HHL as a predictor-corrector

Securing a practical quantum advantage

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Outline

- QEVEC
- Background: ISPH and HHL
- Hybrid Predictor-Corrector
- Quantum Predictor-Corrector
- Results from Taylor-Green-Vortex
- Emphasis on scalability

QEVEC

- ExCALIBUR Cross-Cutting project: potential disruptor: quantum computing
- Goal: Systematic evaluation, identification, and development of relevant quantum algorithms for exascale subroutines
- Use cases:

  - Materials simulations

  - Fluids simulations (this talk)
- Quantum verification, validation and uncertainty quantification (VVUQ)
- Funding and partners:

UK NATIONAL QUANTUM TECHNOLOGIES PROGRAMME · UKRI Engineering and Physical Sciences Research Council · Quantum Computing & Simulation Hub · UKRI National Quantum Computing Centre · CCP-QC

Quantum
Enhanced
Verified
Exascale
Computing

Durham
Strathclyde
UCL
Warwick
London Southbank

https://excalibur.ac.uk/projects/qevec/

Incompressible SPH

NS (Lagrangian form)

$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \frac{1}{\rho}\nabla P + \nu \nabla^2 \mathbf{u} + \mathbf{g}.$$

$$\mathbf{x}_i^* = \mathbf{x}_i^n + \mathbf{u}_i^n \Delta t.$$

$$\mathbf{u}_i^* = \mathbf{u}_i^n + \nu \nabla^2 \mathbf{u}_i^n \Delta t.$$

$$\nabla \cdot \left(\frac{1}{\rho} \nabla P^{n+1} \right)_i = \frac{1}{\Delta t} \nabla \cdot \mathbf{u}_i^*.$$

Poisson equation for pressure. Can be discretised into a system of linear equations

$$\mathbf{u}_i^{n+1} = \mathbf{u}_i^* - \left(\frac{1}{\rho} \nabla P_i^{n+1} + \mathbf{g} \right) \Delta t$$

$$\tilde{\mathbf{x}}_i^{n+1} = \mathbf{x}_i^n + \left(\frac{\mathbf{u}_i^{n+1} + \mathbf{u}_i^n}{2} \right) \Delta t.$$

Linear system of equations

$$\nabla^2 P = \rho \frac{1}{\delta t} \nabla . u_i$$

Apply SPH discretisation:

$$(\nabla^2 P)_i = 2V \sum_j \frac{\mathbf{r}_{ij} . \nabla_i w_{ij}}{|r_{ij}|^2 + \eta^2} P_{ij} = 2 \sum_j \frac{\mathbf{r}_{ij} . \nabla_i w_{ij}}{|r_{ij}|^2 + \eta^2} (P_i - P_j)$$

In the form of $A_{ii} * P_i + A_{ij} * P_j$

$$A_{ii} = 2V \sum_j \frac{\mathbf{r}_{ij} . \nabla_i w_{ij}}{|r_{ij}|^2 + \eta^2}$$

$$A_{ij} = -2V \frac{\mathbf{r}_{ij} . \nabla_i w_{ij}}{|r_{ij}|^2 + \eta^2}$$

→ $\mathbf{A}\vec{x} = \vec{b}$

Can we map the solution to a quantum state?

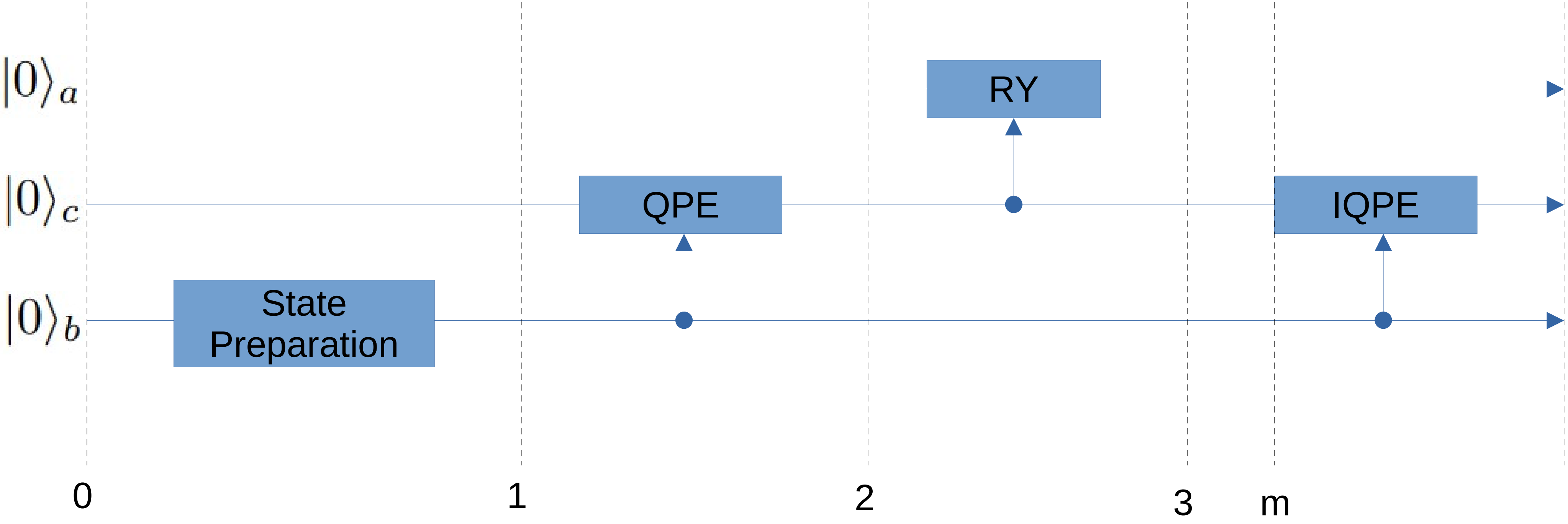
$$\mathbf{A} = \sum_{i=0}^{2^{n_b}-1} \lambda_i |u_i\rangle\langle u_i|$$

$$|b\rangle = \sum_{j=0}^{2^{n_b}-1} b_j |u_j\rangle$$

$$|x\rangle = \mathbf{A}^{-1}|b\rangle = \sum_{i=0}^{2^{n_b}-1} \lambda_i^{-1} b_i |u_i\rangle$$

This is what HHL outputs!

Harrow–Hassidim–Loyd (HHL) Algorithm



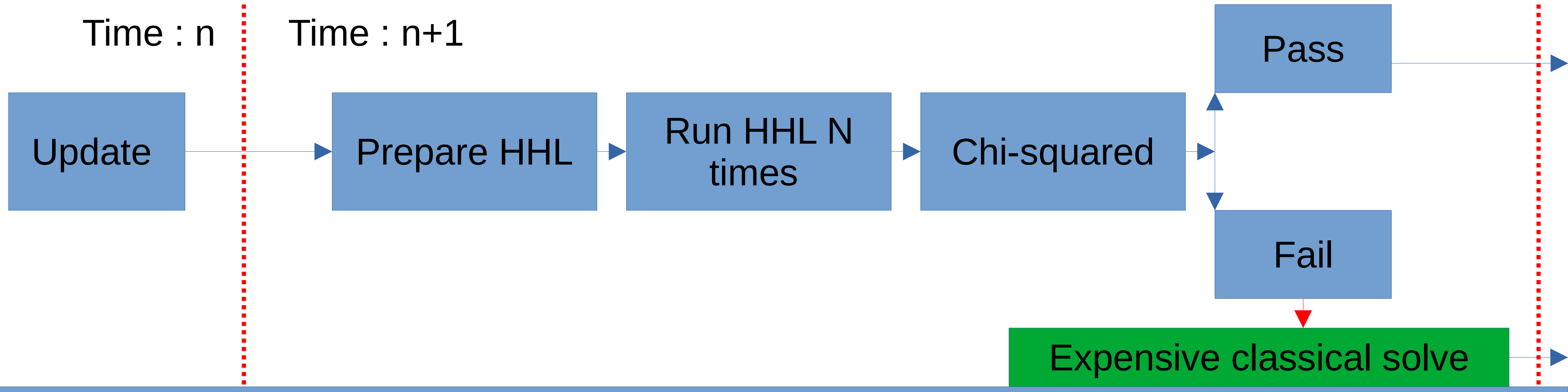
$$\Phi_m = C_2 \sum_{j=0}^{2^{n_b}-1} b_j |u_j\rangle |\tilde{\lambda}_j\rangle \left(\frac{C}{\tilde{\lambda}_j^2} |1\rangle_a \right)$$

Desired state BUT is encoded in the amplitudes!
Will require many samples to read out.

Morrell Jr et. al. arXiv preprint arXiv:2108.09004 (2021).

A hybrid predictor-corrector

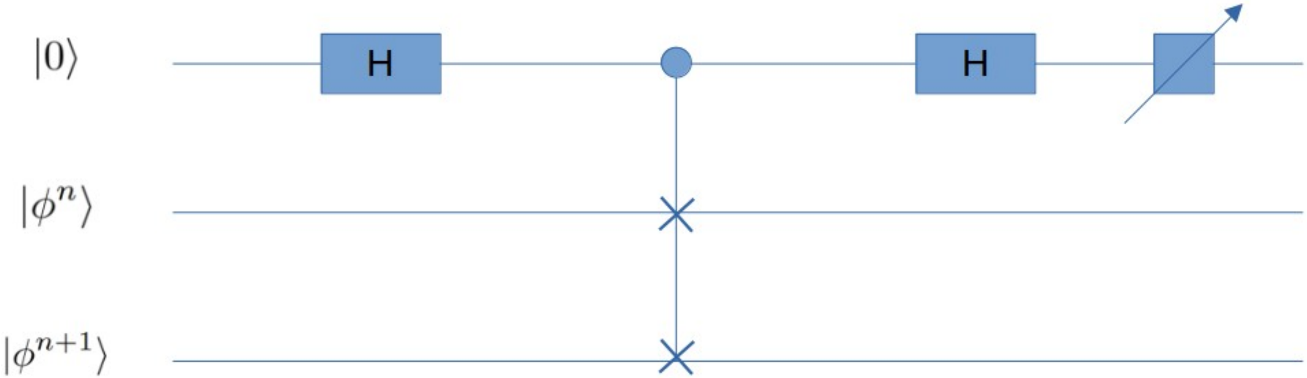
- Known: solution at a previous step
- Unknown: is current step “different enough” to warrant an update
- Goal: estimate likelihood of a given sample (from HHL) having a given distribution (from previous time step)
- Many classical statistical tests exist for this e.g. Chi-squared



A quantum predictor-corrector

- Replace the classical (i.e. chi squared) test with a quantum swap test instead

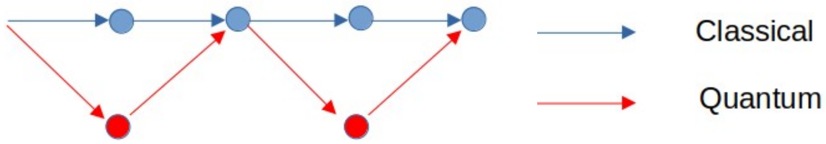
  - A swap test can be used to measure degree of overlap between 2 quantum states
- Only need to measure one ancilla qubit with probability being a function of state overlap
- Drastically reduces required number of samples

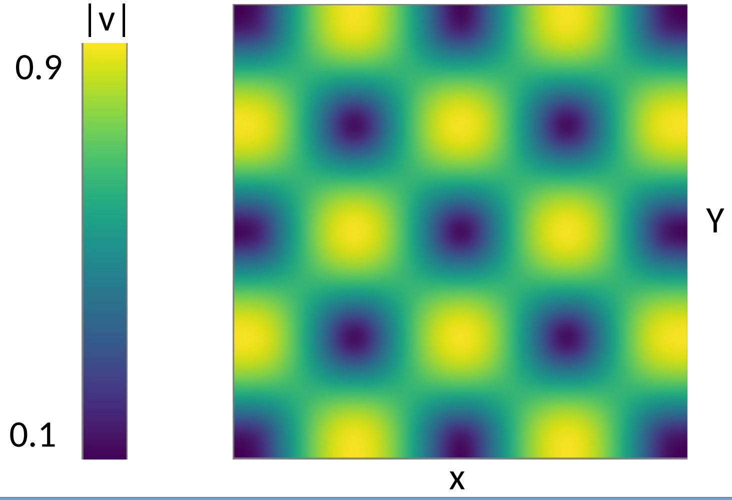


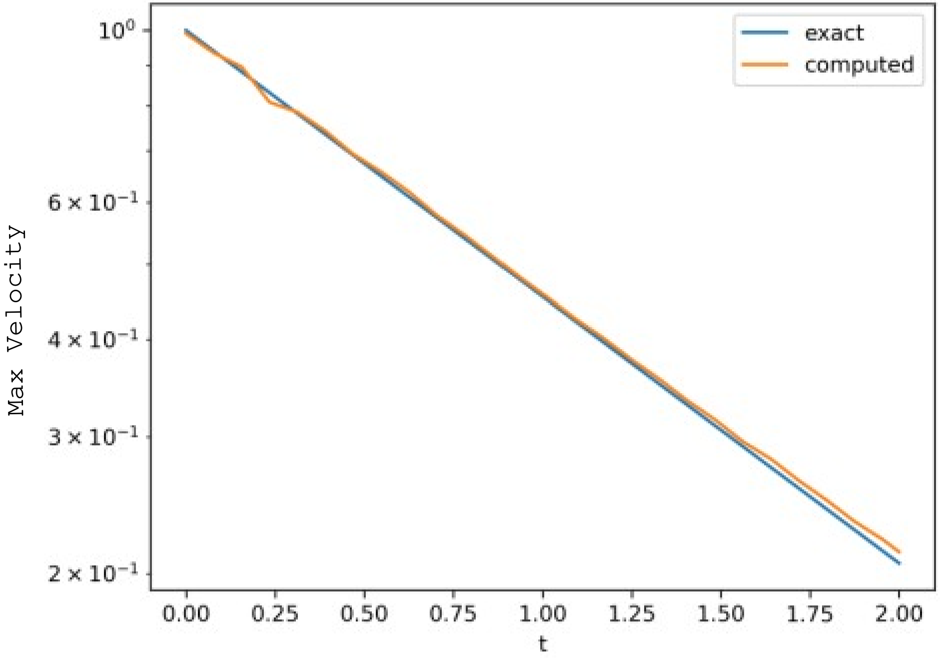
$$P(0) = \frac{1}{2} + \frac{1}{2}|\langle\phi^n|\phi^{n+1}\rangle|^2$$

Taylor Green Vortex (TGV)

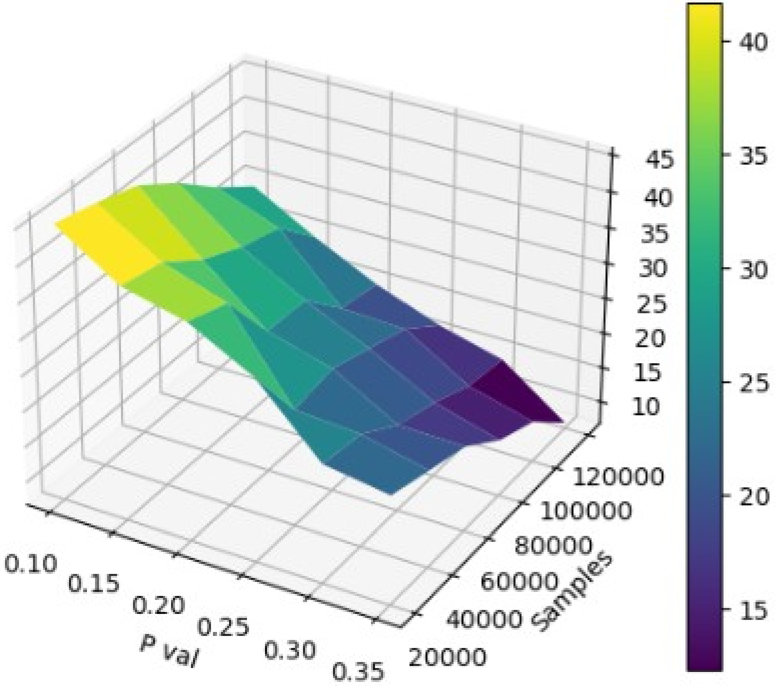
- Asynchronous implementation
- Skips expensive classical solve ~50% of the time
- Negligible impact on global error
- Flexible control via rejection criteria
- Works better than blind skipping

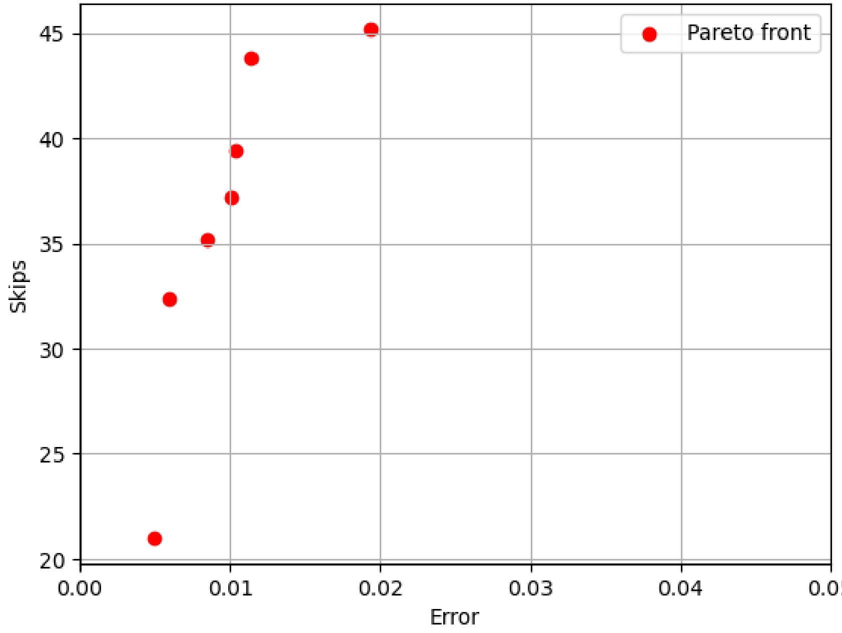






Optimal Skipping?



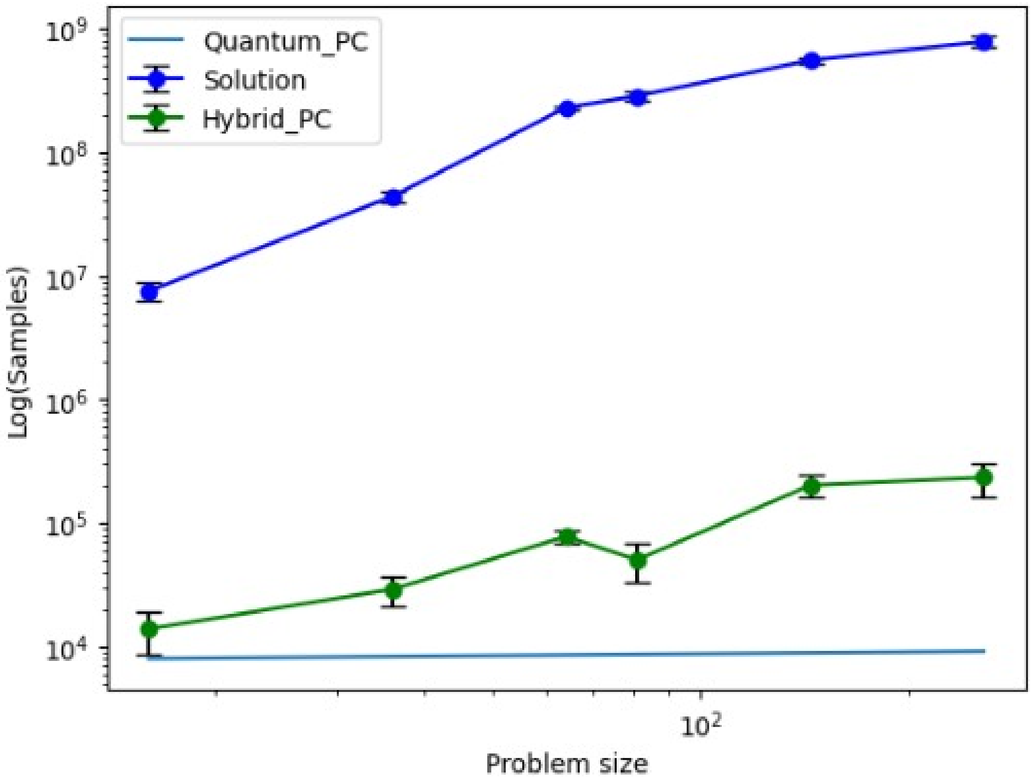


The number of skips can be controlled by changing the rejection criteria of the similarity test

There is a fairly wide region where the number of skips can be increased with little impact on error!

Scalability

- The hybrid PC shows a better scaling with problem size when compared with actually solving using HHL (slope ~1.1 C.F. ~ 1.7)
- The quantum PC further extends this and is close to being independent of problem size
- This greatly minimises the required number of readouts/state preparations and is a strong step towards actually harnessing the “exponential advantage” of HHL in practice



Summary

- Repurposing HHL into a predictor-corrector leverages the quantum advantage while minimising required samples
- Predictor-corrector algorithm scales better with problem size when compared with using HHL to actually “solve” your system
- This comes at the cost of not actually knowing your solution, instead just having an estimate of how different your solution at time n+1 is compared to the solution at time n
- General in scope with other applications including chemistry or plasma simulations and incompressible NS flow solvers etc.