QMC Workshop 2021
Wrap Up & Next Steps

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CPSFM | Center for Predictive Simulation of Functional Materials

Sandia National Laboratories

Argonne NATIONAL LABORATORY

NC STATE UNIVERSITY

BROWN

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Complete the Workshop Survey

Link sent by email this morning. Survey closes next Tuesday.

Make your voice heard and let us know:

How we can improve this workshop

What we should cover next time

What format "next time" should take

How we can improve QMC & QMCPACK for your research

…

Next Steps

Try the workshop examples if you have not already

Run a different set of small molecules in the virtual machine

        e.g. run a hydrocarbon such as methane, examine the charge density

Install QMCPACK, QE, PySCF on local machines

Look at the recent literature

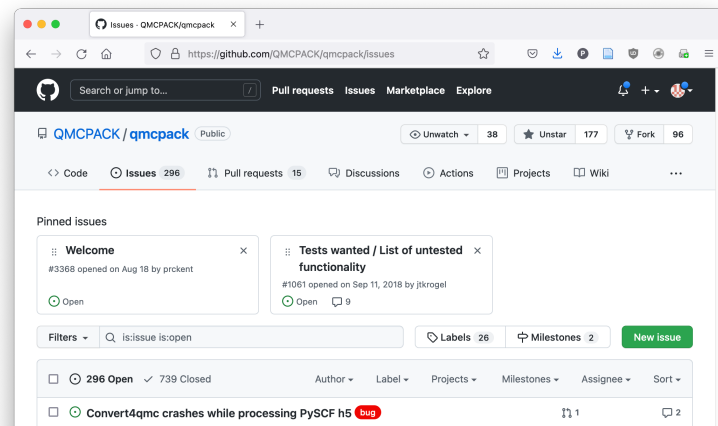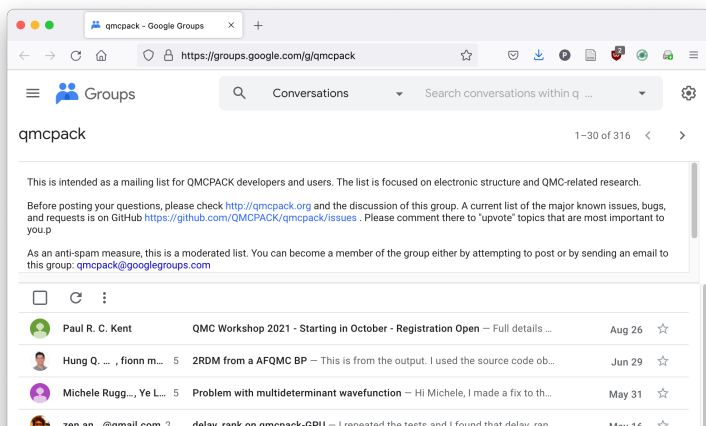Try to setup a research problem

Ongoing Support

Workshop Slack channel will remain open. Workshop image will be updated.

Use the QMCPACK Google Group

Open an issue on QMCPACK GitHub for more technical issues

See https://qmcpack.org for news, updates

Contact us directly

Questions?

Thanks to all