ME618-ST: High Performance Computing and Bio-Inspired Computational Fluid Dynamics
Fall 2024

Instructor: Dr. Peter Balogh
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Office: Mechanical Engineering Center (MEC) 324A

Lectures: Monday 6:00PM – 8:50PM; Faculty Memorial Hall (FMH) 405

Office Hours: Tuesday and Thursday at 1PM

Suggested Readings / Books:
- Engineering Numerical Analysis, by Parvis Moin.
- Parallel and High Performance Computing, by Robey and Zamora.
- Introduction to Theoretical and Computational Fluid Dynamics, by Constantine Pozrikidis.
- Computational Methods for Fluid Dynamics, by Joel Ferziger
- Biomechanics: Circulation, by Y.C. Fung
- The Fluid Dynamics of Cell Motility, by Eric Lauga.

Prerequisites:
- ME 611 – Dynamics of Incompressible Fluids

Course Description:
This course will provide an overview of modern high-performance computing (HPC) systems, with practical real-world applications to modeling a range of bio-inspired phenomena such as blood flow and biological cell transport (e.g. white blood cells, circulating tumor cells). The student will learn the basics of HPC clusters and designing computer code to efficiently leverage resources. The course will heavily emphasize and focus on numerical algorithms for incompressible computational fluid dynamics (CFD), and describe state-of-the-art approaches commonly employed for simulating bio-inspired flows. The course will provide the student with in-depth examples covering a spectrum of topics typically encountered in real-world HPC code development environments for bio-inspired CFD, including numerical methods for low Reynolds number fluid dynamics, coding and parallelizing a Navier-Stokes solver, version control systems for code development, Immersed Boundary Methods and integrating solid mechanics models, and real-world practice with running jobs on a modern HPC cluster.

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<u>Course Policies:</u>

1. <u>Grading</u>
   Total of 100 points:
   - Homework & Computer Projects (60)
   - Tests (10)
   - Final Project (30)

   Scale:

A:	90-100
B+:	85-89
B:	80-84
C+:	75-79
C:	70-74
D:	60-69
F:	0-59

2. Attendance and Lecture Notes
   - Attendance will not be graded. Lecture notes will either be written on the board during class or through PowerPoint presentations. It is extremely important that you attend every class and take good notes.

3. NJIT Canvas
   - https://njit.instructure.com/courses/41709
   - Log in and make sure your email address is correct, as all course notifications will be posted on Canvas
   - HW assignments, projects, test information, and general course announcements will be posted on Canvas

4. Computer Code and Projects
   - The primary code language used by the instructor in this course is Fortran. Knowledge of this language prior to taking the course is not required, but the student is expected to learn the basics of the language during the semester. Fortran will be utilized for in-class examples and demonstrations, as well as with example codes given to the students.
   - There will be multiple computer projects assigned throughout the course. Small-scale projects will cover individual topics as we go through them in class, with one large-scale project due at the end of the course.
   - All computer code must be provided when turning in a project. Acceptable languages are Fortran, C++, or Matlab. Others may be allowed but must be discussed with the instructor prior.

5. Homework
    - Assignments (HW, projects) are due at the beginning of class.
    - Each problem must be worked through in a clear and logical manner with any assumptions clearly stated.
6. Tests
    - All tests and exams will be closed books / closed notes.
    - Failure to show up will result in zero points, and there are no make-ups. The only exceptions are for an officially documented excuse from the Dean of Students.
7. Late Policy
    - All HW and computer projects must be handed in on the due date. Failure to do so will result in zero points, and there are no make-ups. The only exceptions are for an officially documented excuse from the Dean of Students.
8. Academic Integrity
    - "Academic Integrity is the cornerstone of higher education and is central to the ideals of this course and the university. Cheating is strictly prohibited and devalues the degree that you are working on. As a member of the NJIT community, it is your responsibility to protect your educational investment by knowing and following the academic code of integrity policy that is found at: http://www5.njit.edu/policies/sites/policies/files/academic-integrity-code.pdf.
    - Please note that it is my professional obligation and responsibility to report any academic misconduct to the Dean of Students Office. Any student found in violation of the code by cheating, plagiarizing or using any online software inappropriately will result in disciplinary action. This may include a failing grade of F, and/or suspension or dismissal from the university. If you have any questions about the code of Academic Integrity, please contact the Dean of Students Office at dos@njit.edu"
9. Statement on Use of AI
    - This course expects students to work without artificial intelligence (AI) assistance in order to better develop their skills in this content area. As such, **AI usage is not permitted** throughout this course under any circumstance.

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Course Schedule (Tentative)

Lecture	Date	Topics Covered	Due
1	9/9/24	Course Introduction High Performance Computing • Modern Supercomputer Clusters and History • Architecture and Structure • Parallel and Distributed Computing • Hands-On Coding/Demonstrations	
2	9/16/24	Computational Fluid Dynamics • Governing Equations • Dimensionless Numbers and What They Tell Us • PDE's: Hyperbolic, Parabolic, Elliptic • Hands-On Coding/Demonstrations	
3	9/23/24	Numerical Methods for CFD • Discretization and Derivatives • Methods for 1st and 2nd order ODEs • Hands-On Coding/Demonstrations	HW1
4	9/30/24	Numerical Methods for CFD • Solving PDEs & stability • Transient Diffusion • Convection Equation • Hands-On Coding/Demonstrations	HW2
5	10/7/24	Numerical Methods for CFD • Linear systems and solution methods • Multi-dimensional problems • Hands-On Coding/Demonstrations	
6	10/14/24	Numerical Methods for CFD • Iterative schemes • Direct matrix inversion • Solving the incompressible Navier-Stokes Eq. • Hands-On Coding/Demonstrations	Project 1
7	10/21/24	**TEST 1** Coding a 2D Navier-Stokes Solver • Overview and General Considerations	
8	10/28/24	Coding a 2D Navier-Stokes Solver • Projection Method • Advection Diffusion and Poisson Eqns. • Code elements and design considerations • Hands-On Coding/Demonstrations	

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9	11/4/24	Coding a 2D Navier-Stokes Solver • Code Elements and Design Considerations • Hands-On Coding/Demonstrations	
10	11/11/24	Version Control • Overview and Basic Concepts • The Git Version Control System • Hands-On Coding/Demonstrations	Project 2
11	11/18/24	Immersed Boundary Methods • Modeling a Deformable Biological Cell • Integrating the Finite Element Method • Hands-On Coding/Demonstrations	
12	11/25/24	Writing Computer Code to Leverage High Performance Computing • Parallelizing a computer code • Data structures, memory access, and operations • Hands-On Coding/Demonstrations	Project 3
13	12/2/24	• Writing Computer Code to Leverage High Performance Computing • Gauging performance: strong and weak scaling • Understanding limits • Hands-On Coding/Demonstrations	
14	12/9/24	Modern HPC Clusters: Brass Tacks • The command line interface • Bash scripts • Running jobs and job schedulers • Hands-On Coding/Demonstrations	
-	**12/16/24**	**Final Project Due**	