### Research subjects

Recent topics on Computational Science in several fields of physics. Analysis of functions of proteins and biomolecules such as biological sciences and biophysics by Molecular Dynamics simulation, Molecular Orbital method, Monte Carlo method, and Mathematical model in parallel computers and supercomputers.

### Master/Doctor course: Education policy, curriculum, typical activity in the laboratory

Master course students take lectures and join seminars. Conduct research of each research topics and complete master’s theses. Doctor students conduct research under supervisors and complete doctoral theses.

### Daily life in the laboratory, etc.

PC is assign to each student. Students can use supercomputers in other universities and thus carry out large-scale numerical simulation.

### Message or comments by the laboratory faculty staffs

Computational science is the third science in addition to experimental and theoretical sciences. We hope that students conduct research of this new science with special interests.

### Recent Master theses in these 3 years (+ more if appropriate)

<table>
<thead>
<tr>
<th>year.month</th>
<th>Thesis title (including English translation of Japanese thesis title)</th>
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<tbody>
<tr>
<td>2019.3</td>
<td>Theoretical Study of Structural Stability of Plastocyanin Complex by a Coarse-grained model</td>
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<td>Theoretical Study of Structural Stability of Lipid Bilayer Membrane by a Coarse-grained model</td>
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<tr>
<td>2018.3</td>
<td>Theoretical study of diffusion of Plastocyanin by using the Langevin dynamics simulation</td>
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<td>Theoretical study on self-assembly process and shape deformation of lipid membranes by coarse-grained model</td>
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<td>Theoretical study on intermolecular interaction and structural stability of protein complex by using the Go-like model</td>
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<td>Theoretical study of interaction between multilamellar membranes and stability of multilamellar membranes</td>
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<td>Theoretical study on structural dynamics and elasticity of lipid bilayer and mixed membrane</td>
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<td>Theoretical study on the association–dissociation process of metalloproteins in the photosynthetic reaction</td>
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<tr>
<td>2015.9</td>
<td>Prediction of Solvation Free Energy of Proteins and Organic Molecules: Molecular Dynamics Simulation and QSPR Model Approach</td>
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<td>Theoretical study of structure formation of vesicle arising from interactions between lipids by a coarse-grained model</td>
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<td>Molecular Dynamics Study of Human Defensins HNP–1 Binds to DPPC Membrane: Structure and Stability</td>
</tr>
<tr>
<td>2014.3</td>
<td>Development of algorithm for a parallel computing of a excess chemical potential calculation and its application for hydration effect on complex of proteins</td>
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### Division of Mathematical and Physical Sciences | Research field | Computational Biophysics | Lab. ID |
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<tbody>
<tr>
<td>Laboratory web site</td>
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<td>MP21</td>
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<td><a href="http://hal.s.kanazawa-u.ac.jp/">http://hal.s.kanazawa-u.ac.jp/</a></td>
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<td>Theoretical study of dependence of solvent effect of the oxidation-reduction potential on the oxidation of water</td>
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<td>Computational Study of Oxidation Potential Fluctuation of Ketone Molecule</td>
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<td>An Approach for Combining Docking and Molecular Dynamics (MD) Simulation In Protein-Ligand Docking</td>
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Recent Doctoral theses in these 3 years (+ more if appropriate)
(It contains theses of the antecedents of this lab, 'Simulation Science' and 'Applied Computational Mathematics' until March, 2019)

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<tr>
<td>2014.9</td>
<td>Theoretical studies of the formation mechanism of protein complex by using coarse-grained models</td>
</tr>
<tr>
<td>2014.9</td>
<td>Theoretical Studies of the Dependence of Chemical Reaction on Tautomeric Form of His64 in the Active Site of Human Carbonic Anhydrase II</td>
</tr>
<tr>
<td>2012.9</td>
<td>A molecular dynamics study of Hras-GTP complex and Hras-GDP complex</td>
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</table>

Laboratory mail address

Hidemi Nagao <nagao *at* wriron1.s.kanazawa-u.ac.jp>