References for Math 671 (particle methods)

Green's functions

Greenberg, M.D. (2015) Applications of Green's Functions in Science and Engineering, Dover

FFT

Briggs, W.L. and Henson, V.E. (1995) The DFT : an Owner's Manual for the Discrete Fourier Transform, SIAM

Sedgewick, R. (1988) Algorithms, Addison-Wesley

Wickerhauser, V. (1994) Adapted Wavelet Analysis from Theory to Software, A.K. Peters

Edelman, A., McCorquodale, P. and Toledo, S. (1999) The future Fast Fourier Transform?, SIAM J. Sci. Comput., 20:1094-1114

potential theory

Folland, G.B. (1992) Fourier Analysis and its Applications, Wadsworth & Brooks/Cole

Hildebrand, F.B. (1962) Advanced Calculus for Applications, Prentice-Hall

MacRobert, T.M. (1967) Spherical Harmonics; An Elementary Treatise on Harmonic Functions, with Applications, Pergamon Press

Sternberg, W.J. and Smith, T.L. (1961) The Theory of Potential and Spherical Harmonics, University of Toronto Press

Wallace, P.R. (1984) Mathematical Analysis of Physical Problems, Dover

fast summation methods (fast multipole method, treecode, panel clustering)

Anderson, C.R. (1992) An implementation of the fast multiple method without multipoles, SIAM J. Sci. Stat. Comput., 13:923-947

Appel, A.W. (1985) An efficient program for many-body simulation, SIAM J. Sci. Stat. Comput., 6:85-103

Barnes, J. and Hut, P. (1986) A hierarchical O(NlogN) force-calculation algorithm, Nature, 324:446-449

Beatson, R. and Greengard, L. (1997) A short course on fast multipole methods, in Wavelets, Multilevel Methods and Elliptic PDEs, M. Ainsworth, J. Levesley, W. Light and M. Marletta (eds.), pp. 1-37, Oxford University Press

Cheng, H., Greengard, L. and Rokhlin, V. (1999) A fast adaptive multipole algorithm in three dimensions, J. Comput. Phys., 155:468-498

Draghicescu, C.I. and Draghicescu, M. (1995) A fast algorithm for vortex blob interactions, J. Comput. Phys., 116:69-78

Duan, Z.-H. and Krasny, R. (2001) An adaptive treecode for computing nonbonded potential energy in classical molecular systems, J. Comput. Chem., 22:184-195

Greengard, L. (1988) The Rapid Evaluation of Potential Fields in Particle Systems, MIT Press

Greengard, L. and Rokhlin, V. (1987) A fast algorithm for particle simulations, J. Comput. Phys., 73:325-348

Greengard, L. and Rokhlin, V. (1988) The rapid evaluation of potential fields in three dimensions, in Vortex Methods, Lecture Notes in Mathematics 1360, pp. 121-141, Springer-Verlag

Greengard, L. and Rokhlin, V. (1997) A new version of the fast multipole method for the Laplace equation in three dimensions, Acta Numerica, 229-269

Hackbusch, W. and Nowak, Z.P. (1989) On the fast matrix multiplication in the boundary element method by panel clustering, Numer. Math., 54:463-491

Li, P., Johnston, H. and Krasny, R. (2009) A Cartesian treecode for screened Coulomb interactions, J. Comput. Phys., 228:3858-3868

Lindsay, K. and Krasny, R. (2001) A particle method and adaptive treecode for vortex sheet motion in three-dimensional flow, J. Comput. Phys., 172:879-907

Rokhlin, V. (1984) Rapid solution of integral equations of classical potential theory, J. Comput. Phys., 60:187-207

Ying, L., Biros, G. and Zorin, D. (2004) A kernel-independent adaptive fast multipole algorithm in two and three dimensions, J. Comput. Phys. 196:591-626

barycentric Lagrange interpolation

Berrut, J.-P. and Trefethen, L.N. (2004) Barycentric Lagrange Interpolation, SIAM Review 46:501-517

Salzer, H.E. (1972) Lagrangian interpolation at the Chebyshev points $x_{n,\nu} = \cos(\nu\pi/n), \nu = 0(1)n$; some unnoted advantages, Comput. J., 15:156-159

Wilson, L., Vaughn, N. and Krasny, R. (2021) A GPU-accelerated fast multipole method based on barycentric Lagrange interpolation and dual tree traversal, Comput. Phys. Commun. 265:108017

Vaughn, N., Wilson, L. and Krasny, T. (2020) A GPU-accelerated barycentric Lagrange treecode, 2020 IEEE Inter. Para. & Distrib. Process. Symp. Work. (IPDPSW), 701-710.

Wang, L., Krasny, R. and Tlupova, S. (2020) A kernel-independent treecode based on barycentric Lagrange interpolation, Commun. Comput. Phys. 28:1415-1436

Ewald summation

Darden, T., York, D. and Pedersen, L.G. (1993) Particle mesh Ewald: An Nlog(N) method for Ewald sums in large systems, J. Chem. Phys., 98:10089-10092

Duan, Z.-H. and Krasny, R. (2000) An Ewald summation based multipole method, J. Chem. Phys., 113:3492-3495

Essmann, U., Perera, L., Berkowitz, M.L., Darden, T., Lee, H. and Pedersen, L.G. (1995) A smooth particle mesh Ewald method, J. Chem. Phys., 103:8577-8593

Fincham, D. (1993) Optimisation of the Ewald sum, CCP5 Newsletter, 38

Perram, J.W., Petersen, H.G. and de Leeuw, S.W. (1988) An algorithm for the simulation of condensed matter which grows as the 3/2 power of the number of particles, Molec. Phys., 65:875-893

Tosi, M.P. (1964) Evaluation of electrostatic lattice potentials by the Ewald method, in Solid State Physics, Advances in Research and Applications, 16, F. Seitz and D. Turnbull (eds.), Appendix A, 107-113

Toukmaji, A.Y. and Board Jr., J.A. (1996) Ewald summation techniques in perspective: a survey, Comput. Phys. Commun., 95:73-92

particle-in-cell

Hockney, R.W. and Eastwood, J.W. (1988) Computer Simulation Using Particles, Taylor and Francis

radial basis functions

Buhmann, M.D. (2003) Radial Basis Functions, Cambridge University Press

Larsson, E. and Fornberg, B. (2003) A numerical study of some radial basis function based solution methods for elliptic PDEs, Comp. Math. Appl., 46:891-902

Krasny, R. and Wang, L. (2011) Fast evaluation of multiquadric RBF sums by a Cartesian treecode, SIAM J. Sci. Comput., 33:2341-2355

iterative methods

Ciarlet, P.G. (1989) Introduction to Numerical Linear Algebra and Optimisation, Cambridge University Press

multigrid

Brandt, A. (1977) Multi-level adaptive solutions to boundary-value problems, Math. Comp., 31:333-390

Briggs, W.L., Henson, V.E. and McCormick, S.F. (2000) A Multigrid Tutorial, SIAM

applications

Allen, M.P. and Tildesley, D.J. (1987) Computer Simulation of Liquids, Clarendon Press, Oxford

Birdsall, C.K. and Langdon, A.B. (1991) Plasma Physics via Computer Simulation, IOP Publishing

Cottet, G.-H. and Koumoutsakos, P.D. (2000) Vortex Methods Theory and Practice, Cambridge University Press

Koumoutsakos, P.D. (2005) Multiscale flow simulations using particles, Annu. Rev. Fluid Mech., 37:457-487

Li, S and Liu, W.K. (2004) Meshfree Particle Methods, Springer

Liu, G.R. and Liu, M.B. (2003) Smoothed Particle Hydrodynamics. A Meshfree Particle Method, World Scientific Publishing

Pfalzner, S. and Gibbon, P. (1996) Many-Body Tree Methods in Physics, Cambridge University Press

Potter, D. (1973) Computational Physics, John Wiley and Sons

Sagui, C. and Darden, T.A. (1999) Molecular dynamics simulations of biomolecules: Long-range electrostatic effects, Annu. Rev. Biophys. Biomol. Struct., 28:155-179

Schlick, T. (2002) Molecular Modeling and Simulation: An Interdisciplinary Guide, Springer