QMCPACK Workshop 2019

14th-15th May 2019, Oak Ridge National Laboratory

Paul Kent, kentpr@ornl.gov

Wifi: ornl-visitor

Slides: https://github.com/QMCPACK/qmcpack_workshop_2019

Acknowledgments

Local organization: Erica Valentine, ORNL & conference office

Presenters

Anouar Benali, ANL

Raymond Clay, SNL

Paul Kent, ORNL

Jaron Krogel, ORNL

Ye Luo, ANL

Fionn Malone, LLNL

Cody Melton, NCSU

Lubos Mitas, NCSU

Miguel Morales, LLNL

Kayahan Saritas, ORNL

Paul Young, UIUC

Luning Zhao, UC Berkeley

Workshop Goals

Present recent developments to QMCPACK and surrounding ecosystem

See examples of recent research (posters, invited user presentations)

Facilitate discussion among developers and users
- Help new science applications
- Improving ease of use
- Improving the next iteration of this workshop
- …

Tuesday's Schedule

8.30	Paul Kent	Computing Setup
9.00	Cody Melton	Correlation Consistent Pseudopotentials
9.30	Anouar Benali	PySCF for molecules and solids
10.30		Group Photo & Break
11.00	Miguel Morales	Auxiliary Field QMC Part I
12.00	Paul Kent	Working lunch - Recent Developments & Engaging with the QMCPACK project

Tuesday's Schedule

1.00	**Miguel Morales & Fionn Malone**	**Auxiliary Field QMC Part 2**
2.00	**Raymond Clay**	**Development of Forces in QMCPACK**
2.30	**Kayahan Saritas**	**User talk "QMC from benchmarking to understanding nanoscale materials"**
3.00		**Break**
3.30		**Hands-on and discussion**
5.30		**Poster session & reception**

Wednesday's Schedule

8.00	Paul Kent	Recap; Breakfast provided
8.30	Anouar Benali	Select Configuration Interaction with Quantum Package and QMCPACK
9.30	Luning Zhao	Wavefunction Optimization algorithms
10.15		Break
10.45	Jaron Krogel	NEXUS Workflow system
12.00	Paul Kent	Working lunch; Future Workshop and QMCPACK Development Plans

Wednesday's Schedule

1.00	Ye Luo	Running Solids Efficiently at Scale
1.30	Paul Young	User talk "Compton Profile of Solid and Liquid Lithium from QMC"
2.00	Lubos Mitas	Status of Spin in QMC
2.30		Hands-on and discussion
3.00		Break
3.30		Hands-on and discussion
5.00	Paul Kent	Wrap Up

Computing Setup

Use ORNL visitor wifi (ornl-visitor)

Workshop presentations & examples are browsable at
https://github.com/QMCPACK/qmcpack_workshop_2019

Suggestion: Make a local copy on your laptop

git clone https://github.com/QMCPACK/qmcpack_workshop_2019.git

cd qmcpack_workshop_2019; git pull # for updates

This file is day1_Welcome_and_Introduction.pdf

Computational Resources

Each attendee is provided with unique computational resources for the workshop. Discuss with Paul Kent to have access after 5.30pm Wednesday 15th.

Resources are Amazon Web Services c5.4xlarge instances: a recent 16 thread Intel Xeon, 32GB memory and 64GB SSD storage. OS is Ubuntu 18.04.

QMCPACK development version (2019-05-10), Quantum Espresso 6.4, PySCF, and Quantum Package are installed. See qmcpack_workshop_2019/AWS to see how built. We hope to publish a machine image in future.

These resources should only be used for activities related to this workshop and related research calculations

Access

On Monday, everyone should have received an email with key "UserNN.pem"

On Linux and Mac:

chmod 400 User6.pem

ssh –i User6.pem ubuntu@qmcaws.ornl.gov –p 2006 # port is 2000+user number

scp –P 2006 –i User6.pem localfile.txt ubuntu@qmcaws.ornl.gov:

sudo apt-get favorite-editor # Accounts have sudo privs

Applications are installed in $HOME/apps and on PATH, PYTHONPATH:

qmcpack, qmcpack_complex, pw.x, qp_run…

Questions?

Note: Feedback on all aspects of this workshop is appreciated