AME60714: Advanced Numerical Methods

Course logistics

AME60714: Advanced Numerical Methods, 3 units
Lecture: MW 2:20p-3:35p, 138 DeBartolo Hall

Lecture format

All lectures will be broadcast live via Zoom (FA20-AME-60714-01, ID: 935 9119 5729) and recorded. The instructor will deliver all lectures (unless otherwise indicated) from the assigned classroom.

Course description

Theory and implementation of advanced numerical methods to solve and optimize linear and nonlinear partial differential equations (PDEs) with particular emphasis on hyperbolic PDEs and (compressible) computational fluid dynamics. In the first part of the course, the foundational theory of hyperbolic partial differential equations including conservation laws, characteristics, Riemann problems, and Rankine-Hugoniot jump conditions, will be discussed. These concepts will be used to construct numerical methods for approximating solutions of hyperbolic PDEs including finite volume and high-order discontinuous Galerkin methods. The second part of the course will build upon the theory and methods developed in the first part to delve into more advanced topics including Arbitrary Lagrangian-Eulerian (ALE) formulations to solve PDEs on moving domains, optimization problems constrained by partial differential equations including boundary control and shape optimization, and model reduction methods to reduce the computational cost of solving PDEs. Aspects of software design (version control, continuous integration) and verification will also be discussed, as well as advanced programming tools such as automatic and symbolic differentiation and code generation.

Learning goals

Upon successful completion of this course, students will have: (1) fundamental understanding of hyperbolic partial differential equations and their solutions, (2) familiarity with basic and advanced methods for computational fluid dynamics, (3) understanding of advanced numerical methods including PDE-constrained optimization and model reduction, (4) ability to apply and implement the methods introduced in the course to solve relevant problems that arise in research.

Prerequisites

Numerical methods (AME60611 or equivalent)

Instructor

Matthew J. Zahr
300B Cushing Hall
E-mail: mzahr@nd.edu
Office hours: MW 3:35p-5p, or by appointment (all OH virtual via course Zoom meeting)

Course material

Material will not be physically exchanged. All course resources will be provided on Sakai and all deliverables must be submitted via Sakai.

Website: Sakai
Lecture notes: provided by instructor on the website
Recommended textbooks (lecture notes will be taken directly from these book):

- Eleuterio F. Toro. *Riemann Solvers and Numerical Methods for Fluid Dynamics*. Springer Berlin Heidelberg, Berlin, Heidelberg, 1999 (Hyperbolic PDE theory, finite volume methods)
- Randall J. LeVeque. *Finite Volume Methods for Hyperbolic Problems*. Cambridge texts in applied mathematics. Cambridge University Press, Cambridge; New York, 2002 (Hyperbolic PDE theory, finite volume methods)
- J. Hesthaven and T. Warburton. *Nodal Discontinuous Galerkin Methods: Algorithms, Analysis, and Applications*. Springer Science & Business Media, 2007 (Discontinuous Galerkin methods)

- Béatrice Rivière. *Discontinuous Galerkin methods for solving elliptic and parabolic equations: theory and implementation*. Frontiers in Applied Mathematics. Society for Industrial and Applied Mathematics, Philadelphia, PA, 2008 (Discontinuous Galerkin methods)
- Peter Benner, Serkan Gugercin, and Karen Willcox. A Survey of Projection-Based Model Reduction Methods for Parametric Dynamical Systems. *SIAM Review*, 57(4):483–531, January 2015 (Model reduction)
- Peter Benner, Albert Cohen, Mario Ohlberger, and Karen Willcox, editors. *Model Reduction and Approximation: Theory and Algorithms*. Number 15 in Computational Science and Engineering. Society for Industrial and Applied Mathematics, Philadelphia, 2017 (Model reduction)
- Alfio Quarteroni, Andrea Manzoni, and Federico Negri. *Reduced Basis Methods for Partial Differential Equations: An Introduction*. Springer, 2016 (Model reduction)
- Max D. Gunzburger. *Perspectives in Flow Control and Optimization*. Advances in Design and Control. Society for Industrial and Applied Mathematics, Philadelphia, PA, 2003 (PDE-constrained optimization)

Homework

There will 4 homework assignments. They will consist of a combination of theory and programming exercises.

Examinations

There will be one take-home examination near the end of the semester (tentative date: November 2).

Project

The course will culminate with a final project. Students will propose their own project. Project proposals will be due September 7; feedback and approval will be provided by the instructor by September 11. Projects are expected to incorporate some (but not all) topics covered in the course. Students are welcome and encouraged to propose projects based on one's own research or implement a method from a research paper.

Grading

The final score will be calculated as a weighted combination of the homework (40%), exam (20%), and project (40%) scores.

Course topics

The course will be broken into three parts; Part 1-2 will comprise 50% of the semester and Parts 3 and 4 will each comprise 25%.

- Part I: Theory of hyperbolic PDEs
  - Conservation laws: scalar vs. system, linear vs. nonlinear, first- vs. second-order
  - Examples: advection, Burgers', shallow water, Euler, Navier-Stokes
  - Conservation, Riemann problems, Rankine-Hugoniot conditions, numerical fluxes
  - Finite volume and discontinuous Galerkin methods
  - Arbitrary Lagrangian-Eulerian formulations for conservation laws on deforming domains
- Part II: Numerical methods for hyperbolic PDEs
  - Finite volume and discontinuous Galerkin methods
  - Arbitrary Lagrangian-Eulerian formulations for conservation laws on deforming domains
- Part III: PDE-constrained optimization
  - Formulation of PDE-constrained optimization problems: steady vs. unsteady
  - Sensitivity and adjoint methods for computing gradients
  - Gradient-based optimization
- Part IV: Model reduction for linear and nonlinear sytems
  - Reduced basis methods
  - Proper orthogonal decomposition
  - Hyperreduction for nonlinear problems

Sakai

Technical support for Sakai is provided, not by me (instructor) or TAs, but by the OIT Help Desk and the Sakai Team. If you have a question or issue concerning the use of Sakai, please contact the Help Desk at oithelp@nd.edu or phone: 574-631-8111. You can also walk in; they're located in 115 DeBartolo Hall. Support Staff will contact me if they need to discuss the way I've set up our class. Please tell them the web address to our Sakai site, my NetID as your instructor and your NetID, and specifically name the assignment or task you need help with. Technical Tips Before Contacting the OIT Help Desk:

- Access Sakai with a newly opened fresh browser (not one that's been opened for a month and has 47 tabs running across the top).
- Before calling the Help Desk with issues, empty your browser history, close and re-open your browser. Often that's all it takes. (How-To Instructions Here).
- Never login to Sakai twice in two tabs in the same browser, especially when taking a test. You may lose answers.

Policies

Office hours: Students are strongly encouraged to utilize the office hours for assistance with the course material. To make the most out of office hours, students are encouraged to think through the problem on their own and avoid overly generic questions. For example, instead of "How do I do problem 3?", students should explain their thought process, what they have tried, and where they got stuck. If you cannot attend the scheduled office hours, contact the teaching staff directly to schedule an appointment.

Collaboration and honor code: Collaboration is permitted on the homework and project (not exams); however, each student must complete and submit their own assignment. Honor code violations will be handled through appropriate university channels (`http://honorcode.nd.edu`).

Disabilities: Any student who has a documented disability and is registered with Disability Services should speak with me as soon as possible regarding accommodations. More information can be found at `http://disabilityservices.nd.edu`.

COVID19 related accommodations: Students should contact the instructor with any COVID19 related concerns or accommodation requests. The instructor will make every effort to make individualized accommodations as needed while still providing the highest level of instruction possible. **Students that feel comfortable with in-person instruction (and received campus pass based on daily health check) are welcome and encouraged to attend lecture in person. All university rules (detailed below) will be followed including the use of masks and physical distancing. Students are also welcome to engage with the course remotely, either synchronously or asynchronously (synchronous preferred by instructor to promote active engagement with instructor and course content).**

Privacy statement: Course materials (videos, assignments, problem sets, etc) are for use in this course only. You may not upload them to external sites, share with any person outside of this course, or post them for public commentary without my written permission. We are recording class meetings to support remote students and to provide everyone in the class with useful study aids. These recordings will be available for review through Sakai. The University strictly prohibits anyone from duplicating, downloading, or sharing live class recordings with anyone outside of this course, for any reason.

Health and Safety Protocols

In this class, as elsewhere on campus, students must comply with all University health and safety protocols, including:

- Face masks that completely cover the nose and mouth will be worn by all students and instructors;
- Physical distancing will be maintained in all instructional spaces;
- Students will sit in assigned seats throughout the semester, which will be documented by faculty for purposes of any needed contact tracing; and

- Protocols for staged entry to and exit from classrooms and instructional spaces will be followed.

We are part of a community of learning in which compassionate care for one another is part of our spiritual and social charter. Consequently, compliance with these protocols is an expectation for everyone enrolled in this course. If a student refuses to comply with the University's health and safety protocols, the student must leave the classroom and will earn an unexcused absence for the class period and any associated assignments/assessments for the day. Persistent deviation from expected health and safety guidelines may be considered a violation of the University's "Standards of Conduct," as articulated in du Lac: A Guide for Student Life, and will be referred accordingly.

Health Checks and Attendance

Every morning, members of the Notre Dame Community will be asked to complete a daily health check and submit their information via the Return to Campus Advisor application. The health check application will indicate one of the following:

- Student is cleared for class and should attend class in person; or
- Student is advised to stay home to monitor symptoms and should participate in class virtually and complete all assignments and assessments; or
- Student must consult a healthcare provider and should contact University Health Services (UHS) for an assessment. In the meantime, the student should participate in class virtually and complete all assignments and assessments. Depending on the medical assessment, UHS will follow the University's standard protocol for obtaining an excused absence for medical reasons.

Support for student mental health at Notre Dame

Care and Wellness Consultants provide support and resources to students who are experiencing stressful or difficult situations that may be interfering with academic progress. Through Care and Wellness Consultants, students can be referred to The University Counseling Center (for cost-free and confidential psychological and psychiatric services from licensed professionals), University Health Services (which provides primary care, psychiatric services, case management, and a pharmacy), and The McDonald Center for Student Well Being (for problems with sleep, stress, and substance use). Visit care.nd.edu.