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Prospects for calculating plasma transport properties on a quantum computer

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Wait. What?

By now you've probably heard *something* about quantum computing...
You might even be an expert, yourself!

For a while, some of us at Sandia have been looking at how quantum computers might impact plasma physics...

"Classical" dynamics are a plausible but expensive* application area.

We think that strongly coupled plasmas are the most promising application area.

*Relatively expensive. You're going to see some scary numbers, later.

Failures of classical computers.

Why might we want a quantum computer?

Exponential growth in classical resources for *verifiably* accurate solutions.

No exchange-correlation potential. As accurate as the Hamiltonian coefficients.

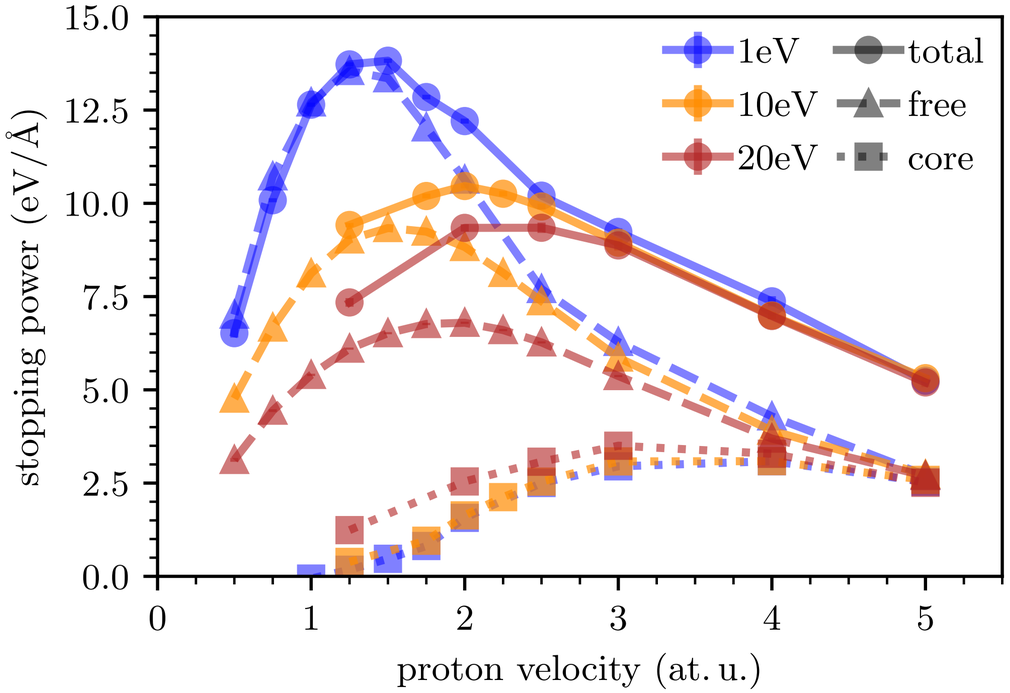
Progress in improving approximate methods isn't consistent or systematic.

No truly satisfying way to treat non-zero temperature, or non-equilibrium, for big basis sets/supercells.

Conspicuous advantage: big reliable classical supercomputers exist...

Setting the scale of the modeling problem.

Lead scientist:
Alina Kononov



Proton stopping powers for warm dense aluminum.

The figure on the left took about 0.25 *billion* CPU hours.

Results like these are benchmarks for more efficient models that can fill out an entire model w/7-8 orders of magnitude fewer resources.

Experiments are actually more expensive than the huge CPU time investment.

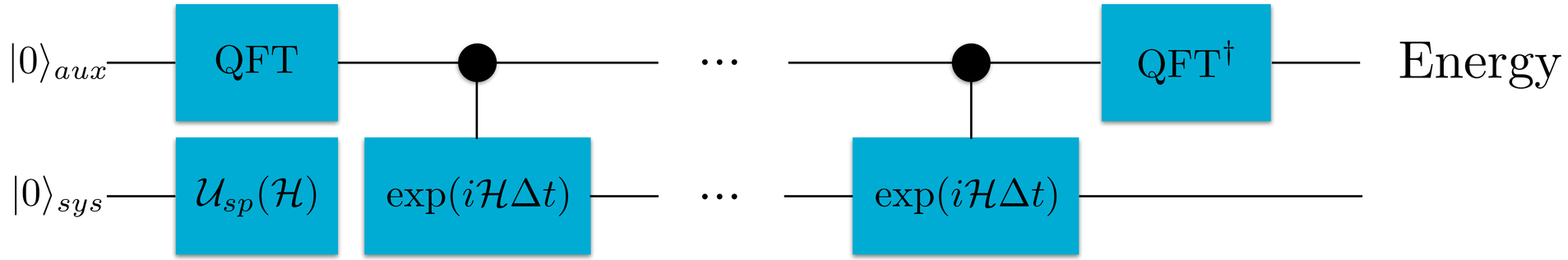
Calculations use Ehrenfest dynamics & time-dependent density functional theory.

First principles, but unknown* approximation error.

*No *rigorous* bounds known, but agreement w/experiments in ambient conditions suggest results are pretty good!

How would a quantum algorithm work?

Surprisingly simple, if you're content to elide details.

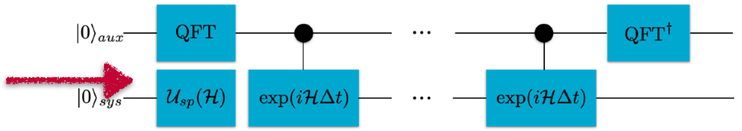


1.) Prepare a state that encodes the system of interest in a register of qubits.
2.) Time evolve said state under the action of the exact many-body Hamiltonian.
3.) Measure observable of interest, e.g., an operator or a 2-point response function.

The above example computes an energy eigenvalue...
It is only a bit more complicated to compute observables with a different eigenbasis.

(Rough) resource estimates.

One of the dominant costs appears to be state preparation.

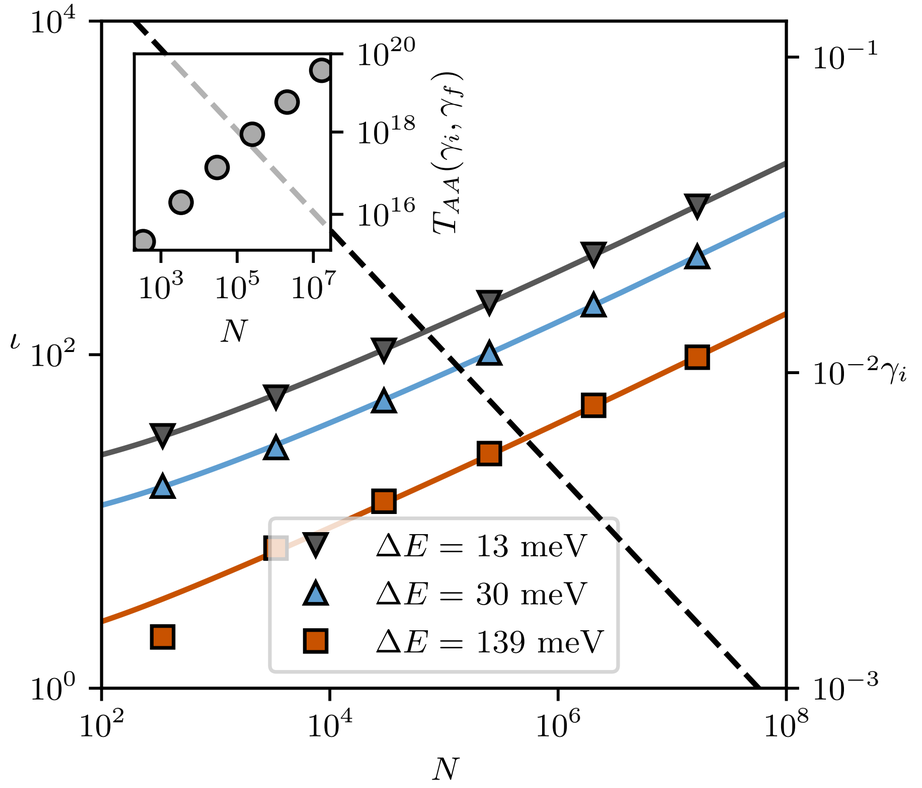


Recent analysis of resource requirements for a near-optimal ground state preparation algorithm* applied to a high-accuracy model of a condensed phase system.

33,275 logical qubits, without T factories.

~100,000,000 physical qubits**

arXiv posting on quant-ph, this week



Lead scientist:

Shivesh Pathak

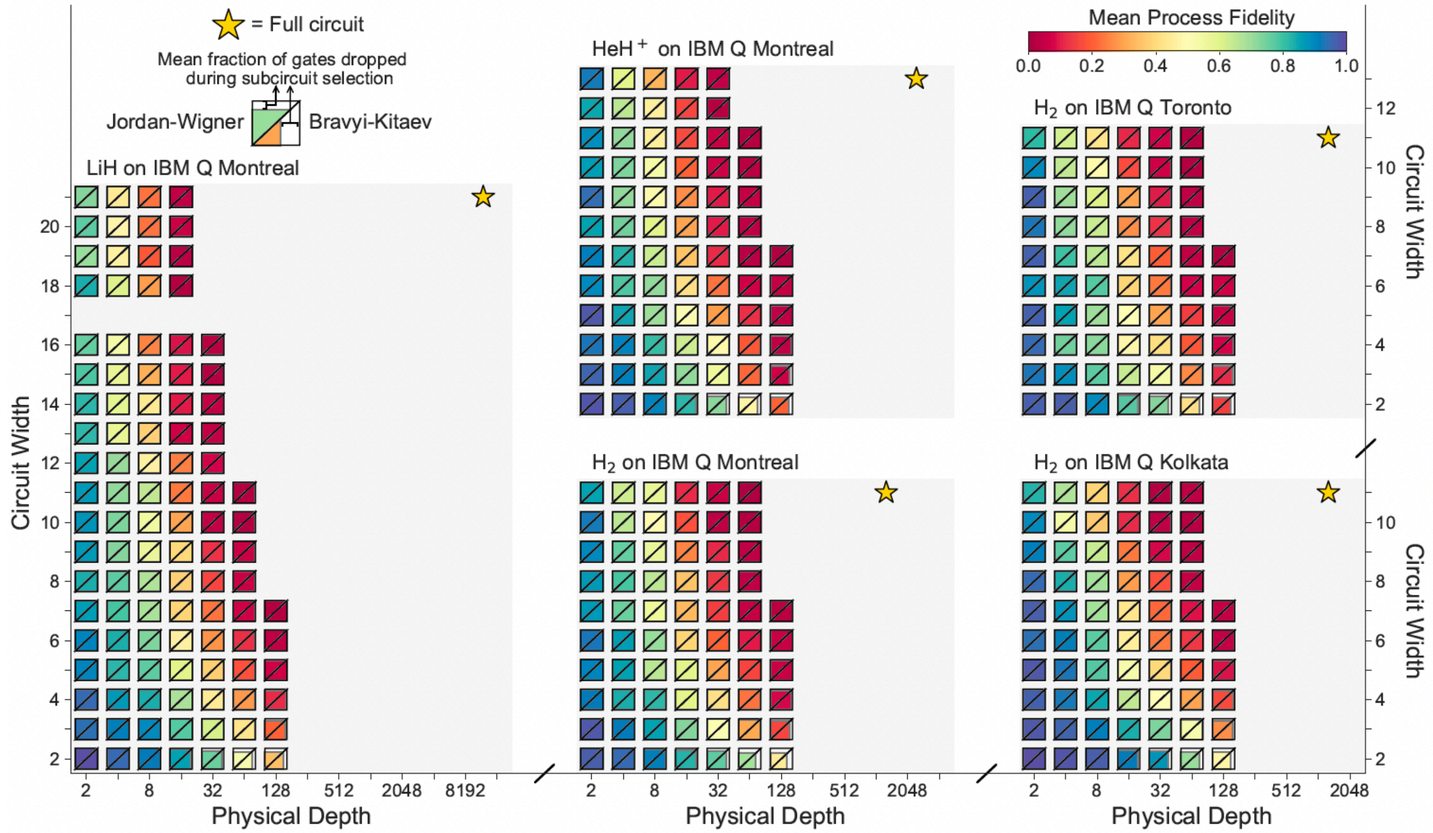
*Lin and Tong, Quantum (2020)

**Fowler, Mariantoni, Martinis, and Cleland, PRA (2012)

Tracking progress towards a useful* QC.

Those are daunting resource estimates - how do we know that we're getting closer?

Lead scientist:
Stefan Seritan



We can turn a subroutine from any algorithm into a volumetric benchmark.

Coming to an arXiv, near you...

*Narrow definition of utility = better than your institutional supercomputer.

Conclusions.

Quantum computers *won't* provide an advantage for every plasma physics problem, but they might *help* solve some niche problems that *we* all care about.

In general, this will likely be true of science applications and quantum computing. Classical computers *help* us do science, and they *don't* replace experiments.

Value added by scientific computation = (Cost of experiment) - (Cost of computer)

As in fusion, the energy balance is currently negative.
But I hope that it won't always be that way.

If you want to chat, or copies of preprints as they become available - adbacze@sandia.gov

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