

Statistics about the Materials Computation Center

NSF-DMR Award 03-25939; Principal Investigators: Duane D. Johnson and Richard M. Martin
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RESEARCH ACTIVITIES

Highlighted research projects

- QMCPACK: a high-performance software package implements advanced quantum Monte Carlo algorithms to solve many-body Schrodinger equation with high accuracy. It is a powerful tool to study a wide range of correlated problems, e.g., the optical properties of semiconductor quantum dots and binding energies of energetic materials. It was used during the QMC 2007 summer school, thereby instructing approximately 70 students in its use.
- Genetic algorithms applied to quantum chemistry problems: Utilizing multi-objective (MO) optimization based upon genetic algorithms (GA), we "machine-learn" approximate yet highly accurate semiempirical method to compute, with about 1000 times decrease in time, excited-state photochemical reactions or decay rates. The MO-GA software, which can interface with Quantum Chemistry codes to produce the accurate semiempirical method, is available through the MCC Software Archive.
- Topology optimization: algorithms which compute the deformation and energy of a structure under loading/stress, and redistributes the material to reduce the energy taken up by the structure. Adaptive mesh refinement and coarsening reduces computational expense. We also use these techniques to design unit cells of advanced materials, such as those with a negative heat index, or negative Poisson ratio.

Highlight

- QMCPACK was selected as a showcase application for NCSA's petascale computing initiative.

Supported students

- Directly supported 29 graduate students and 2 postdoctoral researchers.

Software Archive

- 2,200 users and 5,500 downloads
- 60 titles, 20 are maintained by MCC members and affiliates

Publications

- 171 publications cite our award
- 19% arising from collaborations among MCC's members
- 26% arising from collaborations outside University of Illinois
- 32% published with students
- 27% acknowledge MCC computing resources

SERVICE AND OUTREACH ACTIVITIES

Summer schools (data covering 2005–2007)

- Average number of participants: 80 (24% women applicants)
- Average number of lecturers: 15 (12% women)
- Average amount of educational materials: 30 hours of lecture videos and 1000+ pages of printed course materials and computer tutorials

Participant positions:

- 7% Professor (6% junior, 1% tenured); 3% Research scientist; 15% Post-doc; 72% Graduate student; 1% Undergraduate Student; 2% Other

Highlight

- The lecture videos are accessible through the MCC's website and through Google videos and have been viewed ~1,200 times to date.
- The 2007 summer school was delivered to a satellite location in California, with two-way interaction between remote and local participants via the Access Grid.
- The 2006 summer school included two invited lectures given by participants from underrepresented groups.

Travel Award Program

- Support attendance of US-based researchers to participate in CECAM and Psi-k workshops focused on computational methods in physics, chemistry and materials science.
- 185 applications; 114 awards totaling \$100,210 over 3 years
- Awardees from 52 institutions

Awardee positions:

- 16% Professor (14% junior, 2% tenured); 3% Research scientist; 35% Postdoc; 45% Graduate student; 1% Undergraduate student;

Reported demographic information:

- 20% Female; 17% Hispanic or Latino; 3% Black or African American

Highlight

- "During my career as a graduate student and now as a faculty, I have received invaluable support from the MCC program. I strongly believe that efforts like this one facilitate the communication with our colleagues overseas and aid in integrating our research with that of people from all over the world. Thank you again, MCC!" Alan Aspuru-Guzik, Assistant Professor, Harvard University, Chemistry and Chemical Biology

Workshops

- The MCC contributes yearly to 1) Workshop on Recent Developments in Electronic Structure and 2) Understanding Complex Symposia. The MCC Travel Program supports travel to ~30 workshops in Europe per year.

Highlight

- The MCC created archive of all available materials from 20 years of Electronic Structure workshop.
- In first 7 years, the Complexity Symposium grew to ~300 participants, 100 presentations

Visitor Program

- The MCC has hosted two sabbatical visitors and over 50 lectures.

Highlight

- One MCC sabbatical visitor is Nithaya Chetty, the President of the South African Institute of Physics (SAIP). Dr. Chetty is a local organizer of the African School on Electronic Structure Methods and Applications, 14-25 July 2008, AIMS (African Institute for Mathematical Sciences) near Capetown, South Africa. This school has several sponsors; MCC is sponsoring R. Martin's travel to the school, where he will give tutorials.