BME 538 Engineering Numerical Analysis and Multiscale Modeling
Spring Semester 2022

Time: 2:00 PM-3:15 PM Tuesdays and Thursdays
Location: 227 SEO
Instructor: Zhangli Peng
Email: zhpeng@uic.edu
Zoom: https://uic.zoom.us/j/4594667464?pwd=enAwUEhrV1Ira0RybkJSVWgvOXgxZz09
Office: 820 South Wood Street, Clinical Science North (CSN) 164F

Course description

The goal of this course is to teach graduate students or senior undergraduates the fundamentals of numerical analysis and its applications in science and engineering. We will cover numerical interpolation, differentiation, integration, solution methods for initial value and boundary value problems of ordinary differential equations, solution methods for parabolic, hyperbolic, and elliptic partial differential equations. Besides the mathematical foundations, specific biomedical applications such as modeling various microfluidic systems and cell mechanics using software Matlab, COMSOL, and Abaqus will be demonstrated as hands-on tutorials. Advanced multiscale modeling techniques to bridge cellular and molecular scales with organ and tissue scales by coupling molecular dynamics and continuum modeling will be also introduced.

Textbooks

- Parviz Moin. Fundamentals of Engineering Numerical Analysis, Cambridge University Press; 2nd edition, 2010.
- Belytschko et al., Nonlinear finite elements for continua and structures, Wiley; 2nd edition, 2013.

References

- Pozrikidis, C. (1998, 2008) Numerical Computation in Science and Engineering. Oxford University Press. First Edition (1998), Second Edition (2008).
- Weinan E. Principles of Multiscale Modeling, Cambridge University Press, 2011.

Office hour

- By appointment

Topics

- Interpolation
  General interpolation problem; Lagrange polynomials; piecewise Lagrange interpolation; splines; parametric interpolation; multidimensional interpolation.
- Numerical Differentiation
  Finite differences from interpolation; finite differences from Taylor series; matrix representation of finite difference schemes; Hermitian methods and Pade approximations.
- Numerical Integration
  Newton-Cotes formulas; trapezoidal rule; Simpson's rule; error analysis;

trapezoidal rule with end correction; Richardson's extrapolation and Romberg integration; adaptive quadrature; Gauss quadrature; semi-infinite intervals; infinite intervals; singularities.

- Numerical Solution of Ordinary Differential Equations (ODEs)
  Initial value problems; Runge-Kutta type formulas; multi-step methods; implicit methods; accuracy; stability; model equation; phase and amplitude errors; system of differential equations; stiffness; boundary value problems; shooting; direct methods; non-uniform grids; eigenvalue problems.
- Numerical Solution of Partial Differential Equations (PDEs)
  Method of lines for parabolic and hyperbolic PDEs; modified wave number and von Neumann stability analysis; modified equation analysis; alternating direction implicit methods; approximate factorization; nonlinear equations; iterative methods for elliptic PDEs; conjugate gradient methods; multigrid method; direct methods; method of weighted residuals; Galerkin method; spectral method; finite element method; boundary element method; dissipative particle dynamics.
- Specific Biomedical Applications:
  Modeling various microfluidic systems (inertial, deformability-based, acoustic) and cell mechanics using software Matlab, COMSOL, and Abaqus will be demonstrated as hands-on tutorials.
- Multiscale Modeling
  Coupling molecular dynamics (MD) with finite element simulations; Coupling boundary integral simulations of viscous flow with membrane elasticity; coarse-grained molecular dynamics and dissipative particle dynamics (DPD).

Homework and Grading (Gradescope in Blackboard will be used for homework submission and grading)

While you are allowed and encouraged to discuss the class material with your colleagues and others, everything that you hand in must be your own work. Academic honesty is expected.

GRADES

	Level 1	Level 2	Level 3	Level 4
Homework (30%)	Answer correct and process correct	Answer close and process correct	Answer wrong and process reasonable	Process wrong
Midterm (20%)	Answer correct and process correct	Answer close and process correct	Answer wrong and process reasonable	Process wrong
Final project text (20%), <8 pages.	Method well described, and most important works covered in the literature	Method well described, and some important works covered	Method described in an understandable way	Method and existing works not well described
Final project presentation (15%), 10 mins + 3 mins Q&A	Well organized and well delivered, most audience can understand well	Have a good presentation structure and relative easy to follow	Hard to follow, for example, too many equations	Most people cannot understand
In-class exercises (15%)	Answer correct and process correct	Answer close and process correct	Answer wrong and process reasonable	Process wrong