A Simple Visual Overview of Qiskit-Nature's Components for Ab-Initio Calculations

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Motivation

Quantum technologies are becoming more accessible in the past few years and will soon become a *de facto* alternative to classical *von Neumann* computing alternative for applied research.

Qiskit is an open-source framework for interacting with quantum computers lead by IBM, which consists of multiple sub-projects dealing with hardware, low level algorithms and higher level applications, through a Python API.

One of those high level sub-projects, *Qiskit Nature,* aims at providing an integration with classical codes to enable natural scientists to easily perform their calculations using quantum technologies.

However, despite the quality documentation provided in the project, and general literature, achieving a good understanding of the components and methods involved can become quite challenging.

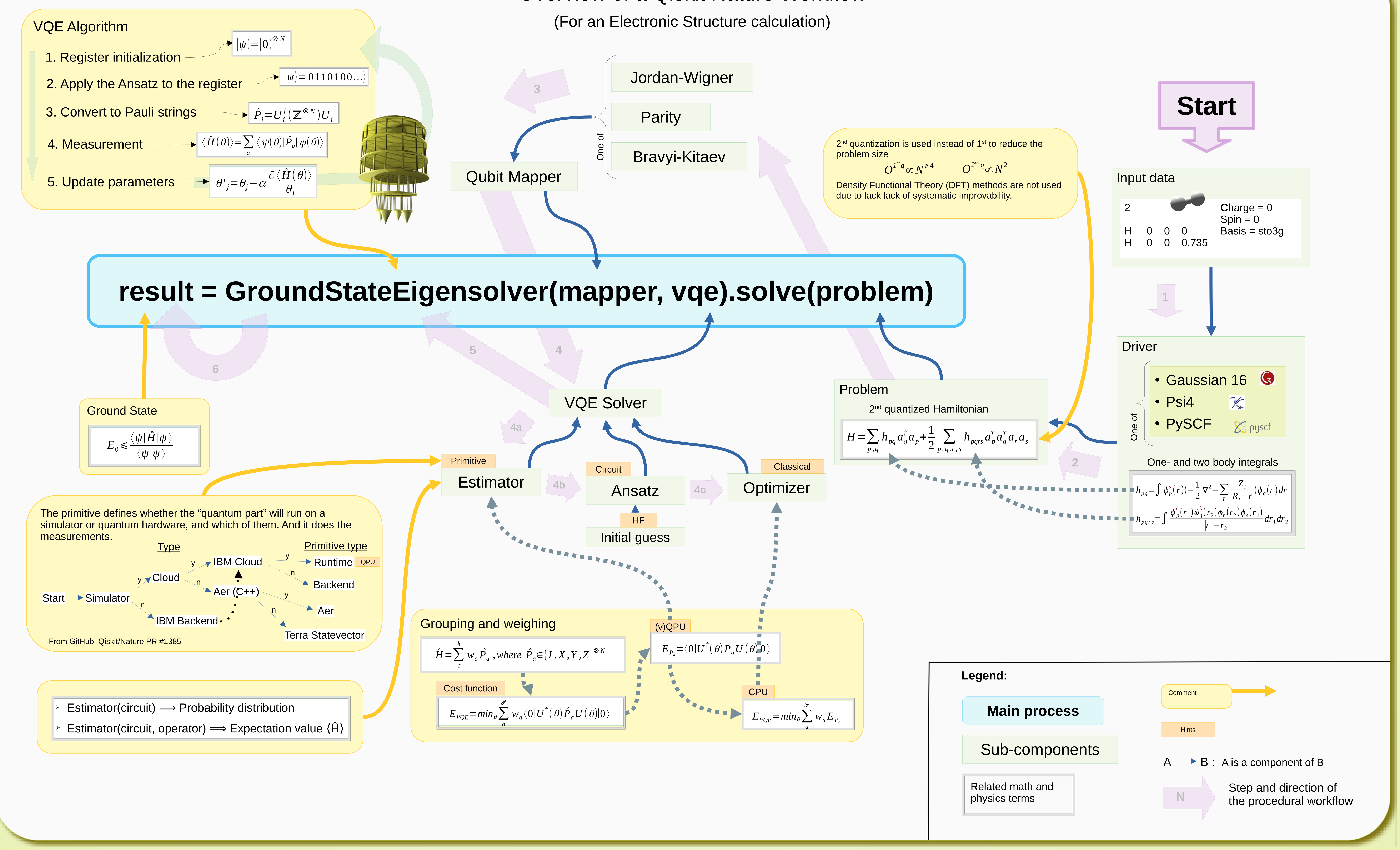
The current poster is an attempt to put the pieces together, in Layman's terms, for those like me, trying to get started on the topic (aiming at electronic structure calculations), who also like to look under the hood.

Concepts

- Qiskit Terra: Qiskit's toolset to create and optimize (quantum) circuits
- Qiskit Nature: Qiskit's framework to run natural science calculations
- Driver: Nature wrapper for the input parameters and classical software
- Problem: Nature element to encode the output of the classical code in the Driver element, including the 2nd quantized Hamiltonian
- Solver: Nature algorithm to find the Eigenvalues of the Hamiltonian operator
- VQE (Variational Quantum Eigensolver): Hybrid quantum algorithm that uses QPU for measuring the expectation value ⟨Ĥ⟩ and CPU for adjusting the parameters $\{\theta_i\}^N_{i=1}$
- Primitive: Terra's class to make the measurements in QPU. There are currently two primitives available: Estimator and Sampler
- Ansatz: The variational form that solves the Problem ($\hat{H}$)
- Optimizer: Classical algorithm to optimize parameters (i.e.)
- Mapper: Converts the Hamiltonian operator into a qubit operator

Overview of a Qiskit Nature Workflow

(For an Electronic Structure calculation)



Workflow summary

1. Define the Driver using one of the (currently) available wrappers for Gaussian 16, Psi4 or PySCF, together with the molecular coordinates and basis set, and optionally additional parameters
2. Run the Driver to obtain the Problem
3. Define the qubit mapper
4. Initialize the VQE solver by providing 3 elements:
   - 4a. Estimator (Primitive): which returns a probability distribution or an expectation value. It defines where the quantum part is going to run
   - 4b. Ansatz: parametrized quantum circuit with a variational form. UCC (UCCSD) is commonly used, together with a (HF) initial state guess
   - 4c. Optimizer: the classical algorithm to (re-)calculate the energy on the CPU
5. Wrap up the VQE solver (and mapper) into the main solver instance
6. Call the *solve()* method on the main solver using the *Problem* as parameter. This will run the main loop until the it the convergency criteria is met, and yield to the results (the ground state)

Useful References

- Peruzzo, A., McClean, J., Shadbolt, P. et al. A variational eigenvalue solver on a photonic quantum processor. Nat Commun 5, 4213 (2014).
- Tilly, J. et al. The Variational Quantum Eigensolver: a review of methods and best practices. Phys Rep 986, 1–128 (2021).
- Qiskit Terra's official documentation at https://qiskit.org/documentation/
- Qiskit Nature's official documentation at https://qiskit.org/ecosystem/nature/

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Disclaimer

The current poster is the author's *own take* on the process of understanding Qiskit Nature's components and workflow. Any comment, correction or explanation will be more than welcome.