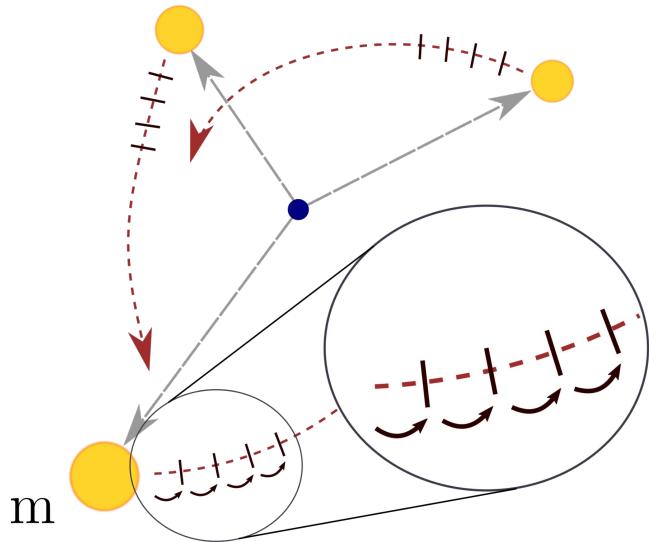
The three-body problem



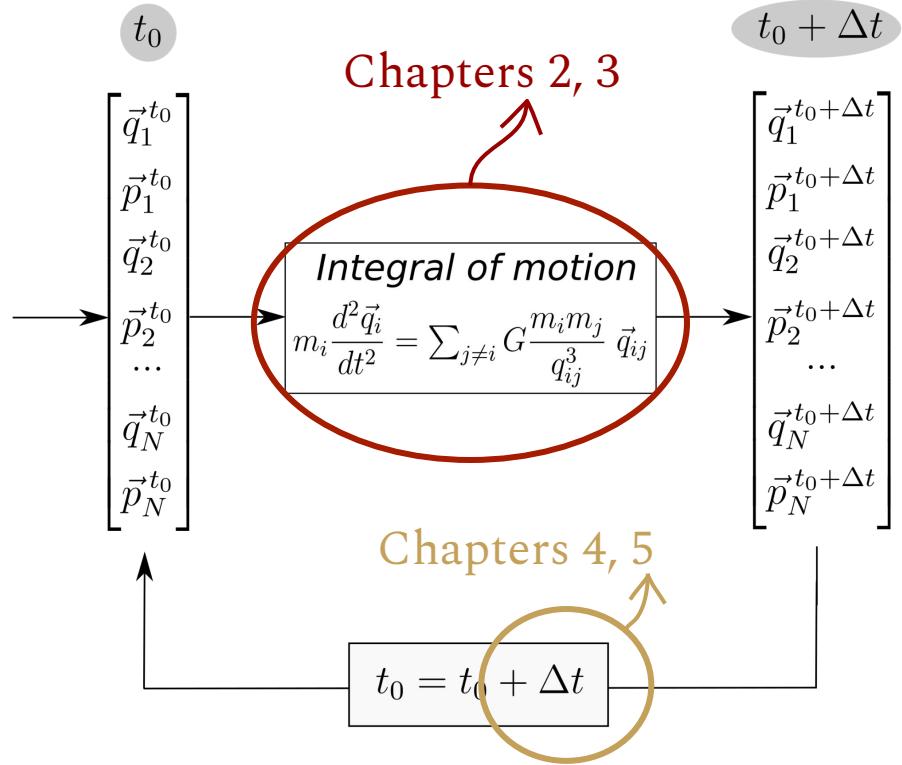
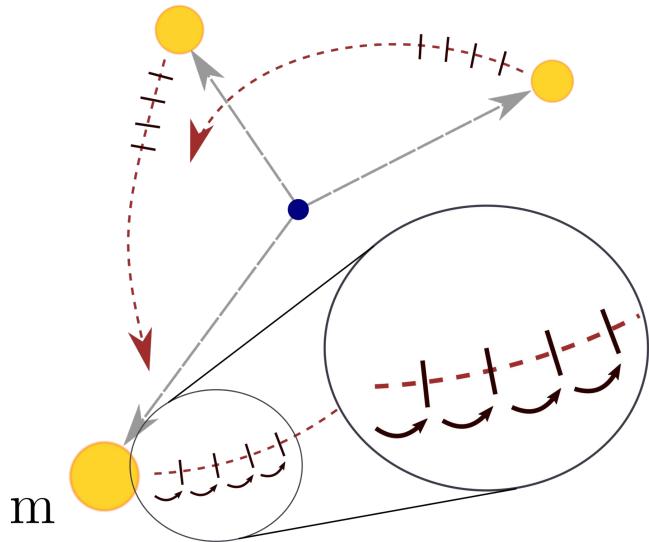
The three-body problem



Numerical integration



Numerical integration

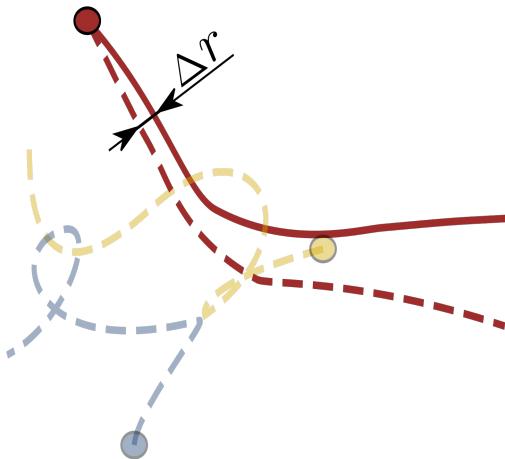


Numerical Error

$$\mathcal{H} = \underbrace{\sum_{i=0}^{N-1} \frac{||\vec{p}_i||^2}{2m_i}}_{\text{Kinetic Energy}} - G \underbrace{\sum_{i=0}^{N-2} m_i \sum_{j=i+1}^{N-1} \frac{m_j}{||\vec{q}_j - \vec{q}_i||}}_{\text{Potential Energy}}$$

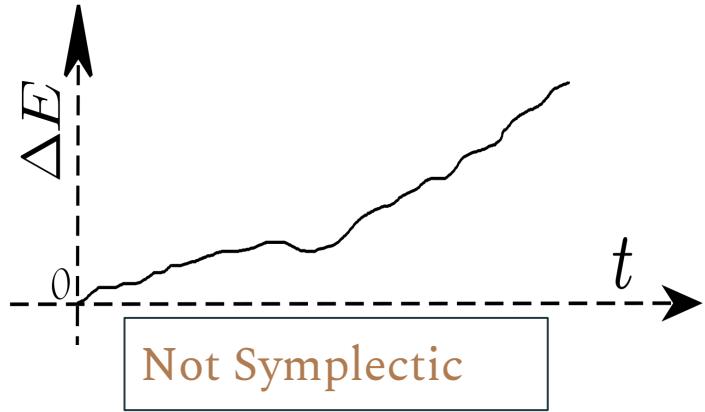
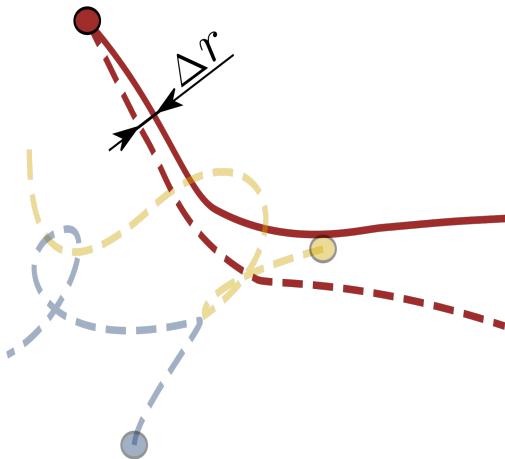
Numerical Error

$$\mathcal{H} = \underbrace{\sum_{i=0}^{N-1} \frac{||\vec{p}_i||^2}{2m_i}}_{\text{Kinetic Energy}} - G \underbrace{\sum_{i=0}^{N-2} m_i \sum_{j=i+1}^{N-1} \frac{m_j}{||\vec{q}_j - \vec{q}_i||}}_{\text{Potential Energy}}$$



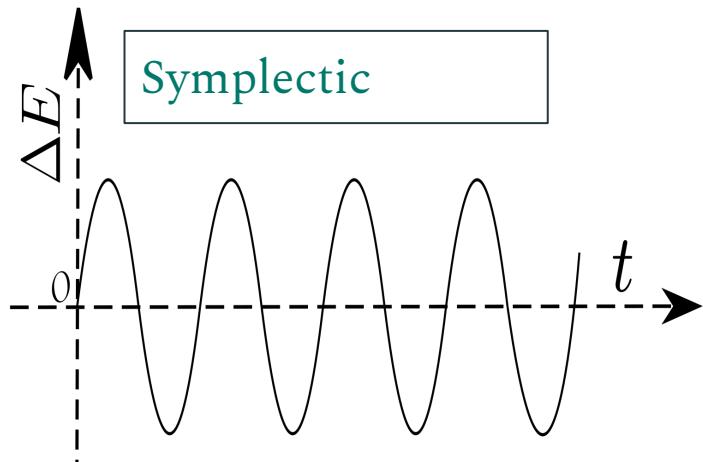
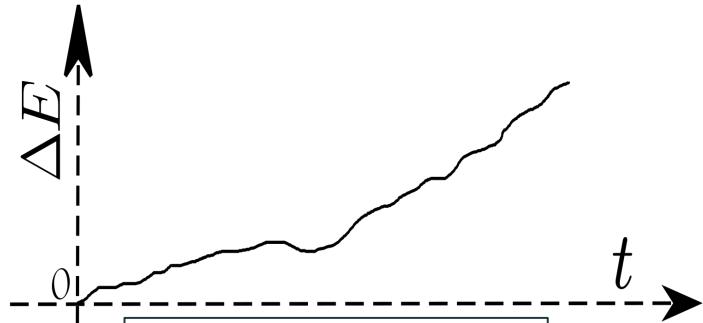
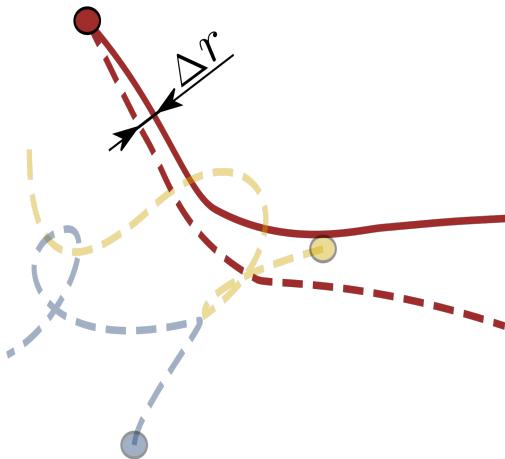
Numerical Error

$$\mathcal{H} = \underbrace{\sum_{i=0}^{N-1} \frac{||\vec{p}_i||^2}{2m_i}}_{\text{Kinetic Energy}} - G \underbrace{\sum_{i=0}^{N-2} m_i \sum_{j=i+1}^{N-1} \frac{m_j}{||\vec{q}_j - \vec{q}_i||}}_{\text{Potential Energy}}$$



Numerical Error

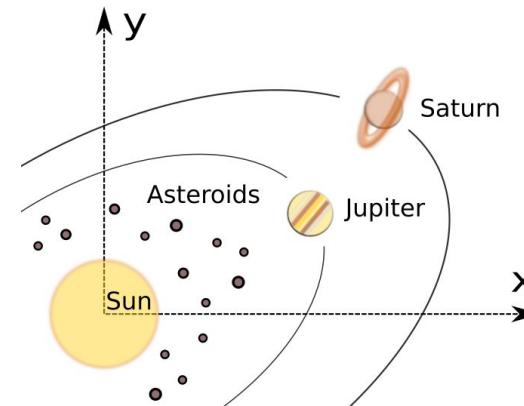
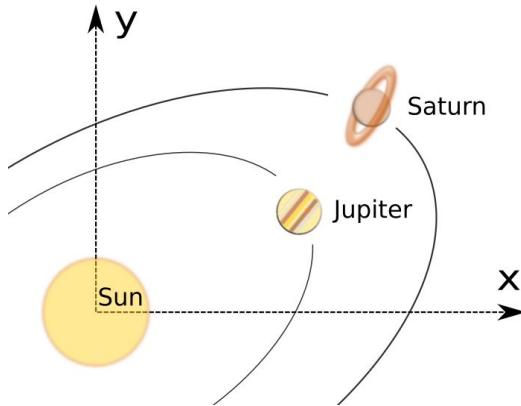
$$\mathcal{H} = \underbrace{\sum_{i=0}^{N-1} \frac{||\vec{p}_i||^2}{2m_i}}_{\text{Kinetic Energy}} - G \underbrace{\sum_{i=0}^{N-2} m_i \sum_{j=i+1}^{N-1} \frac{m_j}{||\vec{q}_j - \vec{q}_i||}}_{\text{Potential Energy}}$$



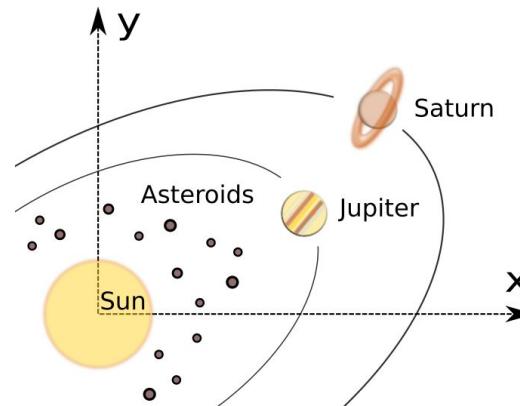
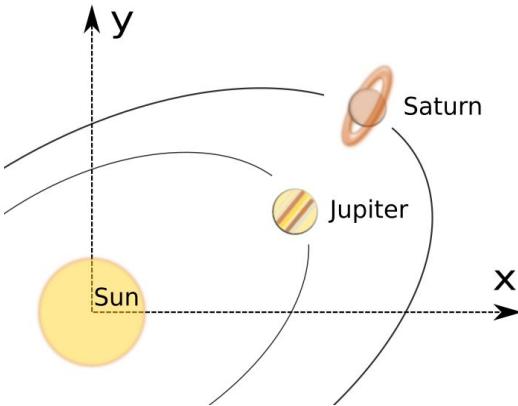
Chapter 2

*A hybrid approach
for solving the gravitational N-body problem
with Artificial Neural Networks*

Planetary Systems

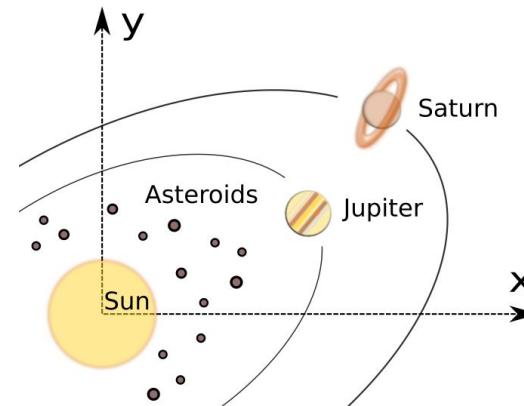
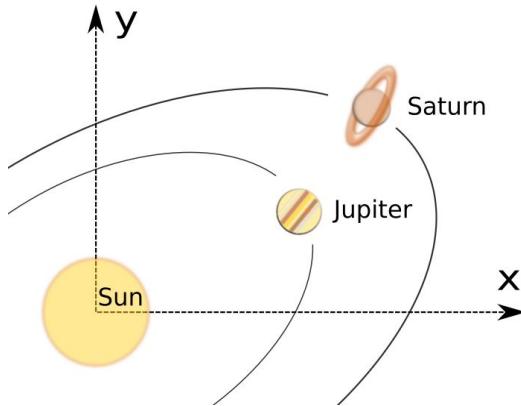


Planetary Systems



$$\mathcal{H} = \underbrace{\sum_{i=0}^{N-1} \frac{||\vec{p}_i||^2}{2m_i}}_{\text{Kinetic Energy}} - G \underbrace{\sum_{i=0}^{N-2} m_i \sum_{j=i+1}^{N-1} \frac{m_j}{||\vec{q}_j - \vec{q}_i||}}_{\text{Potential Energy}}$$

Planetary Systems

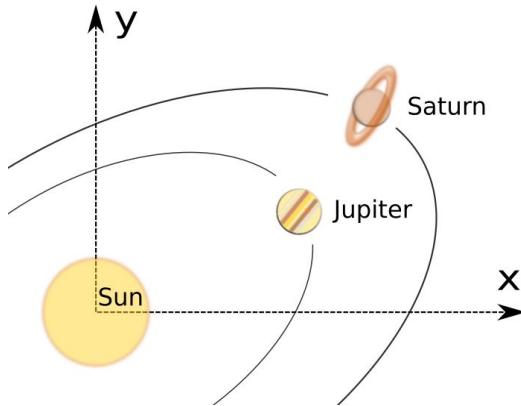


Wisdom-Holman
Integrator

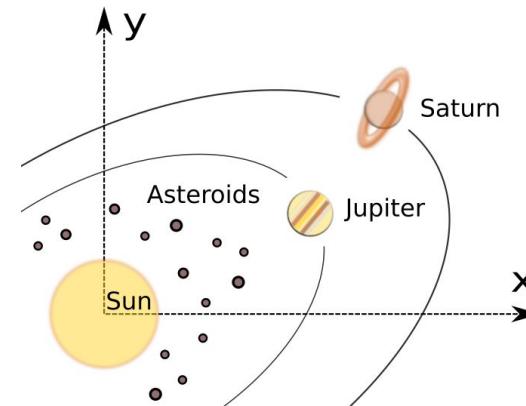
$$\mathcal{H} = \underbrace{\sum_{i=0}^{N-1} \frac{||\vec{p}_i||^2}{2m_i}}_{\text{Kinetic Energy}} - G \underbrace{\sum_{i=0}^{N-2} m_i \sum_{j=i+1}^{N-1} \frac{m_j}{||\vec{q}_j - \vec{q}_i||}}_{\text{Potential Energy}}$$

$$\mathcal{H} = \mathcal{H}_{\text{Kepler}} + \mathcal{H}_{\text{perturbations}}$$

Planetary Systems



a) SJS



b) SJSa

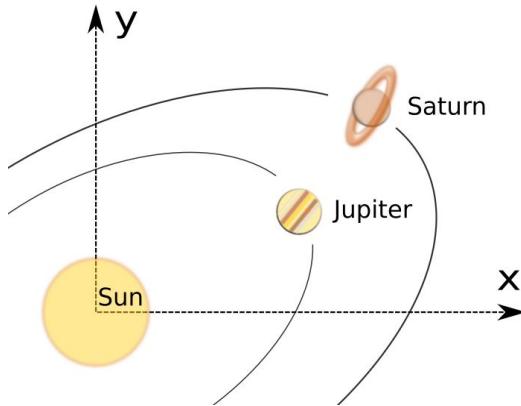
Perturbations

$$\vec{F} = G \frac{m_1 m_2}{|\vec{r}_{12}|^3} \vec{r}_{12}$$

\rightarrow

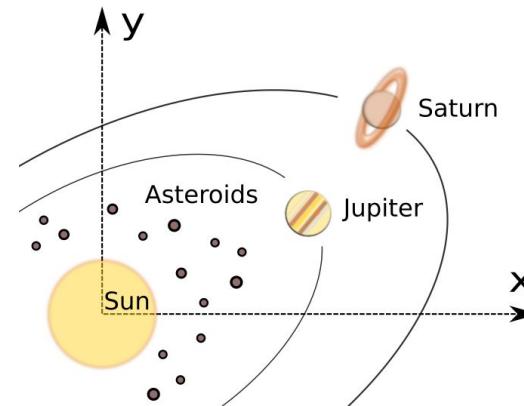
$\mathcal{O}(N^2)$

Planetary Systems



a) SJS

Fast (cheap)



b) SJSa

Expensive as N increases

Perturbations ↵

$$\vec{F} = G \frac{m_1 m_2}{|\vec{r}_{12}|^3} \vec{r}_{12}$$

→

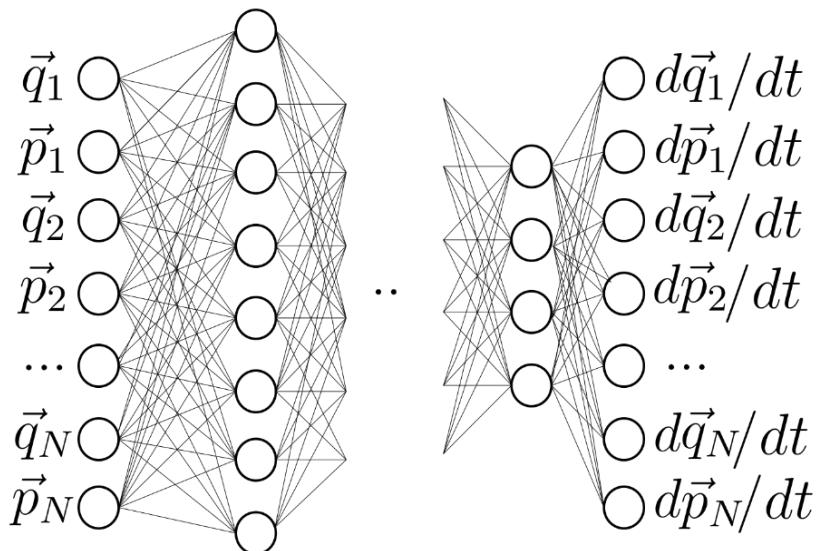
$\mathcal{O}(N^2)$

Neural Networks

Perturbations \rightarrow

$$\vec{F} = G \frac{m_1 m_2}{|\vec{r}_{12}|^3} \vec{r}_{12}$$

Deep Neural Networks

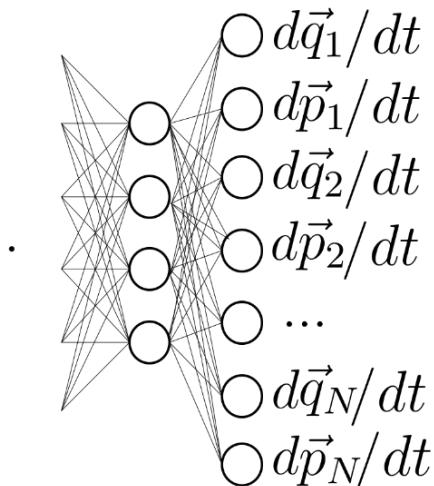
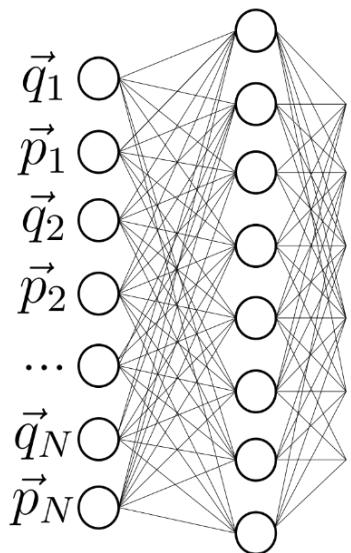


Neural Networks

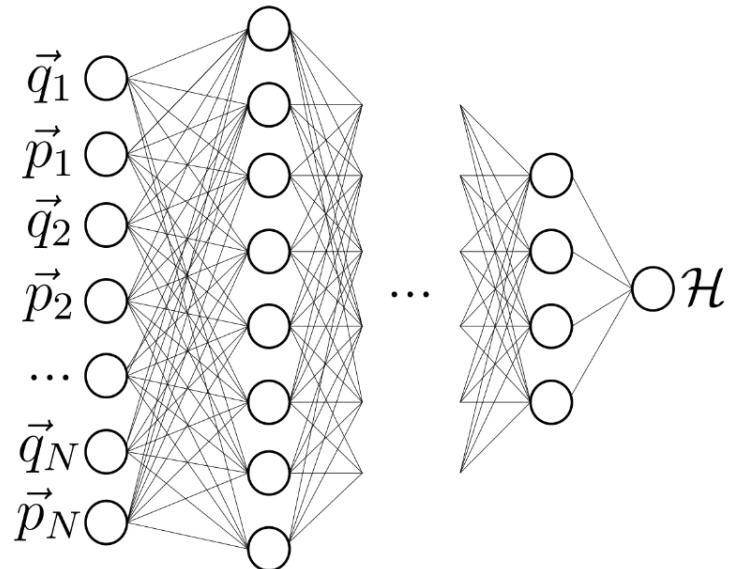
Perturbations $\sim e$

$$\vec{F} = G \frac{m_1 m_2}{|\vec{r}_{12}|^3} \vec{r}_{12}$$

Deep Neural Networks



Hamiltonian Neural Networks

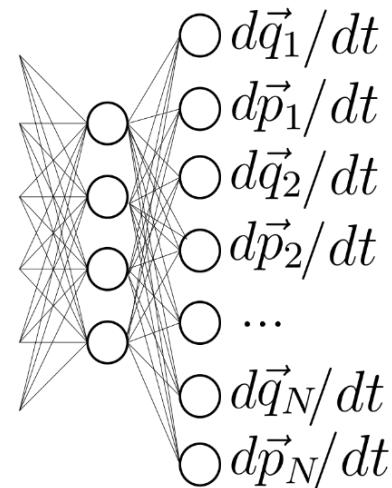
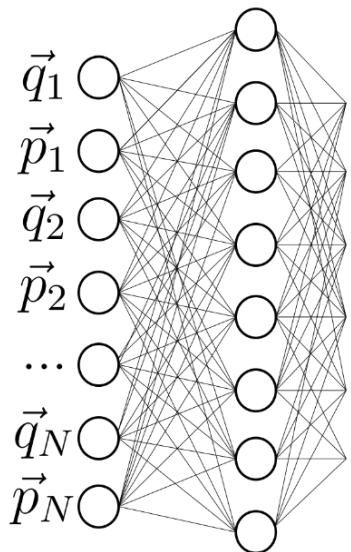


Neural Networks

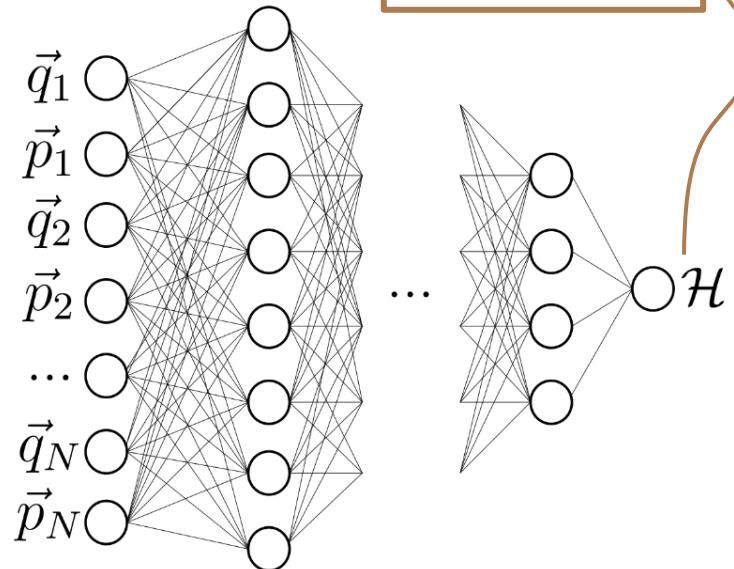
Perturbations $\sim e$

$$\vec{F} = G \frac{m_1 m_2}{|\vec{r}_{12}|^3} \vec{r}_{12}$$

Deep Neural Networks



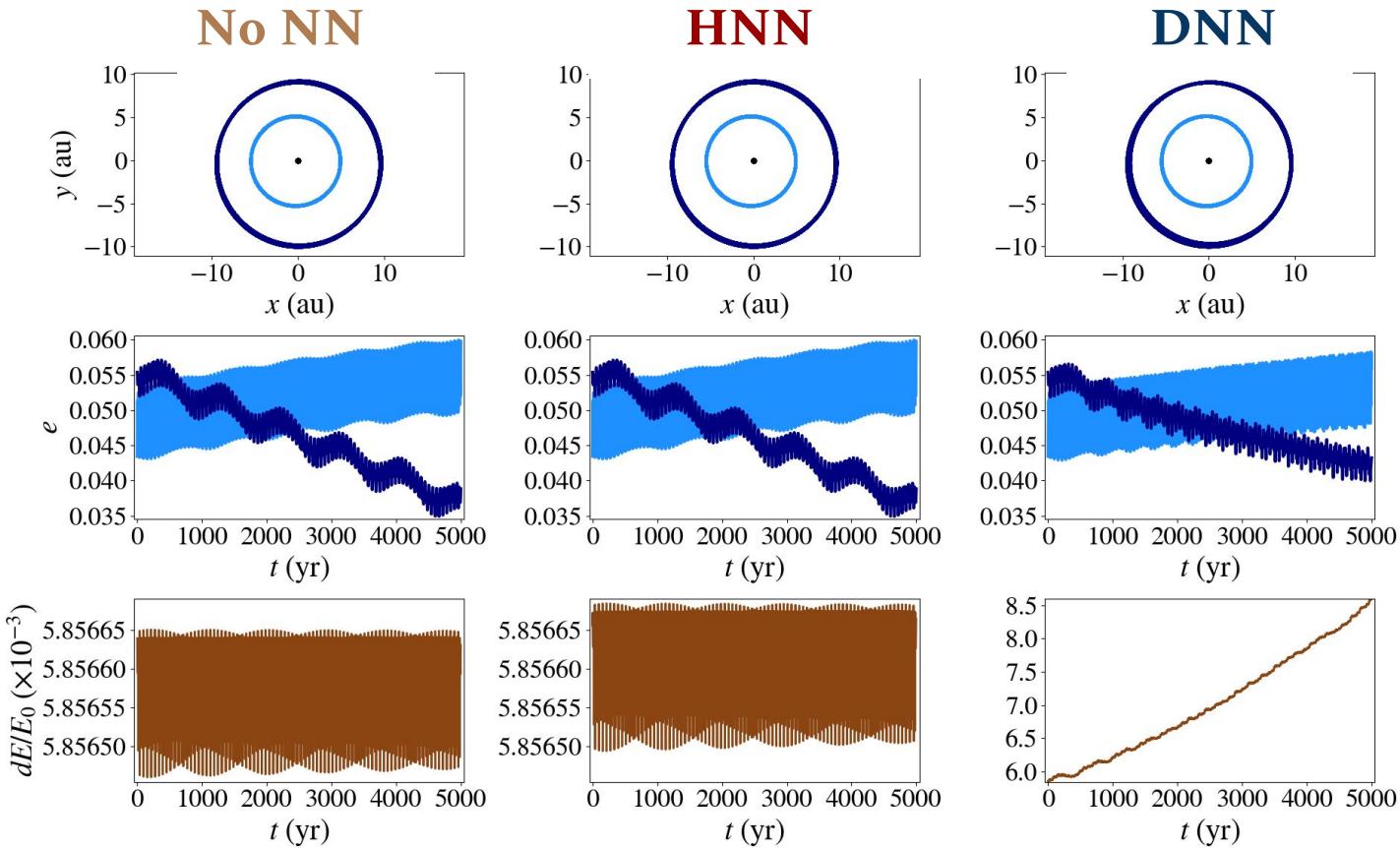
Hamiltonian Neural



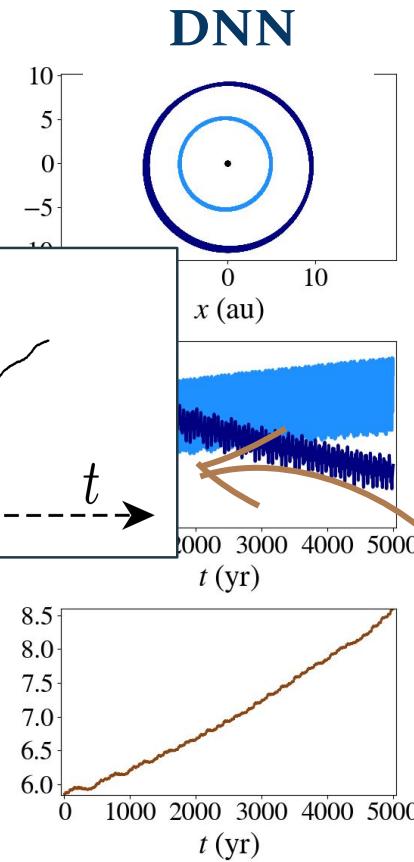
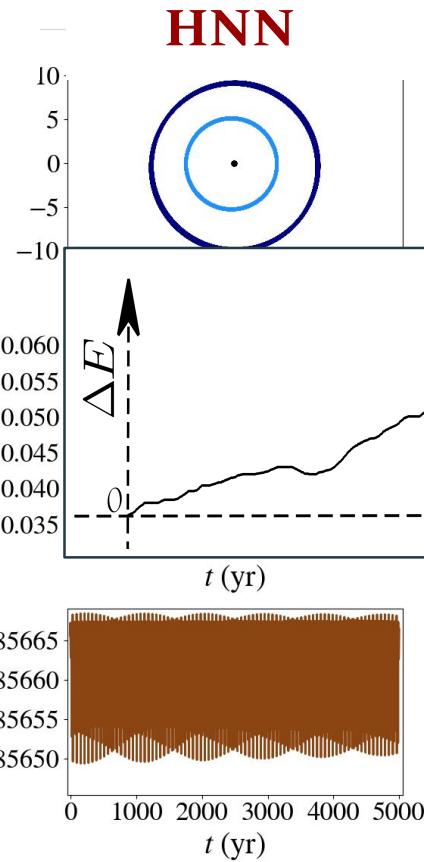
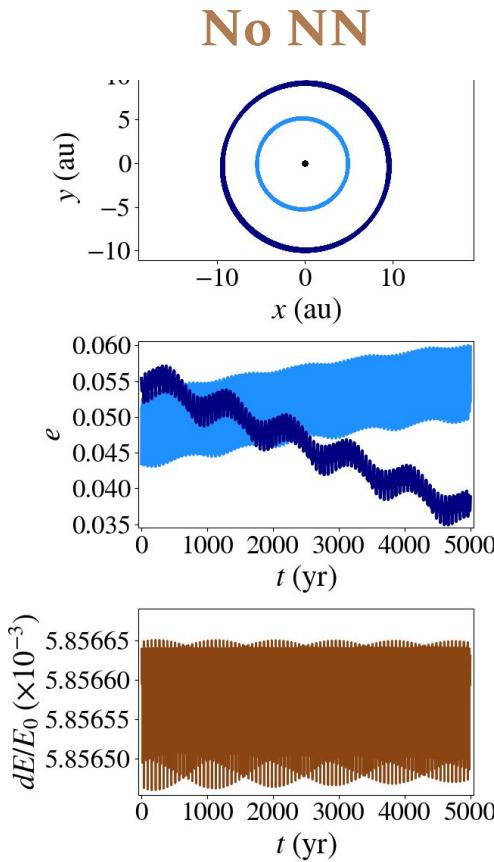
⚠️ Math Alert

$$\begin{aligned}\frac{\partial \mathcal{H}}{\partial \vec{q}} &= \frac{d\vec{p}}{dt} \\ \frac{\partial \mathcal{H}}{\partial \vec{p}} &= \frac{d\vec{q}}{dt}\end{aligned}$$

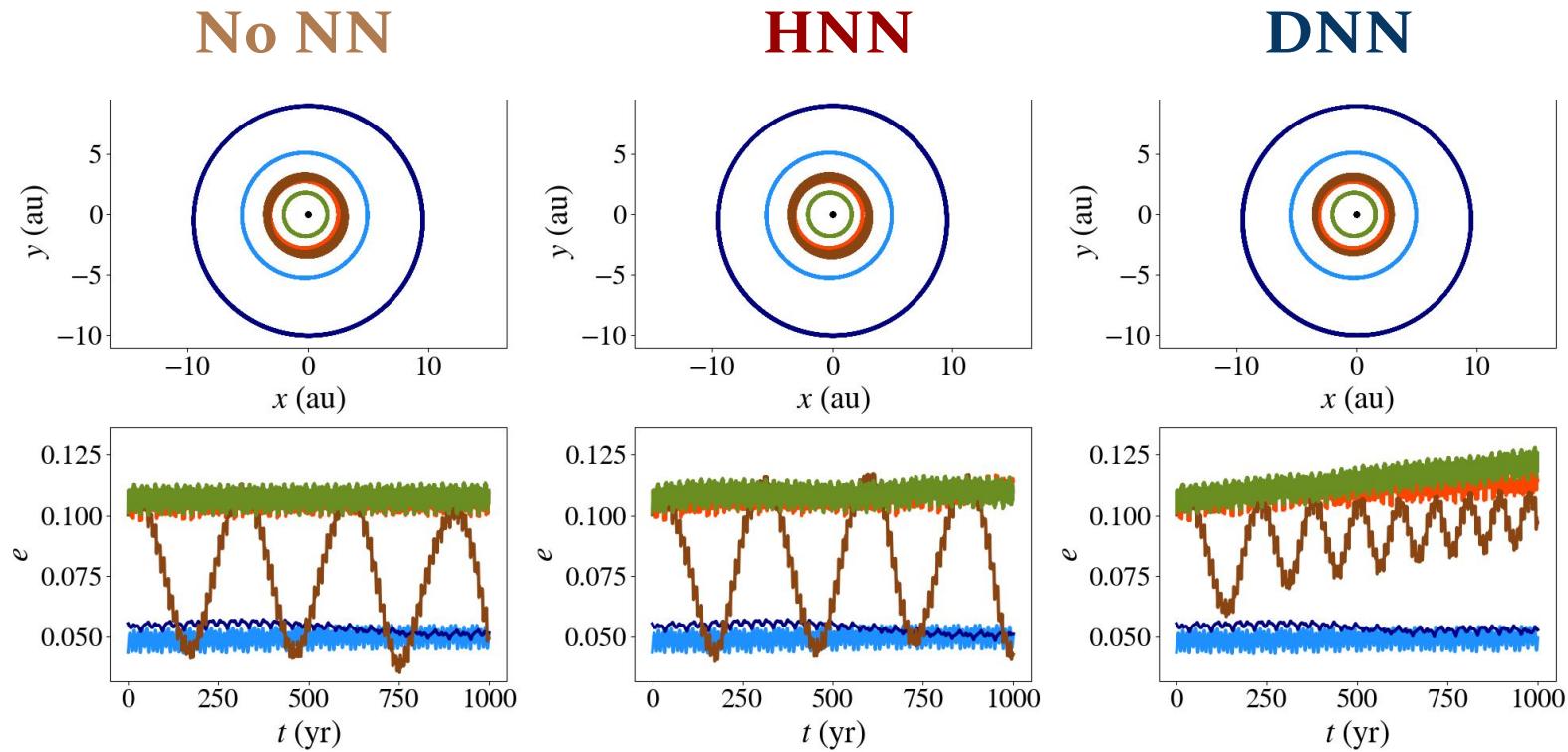
Results



Results

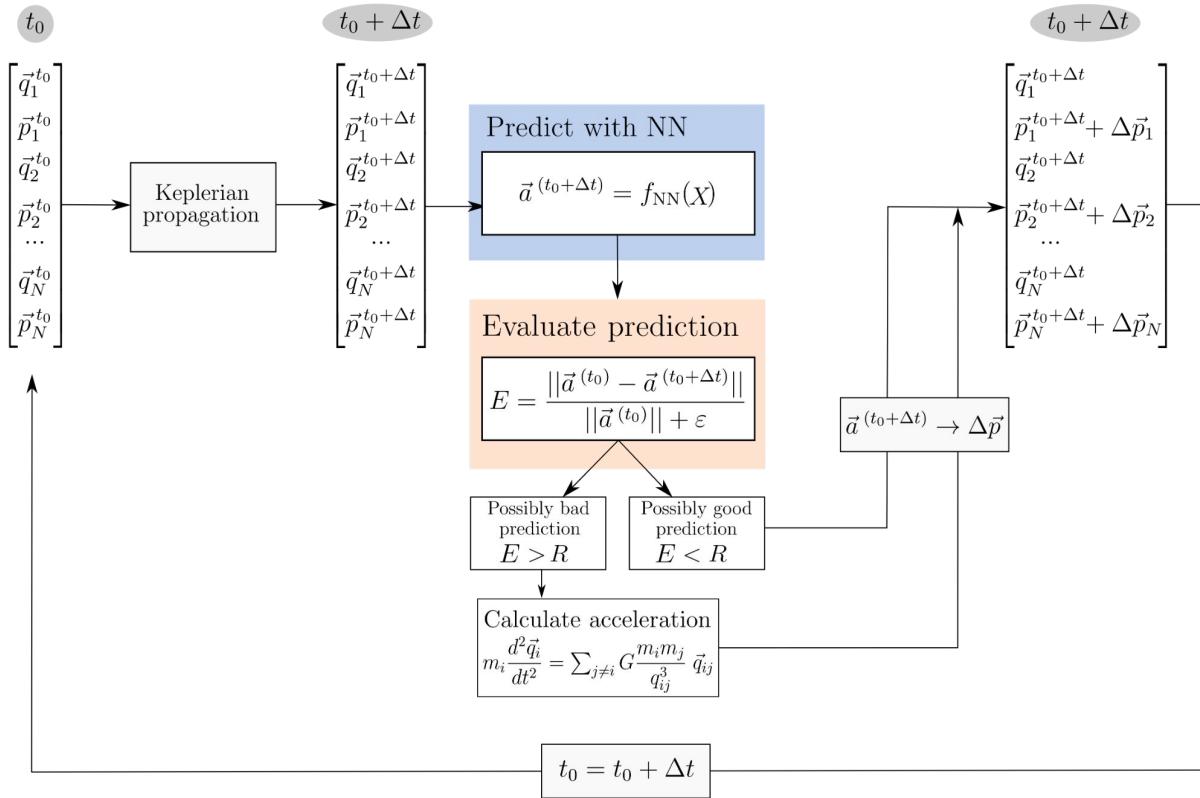


Results

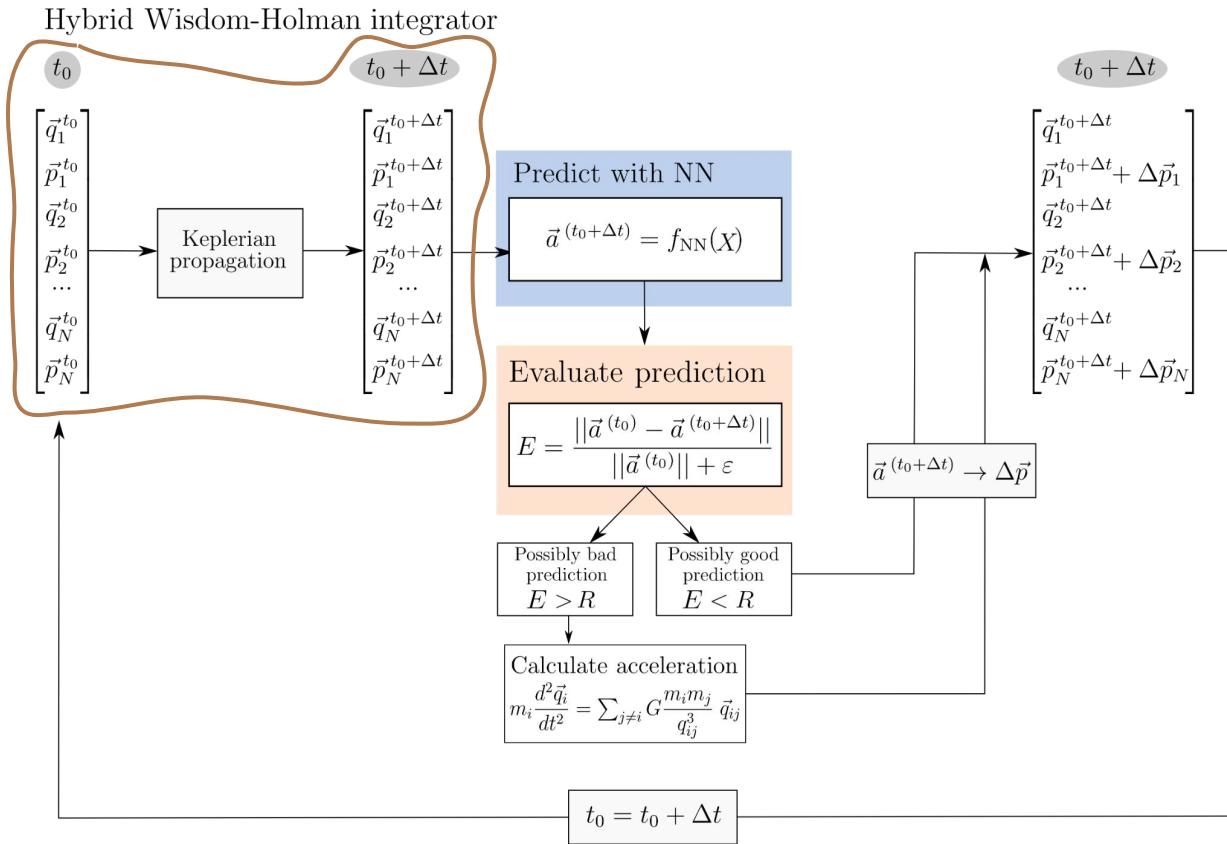


Hybrid method

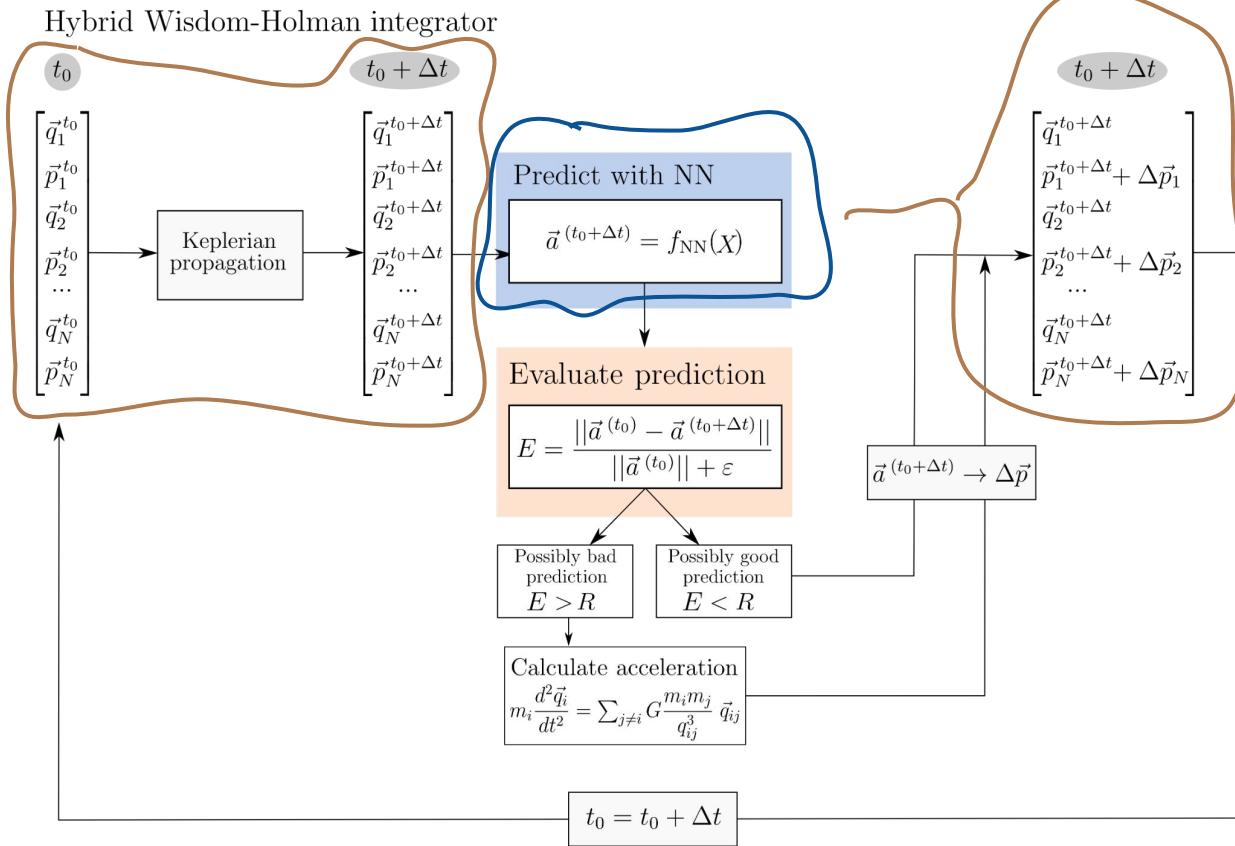
Hybrid Wisdom-Holman integrator



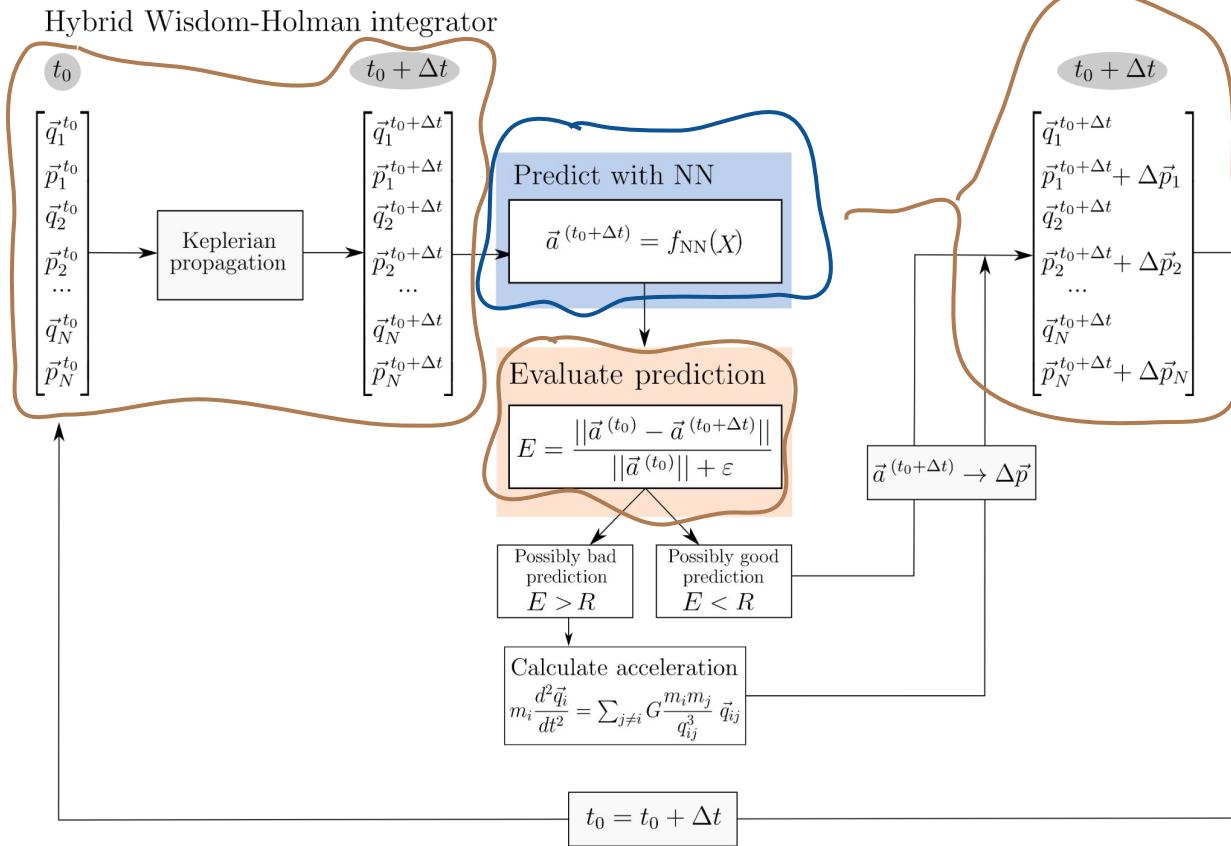
Hybrid method



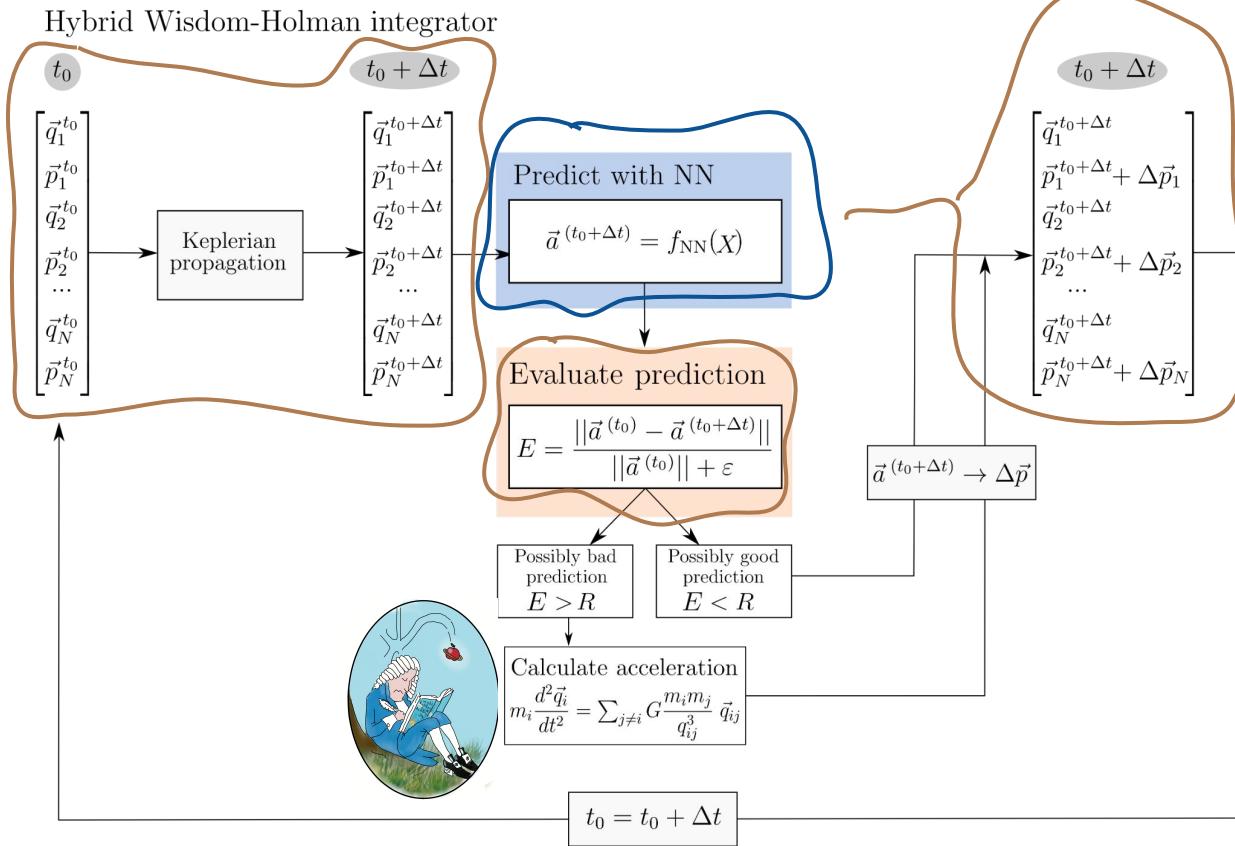
Hybrid method



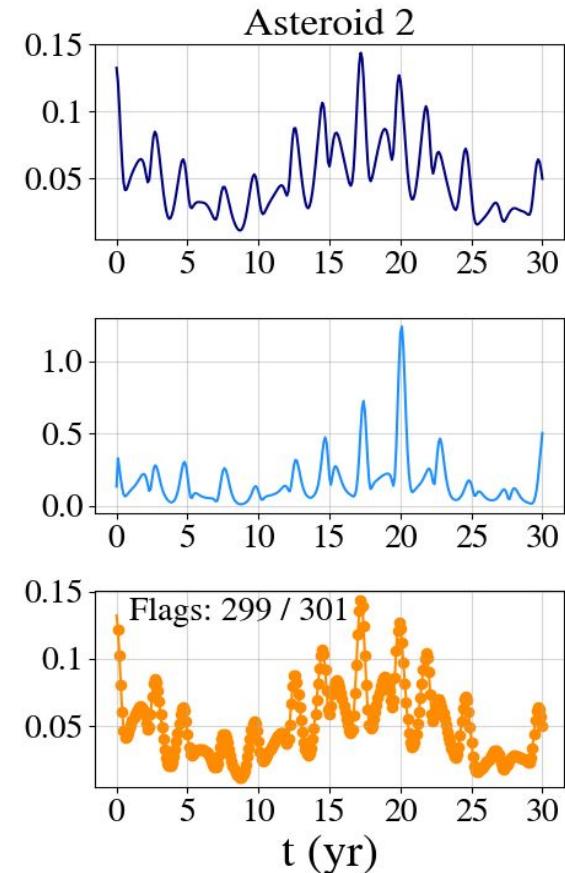
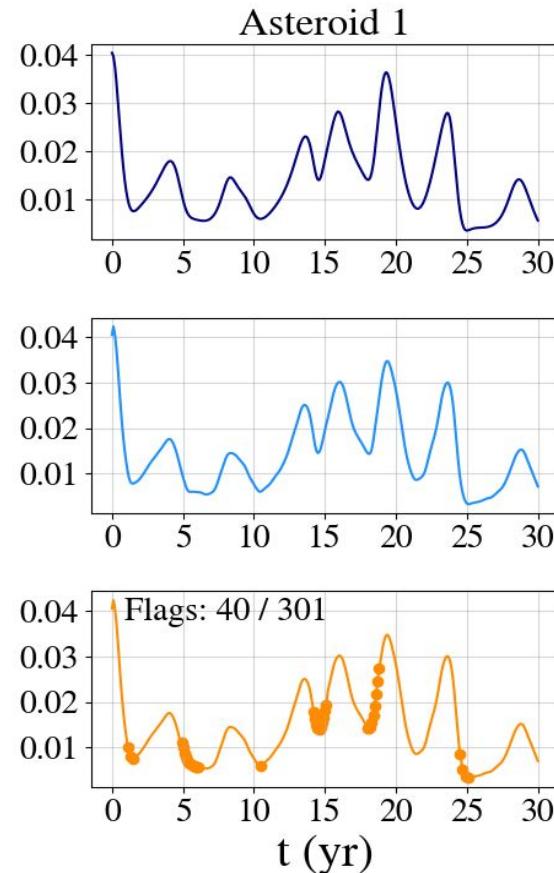
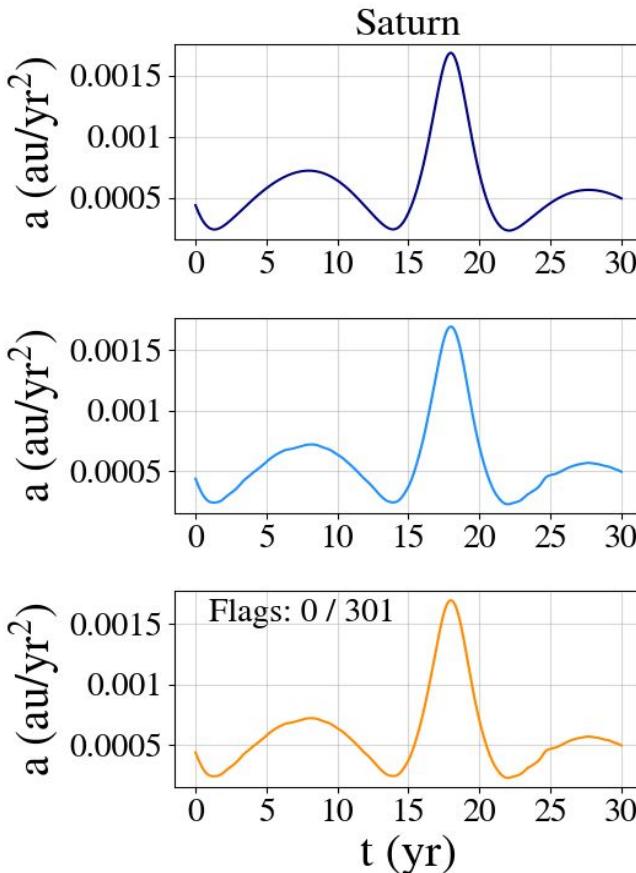
Hybrid method

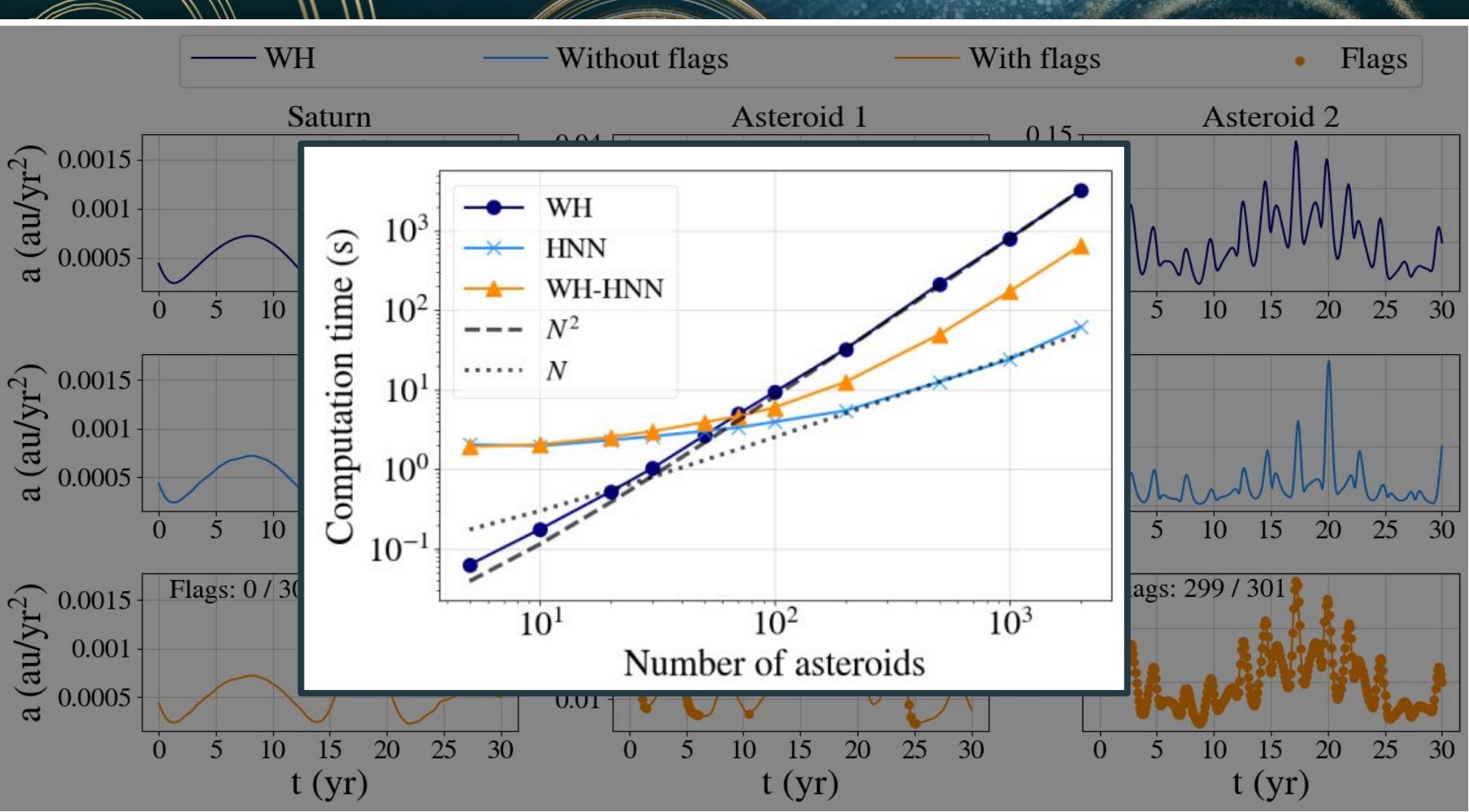


Hybrid method



— WH
 — Without flags
 — With flags
 ● Flags





Conclusions and disclaimers

HNNs can conserve energy error better — DNNs are easier to train

Errors accumulate — Hybrid method

Increasing N implies retraining

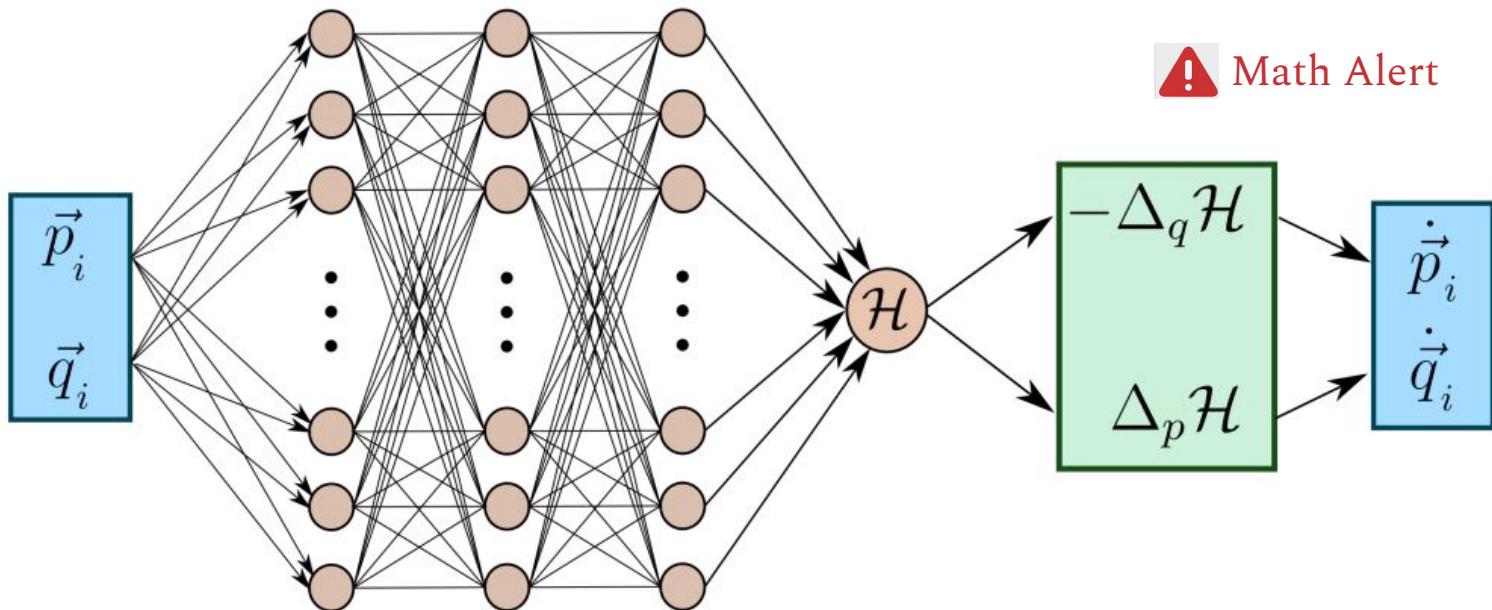
Accuracy of NNs lower than integrators

We need better NNs for complex physics problems

Chapter 3

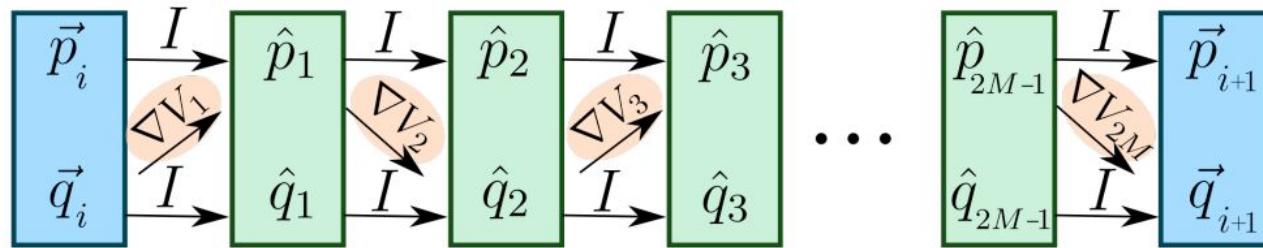
*A Generalized Framework of
Neural Networks for Hamiltonian Systems*

Hamiltonian Neural Network

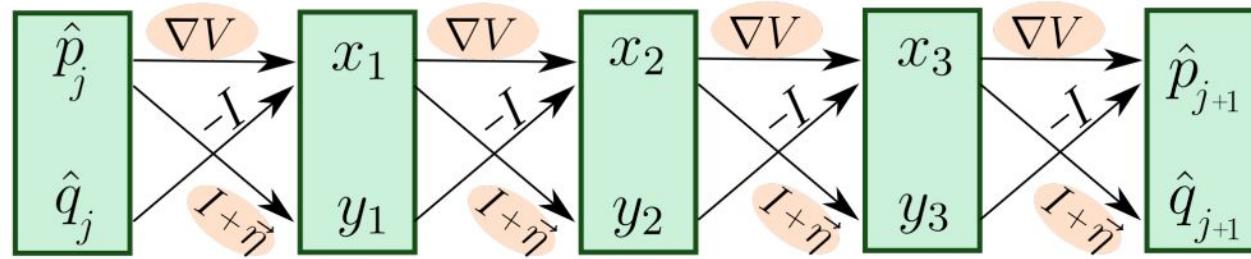


Other physics-aware Neural Networks

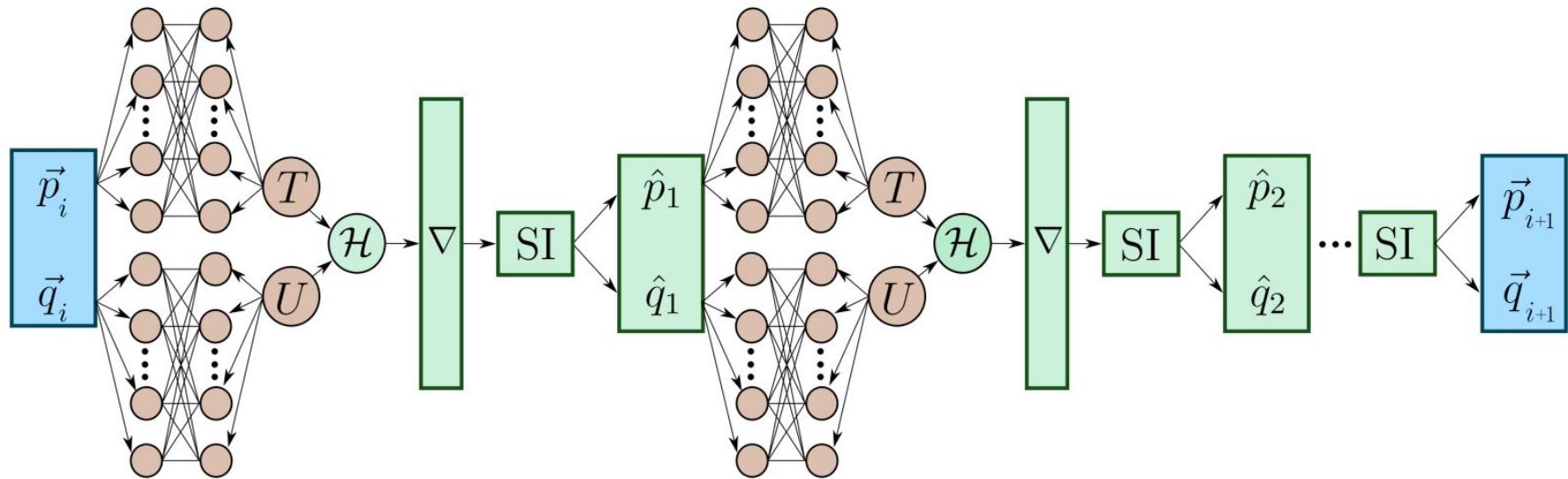
SympNets



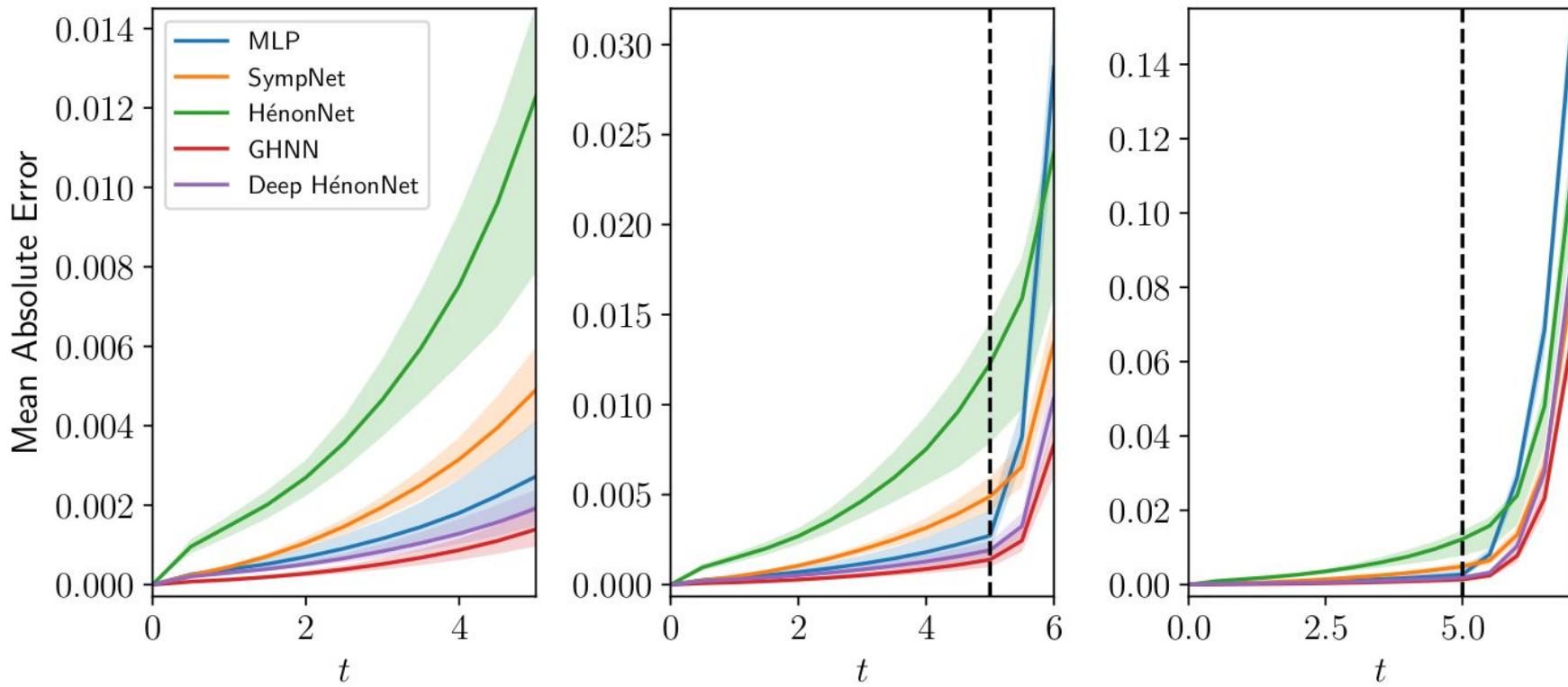
Hénon Nets



Generalized Framework



Results for the 3-body Problem



Conclusions and disclaimers

Physics structure — Better energy conservation — Less flexible

Different methods work for different problems

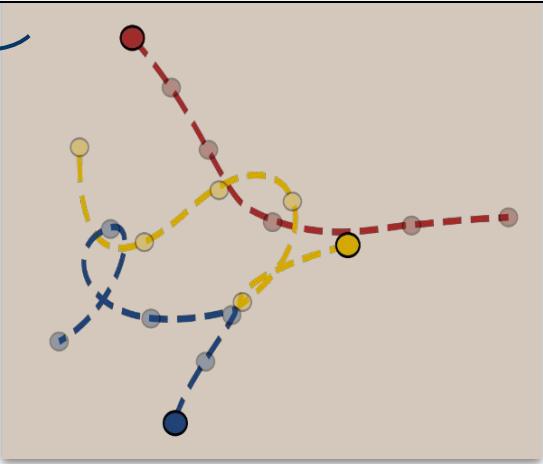
Current algorithms are not yet ready for their application on complex Astrophysics cases

Chapter 4

*Reinforcement Learning for
Adaptive Time-Stepping in the
Chaotic Gravitational Three-Body Problem*

Small $\Delta t \rightarrow$ Accurate - Expensive

Large $\Delta t \rightarrow$ Inaccurate - Cheap

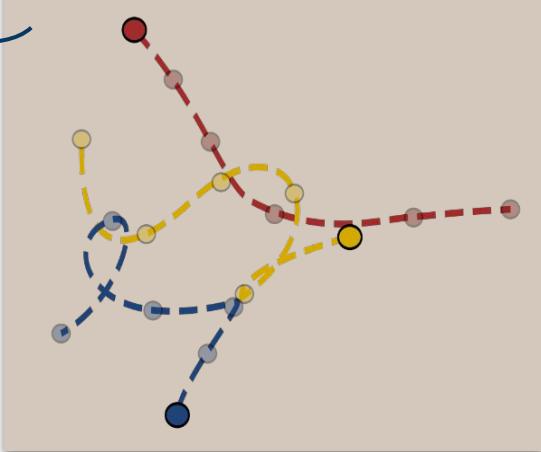


Integrator types

1. Fixed time-step integrators - *Symp*
2. Variable time-step integrators - *Huayno*, *Hermite*, *Brutus*

Small $\Delta t \rightarrow$ Accurate - Expensive

Large $\Delta t \rightarrow$ Inaccurate - Cheap

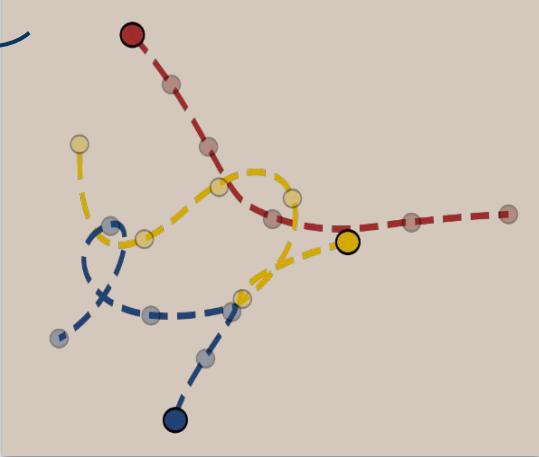


Integrator types

1. Fixed time-step integrators - *Symp*
2. Variable time-step integrators - *Huayno*, *Hermite*, *Brutus* - μ

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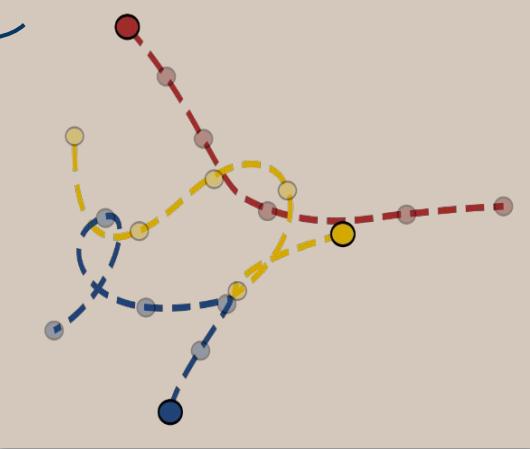
Integrator types

1. Fixed time-step integrators - *Symp*
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Small $\Delta t \rightarrow$ Accurate - Expensive

Large $\Delta t \rightarrow$ Inaccurate - Cheap

Dynamic environment



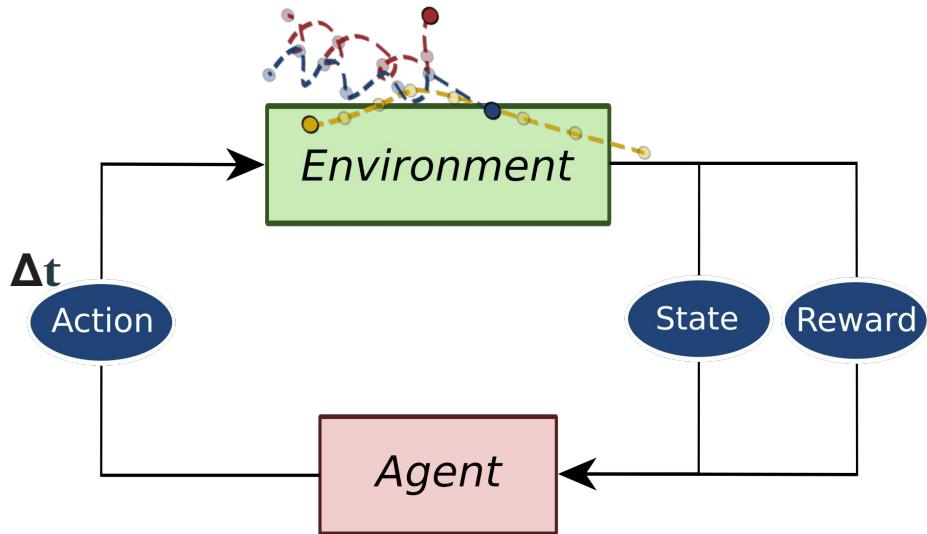
Keep it accurate

Close encounters \rightarrow Smaller Δt

Far away particles \rightarrow Larger Δt

Keep it efficient

Reinforcement Learning

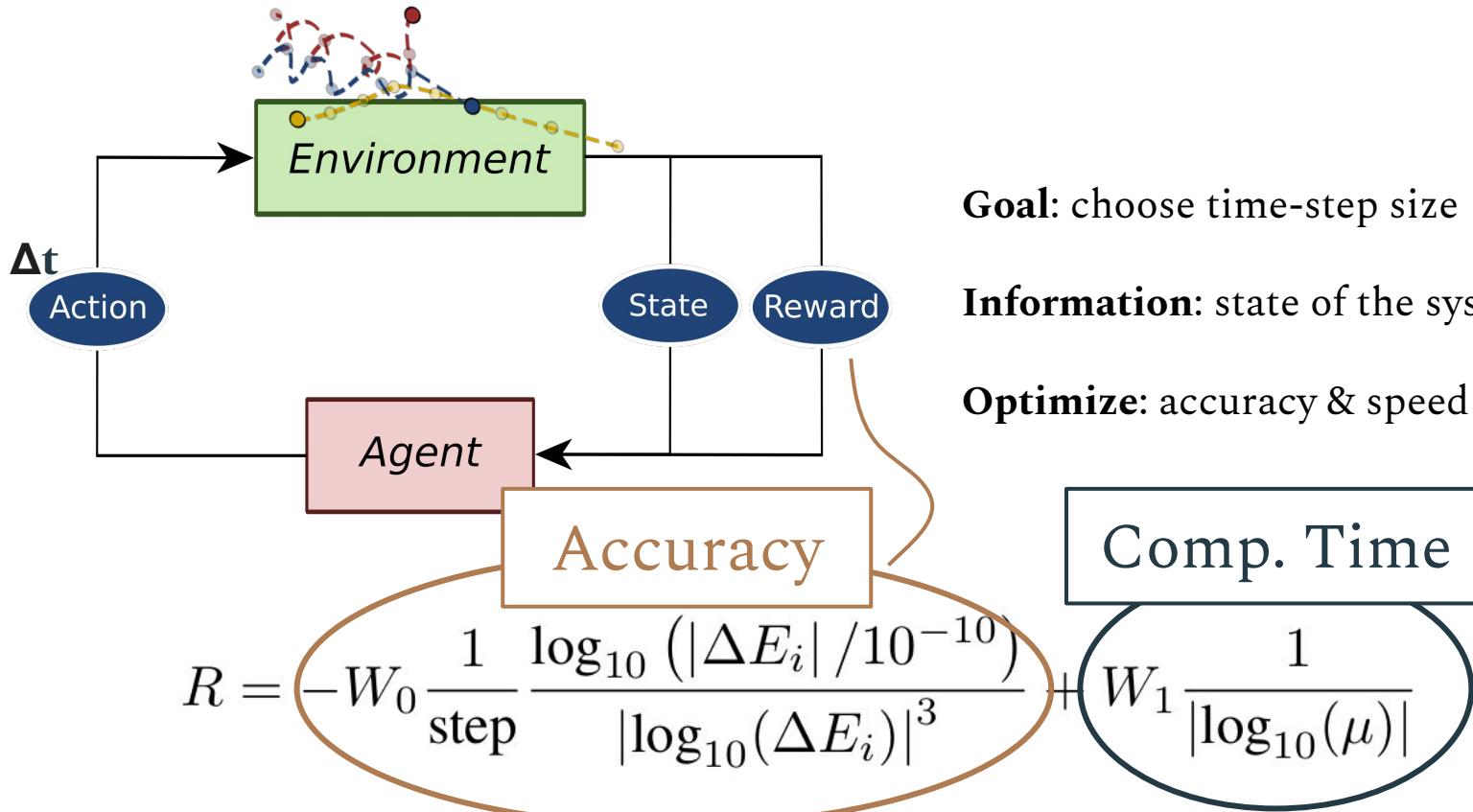


Goal: choose time-step size

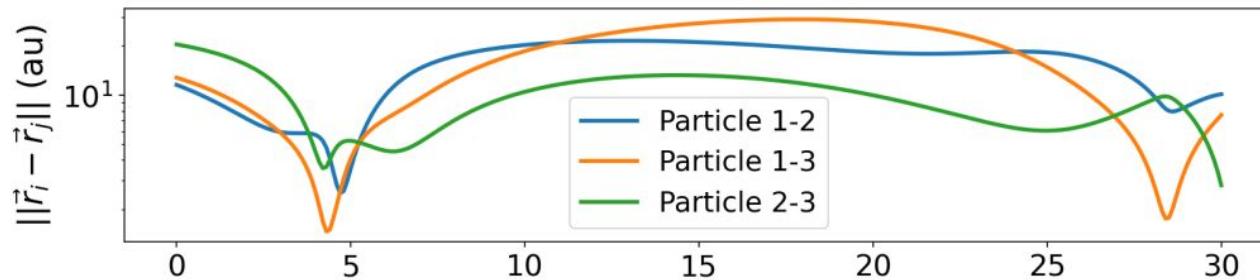
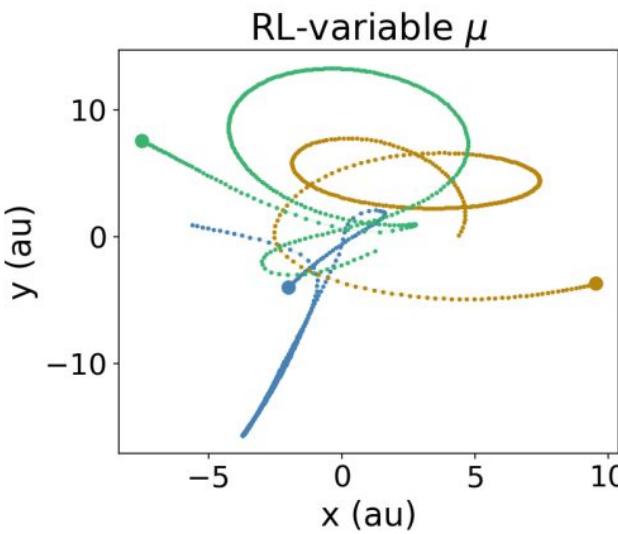
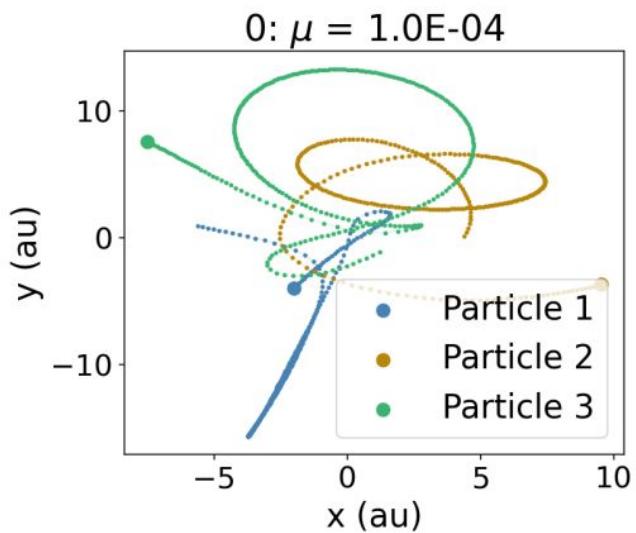
Information: state of the system

Optimize: accuracy & speed

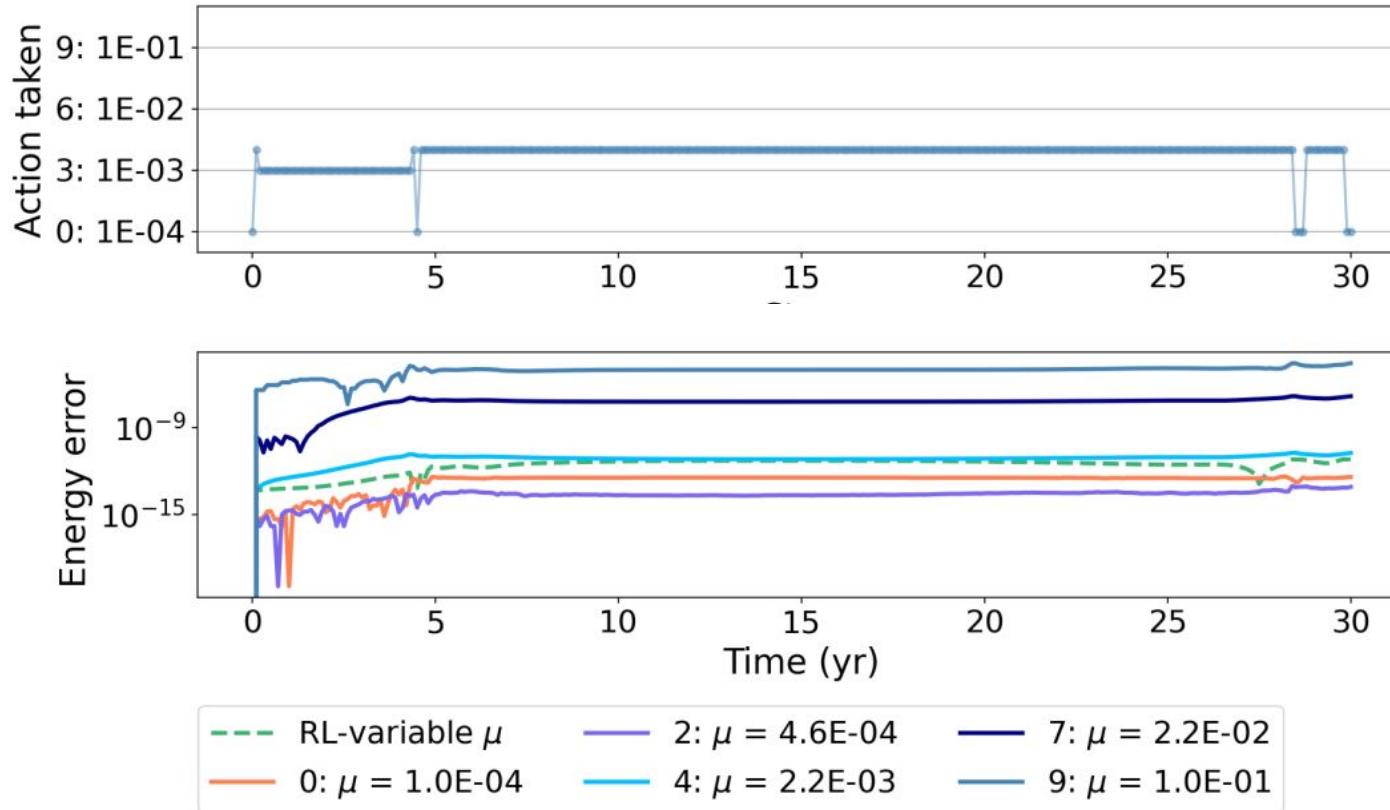
Reinforcement Learning



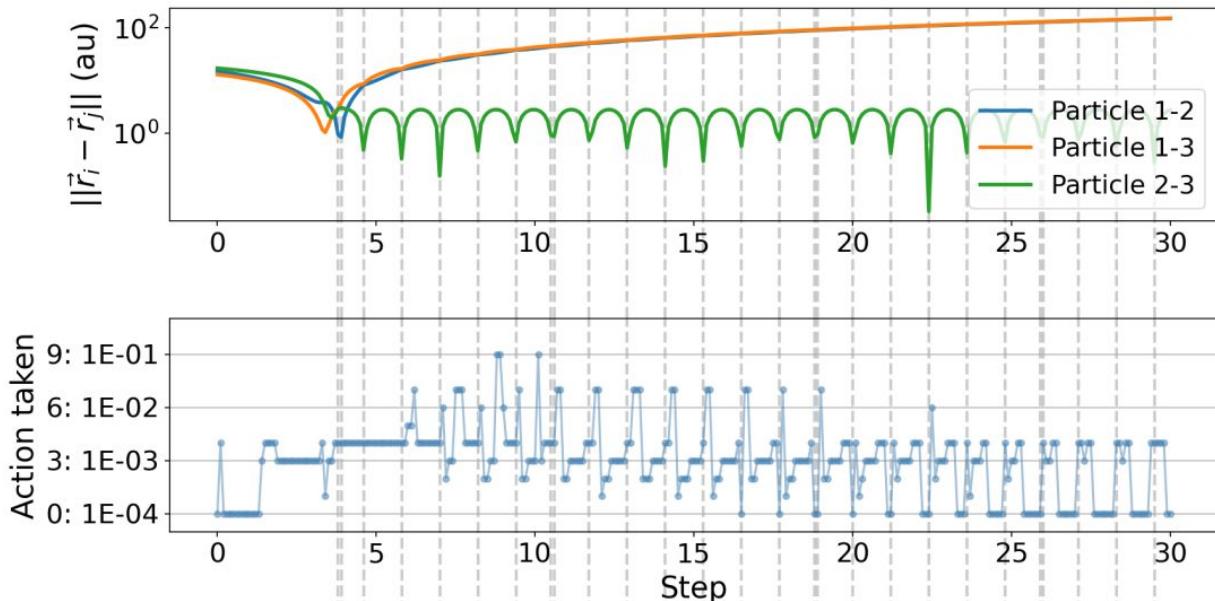
Results



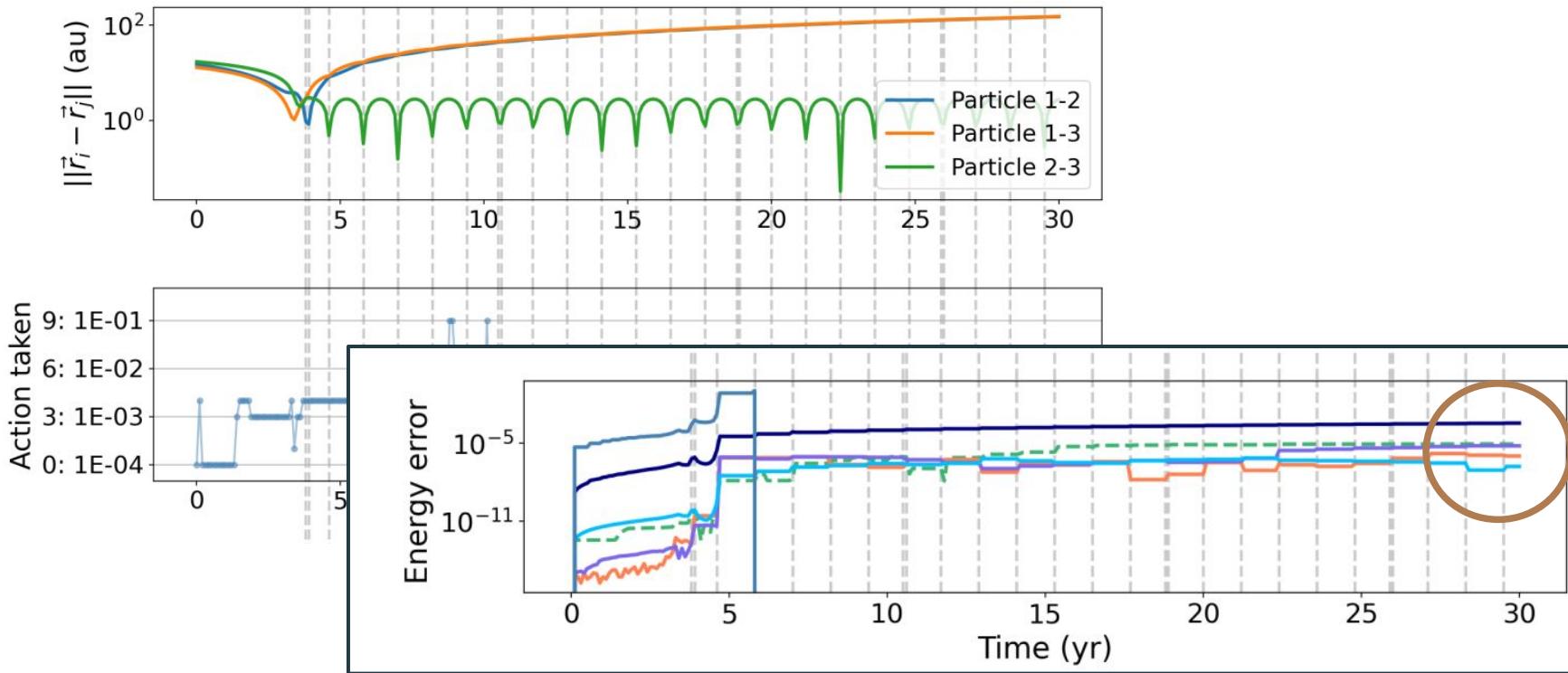
Results



Results



Results



Conclusions and disclaimers

Chapter 5

Easy to extrapolate to other problems

Good results with a preliminary training

Errors in prediction accumulate

Increasing N means retraining

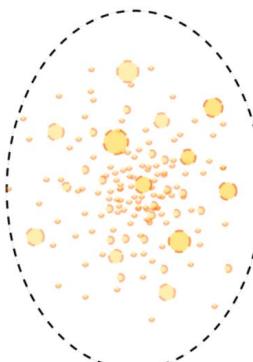
Let's try to apply it to a more complex case

Chapter 5

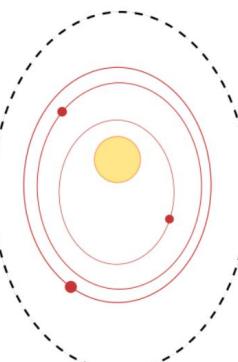
*Reinforcement Learning for the
Determination of the Bridge Time Step in
Cluster Dynamics Simulations*

Bridged Cluster with Planets

Cluster

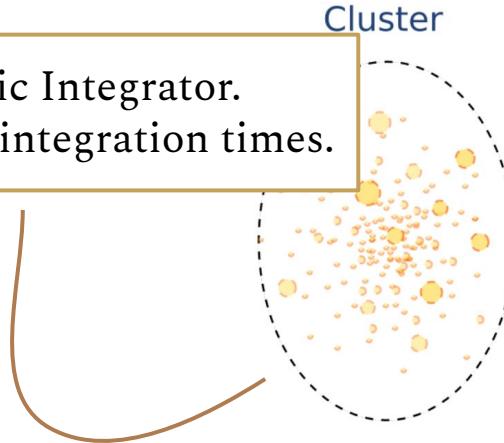


Planetary system



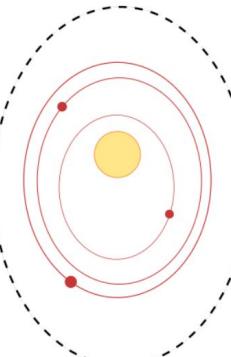
Bridged Cluster with Planets

- Specific Integrator.
- Large integration times.



Cluster Δt

Planetary system

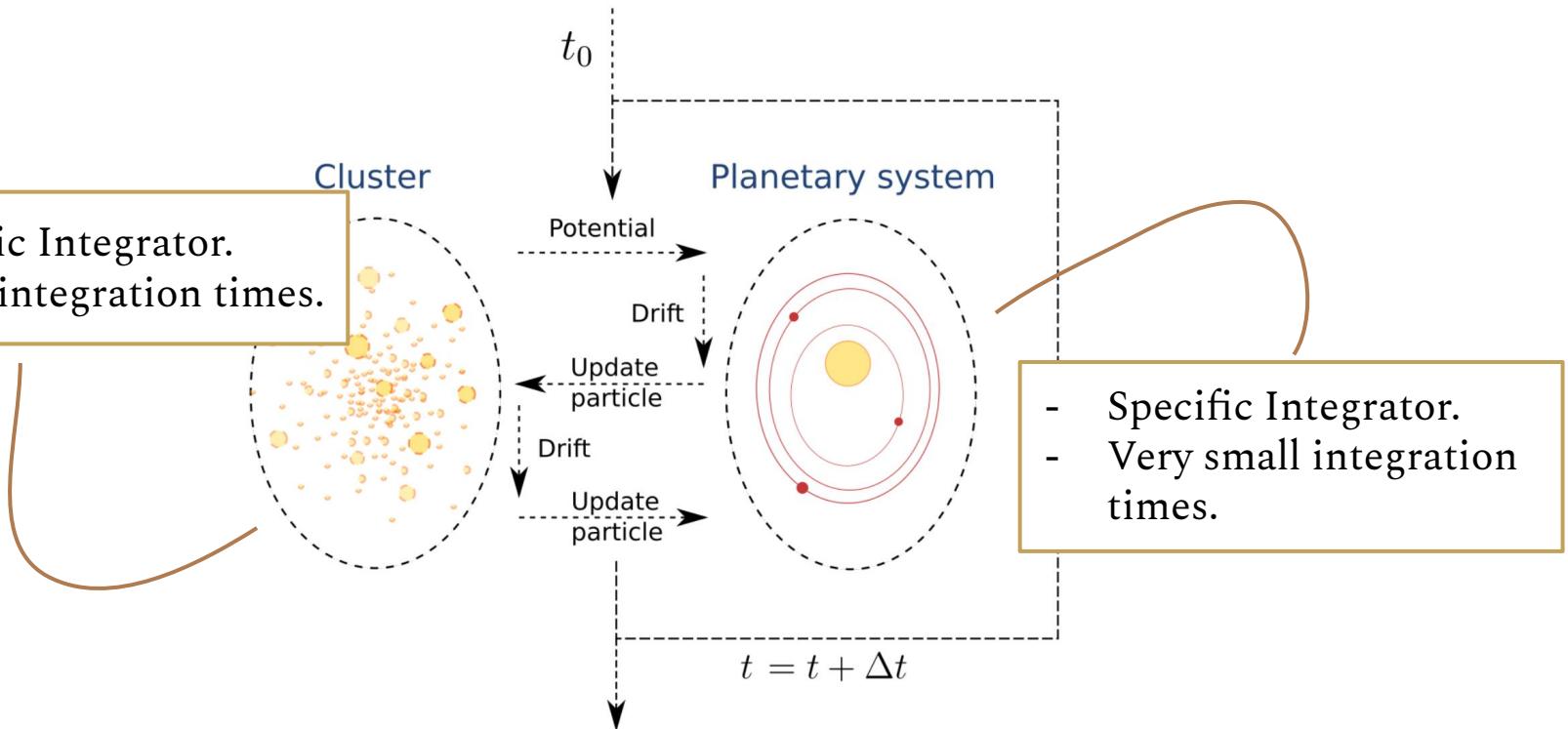


- Specific Integrator.
- Very small integration times.

Planetary System Δt

Bridged Cluster with Planets

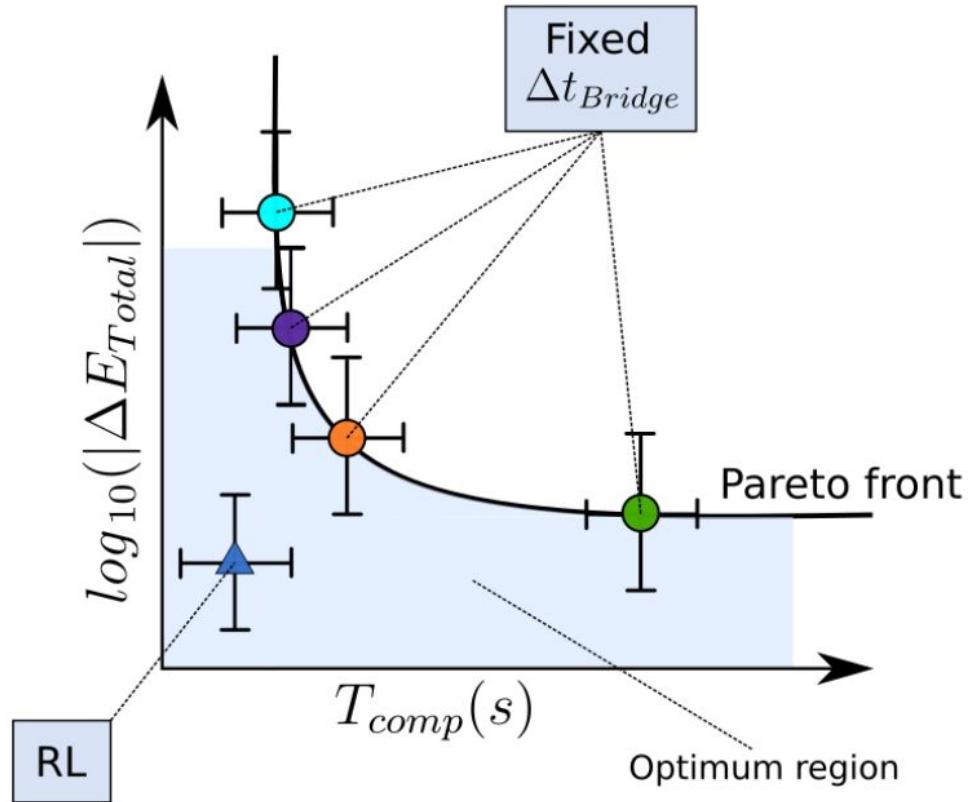
- Specific Integrator.
- Large integration times.



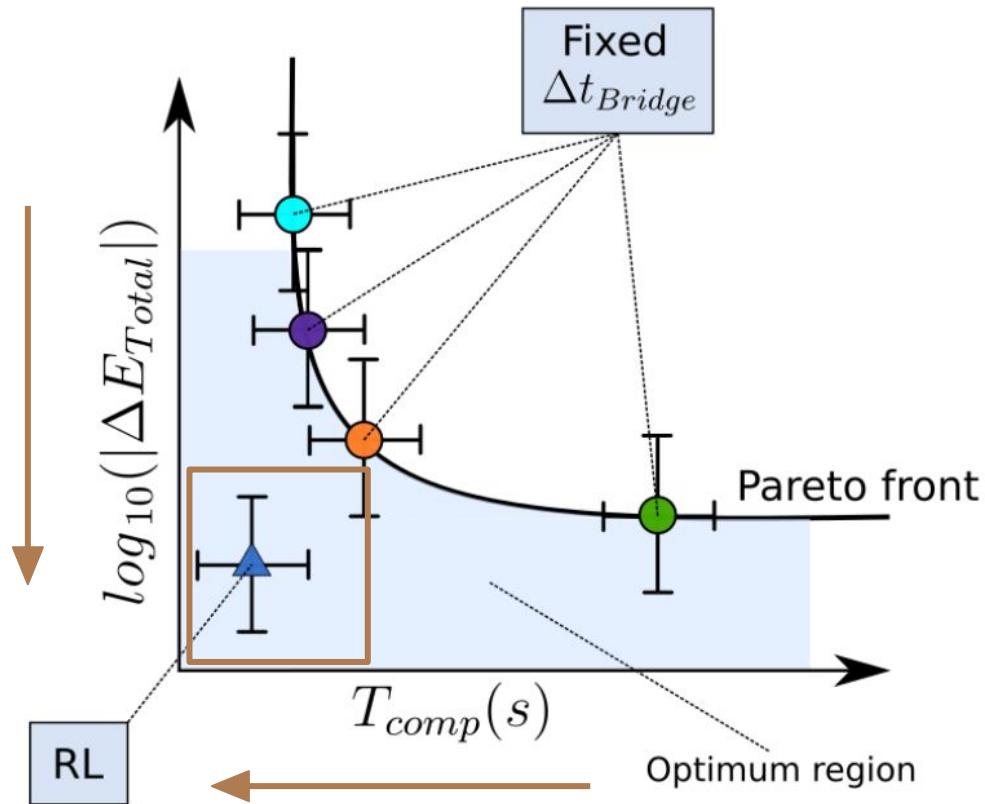
- Specific Integrator.
- Very small integration times.

Cluster Δt | **Bridge** Δt | Planetary System Δt

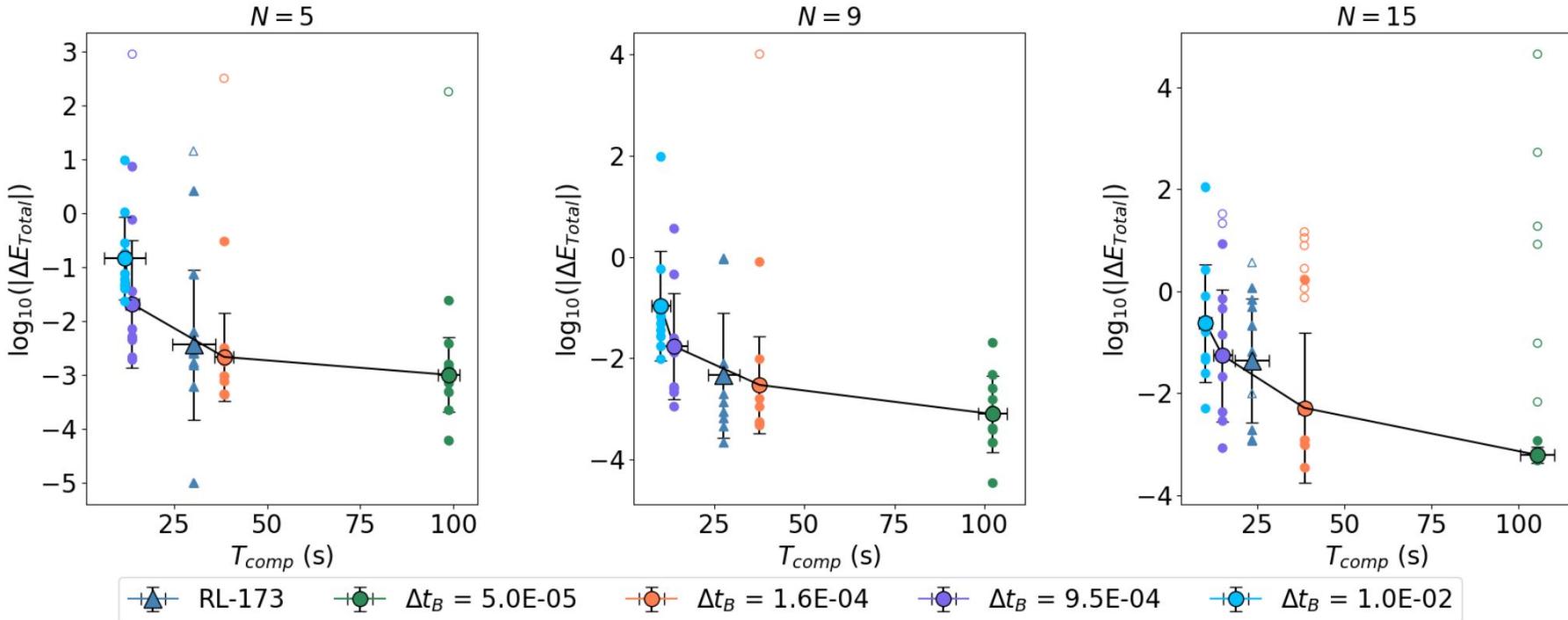
Finding an optimum solution



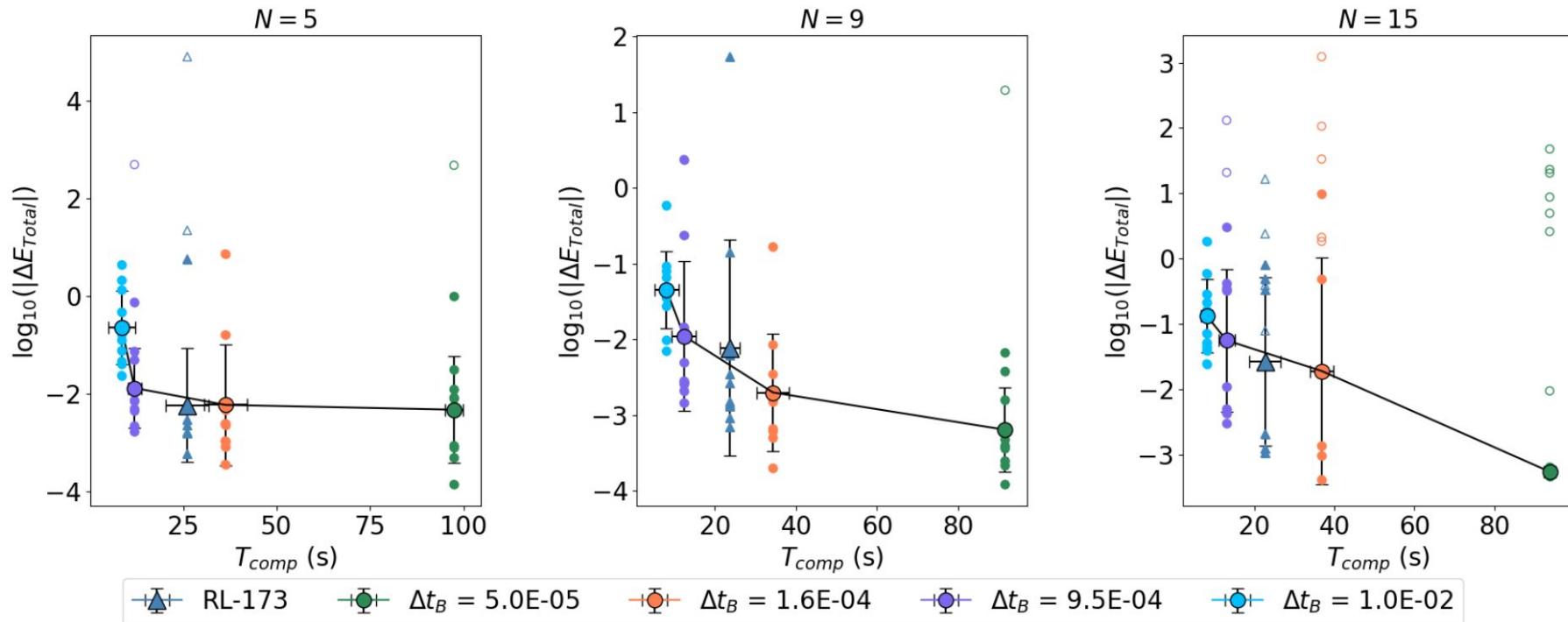
Finding an optimum solution



Finding an optimum solution

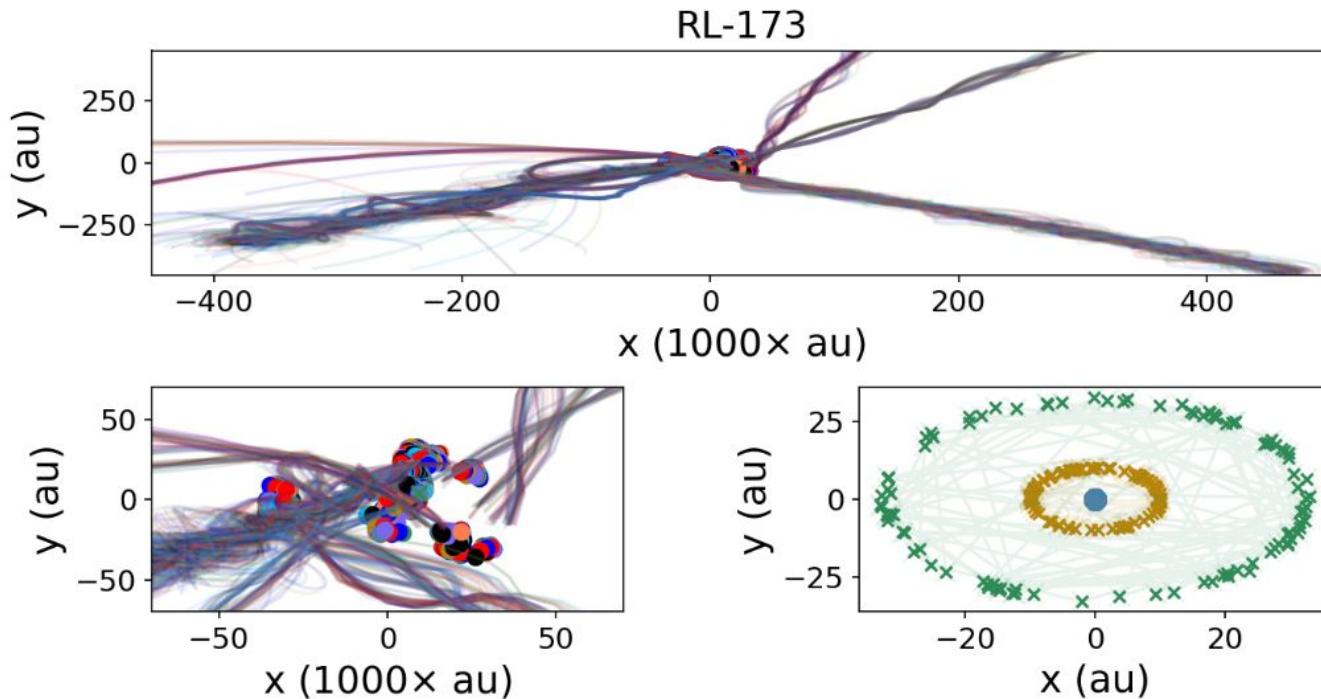


What if we use different integrators?



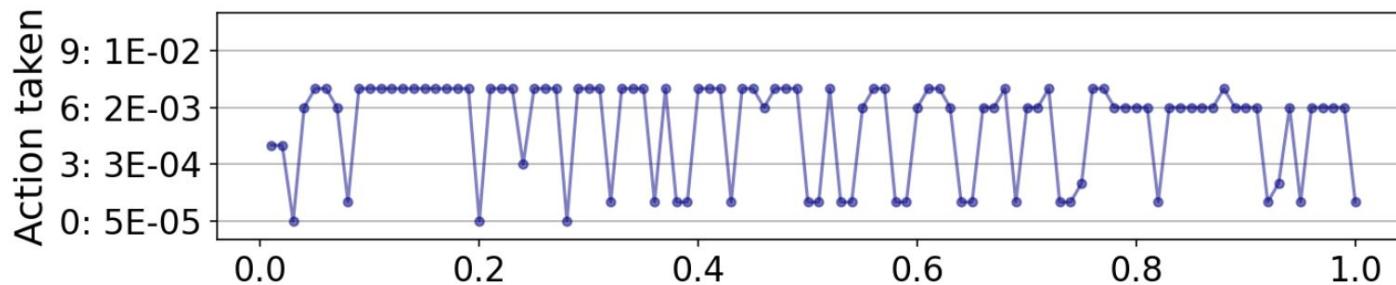
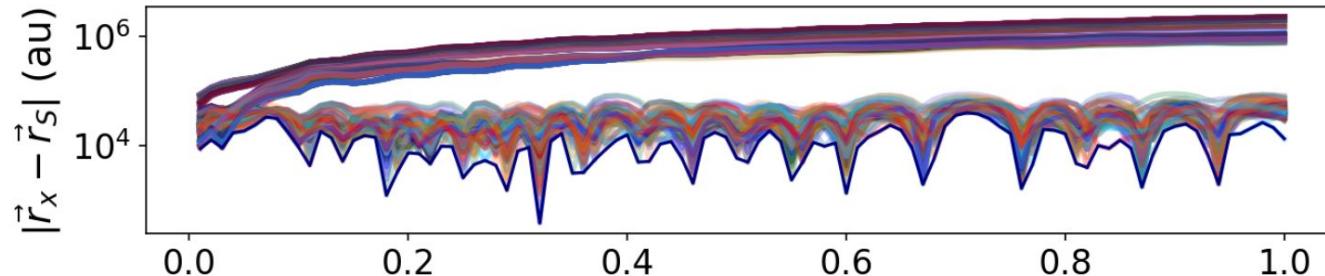
Application to a larger system

$N = 1,000$



Application to a larger system

$N = 1,000$



Conclusions and disclaimers

Input does not depend on N

Energy Error is unreliable for large N

Valid for many problems with small amount of re-training

Hybrid method improves robustness

Final thoughts

1. *In a simulation of the N-body problem **prediction errors accumulate**.*
2. *Complex network topologies help **energy conservation** - but can be hard to adapt to Astrophysics problems.*
3. *We need a better **state representation** for ML than Cartesian coordinates.*
4. *Many times, **integration settings** are left as default without studying the effects of this choice. It is better to **automatize** in a smart way.*

Thank you for your attention