Introduction

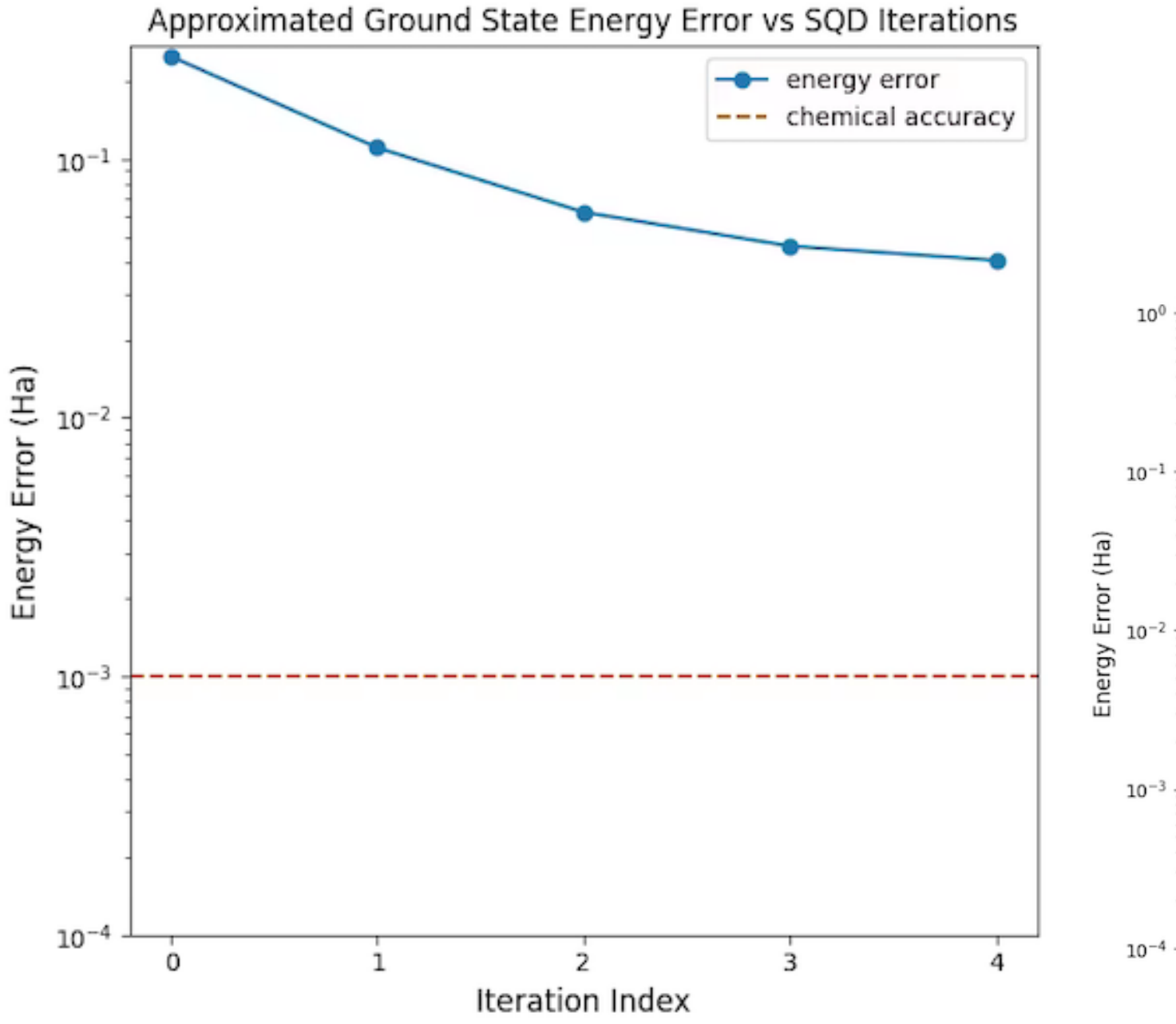
IBM has been shopping their Sample-based Quantum Diagonalization (SQD) method for about a year now, publishing peer reviewed, building on the work, releasing it as an add-on library for Qiskit. It is touted as a method to perform quantum chemistry calculations on a quantum computer, beyond the scale of exact diagonalization on a quantum computer. It does this with a hybrid quantum-classical approach.

The application is in computing molecular energies, the ground state energy being common. The published work studies and says .

Its a simple matter to import the SQD code into an existing Qiskit Python project. An example of use is here: https://quantum.cloud.ibm.com/docs/en/tutorials/sample-based-quantum-diagonalization

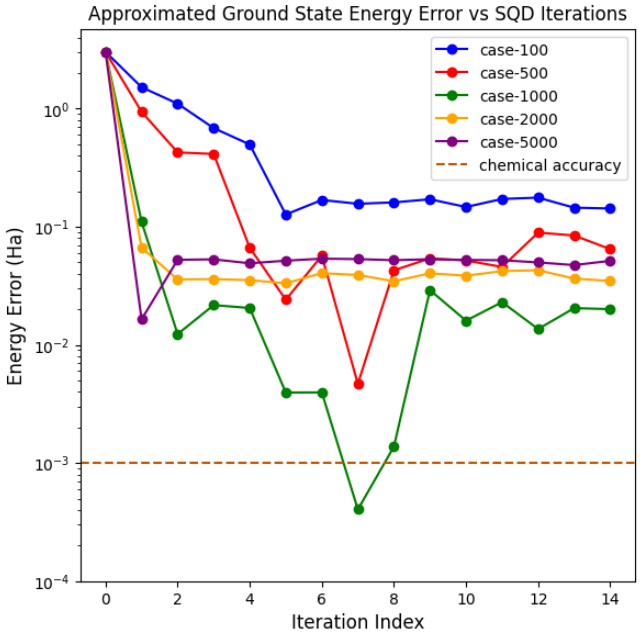
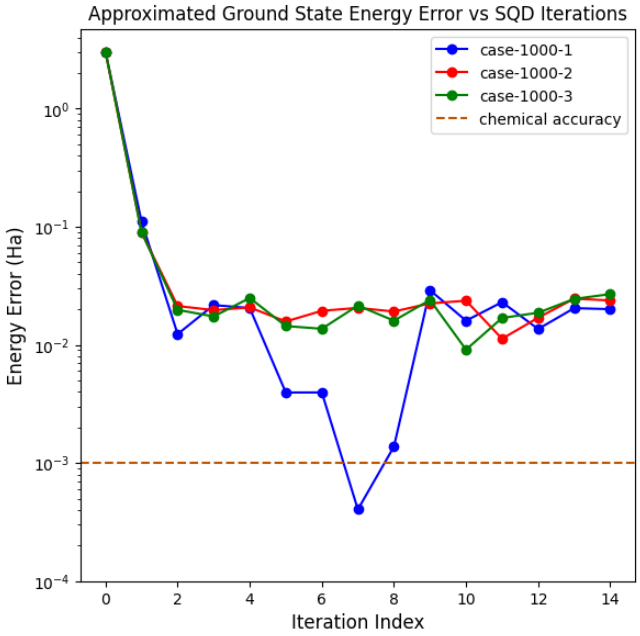
Baselining updated code

Unfortunately this example uses an older version of the SQD library. In the fast moving quantum research space this staleness is common. We modified the example to use the latest version of the SQD library and Qiskit, then ran with the same molecule and SQD parameters. The initial comparison to IBM's example is here, and seems in a similar range:



Varying the SQD parameters

The number of samples in each batch, and the number of batches are two parameters on the algorithm.

Varying #samples,batch=1	Samples=1000, vary #batches
	

Varying other stuff

What fun!