Shadowing the Gravitational N-body Problem

Ph.D. Research Proposal of Wayne Hayes

Abstract

This document outlines my proposed direction of research for my Ph.D., including the specific problems I'd like to solve and how I intend to attempt solving them. It will explain my ideas about rigorous shadowing, how shadowing relates to Boundary Value Problems, and how I intend to apply these ideas to shadowing the gravitational N-body problem. In summary, the main ideas are:

- study the variational equation of the N-body problem to determine if/when it has exponential dichotomy, and if not, if there are ways to get around this (*eg.,* using least-squares fits on the nonhyperbolic directions)
- rigorous shadowing, using interval integration & my new containment algorithm, including accounting for short-time non-hyperbolicity.

Some secondary ideas are:

- if the variational equation has dichotomy, then study if particular integrators produce more or less shadowable trajectories. Clearly bounded energy error is necessary for "long" integrations, so symplectic or energy conserving integrators may be needed, but for shorter integrations any "good" integrator may suffice.
- my cheap implemenation of the rescaling of time has not significantly inreased the reliability of my algorithm in finding shadows; in fact it has been *less* reliable in many cases. I may need to try rescaling time exactly as described by other authors.
- collisionless systems are easier to shadow than collisional ones. I would like to extend my existing collisionless shadowing experiments to larger N. To do it, I will need to implement even faster shadowing algorithms than I presently have. This can include parallelism (*eg.,* using PVM) and the $O(D^3M)$ (as opposed to $O((DM)^3)$) optimization discussed in my M.Sc. thesis.

Note: my Qualifying Depth Paper, in case you don't have a copy handy, can be browsed on the Web at "http://www.cs.utoronto.ca/~wayne/research/thesis/depth/". My M.Sc. thesis is nearby, at "...thesis/msc/". They will be referred to occasionally in this paper.

1 Introduction

A true trajectory of a dynamical system lying close to a numerical trajectory is called a *shadow*. A trajectory $y(t)$ is called *hyperbolic* if the solution of the variational equation along $y(t)$ has an *exponential dichotomy* (Palmer 1988; Chow & Van Vleck 1994). Let $R(t,s)$, called the "resolvent", be the solution of the variational equation along $y(t)$. Then $R(t,s)$ has an exponential dichotomy if, for any given s there exists a constant matrix $P(s)$ and constants K and λ such that $P(s)$ projects into the contracting subspace at time s:

$$
\begin{aligned}
||R(t,s)P(s)|| \leq & \quad Ke^{-\lambda(t-s)} \quad \text{if } t > s, \\
||R(t,s)(I-P(s))|| \leq & \quad Ke^{-\lambda(s-t)} \quad \text{if } t < s.
\end{aligned}
$$

It has a *regular dichotomy* if $\lambda = 0$. A system in which all true trajectories are hyperbolic I will term *globally hyperbolic*, and numerical trajectories in such systems with small, bounded local error always have shadows (Anosov 1967; Bowen 1975). Systems which are not globally hyperbolic, but in which some trajectories are hyperbolic for long periods of time, may still have shadows. The gravitational N-body problem is sometimes such a system. After much meandering in topics, I have come to realize that my main interest is to quantify the word "sometimes" in the previous sentence: to be able to pinpoint precisely why shadowing sometimes fails in N-body systems while at other times it is successful. In order to do this, I need to understand various ways in which shadows can be found, and then apply these concepts specifically to N-body trajectories. The intended end product of this research would be to understand what causes glitches in N-body systems well enough to be able to predict when they will occur without having actually to perform a shadow search; in the words of one committee member, "to be able to look at a phase portrait and be able to point at a particular spot and say 'a glitch will occur *here*.' "

2 Exponential Dichotomies and Boundary Value Problems

It is my belief that the best way to go about studying the properties of shadows of numerical N-body trajectories is to study the behaviour of the variational equation of the N-body problem under various conditions, to determine when it does and does not have an exponential dichotomy. Ascher, Mattheij, and Russel (1988, p.124) state that a boundary value problem is well-conditioned *if and only if* it has a dichotomy (regular or exponential).

The relation between shadowing and boundary value problems has been partly worked out, but not fully. Palmer (1988) deals with shadowing (semi-)infinite periodic trajectories. Let y_n be a noisy trajectory, $n = 0, ..\infty$. We wish to find z_n such that $x_n = y_n + z_n$ is a true trajectory. If $x_{n+1} = f(x_n)$ is the exact map between points on the trajectory (*i.e., f* advances the solution by one timestep) then it can be shown (Palmer 1988) that $\{z_n\}$ is a solution of

$$z_{n+1} = R(t_{n+1}, t_n) z_n - e_{n+1} + g_n(z_n),$$

$$e_{n+1} = y_{n+1} - f(y_n), \text{ the one-step error,}$$

$$g_n(z) = f(y_n + z) - f(y_n) - R(t_{n+1}, t_n) z.$$

Note $g_n(z)$ is the $O(|z|^2)$ term that we usually ignore when implementing shadowing as an iterative Newton-type method. If, instead of being (semi-)infinite, the trajectory is of finite length, then the appropriate boundary conditions (*eg.,* Grebogi *et al.* , Quinlan & Tremaine) seem to be to "pin" the growing components at the right endpoint, and the decaying components at the left endpoint. Formulating these boundary conditions precisely, in the standard language of BVP literature, appears to be easy. Using $P(s)$ as defined above, we want to say

$$P(0)z(0) = (I - P(T))z(T) = 0,$$

where 0 and T are the left and right endpoints of integration, respectively. One of the tasks I am working on currently is to precisely formulate shadowing as a BVP in such a way that current "off-the-shelf" BVP software can handle it. It will be interesting to see how well such BVP software can find shadows.

Finally, Enright (personal communication) believes that there may be ways to handle directions that are neither expanding nor contracting by treating them in some sort of "least-squares" sense, rather than enforcing boundary conditions on them. This may be an area to explore further if there turn out to be eigenvalues λ of the problem that have $\Re\text{e}(\lambda) \approx 0$.

3 Rigorous Shadowing

Grebogi *et al.* (1990) introduce a rigorous method for proving the existence of a shadow in a two-dimensional system. The *containment* process in two dimensions consists of building a parallelogram M_i around each point $\mathbf{p}_i$ of the numerical trajectory such that two sides $E_i^{1,2}$ are parallel to the expanding direction, while the other two sides $C_i^{1,2}$ are parallel to the contracting direction. In order to prove the existence of a shadow, the image of M_i under $f(\cdot)$ must map over M_{i+1} such that $f(M_i)$ makes a "plus sign" with M_{i+1} (Figure 1).

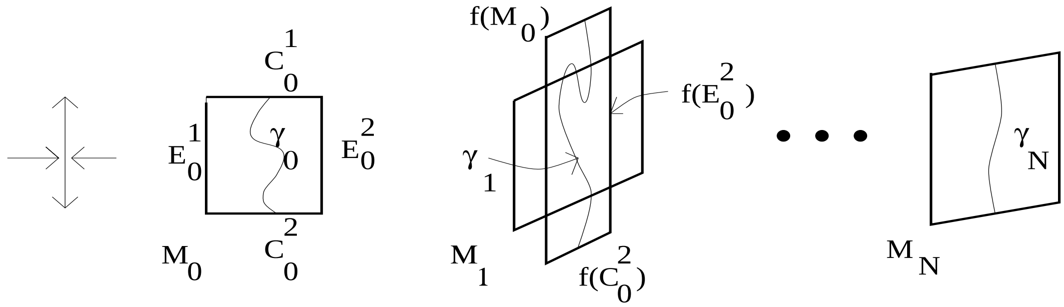

Figure 1: Containment in 2 dimensions, reproduced from Grebogi *et al.*

$$f(E_i^k) \cap C_{i+1}^j \neq \emptyset, \quad j,k = 1,2, \qquad \text{and} \qquad f(C_i^j) \cap E_{i+1}^k = \emptyset, \quad j,k = 1,2. \tag{1}$$

To ensure this occurs, a bound on the second derivative of f is needed, and the expansion and contraction amounts need to be resolvable by the machine precision. The proof of the existence of a true orbit then relies on the following argument. Draw a curve γ_0 in M_0 from one contracting edge to the other, *i.e.,* roughly parallel with the expanding direction. Its image $f(\gamma_0)$ is then stretched such that there is a section of $f(\gamma_0)$ lying wholly within M_1, and in particular $f(\gamma_0)$ leaves M_1 through the contracting sides at both ends. Let γ_1 be the section of $f(\gamma_0)$ lying wholly within M_1. Now look at $f(\gamma_1)$ in M_2. Repeat this process along the orbit, producing γ_N lying wholly within the final parallelogram M_N. Then any point lying along γ_N, traced backwards, represents a true trajectory that stays within M_i, $\ i = N, N-1, \ldots, 1, 0$, and we are done.

The process just described is not directly applicable to systems with more than 2 dimensions, and Grebogi *et al.* provide no argument for how it could be extended beyond 2 dimensions. It turns out, however, not to be too difficult. I will describe the solution in 3 dimensions; the extension to dimensions beyond 3 will then be obvious. With 3 dimensions, there are two cases:

(i) 1 expanding direction, and 2 contracting (Figure 2). Assume that the z direction is expanding, while the x and y directions are contracting. (We assume, for simplicity of exposition and for ease of drawing, that these three directions are roughly orthogonal, although in practice they need only be resolvable from each other.) Then, analogous to the 2 dimensional argument, we draw *cubes* M_i around the noisy points $\mathbf{p}_i$, and require that $f(M_i)$ maps over M_{i+1} so that M_i stretches into a long, thin tube, a length of which lies wholly in M_{i+1}. Then, precisely as in

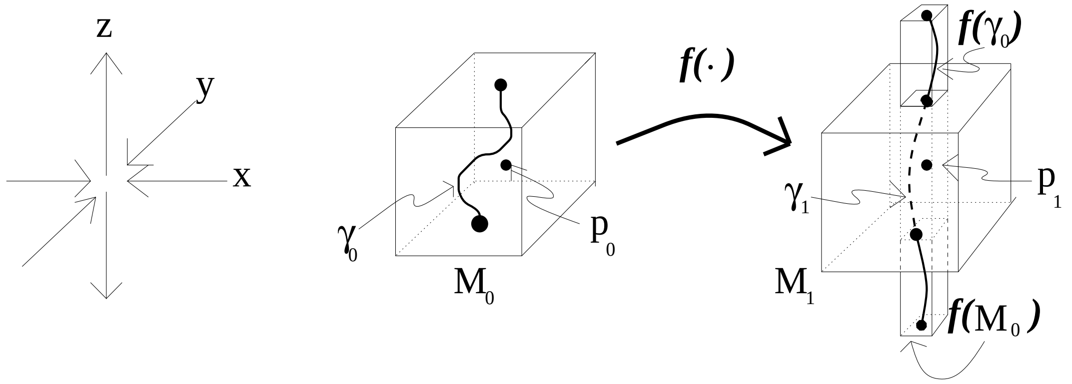

Figure 2: Containment in 3D, case (i): 2 contracting and 1 expanding direction.

the 2-dimensional case, we introduce a curve γ_i that runs approximately along the expanding (vertical) direction from any point on the top contracting side of M_i to its bottom contracting side. Note that γ_i is stretched along the direction in which it has extent (vertically), and is "compressed" in the directions in which it has measure zero (both horizontal directions). If $f(M_i)$ maps over M_{i+1} as in the Figure, then we are guaranteed that a contiguous section of $f(\gamma_i)$ lies inside M_{i+1}, connecting its top and bottom contracting sides along the expanding direction. This becomes γ_{i+1}, and by induction γ_N lies inside M_N, and any point on it can be traced backwards to lie inside every M_i back to M_0, and we are done.

It seems clear to me that the same simple topological argument can be applied to a system of arbitrary dimension, as long as there is only one expanding direction.

(ii) 2 expanding and 1 contracting direction (Figure 3). Assume now that the z (vertical) direction is contracting, while the x and y directions are expanding. We again draw a cube M_i around each noisy point $\mathbf{p}_i$, except now $f(M_i)$ maps over M_{i+1} so that M_i is flattened into a thin slice, cutting M_{i+1} into 3 pieces, the middle piece of which contains a contiguous section of $f(M_i)$. Now, γ_i must be a *surface*, whose boundary connects all the expanding sides, so that under the mapping, $f(\gamma_i)$ is stretched in all the directions it has extent (both horizontal directions), and is "compressed" along the direction it has measure zero (vertical). Then, we are guaranteed that there is a contiguous segment of $f(\gamma_i)$ lying wholly in M_{i+1} and connecting all of its

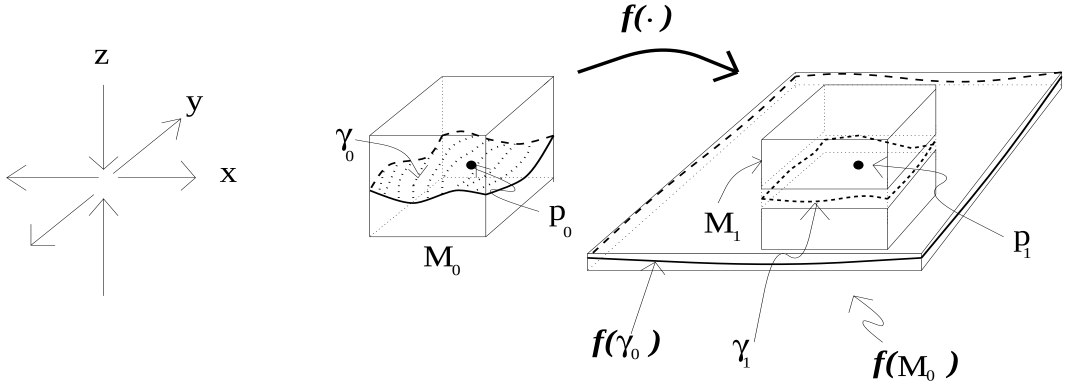

Figure 3: Containment in 3D, case (ii): 1 contracting and 2 expanding directions.

expanding sides. We call this surface γ_{i+1}, and by induction γ_N lies wholly within M_N, and any point on γ_N, traced backwards, always lies within M_i all the way back to M_0.

It seems clear to me that, in the above argument, we can replace "cube" with "hypercube", "surface" with "manifold", and the argument still applies in arbitrarily high dimensions. The crucial point is that γ must have dimension equal to the number of expanding directions, and its border must connect each side of the hypercube that contains a vector parallel to a contracting direction.

Formalizing this argument, especially for dimensions greater than 3, will be part of the thesis.

To rigorously prove that the map satisfies the necessary hyperbolicity criteria at each iteration, interval arithmetic and ODE enclosure methods will be used (*eg.,* Nedialkov).

3.1 Applying containment to non-hyperbolic trajectories

The above arguments can be applied only if the trajectory is hyperbolic at every step. Chow & Palmer (1991; 1992) note that shadowing may still be possible if the trajectory is not hyperbolic at every step, but is hyperbolic in the long run. Assume that the nominal "expanding direction" actually contracts for a few steps, or the nominal "contracting direction" actually expands for awhile. Then, assume that after no more than p steps, the cumulative expansion along the nominal expanding direction is eventually greater than 1, and the cumulative contraction along the nominal contracting direction is eventually less than 1. Then we can apply the above containment argument to the map $f^p(\cdot)$.

4 Integrators

The question of hyperbolicity can be studied independently of the integration scheme used to produce the numerical trajectory. In fact, for the problems I have studied so far (100 particles for about 100 crossing times), I have not seen any difference in shadow lengths between high-order but non-symplectic integrators, and leapfrog (a low-order symplectic integrator). However, for very long integrations of conservative systems we also expect that a numerical trajectory requires bounded global (not just local) energy error in order to have a shadow. If time warrants, and if there is evidence that longer shadows could be found, I may study the influence of various integrators, *eg.,* symplectic ones, on shadow length.

5 Rescaling of time in N-body shadowing

Despite my enthusiasm displayed in my Depth paper for the rescaling of time, my initial numerical implementation has not significantly improved shadow lengths. In fact, in many cases it has proven *less* effective in finding long shadows than the "map method". I cannot explain this, so there are several possibilities for how I can proceed: (i) ignore the rescaling of time; (ii) try to figure out why my implementation doesn't work; (iii) implement it exactly the way somebody else has done it (*eg.,* Van Vleck 1995; Coomes, Koçak, Palmer 1994, 1995). Assuming I can get this to work, there is the possibility of rescaling the time of each particle individually, since different particles can have different time errors, depending mostly upon whether or not the particle is currently undergoing a collision. However, I believe this should be given lower priority than studying exponential dichotomies, BVPs, and high-dimensional containment.

6 Shadowing Collisionless systems

Recall that the gravitational force between simulated particles i and j is

$$F = \frac{Gm_i m_j}{r_{ij}^2 + \varepsilon^2},$$

where ε is the "softening" parameter, designed to artificially smoothen the gravitational potential.

Figure 4 displays the average shadow lengths of 3 types of systems: (i) unsoftened potential with a total of $100M$ particles, M of which move; (ii) unsoftened potential with a total of 100 particles, M of which move; (iii) softened potential (ε = average inter-particle spacing) with a total of 100 particles, M of which move. It is clear that the softened systems are more readily shadowed than the unsoftened ones. In fact, the average shadow length of the unsoftened 100-particle systems are roughly proportional to $1/M^2$. If it turns out that this result is real, and not an artifact of a bad implemenation of shadowing, it means that collisional systems are probably not shadowable. On the other hand, Figure 4 seems to indicate that collisionless systems *are* shadowable for very long times—hundreds of crossing times, almost independent of M. Most interestingly, the $100M$ graph (only plotted out to $M = 10$) seems to be bending upwards, as we might expect since even an unsoftened system has a smoother potential as $N = 100M$ gets larger. I would like to extend the $100M$ graph further as part of my thesis. It is almost a no-brainer, except it is *extremely* compute and memory intensive. There is one more optimization (that is *not* a no-brainer) to the numerical shadowing algorithm of my M.Sc. thesis that I would like to implement, which involves attempting

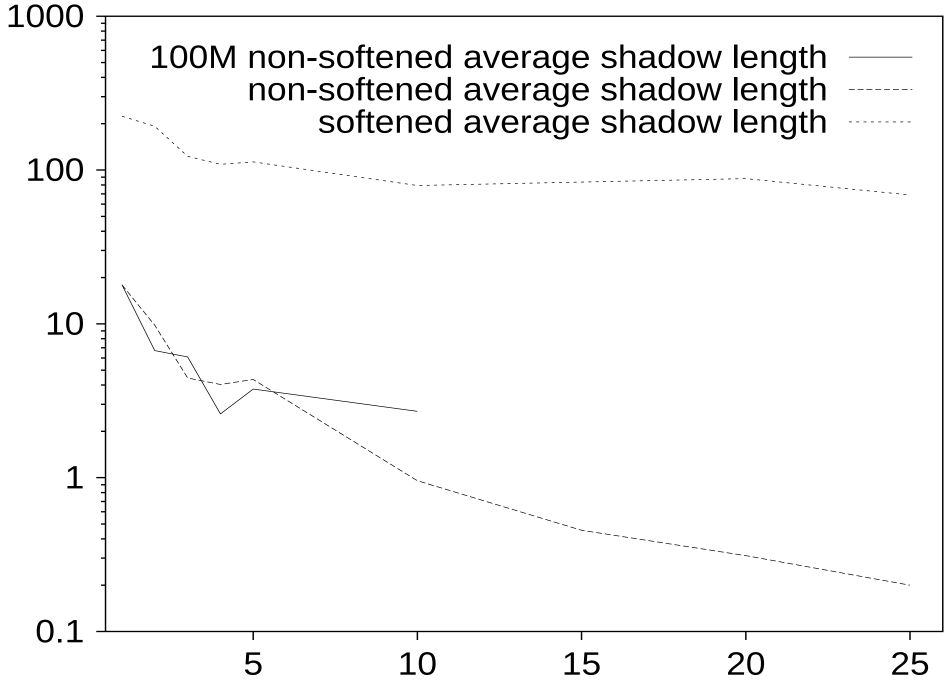

Figure 4: Average shadow lengths, in crossing times, of 3 types of systems as a function of the number of moving particles M. (i) The "$100M$ unsoftened" systems have $100M$ total particles, M of which move—and its graph only goes out to $M = 10$, since it is extremely compute intensive to shadow 10 particles moving amongst 1000. (ii) The "unsoftened" systems have M particles moving out of a fixed total of 100 particles. (iii) The softened systems also have M particles moving out of a total of 100, except the gravitational potential is softened by the average inter-particles distance. Each point on the graph represents the average of between 10 and 50 shadowing runs of trajectories with random initial conditions. More details can be found in Hayes (1995).

to shadow the trajectory of each moving particle *separately*. This gives M variational equations of size D^2 ($D = 6$, the number of phase space dimensions per particle) that would take total time $O(D^3M)$ to solve, rather than one equation of size $(DM)^2$ taking time $O((DM)^3)$ to solve. Thus, each iteration of the numerical shadowing algorithm is asymptotically reduced from $O(M^3)$ time to $O(M)$. However, it is possible that the number of iterations required to converge increases, so it is not clear that there will be a net gain. If there is, however, the "optimization" alone will be a tremendous step forward for shadowing systems with many degrees of freedom.

If this optimization works, it is only a small step to be able to do "fixed-motion shadowing", described in detail in my M.Sc. thesis.

Appendix 1: A conjecture about N-body shadowing

Figure 5 shows two orbits of a single N-body particle moving amongst 99 fixed ones. One orbit has no softening, while the other has softening equal to about the average inter-particle distance. As can be seen, the particle in the softened potential has a much smoother path, compared to the particle in the unsoftened potential. In particular, the motion of the particle in the softened potential is significantly more sinusoidal-like, with the centre of the motion centered roughly at the centre of the cluster (which is not shown, but is at roughly (0.5, 0.5)). The orbit of the softened particle can

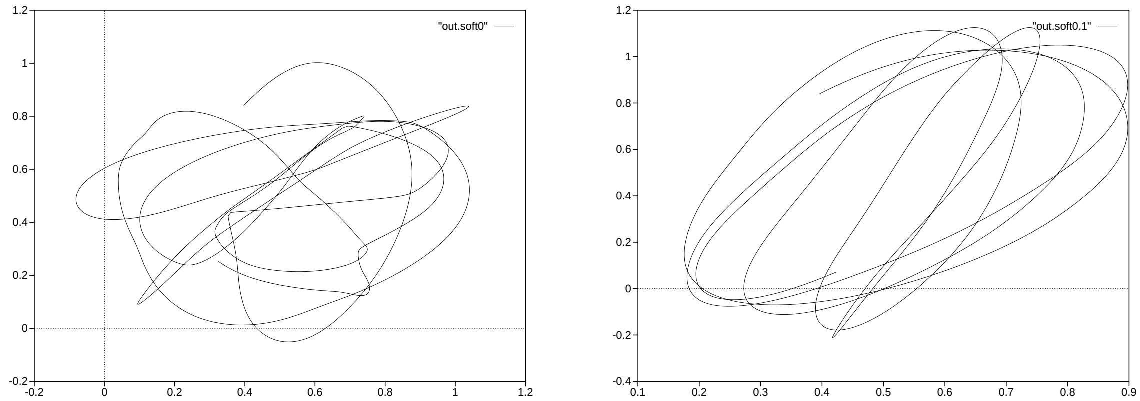

Figure 5: Two N-body orbits: the first in a potential with no softening; the second with softening of 0.1 (about the average inter-particle separation).

be (very roughly) approximated by embedding it in a plane that passes roughly through the centre of the cluster, and whose inclination slowly varies, roughly on the timescale of a crossing time. There is a nice symmetry to such an orbit: there is a well-defined "inward" direction (towards the centre of the cluster), and a well defined "vertical" direction (vertical with respect to the slowly varying plane). If we define a co-ordinate system $\mathcal{T}$ that moves with the particle, with the three axes arranged roughly to be (i) tangential to the trajectory, (ii) "inwards", and (iii) "upwards", then it is plausible that the eigenvectors of the Jacobian along the trajectory, measured in $\mathcal{T}$, will be roughly constant. This means that expanding directions *stay* expanding, contracting directions *stay* contracting, and the trajectory remains hyperbolic for a long time. Conversely, the trajectory of the unsoftened particle has no such well-defined, slowly varying local co-ordinate system, because it frequently and abruptly changes direction, and worse, it frequently and abruptly changes which plane it is orbiting in. So, a direction that is expanding for a short time may suddenly become a contracting one, and vice versa, and there is no guarantee when it will again become contracting, and for how long it will remain so. There seems to be no long-term hyperbolicity. This leads me to the following conjecture:

Conjecture 1 *An N-body trajectory in a bounded system is shadowable, i.e., is hyperbolic for nontrivial lengths of time, if and only if there is a slowly varying local frame, as defined above, for each particle.*

It will be relatively easy to test this conjecture simply by studying the variational equations of various N-body systems. Furthermore, this conjecture seems to make the following predictions:

- glitches occur near close encounters. This has been observed by Quinlan & Tremaine, and by the present author.

- thus, collisional N-body simulations are not shadowable for any appreciable length of time, and the failure to find shadows in collisional systems is not simply a failure of the shadowing algorithm.
- collisionless N-body systems *are* shadowable for appreciable lengths of time.
- long simulations of the Solar System that conserve energy well (using symplectic integrators, for example) should be shadowable, modulo a possible rescaling of time.

Appendix 2: Proposed schedule

I will be working on implementing high-dimensional containment before this summer, in order to present it at the SIAM conference in Toronto in June. Concurrently with this, I will continue studying the relationship between shadowing and boundary value problems, with the assistance of Paul Muir while he is here. I hope to get far enough with these by autumn to be able to make some definitive statements about shadowing N-body systems. For example, I intend to prove rigorously the existence of shadows for systems in which I've already found numerical shadows. If time permits, I may try shadowing of Solar System integrations. If any of these activities prove impossible, unwieldly, or do not lead anywhere (unlikely, in my opinion), then I can resort to the other topics mentioned: studying how shadowability varies as a function of the numerical integration scheme; more studies on the rescaling of time; and the $O(D^3M)$ optimization to my current refinement algorithm.

I aim to finish by December of this year (1998); with luck, this will allow me to *actually* finish by August 1999 (when my funding ends), and I have set for myself an absolute deadline of December 31, 1999. Among the other catastrophes that will be occuring on 1 Jan 2000, I will no longer be able to sleep until noon, because I will no longer be a student.

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