# **QMC**PACK Workshop 2019

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

Paul Kent, kentpr@ornl.gov

Wifi: ornlvisitor

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

Funding: U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, as part of the Computational Materials Sciences Program and Center for Predictive Simulation of Functional Materials.

# Acknowledgments

Local organization: Erica Valentine, ORNL & conference office

Funding: U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, as part of the Computational Materials Sciences Program and Center for Predictive Simulation of Functional Materials.

# 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

| | | |
|---|---|---|
| **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

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|---|---|---|
| **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** |

# Computing Setup

Use ORNL visitor wifi (ornlvisitor)

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*