Multiscale theory and simulation has become an important tool for chemists and biophysicists. In this hands-on workshop, meant for advanced graduate students and postdoctoral scholars, key multiscale theoretical and the computational concepts will be presented.

The goal of the workshop is to train a select group of students and postdocs in multiscale methods that can be used to study biomolecular systems, ranging from the atomic to the mesoscopic scales. The workshop will cover both coarse-graining techniques and rare event sampling, as well as their applications. The relevant physical concepts, mathematical techniques, and computational algorithms used in multiscale simulations will be introduced. Hands-on computer exercises will also be a part of the workshop.

**Dates: June 11-13, 2012**

Center for Multiscale Theory and Simulation
University of Chicago
5735 S. Ellis Ave
Chicago, IL 60637

**Workshop Instructors:**
Gregory A. Voth, Haig P. Papazian Distinguished Service Professor
Department of Chemistry, University of Chicago
Aaron Dinner, Associate Professor
Department of Chemistry, University of Chicago
Benoit Roux, Professor
Department of Biochemistry and Molecular Biology, University of Chicago
Karl Freed, Henry G. Gale Distinguished Service Professor
Department of Chemistry, University of Chicago
Nina Hinrichs, Assistant Professor
Department of Computer Science, University of Chicago
Jonathan Weare, Assistant Professor
Department of Mathematics and the College, University of Chicago

**General Questions:**
NSF-CCI-workshop@uchicago.edu
(773) 702-6805
Lecture sessions will be conducted in the morning followed by hands-on computer lab sessions in which students will be able to set up and run simulations. Enrollment is limited to 15 participants. All participants are required to bring their own laptop for use in workshop tutorial sessions. Housing will be provided for participants, and all course materials will be provided. There is no registration fee. Partial funding is available for participant travel.

The workshop will be held at The Searle Chemistry Laboratory building, University of Chicago, Hyde park campus. It is sponsored by the NSF-funded Center for Multiscale Theory and Simulation (CMTS), which is focused on developing a novel, systematic, and transformative computational capability for the scientific community. The NSF CMTS project combines conceptual advances in statistical mechanics and condensed phase dynamics with computer simulation methodology.

**Significant Dates**

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<thead>
<tr>
<th>Event</th>
<th>Date (in 2012)</th>
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<tbody>
<tr>
<td>Application deadline for full consideration:</td>
<td>March 1</td>
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<tr>
<td>Selection and notification of participants by:</td>
<td>On-going through April</td>
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<tr>
<td>Confirmation of attendance by participants due by:</td>
<td>April 15</td>
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<tr>
<td>Housing check-in date:</td>
<td>June 10</td>
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<tr>
<td>Housing check-out date:</td>
<td>June 13</td>
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