

QMCPACK Users Workshop

Agenda as of (05/07/2019)

Event contact	Paul Kent 865-574-4845 (office); kentpr@ornl.gov Erica Valentine 865-576-3709 (office); valentineem@ornl.gov		
Time	Event	Lead	Place
Tuesday May 14th 2019			
7:30am	Badging at Visitors Center		Building: 5200
8:00am	Welcome - Overview and introduction, <i>Breakfast provided</i>	Paul Kent	Building: 8600 Room: C-156
8:30am	Set up Amazon Web Services	Paul Kent	Building: 8600 Room: C-156
9:00am	Correlation Consistent Pseudopotentials	Cody Melton	Building: 8600 Room: C-156
9:30am	Using PySCF for Molecules and Solids	Anouar Benali	Building: 8600 Room: C-156
10:30am	Break		Building: 8600 Room: C-156
11:00am	Auxiliary Field QMC part I	Miguel Morales	Building: 8600 Room: C-156
12:00pm	Working Lunch - Engaging with the QMCPACK Project, <i>Lunch provided</i>	Paul Kent	Building: 8600 Room: C-156
1:00pm	Auxiliary Field QMC part II	Miguel Morales	Building: 8600 Room: C-156
2:00pm	Development of Forces in QMCPACK	Raymond Clay	Building: 8600 Room: C-156
2:30pm	Invited user talk: “Quantum Monte Carlo from Benchmarking to Understanding Nanoscale Materials”	Kayahan Saritas	Building: 8600 Room: C-156

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Time	Event	Lead	Place
Tuesday May 14th 2019			
3:00pm	Break		Building: 8600 Room: C-156
3:30pm	Hands-on and discussion time	Paul Kent	Building: 8600 Room: C-156
5:30pm	Reception and poster session	Paul Kent	8600 Corridor

Wednesday May 15th 2019			
8:00am	Recap of previous days sessions, <i>Breakfast provided</i>	Paul Kent	Building: 8600 Room: C-156
8:30am	Selected CI Trial Wave Functions with Quantum Package and QMCPACK	Anouar Benali	Building: 8600 Room: C-156
9:30am	Wavefunction Optimization Algorithms in QMCPACK	Luning Zhao	Building: 8600 Room: C-156
10:15am	Break		Building: 8600 Room: C-156
10:45am	NEXUS Workflow System	Jaron Krogel	Building: 8600 Room: C-156
12:00pm	Working Lunch - Future Workshop and QMCPACK Development Plans, <i>Lunch provided</i>	Paul Kent	Building: 8600 Room: C-156
1:00pm	Running Solids Efficiently at Large Scale	Ye Luo	Building: 8600 Room: C-156
1:30pm	Invited user talk: "Compton Profile of Solid and Liquid Lithium from Quantum Monte Carlo"	Paul Yang	Building: 8600 Room: C-156

Wednesday May 15th 2019

2:00pm	Status of Spin in QMC	Lubos Mitas	Building: 8600 Room: C-156
2:30pm	Hands-on and discussion time	Paul Kent	Building: 8600 Room: C-156
3:00pm	Group Photo	Genevieve Martin	SNS Lobby
3:15pm	Break		Building: 8600 Room: C-156
3:30pm	Hands-on and discussion time	Paul Kent	Building: 8600 Room: C-156
5:00pm	Wrap up	Paul Kent	Building: 8600 Room: C-156

Attendees:

Abdulgani Annaberdiyev, North Carolina State University
 Alfredo Correa, Lawrence Livermore National Laboratory
 Alicia Welden, Lawrence Livermore National Laboratory
 Amanda Dumi, University of Pittsburgh
 Anh Pham, Oak Ridge National Laboratory
 Ankit Mahajan, University of Colorado
 Anouar Benali, Argonne National Laboratory
 Can Ataca University of Maryland
 Cancan Huang, Brown University
 Charles Peterson, University of North Texas
 Charles Rendleman, D.E. Shaw Research
 Cody Melton, North Carolina State University
 Daniel Wines, University of Maryland
 Federico Zahariev, Iowa State University / Ames National Laboratory
 Fernando Reboredo, Oak Ridge National Laboratory
 Fionn Malone, Lawrence Livermore National Laboratory
 Gewinner Senderanto Sinaga, Japan Advanced Institute of Science and Technology
 Guangming Wang, North Carolina State University
 Gwangyeong Lee, Konkuk University
 Hongxia Hao, Brown University
 Hyeondeok Shin, Argonne National Laboratory
 Iliya Sabzevari, The University of Colorado at Boulder
 Iuegyun Hong, Konkuk University
 Jaron Krogel, Oak Ridge National Laboratory

Kevin Gasperich, University of Pittsburgh
 Kevin Ly, University of Illinois
 Lubos Mitas, North Carolina State University
 Luke Shulenburger, Sandia National Laboratory
 Luning Zhao, University of California, Berkeley
 Mark Dewing, Argonne National Laboratory
 Miguel Morales, Lawrence Livermore National Laboratory
 P. Ganesh, Oak Ridge National Laboratory
 Paul Kent, Oak Ridge National Laboratory
 Raymond Clay, Sandia National Laboratory
 Ronald Cohen, Carnegie Institution
 Ryo Maezono, Japan Advanced Institute of Science and Technology
 Samuel Greene, University of Chicago
 Shiv Upadhyay, University of Pittsburgh
 Shuai Zhang, Lawrence Livermore National Laboratory
 Tomas Rojas Solorzano, Ohio University
 Tomohiro Ichiba, Argonne National Laboratory
 Ye Luo, Argonne National Laboratory
 Yubo Yang, University of Illinois

Joshua Townsend, Sandia National Laboratory
 Kayahan Saritas, Oak Ridge National Laboratory
 Keishu Uchimura, Japan Advanced Institute of Science and Technology
 Ken Qin, Japan Advanced Institute of Science and Technology
 Kenneth Jordan, University of Pittsburgh