

「3799-299 国際連携特別講義 V」

”International Collaborators' Special Lecture on Engineering V”

2019 年度夏 SNU との短期集中コースプログラム

Short Intensive Course Program between UTokyo and SNU in the summer of 2019 Academic Year



## Introduction to Atomistic Simulations for Nuclear Engineering

(原子力工学のための原子シミュレーション入門)

**Associate Professor Takuji Oda**

Department of Energy Systems Engineering (Nuclear Engineering),  
College of Engineering, Seoul National University

**【Lecture Schedule】 Intensive Lecture Date: Monday, February 10 - Friday, February 14, 2020**

Monday, February 10 : 10:00-12:00, 13:00-17:00  
 Wednesday, February 12: 10:00-12:00, 14:00-17:00  
 Thursday, February 13 : 10:00-12:00, 14:00-17:00  
 Friday, February 14: 10:00-12:00, 14:00-17:00

**【Overview】**

Computer simulations are essential tools for nuclear engineering, such as neutron transport calculations, heat transfer calculations, structural mechanics calculations, reactor physics design, etc. In addition to these applications, atomistic simulations have been attracting increasing attention, which help our understanding of fundamental processes involved in radiation effects on material properties, water chemistry, radionuclide transport, etc. Atomistic simulations are also used to develop new materials, thanks to the advancement in computer sciences including machine learning. In this course, for students who have no/little experience in the atomistic simulations but are interested in future application in a research, basic theories and how-tos of atomistic simulations are provided through lectures and practices. In this course, we mainly learn molecular statics/dynamics calculation and first-principles calculation as atomistic simulation methods, and use them for solid materials in practices, although acquired knowledge/skills would be applied to liquid, solution, molecules, etc. Upon completion of this course, the students will be able to (1) read and understand basic contents of research papers using atomistic simulations, (2) design a research using atomistic simulations, and (3) start preliminary studies using atomistic simulations.

(2 credits)

**【Lecture Room】 To Be Announced Later**

■ Please check the course description in UTAS for details.

- Counterpart at UTokyo: Associate Professor Takumi Saito,  
Department of Nuclear Engineering, Graduate School of Engineering
- Contact information : email: [seut\\_global30.t@gs.mail.u-tokyo.ac.jp](mailto:seut_global30.t@gs.mail.u-tokyo.ac.jp)