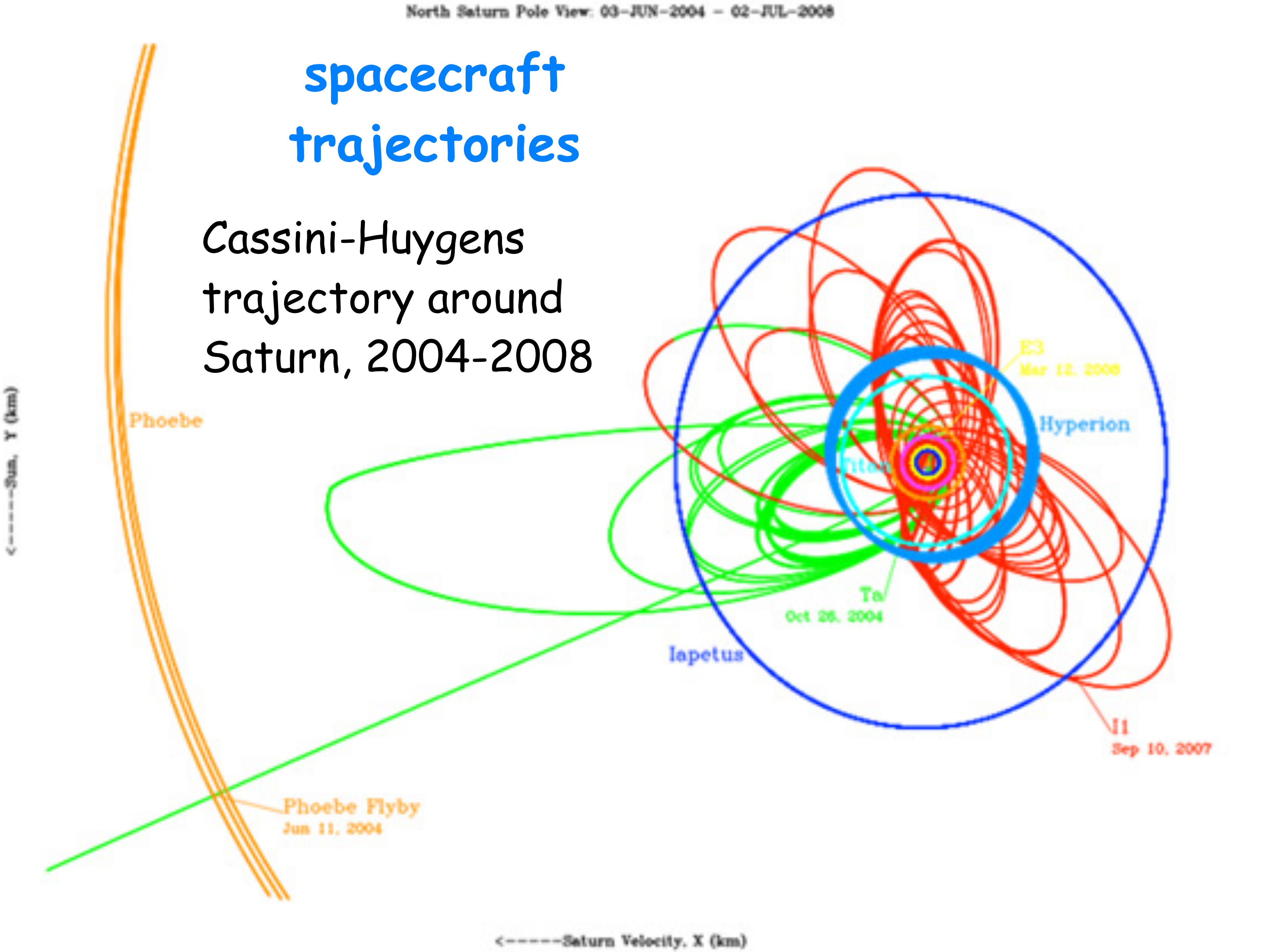
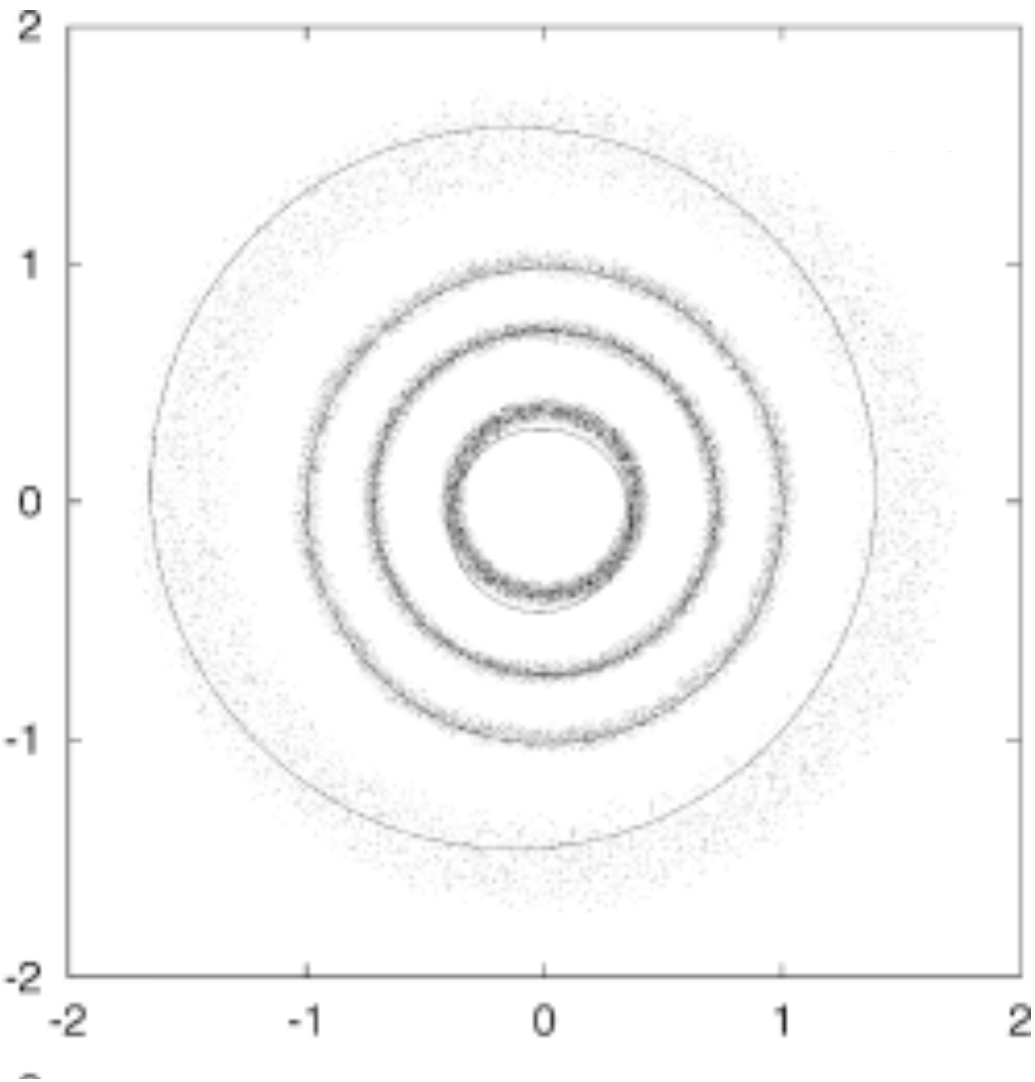
Geometric methods for orbit integration

spacecraft trajectories

Cassini-Huygens trajectory around Saturn, 2004-2008



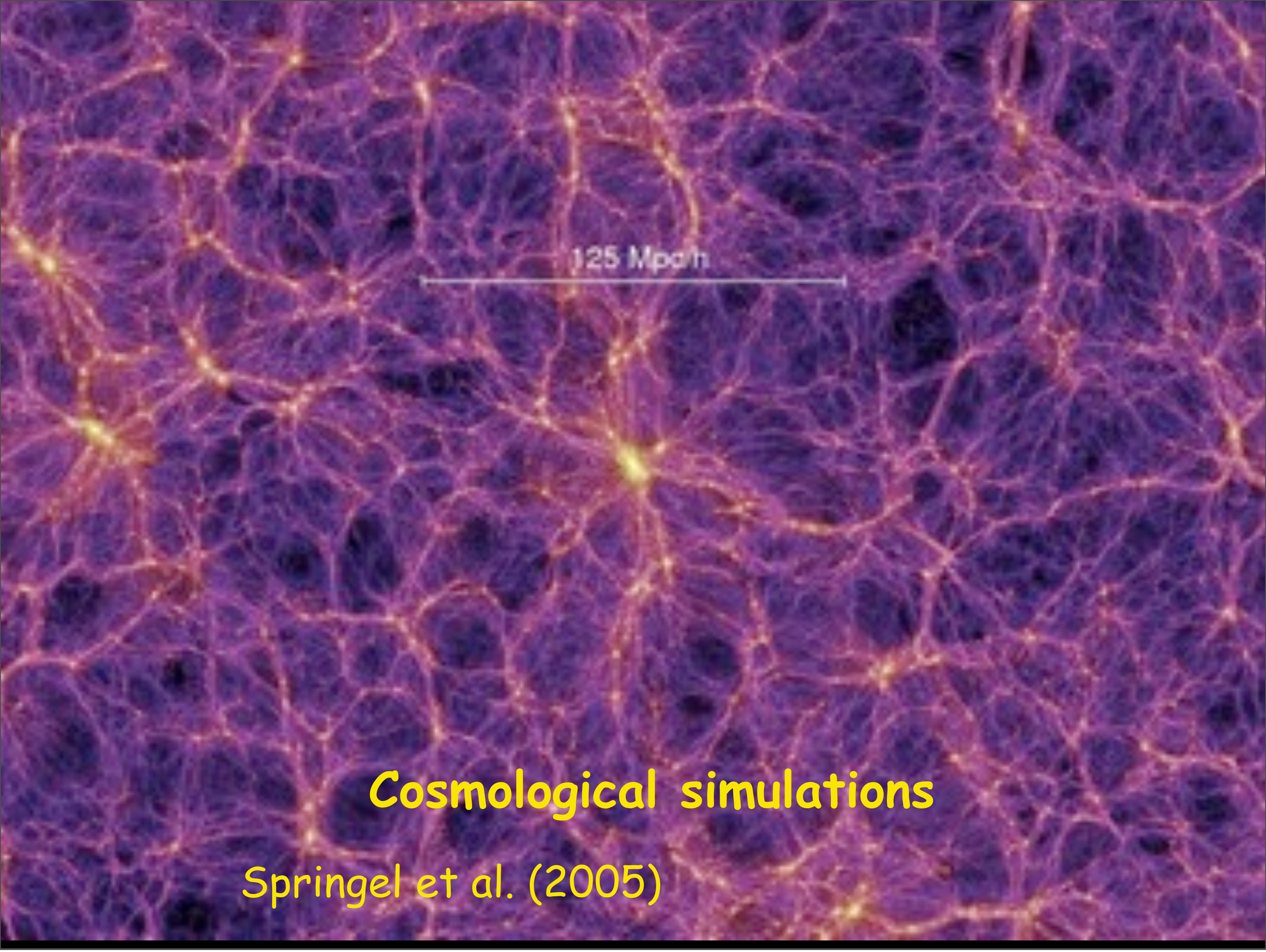


Planetary orbits

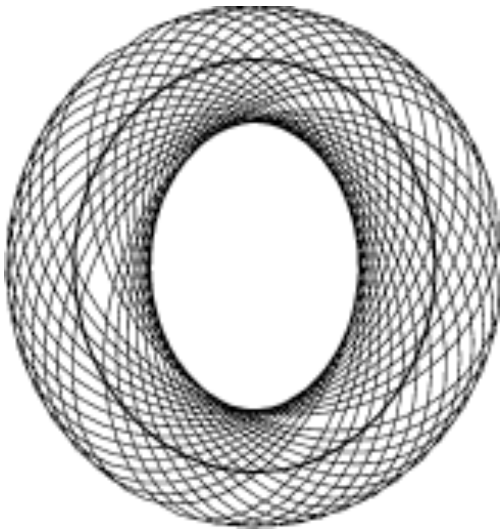
lines = current orbits of the four inner planets

dots = orbits of the inner planets over 50,000 years, 4.5 Gyr in the future

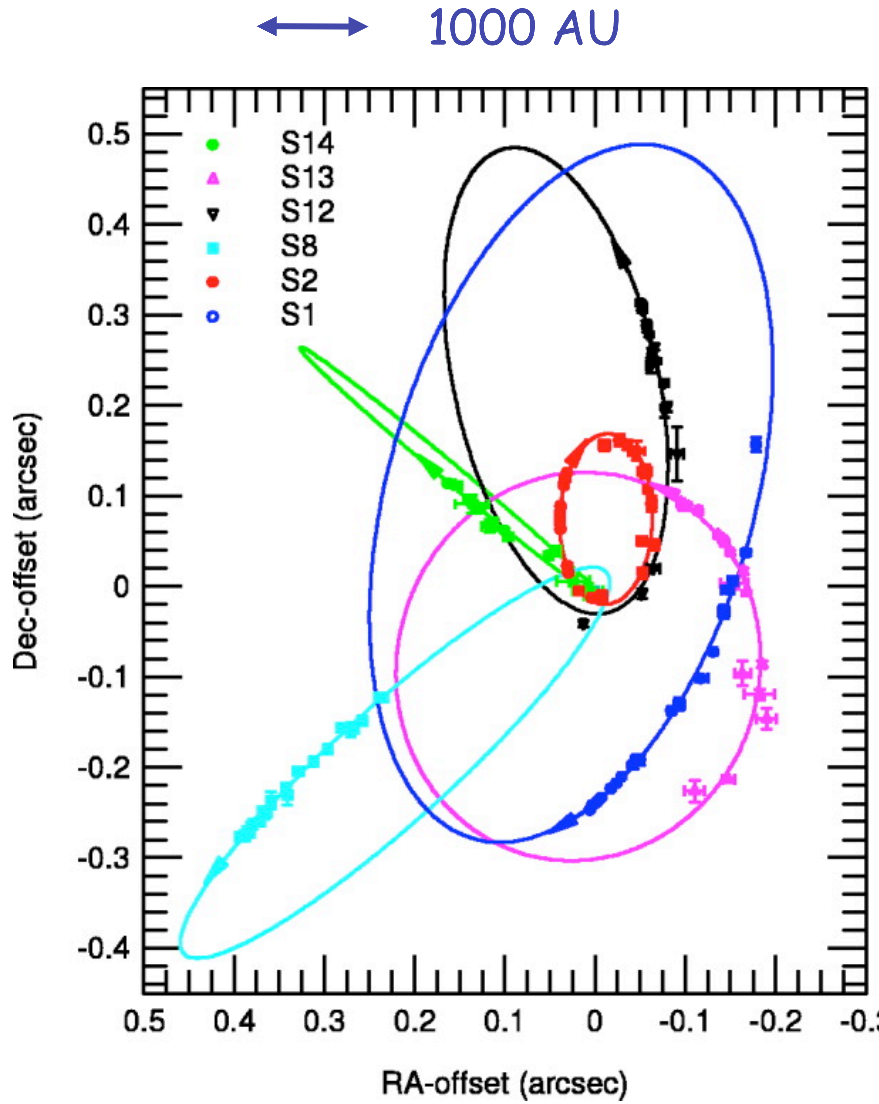
Ito & Tanikawa (2002)


125 Mpc/h
Cosmological simulations
Springel et al. (2005)

Galactic dynamics



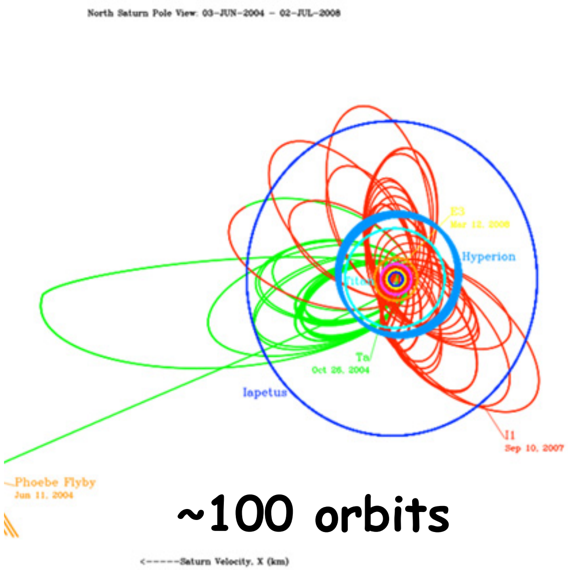
box and tube orbits in a galactic potential



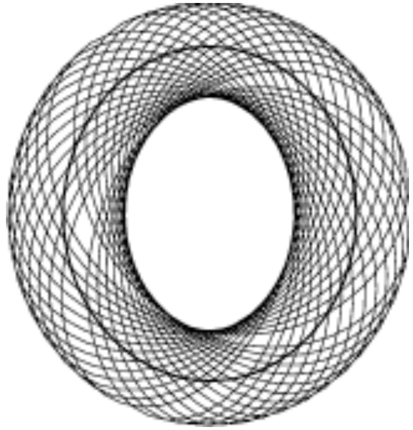
orbits of stars near the Galactic center

Eisenhauer et al. (2005)

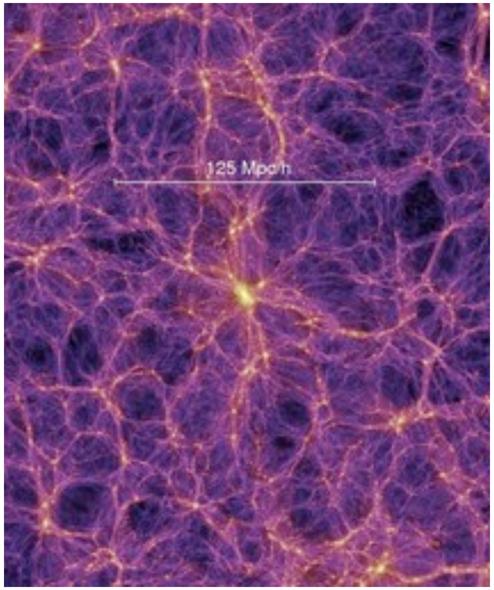

Large Hadron Collider



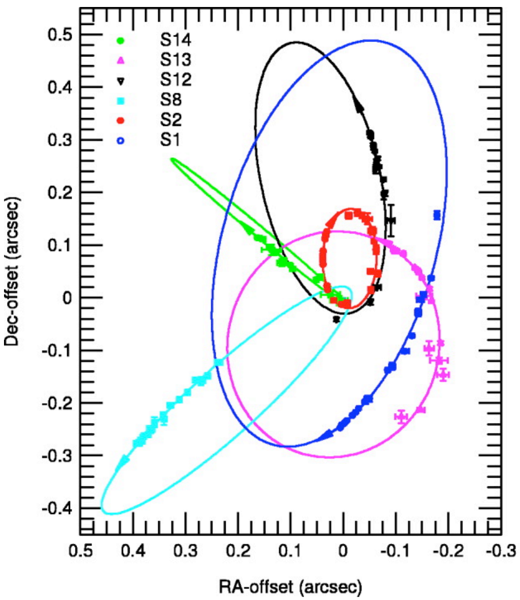
~100 orbits



~100-1000 orbits

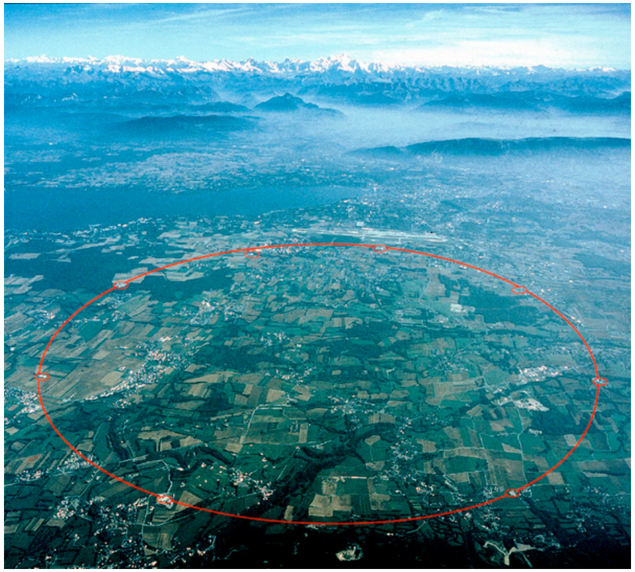


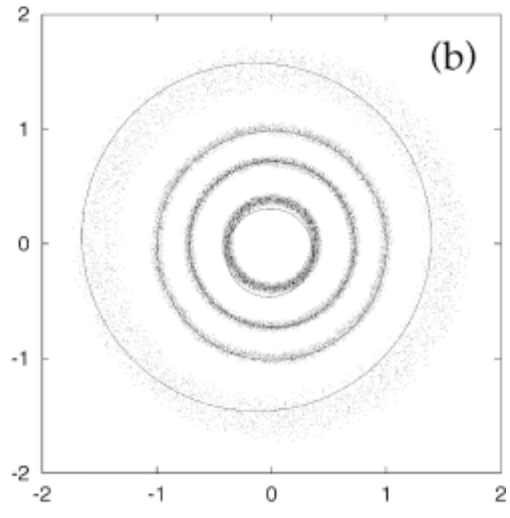
~100-1000 orbits



~10^6 orbits

~10^9 orbits





~10^{10} orbits

Consider following a particle in the force field of a point mass. Set G=M=1 for simplicity. Equations of motion read

$$\dot{\mathbf{r}} = \mathbf{v} \quad ; \quad \dot{\mathbf{v}} = \mathbf{F}(\mathbf{r}) = -\frac{\widehat{\mathbf{r}}}{r^2}$$

Examine three integration methods with timestep h:

$$\mathbf{r}_{n+1} = \mathbf{r}_n + h\mathbf{v}_n \quad ; \quad \mathbf{v}_{n+1} = \mathbf{v}_n + h\mathbf{F}(\mathbf{r}_n)$$

1. Euler's method

$$\mathbf{r}_{n+1} = \mathbf{r}_n + h\mathbf{v}_n \quad ; \quad \mathbf{v}_{n+1} = \mathbf{v}_n + h\mathbf{F}(\mathbf{r}_{n+1})$$

2. modified Euler's

$$\mathbf{r}' = \mathbf{r}_n + \frac{1}{2}h\mathbf{v}_n \ ; \ \mathbf{v}_{n+1} = \mathbf{v}_n + h\mathbf{F}(\mathbf{r}') \ ; \ \mathbf{r}_{n+1} = \mathbf{r}' + \frac{1}{2}h\mathbf{v}_{n+1}$$

3. leapfrog

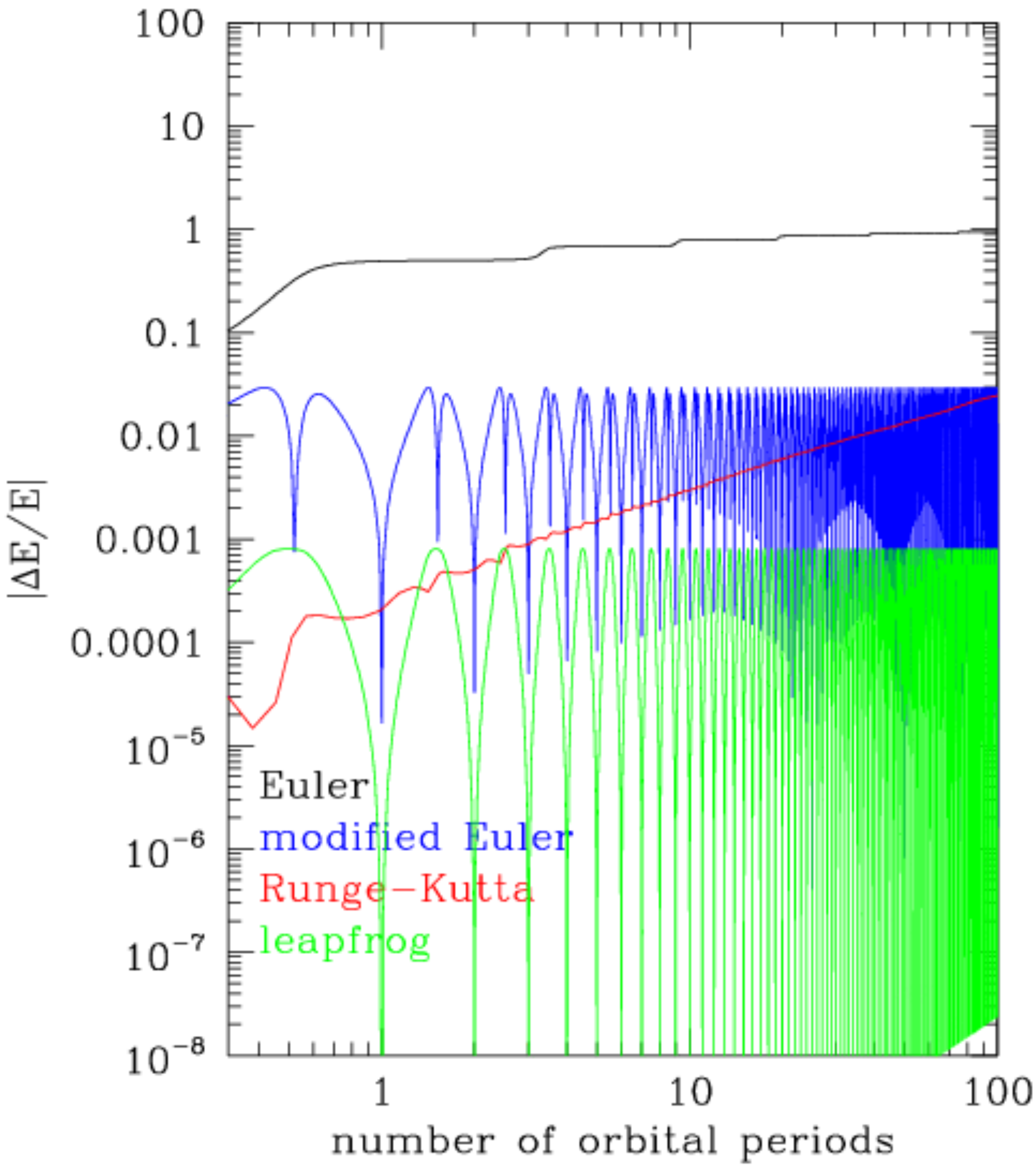
4. Runge-Kutta method

Euler methods are first-order; leapfrog is second-order; Runge-Kutta is fourth order

Use equal number of force evaluations per orbit for each method (rather than equal timesteps) eccentricity = 0.2

200 steps per orbit

plot shows fractional energy error $|\Delta E/E|$

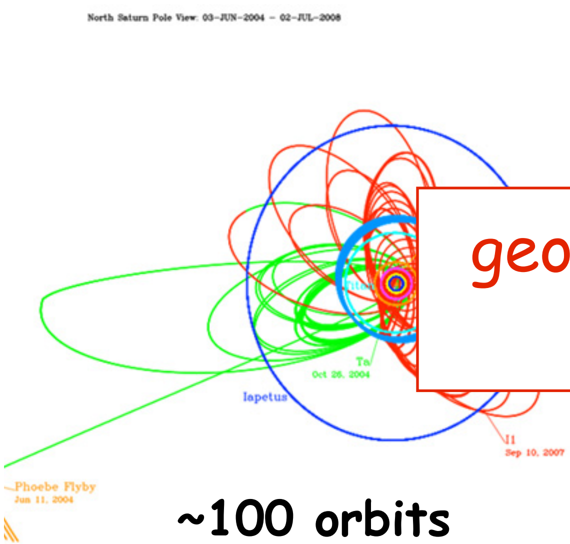


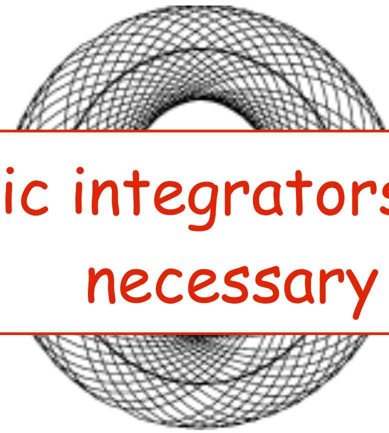
A **geometric integration algorithm** is a numerical integration algorithm that exactly preserves some geometric property of the original set of differential equations

Volume-conserving algorithms:

- conserve phase-space volume, i.e. satisfy Liouville's theorem
- appropriate for Hamiltonian systems
- e.g. modified Euler, leapfrog but not Runge-Kutta

The motivation for geometric integration algorithms is that **preserving the phase-space geometry of the flow determined by the real dynamical system is more important than minimizing the one-step error**



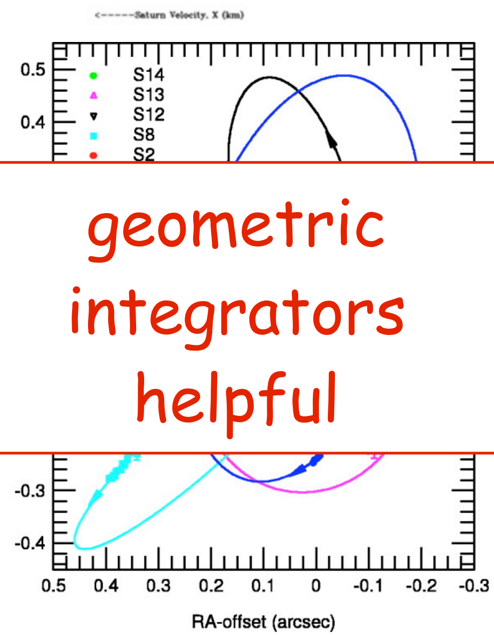


geometric integrators not really necessary

~100 orbits

~100-1000 orbits

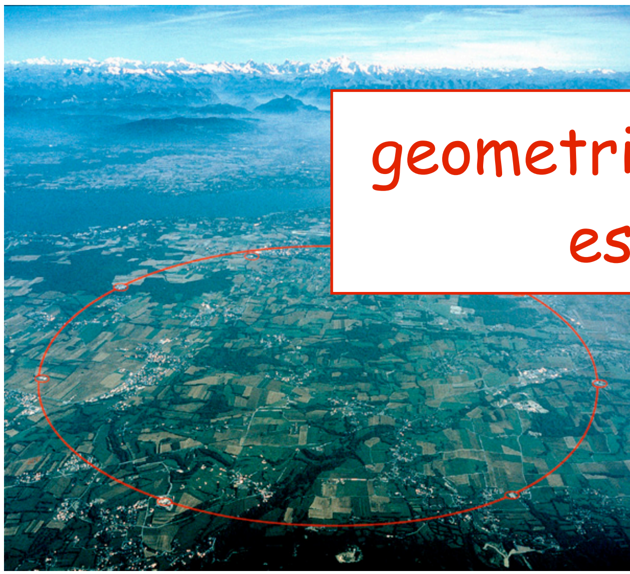
~100-1000 orbits



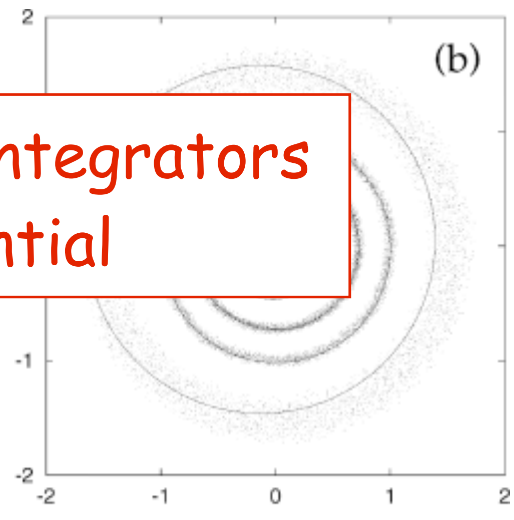
geometric integrators helpful

~10^6 orbits

~10^9 orbits



geometric integrators essential



~10^{10} orbits

Energy-conserving algorithms:

- conserve energy, i.e. restrict the system to a surface of constant energy in phase space
- appropriate for systems with time-independent Hamiltonians, e.g. motion in a fixed potential
- does not include modified Euler, leapfrog, Runge-Kutta

Time-reversible algorithms:

- integrate forward in time for N steps, reverse all velocities, integrate backward in time for N steps, reverse velocities, and the system is back where it started
- appropriate for time-reversible systems, e.g. gravitational N-body problem
- includes leapfrog but not modified Euler or Runge-Kutta

$$\mathbf{r}' = \mathbf{r}_n + \frac{1}{2} h \mathbf{v}_n \; ; \; \mathbf{v}_{n+1} = \mathbf{v}_n + h \mathbf{F}(\mathbf{r}') \; ; \; \mathbf{r}_{n+1} = \mathbf{r}' + \frac{1}{2} h \mathbf{v}_{n+1}$$

Symplectic algorithms:

- if the dynamical system is described by a Hamiltonian H(q,p) then

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{q}} \quad ; \quad \frac{d\mathbf{q}}{dt} = \frac{\partial H}{\partial \mathbf{p}}.$$

- if y(t)=[q(t),p(t)] then the flow from $y(t_0)$ to $y(t_1)$ is a **symplectic** or canonical map
- an integration method is symplectic if the formula for advancing by one timestep

$$y_{n+1}=y_n+g(t_n,y_n,h)$$

  is also a symplectic map
- for one-dimensional systems symplectic = volume-conserving (actually area-conserving)
- for systems of more than one dimension symplectic is more general
- modified Euler and leapfrog are symplectic

Symplectic algorithms for separable Hamiltonians

If the dynamical system is described by a Hamiltonian of the form

$$H = H_D + H_K, \qquad H_D = \frac{1}{2}\mathbf{v}^2,\ H_K = \Phi(\mathbf{x}, t)$$

then the *drift* operator $\mathbf{D}_h$ advances the orbit for time h under the influence of H_D alone:

$$\mathbf{D}_h : (\mathbf{x}, \mathbf{v}) \to (\mathbf{x} + \mathbf{v}h, \mathbf{v}).$$

Similarly the *kick* operator $\mathbf{K}_h$ advances the orbit under the influence of H_K alone:

$$\mathbf{K}_h : (\mathbf{x}, \mathbf{v}) \to (\mathbf{x}, \mathbf{v} - h\nabla\Phi(\mathbf{x})).$$

The modified Euler operator is

$$\mathbf{K}_h\mathbf{D}_h : (\mathbf{x}, \mathbf{v}) \to [\mathbf{x} + \mathbf{v}h, \mathbf{v}\ -\ \nabla\Phi(\mathbf{x} + \mathbf{v}h)].$$

Similarly the leapfrog operator is

$$\mathbf{D}_{h/2}\mathbf{K}_h\mathbf{D}_{h/2} \quad \text{or} \quad \mathbf{K}_{h/2}\mathbf{D}_h\mathbf{K}_{h/2}$$

Symplectic algorithms

An n^{th}-order symplectic integration algorithm for a Hamiltonian H gives the exact trajectory for a nearby Hamiltonian $H+H_{error}$ where H_{error} is $O(h^n)$

This result changes the study of numerical integration from numerical analysis (boring) to dynamics (interesting)

e.g., integrating pendulum Hamiltonian $H=v^2/2+C\cos(x)$ with modified Euler method gives

$$x' = x + hv \quad , \quad v' = v + Ch\sin(x')$$

set $hv=y$

$$x' = x + y \quad , \quad y' = y + K\sin(x') \qquad K=Ch^2$$

This is the Chirikov-Taylor or standard or kicked pendulum map

Symplectic algorithms

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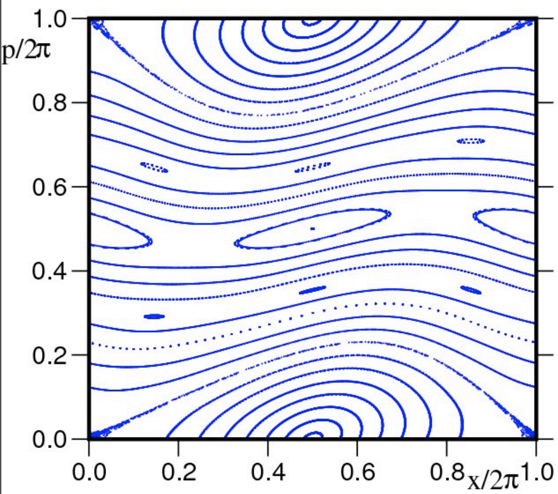
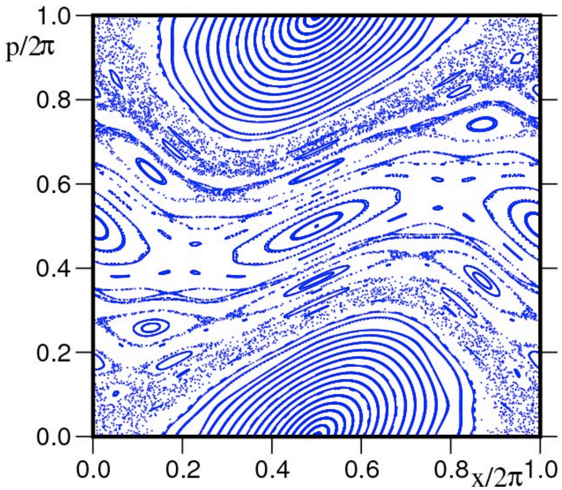
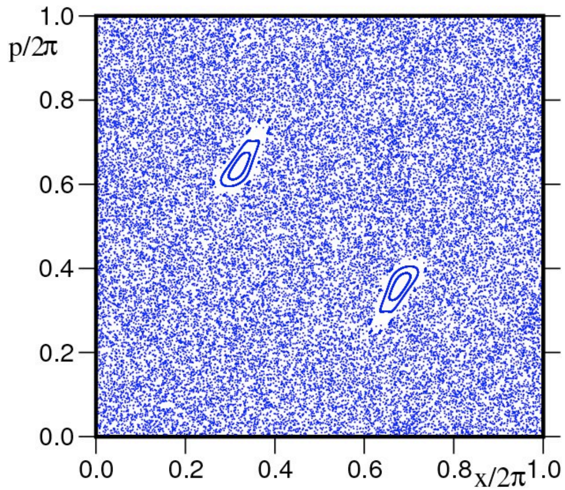
K=0.5



K=0.971635



K=5



Geometric integrators for cosmology

The Lagrangian for a gravitational N-body system is

$$L = \frac{1}{2}\sum_i m_i \dot{\mathbf{r}}_i^2(t) - G\sum_{j>i}\frac{m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|}$$

Introduce comoving coordinates x by r = a(t)x

$$L = \frac{1}{2}\sum_i m_i(\dot{a}\mathbf{x}_i + a\dot{\mathbf{x}}_i)^2 - \frac{G}{a}\sum_{j>i}\frac{m_i m_j}{|\mathbf{x}_i - \mathbf{x}_j|}$$

Momentum is $\mathbf{p}_i = \partial L/\partial\dot{\mathbf{x}}_i = m_i(a\dot{a}\mathbf{x}_i + a^2\dot{\mathbf{x}}_i)$

Hamiltonian is

$$H(\mathbf{q},\mathbf{p},t) = \sum \mathbf{p}_i\cdot\mathbf{q}_i - L = H_A(\mathbf{q},\mathbf{p},t) + H_B(\mathbf{q},\mathbf{p},t)$$

with

$$H_A = \sum_i \frac{\mathbf{p}_i^2}{2m_i a^2(t)}, \qquad H_B = -\sum_{i>j}\frac{Gm_i m_j}{a(t)|\mathbf{x}_i - \mathbf{x}_j|}.$$

Drift and kick operators correspond to motion under H_A and H_B:

$$\mathbf{x}_i' = \mathbf{x}_i + \frac{\mathbf{p}_i}{m_i}\int_t^{t+h}\frac{dt}{a^2(t)}, \qquad \mathbf{p}_i' = \mathbf{p}_i - G\sum_j\frac{\mathbf{x}_i - \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|^3}\int_t^{t+h}\frac{dt}{a(t)}$$

Geometric integrators for planetary systems

To follow motion in the general potential **Φ(r,t)** we may use the Hamiltonian splitting

$$H(\mathbf{q},\mathbf{p},t) = H_A(\mathbf{q},\mathbf{p},t) + H_B(\mathbf{q},\mathbf{p},t)$$

with

$$H_A = \frac{1}{2}p^2, \qquad H_B = \Phi(\mathbf{q},t)$$

Then integrate using the leapfrog operator **$A_{h/2}B_hA_{h/2}$**.

Motion of a test particle in a planetary system is described by

$$\Phi(\mathbf{r},t) = -\frac{GM_*}{r} - \sum_j \frac{Gm_j}{|\mathbf{r}-\mathbf{r}_j|}$$

In this case a much better split is

$$H_A = \frac{1}{2}p^2 - \frac{GM_\star}{r}, \qquad H_B = \sum_j \frac{Gm_j}{|\mathbf{r}_i-\mathbf{r}_j|}$$

The workhorse for long orbit integrations in planetary systems is the mixed-variable symplectic integrator (Wisdom & Holman 1991)

$$H(\mathbf{r}, \mathbf{p}) = H_A + H_B,$$

with

$$H_A = \frac{1}{2}p^2 - \frac{GM_\star}{r}, \qquad H_B = \sum_j \frac{Gm_j}{|\mathbf{r}_i - \mathbf{r}_j|}$$

and the operator **$A_{h/2}B_hA_{h/2}$.**

- motion under H_A is analytic (Keplerian motion) and motion under H_B is also analytic (impulsive kicks from the planets)
- this is a geometric integrator (symplectic and time-reversible)
- errors smaller than leapfrog by of order $m_{planet}/M_* \sim 10^{-4}$

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and the operator $A_{h/2}B_hA_{h/2}$.

This integrator exactly follows the motion in a Hamiltonian $H+H_{error}$ where H_{error} is $O(h^2)$ and oscillatory. Dominant errors can be reduced to $O(m_{planet}/M^*)^2$ by ensuring that the action associated with H_{error} is zero

This can be done by the "warmup" starting procedure (Saha & Tremaine 1992)

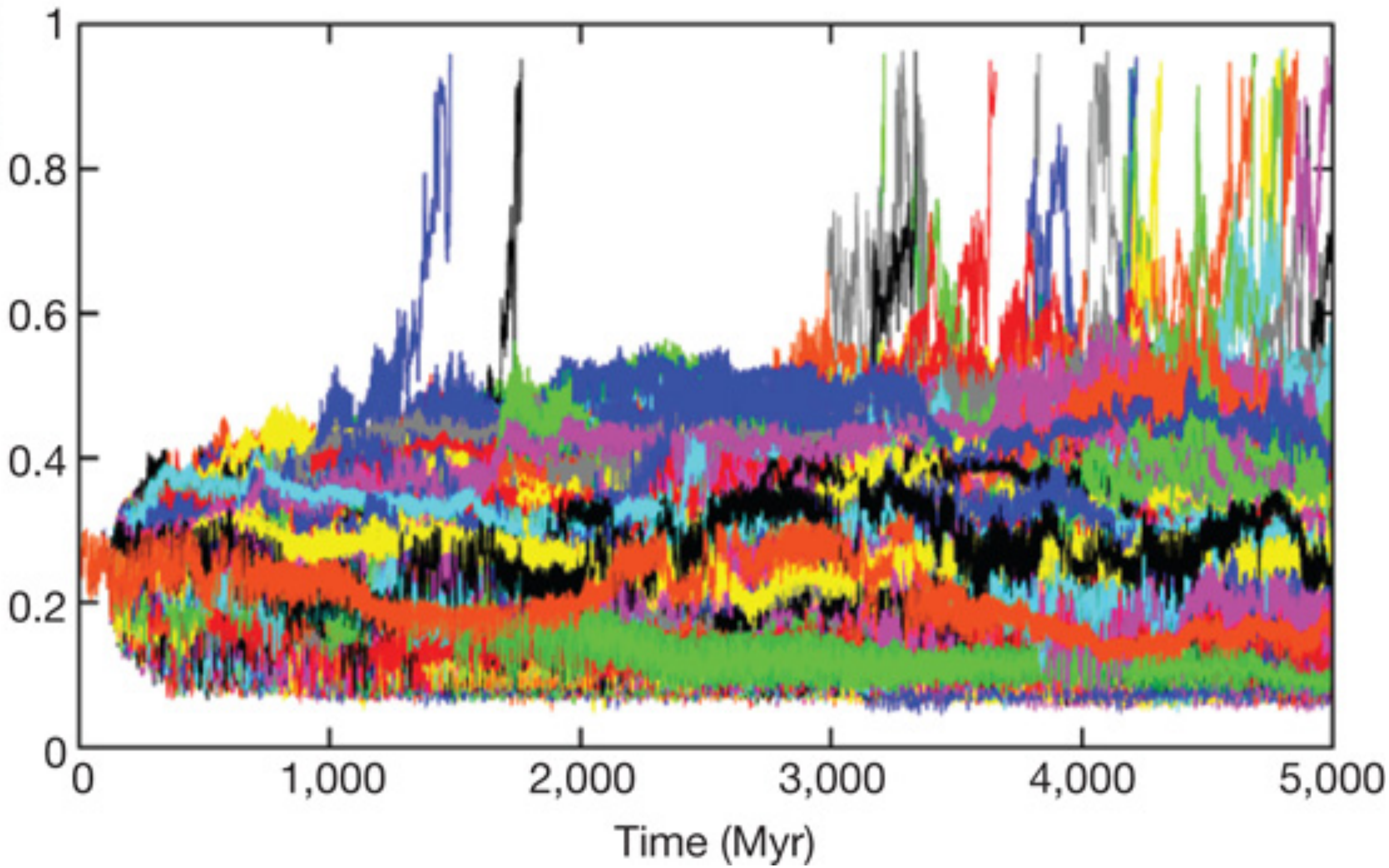
The workhorse for long orbit integrations in planetary systems is the mixed-variable symplectic (MVS) integrator (Wisdom & Holman 1991)

- what it does well: long (up to Gyr) integrations of planets on orbits that are not too far from circular and don't come too close
- what it doesn't do well: close encounters and highly eccentric orbits

The most popular public software packages for solar-system and other planetary integrations are MERCURY (John Chambers) and SWIFT (Hal Levison, Martin Duncan)

- include several integrators: MVS, Bulirsch-Stoer, Forest-Ruth, etc.
- can handle close encounters + test particles
- can include most important relativistic corrections

Following 9 planets for 10^6 yr takes about 30 minutes



eccentricity of Mercury over 5 Gyr from 2,500 integrations differing by < 1 mm in semi-major axis of Mercury

(Laskar & Gastineau 2009)

Higher-order symplectic integrators

"drift" and "kick" operators

$$D_h : \mathbf{q} \to \mathbf{q}' = \mathbf{q} + h\mathbf{p}, \; K_h : \mathbf{p} \to \mathbf{p}' = \mathbf{p} - h\nabla V(\mathbf{q}')$$

- modified Euler method $K_h D_h$ or $D_h K_h$ (first-order integrator)
- leapfrog $D_{h/2} K_h D_{h/2}(z)$ (second-order integrator)
- Forest method $D_a K_a D_b K_c D_b K_a D_a$ (fourth-order integrator)

  if $a = 1.35120h$, $b = -0.3512h$, $c = -1.7024h$

- automatically symplectic since D_h, K_h are symplectic
- any symmetric formula is time-reversible
- only one set of phase-space coordinates has to be stored
- can be generalized to arbitrarily high order (Yoshida 1993)

Leapfrog with variable timestep (1)

- we want to allow a variable timestep that depends on phase-space position, h= τ(r,v)
- time-reversible integrators have almost all the good properties of symplectic integrators
- define a symmetric function s(h,h'), e.g. s(h,h')=(h +h')/2

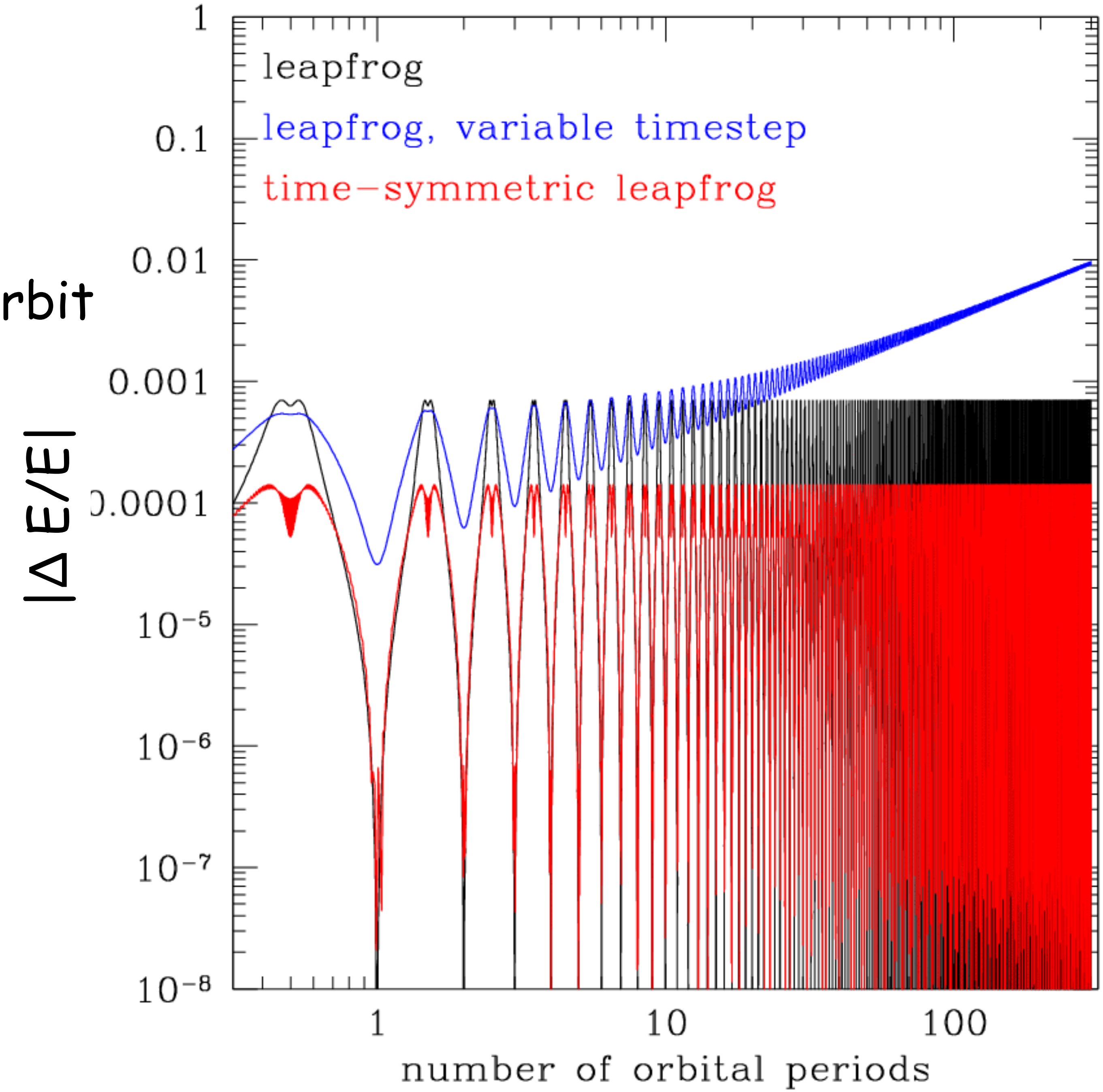
$$\mathbf{r}' = \mathbf{r}_n + \frac{1}{2} h \mathbf{v}_n \quad ; \quad \mathbf{v}' = \mathbf{v}_n + \frac{1}{2} h \mathbf{F}(\mathbf{r}')$$

$$s(h, h') = \tau(\mathbf{r}', \mathbf{v}')$$

$$\mathbf{v}_{n+1} = \mathbf{v}' + \frac{1}{2} h' \mathbf{F}(\mathbf{r}') \quad ; \quad \mathbf{r}_{n+1} = \mathbf{r}' + \frac{1}{2} h' \mathbf{v}_{n+1}$$

This is time-reversible but not symplectic e=0.5

200 steps per orbit



Leapfrog with variable timestep (2)

Time transformation:

- we want to allow a variable timestep that depends on phase-space position $h = \tau(q,p)$
- introduce a new time variable t' by $dt = \tau(q,p)\, dt'$; then unit timestep in t' corresponds to desired timestep in t
- introduce extended phase space $Q=(q_0,q)$ with $q_0=t$ and $P=(p_0,p)$ with $p_0=-H$. Then set

$$H'(Q,P) = \tau(q,p)[H(q,p)+p_0]$$

If (q,p) satisfy Hamilton's equations with Hamiltonian H and time t, then (Q,P) satisfy Hamilton's equations with Hamiltonian H' and time t'

- works very well on eccentric orbits but only for one particle (can't synchronize timesteps of different particles)

Leapfrog with variable timestep (3)

- we have a general differential equation dy/dt = f(t,y) that is known to be time-reversible
- we want an integration scheme that is time-symmetric with a variable timestep that depends on y, h= τ(y)
- define a symmetric function s(h,h'), e.g. s(h,h')=(h+h')/2
- pick your favorite one-step integrator, $y_{n+1}=y_n+g(y_n,h)$ (e.g. Runge-Kutta)
- introduce a dummy variable z and set $z_n=y_n$ at step n

$$\mathbf{y}' = \mathbf{y}_n + g(\mathbf{z}_n, h/2) \quad ; \quad \mathbf{z}' = \mathbf{z}_n - g(\mathbf{y}', -h/2)$$
$$s(h, h') = \tau(\mathbf{y}')$$
$$\mathbf{z}_{n+1} = \mathbf{z}' + g(\mathbf{y}', h/2) \quad ; \quad \mathbf{y}_{n+1} = \mathbf{y}' - g(\mathbf{z}_{n+1}, -h/2)$$

This is time-reversible (Mikkola & Merritt 2006)

Summary

When integrating ordinary differential equations

• short-term quantitative accuracy is not the same as---and is often less important than---long-term qualitative accuracy

• use geometric integrators, which preserve the qualitative features of the physical systems they are describing (symplecticity, time-reversibility, etc.)

• if the physical system is close to one that can be integrated exactly, choose the integration algorithm so that it is exact for the integrable system

• implement variable timestep in a time-reversible algorithm