Math 671, Winter 2007

Particle Methods in Scientific Computing

Instructor: Robert Krasny, 4830 East Hall, 763-3505, krasny@umich.edu

Time and Location: TuTh 10-11:30am, 3096 East Hall

Office Hours: TuTh 11:30am-12:30pm and by appointment or drop in

Course Website: http://www.math.lsa.umich.edu/∼krasny/math671b.html

Topics: fast Fourier transform (FFT), particle-in-cell method (PIC), particle-cluster approximation, Barnes-Hut treecode, spherical harmonics, Greengard-Rokhlin Fast Multipole Method (FMM), Ewald summation, applications to fluids (vortex method, smooth particle hydrodynamics) and plasmas, time permitting: radial basis functions

Prerequisite: some knowledge of numerical methods (e.g. Math 571 or 572) and applied analysis (e.g. Math 555 or 556) is recommended

Text: no required text, lecture notes will be available online, however, a recommended text is "Computer Simulation Using Particles", R.W. Hockney & J.W. Eastwood (1988) Taylor & Francis, ISBN: 0852743920 (on reserve in Science Library)

Course Grade: based on homework

The course will survey particle methods in scientific computing, an active area in applications and research. Particle methods are an alternative to traditional mesh-based methods for solving differential equations. The course will examine fast methods, i.e. methods that require fewer operations than the obvious straightforward approach. A well-known example is the fast Fourier transform (FFT) which reduces the operation count for computing the discrete Fourier transform of a vector of length N from $O(N^2)$ to $O(N \log N)$. This has a huge impact in practice, and as a result, the FFT is a basic tool in signal processing and spectral analysis. We'll start by deriving an FFT algorithm and look at applications to interpolation and boundary value problems. Much of the course will deal with methods for evaluating the potential energy and forces due to long-range particle interactions, an important component in molecular dynamics and Monte-Carlo simulations. Applications arise in many fields including astrophysics (gravitational interaction), chemistry, materials science, and plasma dynamics (electrostatic interaction), and fluid dynamics (vortex interaction). In a system with N particles, $O(N^2)$ operations are required to evaluate the pairwise interactions by direct summation. The FFT can be applied when the particles are uniformly spaced, but different ideas are needed to gain a speedup for nonuniform particle distributions. First we'll consider particle-mesh algorithms such as particle-in-cell (PIC) and P3M (Hockney-Eastwood). We'll also derive the Ewald summation technique and consider particle-mesh Ewald (Darden-York-Pedersen). Then we'll discuss hierarchical algorithms including the particle-cluster treecode (Barnes-Hut) and the cluster-cluster Fast Multipole Method (Greengard-Rokhlin). We'll derive the spherical harmonics expansion for the Coulomb potential, on which these methods are based. There's great interest in optimizing the performance of these algorithms and I'll present some recent developments. Applications in fluid and plasma dynamics will be discussed.