# PHYS 410 Senior Computational Physics Capstone

Fall 2022 Lecture: Monday and Wednesdays 8:30 – 10:20 am Classroom: Exploratory Hall, Room 1004

# Instructor:

- Dr. Fernando E. Camelli
- Phone: 703-993-4073 (Office)
- E-mail: <u>fcamelli@gmu.edu</u>
- Office Hours:
  - In person Wednesdays from 10:30 11:30 am
  - virtual or in person by appointment.
- Course Modality: face-to-face.
- Prerequisites: PHYS 251 and (PHYS 325 or ASTR 401) and PHYS 303 and PHYS 305

# **Course Description:**

This course synthesizes your undergraduate experiences with scientific computing and is designed to prepare you for a career in computational physics and engineering. It focuses on numerical methods for solving all the major problems in scientific computing, including linear and nonlinear equations, least squares, eigenvalues, optimization, interpolation, integration and differentiation, ordinary differential equations, and Fast Fourier transform. You will solidify your skills in constructing computational methods to solve problems as they arise in the sciences and engineering.

#### About this Class:

Each class meeting will be split into two parts. In the first part, new information will be presented. In the second part, students will work on problems that will appear the homework assignment due at the start of the following class.

#### **Objectives:**

- 1. To fulfill the capstone requirement for the Physics major
  - a. physics knowledge integration
  - b. knowledge application
  - c. knowledge reinforcement
- 2. To demonstrate proficiency in computational physics
  - a. numerical methods
  - b. computational techniques
  - c. problem solving
  - d. interpretation
  - e. write your own code
  - f. written and oral communication
- 3. To fulfill the writing-intensive requirement for the Physics major
  - a. writing instruction
  - b. instructor feedback
  - c. writing assignments totaling at least 3500 words

### Writing Intensive Course:

PHYS 410 has been approved by the Faculty Senate Writing Across the Curriculum Committee to fulfill the Writing Intensive requirement of the Physics B.S. degree. Three short papers, all related to a final project, will be required, two of which will undergo a draft-comment-revision process. A first draft of the first paper, 3 to 4 pages (single-space equivalent, or 1500 – 2000 word) research proposal presenting the ideas and justification for the project, is due at the end of week 4, and the final draft is due at the end of week 6. A first draft of the second paper, 3 to 4 pages (single-space equivalent, or 1500 – 2000 word) technical report describing some core aspect of the project, is due at the end of week 8, and the final draft is due at the end of week 10. A minimum 5 pages (single-space equivalent, or 2500 word) research paper summarizing the project is due at the end of the last week of the semester. At least 11 pages (single-space equivalent, or 5500 words) of professional-style writing will be produced.

Competencies: 3 papers, 2 of them with drafts; and presentation: 30%

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1.	Research proposal, draft required:			5%
	a.	Physics:	1%	
	b.	Computation:	1%	
	C.	Writing:	3%	
2.	Technical paper, draft required:			5%
	a.	Context/Motivation:	1%	
	b.	Computation:	2%	
	C.	Writing:	2%	
3.	Research paper:			10%
	a.	Physics:	2%	
	b.	Computation:	2%	
	C.	Integration:	2%	
	d.	Writing:	4%	
4.	Presentations:			10%
	a.		1%	
	b.	Technical talk:	2%	
	C.	Research project:	7%	

# **Course Expectations**

- 1. Review or introduction of computational physics topics
  - a. Computers
  - b. Theory
  - c. Errors and uncertainties
  - d. Interpolation
  - e. Numerical solutions
  - f. Differentiation
  - g. Integration
  - h. ODEs
  - i. PDEs
  - j. Matrices
  - k. Monte Carlo
  - I. Fourier Analysis
  - m. Time Series

Complete lecture notes are available online. The first three topics should be reviewed separately; no class time will be spent on them, but the first homework exercise will be based on them. Each of the remaining topics will be covered in a single class session. Once the topics are covered, no further formal lectures will be given. Class period times will be used for tutorial and help sessions to ensure progress is being made on homework exercises and research projects.

- Homework exercises: Homework exercises reinforce and practice the material methods and techniques of presented above. You should have these in your computational toolbox, particularly as you undertake your research project. Prompt completion of the exercises ensures your comprehension, but also frees up time to work on the research projects.
- 3. Research project: If you are involved in an ongoing project that involves computation, you may continue with or even expand that effort. Otherwise, you will have to come up with one on your own, in consultation with the instructor. Consider as simulator, game, data analysis, etc. For specific ideas of what's been done before in undergraduate courses, consult:

http://phycomp.technion.ac.il/~comphy/projects\_class.html https://www.asc.ohio-state.edu/physics/ntg/780/project\_list.php http://physics.oregonstate.edu/~landaur/nacphy/ComPhys/

Your research project must include writing your own research code. It is allowed to use libraries. If you choose to use an external library, you must show understanding of what is the library doing. It is not acceptable to copy code from others without proper recognition. The final code should be at least 70 percent of your own writing.

- 4. Research proposal: Plan, design, and cost-out (in terms of time) your research project.
- 5. Technical note: Describe, in detail, a computational component of your research project. The description should include a presentation of the problem the component solves, how it solves the problem, code snippets the component, an explanation of how to use the component, and an assessment of how the component solves the problem defined.
- 6. Research paper: A complete report on your research project, include its motivation, design, and outcome.

Final drafts must be submitted in pdf. Preliminary drafts of the research proposal and the technical note are required. Failure to submit a draft result in no credit for the paper. Drafts must be submitted far enough in advance of a final draft due date to allow them to be reviewed and returned, and their comments incorporated into the final draft.

# Notebooks:

Complete records of all activities should be kept as evidence for the veracity of reported results. These records should be permanent and referable in case questions arise either later in an investigation or after publication in any form. Typically, a notebook, of the sort without loose paper, such as a bound composition notebook is preferred. A spiral notebook is acceptable, but a three-ring binder is not. Pages in the notebook should be numbered consecutively, either by the manufacturer or by hand, and never removed from the notebook. Entries should never be erased or blacked/whited out. A single line through a mistake is all that is necessary. The notebook is often left at the site of a running experiment, so that there is no chance that it can be lost or damaged during transport. You should be able to produce such a record for the work you present in this course or else face a grade of zero (0) for the work reported.

# Grading:

- Homework Exercises: up to 6 exercise sets, 30%
- Computational Research Project:
- 3 papers and presentation: 30%

Letter Grades:

- > 97: A+
- 93 to 96.9: A
- 90 to 92.9: A-
- 87 to 89.9: B+
- 83 to 86.9: B
- 80 to 82.9: B-
- 77 to 79.9: C+
- 73 to 76.9: C
- 70 to 72.9: C-
- 60 to 69.9: D
- < 60: F

# Textbooks:

There is not a required textbook for this course. The following list is a sample of the books available in the University Library. Some of these books are available online through the University. The course will not follow any specific book.

40%

- <u>"Numerical Methods in Physics with Python"</u>, A. Gezerlis, 2020. **RECOMMENDED**.
- "Computational Physics", Mark Newman, 1<sup>st</sup> Edition revised and expanded, 2013.
- <u>"Computational Physics: Problem Solving with Python"</u>, Rubin H. Landau, Manuel J. Paez and Cristian C. Bordeianu, 3<sup>rd</sup> Edition, 2015.
- <u>"Elementary Mechanics Using Python"</u>, Anders Malthe-Sørenssen, 2015.
- <u>"A Primer on Scientific Programming with Python"</u>, Hans Petter Langtangen, 4<sup>th</sup> Edition, 2014.
- "Numerical Analysis", Tim Sauer, 2<sup>nd</sup> Edition, 2014.
- "Numerical Analysis", Richard L. Burden and J. Douglas Faires, 1993.
- "Python and Matplotlib Essentials for Scientists and Engineers", Matt A. Wood, 2015.
- <u>"Mastering Matplotlib"</u>, Duncan M. McGreggor, 2015.
- <u>"Introduction to Programming in Python: An Interdisciplinary Approach"</u>, Robert Sedgewick, Kevin Wayne and Robert Dondero, 2015.
- <u>"Numerical Python: A Practical Techniques Approach for Industry"</u>, Robert Johansson, 2015.
- <u>"NumPy: Beginner's Guide"</u>, Ivan Idris, 3<sup>rd</sup> Edition, 2015.
- <u>"NumPy Essentials"</u>, Leo Chin and Tanmay Dutta, 2016.
- <u>"SciPy and NumPy"</u>, Eli Bressert, 2012.
- <u>"Python Data Analytics: Data Analysis and Science Using Pandas, matplotlib, and the Python</u> <u>Programming Language</u>", Fabio Nelli, 2015,

#### Additional references:

The following are additional references covering Computational Physics at the Junior/Senior undergraduate level.

- "Computational Physics", Nicholas Giordano and Hisao Nakanishi, 2<sup>nd</sup> Edition, 2006.
- <u>"Basic Concepts in Computational Physics"</u>, Benjamin A. Stickler and Ewald Schachinger, 2014.
- "A Course on Mathematical Methods for Physicists", Russel L. Herman, 2013.
- "Introduction to Computational Science: Modeling and Simulation for the Sciences", Angela B. Shiflet George W. Shiflet, 2006.

### Other links:

- Finding E-Books at Mason: [1]
- A list of computational physics books: [2]
- Instructor resources for undergraduate computational physics: [3]

# **Email Communication:**

Please send all your question to me via email. Here are a few thinks to remember to make email communication better.

- Please use your name in the salutation so that I do not have to look up your name given only your Mason email address. There is a way of setting up your email, consequently your full name appears in the header - see below.
- If you have a question about a program, copy it inline in the email body, or attach it.
- Always tell me what you tried and read and be very specific about your point of confusion. Otherwise, I may guess incorrectly why you are confused. For example, if you say "I don't know where to start" I may guess that you don't know how to use a keyboard or that you need to be told "at the beginning". You will oftentimes find that if you write out a question, in the process of trying to make yourself clear about your point of confusion, you will realize the answer to your question.

If you want to make any instructor happy, do all the above in all your email communications.

How to show your full name in MasonLive emails:

- 1. Log in to your MasonLive account.
- 2. Click on the 'Settings Gear' at the top right of your window, then select 'Options' from the drop-down list.
- 3. On the left-hand menu click 'General', then click on 'My Account'.
- 4. On the 'My Account' screen, type in your full name in the 'Display Name' area, then click 'Save'.

#### **Collaboration Policy:**

You may collaborate with other students on your homework. *However, the write-up and code that you turn in must be independent.* I suggest starting the homework prior to having any discussion with other students. Turning in a write-up or code that is similar to another student's will be treated as an <u>honor code violation</u>. The best way to avoid an honor code violation is to have someone look at your work when you are stuck and have them suggest modifications (rather than looking at someone else's work). *Plagiarism will not be tolerated.* If you collaborate with another student, you must indicate the name of the student on your write-up and/or code.

#### **Referencing Policy:**

It is quite unlikely that any homework problem will have a solution available on an external website, and you are encouraged to use other resources to help you with parts of a problem. If you used a website or a

book while doing your homework, please reference it. This is a good habit to have when you do any programming or writing.

#### Software:

All software needed for this course is available to GMU students free of charge. Students will build on example code in Python; no prior experience with other languages is expected. We will also experiment with Python during the class.

# Academic Calendar: GMU Academic Calendar

# **University Policy:**

The University Catalog, <u>http://catalog.gmu.edu</u>, is the central resource for university policies affecting student, faculty, and staff conduct in university academic affairs. Other policies are available at <u>http://universitypolicy.gmu.edu/</u>. All members of the university community are responsible for knowing and following established policies.

# Policies in Continuing Pandemic:

All students taking courses with a face-to-face component are required to follow the university's public health and safety precautions and procedures outlined on the university Safe Return to Campus webpage (<u>https://www2.gmu.edu/safe-return-campus</u>). Similarly, all students in face-to-face and hybrid courses must also complete the Mason COVID Health Check daily, seven days a week. The COVID Health Check system uses a color code system and students will receive either a Green, Yellow, or Red email response. Only students who receive a "green" notification are permitted to attend courses with a face-to-face component. If you suspect that you are sick or have been directed to self-isolate, please quarantine or get testing. Faculty are allowed to ask you to show them that you have received a Green email and are thereby permitted to be in class.

#### **Disability Accommodations:**

If you have a learning disability or other condition that may affect academic performance, please: a) make sure documentation is on file with Office of Disability Services (SUB I, Rm. 4205; 993-2474; <u>http://ods.gmu.edu</u>) to determine the accommodations you need; and b) talk with me to discuss your accommodation needs.

#### Counseling and Student Support:

- Counseling and Psychological Services provides confidential psychological services, including 24/7 crisis intervention and consultation to faculty and staff: <u>http://caps.gmu.edu/</u>
- Student Support helps students negotiate life situations by connecting them with appropriate on- and off-campus resources <u>http://studentsupport.gmu.edu/referral-form/</u>

# Celebrating our Diversity:

The College of Science, an intentionally inclusive community, promotes and maintains an equitable and just work and learning environment. We welcome and value individuals and their differences including race, economic status, gender expression and identity, sex, sexual orientation, ethnicity, national origin, first language, religion, age, and disability.

- We value our diverse student body and desire to increase the diversity of our faculty and staff.
- We commit to supporting students, faculty and staff who have been the victims of bias and discrimination.
- We promote continuous learning and improvement to create an environment that values diverse points of view and life experiences.

- We believe that faculty, staff, and students play a role in creating an environment that engages diverse points of view.
- We believe that by fostering their willingness to hear and learn from a variety of sources and viewpoints, our students will gain competence in communication, critical thinking and global understanding, aware of their biases and how they affect their interactions with others and the world.

# Mason University Life religious holiday calendar:

# https://ulife.gmu.edu/religious-holiday-calendar/

It is your responsibility, within the first two weeks of the semester, to let me know the dates of major religious holidays on which you will be absent or unavailable due to religious observances.

#### Student Privacy: https://registrar.gmu.edu/ferpa/

#### Student services:

- Keep Learning, Learning Services (<u>learningservices.gmu.edu/keeplearning/</u>)
- University Libraries (<u>library.gmu.edu</u>)
- Writing Center (writingcenter.gmu.edu)
- Counseling and Psychological Services (<u>caps.gmu.edu</u>)