

# QMCPACK Workshop 2019

14<sup>th</sup>-15<sup>th</sup> May 2019, Oak Ridge National Laboratory

Paul Kent, kentpr@ornl.gov

Wifi: ornlvisitor

Slides: [https://github.com/QMCPACK/qmcpack\\_workshop\\_2019](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

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

# Tuesday's Schedule

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

# Wednesday's Schedule

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

# Wednesday's Schedule

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



# Computing Setup

Use ORNL visitor wifi (ornl-visitor)

Workshop presentations & examples are browsable at  
[https://github.com/QMCPACK/qmcpack\\_workshop\\_2019](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*