

## Syllabus for Computational Physics Laboratory (C-lab)

### Spring semester 2024

Course Name: **5001 Special Topics Physics**

Course Number: **Physics 5001**

Course Credits: **3 hours**

Prerequisites: **Physics 2305 or 2311 (Modern Physics)**

Instructor: **Prof. Julia E. Medvedeva (juliaem@mst.edu)**

Meeting times: **Wednesdays and Fridays, 1pm-3:50pm**

Meeting place: **Physics 128 (CLC)**

### Course Description

Computational project-based studies in the areas of fundamental, applied or data physics, astronomy, quantum chemistry, material science and related fields. All levels of programming skills are welcome. The semester-long individual projects will begin with identifying problems amenable to solution via computations and/or computer simulations and developing a research plan that includes formulation of proper mathematical model, choosing suitable existing computational tools and/or code writing. Atomistic or ab-initio computer simulations using FLAPW, Quantum Espresso, Siesta, or LAMMPS on the S&T HPC cluster, The Foundry, as well as Linux, bash-scripting, Python visualization and data analysis.

In addition to several examples of computational projects with specific methods, algorithms, approaches and their realization on HPC, the following **general topics will be covered in 40-50 minute in a few lectures**: 1) Significance and history (timeline) of scientific computing and algorithm evolution; 2) What is HPC? Top 500 high-performance computers; 3) Campus HPC cluster, The Foundry; 4) Linux operating system; 5) Running Matlab on Foundry: interactive GUI vs parallel mode; 6) Bash scripting in Linux; 7) Using Conda or pip to install python packages; 8) Data science and visualization with Python: matplotlib, numpy, pandas.

### Student Learning Outcomes

Students shall be able to:

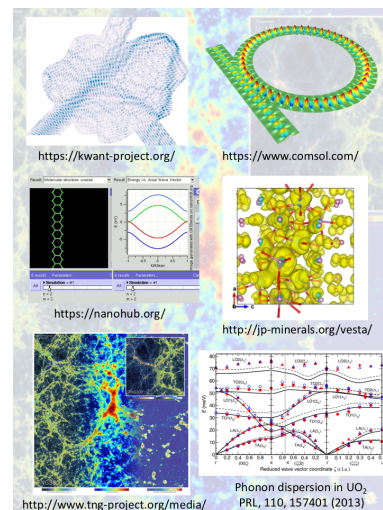
- Know the basics in Linux operating system, bash scripting, HPC, and python visualization
- Prepare and run sequential and parallel jobs on campus HPC cluster, Foundry
- Develop a research plan for a specific computational problem
- Choose appropriate tools, methodologies, and/or programming language to solve scientific problems and determine advantages and limitations of the approach
- Carry out research tasks to achieve project objectives
- Analyze the data, interpret the results, derive conclusions, make predictions
- Articulate the research project and its outcomes in oral/written way

### Learning resources

There is no required textbook. Several books on Python, Linux, MatLab, and Computational Physics are available to borrow from the Instructor on the first-come-first-served basis.

### Evaluation of Student Performance

1. Weekly 10-minute progress report/discussion/troubleshooting: *10% of the grade*
2. Homework assignments: *10% of the grade*
3. Research Project Plan: *20% of the grade*
4. Mid-term Progress Report: *20% of the grade*
5. Final report (presentation or paper): *40% of the grade*



## Statement about Copyright, FERPA, and Use of Video

It is vitally important that our classroom environment promote the respectful exchange of ideas. This entails being sensitive to the views and beliefs expressed during discussions, whether in class or online. Please obtain instructor permission before recording any class activity. It is a violation of University of Missouri policy to distribute such recordings without authorization and the permission of all who are recorded. More information is provided [online](#).

## Accessibility and Accommodations

It is the university's goal that learning experiences be as accessible as possible. Student Accessibility and Testing provides services and accommodations that facilitate full participation in Missouri S&T's learning experience for students with disabilities. If you anticipate or experience physical, academic, and/or digital barriers due to a disability, please contact Student Accessibility and Testing at (573) 341-6655, email [dss@mst.edu](mailto:dss@mst.edu), or visit <https://saat.mst.edu/> for information.

## Student Honor Code and Academic Integrity

- All students are expected to follow the [Honor Code](#).
- [Student Academic Regulations](#) describes the student standard of conduct relative to the University of Missouri System's Collected Rules and Regulations section 200.010, and offers descriptions of academic dishonesty including cheating, plagiarism, sabotage, and **unauthorized use of artificially generated content**, any of which will be reported to the Vice Provost for Undergraduate Education.
- Other resources for students regarding academic integrity can be found [online](#).

## [Student Well-Being](https://wellbeing.mst.edu/) (<https://wellbeing.mst.edu/>)

Your well-being is important, and it contributes to your success in this course. At S&T, we provide resources to support your mental, physical, and social well-being. Any of us can experience challenges that make learning difficult. If you are struggling, take advantage of the following resources offered by the university:

### Student Well-Being

Student Well-Being provides counseling services, health promotion initiatives, and prevention programs to empower the S&T community to thrive and enhance personal, academic, and professional success. Department office hours are Monday-Friday, 8 a.m. – 5:00 p.m. On the website, you can find information related to confidential individual and group counseling, wellness consultations and trainings, resources for many health and wellness topics, and help for mental health crisis situations.

For the National Suicide Prevention Lifeline, call or text 988, or visit [missouri988.org](https://missouri988.org).

[Health and Well-Being Canvas Course](https://umsystem.instructure.com/enroll/G3LY3G) (<https://umsystem.instructure.com/enroll/G3LY3G>) The Health and Well-Being Canvas Course features trainings, presentations, and other health and well-being resources for students. The course is free for all students, is non-credit, and students can enroll at any point in the semester.

[Student Support and Community Standards](#) is your “Google Maps” for support. During your time at S&T, you or a friend may need help navigating their student experience, facing a barrier, or experiencing a challenge. You are not alone!

Student Support has a dedicated team and numerous resources such as [UCARE](#) and the [student emergency fund](#) to help you navigate the S&T experience and support your success. This includes support to address barriers related to academic, personal, emotional, medical, financial, or any other needs. All students can learn and grow from challenges or setbacks, they are stepping stones to success and we are here to help.

### **Nondiscrimination, Equity, and Title IX**

Missouri S&T is committed to the safety and well-being of our campus community, and to creating an environment free from discrimination and harassment.

The University prohibits discrimination and harassment on the basis of race, color, national origin, ancestry, religion, sex, pregnancy, sexual orientation, gender identity, gender expression, age, disability, protected veteran status, and any other status protected by applicable state or federal law. As used in this policy, the word “sex” is also inclusive of the term “gender.”

Additionally, US Federal Law Title IX states that no member of the university community shall, on the basis of sex, be excluded from participation in, or be denied benefits of, or be subjected to discrimination under any education program or activity. Sexual harassment violations of this law include quid pro quo, hostile environment, sexual assault, dating/domestic violence, and stalking. The U.S. Department of Education has stated the prohibition on discrimination on the basis of sex includes sexual orientation and gender identity.

Students who are experiencing pregnancy or pregnancy-related conditions, including the birthing parent and non-birthing parent, have rights protected under Title IX. Students should contact the Office of Equity and Title IX to learn more about their rights and pregnancy-related assistance/accommodations provided by the University to ensure equitable access to University educational programs and activities.

In accordance with the University of Missouri’s Collected Rules and Regulations, all faculty and staff are required to report any information concerning discrimination disclosed through communication including, but not limited to, direct conversation, email, social media, classroom papers and homework exercises to the Equity Officer/Title IX Coordinator.

For more information regarding support for those that have been impacted or to report an incident of discrimination or harassment as defined by [Chapter 600](#) of the University’s Collected Rules and Regulations, visit the Office of Equity and Title IX or visit their website at [equity.mst.edu](http://equity.mst.edu).

### **Office of Equity and Title IX**

Equity Officer and Title IX Coordinator: Dr. Paul Hirtz

Phone: (573) 341-7734 Location: 900 Innovation Drive, Suite 500 E-mail: [equity@mst.edu](mailto:equity@mst.edu)

### **Classroom Egress Maps**

For all in-person instruction, faculty should explain where the classroom emergency exits are located. Classroom egress maps are posted at <http://designconstruction.mst.edu/floorplan/>.

### **Learning Assistance through LEAD**

The Learning Enhancement Across Disciplines (LEAD) program runs Learning Centers and Tutoring which provide an efficient means to improve your understanding and increase your mastery of the material you are studying. Discipline-based faculty and undergrad peer instructors operate open-environment learning centers in nearly every foundational course as well as many upper-level courses. See the schedule for LEAD learning assistance at <https://lead.mst.edu/schedule/>.

### **Writing and Communication Center**

The Writing and Communication Center’s mission is to assist all students in their efforts to become better writers, communicators, and critical thinkers. The Center’s peer consultants and coaches provide free individualized one-on-one and small-group conversations to offer meaningful feedback and guidance to

students across all disciplines. More information can be found on our website, through email: [writing@mst.edu](mailto:writing@mst.edu) or stop by Curtis Laws Wilson Library 314–315.

### **Student Success Center**

The Student Success Center (SSC) supports student development through peer Academic Mentoring focusing primarily on STEM courses, peer-to-peer soft skill coaching which can also act as an accountability buddy, and campus programming – all while providing free coffee and hot beverages! All undergraduate students are encouraged to utilize the SSC's free services to get timely support and to enhance their S&T Miner Experience. Contact us at [success@mst.edu](mailto:success@mst.edu) OR 573-341-7590. To see the course offerings and times for SSC Academic Mentoring, visit <https://studentsuccess.mst.edu/academicmentoring/>.

### **Knack Tutoring (<https://mst.joinknack.com/>)**

Enrolled S&T undergraduate students can receive complimentary **FREE** tutoring assistance from peers who have successfully completed the course, available round the clock. You have the option to connect via the Knack platform online or in person on campus. If you've excelled in a course, consider becoming a Knack Tutor to support your fellow Miners!

### **Student Veterans Resource Center**

The Student Veterans Resource Center (SVRC) is the nexus of resources and support for student veterans at S&T. The SVRC provides student veterans with a “safe space” and a familiar atmosphere. The center's Veteran Consuls provide one-on-one consultations to guide students to various resources on campus, while its advisor provides students with VA health and benefits resources. Visit the SVRC at Harris Hall, Suite G10, and contact us at [svrc@mst.edu](mailto:svrc@mst.edu).