Institute for Advanced Study

How to get a particle simulation running on your computer in 30 seconds. (+Science)

Hanno Rein @ Cornell, July 2012

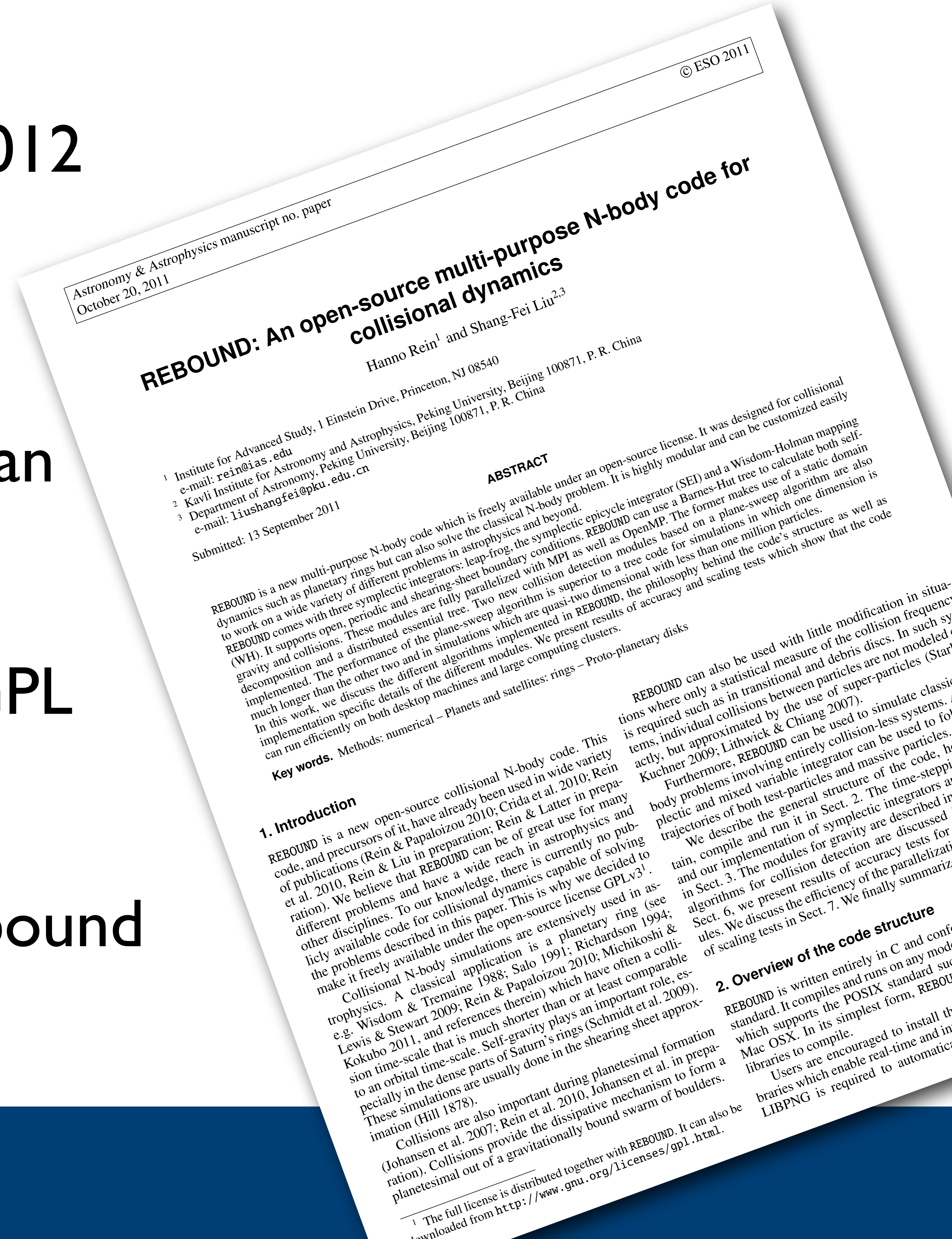
Part I: REBOUND
Part II: Science

Take home message I

Please make your codes public!

REBOUND

- Code description paper published by A&A, Rein & Liu 2012
- Multi-purpose N-body code
- First public N-body code that can be used for granular dynamics
- Written in C99, open source, GPL
- Freely available at http://github.com/hannorein/rebound



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October 20, 2011

REBOUND: An open-source multi-purpose N-body code for collisional dynamics

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ABSTRACT

REBOUND is a new multi-purpose N-body code which is freely available under an open-source license. It was designed for collisional dynamics such as planetary rings but can also solve the classical N-body problem. It is highly modular and can be customized easily to work on a wide variety of different problems in astrophysics and beyond.
REBOUND comes with three symplectic integrators: leap-frog, the symplectic epicycle integrator (SEI) and a Wisdom-Holman mapping (WH). It supports open, periodic and shearing-sheet boundary conditions. REBOUND can use a Barnes-Hut tree to calculate both self-gravity and collisions. These modules are fully parallelized with MPI as well as OpenMP. The former makes use of a static domain decomposition and a distributed essential tree. Two new collision detection modules based on a plane-sweep algorithm are also implemented. The performance of the plane-sweep algorithm is superior to a tree code for simulations in which one dimension is much longer than the other two and in simulations which are quasi-two dimensional with less than one million particles.
In this work, we discuss the different algorithms implemented in REBOUND, the philosophy behind the code's structure as well as implementation specific details of the different modules. We present results of accuracy and scaling tests which show that the code can run efficiently on both desktop machines and large computing clusters.

Key words. Methods: numerical – Planets and satellites: rings – Proto-planetary disks

1. Introduction

REBOUND is a new open-source collisional N-body code. This code, and precursors of it, have already been used in wide variety of publications (Rein & Papaloizou 2010; Crida et al. 2010; Rein et al. 2010, Rein & Liu in preparation; Rein & Latter in preparation). We believe that REBOUND can be of great use for many different problems and have a wide reach in astrophysics and other disciplines. To our knowledge, there is currently no publicly available code for collisional dynamics capable of solving the problems described in this paper. This is why we decided to make it freely available under the open-source license GPLv3[1].

Collisional N-body simulations are extensively used in astrophysics. A classical application is a planetary ring (see e.g. Wisdom & Tremaine 1988; Salo 1991; Richardson 1994; Lewis & Stewart 2009; Rein & Papaloizou 2010; Michikoshi & Kokubo 2011, and references therein) which have often a collision time-scale that is much shorter than or at least comparable to an orbital time-scale. Self-gravity plays an important role, especially in the dense parts of Saturn's rings (Schmidt et al. 2009). These simulations are usually done in the shearing sheet approximation (Hill 1878).

Collisions are also important during planetesimal formation (Johansen et al. 2007; Rein et al. 2010, Johansen et al. in preparation). Collisions provide the dissipative mechanism to form a planetesimal out of a gravitationally bound swarm of boulders.

[1] The full license is distributed together with REBOUND. It can also be downloaded from http://www.gnu.org/licenses/gpl.html.

REBOUND modules

Geometry

- Open boundary conditions
- Periodic boundary conditions
- Shearing sheet / Hill's approximation

Integrators

- Leap frog
- Symplectic Epicycle integrator (SEI)
- Wisdom-Holman mapping (WH)
- 15th order RADAU integrator

Gravity

- Direct summation, $O(N^2)$
- BH-Tree code, $O(N \log(N))$
- FFT method, $O(N \log(N))$
- GRAPE, hardware accelerated, $O(N^2)$

Collision detection

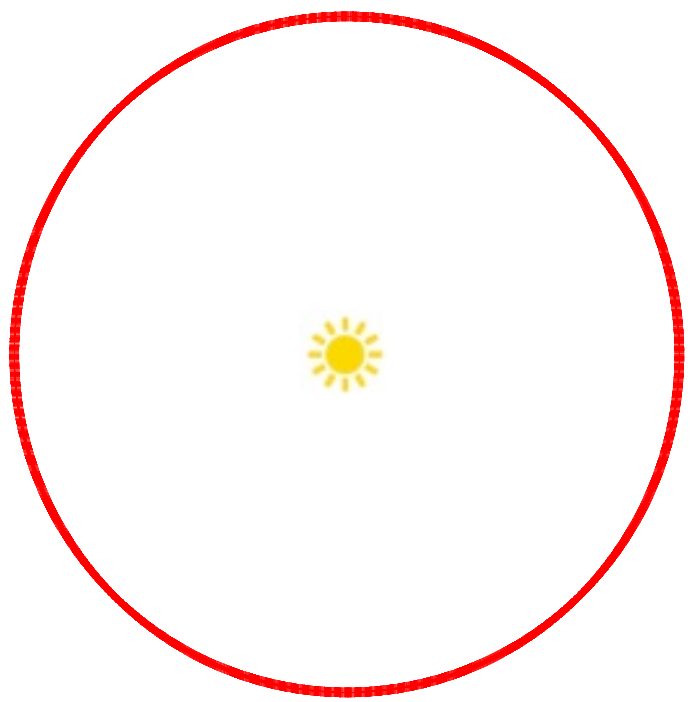
- Direct nearest neighbor search, $O(N^2)$
- BH-Tree code, $O(N \log(N))$
- Plane sweep algorithm, $O(N)$ or $O(N^2)$

Real-time visualization

- OpenGL

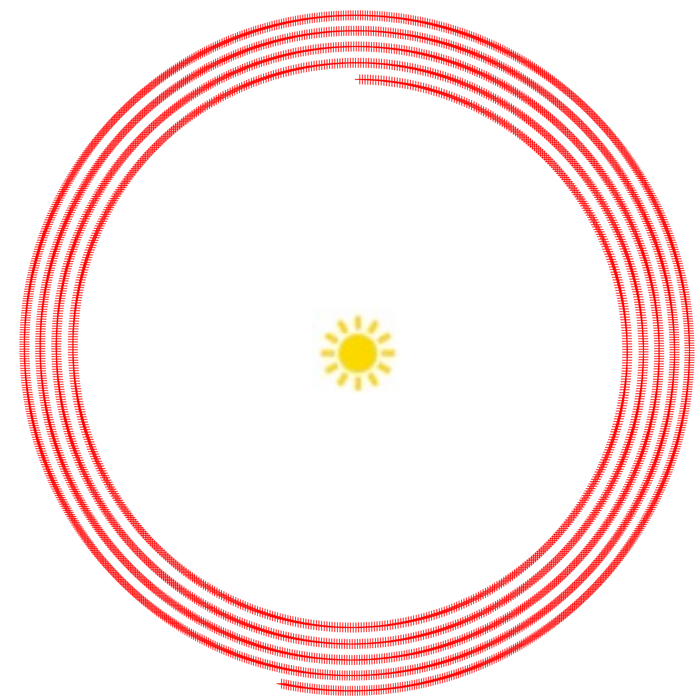
Integrators

Symplectic Integrators



Symplectic integrator

- REBOUND uses three symplectic integrators
- Mimic symmetries that are manifest in the Hamiltonian such as energy, momentum, angular momentum



Non-symplectic integrator

- REBOUND can also use a 15th order non-symplectic integrator
- Good for non-Hamiltonian systems

Symplectic integrator: Leap-frog

$$H = \frac{1}{2}p^2 + \Phi(x)$$

Drift Kick

$$x \longrightarrow x + v\,\frac{\Delta t}{2}$$

$$v \longrightarrow v + \nabla\Phi\,\Delta t$$

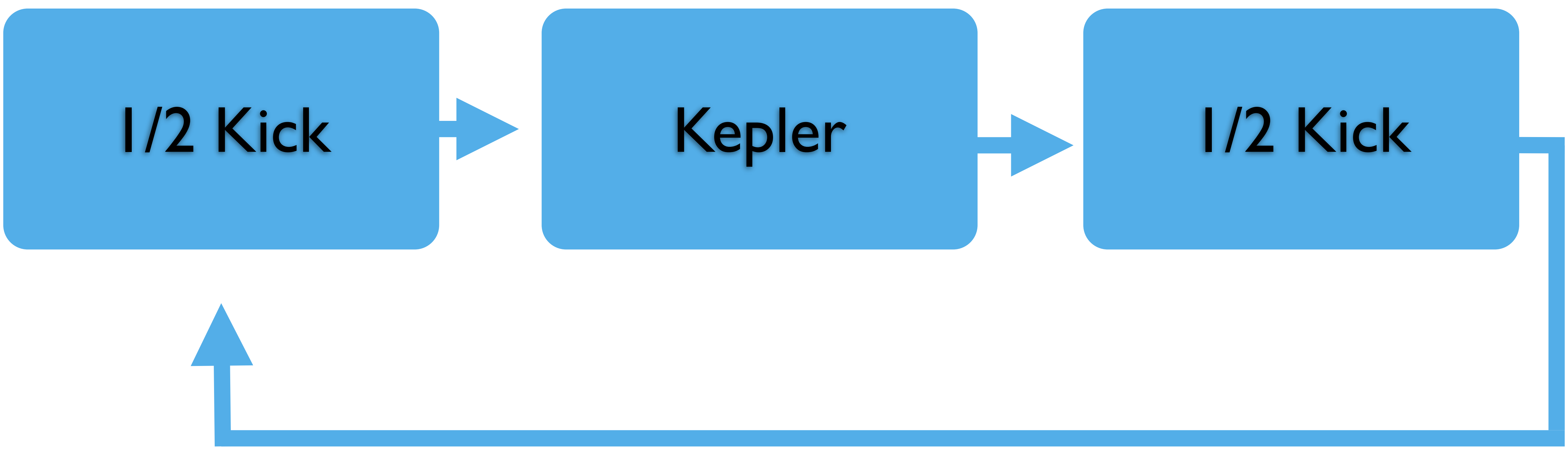
$$x \longrightarrow x + v\,\frac{\Delta t}{2}$$

Mixed variable symplectic integrator

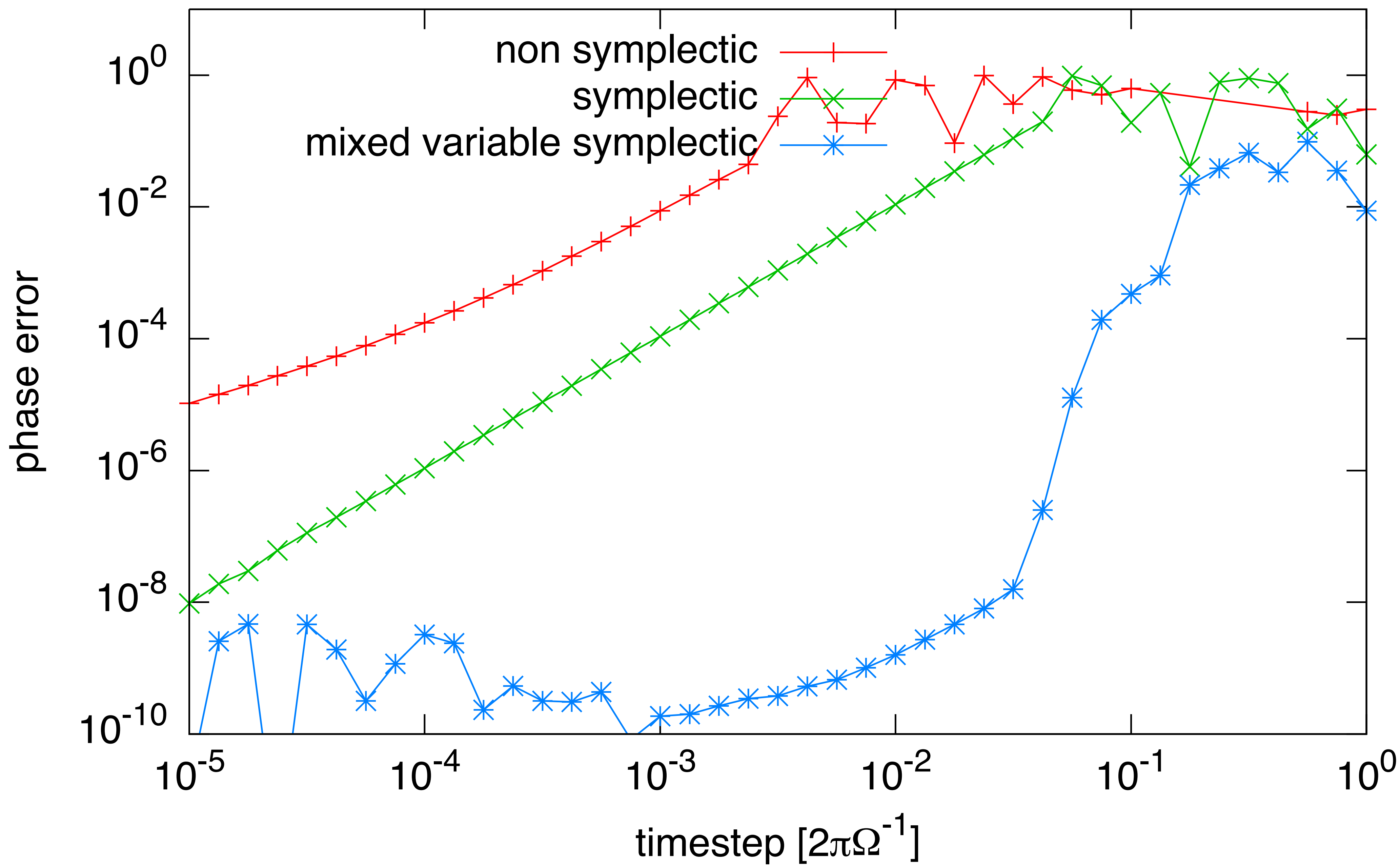
$$H = \frac{1}{2}p^2 + \Phi_{\rm Kepler}(x) + \Phi_{\rm Other}(x)$$

Kepler

Kick

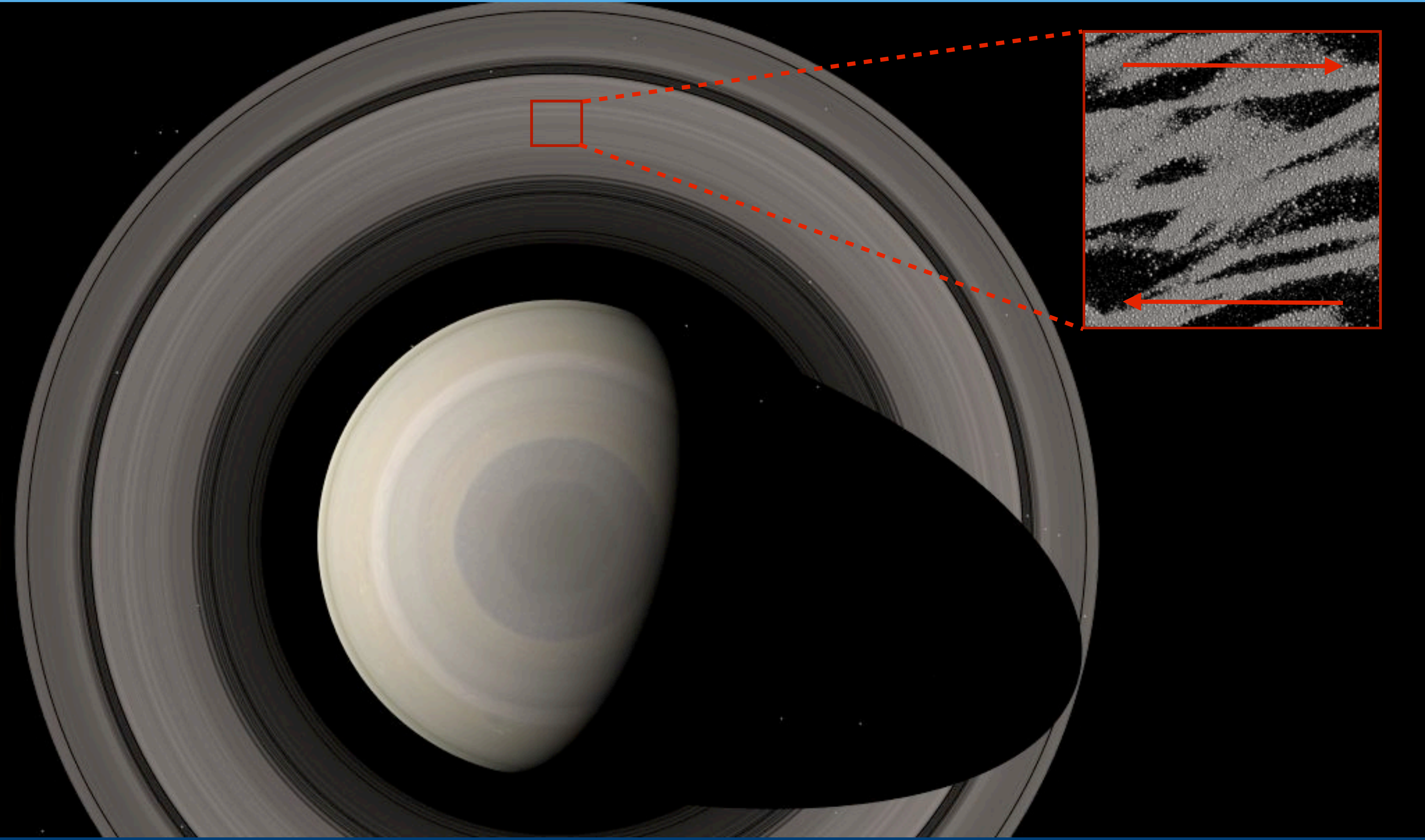


Mixed variable symplectic (MVS) integrator



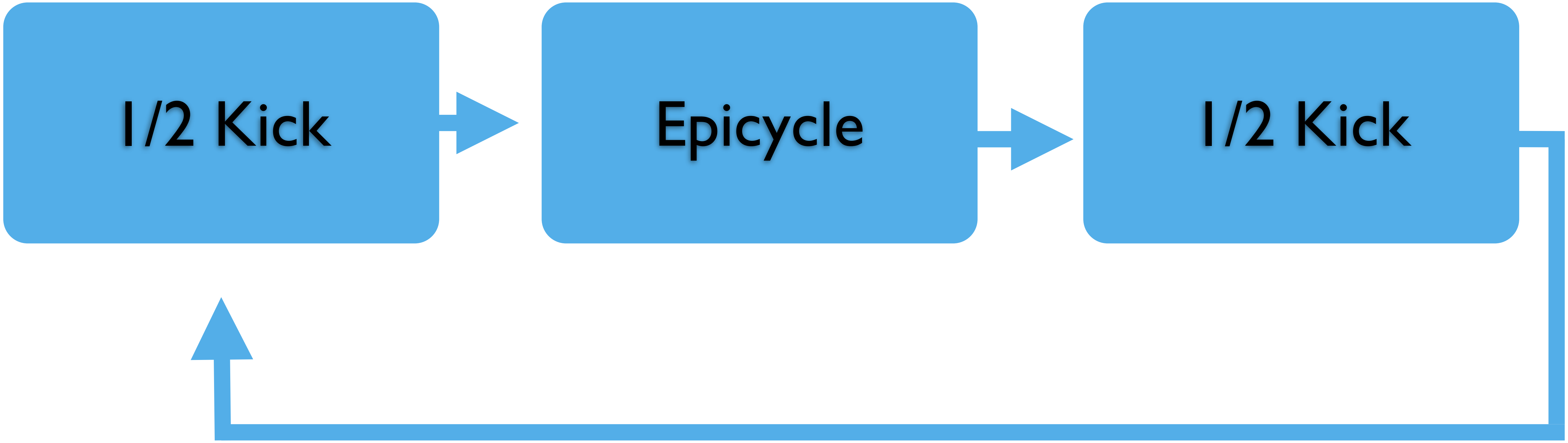
Rein & Tremaine 2011

A new integrator for the shearing sheet



Symplectic Epicycle Integrator

$$H = \underbrace{\frac{1}{2}p^2 + \Omega(p \times r)e_z + \frac{1}{2}\Omega^2\left[r^2 - 3(r \cdot e_x)^2\right]}_{\text{Epicycle}} + \underbrace{\Phi(r)}_{\text{Kick}}$$

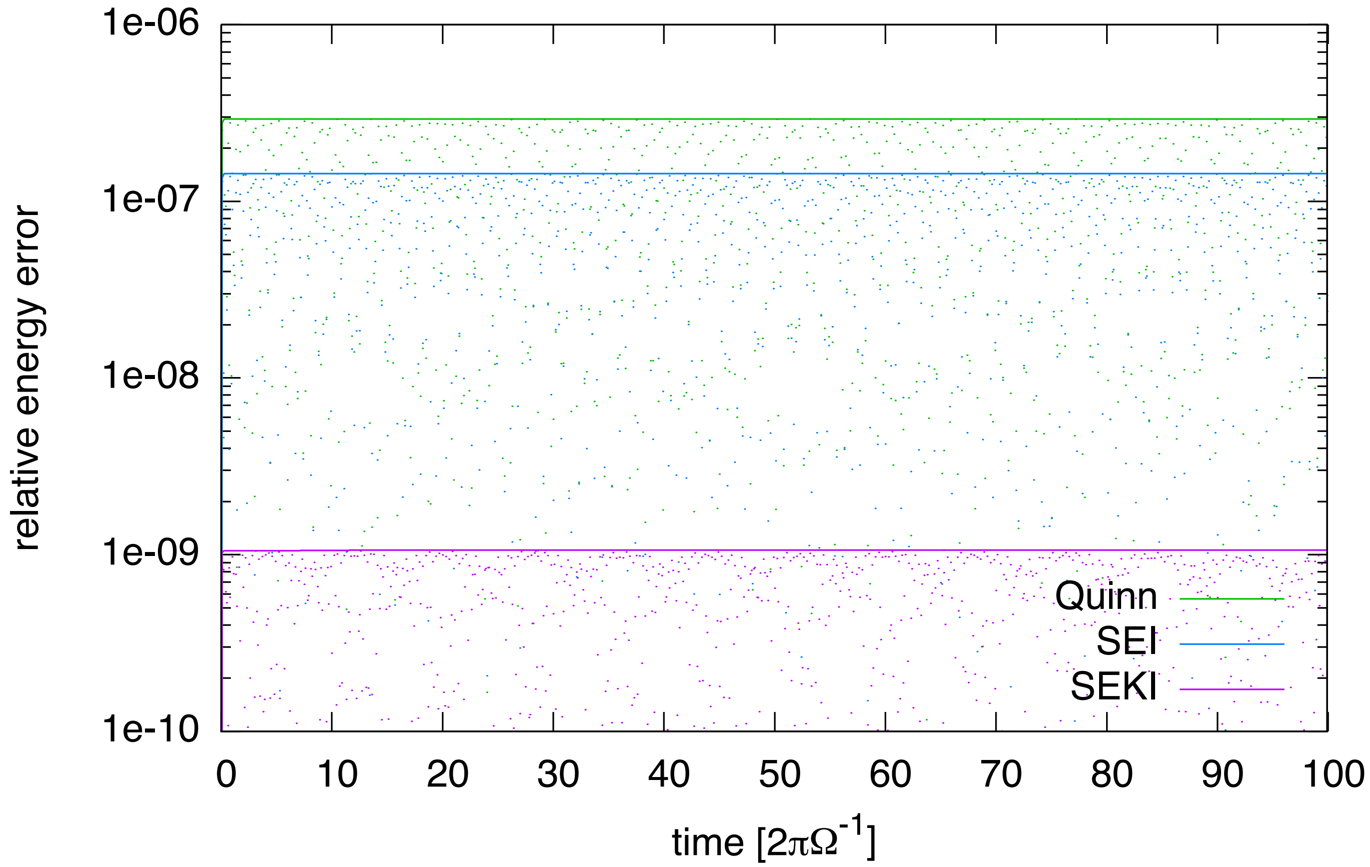


Symplectic Epicycle Integrator: Rotation

- Solving for the orbital motion involves a rotation.
- Formally $\det(D) = 1$, but due to floating point precision $\det(D) \sim 1$ only.
- Trick: Use three shear operators instead of one rotation.

$$\begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -\tan\frac{1}{2}\phi & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & \sin\phi \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ -\tan\frac{1}{2}\phi & 1 \end{pmatrix}$$

- $\det(D) = 1$ exactly for each shear operator, even in floating point precision.
- No long term trend linear trend anymore!

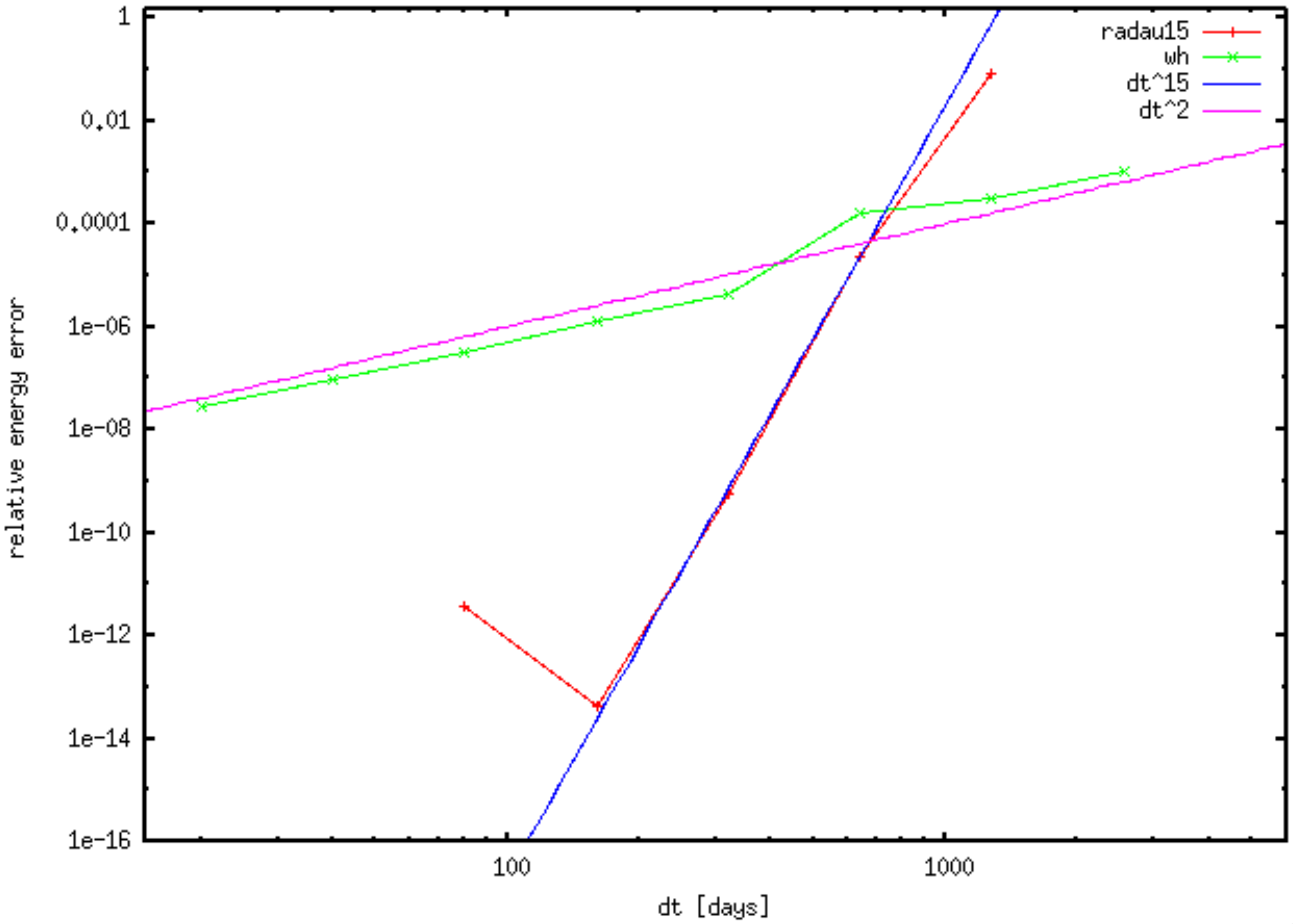


Take home message II

Symplectic integrators are awesome.

Non-Hamiltonian systems

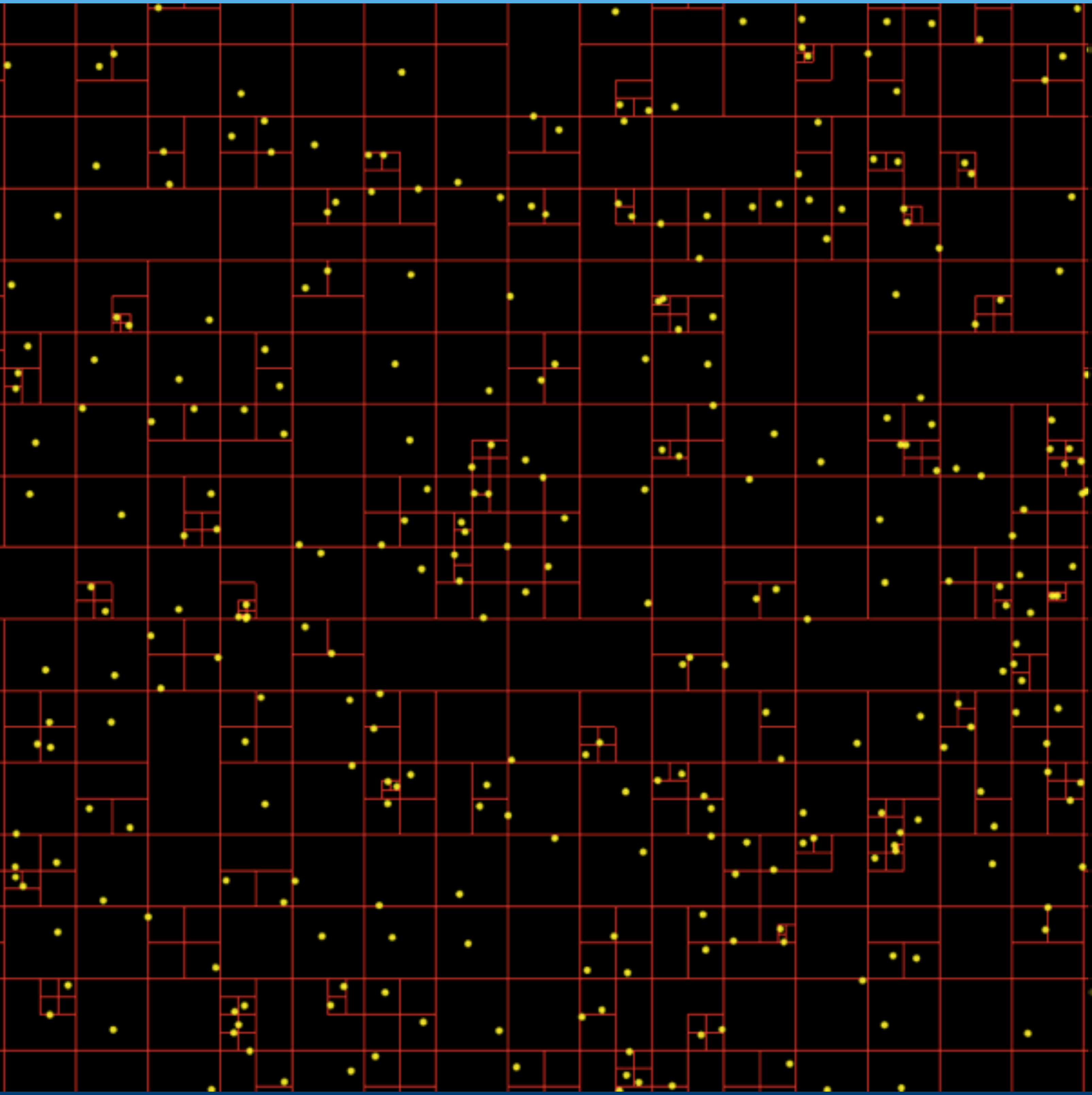
- If the system is not Hamiltonian, the advantages of a symplectic integrator mostly disappear
- Examples: drag-forces, radiation-forces, migration
- Simply use a high accuracy integrator such as RADAU15.



Everhart 1985

Collisions

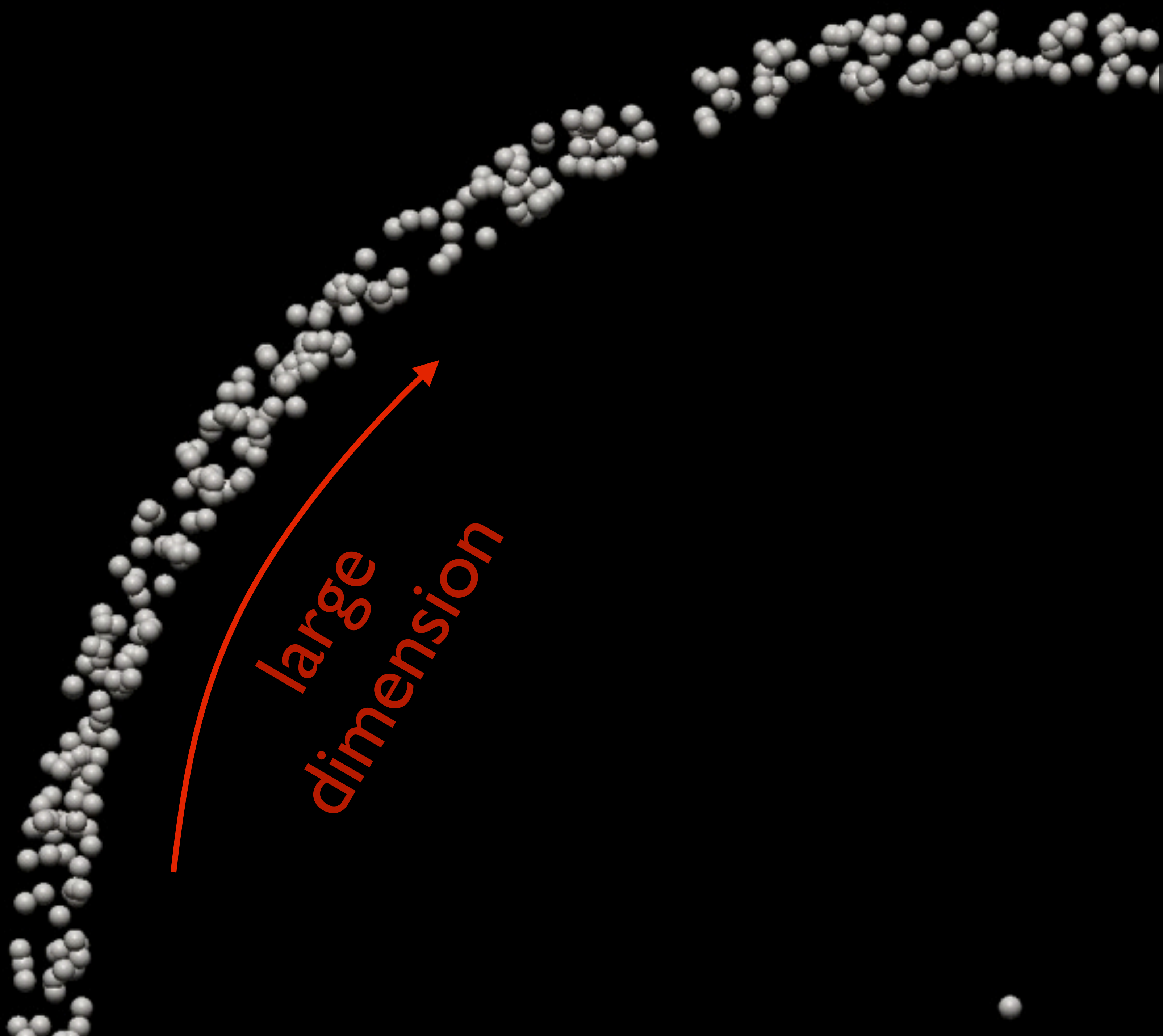
Collision Detection: Tree



- Using the same tree as for the gravity calculation, one can search for neighboring particles
- Tree is local to every node and only the essential parts are shared with other nodes
- Scales as O(N log(N))

Barnes & Hut 1986

Collision Detection: Plane-Sweep algorithm



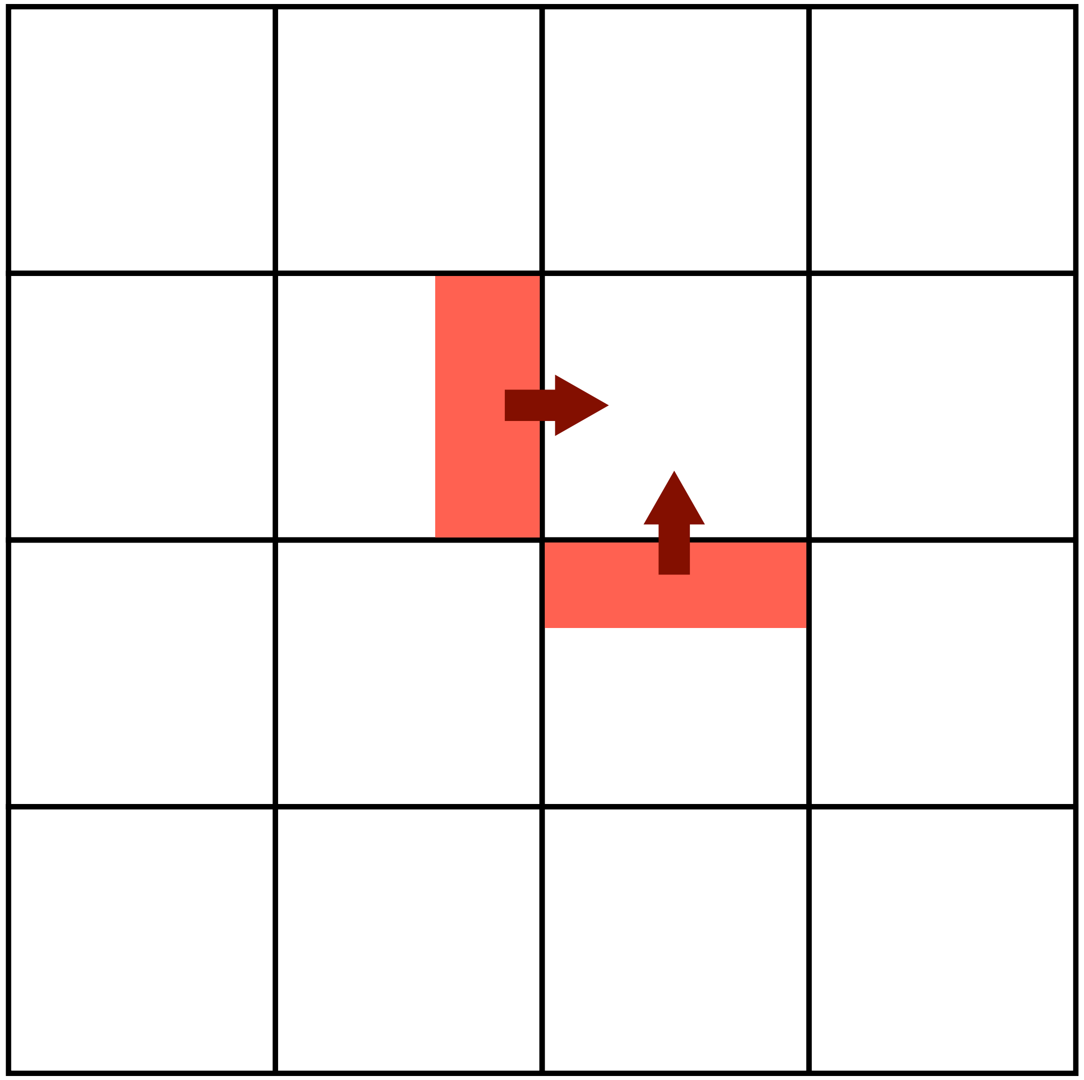
- Very efficient if one dimension is much larger than all the others
- No complicated data-structure needs to be maintained
- Scales as O(N) in the ideal case

Take home message III

Efficient collision detection is hard.

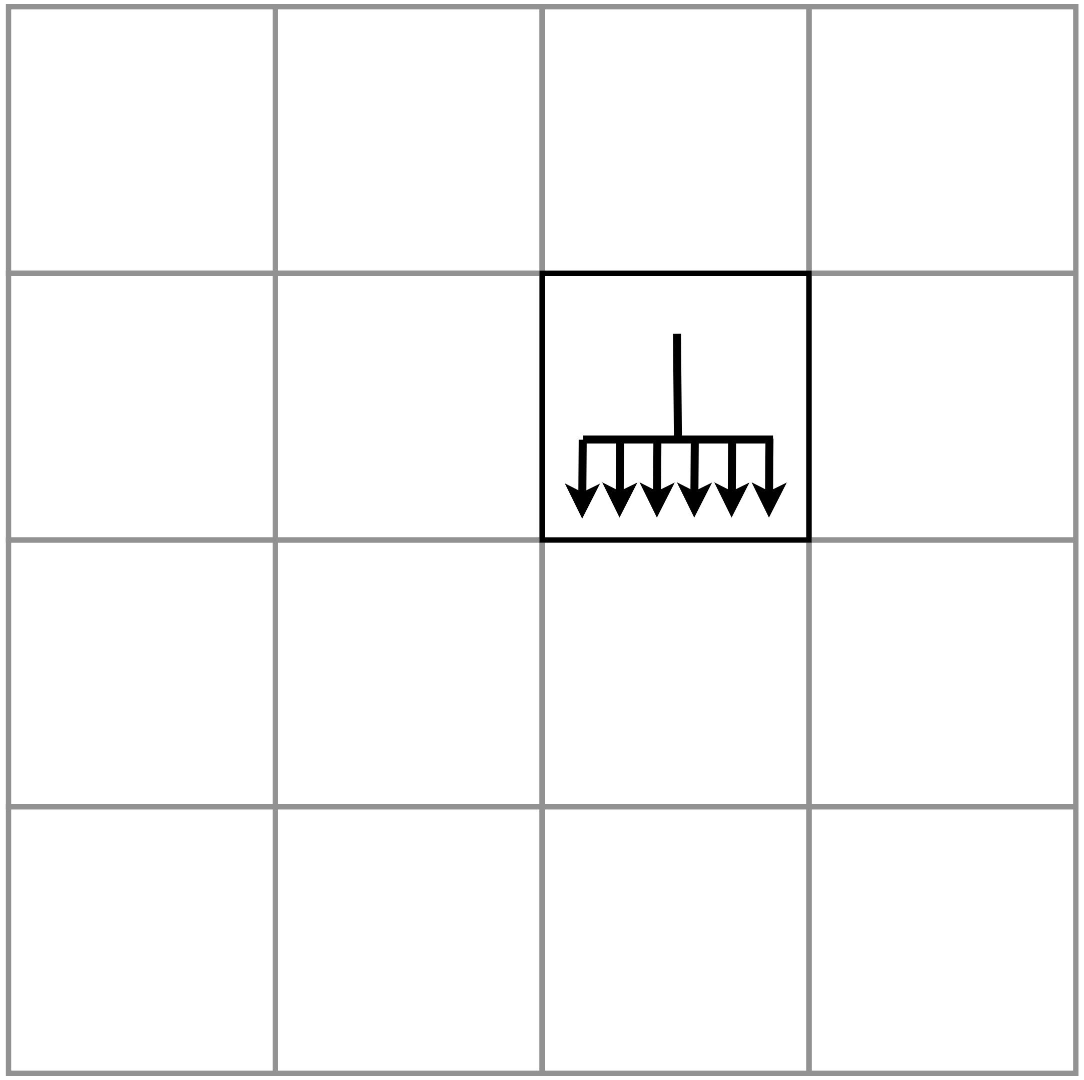
Parallelization

Parallelization Strategies



- Static domain decomposition on distributed memory systems
- Nodes communicate via MPI and share the essential tree with each other prior to gravity and collision calculations.
- MPI is a really bad framework for this sort of algorithm. But there's not much that can be done about it.

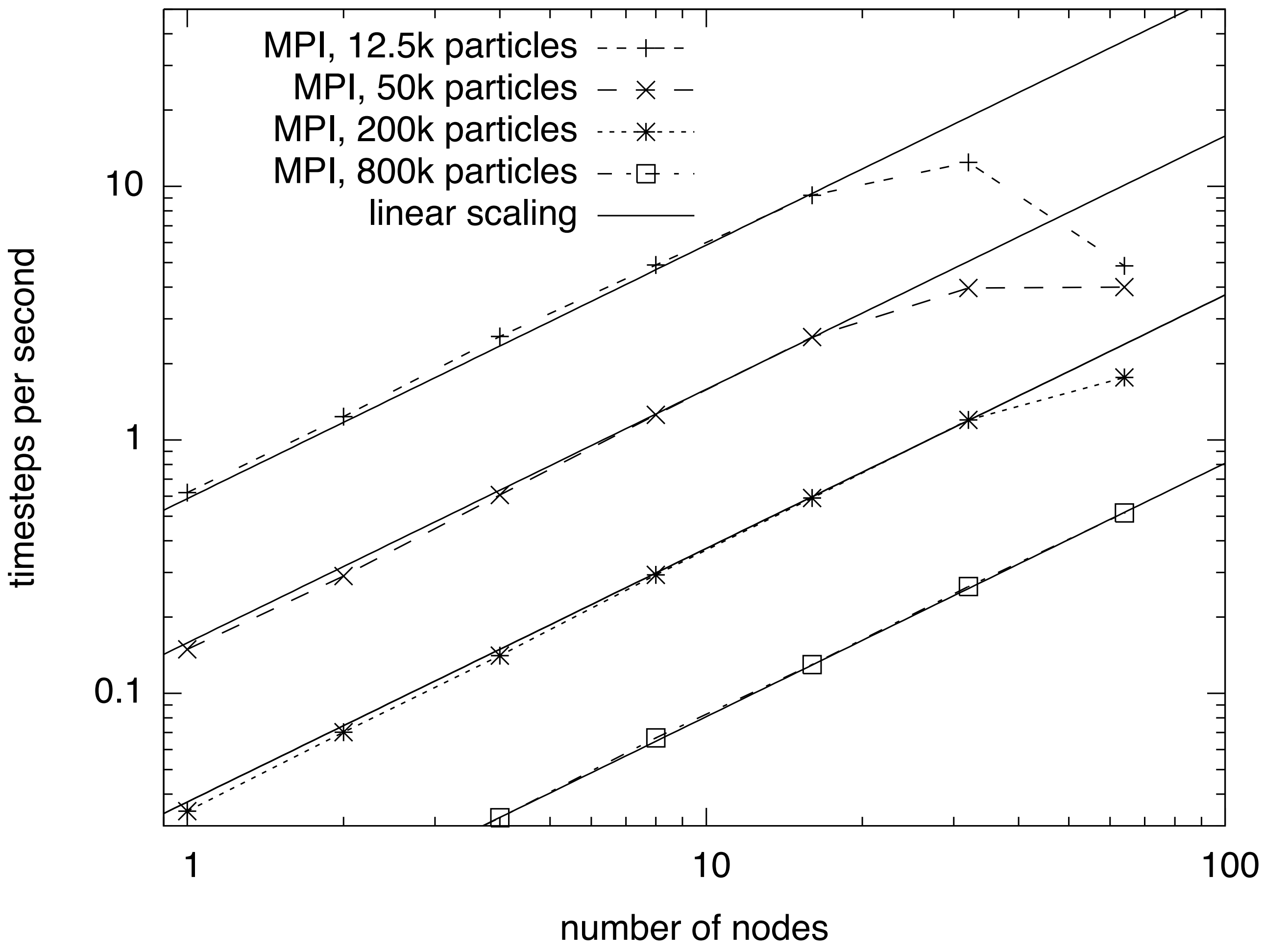
Parallelization Strategies II



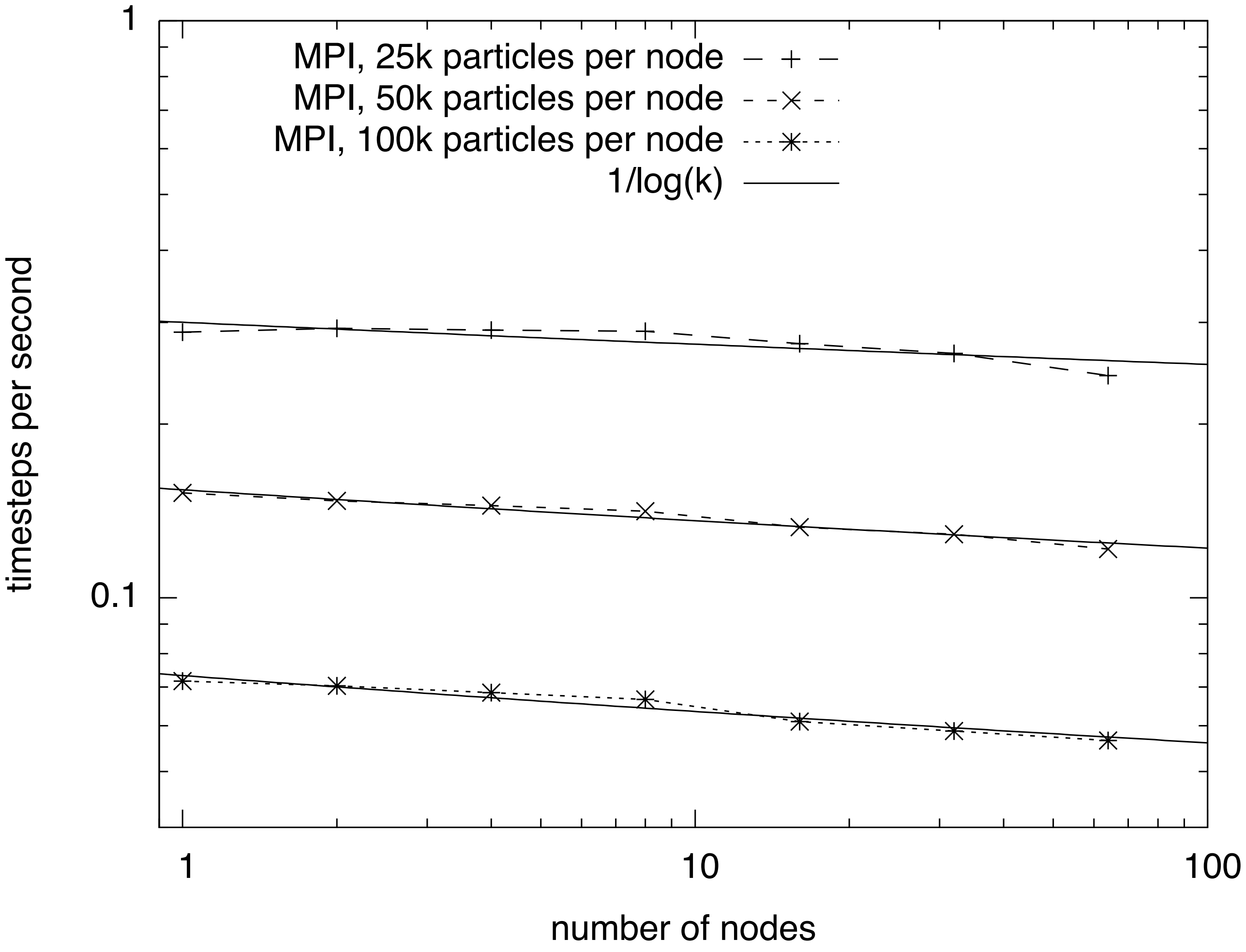
Locally (on each node or on your laptop), OpenMP is used for parallelization.

Scalings using a tree

strong



weak



REBOUND Demo

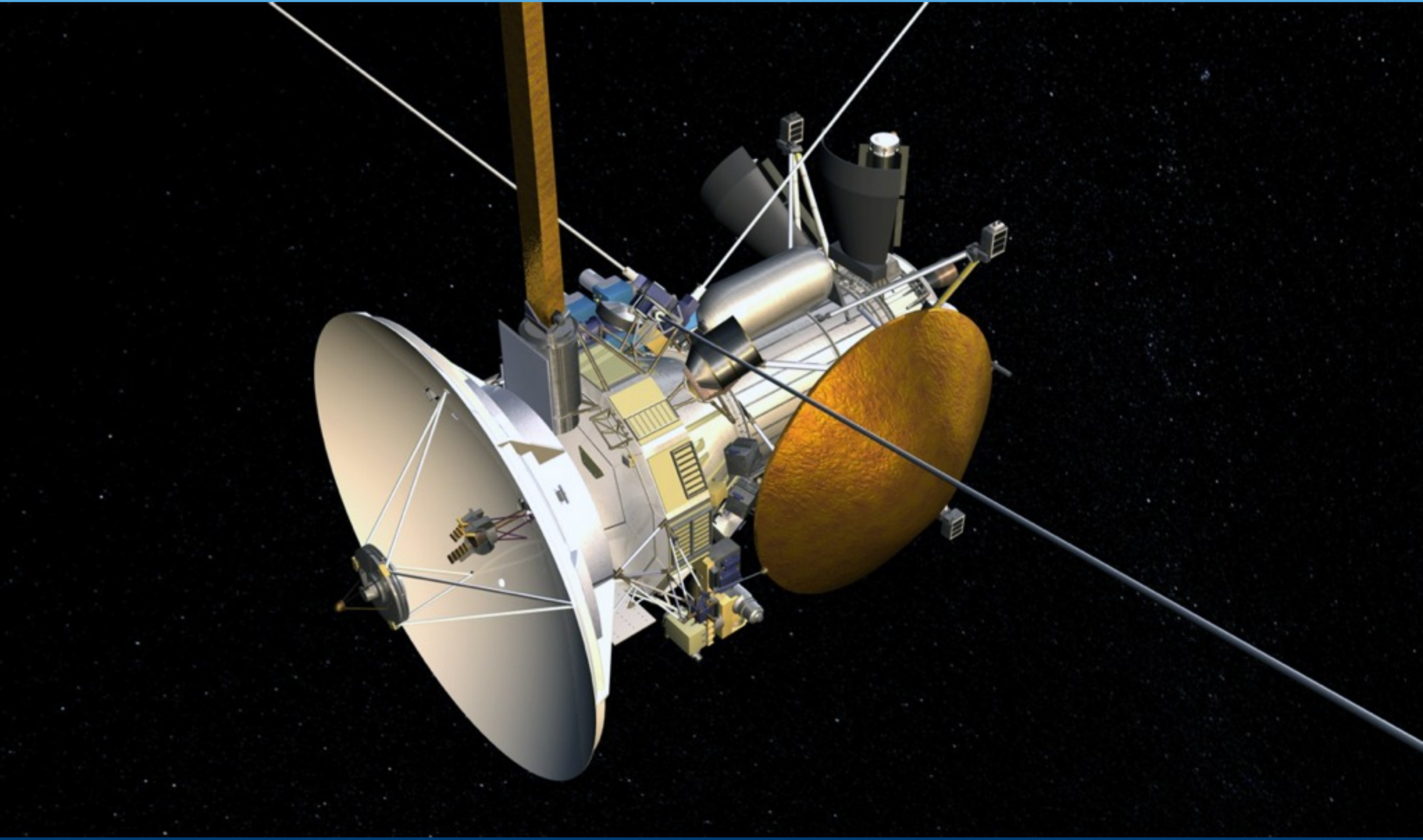
Take home message IV

Download and play with REBOUND.*

*Let me know if you run into a problem!

Science!

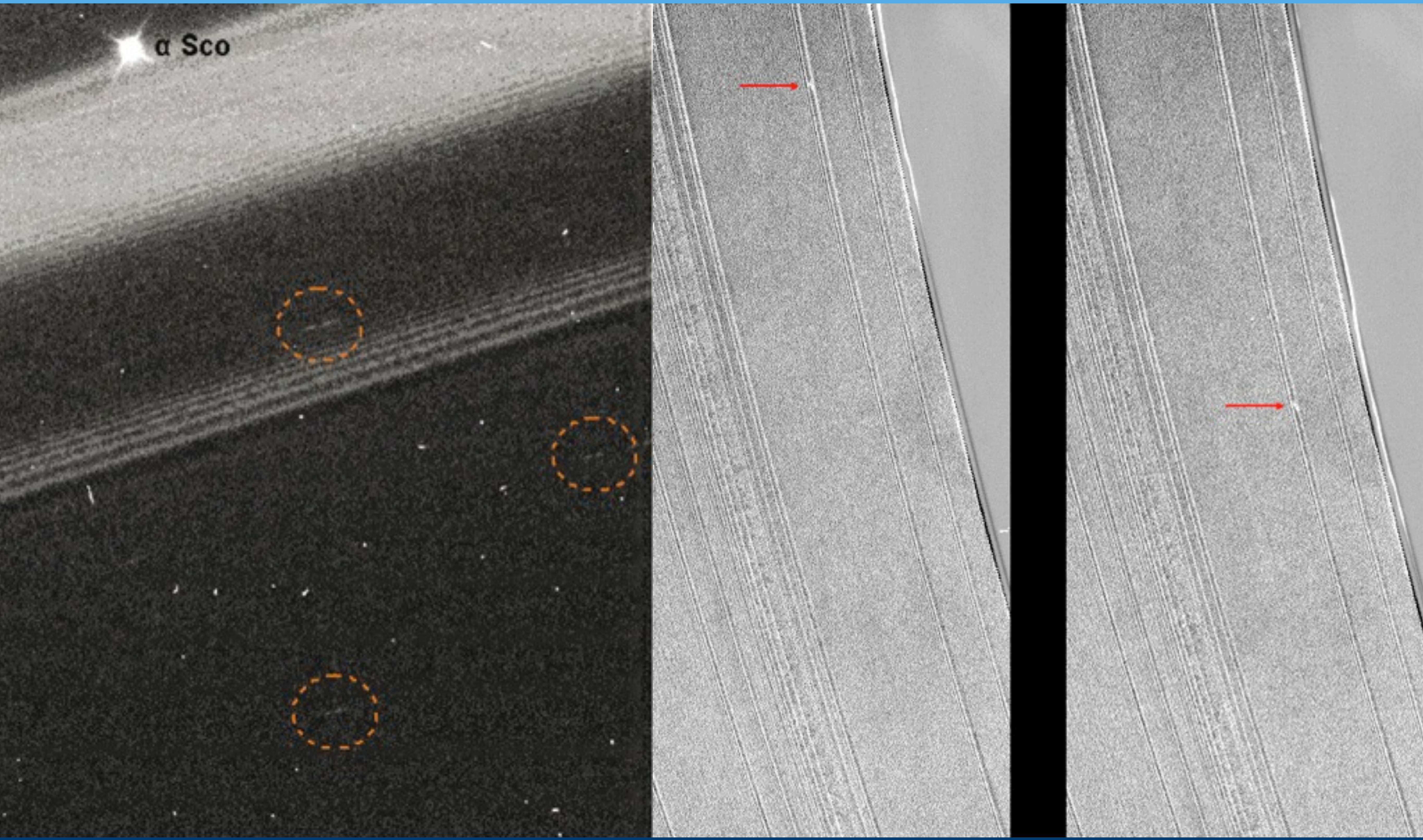
Cassini spacecraft



Credit: JPL/Gordon Morrison

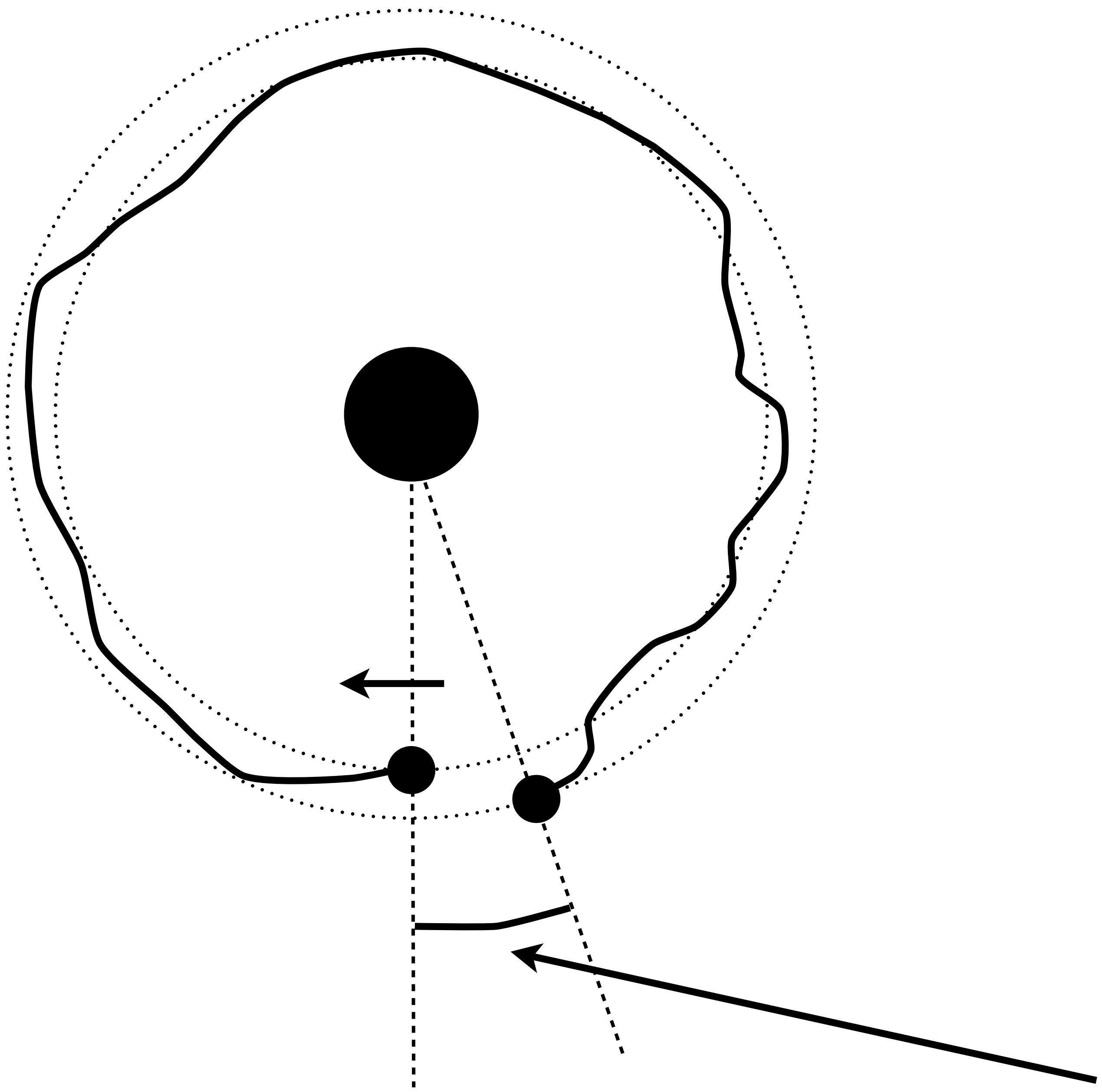
Moonlets in Saturn's Rings

Propeller structures in A-ring



Porco et al. 2007, Sremcevic et al. 2007, Tiscareno et al. 2006, NASA/JPL-Caltech/Space Science Institute

Longitude residual



Mean motion [rad/s]

$$n = \sqrt{\frac{GM}{a^3}}$$

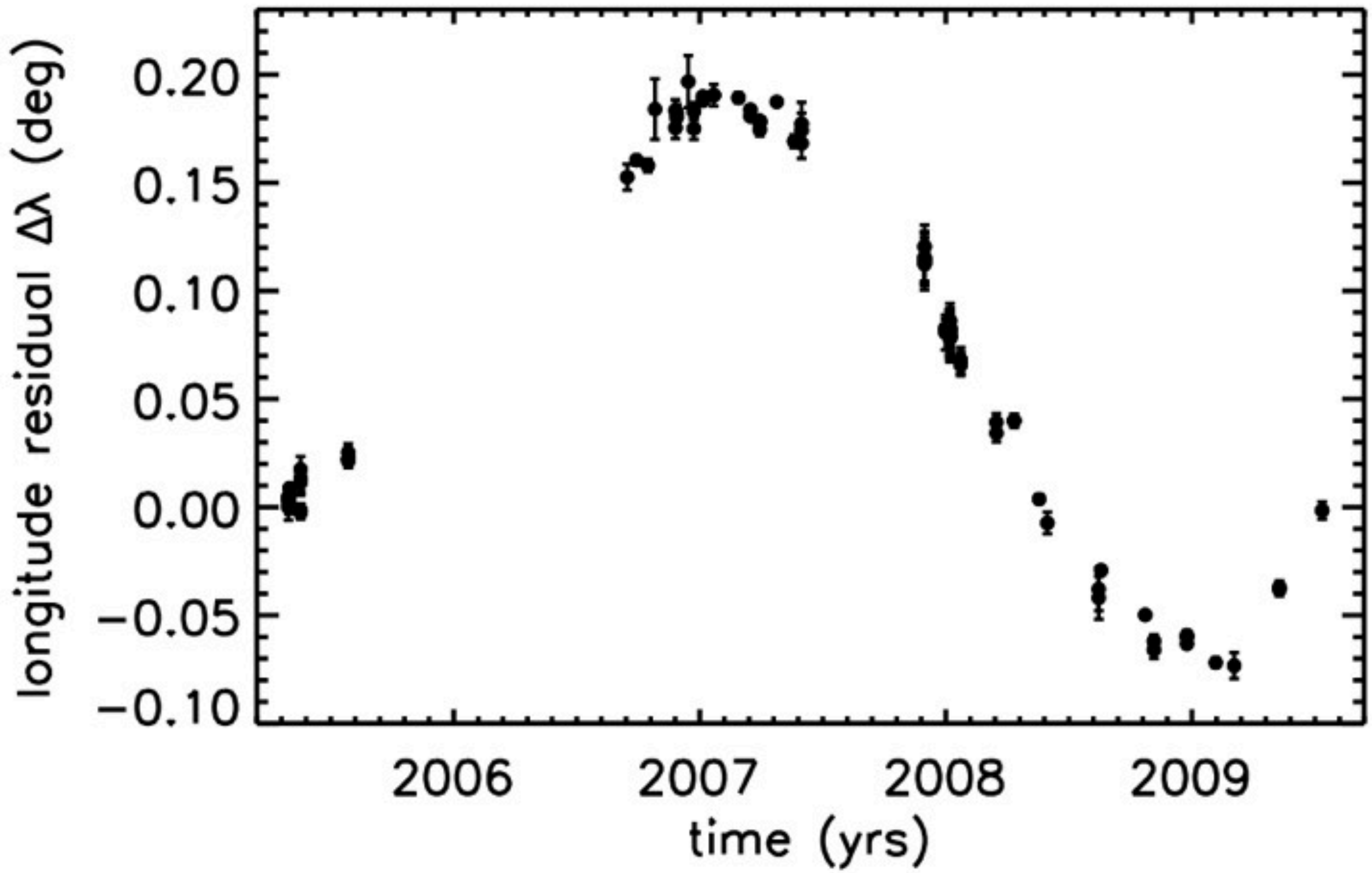
Mean longitude [rad]

$$\lambda = n\, t$$

Longitude residual [rad]

$$\Delta\lambda$$

Observational evidence of non-Keplerian motion



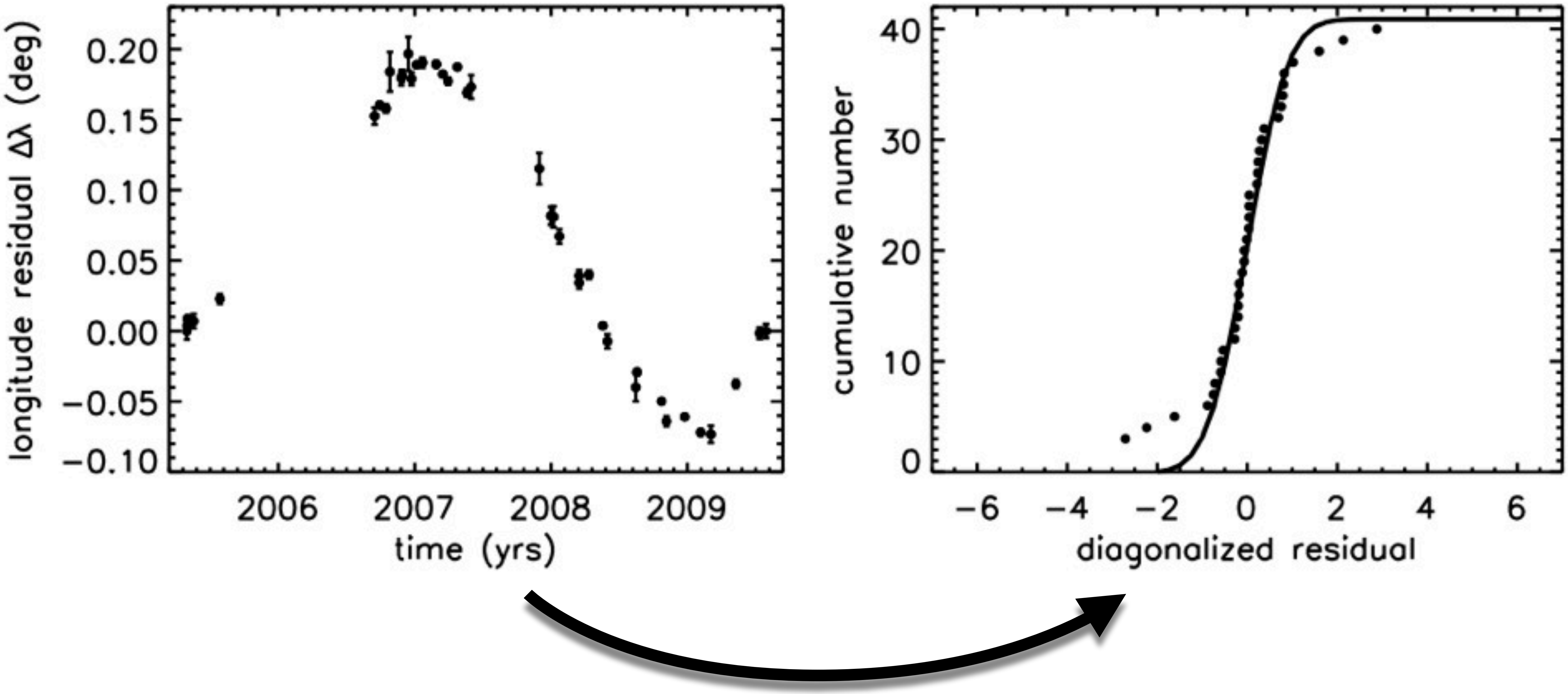
Tiscareno et al. 2010, Pan et al. 2012

Random walk?

$$\Delta\lambda(n\delta t) = -\sum_{i=1}^{n} \frac{3\Omega}{2a} \Delta a(i\delta t)\delta t$$
$$= -\frac{3\Omega\delta t}{2a} \sum_{i=1}^{n} \sum_{j=0}^{i-1} \xi_j$$
$$= -\frac{3\Omega\delta t}{2a} \sum_{j=0}^{n-1} (n-j)\xi_j$$

- The observed longitude residual is a double integral
- Linear combination of individual kicks

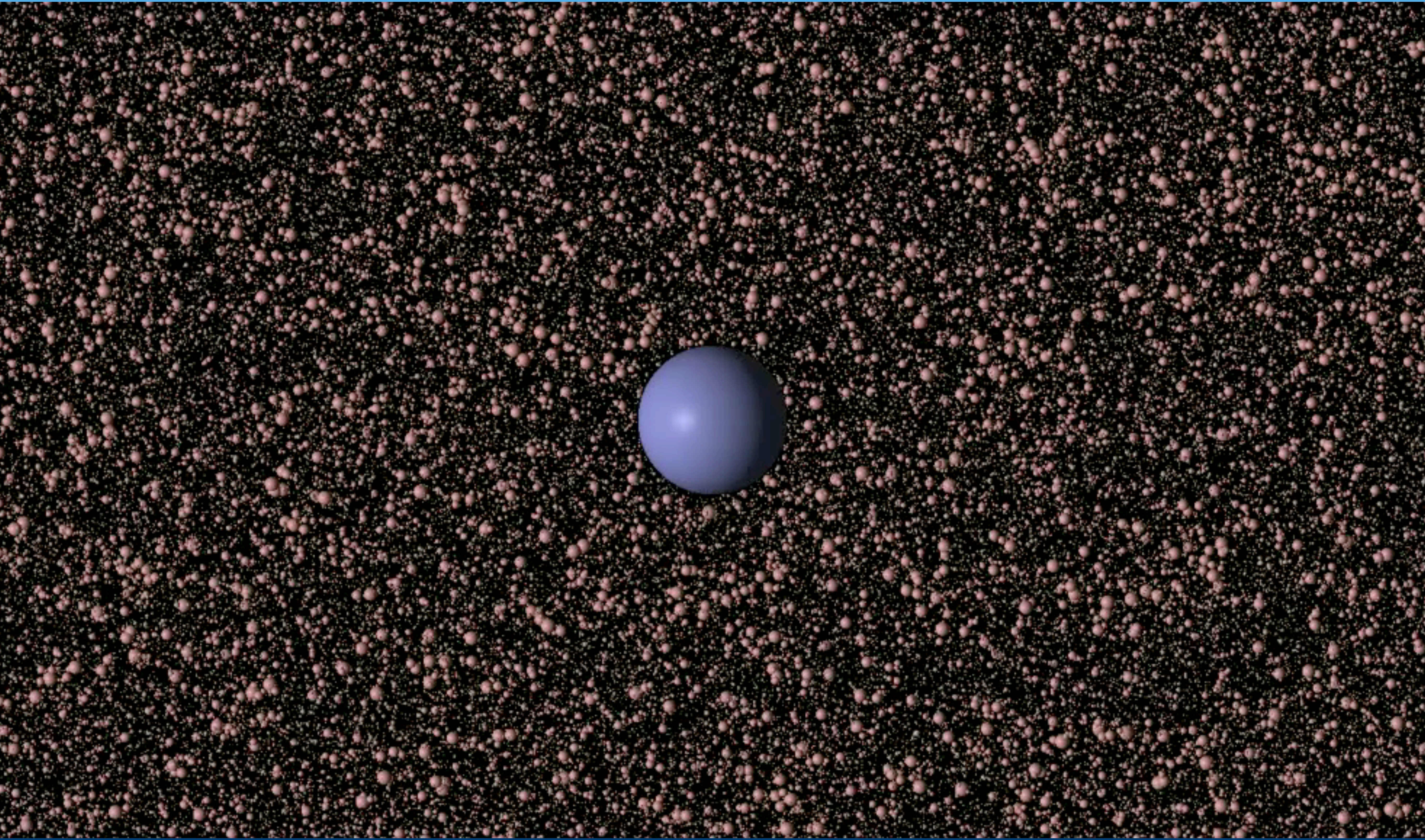
Random walk?



Diagonalization

Pan et al. 2012

Random walk



REBOUND code, Rein & Papaloizou 2010, Crida et al 2010

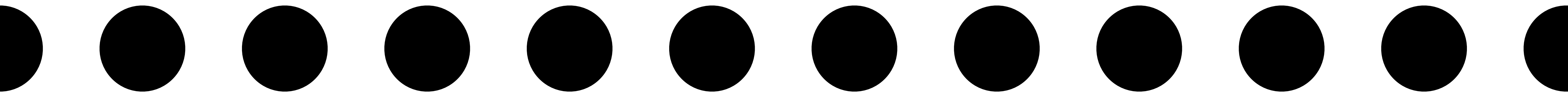
Take home message V

Moonlets in Saturn's Rings show direct evidence of disk satellite interaction.

Gravitational instability in a narrow ring

Gravitational instability in a narrow ring

- First studied by Maxwell 1859
- Idealized setup
- Equal mass, equally spaced particles
- Initially on circular orbits around central object



- Seed perturbations grow if the mass is above a critical value
- Two different modes, depending on particle mass and spacing

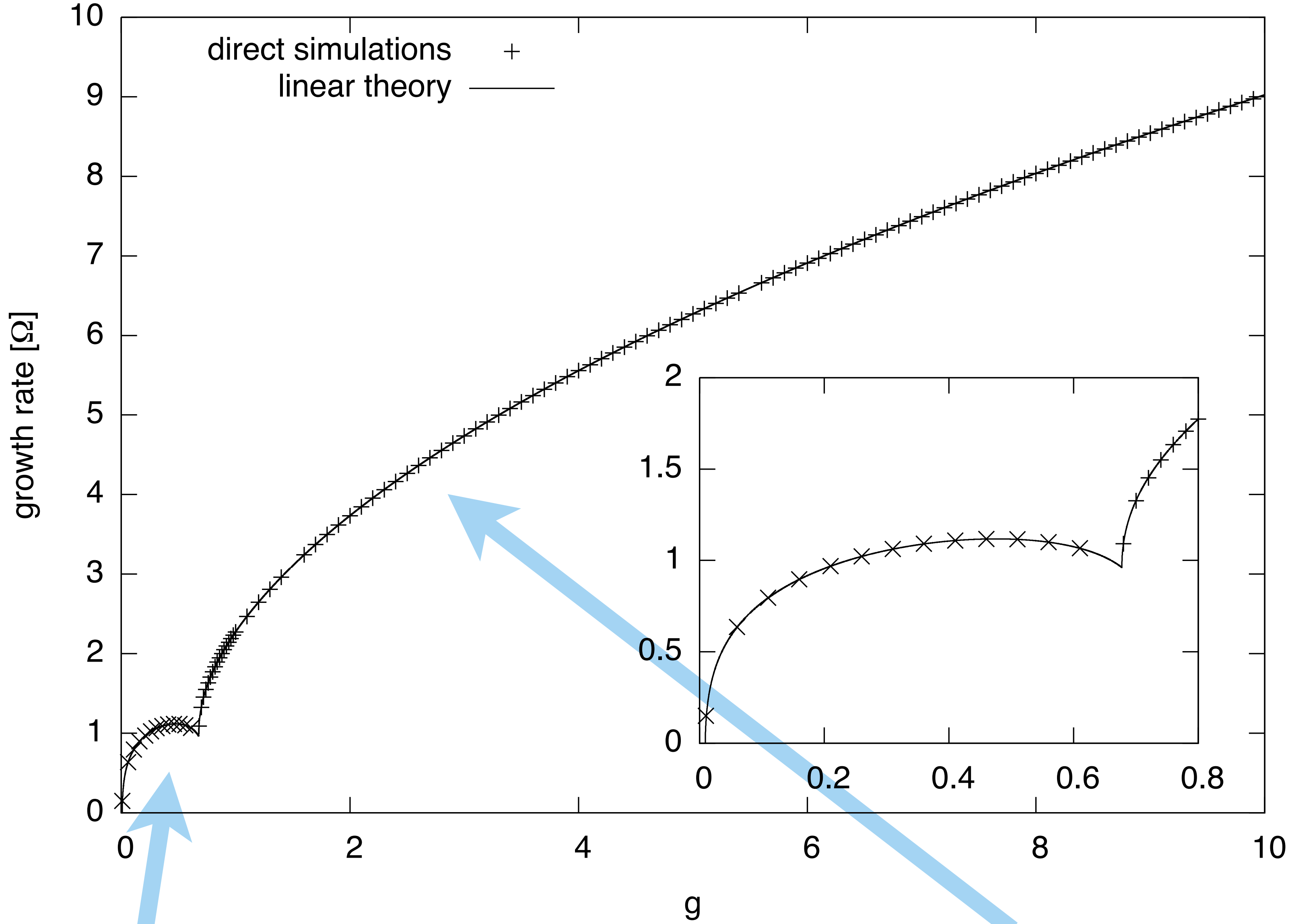
Growing epicycles

Longitudinal clumping

Latter, Rein & Ogilvie (2012)

Latter, Rein & Ogilvie (2012)

Analytic and numerical growth rates of the GI



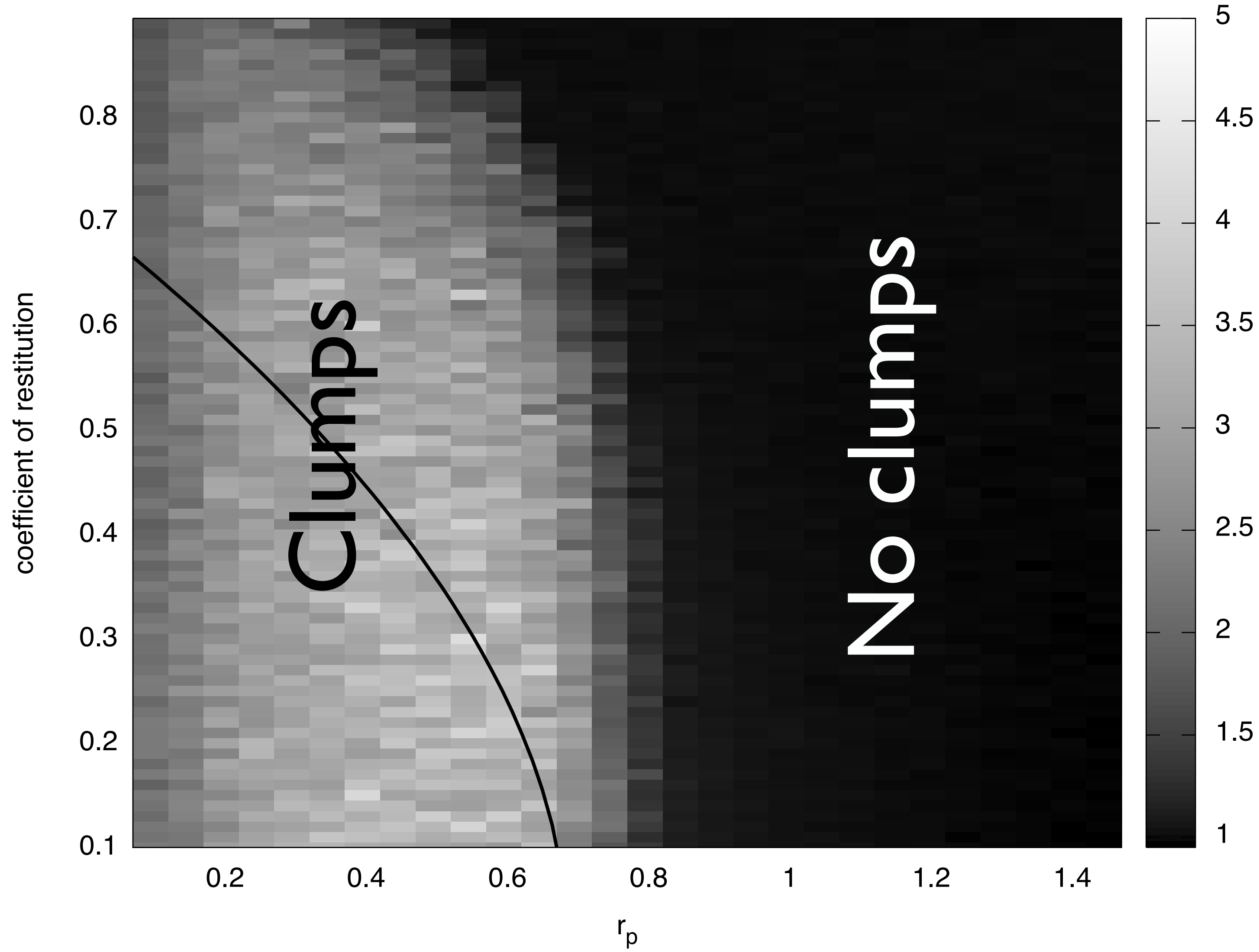
Growing epicycles

Longitudinal clumping

Latter, Rein & Ogilvie (2012)

Long term evolution

- Hot ring or clumps
- Independent of initial mode of the instability
- Determined by coefficient of restitution and particle density



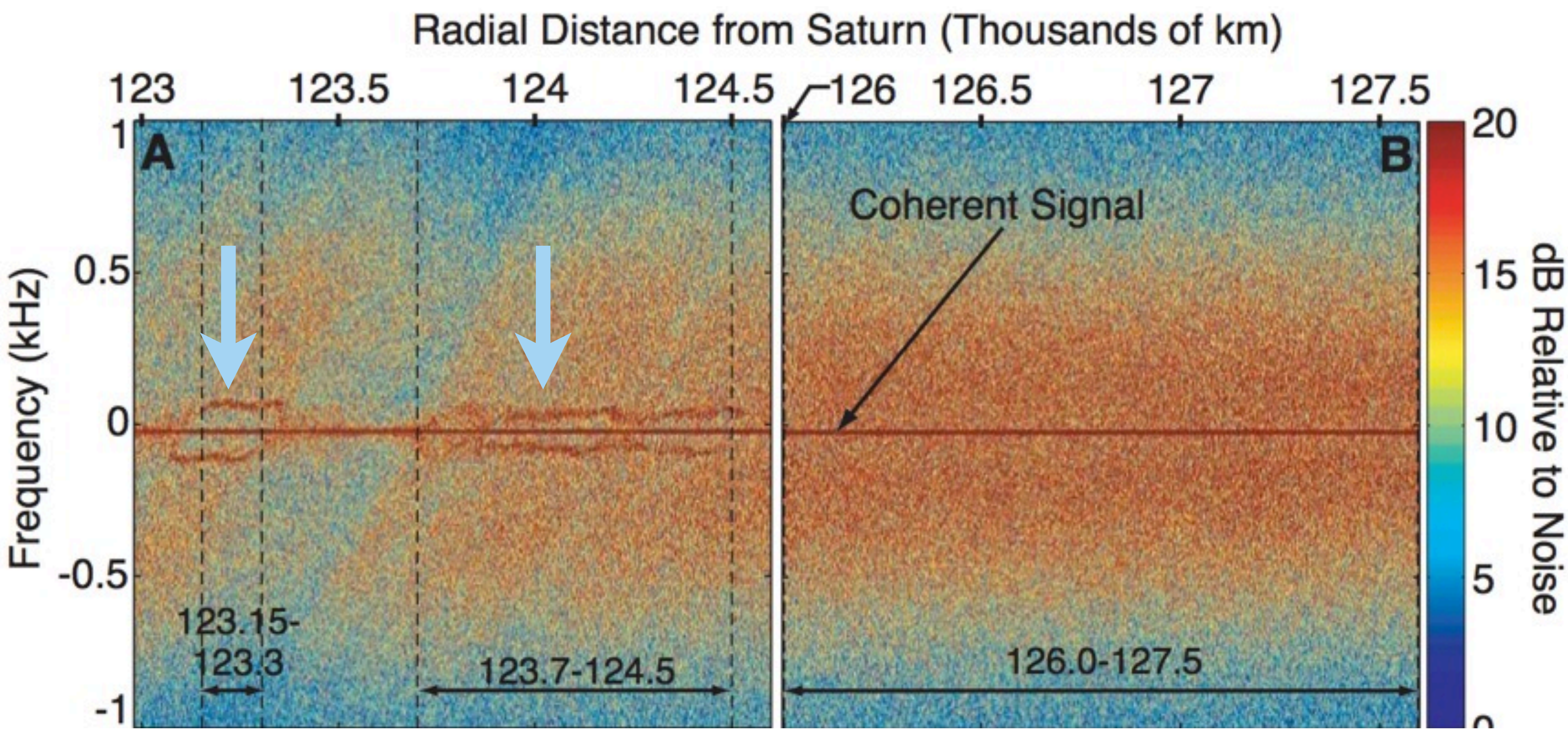
Take home message VI

Maxwell was right.

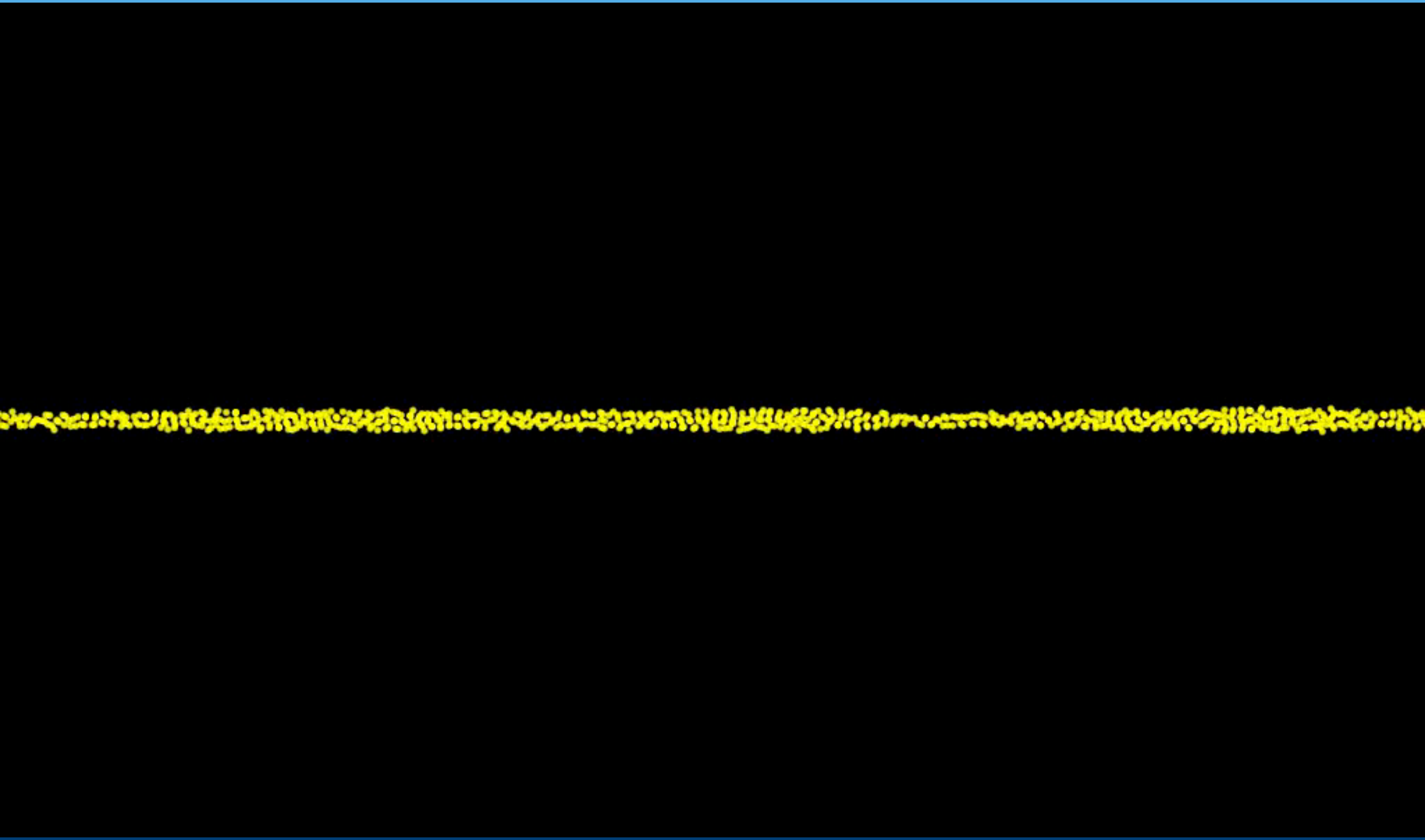
Viscous over-stability in Saturn's rings

Observations

- Observational evidence for small scale structures
- Typical size ~100m



Close-up view of the viscous over-stability



Rein & Latter (in prep)

Numerical simulations with REBOUND

Symplectic Epicycle Integrator

- Fast
- High accuracy
- No long term drifts (important)

Plane-sweep algorithm

- Fast
- O(N) for elongated boxes

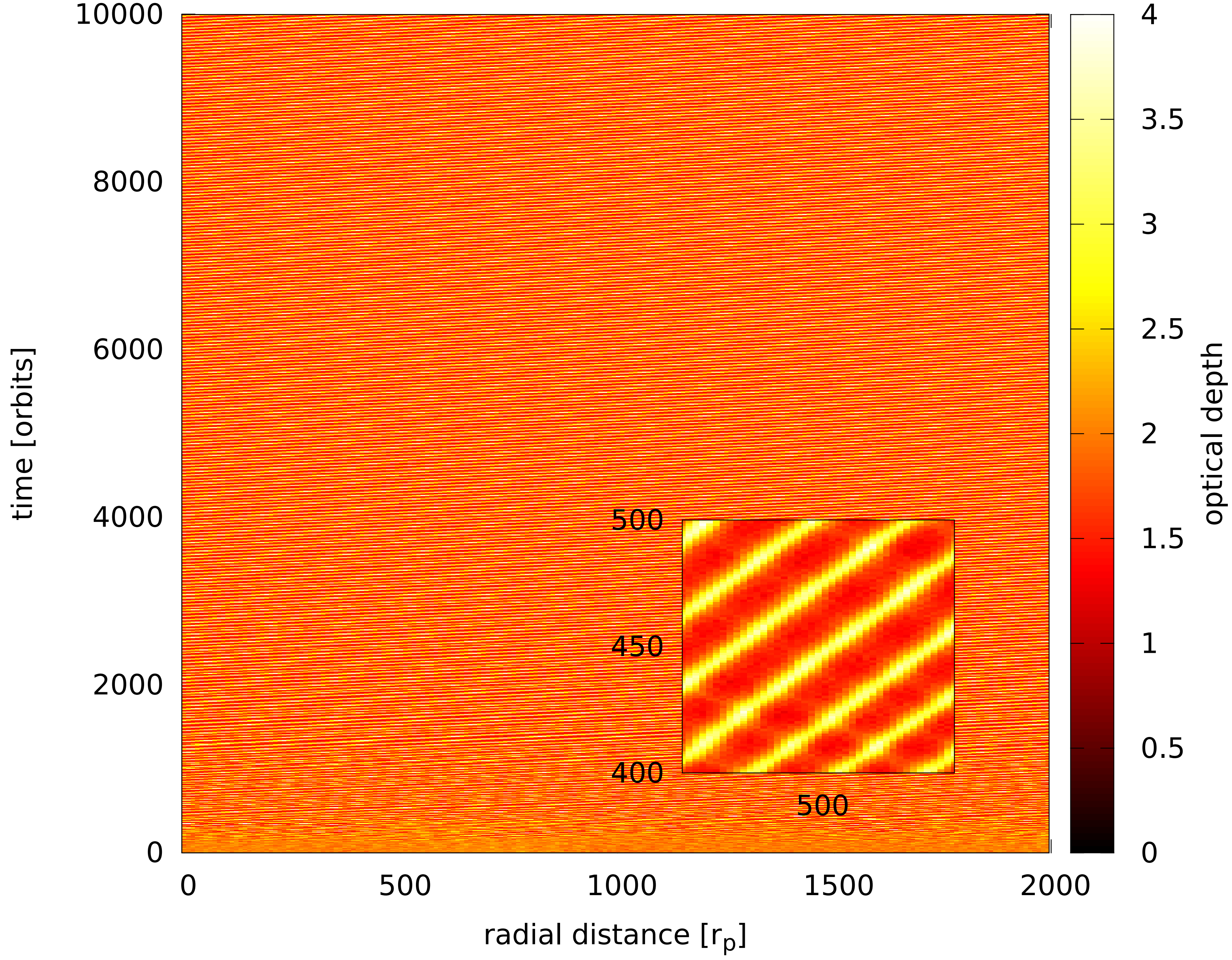
↓ ↓

Direct particle simulations of Saturn's Rings

- Longest integration time ever done*
- Widest boxes ever done*

* to my knowledge, Rein & Latter (in prep)

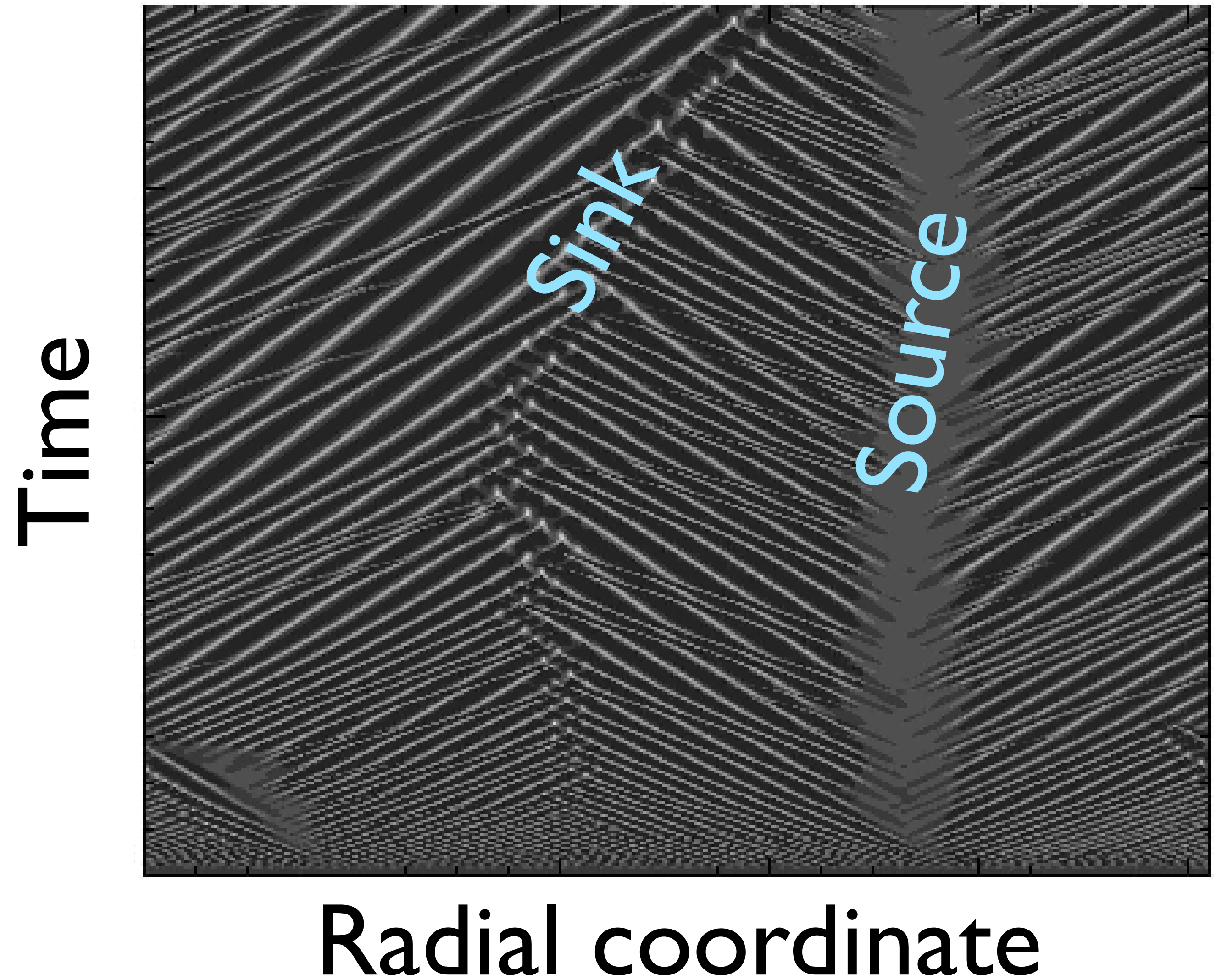
Long-term evolution (direct integration)



Rein & Latter (in prep)

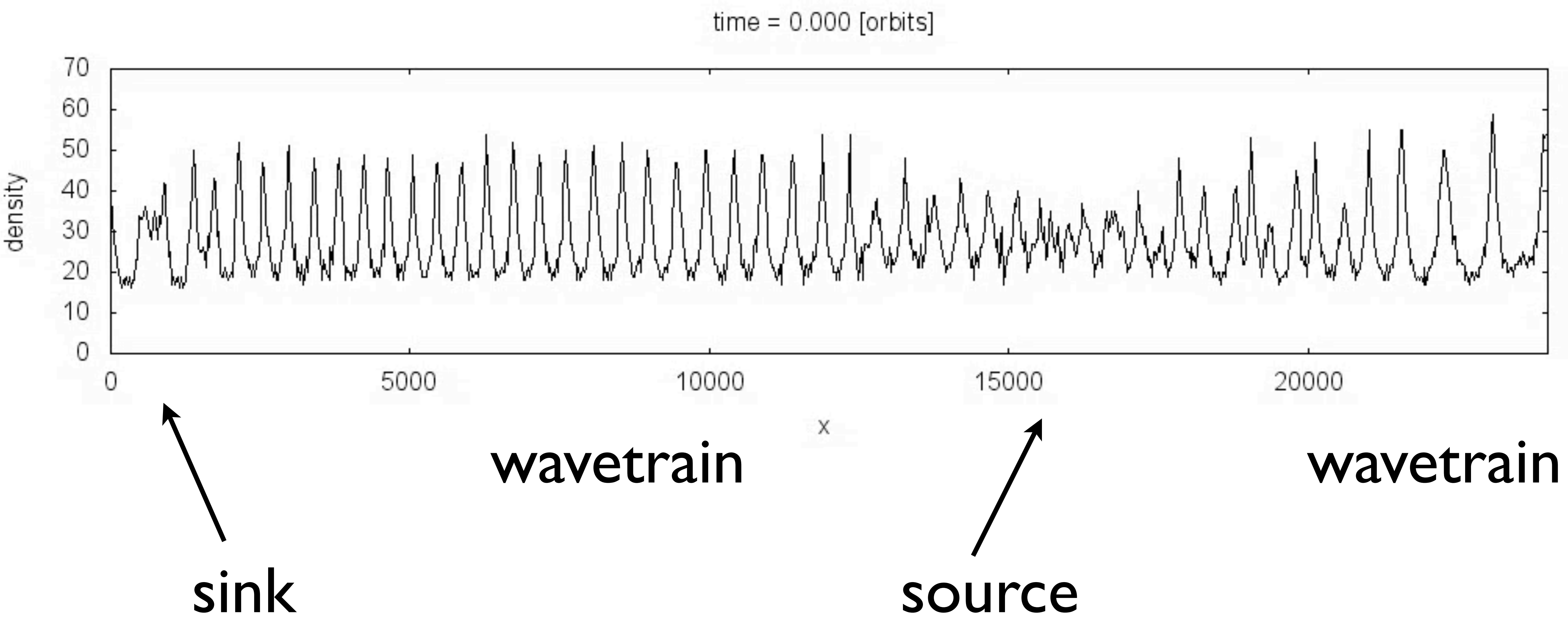
Previous work

- Both analytic calculations and hydrodynamic simulations show non-linear wave-train solutions.
- Rich dynamics with sources and sinks of wave-trains.



Latter & Ogilvie 2009, Salo (in press), etc

Non-linear evolution (direct integration)



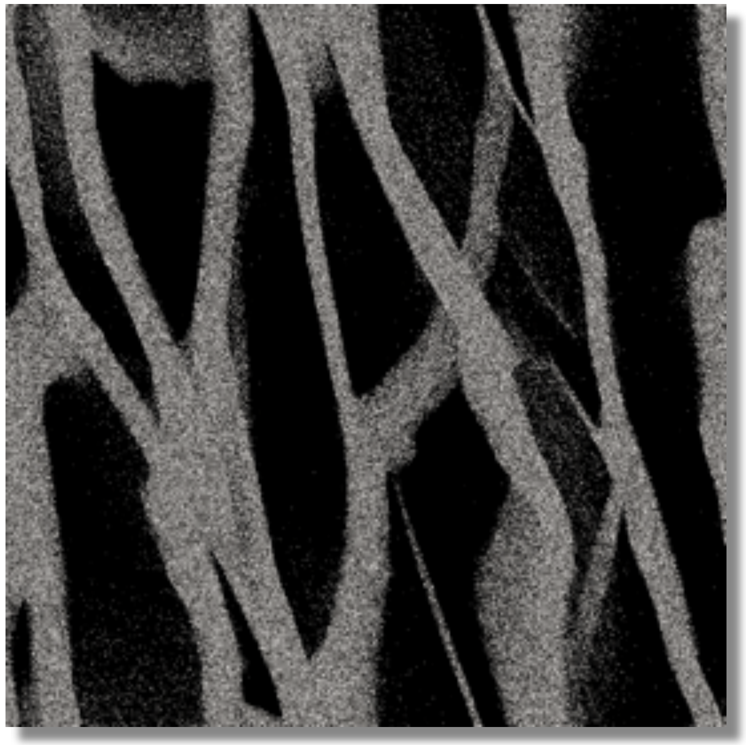
Take home message VII

Simulations are now big enough to directly study the non-linear evolution of the viscous over-stability.

Dense rings

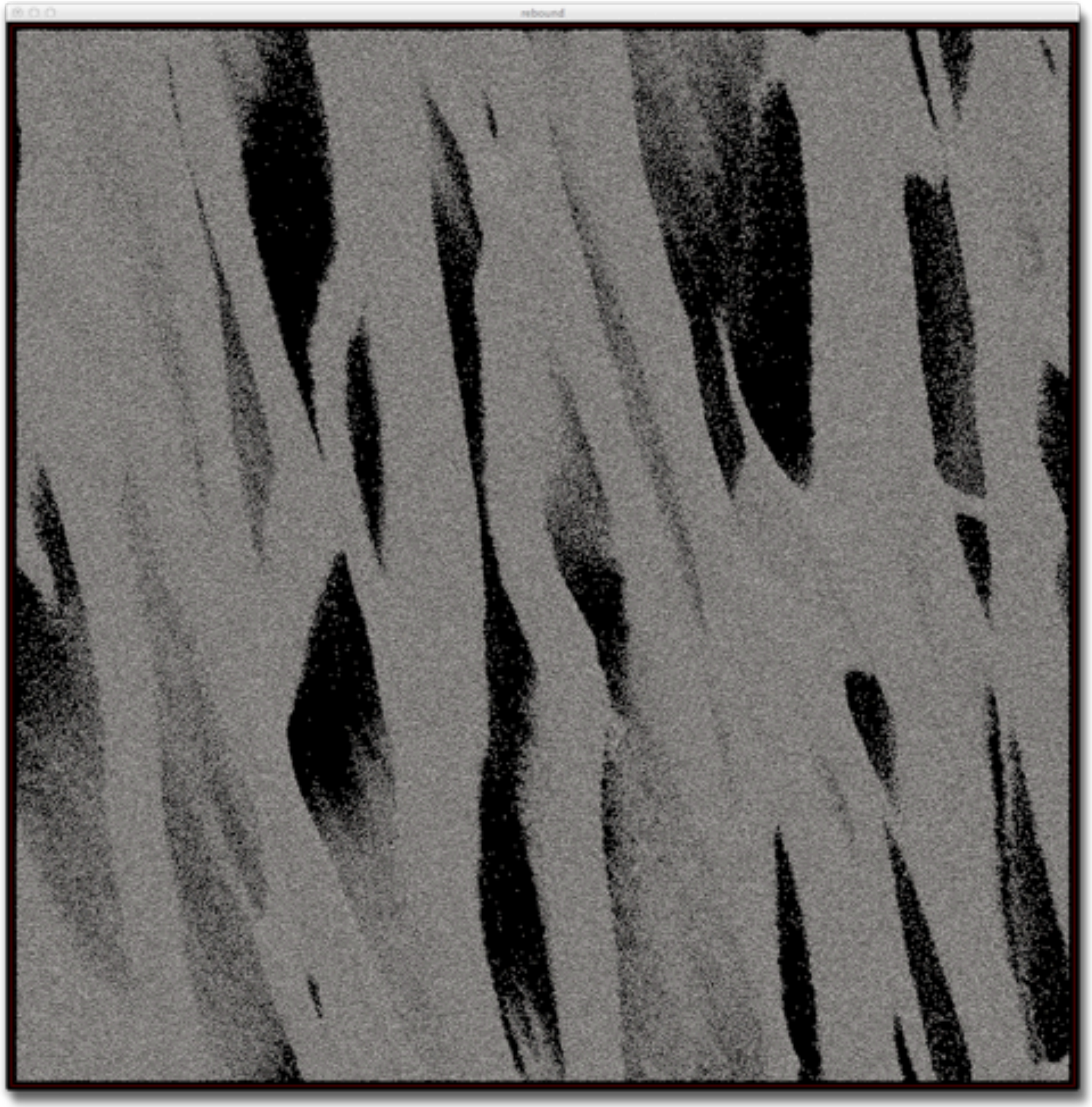
Comparison to previous work

- Robbins et al. (2010)
- Largest simulation
  N = 524.000
- Runtime ~17 days

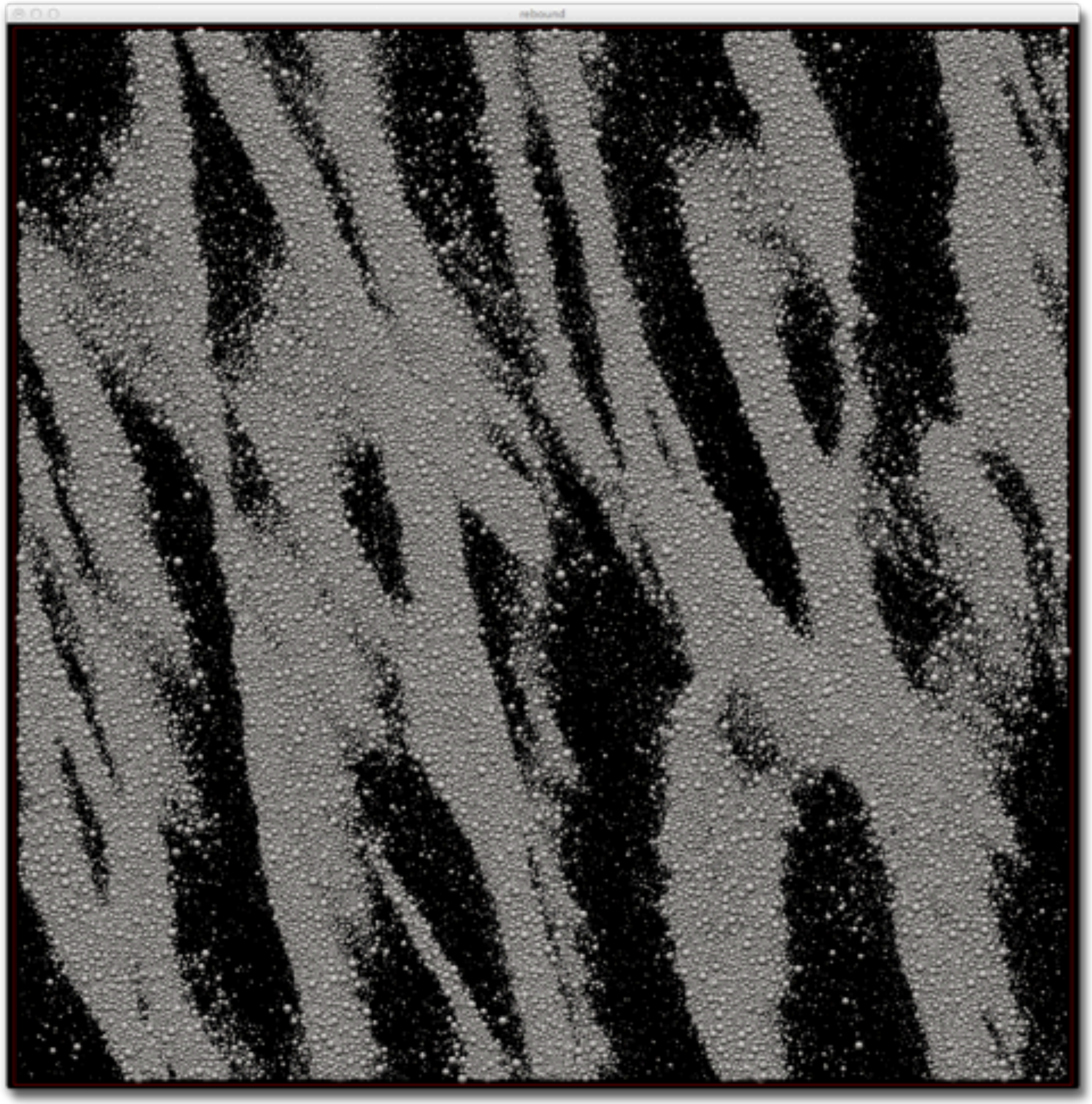


- Rein & Kokubo (in prep)
- Largest simulation (so far)
  N = 10.185.912
- Runtime ~2 days

Dense Rings

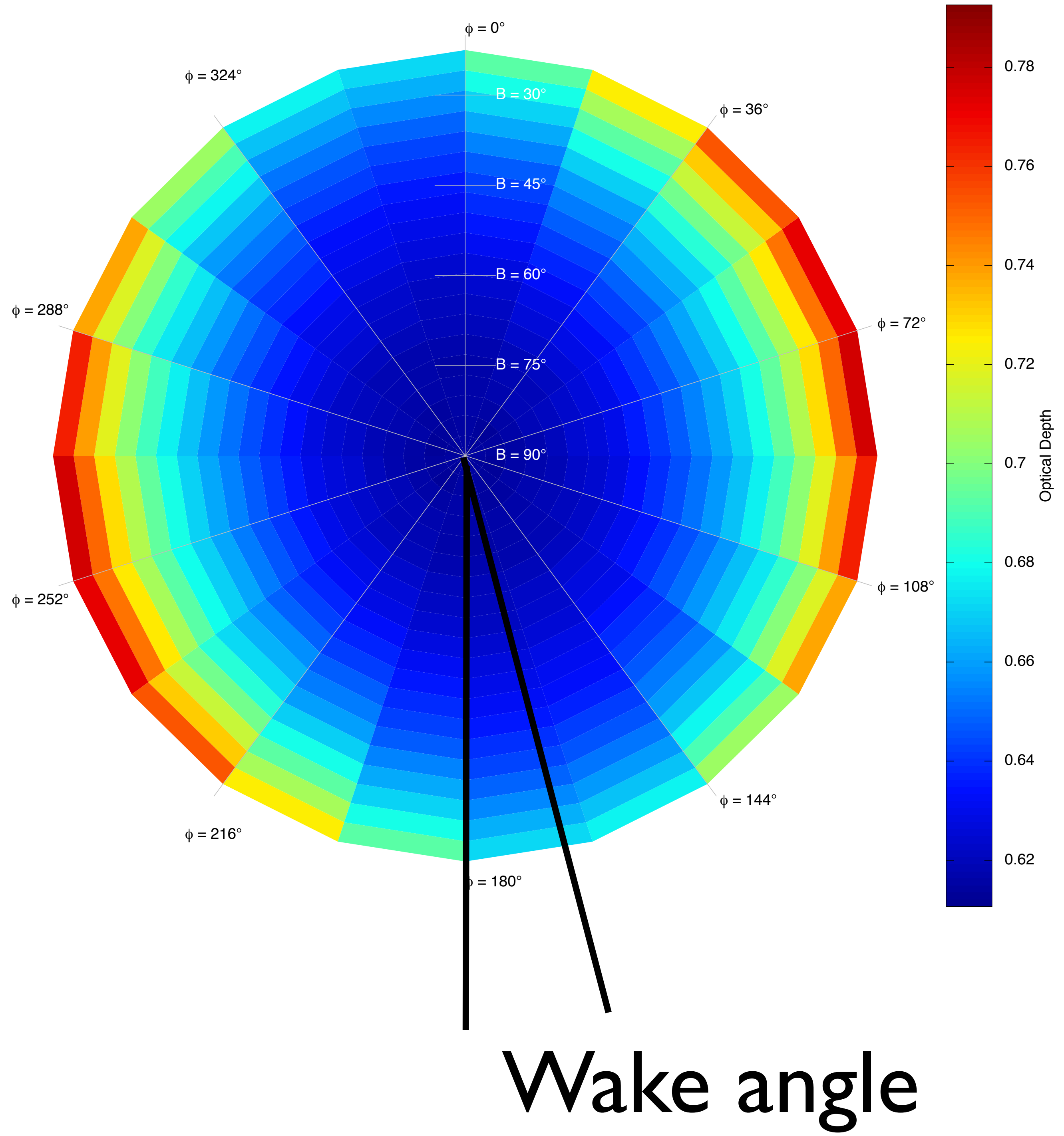


- Geometric optical depth ~ 8



- Geometric optical depth ~ 2
- Realistic size distribution

Actual Optical Depth



Take home message VII

Bigger is better (sometimes).

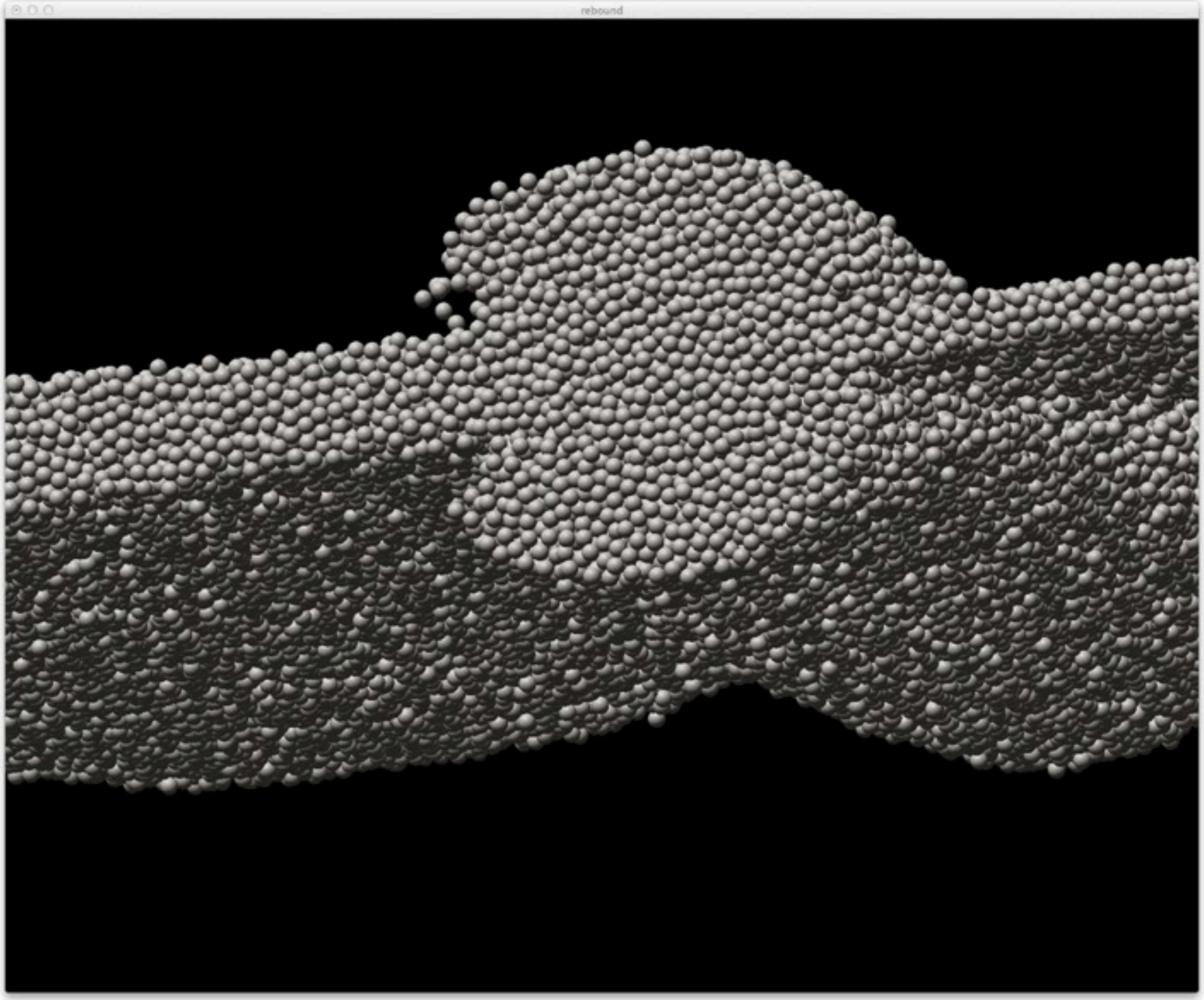
Conclusions

Conclusions / Take home messages

I. Please make your codes public!
II. Symplectic integrators are awesome.
III. Efficient collision detection is hard.
IV. Download and play with REBOUND.*
*Let me know if you run into a problem!
V. Moonlets in Saturn's Rings show direct evidence of disk satellite interaction.
VI. Simulations are now big enough to directly study the non-linear evolution of the viscous over-stability.
VII. Bigger is better (sometimes).

Backup Slides

Dense rings



Rein & Kokubo (in prep)