

On Simulation Reliability: Shadowing the Gravitational N -body Problem

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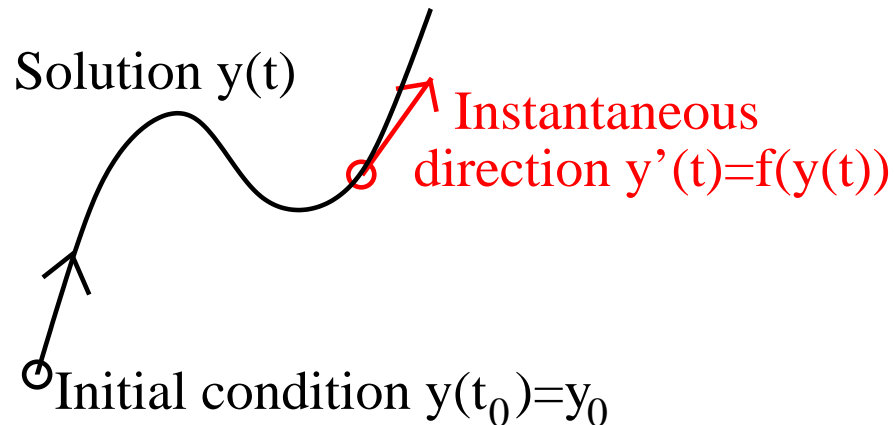
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Physical simulation and Ordinary Differential Equations

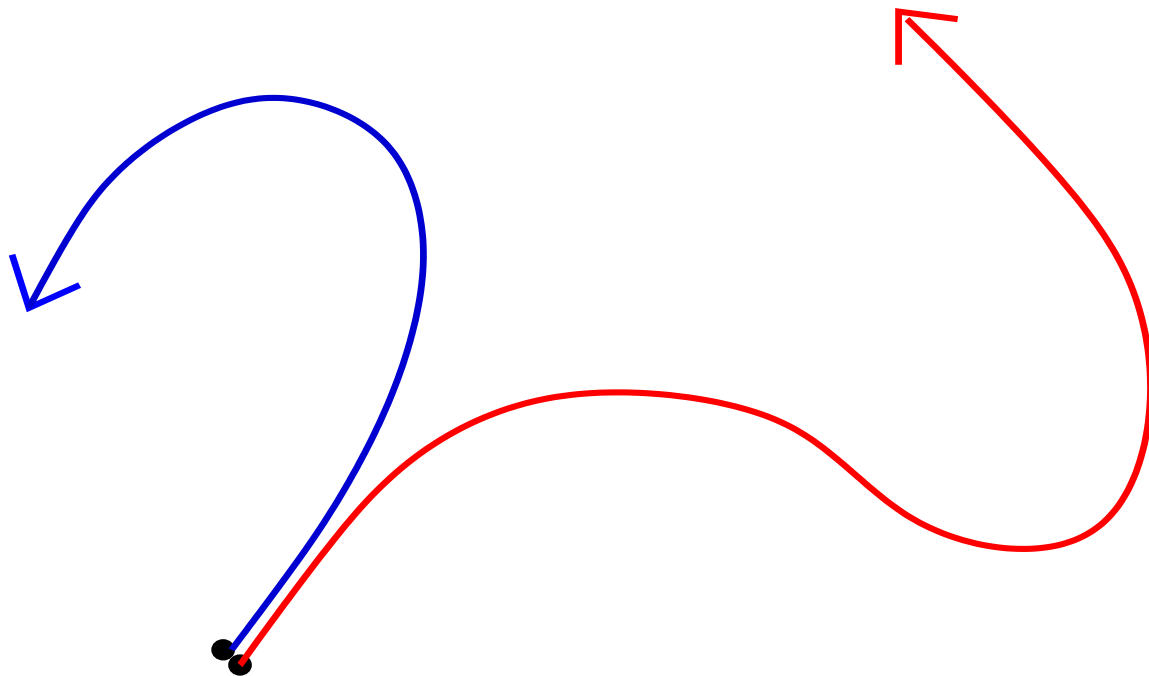


- deterministic (no randomness)
- time t is continuous
- $y(t)$ = state of system (e.g., position and velocity)
- given initial condition $y(t_0) = y_0$
- $y'(t) = f(y)$ defines how system evolves
- solve for $y(t)$, $t \geq t_0$ (exists and is unique if f is Lipschitz)

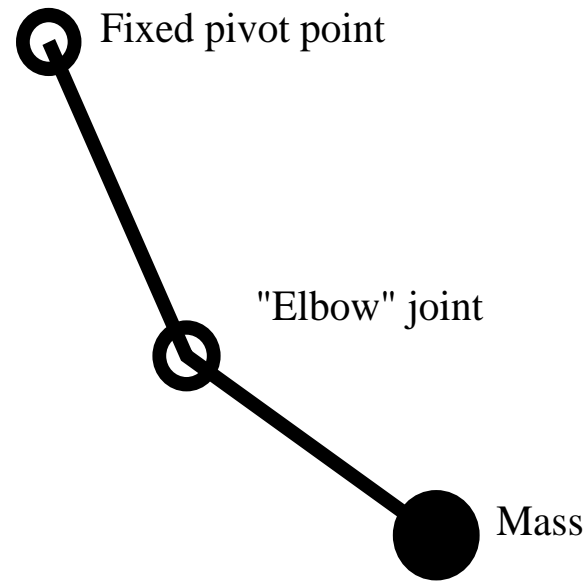
Some Systems Exhibit “Chaos”

- “Sensitive Dependence on Initial Conditions”

⇒ exponential divergence of nearby trajectories



Example of a Chaotic System: The Double Pendulum



- next: two double-pendula start at **almost** same position
- observe divergence

Numerical Solution of Ordinary Differential Equations

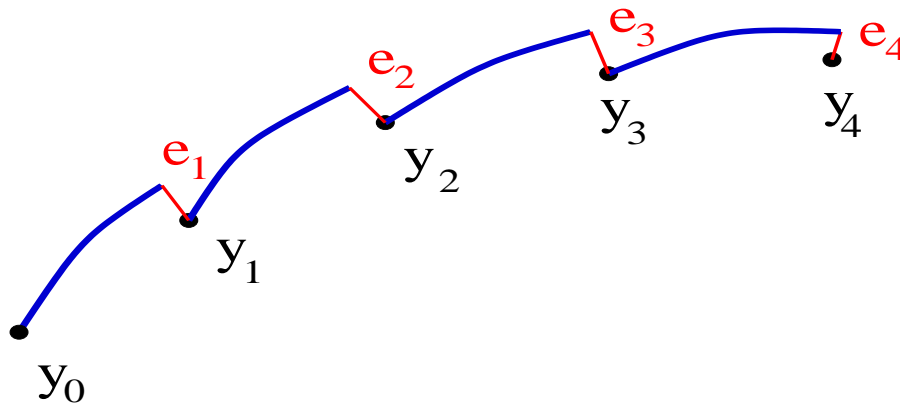
Definition: $\varphi_h(\mathbf{y})$ is the “time- h ” solution operator

– tells us **exactly** where \mathbf{y} will be h time units in the future

- numerical method $\tilde{\varphi}$ **approximates** solution at time $t + h$

$$\mathbf{y}_{i+1} = \tilde{\varphi}(\mathbf{y}_i) \approx \varphi_h(\mathbf{y}_i)$$

- produces discrete, approximate (“**noisy**”) solution $\{\mathbf{y}_0, \mathbf{y}_1, \dots, \mathbf{y}_S\}$

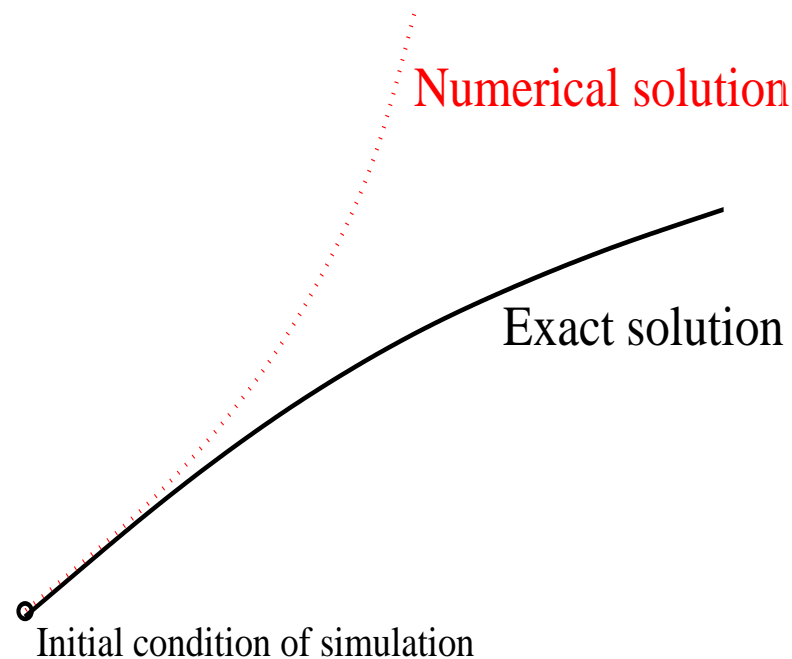


- assume one-step error $\mathbf{e}_i = \mathbf{y}_i - \varphi_h(\mathbf{y}_{i-1})$ is small

Problem: Exponential Divergence of Simulated and Exact Trajectories

- numerical simulation injects small errors *e.g.*, roundoff error, numerical integration error

⇒ numerical trajectory diverges from the exact trajectory (**rosette**)



The Dilemma of Chaotic System Simulation

FACT: the numerical solution diverges exponentially away from the exact solution starting at the same initial condition.

QUESTIONS

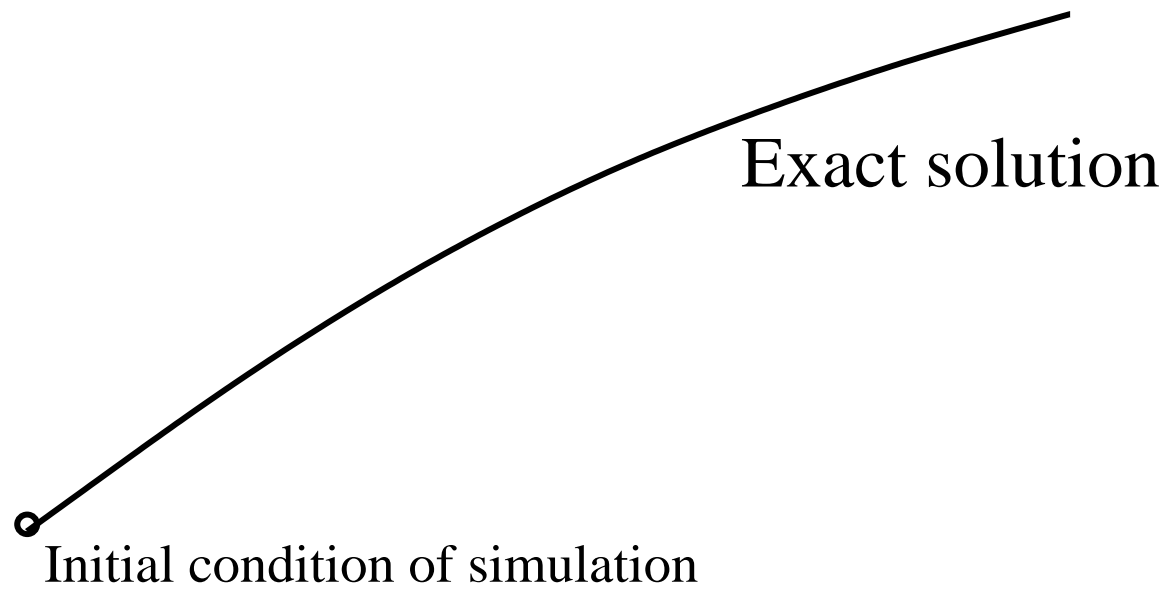
- How reliable is such a numerical solution?
- What does “reliability” **mean** when simulation diverges so far from true?
- Are numerical solutions just magnified noise?

Maybe it's not so bad...

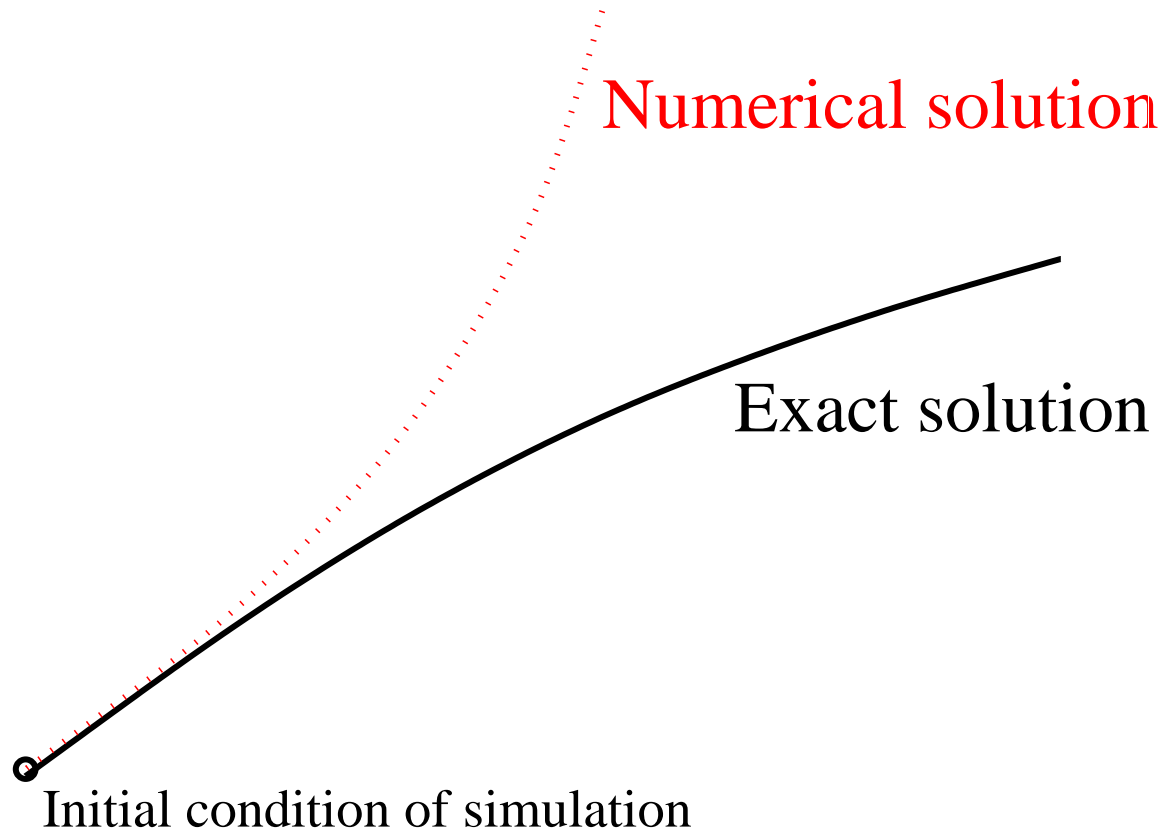
Observation: physicists are usually interested in *the nature of trajectories*, not a particular trajectory

- eg., maybe triple star systems are unstable
- exact init. conds. not important
- randomly sample init. conds. to observe dynamics
- happy if numerical solution follows **any** exact solution
- if exact solution exists, called a **shadow**

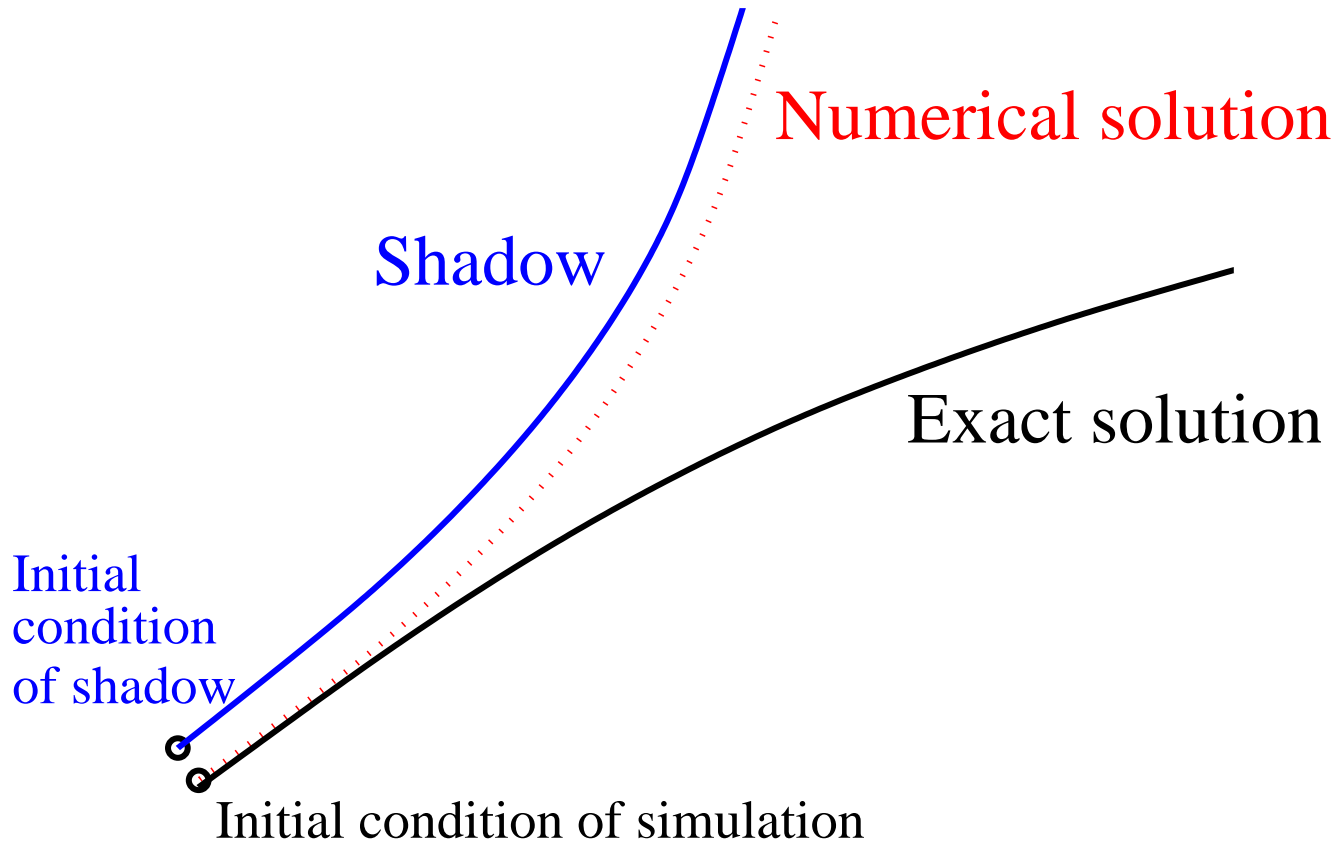
Recap: The exact solution goes one way...



Recap: The numerical (“noisy”) solution goes another...

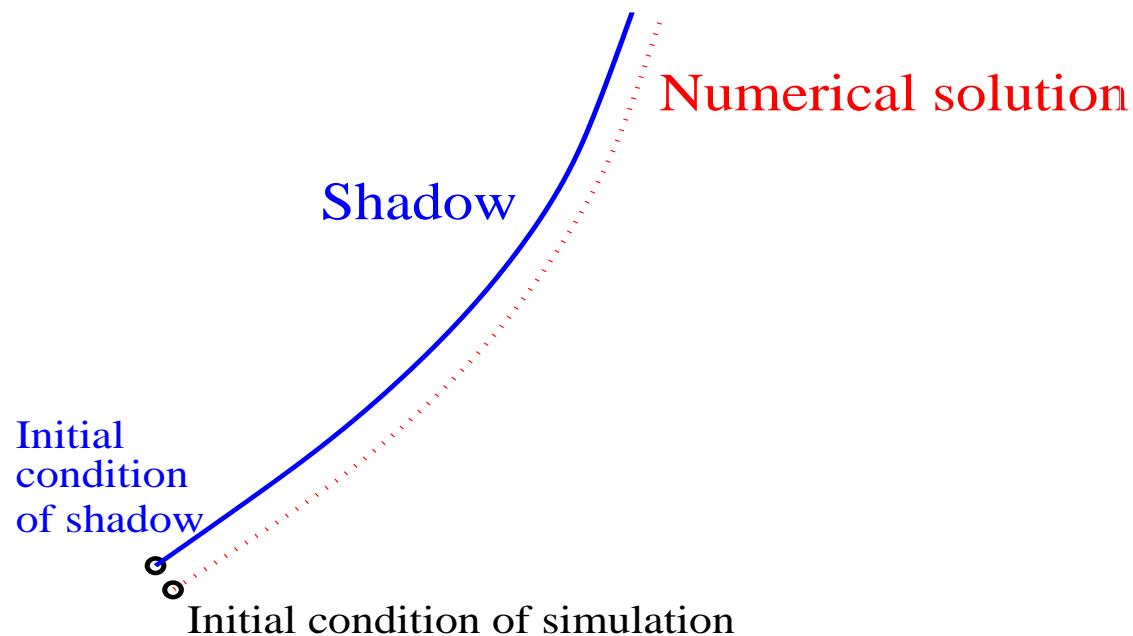


Recap: but a nearby exact solution may exist, called a **shadow**



The Meaning of Shadowing

- existence of a shadow is a **strong** property
- noisy solution is **experimental observation** of exact trajectory
- distance to shadow is “observational error”
- within observational error, observed dynamics are real



Previous Work

For iterated maps (*i.e.*, discrete time)

- Grebogi, Hammel, Yorke & Sauer 1988, 1990
 - refinement (like Newton's Method) + containment
- Rigorous refinement (Sauer & Yorke 1991)
 - prove convergence of refinement
- Proofs by fixed-point iteration (Chow & Palmer 1992)

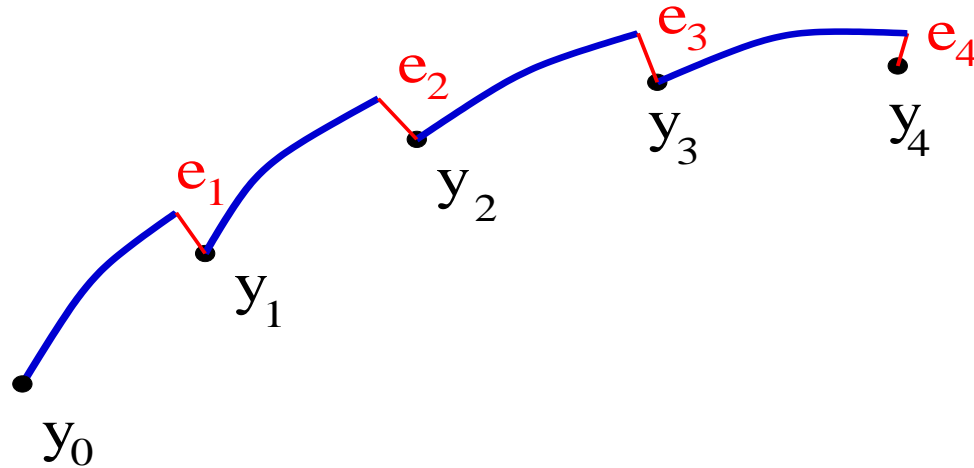
For ODEs (continuous time):

- Rigorous fixed-point method (Coomes, Koçak, Palmer 1994, 1995)
- Non-rigorous Newton's method (Van Vleck 1995)

Existence of periodic orbits from approximately periodic ones:

- Coomes, Koçak & Palmer (1994, 1997) (rigorous)
- Van Vleck (1995) (non-rigorous)

Finding Shadows: Refinement



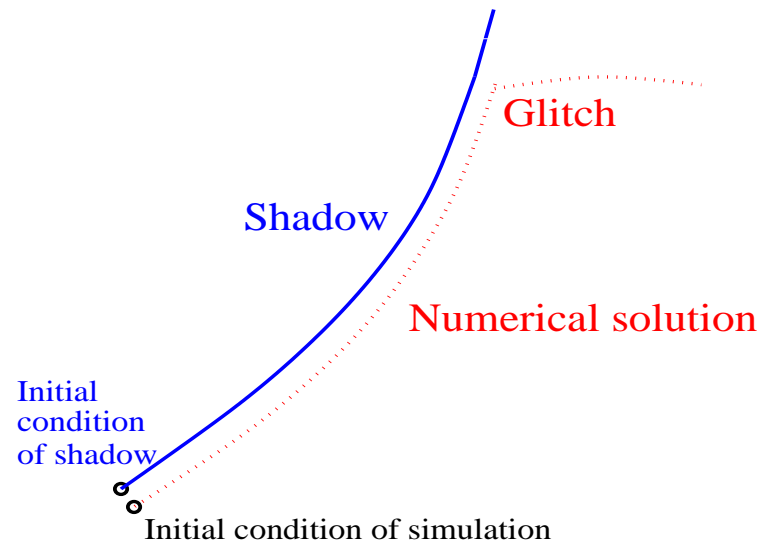
- $\mathbf{Y} = \{y_0, y_1, y_2, \dots, y_n\}$ = entire discrete trajectory
- $\mathbf{E} = \{e_1, e_2, \dots, e_n\}$ = sequence of local errors
- let $g(\mathbf{Y}) = \mathbf{E}$
- Newton's method applied to g drives errors to zero
- trajectory with zero error is exact \Rightarrow shadow of \mathbf{Y}

Discussion of Refinement

- shadows don't always exist

⇒ iteration doesn't always converge

- to find longest shadow length L starting from y_0
 - refine longer-and-longer segments
- end of longest shadow defines a “glitch”



The Gravitational N -body problem

- N particles moving under mutual gravitational forces
- particle i has mass m_i
- distance between two particles is r_{ij} , direction $\bar{\mathbf{r}}_{ij}$
- total force on particle i is

$$\mathbf{F}_i = - \sum_{j \neq i} G \frac{m_i m_j}{r_{ij}^2} \bar{\mathbf{r}}_{ij}.$$

Why the N -body Problem?

“The gravitational N -body problem is a simple problem that remains fascinating and incompletely understood after three centuries of intense study by generations of illustrious physicists and mathematicians including Laplace, Lagrange, Gauss and Poincaré. It inspired the modern subjects of nonlinear dynamics and chaos theory, and remains one of the oldest unsolved problems in physics.”

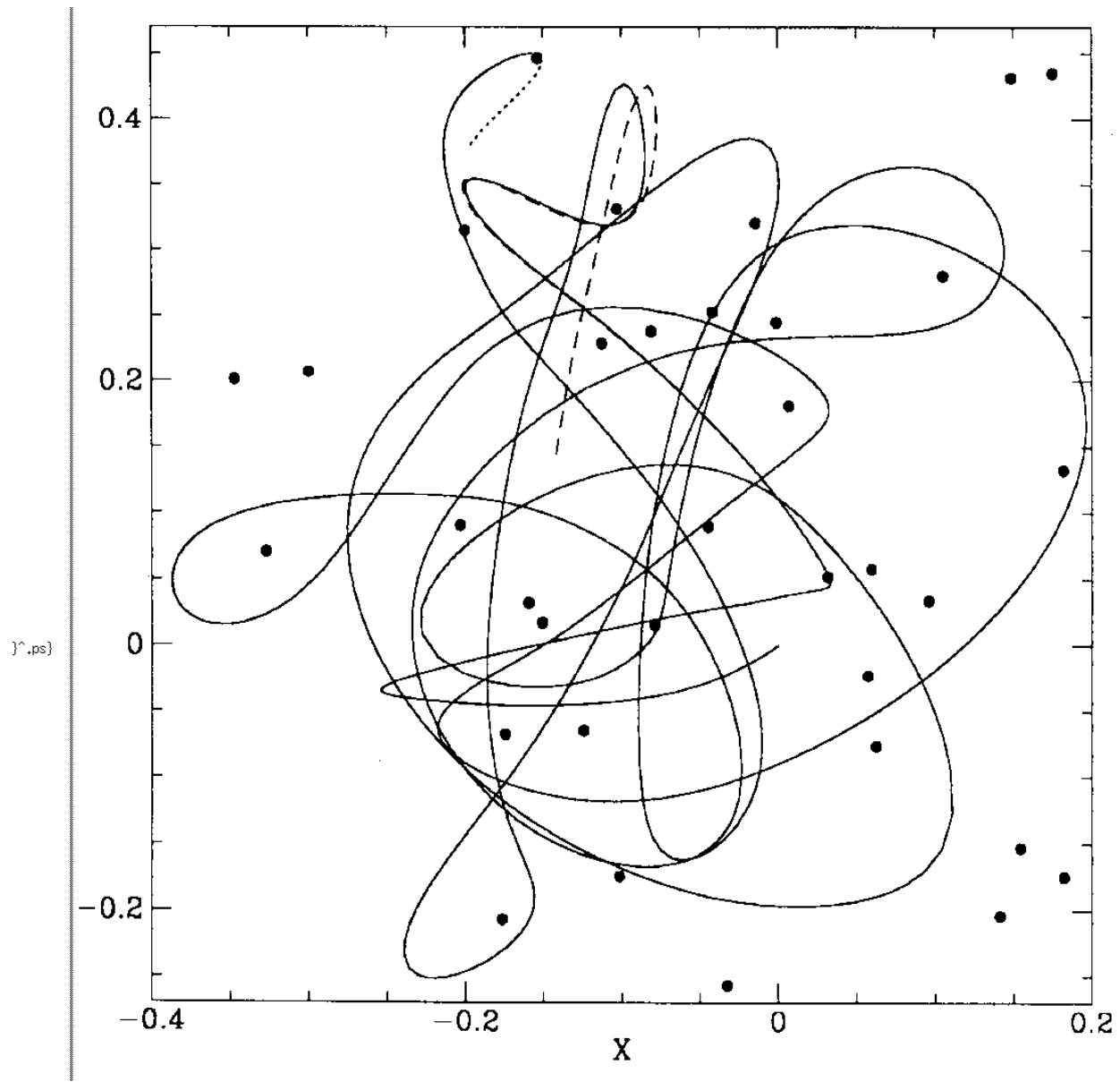
– Scott Tremaine

Shadowing the N -body Pinball Machine

Quinlan & Tremaine (1992) (hereafter called QT)

- shadowing N -body problem is expensive: $O(SN^3)$
 - N = number of particles
 - S = number of steps in trajectory

⇒ shadowed one particle moving amongst 99 fixed particles



Shadowing the N -body Pinball Machine

Quinlan & Tremaine (1992) (continued...)

- particle could be shadowed for a few tens of “crossing times”
- more accurate simulation \Rightarrow closer, longer shadows
- allowing more than one particle to move was too expensive

More Moving Particles (*beginning of my contribution*)

- single particle pinball is not very realistic
- how does shadow length scale as more particles move?
- first, must make algorithm **MUCH** faster!
 - added several heuristics to QT refinement algorithm
 - ⇒ speedup factor of 100 for one-particle systems
 - software provides API to shadow any ODE system
- now allow M particles out of 100 to move, for $M = 1, \dots, 35$
- **Result**: average shadow length scales as $1/M$ — **bad news!**
(Hayes, *Physics Review Letters* 2003)
- $1/M$ scaling is not surprising in retrospect

But is this the right way to think about it?

Crash Course in Galactic Dynamics

Fact 1: Even modest sized galaxy contains about 10^{11} stars

Fact 2: Stars are *extremely* far away from each other.

(Proof: compare day + night sky on Earth.)

Consequence: Galaxies are strictly “collisionless”:

- stars remain far apart
- motion is governed *entirely* by “global galactic potential”
- no star has strong influence on any other
- trajectories are virtually independent in the global potential

Trajectories of individual stars are virtually independent ...

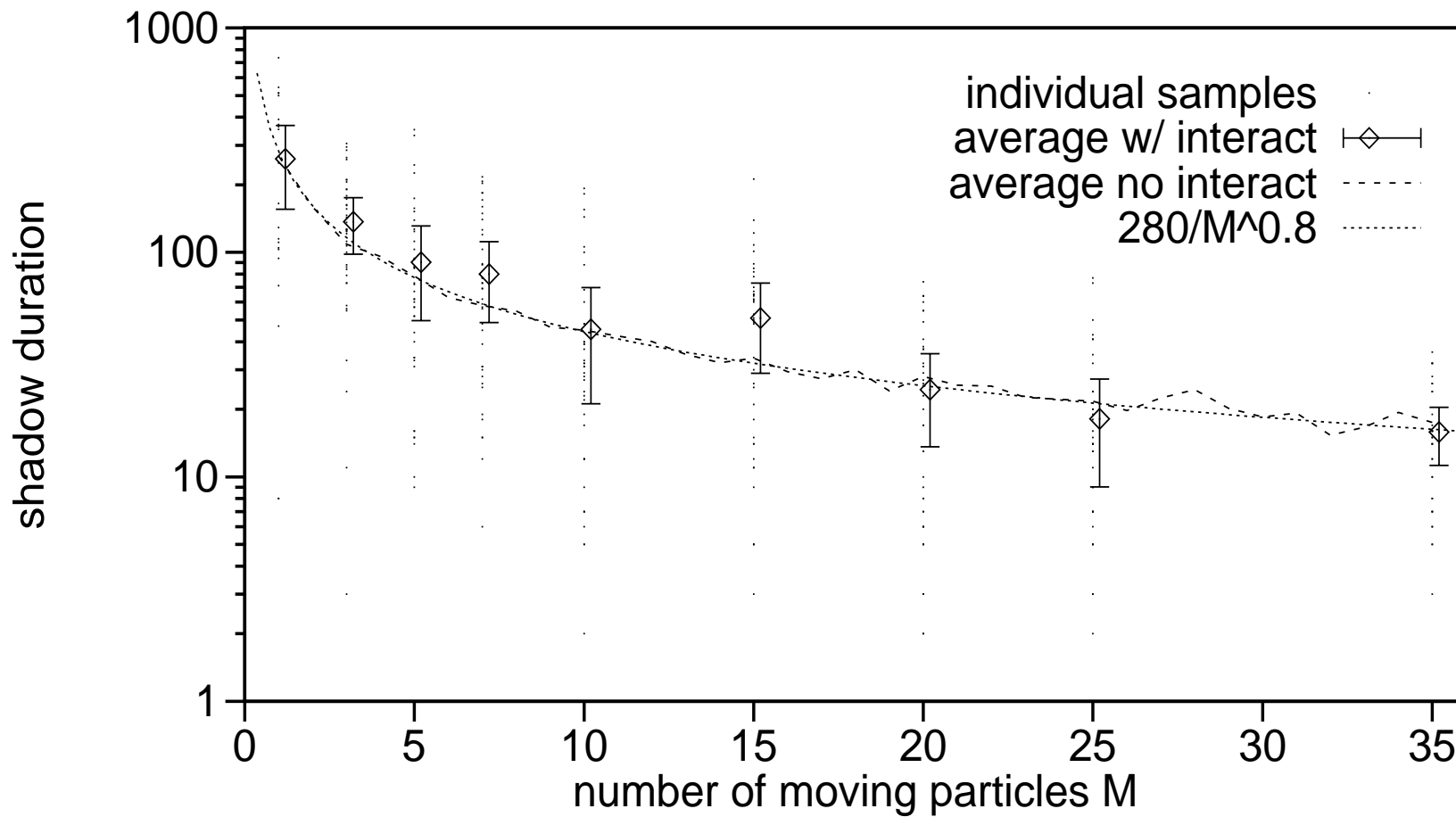
So if **one** simulated star encounters a glitch...

its errant motion has negligible impact on motion of other stars.

PREDICTION:

- particles encounter glitches independently of one another
- ⇒ shadow lengths independent of whether moving particles interact or not

N -body pinball with multiple moving particles



Shadow durations are unchanged whether or not moving particles interact.

Implications for large N -body simulations

Consider:

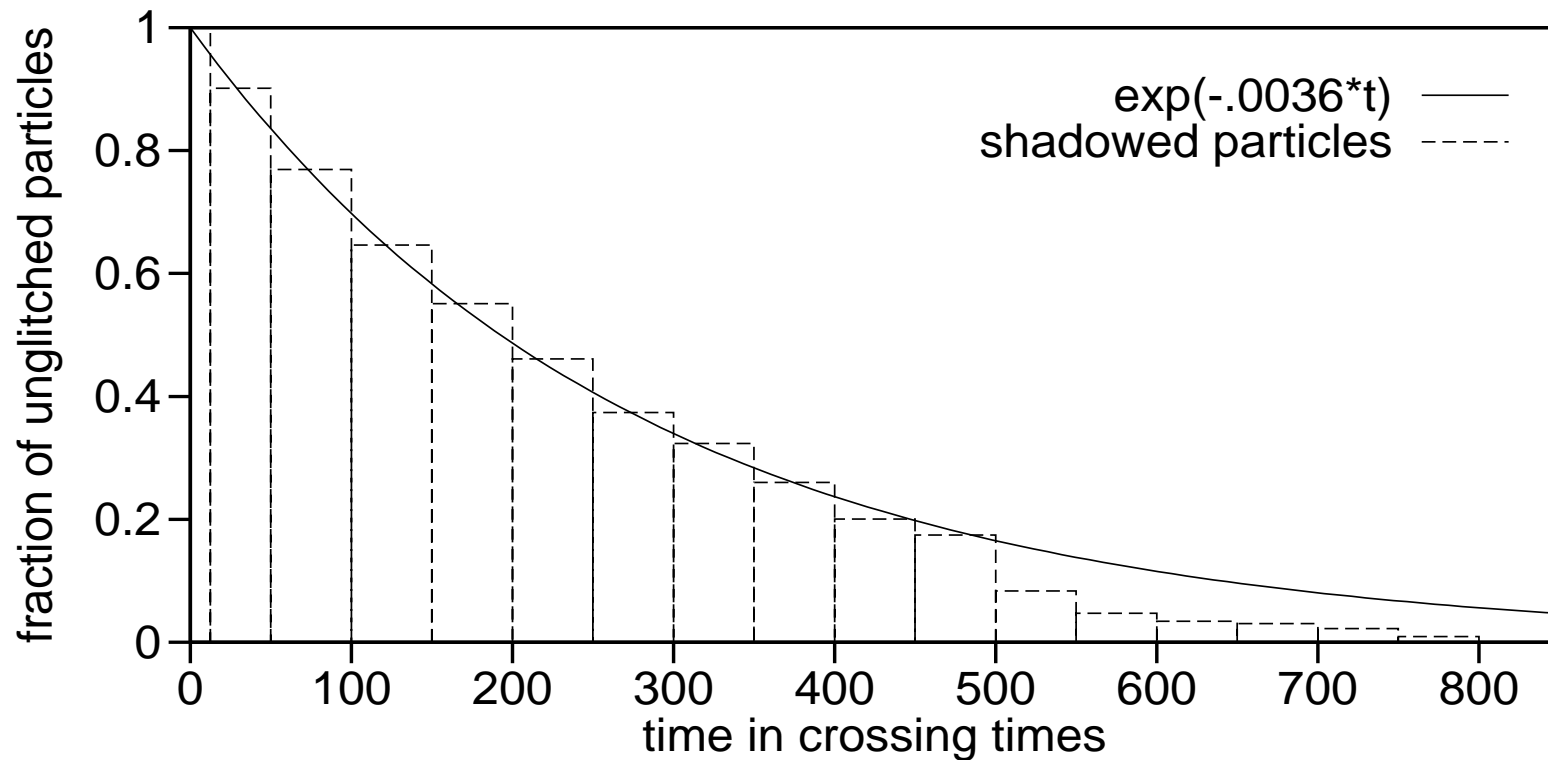
- particles encounter glitches independently of one another
- early in simulation, number of glitched particles is small
- individual stars have little influence on galactic potential

⇒ early in simulation, global potential is substantially valid

⇒ “unglitched” particles remain on valid trajectories

⇒ How many unglitched particles remain, as a function of time?

Fraction of unglitched particles vs. time.
for an N -body simulation of typical accuracy



Note: Milky Way Galaxy is only about 100 crossing times old.
[Hayes, Phys. Rev. Letters (2003)]

Crash Course in Galaxy Simulation

- real galaxies have $\sim 10^{11}$ stars or more
- simulations use far fewer particles ($N = 10^8$ is typical today)

⇒ gravitational potential must be artificially “softened” using

$$F = G \frac{m_1 m_2}{r^2 + \varepsilon^2},$$

where $\varepsilon \approx$ average inter-particle distance

- faster computer ⇒ use bigger N , smaller ε

Question: how to scale these parameters to maintain shadowing?

A scaling that keeps “shadowing accuracy” constant

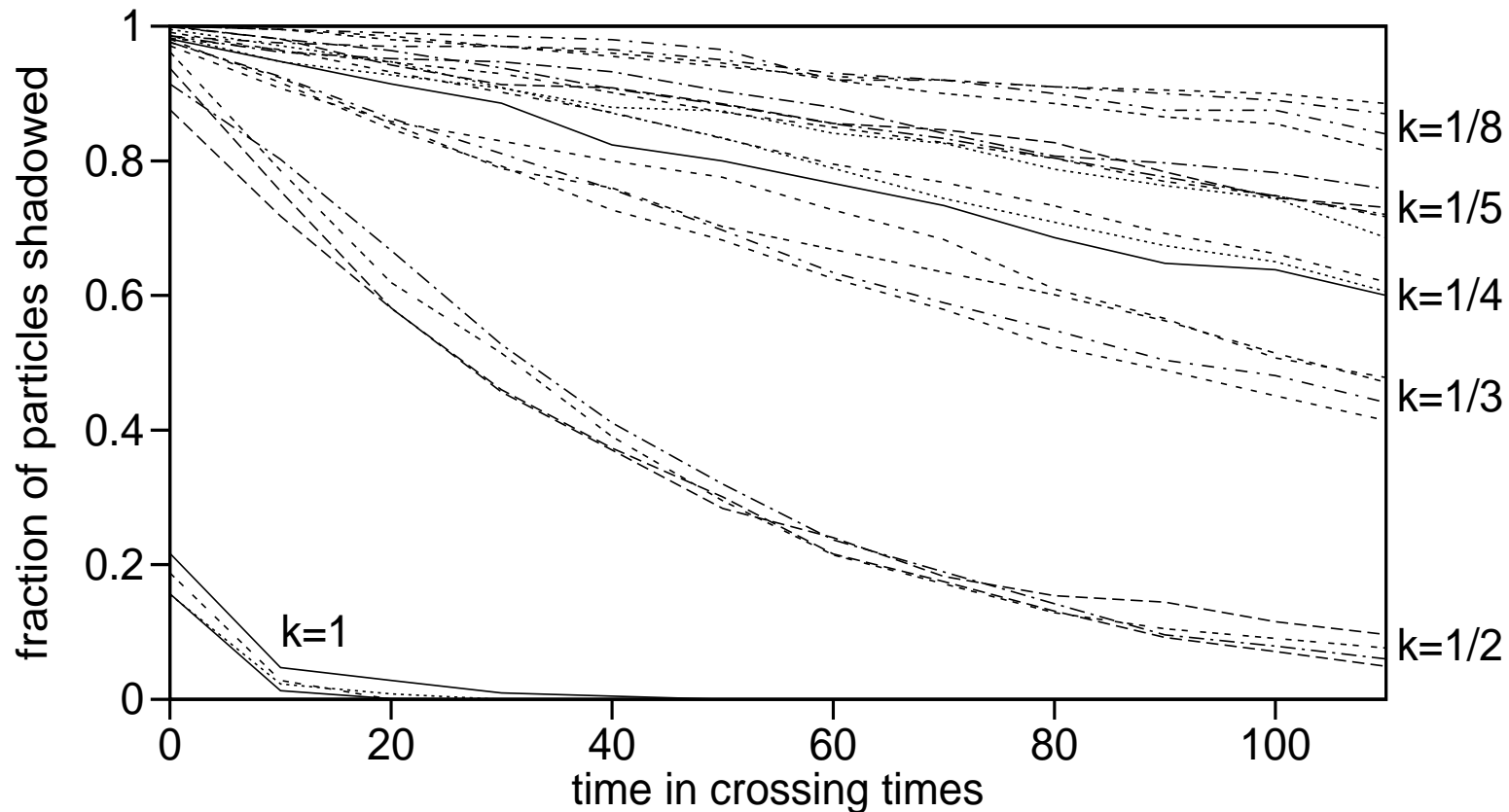
Answer (Hayes, *Astrophysical Journal Letters* 2003):

Scale parameters as

$$h^2 = k^2 \varepsilon^2 N^{1/3} \quad (1)$$

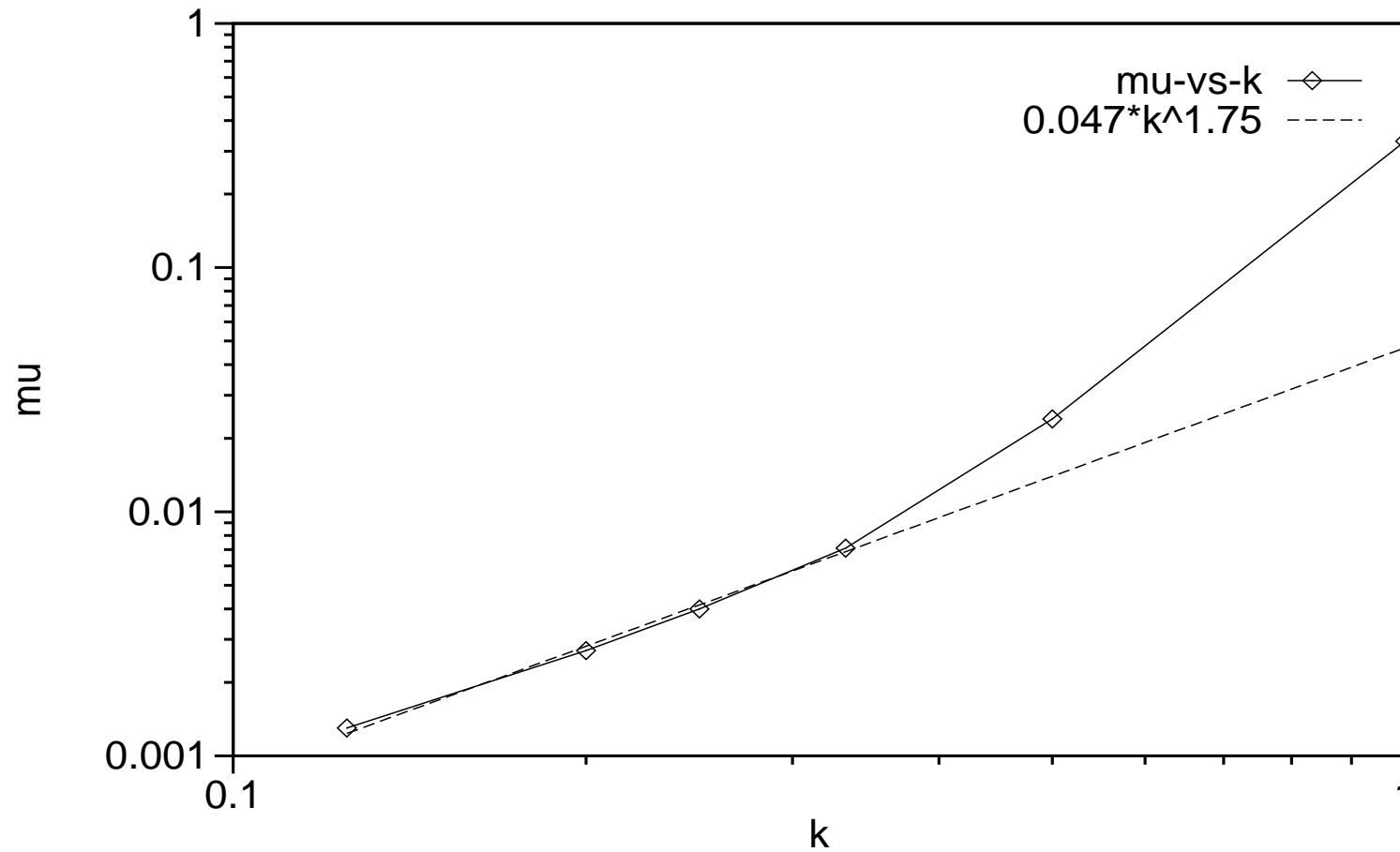
- ε is gravitational “softening” parameter
- N is number of simulated particles
- h = integration timestep (using “leapfrog” integrator)
- k = “shadowing accuracy parameter”
- smaller k gives smaller $h \Rightarrow$ more accurate simulation

Fraction of unglitched particles vs. time for various k



Each cluster of lines depicts a given accuracy parameter k .
A given cluster has various N, ϵ, h scaled via (1) for fixed k .
For a given k , lines fit curves $F(t) = e^{-\mu t}$. (24,000 CPU hours)

Fitting decay constant μ to accuracy parameter k



Fit for $k \lesssim 1/3$ ($> 50\%$ shadowed) [Hayes, *Astrophys. J. Letters* (2003)]

A practical timestep criterion for galaxy simulations

To choose the timestep h for a given simulation:

- given # particles N , total simulation time T and softening ε
- choose F =desired fraction of unglitched particles at T
- solve for corresponding decay constant μ in $F = e^{-\mu T}$
- solve for required accuracy parameter k in $\mu = 0.047k^{1.75}$
- solve for required timestep h in Eq. (1),

$$h^2 = k^2 \varepsilon^2 N^{1/3}$$

Then sit back and enjoy the show.

Galaxy cluster simulation afterwards

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- John Pryce (Royal Military College, U.K.) [proving theorems]

References to some of Wayne Hayes's work

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All references can be found on my webpage

www.cs.toronto.edu/~wayne