

IUPAB2024 Hands-on Training Program

CHARMM-GUI/GENESIS MD Tutorial

June 30 (Sunday) – July 02 (Tuesday), 2024
Integrated Innovation Building (IIB), RIKEN Kobe

Invited Speakers

- Bernard Brooks
NIH
- Jianhan Chen
University of Massachusetts
- Ben Corry
Australian National University
- Michael Feig
Michigan State University
- Helmut Grubmüller
Max Planck Institute for Multidisciplinary Sciences
- Gerhard Hummer
Max Planck Institute of Biophysics
- Naoto Hori
University of Nottingham
- Yasuhiro Matsunaga
Saitama University
- Kei Moritsugu
Osaka Metropolitan University
- Kwangho Nam
The University of Texas at Arlington
- Alberto Perez
University of Florida
- Youngmin Rhee
KAIST
- Jana Shen
University of Maryland
- Chen Song
Peking University
- Florence Tama
RIKEN

Hands-on Lecturers

- **GENESIS** *RIKEN*
Shingo Ito, Jaewoon Jung,
Chigusa Kobayashi, Cheng Tan
TA: Diego Ugarte La Torre, Kiyoshi Yagi, Yangyang
Zhang, Azuki Mizutani, Masahiro Motohashi *RIKEN*
Song-Ho Chong *Kumamoto University*
- **CHARMM-GUI** *Lehigh University*
Wonpil Im, Nathan Kern, Donghyuk Suh
TA: Turner Brown, Seonghoon Kim *MolCube Inc.*

Organizers

Yuji Sugita *RIKEN*, Wonpil Im *Lehigh University*, Florence Tama *RIKEN*,
Yasuhiro Matsunaga *Saitama University*, Kei Moritsugu *Osaka Metropolitan University*



IUPAB2024

CHARMM-GUI/GENESIS Workshop

PROGRAMME

Sunday, 30 June 2024

8:40 – 9:00 Registration
9:00 – 9:10 Wonpil Im
Lehigh University
Welcome address

Session 1. Molecular Dynamics Theories and Methods

(chair: Yasuhiro Matsunaga)

9:10 – 9:40 Helmut Grubmüller
Max Planck Institute for Multidisciplinary Sciences
Constant pH Simulations with FMM and solvation shell entropies

9:40 – 10:10 Kei Moritsugu
Osaka Metropolitan University
Weighted Ensemble for Biomolecules

10:10 – 10:40 Ana Damjanovic, Juyong Lee, Bernard Brooks (Speaker)
NIH
Constant pH Replica-Exchange Methods

10:40 – 11:00 COFFEE BREAK

Session 2. Enzyme Mechanisms (chair: Kiyoshi Yagi)

11:00 – 11:30 Kwangho Nam
The University of Texas at Arlington

Advancements in multiscale QM/MM and free simulation methods for enzyme modeling

11:30 – 12:00 Youngmin Rhee
KAIST
Following photodynamics in biology: non-adiabatic dynamics simulations with conventional MD packages

12:00 – 13:30 LUNCH

13:30 – 18:00 Scientific Discussion (6F, 8F)

Tutorial students:

GENESIS Hands-on Part 1

13:30 – 14:30 Lecturer: Chigusa Kobayashi (RIKEN)
GENESIS basics and GENESIS on Fugaku

14:30 – 15:00 Hands-on GENESIS

15:00 – 15:20 BREAK

CHARMM-GUI Hands-on Part 1

15:20 – 16:20 Wonpil Im (Lehigh University)
Introduction of CHARMM-GUI and Membrane Builder

16:20 – 17:20 Hands-on CHARMM-GUI

17:20 – 18:00 BREAK

18:00 BANQUET

Monday, 01 July 2024

Session 3. Membrane Biology (chair: Florence Tama)

- 9:00 – 9:30 Chen Song
Peking University
Gating mechanism of the mechanosensitive ion channel NOMPC: new insights from molecular dynamics simulations
- 9:30 – 10:00 Jana Shen
University of Maryland
Drug-membrane partitioning and crossing from unbiased molecular dynamics coupled with proton titration
- 10:00 – 10:30 Ben Corry
Australian National University
Molecular simulation of membrane channels, transporters, and receptors
- 10:30 – 10:50 COFFEE BREAK

Session 4. Modeling of Cellular Components, Part I

(chair: Yasuhiro Matsunaga)

- 10:50 – 11:20 Jianhan Chen
University of Massachusetts
Coarse-grained simulations of protein and RNA phase separation
- 11:20 – 11:50 Michael Feig
Michigan State University
Multi-scale modeling of biomolecular condensates.

11:50 – 13:15 LUNCH

13:15 – 18:00 Scientific Discussion (6F, 8F)

Fugaku Tour (Instructor: Chigusa Kobayashi)

13:15 – 14:20 GROUP 1

13:55 – 14:55 GROUP 2

Tutorial students:

GENESIS Hands-on Part 2

- 14:30 – 15:30 Cheng Tan (RIKEN)
Coarse-grained simulations in GENESIS (Lecture and Hands-on)
- 15:30 – 16:30 Jaewoon Jung (RIKEN)
High-performance computation with GENESIS (Lecture and Hands-on)
- 16:30 – 16:45 BREAK

CHARMM-GUI Hands-on Part 2

- 16:45 – 17:15 Nathan Kern (Lehigh University)
Multi-component assembler
- 17:15 – 18:00 **Hands-on multi-component assembler**

Tuesday, 02 July 2024

Session 5. Modeling of Cellular Components, Part II

(chair: Kei Moritsugu)

- 9:00 – 9:30 Gerhard Hummer
Max Planck Institute of Biophysics
Integrating molecular dynamics simulations and experiments
- 9:30 – 10:00 Naoto Hori
University of Nottingham
Coarse-grained simulations of RNA folding and misfolding
- 10:00 – 10:20 COFFEE BREAK
- 10:20 – 10:50 Alberto Perez
University of Florida
Synergizing simulations and experiments: faster exploration of biologically relevant states
- 10:50 – 11:20 Florence Tama
RIKEN
Unraveling the Structure and Dynamics of Biomolecules via Integrative Modeling
- 11:20 – 11:50 Yasuhiro Matsunaga
Saitama University
Integrative Modeling of Protein Dynamics from High-speed Atomic Force Microscopy and Molecular Dynamics Simulations

Closing of the Morning Sessions

- 11:50 – 12:00 Yuji Sugita
RIKEN
Closing Remarks to the morning sessions

12:00 – 13:30 LUNCH

13:30 – 17:10 Scientific Discussion (6F, 8F)

Tutorial students:

GENESIS Hands-on Part 3

13:30 – 15:00 Shingo Ito (RIKEN)
Generalized-ensemble simulations using GENESIS

15:00 – 15:30 BREAK

CHARMM-GUI Hands-on Part 3

15:30 – 16:00 Donghyuk Suh (Lehigh University)
Enhanced sampler

16:00 – 17:00 **Hands-on Enhanced sampler**

17:00 – 17:10 Yuko Okamoto
Nagoya University

Closing Remarks

Food Map 1

Nearest Station: Iryo Center Station



2F, Restaurant
Kazokutei Port Island



2F, Restaurant
Compass



1F, Convenience
Store (Inside of
hospital building)



1F, Kitchen &
Coffee matros



2F, みなと庵縁



1F, Convenience
Store



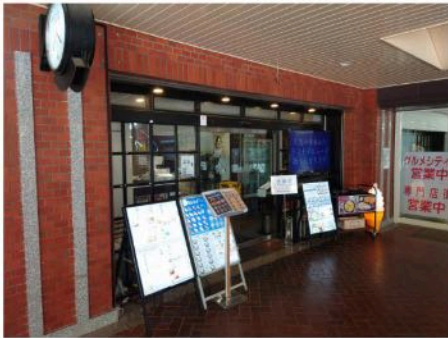
In this building

Food Map 2

Next 2 Neighboring Stations: **Shiminhiroba** and **Minatojima**

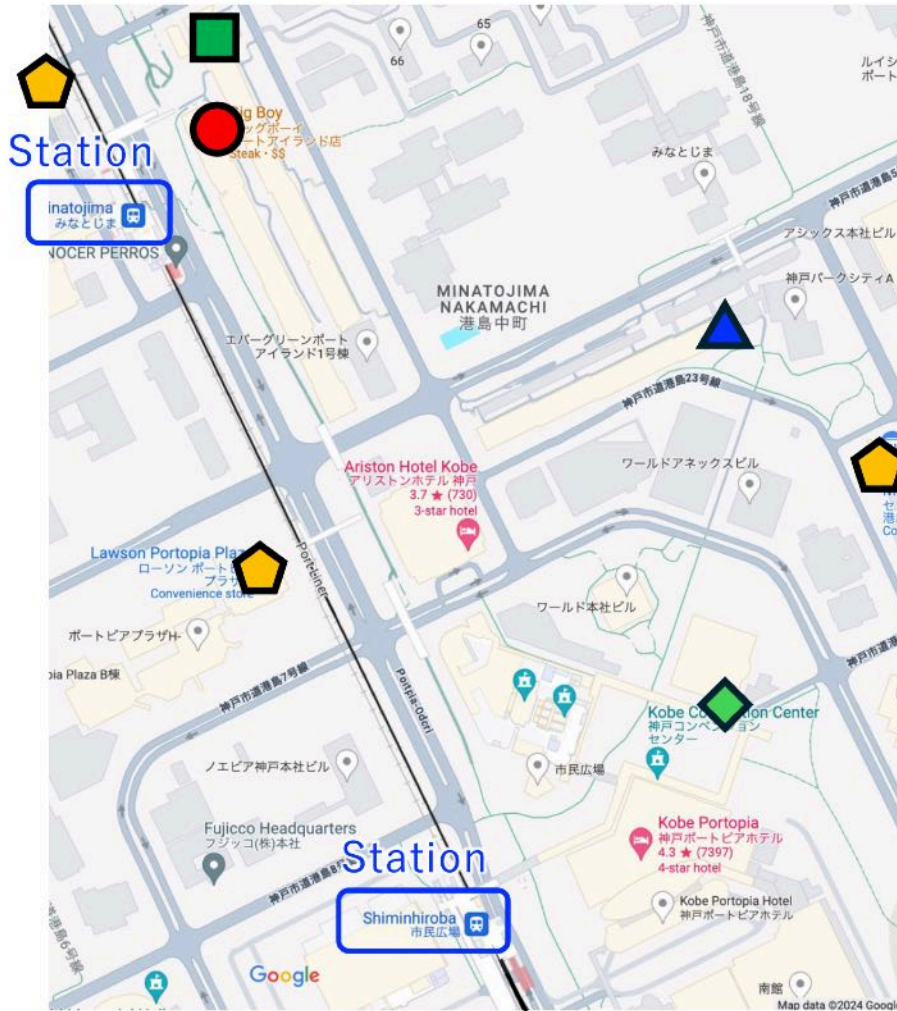


1F, Big Boy
(Steaks)



1F, ごはん家
(Japanese food)

 Convenience Store



 Iryo Center
Station

* Closed on Monday



1F, Chiriken
(Chinese food)



1F, うどんのことは
(Udon noodle)

Note that there are several restraints in the “Kobe Portopia Hotel” and “Ariston Hotel Kobe”, but they are little expensive.