# Current topics in Computer Science: Computational Tools for Multiscale Problems

## Logistics

**Course**: CSCI 7000, Fall 2024

**Time**: Monday, Wednesday, Friday 3:35–4:25 PM

**Location**: ECEE 283

**Instructor**: Fruzsina Agocs

**Email**: fruzsina.agocs@colorado.edu

**Office hours**: Fridays 4:30–5:30pm, ECOT 614 (or by appointment)

**Course website**: https://cu-comptools.github.io/fall2024

## 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
- Familiarity with Python 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 software and (unit, convergence) test it.
- Distill information from numerical analysis research; summarize, communitate results by presentation.
- Deliver constructive feedback on presentations.

# Grading

Your grade will be calculated as follows:
- Homework (60%, 15% each)
  - Will discuss rubric in class
- Paper presentation (30%, 15% each)
  - Will discuss rubric in class
- Reading and reading questions (10%)

# 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 [PDF](#)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/homework sheets

# Course plan (subject to change)

| Week | Topics | Assignment |
|---|---|---|
| 1 Aug 26–Aug 30 | Condition number, backwards stability, Vandermonde matrix & instability | HW1 (due Sept 3) |
| 2 Sept 2–Sept 6 | Polynomial interpolation and its error, quadrature | |
| 3 Sept 9–Sept 13 | ODEs: when polynomials go wrong (asymptotic methods, hybrid solvers) | HW2 (due Sept 23) |
| 4 Sept 16–Sept 20 | ODEs ctd.: Stability/stiffness/control | |
| 5 Sept 23–Sept 27 | Special quadrature methods: singularity nearby, oscillatory funcs | Choose pres time, papers assigned |
| 6 Sept 30–Oct 4 | Linear PDEs, SVD, numerical rank | Prepare for paper pres |
| 7 Oct 7–Oct 11 | Student paper presentations (1+2) | Prepare for paper pres |
| 8 Oct 14–Oct 18 | Student paper presentations (3) | Prepare for paper pres |
| 9 Oct 21–Oct 25 | Integral equations, Nystrom method, (compact operators), Fredholm Alternative | HW3 (due Nov 4) |
| 10 Oct 28–Nov 1 | Laplace's eq, fundamental solution, Green's representation formula, properties of | |

| | harmonic functions, boundary repr | |
|---|---|---|
| 11 Nov 4–Nov 8 | Layer potentials, jump relations, non-uniqueness | HW4 (due Nov 18) |
| 12 Nov 11–Nov 15 | Helmholtz, Maxwell's eqs, scattering formalism | |
| 13 Nov 18–Nov 22 | Panel quadrature, close evaluation, special quadrature | Choose pres time, papers assigned |
| 14 Nov 25–Nov 29 Fall break, 1 class | Student paper presentation (1) | Papers assigned, prepare for paper pres |
| 15 Dec 2–Dec 6 | Student paper presentations (3) | Prepare for paper pres |
| 16 Dec 9–Dec 13 End of semester, 2 classes | Student paper presentations (2) | Prepare for paper pres |

# Programming languages and use of ML tools

I will primarily use Python/Jupyter for coding demos, but we may make use of libraries written in several languages. You don't need prior experience in any particular language, but please bring a growth mindset and ask for help as needed. You may submit code written in any non-esoteric language you are comfortable with.

Most HPC facilities use a Linux operating system and many open source software packages and libraries will have the best documentation and testing on Linux systems. You can use any environment for your local development environment, or use the CS Department's JupyterHub coding.csel.io to experiment and develop without a local install.

You may use LLMs and other ML-based tools (e.g. ChatGPT, GitHub copilot) for assistance in your assignments, but I ask that you do so carefully and treat their output with some skepticism. For your sake, do not turn in untested code or unedited

LLM output. Note on your assignment (or verbally, during a presentation) what tool you used and your prompt(s).

# 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 [classroom behavior policy](#), the [Student Code of Conduct](#), and the [Office of Institutional Equity and Compliance](#).

# 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 doesn't always align with how they identify. Students may update their preferred names and pronouns via the student portal; those preferred names and pronouns are listed on instructors' class rosters. In the absence of such updates, the name that appears on the class roster is the student's legal name.

# 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 in 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 the Student Conduct & Conflict Resolution as well as 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 [protected-class]() 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

CUreport@colorado.edu. Information about university policies, [reporting options](), and [support resources]() including confidential services can be found on the [OIEC website](). Please know that faculty and graduate instructors must inform OIEC when they are made aware of incidents related to these policies regardless of when or where something occurred. This is to ensure that individuals impacted receive outreach from OIEC about resolution options and support resources. To learn more about reporting and support for a variety of concerns, visit the [Don't Ignore It]() page.

# 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, {Faculty: insert your procedures here}.
See the [campus policy regarding religious observances]() 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 [Counseling and Psychiatric Services (CAPS)]() located in C4C or call (303) 492-2277, 24/7.

Free and unlimited telehealth is also available through [Academic Live Care](). The [Academic Live Care]() site also provides information about additional wellness services on campus that are available to students.