Computational Tools for Multiscale Problems

Logistics

Course: CSCI 5526, Fall 2025

Time: Tuesday & Thursday 11:00 AM-12:15 PM

Location: CMDI Dept of Info Science 158

Instructor: Fruzsina Agocs

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Office hours: Wednesday & Friday 1-2 PM, ECOT 614

Course website: https://cu-comptools.github.io/fall2025

Course description

Physical phenomena are often described in terms of ordinary and partial differential equations (ODEs and PDEs) with interactions and features on multiple scales. Some of these systems are notoriously hard to solve but abound in scientific and engineering applications. In this course you will learn about state-of-the-art methods and software for the fast and accurate numerical solution of such systems, starting from their fundamental components (linear solve, interpolation, differentiation, quadrature) and building up to hybrid ODE solvers and boundary integral equation methods for PDEs.

Prerequisites

- Basic linear algebra, calculus, basic complex analysis
- CSCI 3656 (3) Numerical Computation encouraged
- CSCI 5636 Numerical Solution of Partial Differential Equations encouraged
- Familiarity with Python (or some other programming language) encouraged

Learning goals

- Be familiar with established and novel numerical tools (methods and software)
 for fundamental computational tasks: interpolation, quadrature, solution of
 ODEs, solution of linear PDEs with boundary integral equation methods.
- Understand how to assess whether a numerical solution is satisfactory, learn to evaluate what accuracy one can reasonably demand.
- Learn to build robust numerical code and (unit, convergence) test it.

Grading

Your grade will be calculated as follows:

- In-class quizzes (90% total, equally weighed)
 - There will be **7** of them total, see the lesson plan for dates.
 - Some will include coding (in Python). During the quiz, I will go around and help with coding-related questions. We can discuss in class if there's a need for exercises in a different programming language.
 - Your lowest scoring quiz will not count towards your grade.
 - Optional presentation on the last couple of days of the semester if you'd like to improve your grade, counts as a quiz.
 - Each quiz will have about 80% "bookwork" (so you can get at least a B
 if you've been keeping up with the classes) and 20% "unseen"
 problems (an exercise, of part of an exercise, that requires some
 independent thinking or creativity)
 - "Bookwork" exercises are posted at the end of each class, the quiz will have pretty much exactly those exercises. Solutions may be discussed at office hours.
- Attendance (10% total)
 - This is a pass/fail criterion, you're required to attend 80% of classes
 (22 out of 28)

Resources

- Trefethen, L. N. (2019). Approximation theory and approximation
 practice. (available online through author)
- Driscoll, T. A., & Braun, R. J. (2017). Fundamentals of Numerical Computation. (available online through author)
- Corless, R. M., & Fillion, N. (2013). A graduate introduction to numerical methods. (PDF through publisher)
- Hairer, E., Nørsett, S. P., & Wanner, G. Solving Ordinary Differential
 Equations I-II. (PDF I and PDF II through publisher)
- Trefethen, L. N. (2000). Spectral methods in MATLAB. (Chapter-by-chapter <u>PDF</u>s through publisher)
- Alex Barnett's Math 126 Numerical analysis for PDEs and wave scattering lecture notes (hand-written notes online)
- Kress, R. (1999). **Linear integral equations**. (PDF through publisher)
- Further resources will be listed in the lecture notes

Course plan (subject to change)

- Fundamentals of computation
 - Condition number, backwards stability
 - GitHub for version control, docstrings and unit tests
 - o Quiz: Sept 2
- Components of differential equations
 - Interpolation, numerical differentiation, (smooth) quadrature
 - o Quiz: Sept 18
- ODEs
 - Runge–Kutta methods, Butcher tableaus, stability and stiffness, spectral methods, asymptotic acceleration (non-examinable)
 - o Quiz: Oct 7
- Integral equations I
 - What are integral equations? Nyström method, SVD, compact operators
 - Quiz: Oct 21

- Integral equations II
 - Laplace's equation, fundamental solution, properties of harmonic functions, Green's representation theorem, boundary parameterization
 - o Quiz: Nov 4
- Integral equations III
 - Layer potentials, jump relations, interior/exterior Neumann/Dirichlet problems, complementary boundary value problem
 - o Quiz: Nov 18
- Integral equations IV
 - Helmholtz equation, scattering formulation, combined field integral equation, transmission formulation, low-rank interactions
 - o Quiz: Dec 4 (take-home
- Fast algorithms
 - The fast multipole method, iterative methods and their convergence, singular / near-singular quadrature
 - No quiz
- Guest lectures
 - Maxwell's equations, special quadratures ctd... to be confirmed
 - No quiz

Acceptable use of AI in this class

You may not, under any circumstances, use LLMs or other ML-based tools (e.g. ChatGPT, GitHub copilot, Cursor) for assistance in your assignments. Doing so will count as cheating and will be reported, and you will get a zero on your assignment.

Classroom Behavior

Students and faculty are responsible for maintaining an appropriate learning environment in all instructional settings, whether in person, remote, or online. Failure to adhere to such behavioral standards may be subject to discipline. Professional courtesy and sensitivity are especially important with respect to individuals and topics dealing with race, color, national origin, sex, pregnancy, age, disability, creed,

religion, sexual orientation, gender identity, gender expression, veteran status, marital status, political affiliation, or political philosophy.

For more information, see the <u>classroom behavior policy</u>, the <u>Student Code of Conduct</u>, and the <u>Office of Institutional Equity and Compliance</u>.

Accommodation for Disabilities, Temporary Medical Conditions, and Medical Isolation

If you qualify for accommodations because of a disability, please submit your accommodation letter from Disability Services to your faculty member in a timely manner so that your needs can be addressed. Disability Services determines accommodations based on documented disabilities in the academic environment. Information on requesting accommodations is located on the Disability Services website. Contact Disability Services at 303-492-8671 or DSinfo@colorado.edu for further assistance. If you have a temporary medical condition, see Temporary Medical Conditions on the Disability Services website.

If you have a temporary illness, injury or required medical isolation for which you require adjustment, please contact the instructor in person or via fruzsina.agocs@colorado.edu (you are **not** required to state the nature of your illness/injury or provide a doctor's note).

Preferred Student Names and Pronouns

CU Boulder recognizes that students' legal information does not always align with how they identify. If you wish to have your preferred name (rather than your legal name) and/or your preferred pronouns appear on your instructors' class rosters and in Canvas, visit the Registrar's website for instructions on how to change your personal information in university systems.

Honor Code

All students enrolled in a University of Colorado Boulder course are responsible for knowing and adhering to the Honor Code. Violations of the Honor Code may include but are not limited to: plagiarism (including use of paper writing services or technology [such as essay bots]), cheating, fabrication, lying, bribery, threat, unauthorized access to academic materials, clicker fraud, submitting the same or similar work in more than one course without permission from all course instructors involved, and aiding academic dishonesty. Understanding the course's syllabus is a vital part of adhering to the Honor Code.

All incidents of academic misconduct will be reported to Student Conduct & Conflict Resolution: StudentConduct@colorado.edu. Students found responsible for violating the_Honor Code will be assigned resolution outcomes from Student Conduct & Conflict Resolution and will be subject to academic sanctions from the faculty member. Visit Honor Code for more information on the academic integrity policy.

Sexual Misconduct, Discrimination, Harassment and/or Related Retaliation

CU Boulder is committed to fostering an inclusive and welcoming learning, working, and living environment. University policy prohibits <u>protected-class</u> discrimination and harassment, sexual misconduct (harassment, exploitation, and assault), intimate partner abuse (dating or domestic violence), stalking, and related retaliation by or against members of our community on- and off-campus. The Office of Institutional Equity and Compliance (OIEC) addresses these concerns, and individuals who have been subjected to misconduct can contact OIEC at 303-492-2127 or email OIEC@colorado.edu. Information about university policies, <u>reporting options</u>, and <u>OIEC support resources</u> including confidential services can be found on the <u>OIEC</u> website.

Please know that faculty and graduate instructors are required to inform OIEC when they are made aware of incidents related to these concerns regardless of when or where something occurred. This is to ensure the person impacted receives outreach from OIEC about resolution options and support resources. To learn more about reporting and support a variety of concerns, visit the <u>Don't Ignore It page</u>.

Religious Accommodations

Campus policy requires faculty to provide reasonable accommodations for students who, because of religious obligations, have conflicts with scheduled exams, assignments, or required attendance. Please communicate the need for a religious accommodation in a timely manner. In this class, please give advance notice to the instructor in person or via fruzsina.agocs@colorado.edu.

See the <u>campus policy regarding religious observances</u> for full details.

Mental Health and Wellness

The University of Colorado Boulder is committed to the well-being of all students. If you are struggling with personal stressors, mental health or substance use concerns that are impacting academic or daily life, please contact <u>Counseling and Psychiatric Services (CAPS)</u> located in C4C or call (303) 492-2277, 24/7.

Free and unlimited telehealth is also available through <u>Academic Live Care</u>. The <u>Academic Live Care</u> site also provides information about additional wellness services on campus that are available to students.