Quantum Statistical Simulations with Julia

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“Quantum Simulations?”

- Condensed matter systems: lots of electrons
- Classical mechanics fails
- Off-diagonal/non-commuting terms in the action
- We don't know the eigenbasis of the Hamiltonian
- Use a computer to find eigenstates:
  - Either just the groundstate
  - Or many states deep in the band

Techniques

- Density Matrix Renormalization Group
  - Approximate system as matrix product state
  - Optimize the MPS towards the groundstate
  - Works in 1- and quasi 1-D
- Quantum Monte Carlo
  - Importance sample wavefunctions or diagrams or path through configuration space
  - Approximate partition function, make measurements
- Exact Diagonalization
  - Says on the tin

Why is quantum simulation hard?

- Options for high performance languages:
  - C
  - C++
  - FORTRAN
  - All are hard to learn and reason about
- Options for easy-to-learn/teach languages:
  - Python
  - ?????
- Can we have both?

We like Julia because...

- Does 80% of what C++/MPI does for us...
- ...with 20% of the work and care
- Much faster than Python
- Just as easy to write **and** teach
- Hard to accidentally hurt yourself
- Most scientists don't want to learn move semantics

We like Julia because..

- Active development
- Parallelism: hope for the future
- GPU programming with C is painful
- GPGPU in Julia removes 80% of the friction
- Dealing with a variety of clusters is so easy
- MPI and HDF5 integration

More on Parallelism

- Most scientists don't need all (or most) of MPI
- Teaching someone parallel computing with C or C++ takes >1/2 a year
- Julia may cut that down by a lot
- Julia is still performant and will run “anywhere”
- Compiled binaries are coming?

Summary

- Julia can improve the user/dev experience for almost all our work
- Lots of new features and development to be excited about
- Parallelism features will make my life better
- Questions?