Syllabus (Link to latest version)

PHYS 5v48.002 – High Performance Scientific Computing (Spring 2025)

Instructor: Aaron Smith, SCI 3.118, asmith@utdallas.edu
Lectures: Tu/Th 10:00 – 11:15 AM, SCI 2.240
Office Hours: After class until noon, or by appointment

Course Description

This course introduces the principles and practice of high-performance scientific computing with an emphasis on numerical methods relevant for physics. We will cover a broad range of topics:

- **Fundamentals of HPC:** Environments, compilers, CPU/GPU parallel programming.
- **Software Engineering & Optimization:** Modern C++ and Python for high-performance computing (HPC), code profiling, debugging, documentation, and version control.
- **Numerical Methods & Applications:** Finite difference and finite volume methods, boundary conditions, direct/iterative solvers, stability analysis, preconditioning, multigrid methods, explicit/implicit time-stepping. Fluid dynamics (shock waves, advection-diffusion), N-body solvers, Monte Carlo simulations, and more.

The course will be taught by example using standard libraries or proof-of-concept implementations. Materials are drawn from the internet, textbooks, and personal experience. Students will complete regular programming assignments and a major computational project and final presentation, applying techniques relevant to their research interests.

Prerequisites

This course is designed for students engaged in or preparing for research. Expectations:

- Strong background in physics and mathematics (calculus and differential equations).
- Programming experience in Python and willingness to learn C++.

Course Objectives

Upon successful completion of this course, students will be able to:

- **Select** and **implement** appropriate **numerical methods** for solving scientific problems.
- **Use** Python and C++ effectively for high-performance applications for their research.
- **Optimize** code performance with parallel programming (CPU and GPU) strategies.
- **Employ** software engineering best practices for robust, maintainable scientific codes.
- **Present** results clearly using established scientific visualization tools.
- **Collaborate** effectively on code development and large-scale computational projects.

Grading

The course will consist of lectures and hands-on computational labs. There will be in-class pop quizzes for participation credit (5%) and informal assessments to gauge understanding. There will be regular coding assignments due 1-2 weeks after being posted (60%), group presentations on specific numerical techniques or applications (15%), and a major computational project (20%). The project will be individual and involve a research topic that is complementary to each student's research area. Students will propose a topic, provide an interim progress report, and submit a final project with accompanying code and results.

Course Schedule

Below is an outline of topics. Some adjustments to pacing may occur based on class progress.

Topic 1: Introduction to High Performance Computing

- Course overview – goals, expectations, grading, project guidelines.
- What is high-performance computing? – history, possibilities, estimating costs
- Importance for academia and industry – numerical experiments, beyond analytics
- Philosophies of discretization – resolution vs. problem size vs. physical accuracy
- Introduction to programming – pros/cons, ecosystems, template scripts
- Example: Simple Python and C++ "Hello World" + GitHub setup

Topic 2: Fast-Track through Programming Environments

- Command line – Shell scripting, environment configuration, job submission scripts
- Python ecosystem – numpy, scipy, plots, files, notebooks, libraries, package managers
- Build systems and editors – compiling, Makefile, CMake, IDEs, terminal editors (vim)
- Introduction to C++ – variables, operators, logic, functions, imports, data types, memory
- Object oriented programming – classes, memory allocation, modularity, encapsulation
- Speeding up Python – numba (just in time compiler), cython (calling C++ from python), ProcessPoolExecutor, threads, multiprocessing, Joblib, Dask, mpire, JAX, julia, Rust
- Github – version control, asynchronous development, ssh keys, AI copilots and LLMs
- Example: Bash scripting for automating tasks and gather timing information

Topic 3: Parallel Programming + GPU Preview

- Introduction – multiple data, concurrency, strong/weak scaling, timing prediction
- OpenMP – shared memory, multi-threading, clauses, fine-tuning
- MPI – distributed memory, communication, synchronization, data reduction
- GPU – Basic architecture, data transfers, simple kernel examples
- Example: N-Body problems using the different strategies, measure speedups

Topic 4: Numerical Methods Foundations

- Important data structures – trees, (sparse) matrices, hash tables, data frames
- Miscellaneous – interpolation, quadrature integration, root finding, series convergence

- Difference approximations – forward, backward, centered, truncation, accuracy
- Boundary conditions – Dirichlet, Neumann, Robin, periodic
- Integration of ODEs – Runge-Kutta, symplectic operators, implicit/explicit
- Monte Carlo methods – sampling, integration, transport and diffusion
- Fast Fourier transforms – applications, libraries, nested grids, spectral methods
- Example: Adaptive quadrature, root finding, nearest neighbors, 1D heat equation

Topic 5: Direct and Iterative Solvers

- Direct methods – Gaussian elimination, LU decomposition, Cholesky
- Iterative Methods – Jacobi, Gauss-Seidel, Conjugate gradient
- Stability analysis – CFL condition, explicit vs. implicit time-stepping
- Accelerating convergence – Preconditioning, multigrid
- Example: Compare solver performance on a small 2D Poisson equation
- Example: Explicit vs. implicit time-stepping for general ODEs and advection-diffusion

Topic 6: GPU Computing in Depth

- Programming – philosophy, hardware, throughput, advantages, limitations, future plans
- Memory hierarchy – levels of memory, performance characteristics, warps, coalescence
- Performance tuning – data organization, bottlenecks, asynchronous communication, strides, number of threads, memory layout, shared memory, avoiding branching, etc.
- Example: Accelerate a finite difference PDE solver on the GPU, analyze performance

Topic 6: Computational Fluid Dynamics

- Euler equations – conservation laws, advection formalism, Eularian/Lagrangian
- Overview of methods – finite volume, finite element, particles, etc. hydrodynamics
- Flux computations – Godonov methods, Riemann solvers (conceptual), interfaces
- Shock waves – development, jump conditions, capturing vs. tracking
- Example: Implement a 1D finite volume solver for the advection equation
- Example: 1D Sod shock tube test (and potentially 2D Kelvin–Helmholtz instability)

Bonus Topic: Software Engineering

- Unit testing – reproducibility, maintainability, continuous integration
- Tools – debugging, profiling, security, Makefiles, configuration, installation
- Deployment – documentation, collaboration, cloud, supercomputers
- Load balancing – domain decomposition, communication strategies
- Example: Extend previous projects to run on a distributed cluster (MPI)

Bonus Topic: Applicable but taught by other courses

- Statistics – Bayesian inference, Monte Carlo Markov Chains (MCMC)
- Machine learning – Gaussian processes, regression, non-parametric methods
- Deep learning and generative AI – convolutional neural networks

Recommended Textbooks and Resources

There is no official required textbook for this course since there are many high-quality online materials available. However, here is a list of relevant books that we may refer to at times:

- **Effective Computation in Physics: Field Guide to Research with Python**, 1st Edition by Anthony Scopatz and Kathryn Huff (Web version: https://github.com/physics-codes)
- **Numerical Methods for Partial Differential Equations: Finite Difference and Finite Volume Methods**, 1st Edition by Sandip Mazumder
- **Computational Methods for Fluid Dynamics**, 4th Edition by Joel Ferziger, Milovan Perić, and Robert Street
- Scientific Computing with Python: High-performance scientific computing with NumPy, SciPy, and pandas, 2nd Edition by Claus Führer, Jan Erik Solem, Olivier Verdier
- Numerical Recipes: The Art of Scientific Computing, 3rd Edition by William Press, Saul Teukolsky, William Vetterling, and Brian Flannery
- Finite Difference Methods for Ordinary and Partial Differential Equations: Steady-State and Time-dependent Problems, 1st Edition by Randall LeVeque
- Riemann Solvers and Numerical Methods for Fluid Dynamics: A Practical Introduction, 3rd Edition by Eleuterio Toro
- Websites: python website (www.python.org), numpy (numpy.org), scipy (scipy.org), pandas (pandas.pydata.org), matplotlib (matplotlib.org), h5py (h5py.org), GitHub (github.com), Stack Overflow (stackoverflow.com), ChatGPT (chat.openai.com) Bayesian Methods for Hackers (website) **Art of HPC** (website) UW HPSC (website)

General Notes

Inclusion & Diversity

I value all students regardless of their background, country of origin, race, religion, ethnicity, disability status, etc., and am committed to providing a climate of excellence and inclusiveness within all aspects of the course. If there are aspects of your culture or identity that you would like to share with me as they relate to your success in this class, I am happy to meet to discuss. Likewise, if you have any concerns in this area or facing any special issues or challenges, you are encouraged to discuss the matter with me (set up a meeting by email) with an assurance of full confidentiality (only exception being mandatory reporting of academic integrity/code violations, and/or sexual harassment).

Attendance

Students are expected to attend class meetings regularly and to abide by the attendance policy established for the course. It is important that you communicate with the professor and the instructional team prior to being absent, so you, the professor, and the instructional team can discuss and mitigate the impact of the absence on your attainment of course learning goals. Please inform the professor and instructional team if you are unable to attend class meetings because you are ill, in mindfulness of the health and safety of everyone in our community.

If you are experiencing any symptoms of COVID-19 (CDC) please seek medical attention from the Student Health Center or your health care provider PRIOR to coming to campus.

Student Conduct & Discipline

The University of Texas System and The University of Texas at Dallas have rules and regulations for the orderly and efficient conduct of their business. It is the responsibility of each student and each student organization to be knowledgeable about the rules and regulations which govern student conduct and activities. General information on student conduct and discipline is contained in the UTD publication, *A to Z Guide*, which is provided to all registered students each academic year.

The University of Texas at Dallas administers student discipline within the procedures of recognized and established due process. Procedures are defined and described in the *Rules and Regulations, Board of Regents, The University of Texas System, Part 1, Chapter VI, Section 3*, and in Title V, Rules on Student Services and Activities of the university's Handbook of Operating Procedures. Copies of these rules and regulations are available to students in the Office of the Dean of Students, where staff members are available to assist students in interpreting the rules and regulations (SU 1.602, 972/883-6391).

A student at the university neither loses the rights nor escapes the responsibilities of citizenship. He or she is expected to obey federal, state, and local laws as well as the Regents' Rules, university regulations, and administrative rules. Students are subject to discipline for violating the standards of conduct whether such conduct takes place on or off campus, or whether civil or criminal penalties are also imposed for such conduct.

Religious Holy Days

The University of Texas at Dallas will excuse a student from class or other required activities for the travel to and observance of a religious holy day for a religion whose places of worship are exempt from property tax under Section 11.20, Tax Code, Texas Code Annotated.

The student is encouraged to notify the instructor or activity sponsor as soon as possible regarding the absence, preferably in advance of the assignment. The student, so excused, will be allowed to take the exam or complete the assignment within a reasonable time after the absence: a period equal to the length of the absence, up to a maximum of one week. A student who notifies the instructor and completes any missed exam or assignment may not be penalized for the absence. A student who fails to complete the exam or assignment within the prescribed period may receive a failing grade for that exam or assignment.

If a student or an instructor disagrees about the nature of the absence [i.e., for the purpose of observing a religious holy day] or if there is similar disagreement about whether the student has been given a reasonable time to complete any missed assignments or examinations, either the student or the instructor may request a ruling from the chief executive officer of the institution, or his or her designee. The chief executive officer or designee must take into account the legislative intent of TEC 51.911(b), and the student and instructor will abide by the decision of the chief executive officer or designee.

Academic Dishonesty – Plagiarism and Cheating

Academic misbehavior means any activity that tends to compromise the academic integrity of the institution or subvert the education process. All forms of academic misbehavior are prohibited at the University of Texas at Dallas, as outlined in the Student Code of Conduct (https://policy.utdallas.edu/utdsp5003). Students who commit or assist in committing dishonest acts are subject to **downgrading** (to a failing grade for the test, paper, or other course-related activity in question, or for the entire course) and/or **additional sanctions** as described in the Student Code of Conduct.

Cheating: Intentionally using or attempting to use, or intentionally providing or attempting to provide, unauthorized materials, information or assistance in any academic exercise. Examples include: (a) copying from another student's test paper; (b) allowing another student to copy from a test paper; (c) using unauthorized material such as a "cheat sheet" during an exam.

Fabrication: Intentional and unauthorized falsification of any information or citation. Examples include: (a) citation of information not taken from the source indicated; (b) listing sources in a bibliography not used in a research paper.

Plagiarism: To take and use another's words or ideas as one's own. Examples include: (a) failure to use appropriate referencing when using the words or ideas of other persons; (b) altering the language, paraphrasing, omitting, rearranging, or forming new combinations of words in an attempt to make the thoughts of another appear as your own.

Other forms of academic misbehavior include, but are not limited to: (a) unauthorized use of resources, or any attempt to limit another student's access to educational resources, or any attempt to alter equipment so as to lead to an incorrect answer for subsequent users; (b) enlisting the assistance of a substitute in the taking of examinations; (c) violating course rules as defined in the course syllabus or other written information provided to the student; (d) selling, buying or stealing all or part of an un-administered test or answers to the test; (e) changing or altering a grade on a test or other academic grade records.

The faculty expects from its students a high level of responsibility and academic honesty. Because the value of an academic degree depends upon the absolute integrity of the work done by the student for that degree, it is imperative that a student demonstrate a high standard of individual honor in his or her scholastic work.

Legal Notice Regarding Lecture Notes

My lectures and notes are protected by state common law and federal copyright law. You are authorized to take notes in class thereby creating a derivative work from my lecture, but the authorization extends only to making one set of notes for your own personal use and no other use. You are not authorized to record my lectures, to provide your notes to anyone else (hard copy or electronic), or to make any other use of those notes without express prior written permission from me.

Email Use

The University of Texas at Dallas recognizes the value and efficiency of communication between faculty/staff and students through electronic mail. At the same time, email raises some issues concerning security and the identity of each individual in an email exchange. The university encourages all official student email correspondence be sent only to a student's U.T. Dallas email address and that faculty and staff consider email from students official only if it originates from a UTD student account. This allows the university to maintain a high degree of confidence in the identity of all individual corresponding and the security of the transmitted information. UTD furnishes each student with a free email account that is to be used in all communication with university personnel. The Department of Information Resources at U.T. Dallas provides a method for students to have their U.T. Dallas mail forwarded to other accounts. My policy in this class is to **not** communicate any details regarding your grade through email. I will only discuss these details in person with a student.

Withdrawal from Class

The administration of this institution has set deadlines for withdrawal of any college-level courses. These dates and times are published in that semester's course catalog. Administration procedures must be followed. It is the student's responsibility to handle withdrawal requirements from any class. In other words, I cannot drop or withdraw any student. You must do the proper paperwork to ensure that you will not receive a final grade of "F" in a course if you choose not to attend the class once you are enrolled.

Incomplete Grade Policy

As per university policy, incomplete grades will be granted only for work unavoidably missed at the semester's end and only if 70% of the course work has been completed. An incomplete grade must be resolved within eight (8) weeks from the first day of the subsequent long semester. If the required work to complete the course and to remove the incomplete grade is not submitted by the specified deadline, the incomplete grade is changed automatically to a grade of **F**.

Acceptable Student Behavior

Student behavior that interferes with an instructor's ability to conduct a class or other students' opportunity to learn is unacceptable and disruptive and will not be tolerated in any instructional forum at UTD. Students engaging in unacceptable behavior will be directed to leave the classroom and the instructor may refer the student to the Dean of Students to consider whether the student's conduct violated the Code of Student Conduct. The university's expectations for student conduct apply to all instructional forums, including university and electronic classroom, labs, discussion groups, field trips, etc. The Code of Student Conduct can be found at https://conduct.utdallas.edu/handbook/.

Retention of Student Records

Student records pertaining to this course are maintained in a secure location by the instructor of record. All records such as exams, answer sheets (with keys), and written papers submitted during the duration of the course are kept for at least one calendar year after course completion. Course work completed via the Blackboard online system, including grading information and comments, is also stored in a safe electronic environment for one year. You have a right to view your individual record; however, information about your records will not be divulged to other individuals without the proper written consent. You are encouraged to review the Public Information Policy and the Family Educational Rights and Privacy Act (FERPA) laws and the university's policy in accordance with those mandates at the following link: https://registrar.utdallas.edu/legislative-policies/ferpa/

Universal Evaluation System Class Evaluation

Student feedback is important and an essential part of participation in this course. The UES Class evaluation is a requirement for all organized classes at UTD. This short survey will be made available at the end of the semester to provide you with an opportunity to evaluate how this course is taught.

Disability Services

The goal of Disability Services is to provide students with disabilities educational opportunities equal to those of their non-disabled peers. Disability Services is located in room 1.610 in the Student Union. Office hours are Monday and Thursday, 8:30 a.m. to 6:30 p.m.; Tuesday and Wednesday, 8:30 a.m. to 7:30 p.m.; and Friday, 8:30 a.m. to 5:30 p.m. The contact information for the Office of Disability Services is:

The University of Texas at Dallas, SU 22
PO Box 830688
Richardson, Texas 75083-0688
(972) 883-2098 (voice or TTY)

Essentially, the law requires that colleges and universities make those reasonable adjustments necessary to eliminate discrimination on the basis of disability. For example, it may be necessary to remove classroom prohibitions against tape recorders or animals (in the case of dog guides) for students who are blind. Occasionally an assignment requirement may be substituted (for example, a research paper versus an oral presentation for a student who is hearing impaired). Classes enrolled students with mobility impairments may have to be rescheduled in accessible facilities. The college or university may need to provide special services such as registration, note-taking, or mobility assistance.

It is the student's responsibility to notify his or her professors of the need for such an accommodation. Disability Services provides students with letters to present to faculty members to verify that the student has a disability and needs accommodations. Individuals requiring special accommodation should contact the professor after class or during office hours.

Off-Campus Instruction and Course Activities

Off-campus, out-of-state, and foreign instruction and activities are subject to state law and University policies and procedures regarding travel and risk-related activities. Information regarding these rules and regulations may be found at the website address given below. Additional information is available from the office of the school dean.
(http://www.utdallas.edu/Business Affairs/Travel_Risk_Activities.htm)

These descriptions and timelines are subject to change at the discretion of the Professor.