1 Introduction

The study of physical systems by particle simulation is well-established in a number of fields. It is becoming increasingly important in others. A classical example is celestial mechanics, but much recent work has been done in formulating and studying particle models in plasma physics, fluid dynamics, and molecular dynamics [24].

There are two major classes of simulation methods. Dynamical simulations follow the trajectories of N particles over some time interval of interest. Given initial positions $\{x_i\}$ and velocities, the trajectory of each particle is governed by Newton's second law of motion:

$$m_i \frac{d^2 x_i}{dt^2} = -\nabla_i \Phi \qquad \text{for } i = 1, ..., N \ ,$$

where m_i is the mass of i^{th} particle, and the force is obtained from the gradient of a potential function Φ. When one is interested in an equilibrium configuration of a set of particles rather than their time-dependent properties, an alternative approach is the Monte Carlo method. In this case, the potential function Φ has to be evaluated for a large number of configurations in an attempt to accurately describe the potential surface.

In a typical application, the potential has the form

$$\Phi = \Phi_{near} + \Phi_{external} + \Phi_{far} \ ,$$

where Φ_{near} is a rapidly decaying function of distance (e.g. the Van der Waals potential in chemical physics), $\Phi_{external}$ is independent of the number of particles (e.g. an applied external electrostatic field), and Φ_{far}, the far-field potential, is Coulombic or gravitational. Such models describe classical celestial mechanics and many problems in plasma physics and molecular dynamics. In the vortex method for incompressible fluid flow calculations [12], an important and expensive portion of the computation has the same formal structure (the stream function and the vorticity are related by Poisson's equation).

In a system of N particles, the calculation of Φ_{near} requires an amount of work proportional to N, as does the calculation of $\Phi_{external}$. The decay of the Coulombic or gravitational potential, however, is sufficiently slow that all interactions must be accounted for, resulting in CPU time requirements of the order $O(N^2)$. In this dissertation, a method is presented for the rapid (order $O(N)$) evaluation of these interactions for all particles to within round-off error.

1.1 Brief History

There have been a number of previous efforts aimed at reducing the computational complexity of the N-body problem. Particle-in-cell methods [24] have received careful study and are used with much success, most notably in plasma physics. Assuming the potential satisfies Poisson's equation, a regular mesh is layed out over the computational domain and the method proceeds by:

1. interpolating the source density at mesh points,
2. using a "fast Poisson solver" to obtain potential values on the mesh,
3. computing the force from the potential and interpolating to the particle positions.

The complexity of these methods is of the order $O(N + M\ logM)$, where M is the number of mesh points. The number of mesh points is usually chosen to be proportional to the number of particles, but with a small constant of proportionality so that $M \ll N$. Therefore, although the asymptotic complexity for the method is $O(N\ logN)$, the computational cost in practical calculations is usually observed to be proportional to N. Unfortunately, the mesh provides limited resolution, and highly non-uniform source distributions cause a significant degradation of performance. Further errors are introduced in step (3) by the necessity for numerical differentiation to obtain the force.

To improve the accuracy of particle-in-cell calculations, short-range interactions can be handled by direct computation, while far-field interactions are obtained from the mesh, giving rise to so-called particle-particle/particle-mesh (P^3M) methods [24]. For an implementation of these ideas in the context of vortex calculations, see [5]. While these algorithms still depend for their efficient performance on a reasonably uniform distribution of particles, in theory they do permit arbitrarily high accuracy to be obtained. As a rule, when the required precision is relatively low, and the particles are distributed more or less uniformly in a rectangular region, P^3M methods perform satisfactorily. However, when the required precision is high (as, for example, in the modeling of highly correlated systems), the CPU time requirements of such algorithms tend to become excessive.

Appel [7] introduced a "gridless" method for many-body simulation with a computational complexity estimated to be of the order $O(N\ logN)$. It relies on using a monopole (center-of-mass) approximation for computing forces over large distances

and sophisticated data structures to keep track of which particles are sufficiently clustered to make the approximation valid. For certain types of problems, the method achieves a dramatic speed-up compared to the naive $O(N^2)$ approach. It is less efficient when the distribution of particles is relatively uniform and the required precision is high.

1.2 Outline of the Dissertation

The algorithms presented here make use of multipole expansions to compute potentials or forces to whatever accuracy is required. Portions of the work described below have been published previously [20,21,11]. The approach taken is similar to the one introduced in [36] for the solution of boundary value problems for the Laplace equation.

In chapter 2, we consider potential problems in two dimensions and begin with the introduction of the necessary mathematical preliminaries. A fast multipole algorithm is then developed for the evaluation of the potentials and forces in large-scale systems of particles randomly distributed in a square domain. This method requires an amount of work proportional to N to evaluate all pairwise interactions in a system of N charges. The chapter ends with a description of an adaptive version of the algorithm whose CPU time requirements are proportional to N and independent of the statistics of the charge distribution.

In Chapter 3, three-dimensional systems of particles are considered. The mathematical foundation of the method in this case is the theory of spherical harmonics, which is developed in some detail. In particular, two generalizations of the classical addition theorem for Legendre polynomials (Theorems 3.5.1 and 3.5.2) are formulated and proved. They appear to have been previously unknown, and are needed for the development of efficient translation operators which are critical features of the algorithm. It should be noted, however, that despite the increased mathematical complexity of the three-dimensional case, the framework of the fast multipole algorithm is the same as in two dimensions.

In chapter 4, we present numerical results demonstrating the actual performance of the method, and in chapter 5, we briefly outline some applications and generalizations.