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Curriculum Construction of "Soft Matter and Molecular Simulation" Integrating Computational Physics and Artificial Intelligence in Graduate Education

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ABSTRACT

Molecular simulation plays an increasingly important role in the study of soft matter and biomolecular systems, driven in part by the growing use of computational physics and artificial intelligence (AI). In response to the need for interdisciplinary training at the graduate level, a new course entitled Soft Matter and Molecular Simulation was developed and offered to physics graduate students at our university. The course is organized around statistical physics and soft matter theory, and systematically introduces molecular dynamics simulations, free energy perturbation methods, and selected AI-assisted approaches for molecular modeling and protein-related studies. A progressive teaching framework is employed to link theoretical instruction with hands-on computational practice and research-oriented examples. Based on classroom implementation and student learning activities, the course has been found to support the development of fundamental modeling skills and to help students gain a clearer understanding of interdisciplinary research workflows. The curriculum design and teaching practices described in this paper also reflect a broader attempt to align graduate physics education with emerging computational and intelligent research paradigms.

KEYWORDS

Graduate curriculum construction; Soft matter and molecular simulation; Computational physics education; Artificial intelligence in teaching; Interdisciplinary graduate training

1 Introduction

Computational modeling has become an increasingly important component of contemporary research in physics, chemistry, and the life sciences. In studies of soft matter and biomolecular systems, molecular simulation offers a practical way to examine microscopic mechanisms that are often difficult to access through direct experimental approaches. In particular, molecular dynamics simulations enable researchers to explore conformational changes, interaction patterns, and thermodynamic properties at the atomic level, thereby complementing experimental techniques such as cryo-electron microscopy, X-ray crystallography, and other approaches in structural biology. As a result, simulation-based methods have gradually evolved from auxiliary tools into essential components of modern scientific inquiry.

The recognition of computational modeling by the 2013 Nobel Prize in Chemistry further underscored its importance in molecular science. Since then, free energy calculation methods, including free energy perturbation (FEP) and MM/PBSA, have been widely applied to studies of molecular recognition, protein mutation effects, and drug design. When combined with molecular dynamics simulations, these approaches provide quantitative insights into interaction energetics and thermodynamic behavior, making them particularly valuable for research areas that require predictive modeling and mechanism-oriented analysis.

In parallel with advances in physics-based simulations, artificial intelligence has provided additional tools for molecular modeling. Machine learning techniques have been explored in areas such as structure prediction, force field development, and mutation screening. Representative examples, including AlphaFold, illustrate how data-driven approaches can work alongside physics-based models, offering complementary perspectives rather than acting as direct substitutes. More recently, AlphaFold 3 extended structure prediction to protein-ligand, protein-nucleic acid, and protein-protein complexes, further broadening the scope of AI-assisted molecular modeling. These developments have not only influenced research practice but have also reshaped expectations for graduate education, particularly for students engaged in computational and theoretical research.

From an educational perspective, however, the rapid development of computational and AI-based methods has introduced new challenges. Graduate students in physics often possess strong theoretical backgrounds but may lack systematic training in molecular modeling workflows, simulation software, and data-driven approaches. Conversely, the increasing complexity of simulation tools and algorithms can make it difficult for students to connect computational results with underlying physical principles. These gaps highlight the need for carefully designed curricula that integrate

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theoretical foundations, computational practice, and emerging intelligent methods in a coherent manner.

Based on this background, the course *Soft Matter and Molecular Simulation* was established as a graduate-level elective. As a newly developed course, its primary goal is to provide students with foundational knowledge and practical skills in molecular simulation, while offering a preliminary introduction to AI-assisted modeling methods within a physics-oriented framework. The course was designed not only to develop technical proficiency but also to foster critical evaluation of modeling assumptions, informed interpretation of simulation results, and a broader understanding of the role of computation in interdisciplinary research.

2 Course Objectives and Design Considerations

The course is designed for graduate students majoring in physics or related disciplines, particularly those who are beginning to engage in computational or interdisciplinary research. Its objectives are threefold. First, the course aims to help students develop a physical understanding of soft matter systems, including polymers, colloids, and biomolecular assemblies. Second, it seeks to provide students with hands-on experience in molecular simulation tools and workflows that are commonly used in contemporary research. Third, the course introduces students to the basic concepts of artificial intelligence in molecular modeling, with the goal of fostering awareness rather than technical mastery at this stage.

During curriculum design, careful attention was given to balancing theoretical explanation and computational practice. Instead of treating simulation software as isolated technical tools, the course emphasizes the physical assumptions behind simulation methods, the interpretation of numerical results, and the limitations of different computational approaches. For example, students are encouraged to analyze how choices of force fields, ensemble conditions, and sampling strategies influence simulation outcomes.

Another important consideration was the diversity of academic backgrounds among course participants. While some students enter the course with prior experience in numerical methods or programming, others may have limited exposure to large-scale simulations. To address this issue, the course adopts a progressive structure in which conceptual understanding is developed before complex computational tasks are introduced. This design allows students to gradually build confidence and competence, while maintaining a clear connection between physical theory and computational implementation.

Overall, the course is intended to support the development of scientific reasoning skills, helping students view molecular simulations as part of an integrated research process rather than as purely technical procedures.

3 Curriculum Structure and Content Organization

The course content is organized into three interconnected modules: theoretical foundations, computational methods with practical training, and research-oriented applications. This modular structure was designed to guide learners progressively from fundamental physical concepts to practical simulation workflows and, finally, to representative research scenarios. The arrangement allows flexibility in teaching while maintaining coherence across different levels of difficulty.

3.1 Theoretical Foundations

The first module introduces essential concepts in soft matter physics, including polymers, colloids, and biomolecular systems. These topics are selected to illustrate how soft matter systems can be described using statistical physics and continuum concepts. Fundamental principles of molecular dynamics simulations are also covered, such as equations of motion, statistical ensembles, and commonly used temperature and pressure control techniques.

Rather than providing a purely mathematical treatment, this module emphasizes physical interpretation. Key simulation parameters are discussed in relation to real physical systems, helping learners understand how modeling choices influence simulation outcomes. This theoretical grounding is intended to prepare participants for later computational work by clarifying the assumptions and limitations underlying molecular simulations.

3.2 Computational Methods and Practical Training

The second module focuses on hands-on training using widely adopted molecular simulation software packages, including GROMACS and NAMD. Practical sessions guide participants through typical simulation workflows, covering system preparation, force field selection, equilibration procedures, production simulations, and trajectory analysis.

Free energy calculation methods receive particular attention in this module. Free energy perturbation (FEP) is introduced as a representative and rigorous approach, with emphasis placed on thermodynamic cycle construction,

mutation pathway design, and uncertainty estimation. Through guided exercises, participants learn how methodological choices affect numerical stability and result reliability. This module aims to strengthen practical competence while reinforcing connections between computational procedures and underlying physical principles.

3.3 Applications and AI-Related Topics

The final module presents selected application scenarios to demonstrate how molecular simulation methods are used in current research. Typical examples include protein – ligand interactions, mutation-induced stability changes, and binding affinity estimation. These cases are chosen to reflect common research questions encountered in biophysics and related fields.

In addition, introductory discussions on machine learning applications in molecular modeling are incorporated. Topics such as structure prediction and mutation screening are used to illustrate how AI-based tools can complement physics-based simulations. The focus remains on conceptual understanding and appropriate usage, rather than detailed algorithmic implementation, helping participants develop a balanced perspective on emerging computational approaches.

4 Teaching Practice and Learning Activities

Teaching activities are closely linked to research practice. Case studies are primarily drawn from published work and ongoing research projects, allowing students to engage with realistic simulation workflows. Computational assignments are designed as modular tasks that reflect the structure of actual research projects, guiding students through complete simulation processes from model construction to data analysis.

In addition to structured assignments, participants are encouraged to undertake a small independent project related to their own research interests. Each project requires a short-written report and an oral presentation. This process supports the development of scientific communication skills alongside technical competence and reinforces the integration of computational tools into broader research activities.

5 Observed Outcomes and Discussion

Based on classroom observations, student feedback, and performance in assignments, the course appears to support improved confidence in the use of molecular simulation tools and a clearer understanding of computational modeling strategies. Many participants report greater familiarity with simulation workflows and an enhanced ability to interpret numerical results within a physical framework.

At the same time, several challenges were identified. Differences in prior computational experience required additional guidance during early practical sessions. Moreover, the rapid development of AI-related methods necessitates continuous updates to course content to remain current. These observations highlight the need for ongoing refinement of teaching materials and support mechanisms in future course offerings.

6 Conclusion

The *Soft Matter and Molecular Simulation* course represents an attempt to integrate computational physics and artificial intelligence into graduate education through a structured and practice-oriented curriculum. By emphasizing theoretical understanding, computational skills, and research relevance, the course supports interdisciplinary training for physics graduate students. The experience reported here reflects a pragmatic approach to curriculum construction at the intersection of computational modeling and emerging intelligent techniques. While further improvements are needed, the course provides a useful reference for similar educational initiatives in computational and physical sciences.

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