

NUCL 497
Introduction to Computational Physics
Spring 2025

CRN: 13213

Course Credits: 3

Meeting day(s) and time: TR 10:30-11:45 am

Instructional Modality: In person and one-on-one interaction with Professor

INSTRUCTOR: Prof. A. Hassanein POTR 376C 49-69731
hassanein@purdue.edu

Office Hours: Anytime in arrangement with the professor
Various days or times are available to accommodate students' schedule for consultation either by email or in person

Textbook: No specific textbook is required

Reference books

Recommended: Numerical Recipes (W. H. Press, et al., Cambridge University Press)

Additional Reading Material

Radiation Effects on Reactor Materials
Fortran 90/95 For Scientists and Engineers (S. Chapman)
<http://www.fortran90.org/index.html>

ONLINE COURSE INFO: **Brightspace.** <https://purdue.brightspace.com/>

Notes. Materials if provided in class and **Brightspace** are only for your personal use. Please do not distribute them to public domain.

Course Description

This course requires knowledge of radiation effects on reactor materials (e.g., NUCL 420 or equivalent) and computer programming languages, preferably FORTRAN 90. The course provides an introduction to computational radiation effects on materials. These may include introduction to analytical methods, Monte Carlo, and Molecular Dynamics techniques for solving of various problems such as particles interaction and transport. The course will be based on project-oriented problems and could be different for each student and several individual lectures depending on each student's project. Each student may work individually with the professor regarding their homework progress and their projects and meet separately at agreeable times to learn details of computational methods for their own project and homework assignments.

Learning Outcomes

- 1) Learn about numerical algorithms (e.g., Monte Carlo and Molecular Dynamics) for the analysis of fundamental physics processes in engineering systems;
- 2) Acquire experience in implementation of these algorithms for the analysis of different problems related to nuclear engineering and particularly in radiation effects;
- 3) Develop/run computer codes to study engineering and physics problems, for example, particles diffusion and retention in various materials considered in nuclear fission/fusion reactors; heat transfer in nuclear reactor components; heating of plasma facing materials; Monte Carlo (MC) and Molecular dynamics (MD) modeling of energy deposition and erosion of materials by energetic particles.

GRADING:

50%	Homework Progress
50%	Final Project & Presentation

The course grade will be based on homework and final project performance as:

A:	90-100
B:	80-89
C:	70-79
D:	60-69
F :	< 60

HOMEWORK:

Homework assignments are intended to help students in gaining experience in code analysis to prepare for their final project. Students are expected to work independently on the assignments and each working individually with the professor. Discussions and some cooperation between students are allowed on a general level but computer codes and reports should be independently run and analyzed.

Final Project & Presentation

Each student may choose a subject/case to study. The project topics include, but are not limited to, particles diffusion and retention in various materials considered for nuclear reactors; heat transfer in reactor components; heating of plasma facing materials in fusion reactor; Monte Carlo/Molecular Dynamics modeling of energy deposition and interactions in materials by energetic particles.

Students will make several 15-20 minutes PowerPoint presentation with the discussion of methods implemented, a short description of engineering problems solved using developed codes and analysis of obtained results utilizing visualization methods.

The final presentations will be scheduled during the final week of the class.

Schedule

The course schedule is for each student to study:

- (1) Radiation effects on reactor materials and materials under extreme conditions
- (2) Monte Carlo (MC) methods and codes for the solution of different problems
- (3) Molecular Dynamics (MD) methods and codes for the solution of different problems

Schedule and assignments subject to change. Any changes will be communicated to the students or posted in Brightspace

Academic Integrity

Purdue honors pledge: “As a boilermaker pursuing academic excellence, I pledge to be honest and true in all that I do. Accountable together - we are Purdue.”

Academic integrity is one of the highest values that Purdue University holds. Individuals are encouraged to alert university officials to potential breaches of this value by either emailing integrity@purdue.edu or by calling 765-494-8778. While information may be submitted anonymously, the more information is submitted the greater the opportunity for the university to investigate the concern. More details are available on our course Brightspace table of contents, under University Policies.

Course materials on Brightspace considered to be derivative works and cannot be distributed without my express written permission.

Accessibility

Purdue University strives to make learning experiences as accessible as possible. If you anticipate or experience physical or academic barriers based on disability, you are welcome to let me know so that we can discuss options. You are also encouraged to contact the Disability Resource Center at: drc@purdue.edu or by phone: 765-494-1247.

Mental Health Statement

If you find yourself beginning to feel some stress, anxiety and/or feeling slightly overwhelmed, try [WellTrack](#). Sign in and find information and tools at your fingertips, available to you at any time.

If you need support and information about options and resources, please contact or see the [Office of the Dean of Students](#). Call 765-494-1747. Hours of operation are M-F, 8 am- 5 pm.

If you find yourself struggling to find a healthy balance between academics, social life, stress, etc. sign up for free one-on-one virtual or in-person sessions with a [Purdue Wellness Coach at RecWell](#). Student coaches can help you navigate through barriers and challenges toward your goals throughout the semester. Sign up is completely free and can be done on BoilerConnect. If you have any questions, please contact Purdue Wellness at evans240@purdue.edu.

If you're struggling and need mental health services: Purdue University is committed to advancing the mental health and well-being of its students. If you or someone you know is feeling overwhelmed, depressed, and/or in need of mental health support, services are available. For help, such individuals should contact [Counseling and Psychological Services \(CAPS\)](#) at 765-494-6995 during and after hours, on weekends and holidays, or by going to the CAPS office on the second floor of the Purdue University Student Health Center (PUSH) during business hours.

Emergency Preparation

In the event of a major campus emergency, course requirements, deadlines and grading percentages are subject to changes that may be necessitated by a revised semester calendar or other circumstances beyond the instructor's control. Relevant changes to this course will be posted onto the course website or can be obtained by contacting the instructors or TAs via email or phone. You are expected to read your @purdue.edu email on a frequent basis.