Hamiltonian simulation algorithms for near-term quantum hardware

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Problem statement

Definition

Hamiltonian simulation:
"Given a description of a Hamiltonian H, and evolution time t, some initial state $|\psi(0)\rangle$ produce the final state $|\psi(t)\rangle$ (to some error ϵ)"

- "The Hamiltonian of a system is the sum of the kinetic energies of all the particles, plus the potential energy of the particles associated with the system

Why is this a difficult problem?

Definition

We assume that the quantum state is loaded into memory

- a classical computer can't store the state efficiently
- a classical computer cannot produce a complete description of the state

Schrödinger equation

Definition

$$H|\psi(t)\rangle = i\hbar\frac{\delta}{\delta t}|\psi(t)\rangle$$

integrate both sides:

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi(0)\rangle$$

break H down into potential and kinetic energy:

$$E_{kin} = \frac{p^2}{2m}$$

$e^{\frac{-ip^2t}{2m\hbar}}$ and $e^{\frac{-iE_{pot}t}{\hbar}}$ don't commute, so $e^{-iHt/\hbar} = e^{\frac{-ip^2t}{2m\hbar}}e^{\frac{-iE_{pot}t}{\hbar}}$ doesn't hold

Lie-Trotter product formula

Definition

$e^{A+B} = \lim_{n\to\inf}(e^{A/n}e^{B/n})^n$

- product formula: simulate the sum-terms of a Hamiltonian by simulating each one separetly for a small time slice
- $H = A + B + C$
- $U = e^{-i(A+B+C)t} = (e^{-iCt/r}e^{-iBt/r}e^{-iCt/r})^r$
- switching between kinetic and potential energy terms

we arrive at: $e^{\frac{-i\hat{H}t}{\hbar}} = \lim_{N\to\infty}(e^{\frac{-ip^2t}{2m\hbar N}}e^{\frac{-\hat{V}(\hat{x})t}{\hbar N}})^N$

Definition

Split operator

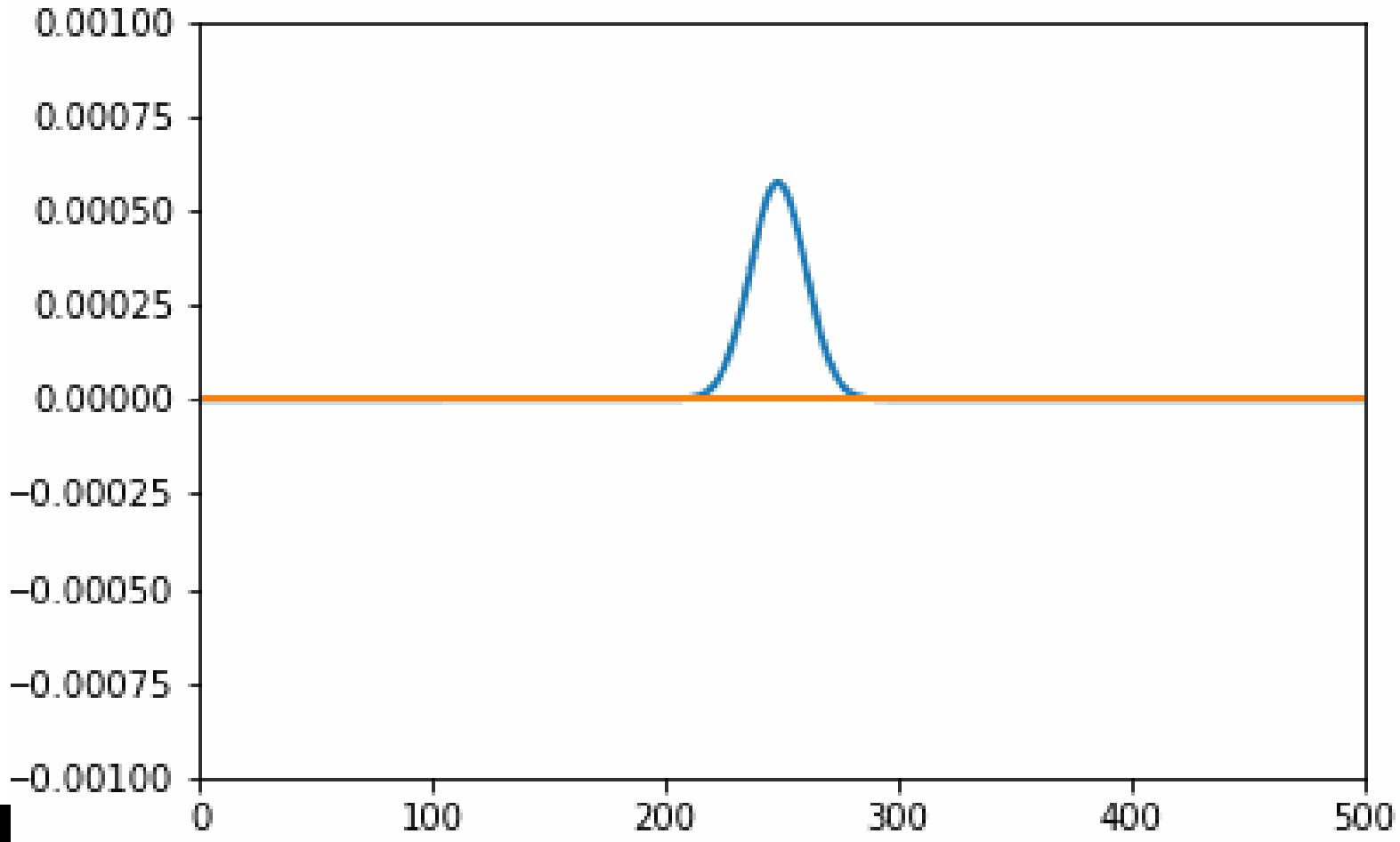
Algorithm:

1. Apply a half step of the potential propagator to $\psi(0)$
2. Apply the Fourier transform: momentum basis
3. Apply a full step of the kinetic propagator on the momentum basis
4. Apply the Inverse Fourier transform: back to coordinate basis
5. Apply the second half step of the potential propagator

this algorithm results from splitting the propagator, substituting into the Schrödinger equation and projecting onto a coordinate basis $|x\rangle$

Simulating a wavefunction

- blue line: $\langle \Psi | \Psi \rangle$
- orange line: potential energy, $\hat{V}$



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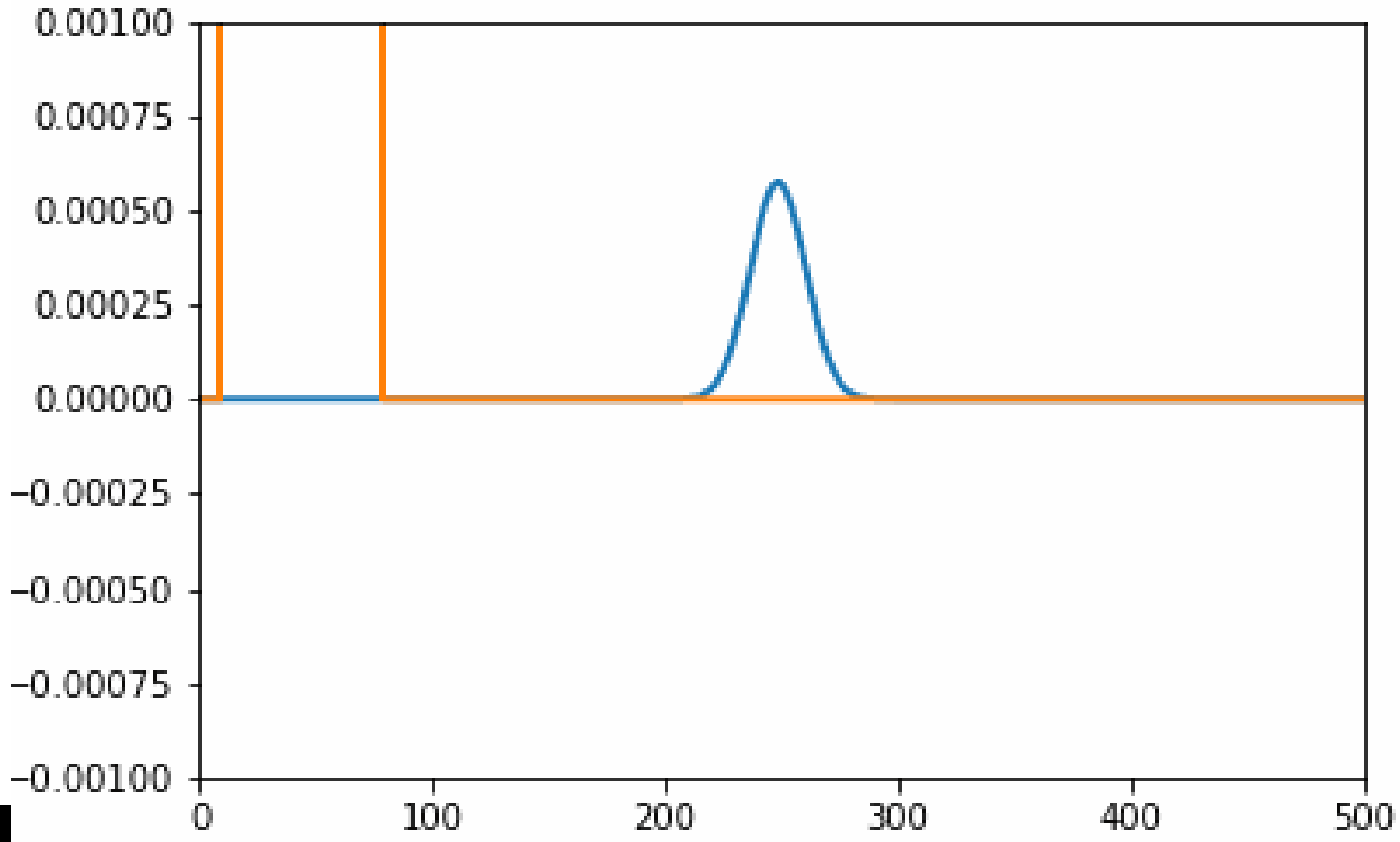
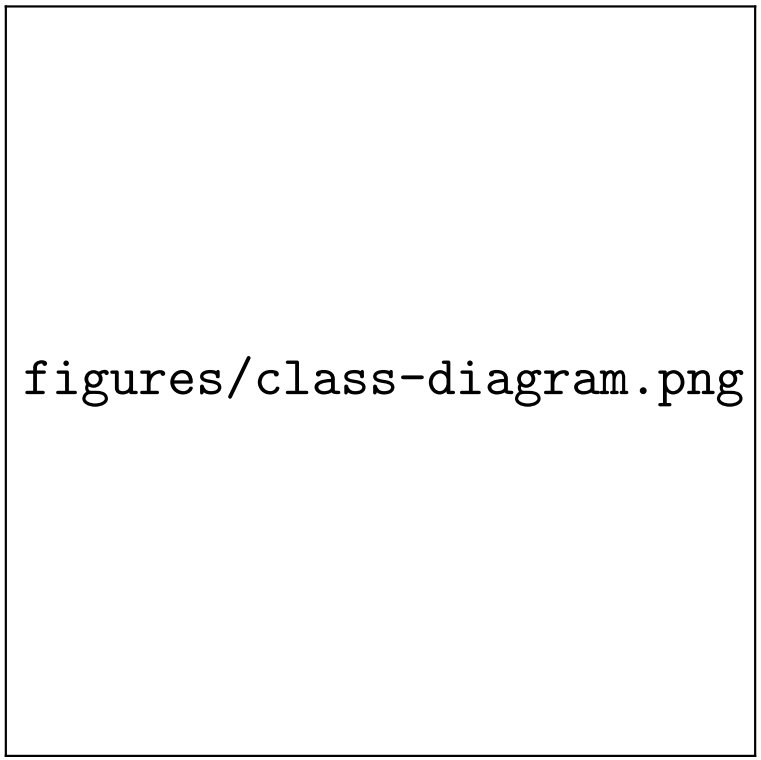
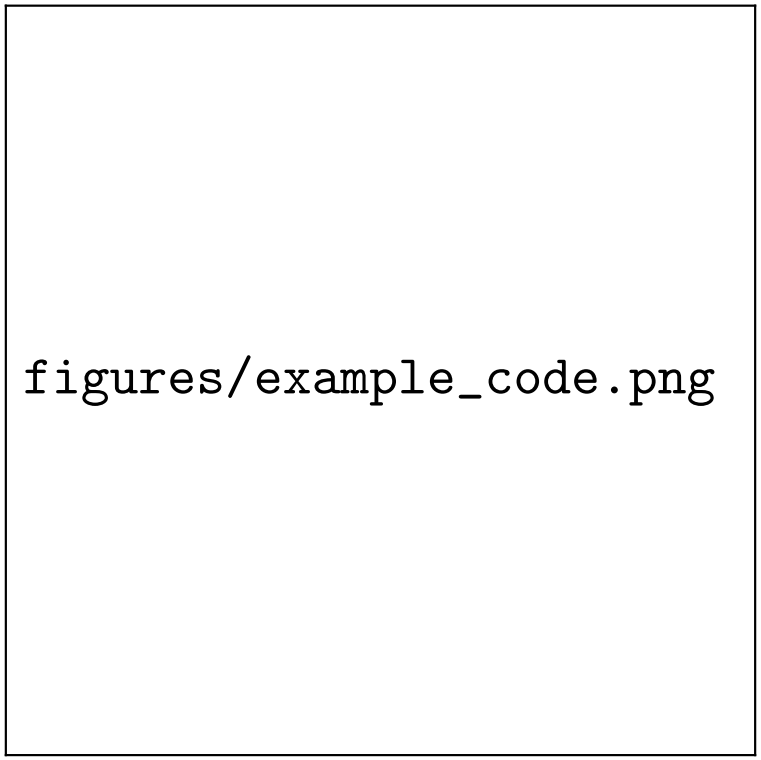


Data Structures

- object-oriented
- modularized
- expandable
- built on top of the Scan framework



Example Code



Setup Function

figures/setup_code.png

figures/setup1.png

Run the Algorithm

figures/run_code.png

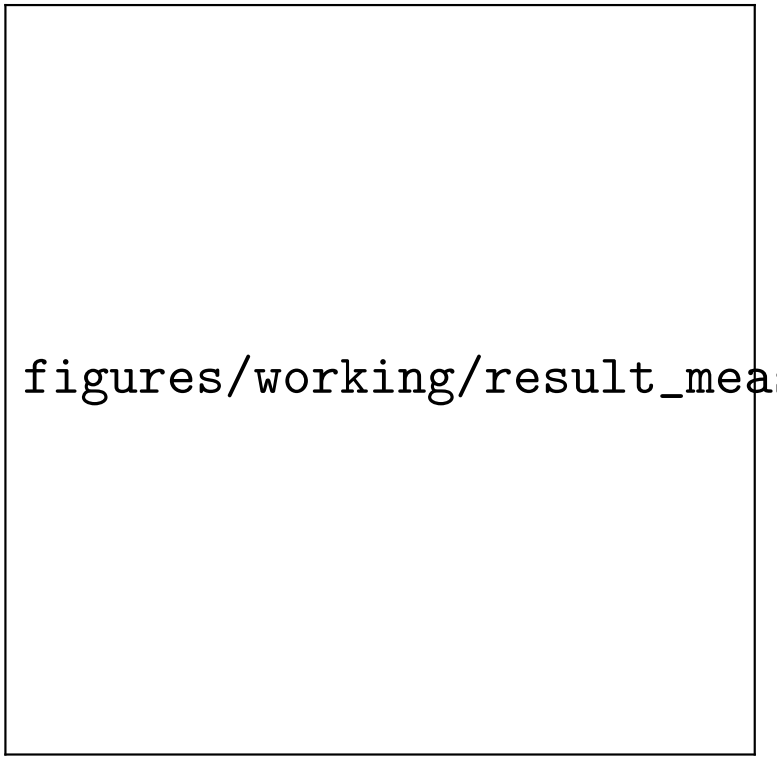
figures/lsgpa_1.png

Results: synthesized data

figures/working/results_synthesized_2.png

$$\text{Merit} = \sqrt{\sum_{i=1}^{N_\epsilon} |S_{1,i} - IFFT(\tilde{S}_{2,i})|^2}$$

Results: measured data



$$\text{Merit} = \sqrt{\sum_{i=1}^{N_\epsilon} |S_{1,i} - IFFT(\tilde{S}_{2,i})|^2}$$

Outlook

- Make the algorithm run perfectly, fix the bug
- Research Interest: get the delays between two traces

Thank you for your attention!