The Complexity of $N$-body Simulation*

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Abstract. The $n$-body simulation problem is stated as follows: Given initial positions and velocities of $n$ particles that have pair-wise force interactions, simulate the movement of these particles so as to determine the positions of the particles at a future time.

In this paper, we give the first known $n$-body simulation algorithms with rigorous proofs of bounded error. The reachability problem is to determine if a specific particle will reach a certain region at some specified target time. In the case we require $\text{poly}(n)$ bits of accuracy and where the target time is $\text{poly}(n)$, our complexity bounds are surprisingly PSPACE.

We also have matching lower bounds for $n$-body simulation problem (in comparison all previous lower bound proofs required either artificial external forces or obstacles). We show that the reachability problem for a set of interacting particles in three dimensions is PSPACE-hard.

1 Introduction

The $n$-body problem, is the problem of simulating a set of $n$ charged particles in three dimensions, where the particles interact under the induced electrostatic or gravitational potential field. Generally the simulations are done by time stepping. See [1, 6, 7, 8, 10] for details. These simulations are one of the heaviest users of super computer cycles (for example at the CRAY-YMP, at RTP, a study by MCNC recent showed that over 30 percent of all compute time was used for $n$-body simulation by molecular chemists), and are widely used by astronomers, chemists, and biochemists, and to a lesser degree physicists (note: certain physicists prefer other methods based on energy minimization).

The equations of motion for each body are in fact given by Newton's second law of motion applied to each body; this results in a system of $n$ ordinary differential equations. These equations can be approximately solved from initial positions and velocities by stepping in time, using the equations of motion and numerical integration to determine approximations to incremental movements and velocity changes of the bodies due to the forces exerted by the other particles. The force vector associated with these potentials is calculated by taking the partial derivatives of the potential in each direction. This is the basis for most computer simulations of $n$-body systems. The main computational task

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is the calculation of the potential field due to all other bodies, at the current location of each body. The naive algorithm for this potential computation requires quadratic work; however, the potential can be approximated to \( p \) bits of accuracy in \( O(np^2 \log p) \) time using the multipole method of Greengard and Rokhlin [4, 5], or by the recent modified multipole method of Reif and Tate [11] that has time complexity \( O(np^2) \).

1.1 The \( n \)-body Reachability Problem

In this paper, we consider the complexity of simulating a set of \( n \) charged particles in three dimensions, where the particles interact under the induced electrostatic potential field.

Throughout this paper, \( n \) denotes the number of bodies. We require that the number of bits of the input description is polynomial in \( n \). A \( k \)-bit rational is a ratio of two \( k \)-bit integers. Consider a set of \( n \) points satisfying a fixed electrostatic potential law. We assume that we are given an initial \( \text{poly}(n) \)-bit rational position and velocity as well as a destination position, given by a ball, where the ball’s position and radius is \( n \)-bit rational. The \( n \)-body reachability problem concerns the trajectories of these bodies; in particular we wish to determine if a given particle reaches a position within the given destination ball within a given time bound, where the ball’s position and radius are \( \text{poly}(n) \)-bit rationals.

We give the first known \( n \)-body simulation algorithms with rigorous proofs of bounded error. In the case we require \( \text{poly}(n) \) bits of accuracy and where the target time is \( \text{poly}(n) \), our complexity bounds are surprisingly PSPACE.

Our algorithm requires the additional assumption that there is at least an exponentially small separation between all pairs of particles at all times during the simulation.

Molecular Computers, Molecular Castles, and Our Lower Bounds for the \( n \)-body Simulation Problem. We also give the first lower bounds for these simulations, and show that the reachability problem for \( n \)-body simulations is PSPACE-hard. We prove this lower bound for the most practical version of this problem: inverse-square law forces in three dimensions.

The hardness proof is via a reduction to machine simulation, and is novel due to the nature of the problem under study. In particular, non-trivial problems to overcome include the fact that machines work in discrete time steps and particle simulations are continuous, and the fact that realistic machines perform transitions based on local state whereas the particle simulations have the property that all particles induce a force on all other particles (so all effects are global). To our knowledge, this is the first hardness proof to overcome these problems.

The techniques involved in our lower bound proof include constructions in which the time-averaged potential of a small set of particles is almost identical to the potential due to solid, uniformly-charged plates which persists for exponential time. A side effect of this construction is a proof that given any set of polygons fixed at rational positions in 3D with \( f \) faces and sides (say a castle),