QMCPACK
Development Plans

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Question:

What are the “non-research” developments - both large and small - that would most help us do our sciences with QMCPACK? Or reduce barriers for others?

Develop a single code version

One focus of our DOE funded Exascale project is making a single “version” of the real space code where all features run on all platforms. Optimizations can be done for specific platforms. AFQMC is ~already there.

Today:

CPU Array-of-structures build	Legacy, largely feature complete
CUDA GPU build	Fast, but a fork with very limited feature coverage
CPU Structures-of-arrays build	(Default today) 2x as fast on modern CPU architectures, but an internal fork, most but not all features supported

Simplifying Trial Wavefunction Generation & Usage

Keep improving NEXUS!

Try to minimize number of steps between scf calculation and a runnable QMC calculation

Quantum Espresso – As the QE HDF5 support matures we hope to avoid a custom pw2qmcpack and use the native QE files directly. Conversions will then be like the quantum chemistry codes and patching QE won't be necessary.

Also generate example inputs as per convert4qmc

Improving inputs

Feedback needed – very subjective!

1. Recommended and logically consistent sample inputs for different “routes”
2. Provide a new parallel set of input parameters specifying “total work” to be performed and infer other parameters where not specified. E.g. Total number of walkers in VMC! Many “legacy” parameters hide/don’t specify normalization.
3. Improved validation of inputs will require an overhaul of the input system ☹ , but we are adding error checks based on real-world experience. E.g. Missing files, typos should result in meaningful error message.
4. “Stop on target error bar” -> facilitate via workflow system initially
5. AFQMC<>real-space consistency

Increasing examples

Many calculations start by recycling existing inputs ☺

Expand provided example files to have >= 1 per main feature

> Currently we have lots of tests and only a few real examples with READMEs etc.

Workshops

Holding annual 2 day workshops should be feasible. Weeklong schools and workshops are more challenging (location, time commitment, $).

Should we continue with this 2 day format? How should it change?