

# NE 491/591 Monte Carlo Methods and Applications

## Fall 2024, 3 Credit Hours

## **1** Course Information

 Note: This course is expected to become a permanent course by the end of 2024: NE 470/570 Monte Carlo Methods for Radiation Transport Graduate students will be able to claim this course for Qualification Exam Part 1 (QE1) using the course number "NE 591". "NE 570" may work as well for QE1 but please confirm with Mario.

### • Schedule

- Time: Tuesdays and Thursdays, 1:30 PM 2:45 PM
- Location: Room 331, 111 Lampe Drive
- *Course website:* **Moodle** will be used to post lecture notes, homework, computer projects and other materials.
  - https://moodle-courses2425.wolfware.ncsu.edu/course/view.php?id=4252
- Lecture recordings: Panopto will be used to host the lecture recordings. https://ncsu.hosted.panopto.com/Panopto/Pages/Sessions/List.aspx#folderID=%2 2a9751aa0-199a-458d-bf9f-b1c200c535b1%22
- Instructor 1
  - Instructor: Dr. Xu Wu, Assistant Professor of Nuclear Engineering
  - Office: Burlington Laboratory 2110
  - Office Hours: Tuesdays, 3:00 5:00 PM, in-person, or Zoom (by appointment)
  - Phone: 919-515-6570
  - Email: xwu27@ncsu.edu
  - Website: https://www.ne.ncsu.edu/people/xwu27
- Instructor 2
  - Instructor: Dr. John Zino, Associate Teaching Professor of Nuclear Engineering
  - Office Hours: TBD
  - Phone: (910) 398-2832
  - Email: jfzino@ncsu.edu, John.Zino@ge.com
  - Website: https://www.ne.ncsu.edu/people/jfzino
- Teaching Assistant
  - TA: Mahmoud Yaseen
  - Email: mqyaseen@ncsu.edu
  - Office Hours: Wednesdays 1:00 3:00 PM



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# 2 Course Description

- This course provides a detailed discussion over the fundamental concepts associated with the Monte Carlo (MC) method for particle/radiation transport. Students will be able to learn the fundamental and advanced topics on the application of MC to solve radiation transport problems in nuclear engineering.
- Applications of generalized MC techniques using the MCNP code to solve neutron, photon, and electron radiation transport problems typically encountered in reactor physics, shielding, criticality safety, and radiation dosimetry will be addressed. The students will also learn how to use the MCNP code to solve these problems.

# 3 Student Learning Outcomes

- The students completing this course will be able to:
  - analyze random variables and their relation to random numbers;
  - develop codes to sample random numbers using the fundamental formulation of MC;
  - generate random numbers using Pseudo-Random Number Generators (PRNGs) and test their randomness;
  - apply the fundamentals of probability and statistics to the design and interpretation of MC techniques for particle transport problems;
  - evaluate numerical integrals and reduce their variances using different MC approaches;
  - build MC models and write numerical codes to solve the fixed-source MC particle transport problem, and reduce the variance using various approaches;
  - apply MC in particle transport problems, such as geometry modeling, particle tracking, data, physical processes, scoring and tallying, and eigenvalue/criticality calculations;
  - use the MCNP v6.2 code for several representative real-world neutron transport problems, including building input decks, running the simulations, and interpreting the simulation results.
- Additionally, the graduate students completing this course (NE 570) will be able to:
  - implement advanced variance reduction techniques for fixed source MC particle transport, such as PDF biasing with Russian roulette, particle splitting with Russian roulette, weightwindow technique, integral biasing, and hybrid method (CADIS and FW-CADIS). This will be evaluated in Homework 5.
  - solve more advanced radiation transport problems using the MCNP code, such as the deep penetration streaming problem with MC particle transport. This will be evaluated in computational project 6.
  - employ various types of advanced Monte Carlo particle biasing techniques to reduce the tally variance using a deep penetration streaming problem where students simulate gamma-ray radiation transport through a narrow streaming path from the source to a detector.
  - simulate an actual detector response and makes direct comparison between calculated and measured values for a benchmark calibration experiment.
  - build the entire 3-D radiation transport model in the MCNP code from scratch.



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## 4 Prerequisites

- A basic understanding of nuclear reactor physics is needed, as in NE 301 (Fundamentals of Nuclear Engineering), or an equivalent undergraduate course.
- Background in Probability and Statistics is desirable, equivalent to ST 311 (Introduction to Statistics) and ST 371 (Introduction to Probability and Distribution Theory).
- Programming experience (e.g., Python, MATLAB) will be required.

# 5 Outline of Topics

### Part 1: Monte Carlo Theories for Radiation/Particle Transport

- 1. Random Variables and Sampling (1 week)
  - Discrete and Continuous Random Variables
  - Random Numbers
  - Fundamental Formulation of Monte Carlo (FFMC)
  - Sampling Procedures for One-dimensional and Multi-dimensional Density Functions
- 2. Random Number Generator (RNG) (1 week)
  - Random Number Generation Approaches
  - Pseudo-Random Number Generators (PRNGs)
  - Randomness Testing
- 3. Fundamentals of Probability and Statistics (2.5 weeks)
  - Statistical Moments
  - Sample Statistics
  - Common Discrete and Continuous Distribution Functions
  - Limit Theorems
  - Relative Uncertainty and Confidence Levels
  - Normality Tests
- 4. Monte Carlo Integrals and Variance Reduction Techniques (1.5 weeks)
  - Numerical Integrals with Monte Carlo
  - Variance Reduction Techniques
    - Importance sampling
    - Control variates
    - Stratified sampling
    - Combined sampling
- 5. Fixed-Source Monte Carlo Particle Transport (2 weeks)



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- The Linear Boltzmann Equation (LBE)
- MC for Simplified Particle Transport
- Perturbation via Correlated Sampling
- Statistical Reliability of MC Results
- Variance Reduction for Fixed-Source Particle Transport
  - PDF biasing with Russian roulette
  - Particle splitting with Russian roulette
  - Weight-window technique
  - Integral biasing
  - Hybrid method (CADIS and FW-CADIS)

### Part 2: Monte Carlo Applications with the MCNP Code

6. Geometry Modeling and Particle Tracking (2 weeks)

- Generalized Geometry
- Surfaces
- Repeated structures geometry
- Particle Tracking
- 7. Physics & Data in MCNP (2 weeks)
  - Source definition
  - Materials/Physics Input
  - Cross-sections
  - Scattering tables *S*(*α*, *β*)
- 8. Scoring/Tallying (2 weeks)
  - Major Physical Quantities in Particle Transport
    - Flux (surface, volume), current, track-length, dose, energy deposition, pulse height, point detector, reaction rates
  - Tallying in Steady-state System
  - Tallying in Time-dependent System
  - Variance reduction techniques in MCNP
- 9. Eigenvalue (Criticality) Monte Carlo Method (2 weeks)
  - Power Iteration for Eigenvalue Problems
  - Eigenvalue Calculation with MC
  - Derivation and Formulation of the Fission-Matrix (FM) Methodology
  - Application of the FM Method



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## 6 Course Schedule

• Detailed course schedule will be available in a separate document, including dates for each section/topic, homework/project assignment dates and deadlines, midterm exam date, etc.

# 7 Assignments and Grading Policy

(1) Homework problems (30%), see Table 1.

- Homework will be assigned periodically throughout the semester, typically every 2 weeks.
- Homework will be assigned and submitted via Moodle.
- Homework 5 will include two problems only for students taking NE 570. These problems will be based on advanced variance reduction techniques for fixed source MC particle transport.

Tuble 1. List of homework and topics.			
Homework	Weights	Topics	
1	5%	Random variables, random numbers, FFMC and sampling	
2	5%	RNG/PRNG and randomness testing	
3	5%	Statistical moments, limit theorems, confidence level, normal-	
		ity testing	
4	5%	MC integrals and variance reduction	
5	10%	Fixed-source MC particle transport and its variance reduction	
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(2) Mid-term exam (25%) - The midterm exam will be in-class closed book, closed notes.

### (3) Computational projects (45%), see Table 2.

- Project 6 is only for students taking NE 570. For undergraduates taking NE 470, the weights (10%) will be evenly distributed to projects 1-5.
- Computational project reports are short (4-5 pages) technical summary describing the details of an engineering analysis. These are not full technical reports but rather abbreviated technical notes which summarizes the key aspects of a study and provide enough detail that a knowledgeable person could re-create the results of the study given the same input and description.
- The basic elements of a computational project report include:
  - Introduction: problem background, definition, and objective statement
  - Input: document all input assumptions, sources, describe MCNP calculation model
  - Analysis: describe calculations performed, show geometry plot
  - Results: present results, show graphs, tables, comparison to measurement, etc.
  - Conclusions: provide a summary of findings.

### (4) Grading



Project	Weights	Topics
1	5%	Godiva Neutron Leakage benchmark problem: Modeling of Godiva bare spherical reactor and comparison of measured and calculated neutron energy leakage spectra.
2	5%	Photon Build-up Calculations: Use MCNP to model unit photon shielding problem and generate gamma-ray buildup factors. Then use BU factors to compare point-kernel results to MCNP.
3	7%	Lead/Poly Shielding Optimization Problem: Model Cf-252 spon- taneous fission source (n,p) and calculate optimum Pb/Poly thick- nesses to minimize total neutron and gamma-ray dose rate on other side of shield.
4	8%	Photon-Electron Dosimetry Problem: Model a series of photon- electron internal dosimetry calculations simulating absorbed frac- tions for different photon energies and compare results to ICRP-23.
5	10%	Valduc Critical Benchmark Experiments: Model a series of pin- lattice critical experiments using $UO_2$ (4.7%) fuel rods in water for different fuel pin-lattice configurations.
6	10%	Deep penetration streaming problem: Cs-137 calibration well deep penetration streaming benchmark problem and comparison to measured data.

Table 2:	List of	computational	projects	and topics.
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- The course will be graded on the letter grading scale listed in Table 3 and will count toward your GPA. More information can be found at https://studentservices.ncsu.edu/your-g rades/general-info/.
- *Requirements for Credit-Only (S/U) Grading*: In order to receive a grade of S, students are required to take all exams and quizzes, complete all assignments, and earn a grade of C- or better. Conversion from letter grading to credit only (S/U) grading is subject to university deadlines. Refer to the Registration and Records calendar for deadlines related to grading. For more details refer to http://policies.ncsu.edu/regulation/reg-02-20-15.
- *Requirements for Auditors (AU)*: Information about and requirements for auditing a course can be found at http://policies.ncsu.edu/regulation/reg-02-20-04.
- *Policies on Incomplete Grades*: If an extended deadline is not authorized by the instructor or department, an unfinished incomplete grade will automatically change to an F after either (a) the end of the next regular semester in which the student is enrolled (not including summer sessions), or (b) the end of 12 months if the student is not enrolled, whichever is shorter. Incompletes that change to F will count as an attempted course on transcripts. The burden of fulfilling an incomplete grade is the responsibility of the student. The university policy on incomplete grades is located at http://policies.ncsu.edu/regulation/reg-02-50-3.



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Table 3: Letter grades.			
Low	Grade	High	
97 ≤	A+	≤ 100	
93 ≤	А	< 97	
$90 \leq$	A-	< 93	
$87 \leq$	B+	< 90	
83 ≤	В	< 87	
$80 \leq$	B-	< 83	
$77 \leq$	C+	< 80	
$73 \leq$	С	< 77	
$70 \leq$	C-	< 73	
$67 \leq$	D+	< 70	
63 ≤	D	< 67	
$60 \leq$	D-	< 63	
$0 \leq$	F	< 60	

# 8 Computational Code - MCNP v6.2

- The MCNP v6.2 computer code will be used to perform all analyses for the computational projects. The MCNP executable (or source code if necessary) and data library can be requested (free of charge for students) at the RSICC website: https://rsicc.ornl.gov/Default.aspx
- The RDFMG cluster will be available for the computer projects. Training will be provided on accessing the cluster and running MCNP. https://www.ne.ncsu.edu/rdfmg/rdfmg-guide/

## 9 Recommended Texts

- 1. Textbook
  - Haghighat, A. (2020). Monte Carlo methods for particle transport. Second Edition, ISBN 9780367188054, CRC Press.
  - Estimated cost of book at Amazon: new hardcover \$150.00, eTextbok \$31.26 \$48.99.
  - The lecture notes will cover the most important materials in the textbook above. Purchasing the textbook is high recommended, but not required.
- 2. Reactor physics books (for reference only)
  - Prinja, A. K., & Larsen, E. W. (2010). General principles of neutron transport. In Handbook of nuclear engineering.
  - Lewis, E. E., & Miller, W. F. (1984). Computational methods of neutron transport. ISBN: 978-0-89448-452-01993, 1st Edition



- Carter, L. L., & Cashwell, E. D. (1975). Particle-transport simulation with the Monte Carlo method (No. TID-26607). Los Alamos Scientific Lab., N. Mex.(USA).
- Schaeffer, N. M. (1973). Reactor shielding for nuclear engineers (No. TID-25951). Radiation Research Associates, Inc., Fort Worth, Tex.(USA).
- 3. Statistical books (for reference only)
  - Casella, G., & Berger, R. L. (2002). Statistical inference. Pacific Grove, CA: Duxbury.
  - Liu, J. S. (2008). Monte Carlo strategies in scientific computing. Springer Science & Business Media.
- 4. Further readings (for reference only)
  - Turner, J. E., Wright, H. A., & Hamm, R. N. (1985). A Monte Carlo primer for health physicists. Health physics, 48(6), 717-733.
  - Werner, C. J. (2017). MCNP Users Manual-Code Version 6.2. Los Alamos National Laboratory, LA-UR-17-29981.
  - Zino, J. F. (1992). The need of coupled differential and integral spectral radiation measurements (No. WSRC-MS-92-408; CONF-930907-4). Westinghouse Savannah River Co., Aiken, SC (United States).
  - Peterson, R. E., & Newby, G. A. (1956). An unreflected U-235 critical assembly. Nuclear Science and Engineering, 1(2), 112-125.
  - Zino, J. F. (1995). Exposure rate response analysis of criticality accident detector at Savannah River Site (No. WSRC-MS-94-0544). Westinghouse Savannah River Co.

## 10 Others

### (1) Late Assignments Policy

- Unless stated otherwise, assignments are due by the end of day on the designated due date. Assignments turned in within 24 hours of this time are considered late and will be assessed a 25% penalty. Assignments turned in after 24 hours will be marked and returned to the student, but no credit will be assigned.
- To allow for unforeseen circumstances, each student will be granted a **one-time exemption**. The student should contact the course instructor **at least three days** before the original dead-line and explain the situation in order to get an extension. The assignment must be turned in by the end of the new designated due date.

### (2) Course Attendance/Absence Policy

- Active class participation is strongly encouraged.
- Attendance does not count towards the final grade.
- NC State attendance policies can be found at: REG 02.20.03 Attendance Regulations Policies, Regulations & Rules (https://policies.ncsu.edu/regulation/reg-02-20-03-a ttendance-regulations/). Please refer to the course's attendance, absence, and deadline policies for additional details.



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• *Absences Policy*: Personal Problems: We understand that sometimes life makes it difficult to focus on schoolwork. If you are having a personal problem that affects your participation in this course, please talk to us to create a plan. Please do not wait until the end of the semester to share any challenges that have negatively impacted your engagement and academic performance. The sooner we connect, the more options we will have available to us to support your overall academic success. If you are not comfortable speaking with us directly, please utilize the other student resources provided below in order to understand how to best approach success in this course given your personal needs as soon as possible.

### (3) Transportation

• This course will not require students to provide their own transportation. Non-scheduled class time for field trips or out-of-class activities is NOT required for this class.

### (4) Safety & Risk Assumptions

• N/A

### (5) Digital Course Components

- This on campus course will be captured and distributed via the Internet and/or electronic media as part of the Engineering Online (EOL) program for the distance students.
- These video recordings may contain an image of you entering the classroom, asking a question or being a part of the studio class.
- Please notify Dr. Linda Krute, Director of EOL, at ldkrute@ncsu.edu if you do NOT want your image to be included in the lecture presentation. If EOL does not hear from you after the first week of the class, we will assume that you are in agreement with this procedure.
- Students may be required to disclose personally identifiable information to other students in the course, via digital tools, such as email or web-postings, where relevant to the course. Examples include online discussions of class topics, and posting of student coursework. All students are expected to respect the privacy of each other by not sharing or using such information outside the course.

### (6) Academic Integrity

- Students are required to comply with the university policy on academic integrity found in the Code of Student Conduct found at https://policies.ncsu.edu/policy/pol-11-35-01/
- Absolutely no collaboration is permitted during closed-book tests. All the tests are closed book unless otherwise specified.
- Collaboration on homework assignments is allowed, but the submitted work must be your own individual work. Homework assignments must not be treated as group assignments. Zero grade will be assigned for particular homework for the first offense. Second offense will be reported to the Office of Student Conduct.
- Violations of academic integrity will be handled in accordance with the Student Discipline Procedures (NCSU REG 11.35.02) at https://policies.ncsu.edu/regulation/reg-11-3 5-02/. 11.35.02)

### (7) Additional NC State Rules and Regulations



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- Students are responsible for reviewing the NC State University Policies, Rules, and Regulations (PRRs) which pertain to their course rights and responsibilities, including those referenced both below and above in this syllabus:
  - Equal Opportunity and Non-Discrimination Policy Statement https://policies.ncs u.edu/policy/pol-04-25-05/ with additional references at https://oied.ncsu.edu/ divweb/policies/.
  - Code of Student Conduct Policy https://policies.ncsu.edu/policy/pol-11-35-01/

### (8) Use of Electronic Devices in Class

- Cell phones are to be turned OFF prior to entering the classroom/lab. No exceptions.
- Use of laptops/other electronic devices during class is permitted only for the purpose of following the posted lecture materials/taking electronic notes.

### (9) Accommodations for Students with Disabilities

- Reasonable accommodations will be made for students with verifiable disabilities. In order to take advantage of available accommodations, students must register with Disability Services for Students at 1900 Student Health Center, Campus Box 7509, 515-7653.
- For more information on NC State's policy on working with students with disabilities, please see the "REG 02.20.01 Academic Accommodations for Students with Disabilities" at https://policies.ncsu.edu/regulation/reg-02-20-01/.

### (10) Non-Discrimination Policy

- NC State provides equal opportunity and affirmative action efforts, and prohibits all forms of unlawful discrimination, harassment, and retaliation ("Prohibited Conduct") that are based upon a person's race, color, religion, sex (including pregnancy), national origin, age (40 or older), disability, gender identity, genetic information, sexual orientation, or veteran status (individually and collectively, "Protected Status").
- Additional information as to each Protected Status is included in NCSU REG 04.25.02 (Discrimination, Harassment and Retaliation Complaint Procedure). NC State's policies and regulations covering discrimination, harassment, and retaliation may be accessed at http://policies.ncsu.edu/policy/pol-04-25-05 or https://oied.ncsu.edu/divweb/.
- Any person who feels that he or she has been the subject of prohibited discrimination, harassment, or retaliation should contact the Office for Equal Opportunity (OEO) at 919-515-3148.

### (11) Student Mental Health

• As a student you may experience a range of personal issues that can impede learning, such as strained relationships, increased anxiety, alcohol/drug concerns, feeling down, difficulty concentrating and/or lack of motivation. These mental health concerns or stressful events may lead to diminished academic performance and may impact your ability to participate in daily activities. It is very important that you have a support system and that you ask for help when you are struggling. The Counseling Center at NC State offers confidential mental health services for full time NC State students, including same-day emergency services. Please visit https://counseling.dasa.ncsu.edu/ to get connected.