



RIKEN Center for Computational Science,
Institute for Transformative Biomolecules
(Nagoya university), Nano Life Science
Institute (Kanazawa university)

Workshop “Trends in Computational Molecular Biophysics”

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The Fourth High School Memorial Museum
of Cultural Exchange, Kanazawa

<https://nanolsi.kanazawa-u.ac.jp/en/en-workshop-201811/>

Saturday, November 3rd

10:30 Opening

10:45 J. Yu (Beijing Computational Science Research Center) jinyu@csrc.ac.cn
Transcription studied in a nutshell on T7 RNA polymerase ratcheting along DNA with fidelity control and bursting activity

11:20 T. Uchihashi (Nagoya university) uchihast@d.phys.nagoya-u.ac.jp
Connection between AFM data and computational simulation

11:55 T. Komatsuzaki (Hokkaido university) tamiki@es.hokudai.ac.jp
Revisit transition state theory: Past, Present, Future

12:30 – 14:30 Lunch

14:30 S. Takada (Kyoto university) takada@biophys.kyoto-u.ac.jp
Towards integration of high-speed AFM data with biomolecular simulations

15:05 H. Kodera (Kanazawa university) nkodera@staff.kanazawa-u.ac.jp
Interpretation of HS-AFM images using coarse-grained molecular dynamics simulation

15:40 L. Dai (Beijing Computational Science Research Center) dailiq@csrc.ac.cn
Deciphering intrinsic inter-subunit couplings that lead to sequential hydrolysis of F1-ATPase ring

16:00 – 16:30 Break

16:30 N. Koga (Institute of Molecular Science) nkoga@ims.ac.jp
DBTL in protein design

17:05 K. Okazaki (Institute of Molecular Science) keokazaki@ims.ac.jp
Mechanism of Na⁺/H⁺ antiporter from transition-path simulations: Making faster transporter based on mechanism

17:40 Y. Kawasaki (Kyushu University) y-kawasaki@bioreg.kyushu-u.ac.jp
Integrative approach combining electron microscopy and high-speed AFM revealed the dynamic conformational exchange of the oligosaccharyltransferase in lipid bilayers

18:00 C. Tan (Kyoto University) tan@nick.biophys.kyoto-u.ac.jp
Interaction between transcription factors and the nucleosome studied by molecular dynamics simulations.

Sunday, November 4th

9:00 J. Noel (Max Delbrück Center for Molecular Medicine, Berlin) jknoel@gmail.com
Mesoscopic polymer-like model for dynamics of dynamin filaments on deformable membrane tubes

9:35 Y. Togashi (Hiroshima university) togashi@hiroshima-u.ac.jp
Toward mesoscale models of chromatin: considering the state and shape of molecules

10:10 G. Brandani (Kyoto University) g.brandani88@gmail.com
Molecular dynamics simulations of spontaneous and active nucleosome assembly

10:30 – 11:00 Break

11:00 H. Kitahata (Chiba university) kitahata@chiba-u.jp
Hydrodynamic collective effects of active proteins in biological systems

11:35 T. Nagai (Nagoya university) tnagai@nagoya-u.jp
Toward hybrid modeling of XFEL single particle experiment by Gaussian mixture model

12:10 B. Dasgupta (Nagoya University) dasgupta.bhaskar@k.mbox.nagoya-u.ac.jp
Modelling low-resolution molecular volume of proteins from Atomic-Force Microscopy image by adaptive Gaussian kernels

12:30 – 14:00 Lunch

14:00 H. Flechsig (Kanazawa university) flechsig@staff.kanazawa-u.ac.jp
A reduced model of myosin V motor dynamics to understand the mechanism of processive stepping observed in high-speed AFM experiments

14:35 T. Sumikama (Kanazawa university) sumi@staff.kanazawa-u.ac.jp
Towards elucidating the physical origin of force in AFM measurements and a method analyzing dynamics observed by HS-AFM

15:10 L. Yang (Kanazawa university) l.yang@staff.kanazawa-u.ac.jp
A general approach combining molecular dynamics and machine learning to bridge the gap between AFM image and real structure

15:45 Y. Koyano (Chiba university) y.koyano@chiba-u.jp
Cooperative Dynamics of Active Dimers

16:05 Closing

The workshop will take place in the historical building of the Fourth High School constructed in 1891. Today it accomodates The Fourth High School Memorial Museum of Cultural Exchange and The Ishikawa Modern Literature Museum. This building is located in the center of the city, next to the Kanazawa castle. The conference room is Room 4 on the second floor.

Please take a KANAZAWA LOOP BUS (Left Loop) at Kanazawa Station East Gate Bus Terminal #7, or Line 18 (Terminal #3), Line 13 or 90 or 92-95 (Terminal #6), Line 30-33 or 35 (Terminal #8), Line 41 or 42 or 44-46 (Terminal #9), Line 20-22 (Terminal #10) , or Line 51 or 54 or 56 (Terminal #11), and get off at the Korinbo bus stop. The trip is about 10 minutes and the fare is 200 yen.