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Prospects for simulating warm dense matter on a quantum computer

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High Energy Density Science

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Basics of fusion energy.

Controlled Fusion Research—An Application of the Physics of High Temperature Plasmas

Richard F. Post

University of California Radiation Laboratory, Livermore, California

Table I. Fusion reactions.

(1)	D+D→He^3	+n+	3.25	Mev
(2)	D+D→T	+p+	4	Mev
(3)	T+D→He^4	+n+	17.6	Mev
(4)	He^3+D→He^4	+p+	18.3	Mev
(5)	Li^6+D→2 He^4+		22.4	Mev
(6)	Li^7+p→2 He^4+		17.3	Mev

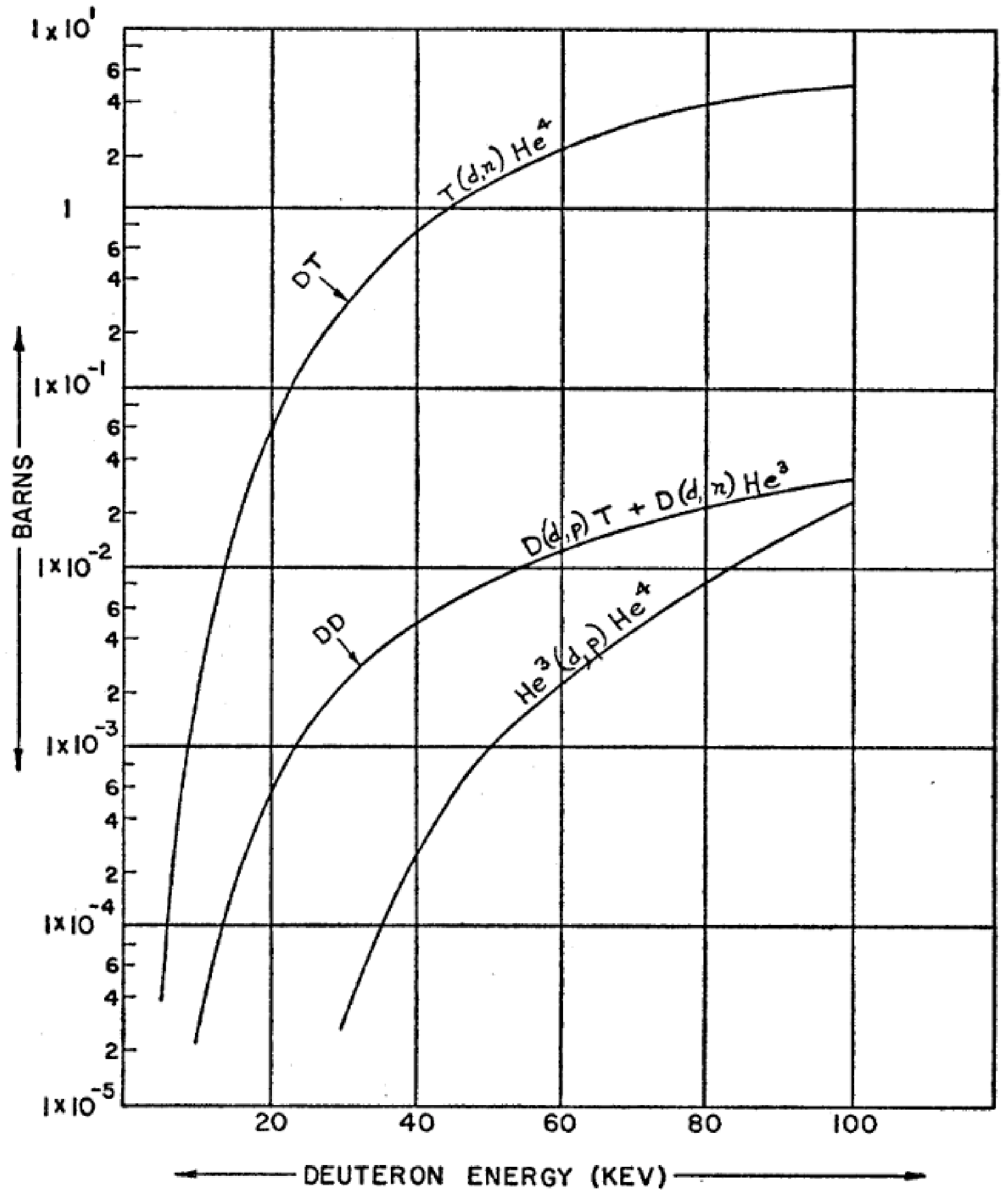


Fig. 1. Nuclear fusion reaction cross sections as a function of relative particle energy.

DT fusion - 10 MeV per reaction with a large cross section at 10 keV*

*Augment with factors of "about" or "ish" as needed

O(1 eV) = O(10,000 K), so O(10 keV) = O(100,000,000 K)

Two approaches to fusion.

Most material containers have a tendency to melt around 1 eV...

We need *something* to keep a fusion plasma confined

	Magnetic	**Inertial**
Key idea	Charged particles don't cross B field lines	Matter stays put for a time ~(size/sound speed)
Temperature	10 keV, e.g., a star	10 keV, e.g., a star
Density	10^{14} parts./cm^3, e.g., 100,000x sparser than air	10^{25} parts./cm^3, e.g., 100x denser than water
Pressure	10^6 Pa, e.g., 10x the room you're in	10^{12} Pa, e.g., 10x the Earth's inner core

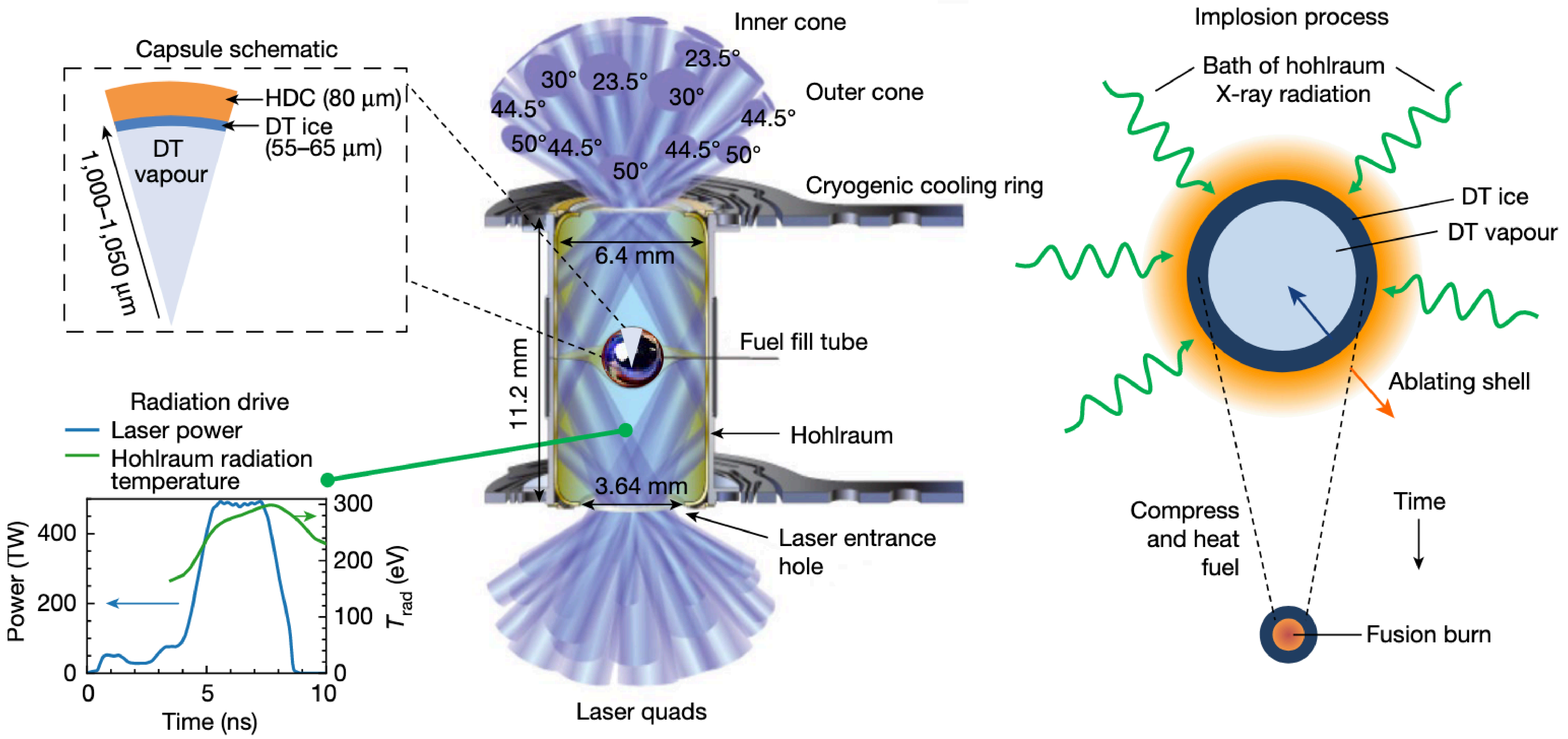
Inertial confinement fusion (ICF) requires us to control matter in conditions that we don't commonly encounter

Reminder, O(1 eV) = O(10,000 K)

ICF research platforms.

nature

Burning plasma achieved in inertial fusion



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Experimental Demonstration of Fusion-Relevant Conditions in Magnetized Liner Inertial Fusion

M. R. Gomez, S. A. Slutz, A. B. Sefkow, D. B. Sinars, K. D. Hahn, S. B. Hansen, E. C. Harding, P. F. Knapp, P. F. Schmit, C. A. Jennings, T. J. Awe, M. Geissel, D. C. Rovang, G. A. Chandler, G. W. Cooper, M. E. Cuneo, A. J. Harvey-Thompson, M. C. Herrmann, M. H. Hess, O. Johns, D. C. Lamppa, M. R. Martin, R. D. McBride, K. J. Peterson, J. L. Porter, G. K. Robertson, G. A. Rochau, C. L. Ruiz, M. E. Savage, I. C. Smith, W. A. Stygar, and R. A. Vesey

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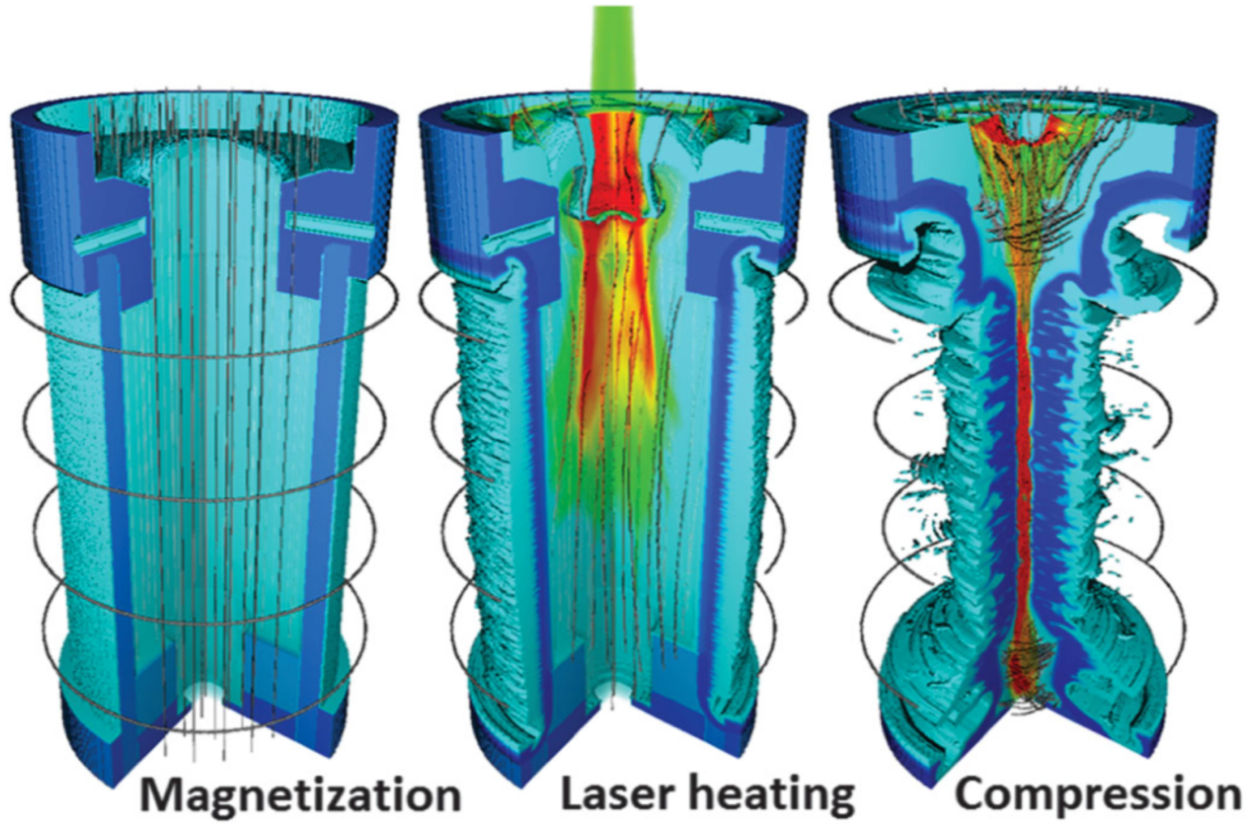
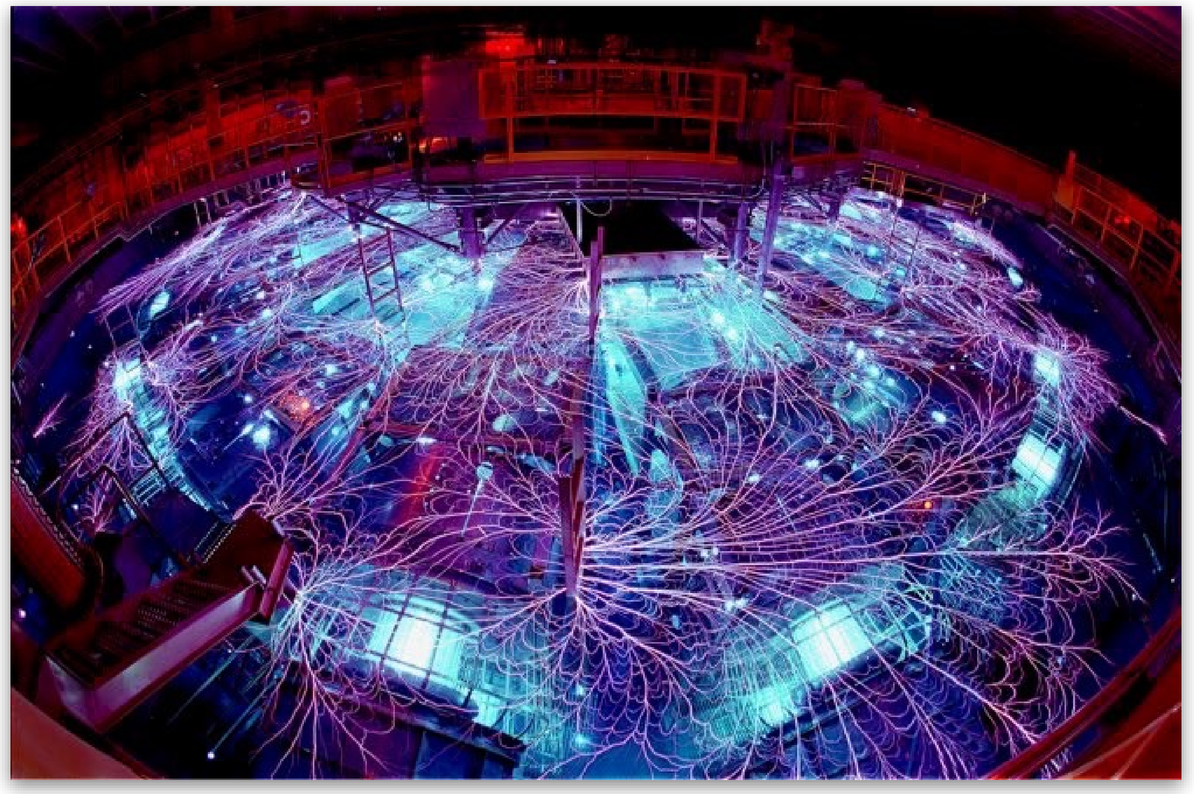
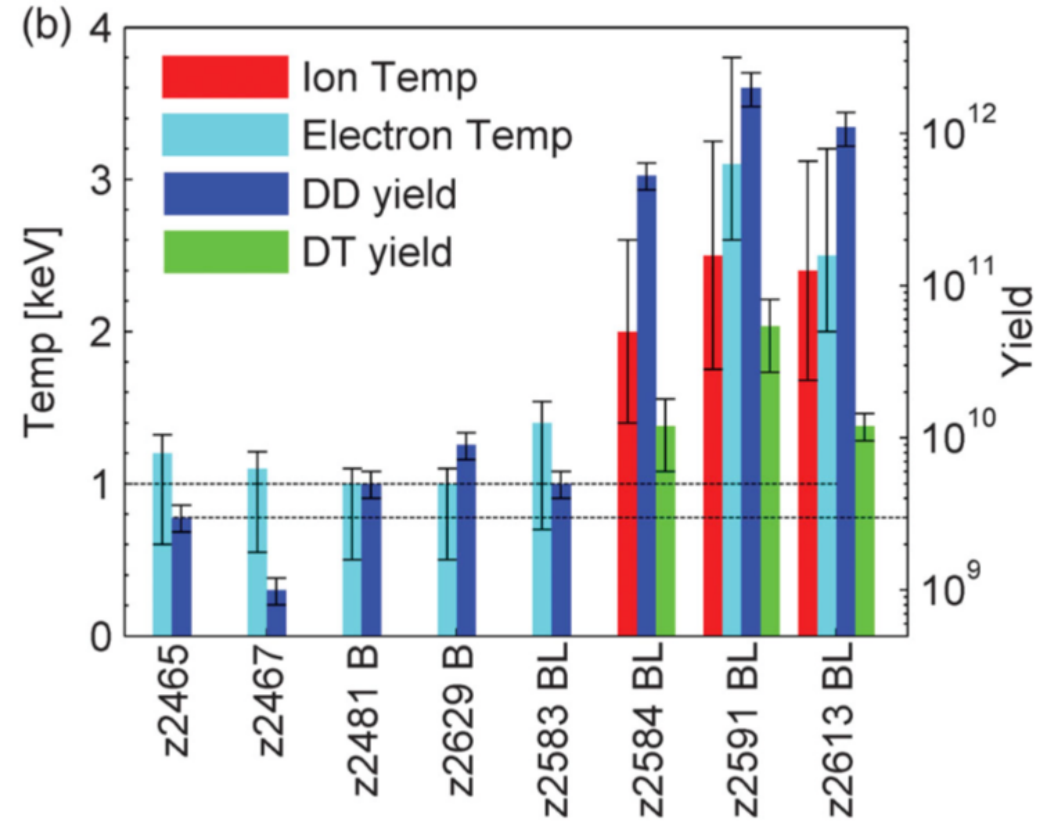
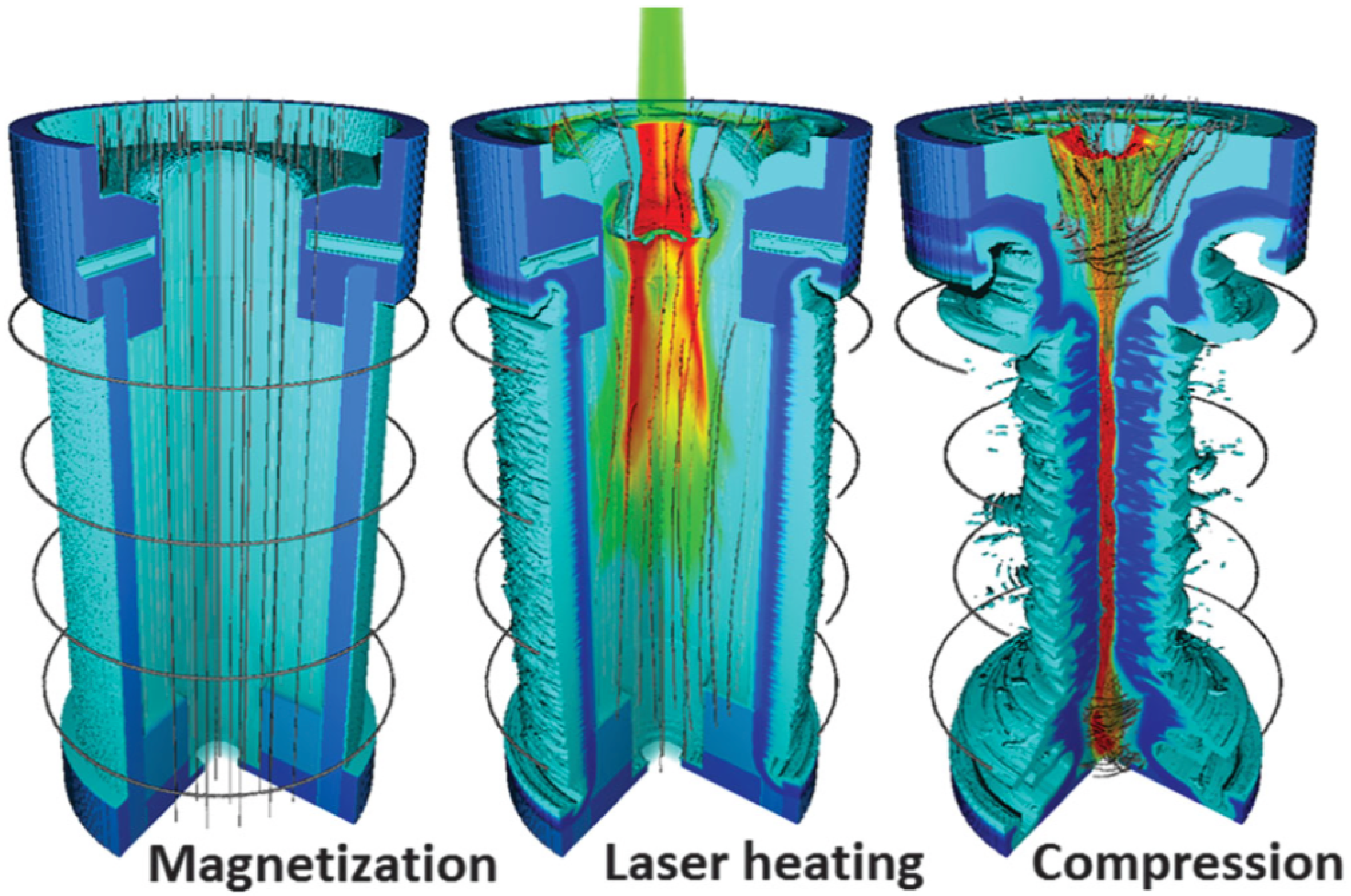






Challenges of multiphysics modeling.

What physics needs to be modeled?



Current in walls drives implosion via Lorentz force

Laser coupling to fuel and window

Magnetic inhibition of transport

Alpha particle self-heating,
balance against radiation and conduction loss

X-rays generated in plasma propagate
through surrounding matter

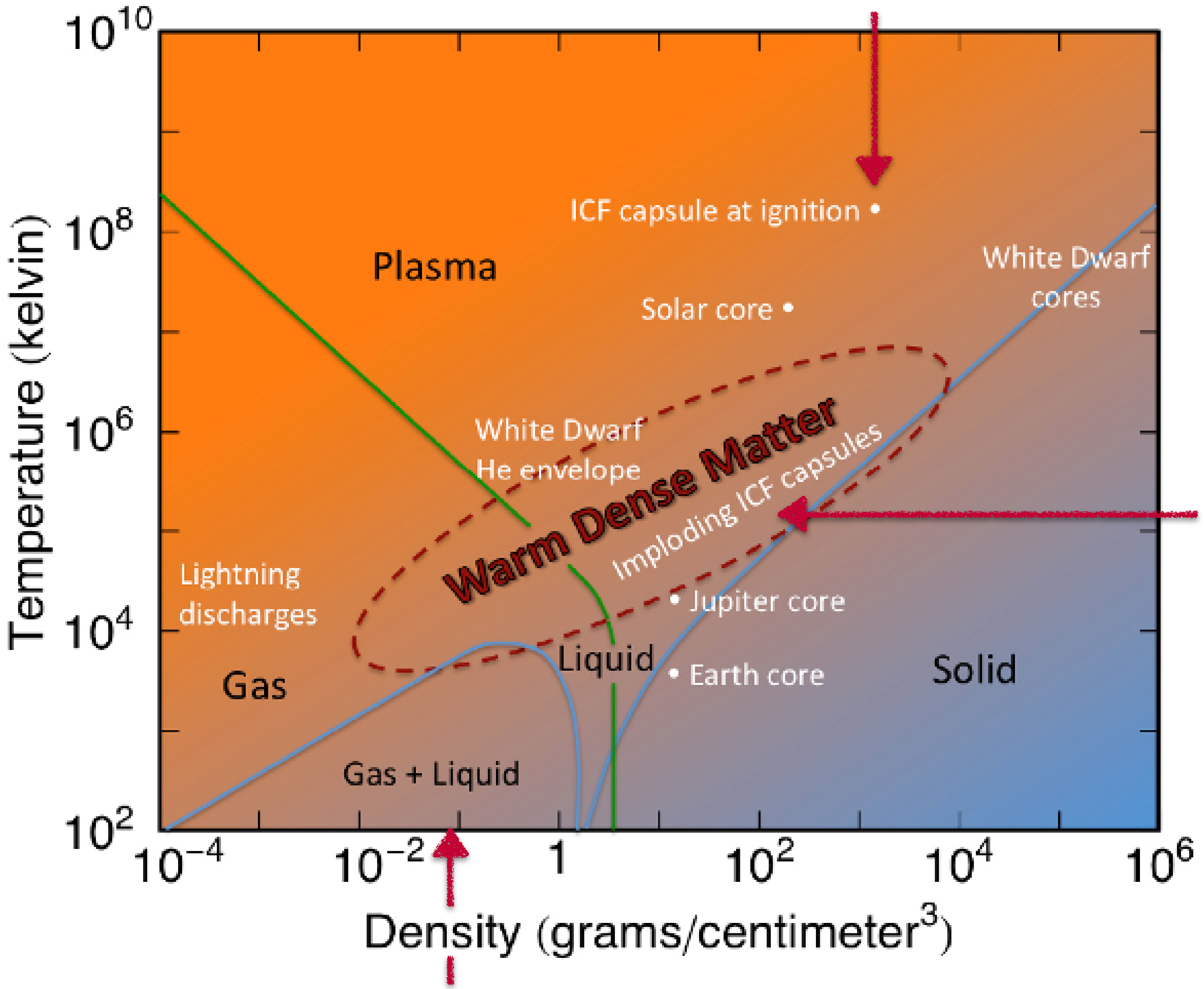
There is vast multidisciplinary expertise in capturing all of this
in a large system of coupled partial differential equations (PDEs).

My expertise is in developing high-fidelity models of the *coefficients* of those PDEs.

This *seems* to be the place where quantum computers might help ICF, soonest.

Materials in extreme conditions.

Fusion happens here



Hard to constrain materials models here

But the fuel starts here

Figure credit: Mike Desjarlais

How *might* a quantum computer help?

Recall various effects that must be modeled

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Conductivity

Stopping power

"Optical" response

Comedic insight: Stephanie Hansen

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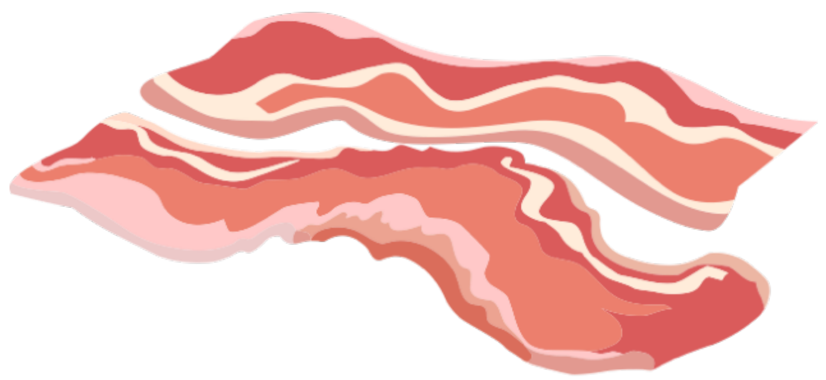
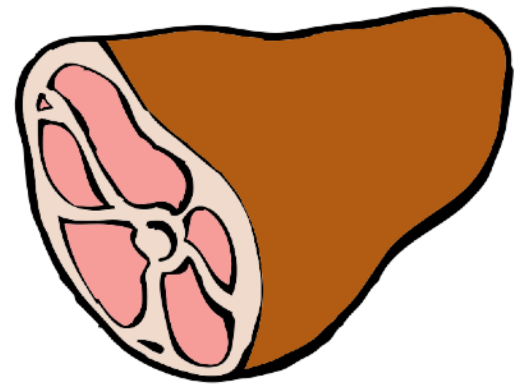
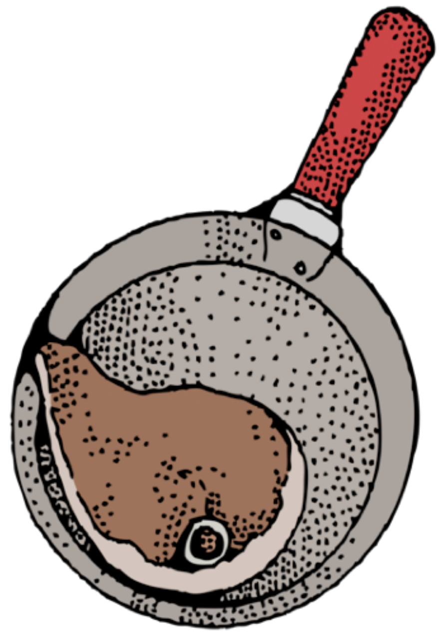


Conductivity



Stopping power

“Optical” response



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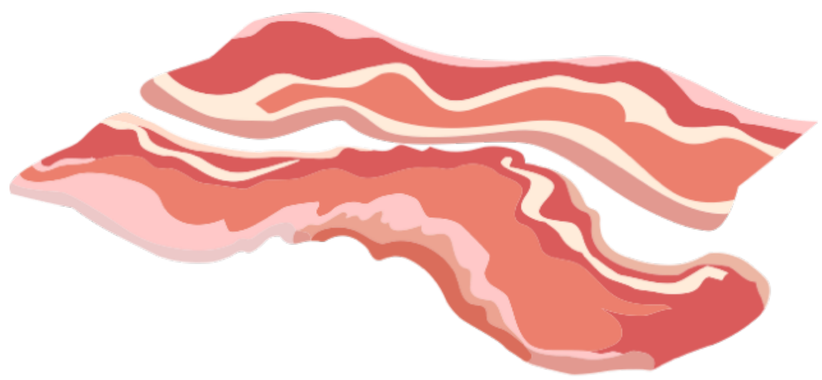
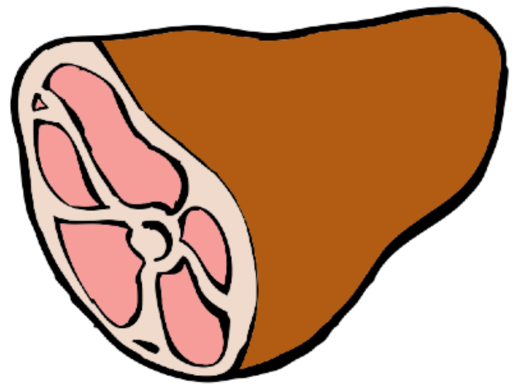


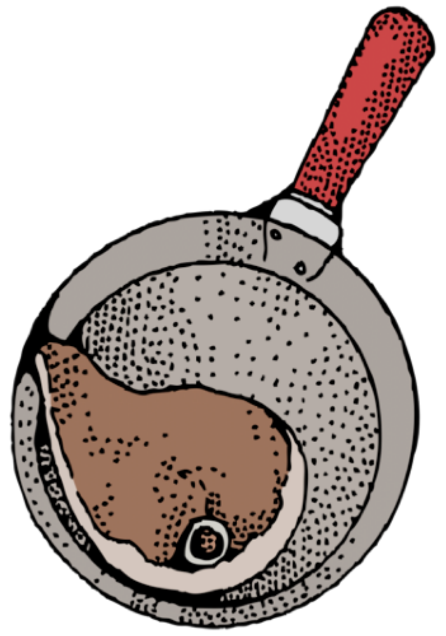
Conductivity



Stopping power

Dielectric function

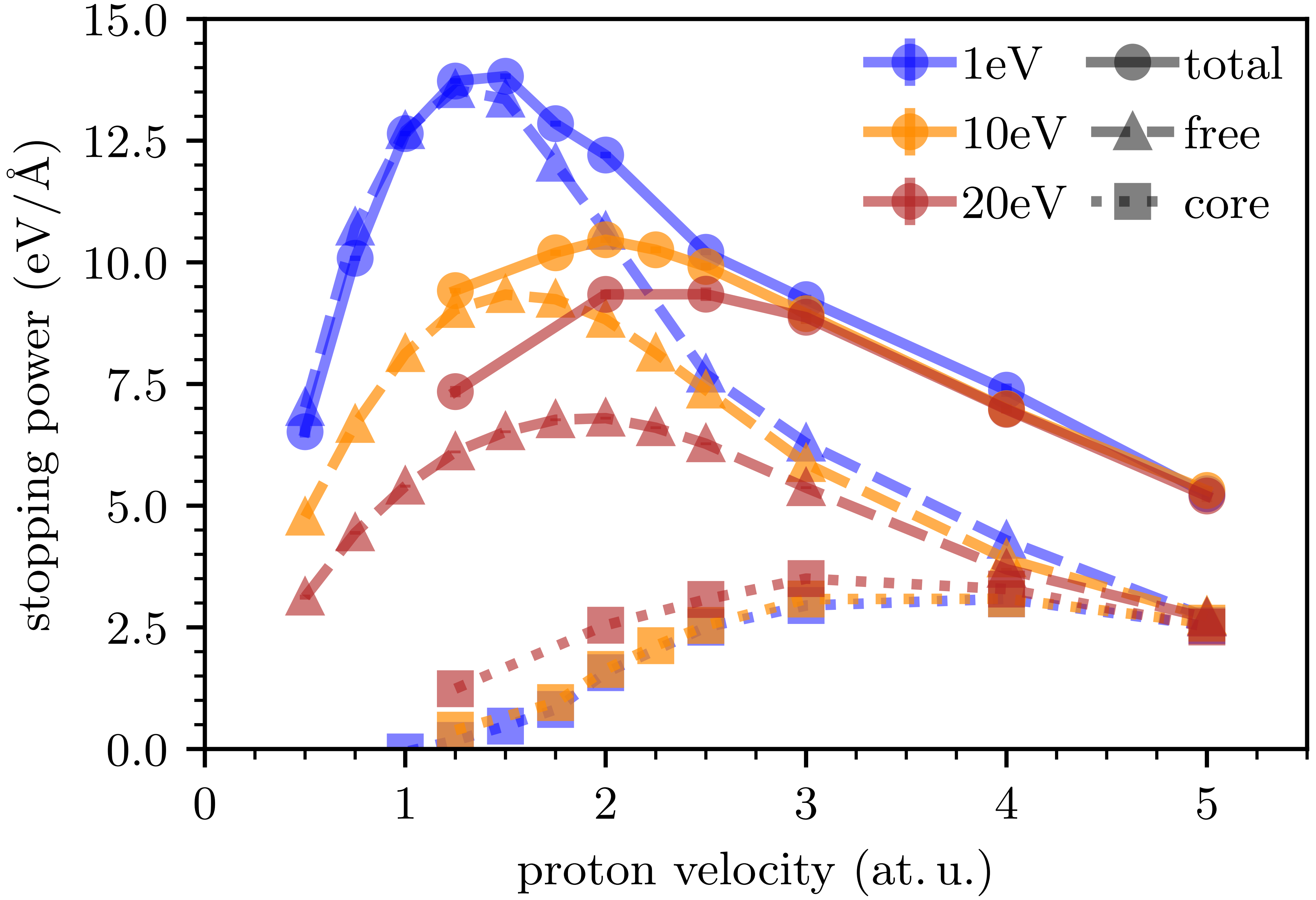
"Optical" response



Comedic insight: Stephanie Hansen

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.

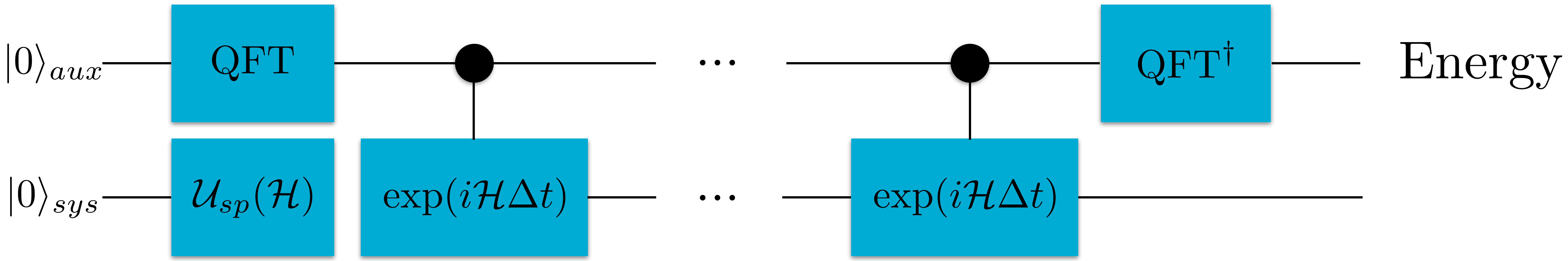
Calculations use Ehrenfest dynamics & time-dependent density functional theory.

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.

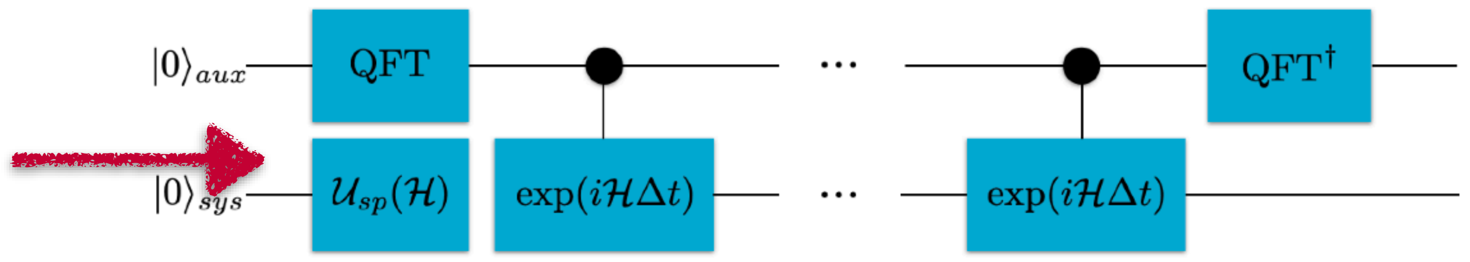


1.) Prepare a state that encodes the system of interest in a register of qubits.
2.) Time evolve said state under the action of the exact many-body Hamiltonian.
3.) Measure observable of interest, e.g., an operator or a 2-point response function.

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

(Rough) resource estimates.

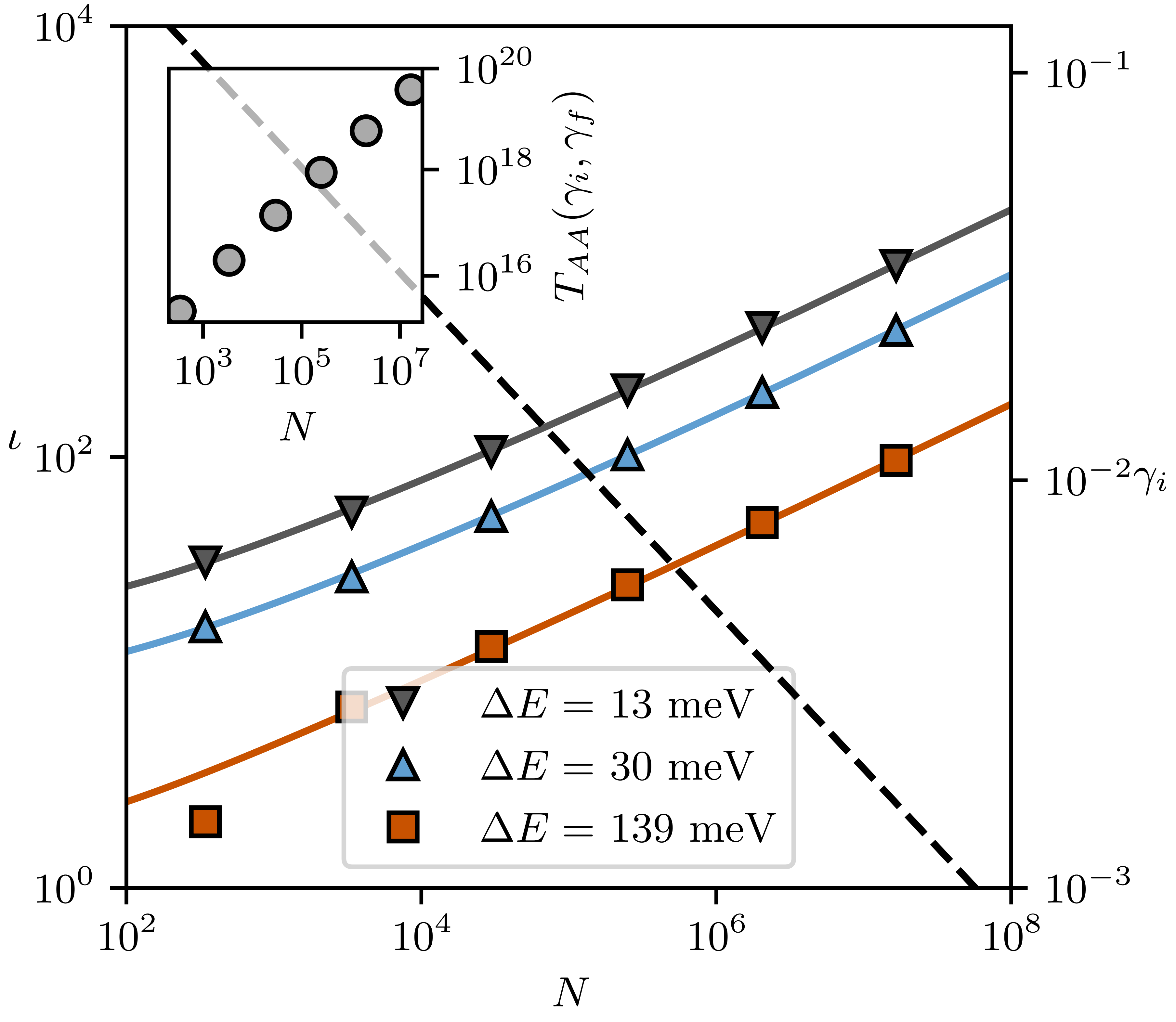
One of the dominant costs appears to be state preparation.



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**

Appearing on arXiv, tonight



Lead scientist:
Shivesh Pathak

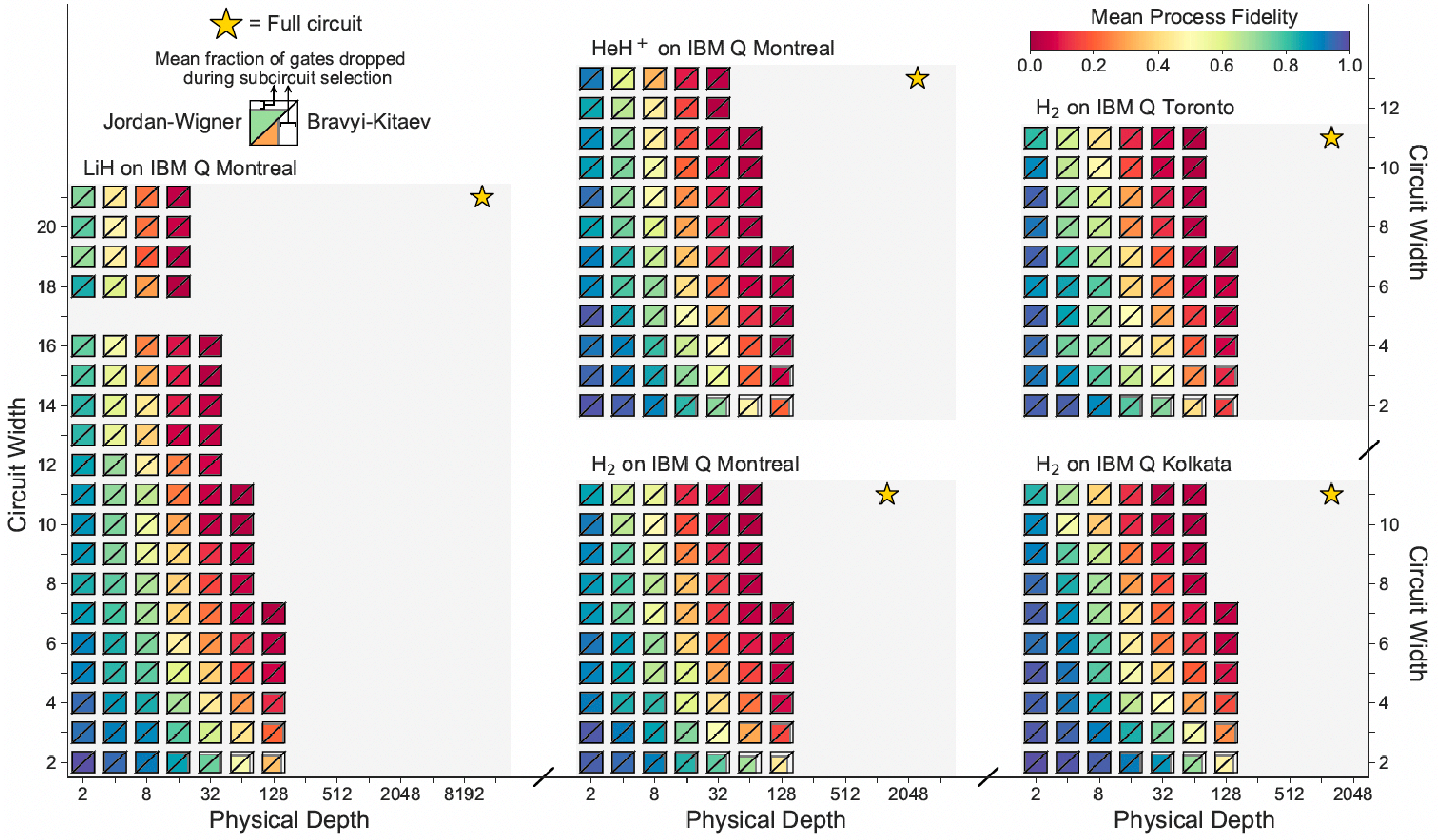
*Lin and Tong, Quantum (2020)

**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 *aren't* going to uniquely enable fusion energy production, but they might *help* solve very specific niche problems along the way.

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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