Math 671, Winter 2022, Topics in Scientific Computing: Particle Methods

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

Time and Location: TuTh 10-11:30am, 3088 East Hall

Office Hours:

TuTh 5-6:30pm or by appointment or just drop in when my office door is open

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

Prerequisites: it is not assumed that students have taken Math 571/572, but they should have some familiarity with differential equations, multivariable calculus, linear algebra, numerical methods, complex variables, Fourier series, and Matlab or a similar tool

Textbook: There is no required textbook; lecture notes will be posted on the course website after each class. A good text for supplementary reading is "Computer Simulation Using Particles", by R.W. Hockney & J.W. Eastwood (1988) Taylor & Francis ISBN: 0852743920.

Description: This course surveys topics related to particle methods in scientific computing. Particles interact with each other through fields, and we'll start by considering boundary value problems for fields. Specifically we'll consider finite-difference methods, spectral methods, and Green's function methods. Examples of particle systems will be given from fluid dynamics (point vortices) and electrostatics (point charges). Much of the course will deal with fast summation methods for evaluating the potential energy and forces due to long-range particle interactions, an important component in molecular dynamics and Monte-Carlo simulations. In a system with N particles, $O(N^2)$ operations are needed to evaluate the pairwise interactions by direct summation. Faster methods have been developed such as the fast Fourier transform (FFT), which reduces the operation count to $O(N \log N)$. The FFT can be applied when the particles are uniformly spaced, but different ideas are needed for nonuniform distributions, and in this context we'll consider hierarchical algorithms such as the Barnes-Hut treecode and Greengard-Rokhlin fast multipole method (FMM).

Syllabus: discrete Fourier transform, fast Fourier transform, finite-difference schemes for boundary value problems, spectral method, Green's function method, particle-in-cell method (PIC) for electrostatic plasmas described by the Vlasov-Poisson equations, vortex method for incompressible fluids described by the Euler equations, spherical harmonics, treecode, fast multipole method, Ewald summation for triply periodic charged particle systems, kernel-independent methods based on barycentric Lagrange interpolation
possible additional topics: multigrid method, single and double layer potentials, boundary element methods

Course Grade: based on several homework sets involving some analysis and computing