QMC Training Program

14th-18th July 2014

Paul Kent (ORNL)

Funding: Predictive Theory and Modeling Program for Materials and Chemical Science Program, Office of Basic Energy Sciences, US Department of Energy, and "QMC Calculations of Deep Earth Materials", DMS-1024936, National Science Foundation

Hosts: ALCF, Argonne National Laboratory

Program Goals

1. Introduce fundamentals of QMC theory
2. Introduce current QMC methods & their applications in physics, chemistry and materials science
3. Introduce the **QMC**PACK code and **QMC**PACK developers

We aim that by the end of week you have the knowledge to plan and run a research level QMC calculation.

Provide on-going support and assistance in your QMC research. Please discuss with us! (Optional)

Lecturers and lab instructors

Anouar Benali (ANL)

David Ceperley (UIUC)

Raymond Clay (UIUC)

Paul Kent (ORNL)

Jaron Krogel (ORNL)

Miguel Morales (LLNL)

William Parker (ANL)

Nichols Romero (ANL)

Luke Shulenberger (SNL)

Norm Tubman (UIUC)

Logistics - Shuttles

See schedule at http://events.alcf.anl.gov/qmc-2014/schedule/

7.40, 8.00, 8.20am Shuttles depart from guesthouse

5pm Shuttles return to guesthouse

Walking or personal car are also options

Logistics – Dining & Breaks

See schedule at http://events.alcf.anl.gov/qmc-2014/schedule/

8am+	Continental breakfast (this room)
~10.45am	Break
12-1pm	Lunch at ANL cafeteria
~3.15pm	Break
6pm+	Dinner at ANL Guest House with guest speakers
	Tuesday: Paul Messina, Director of Science ALCF
	Thursday: Giulia Galli, U. Chicago & Senior ANL scientist

Logistics – Wifi access

Use ArgonneA-guest / ArgonneG-guest

Fill in form that appears on visiting a web page

Schedule and Lecture materials

Linked at http://events.alcf.anl.gov/qmc-2014/schedule/

Check for updates. Please download lecture materials

Morning	Afternoon
Introduction Variational Monte Carlo	QMCPACK Intro / Lab: Monte Carlo Statistics & Data analysis
Diffusion Monte Carlo Wavefunction Optimization	Lab: Running simple QMC calculations (oxygen atom and dimer)
Molecular Calculations	Lab: Molecular calculations
Solid State Calculations	Lab: Solid state calculations
Choosing a QMC Project Obtaining Computational Resources Advanced topics: Forces and Non-adiabatic calculations	Discussion with instructors & ongoing lab

Questions?

Note: Feedback on all aspects of this training is appreciated

Welcome to ALCF & Safety Reminders

Richard Coffey, Director of User Experience ALCF