Annual Report for Blue Waters Allocation

January 2016

Project Information

- Title: Quantum Simulations
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Executive summary (150 words)

Much of our research on Blue Waters is related to the "Materials Genome Initiative," the federally supported cross-agency program to develop computational tools to design materials. We employ Quantum Monte Carlo calculations that provide nearly exact information on quantum many-body systems and are also able to use Blue Waters effectively. This is the most accurate general method capable of treating electron correlation, thus it needs to be in the kernel of any materials design initiative. Ceperley's group has a number of funded and proposed projects to use Blue Waters as discussed below. In the past year, we have been running calculations for dense hydrogen in order to make predictions that can be tested experimentally. We have also been testing a new method that can be used to solve the fermion sign problem and to find dynamical properties of quantum systems.

Description of research activities and results

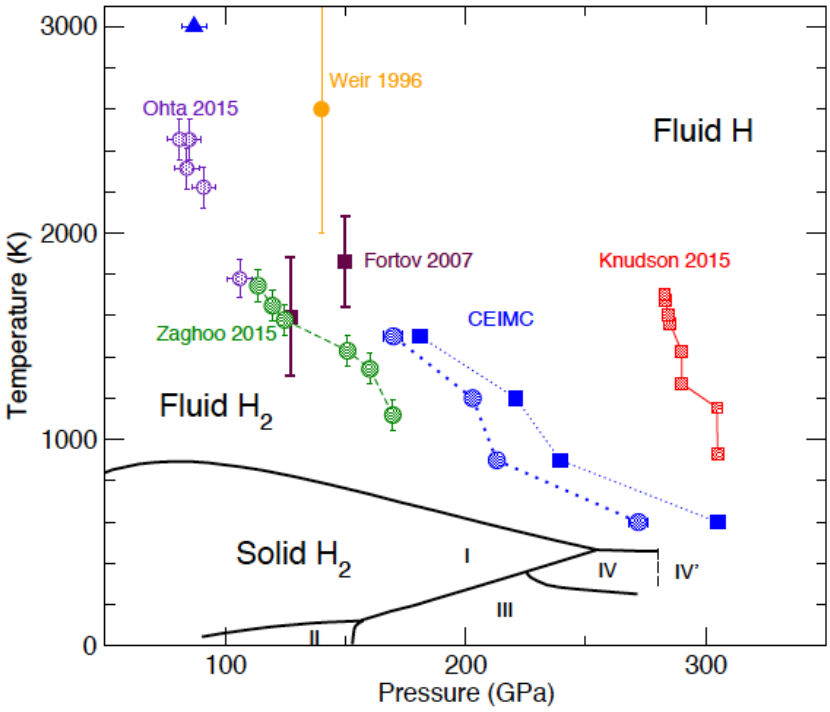
During the past year, the following 4 grants of which Ceperley is a PI or CoPI, and that involve Blue Waters usage, have had their funding renewed. Access to Blue Waters is crucial for success of these projects.

- "Warm dense matter"DE-NA0001789. Computation of properties of hydrogen and helium under extreme conditions of temperature and pressure. Ceperley is sole PI. This is the funding that supported computations in 2014-2015 and it is renewed for 2015-2018.
- SCIDAC, Predictive Computing for Condensed Matter DE-SC0008692. So Hirata is the PI, involves 5 other UIUC faculty. It was recently renewed for 2 more years.
- Network for Ab Initio Many-body Methods: for development of the QMC software, QMCPACK. Kent at Oak Ridge is the PI, involves scientists at 4 national labs as well as UIUC. It was recently renewed for 2 more years.
- EFRC: Center for Emergent Superconductivity. A very ambitious project to discover new superconducting materials using computation and experimental validation. This grant was funded in July 2014. The PI is Peter Johnson at Brookhaven National Lab and involves other faculty at UIUC.

One ongoing project on Blue Waters during 2015 has focused on a "multiscale" project: a way to use highly accurate energies from quantum Monte Carlo to treat larger systems at longer length scales. Atomistic simulations are widely used across many different scientific disciplines, including physics, material science, chemistry, and biology. Large-scale simulations and highly accurate simulations cannot generally be performed simultaneously. *Ab initio* simulations are limited to small system sizes. Despite its

cost, Quantum Monte Carlo is important, since high accuracy is needed. In high-pressure hydrogen simulations, we have recently shown that various density functionals differ significantly from benchmark quantum Monte Carlo simulations. We have made significant progress on the following two projects:

1. Liquid-liquid phase transition in hydrogen by Coupled Electron-Ion Monte Carlo Simulations C. Pierleoni, M. A. Morales, G. Rillo, M. Holzmann, D. M. Ceperley. under review at PNAS (2106). The phase diagram of high pressure hydrogen is of great interest both for fundamental research, such as planetary physics, and for energy applications. The existence and precise location of a phase transition in the liquid phase between a molecular insulating fluid and a monoatomic metallic fluid is relevant for planetary models. Recent experiments reported contrasting results about its location. Theoretical results based on Density Functional Theory are also very scattered. During 2015, we have performed highly accurate Coupled Electron-Ion Monte Carlo calculations of this transition, finding results that lie between the two experimental predictions, close to that measured in Diamond Anvil Cell experiments but at 25-30 GPa higher pressure. The transition along an isotherm is signaled by a discontinuity in the specific volume, a sudden dissociation of the molecules, a jump in electrical conductivity and in electron localization.



The hydrogen phase diagram with experimental liquid-liquid transition lines and CEIMC predictions. Black continuous lines indicate the melting line as well as the transition lines between different experimentally detected crystalline phases: I to IV'. Blue circles and squares are CEIMC predictions for the liquid-liquid transition line in hydrogen and in deuterium, respectively. DAC experimental results for hydrogen are indicated by green circles and purple circles, while red squares indicate shock wave experimental data for deuterium.

2. How do exact quantum Monte Carlo projection methods behave in the thermodynamic limit? D. M. Ceperley and M. Holzmann, paper in preparation. The release-node procedure uses imaginary time projection of a trial wavefunction to obtain "in principle" exact properties of quantum systems. However, for general fermion systems, the signal to noise ratio decreases exponentially fast with respect to the imaginary time projection. We have done calculation on Blue Waters for charged bosons and fermions on

the behavior of the projection versus the number of particles. Methods for finding better estimates of the exact energy of quantum systems in the thermodynamic limit have been discovered.

Talks by D. M. Ceperley on this research in 2015-2016:

- Progress in Quantum Monte Carlo, Telluride CO, 6/2015
- Dense Hydrogen, Tampere, Finland 7/2015
- Problems in the Computation of Dense Hydrogen, International Workshop on Many-Body Theory, Niagara Fall, NY, 8/2015
- Quantum Monte Carlo Simulations in Dense Hydrogen, University of Michigan, 9/2015
- How do exact QMC methods behave in the thermodynamic limit? Honolulu, HI, 12/2015
- The liquid-liquid transition in dense hydrogen, Berkeley CA, 1/2016

Plans for next year

As mentioned above we have several projects underway. Blue Waters capability is needed to take the research from the model level to realistic description of materials where electron correlation is important. Typical materials require simulation of a unit cell with at least one thousand electrons. Just holding the single-body orbitals in memory for a realistic material requires a multiprocessor computer. Relevant accuracy for materials design will definitely require petascale computational access.

J. Kim, D. Ceperley and his colleagues have devised algorithms and software (QMCPACK) where the computation is shared across processors within a node using Open-MP and across nodes with MPI. In addition, parts of the calculation can be done very effectively on GPUS with speed-ups over the CPUs of more than an order of magnitude. The QMCPACK software, which was one of the benchmark algorithms for Blue Waters, is one of the few codes that can take full advantage of its architecture. Our implementation is mature, well optimized, already installed on the Blue Waters; we have demonstrated 90% parallel efficiency on up to 216,000 processor cores for production runs. Development of QMCPACK is now supported by a 5 year DOE grant mentioned above; Ceperley is one of the PIs on this grant. We are planning a summer school at NCSA in June 2016 to teach the usage of QMCPACK.

We plan to continue the current project on hydrogen, in particular examining the phases at lower temperature. Also we plan to initiate several new projects. We expect to submit the results from the second project mentioned above within the next few months. We request 240,000 node hours on Blue Waters, for the period Feb 2016-Jan 2017. We expect to be using the time uniformly throughout the year. The data transfer, data storage and access requirements should be similar to our usage in 2015.