Solving the Navier-Stokes Equations using Qiskit with Water Management Challenges

Date: 10/07/2021

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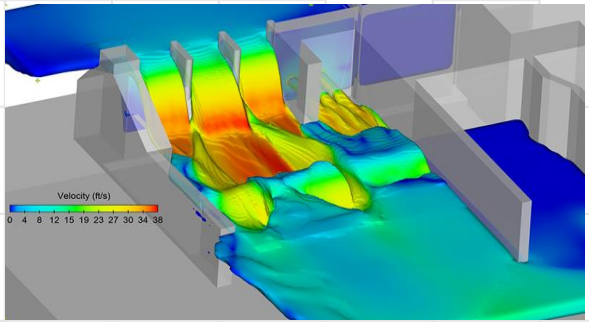
Qiskit

The Navier Stokes Equations

- Fluid simulations are in general very difficult tasks due to the *nonlinearity* of Navier-Stokes equations and *complex geometry + boundary conditions*
- Numerical solutions can be applied to many areas such as water management



MASS Density of the fluid

ACCELERATION How velocity experienced by a particle changes with time

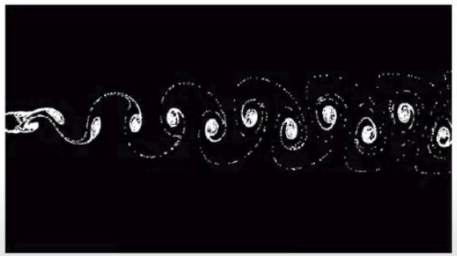
FORCE All the forces that are acting on the fluid

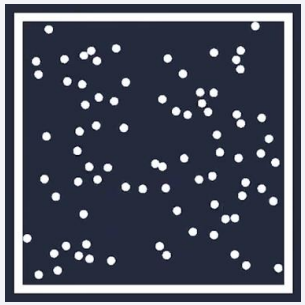
$$\rho\left(\frac{\partial V}{\partial t} + V\cdot\nabla V\right) = \nabla P + \rho g + \mu\nabla^2 V$$

- $\frac{\partial V}{\partial t}$: Change in velocity over time
- $V\cdot\nabla V$: The speed and direction which the fluid is moving
- ∇P: **Internal pressure gradient** of the fluid (the change in pressure)
- ρg: **External forces** acting on the fluid (such as gravity)
- $\mu\nabla^2 V$: **Internal stress forces** acting on the fluid (taking into consideration viscous effects)

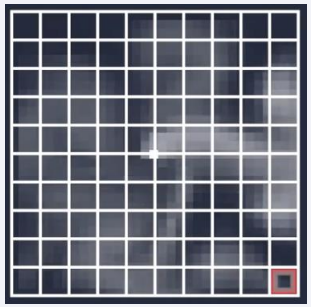
Computational Fluid Dynamics (CFD)

- N-S Equations give *specifications* from physical laws but *no implementations* of fluid simulation
- The art of CFD is to replace such PDE systems with *a set algebraic equations* by discretization methods
- HHL as a quantum linear solver could offer potential *exponential speedup*, but not easily accessible in NISQ devices



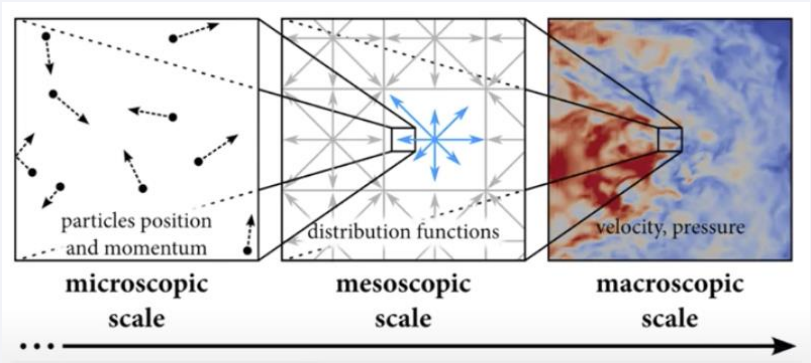


Directly simulating particle dynamics



Finite Element Methods (FEM)

Lattice Boltzmann Methods (LBM)



Traditional CFD Methods and the Navier-Stokes Equation

- ✓ FDM
- ✓ FVM
- ✓ FEM
- ✓ LBM

Sep. 2021

Literature review for existing quantum solutions

- ✓ HHL
- ✓ VQLS
- ❑ QLBM*
- ✓ *QML*

Sep.-Oct. 2021

Develop necessary platform with Qiskit

- ❑ Feature Maps
- ❑ Gradient Calculator
- ❑ Loss functions
- ❑ *Boundary Conditions**
- ❑ Benchmark*

Oct.-Dec. 2021

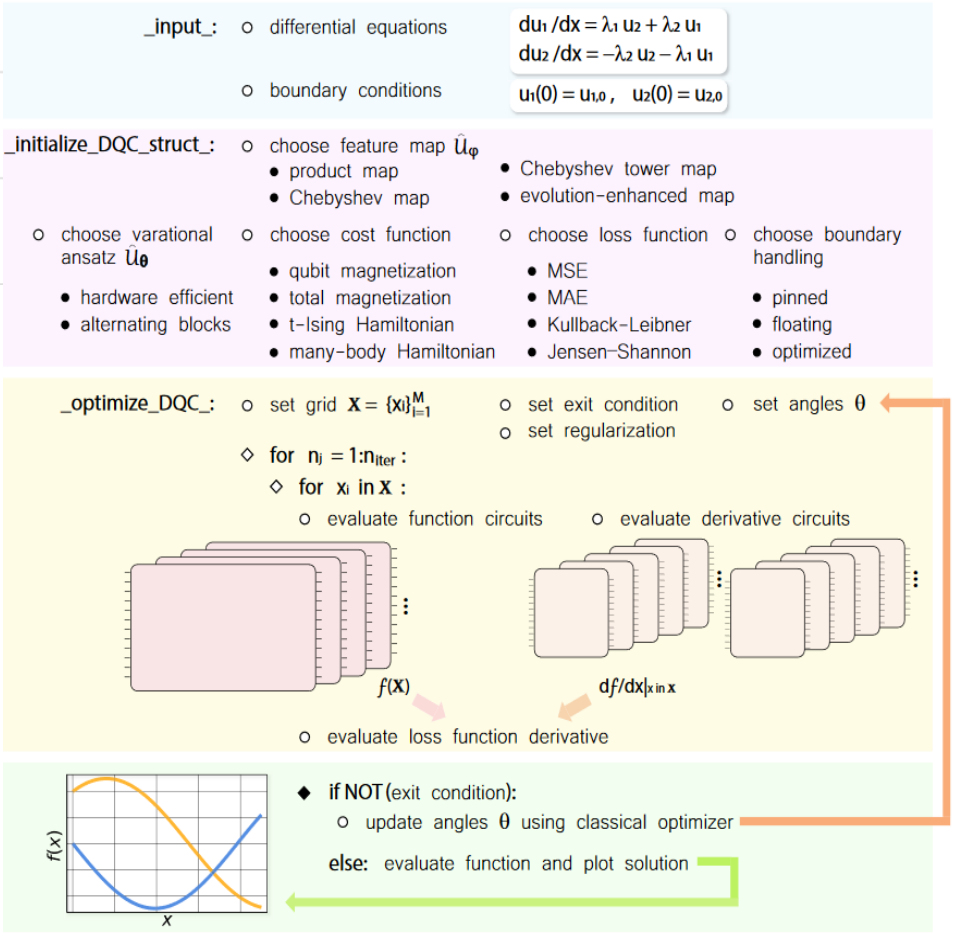
Experiments and Summary

- ❑ Demos
- ❑ Simulations
- ❑ Run on backends*
- ❑ Noise models
- ❑ Barren Plateau*
- ❑ Summary Report

Nov.-Dec. 2021

Quantum Machine Learning Approach

- Key idea is to use the *spectral methods* to solve PDE systems like a polynomial fitting
- Encode differentiable trial function (*a basis set*) in *quantum feature maps*
- Evolve state using parameterized variational ansatz
- Apply cost function: expectation value of some Hermitian operator on the state
- Apply lost function to compare trial superposed quantum state to *desired result*
- Use classical optimizer to tune variational parameters, which correlates *the coefficients in the polynomial fitting*



Challenges

- Dimensionality
- Data Encoding
- Benchmarks

Dimensionality

Mostly 1D problems are considered in the current literature.

Can we do better?

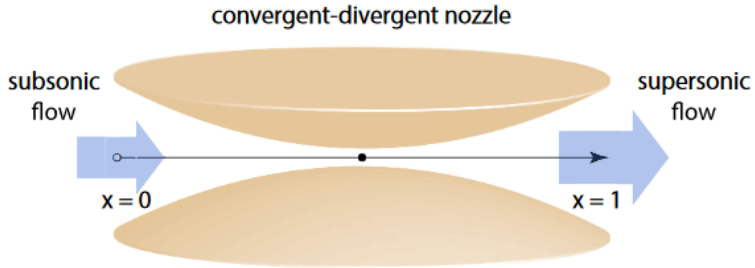
Data Encoding

What's the difference of using different quantum feature maps as basis functions?

Noise models?

Benchmarks

Can we get a little bit closer to modern CFD solvers?



Kyriienko, O., Paine, A. E., & Elfving, V. E. (2021). Solving nonlinear differential equations with differentiable quantum circuits. *Physical Review A*, *103*(5), 052416.

Expected Deliverables

By Dec. 2021

Baseline

- Qiskit Code
- Demo Problem
- Solution in Jupyter Notebooks
- Summary Report

TBD

- Medium Blog Post
- Research Paper (?)
- Other Applications