

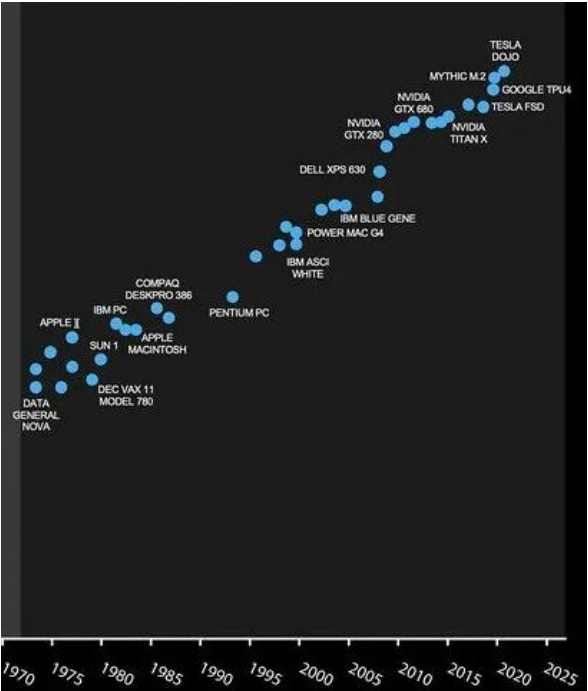


Is the future of HPCSE quantum?

Matthias Möller | HPCSE 2026 | May 18-21, 2026 | Hotel Soláň

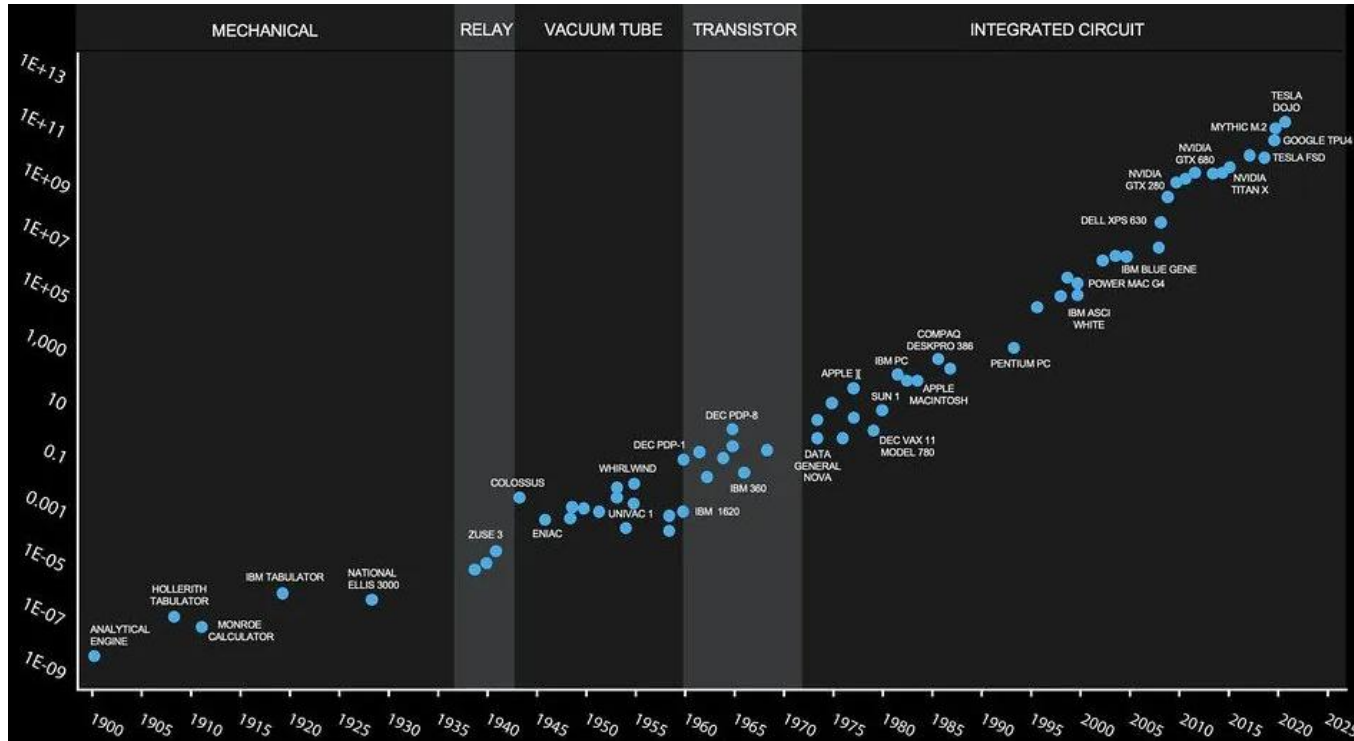


Moore's law

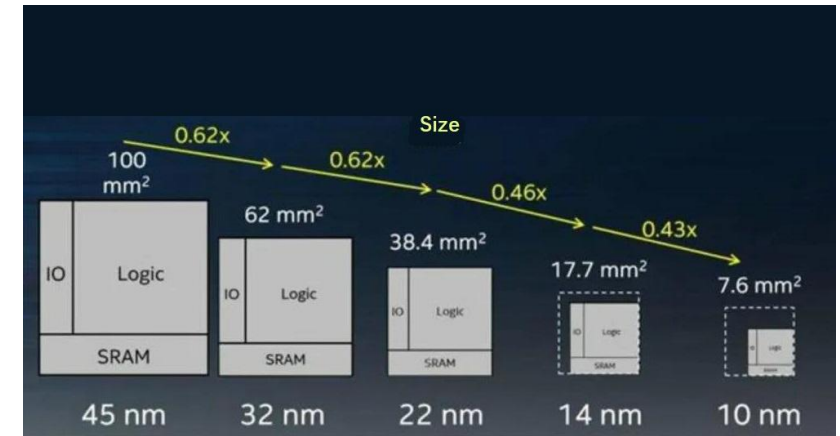


Moore's law

Enabled by changes in the computer technology

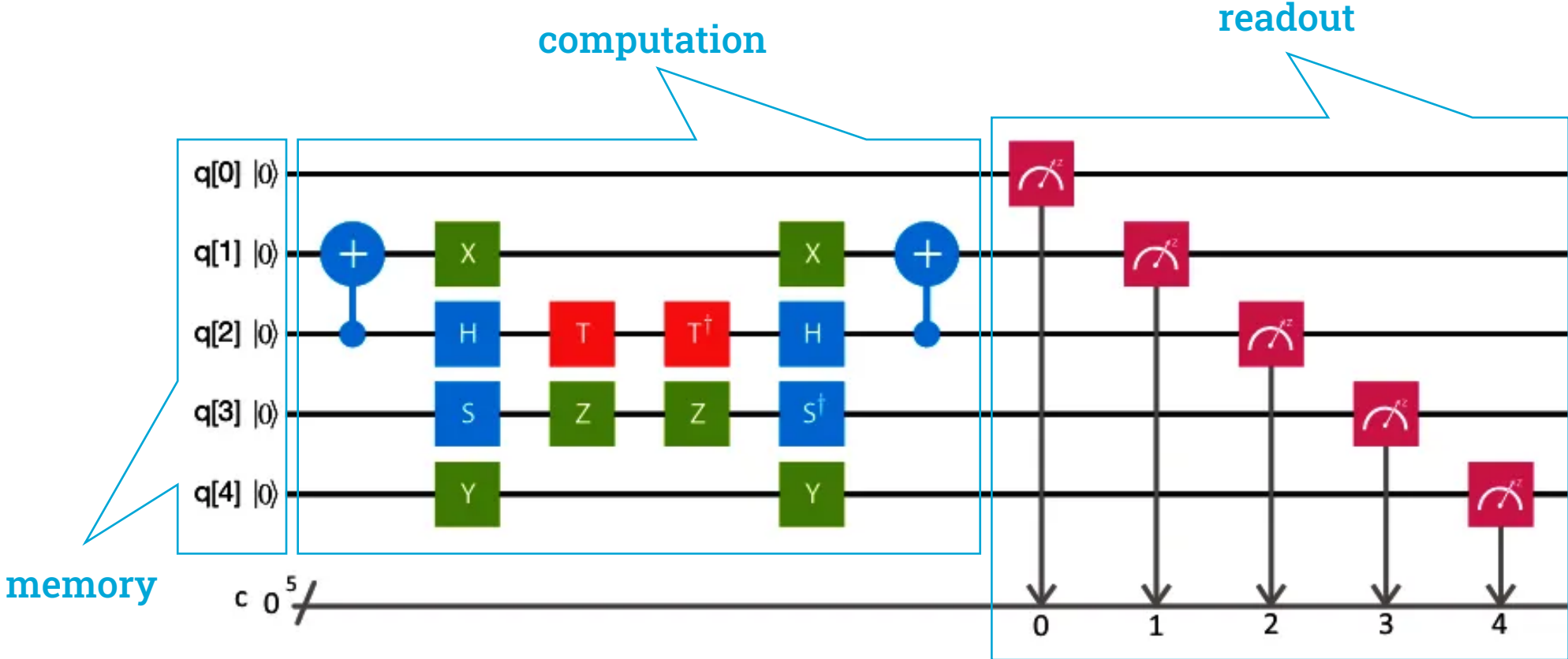


Enabled by technology improvements



Left: <https://www.unite.ai/mooreslaw/>, right: <https://www.utmel.com/blog/categories/integrated%20circuit/is-there-a-limit-to-the-chip-process-node>

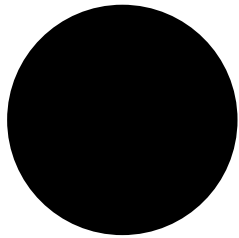
Components of a quantum 'program'



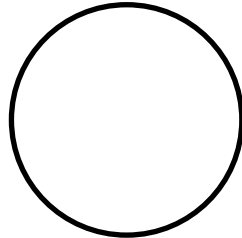
From bits to quantum bits

Classical bit

exclusive state 0 or 1



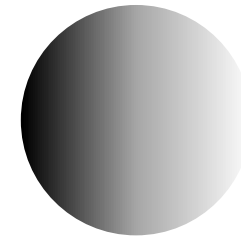
0



1

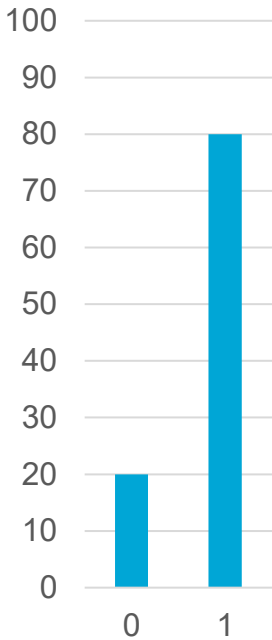
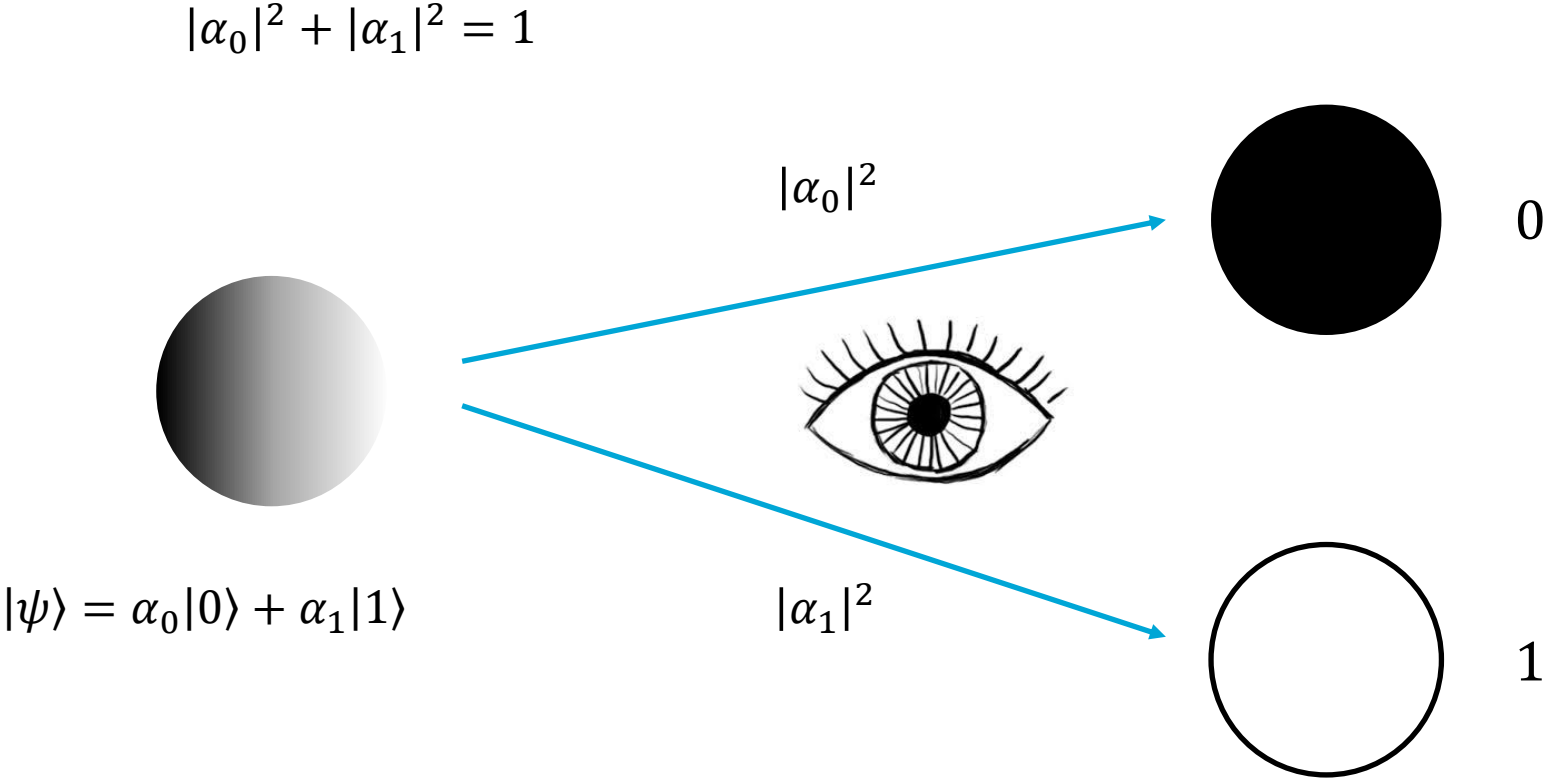
Quantum bit (qubits)

superposition of $|0\rangle$ and $|1\rangle$



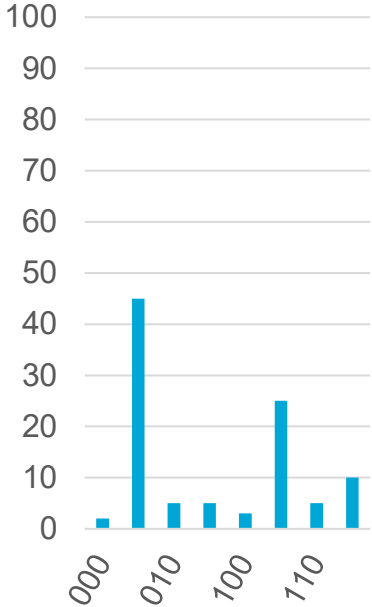
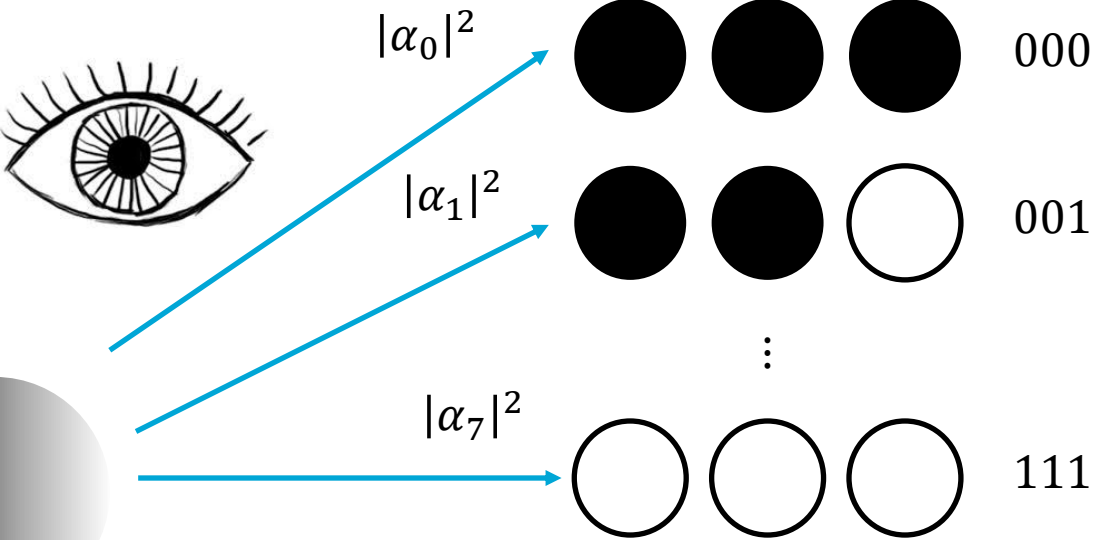
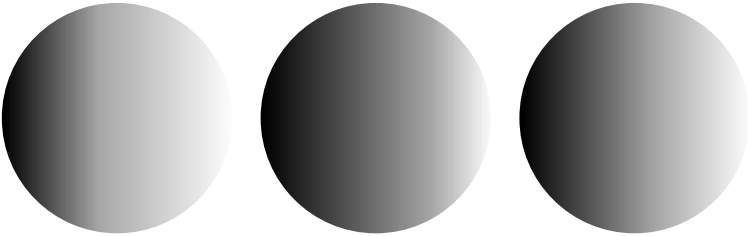
$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle$$

Reading out quantum information



Superposition

$$|\alpha_0|^2 + \dots + |\alpha_7|^2 = 1$$



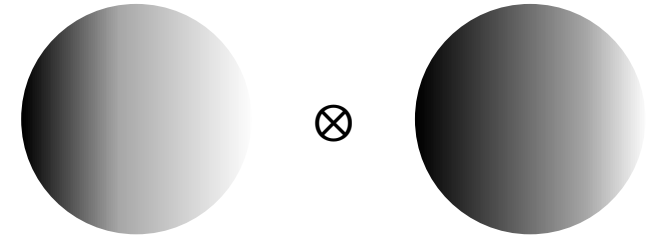
$$|\psi\rangle = \alpha_0|000\rangle + \alpha_1|001\rangle + \alpha_2|010\rangle + \alpha_3|011\rangle + \alpha_4|100\rangle + \alpha_5|101\rangle + \alpha_6|110\rangle + \alpha_7|111\rangle$$

n qubits can hold a **superposition** of 2^n values in their amplitudes $\alpha_i \in \mathbb{C}$; $|\alpha_i|^2$ is the **probability** of reading out the i -th basis state upon measurement

Entanglement

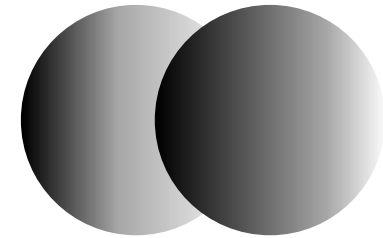
Product of two qubits (= separable quantum state)

$$\begin{aligned} |\psi\rangle &= (\alpha_0|0\rangle + \alpha_1|1\rangle) \otimes (\beta_0|0\rangle + \beta_1|1\rangle) \\ &= \alpha_0\beta_0|00\rangle + \alpha_0\beta_1|01\rangle + \alpha_1\beta_0|10\rangle + \alpha_1\beta_1|11\rangle \end{aligned}$$



Non-separable (= entangled) quantum state

$$|\psi\rangle = \gamma_{00}|00\rangle + \gamma_{01}|01\rangle + \gamma_{10}|10\rangle + \gamma_{11}|11\rangle$$

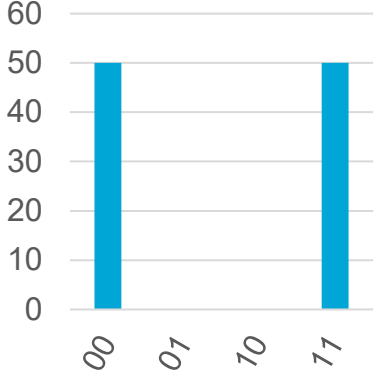


Quantum gates – the assembly of quantum computers

Example

$$|\psi\rangle = \text{CNOT}(\text{H}\otimes\text{I})(|0\rangle\otimes|0\rangle)$$

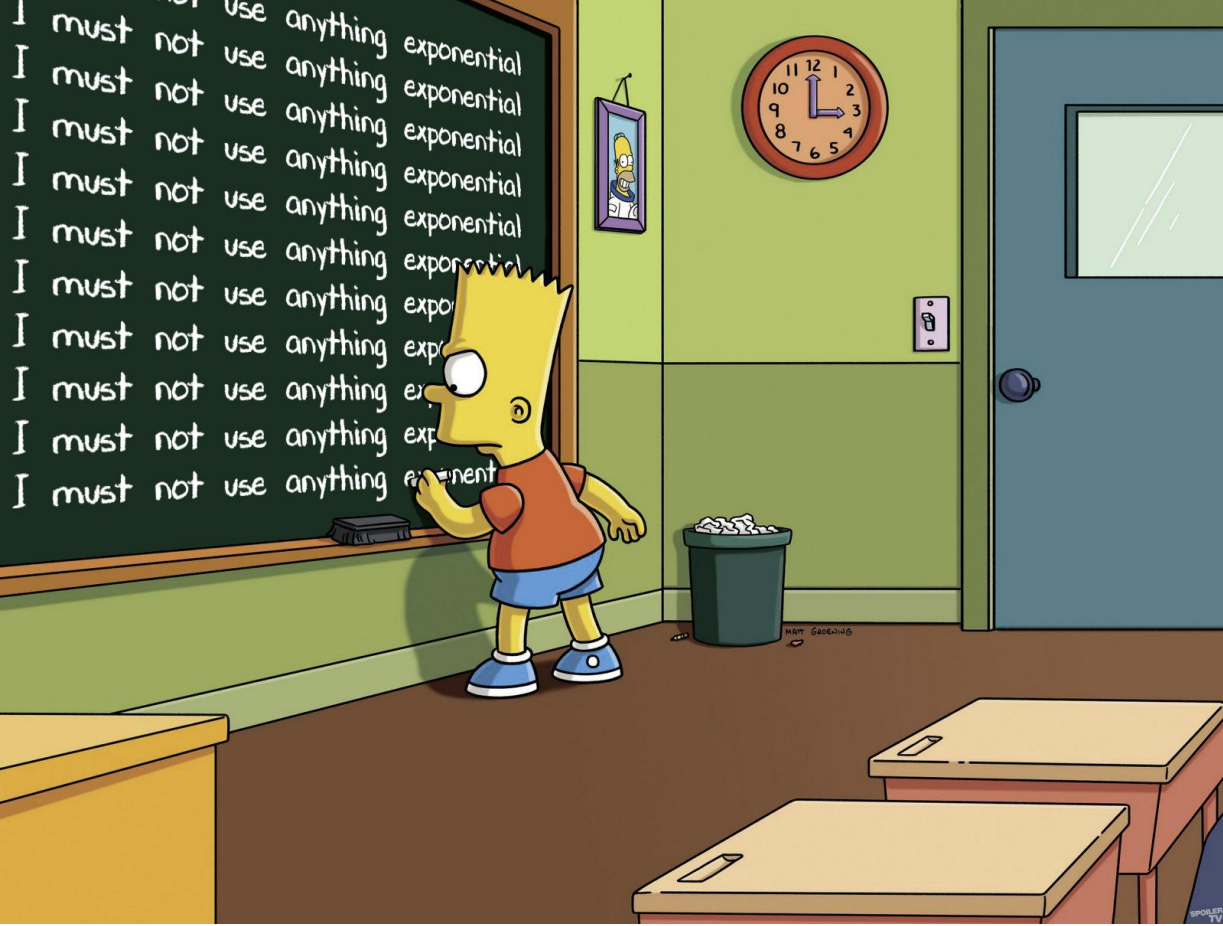
$$\begin{aligned} \text{H}|0\rangle &= \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \\ &= \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle \end{aligned}$$



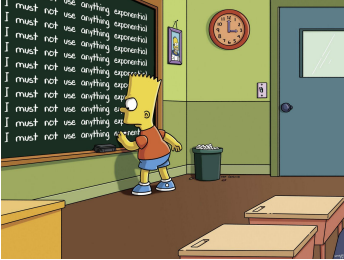
$$\text{CNOT}|10\rangle = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

$|10\rangle$
 $|11\rangle$

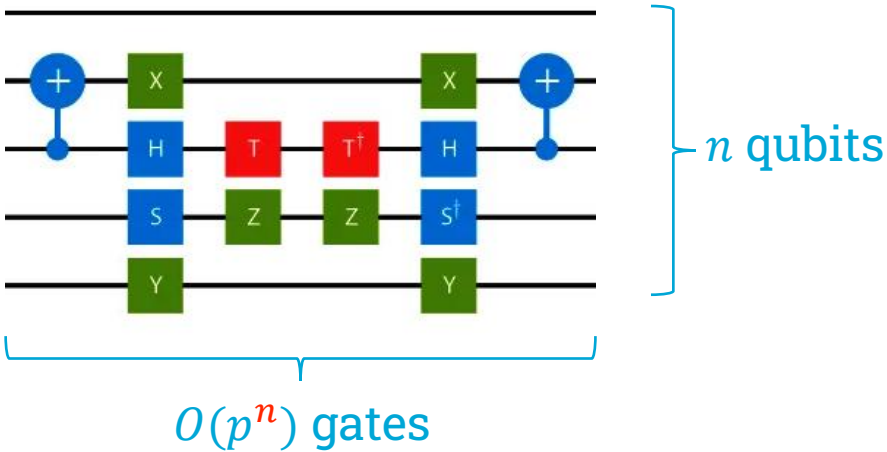
Common pitfalls



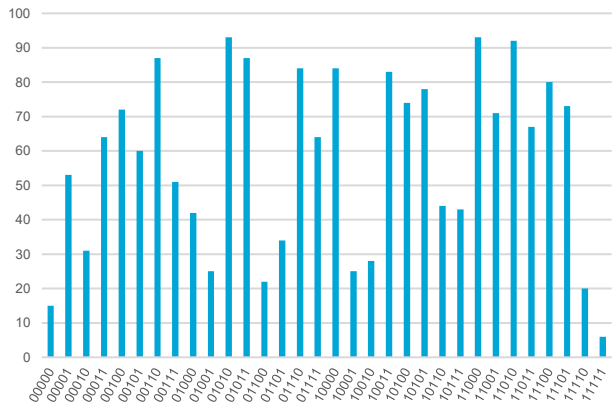
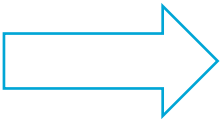
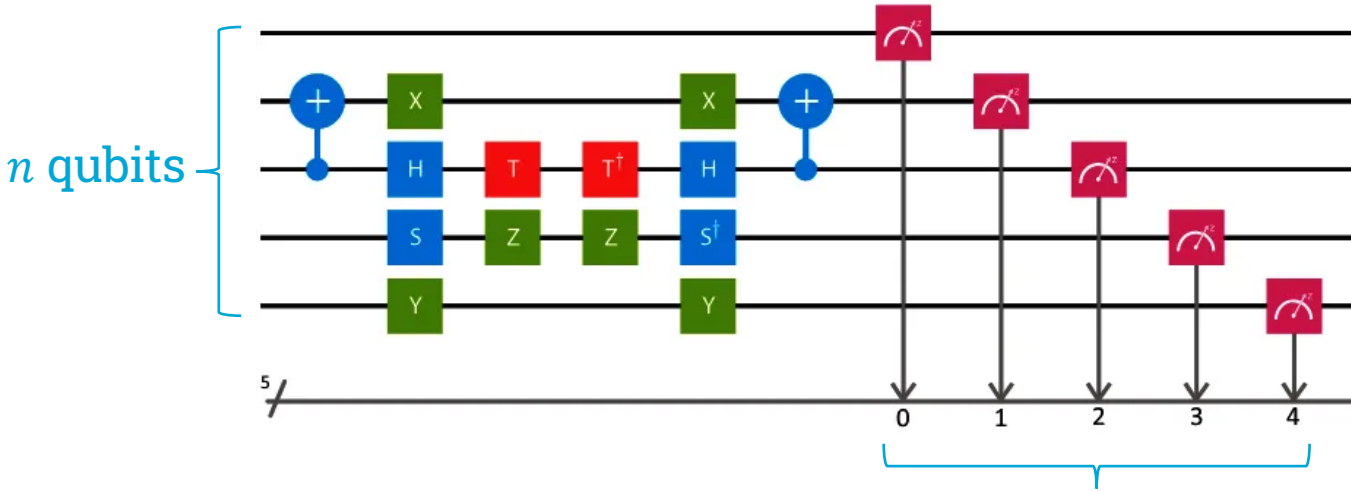
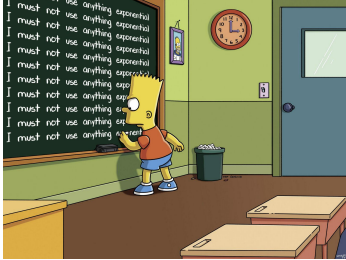
Common pitfalls – exponentially large ‘programs’



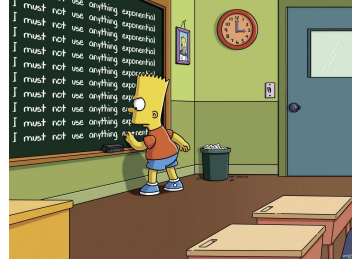
$$|\psi\rangle = U|0\rangle$$



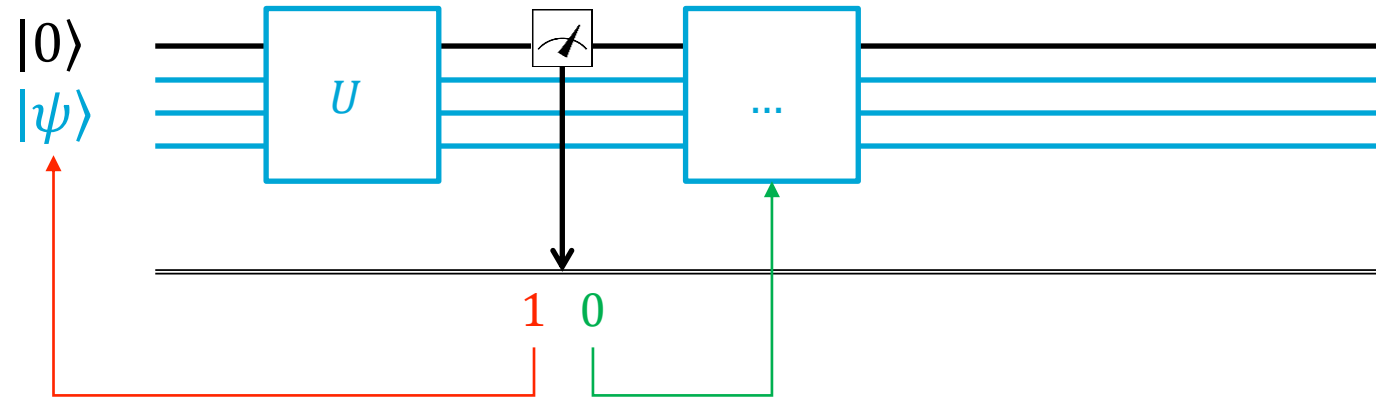
Common pitfalls – exponentially many readouts



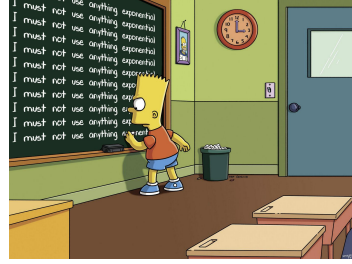
Common pitfalls – probabilistic successes



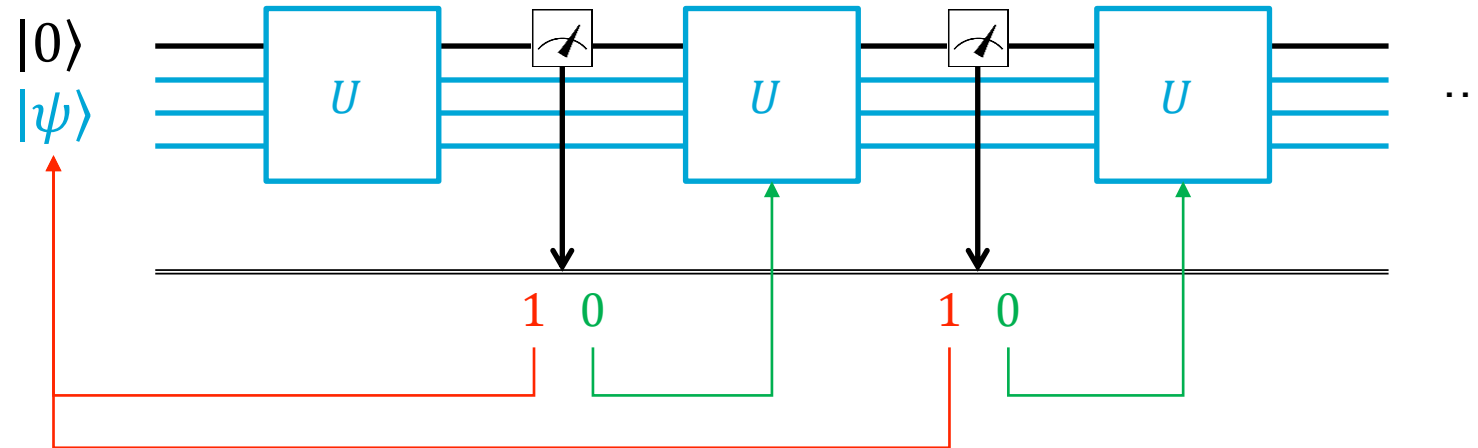
$$U|\psi\rangle|0\rangle = \sqrt{\delta}|\psi_{\text{good}}\rangle|0\rangle + \sqrt{1-\delta}|\psi_{\text{bad}}\rangle|1\rangle$$



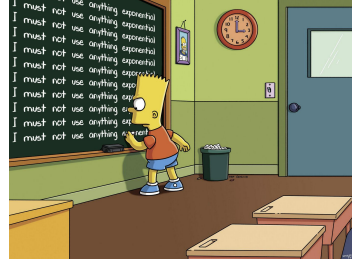
Common pitfalls – probabilistic successes



$$U^m |\psi\rangle |0\rangle = \sqrt{\delta} |\psi_{\text{good}}\rangle |0\rangle + \sqrt{1 - \delta} |\psi_{\text{bad}}\rangle |1\rangle$$



Common pitfalls – probabilistic successes



$$U^m |\psi\rangle |0\rangle = \sqrt{\delta} |\psi_{\text{good}}\rangle |0\rangle + \sqrt{1 - \delta} |\psi_{\text{bad}}\rangle |1\rangle$$

m	$\delta = 0.9$	$\delta = 0.99$	$\delta = 0.999$
10	0.349	0.904	0.990
100	$2.66 \cdot 10^{-5}$	0.366	0.905
1,000	$1.75 \cdot 10^{-48}$	$4.32 \cdot 10^{-5}$	0.368
10,000	n/a	$2.52 \cdot 10^{-44}$	$4.52 \cdot 10^{-5}$

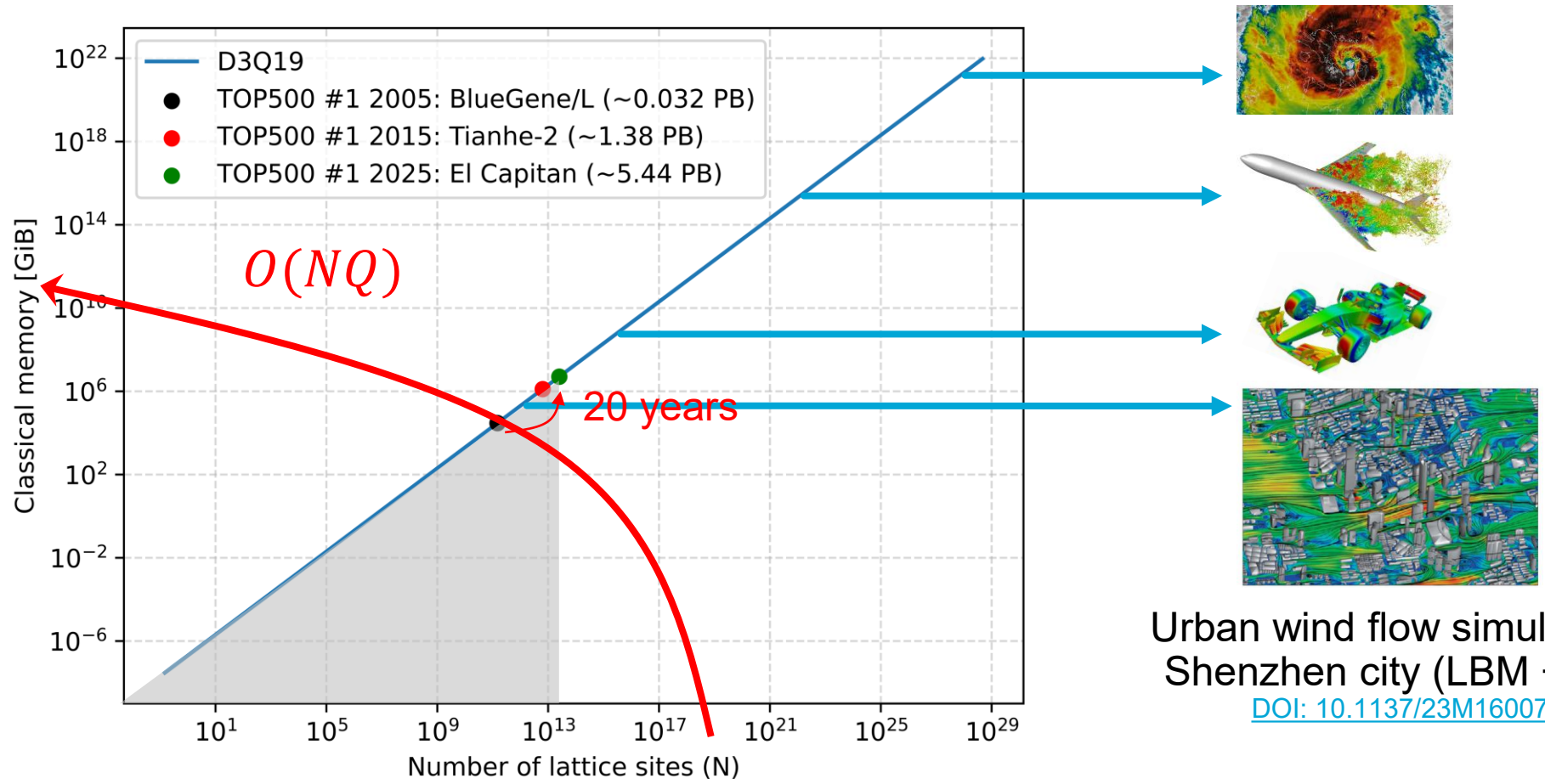
Take-home lessons

$$|0\rangle + \sum_{i=1}^{2^n-1} 0|i\rangle \xrightarrow{\text{unitary operations}} \sum_{i=0}^{2^n-1} \alpha_i|i\rangle \xrightarrow{\text{measurement}} i \text{ with probability } |\alpha_i|^2$$

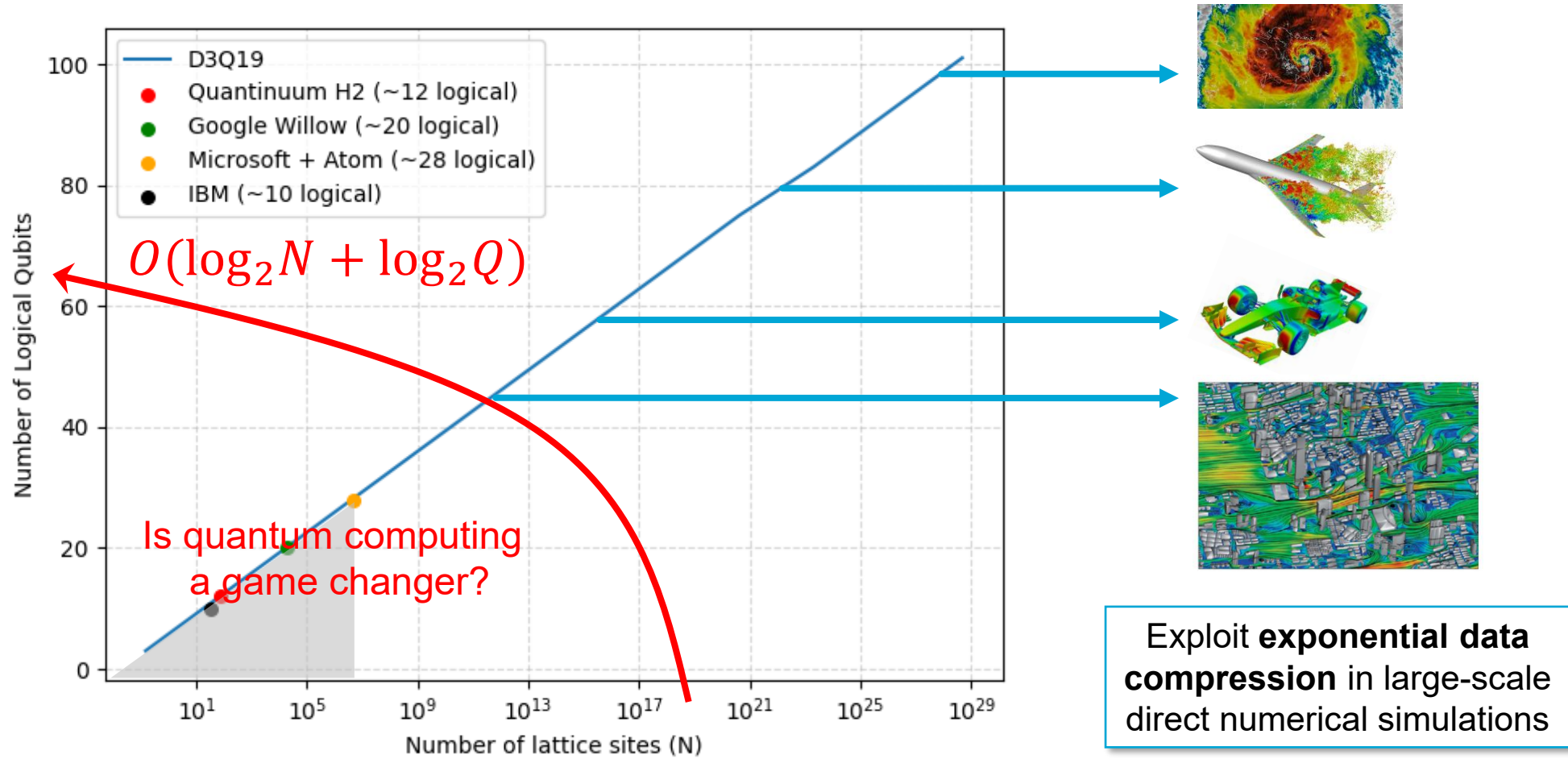
If quantum computing shall become the future of HPCSE we need to ...

- ... identify **applications** that cannot be solved (efficiently) with classical computers
- ... develop **algorithms** that exploit the strengths of quantum computers (and avoid their limitations)
- ... (most probably) change the **workflows** that were designed for classical computers

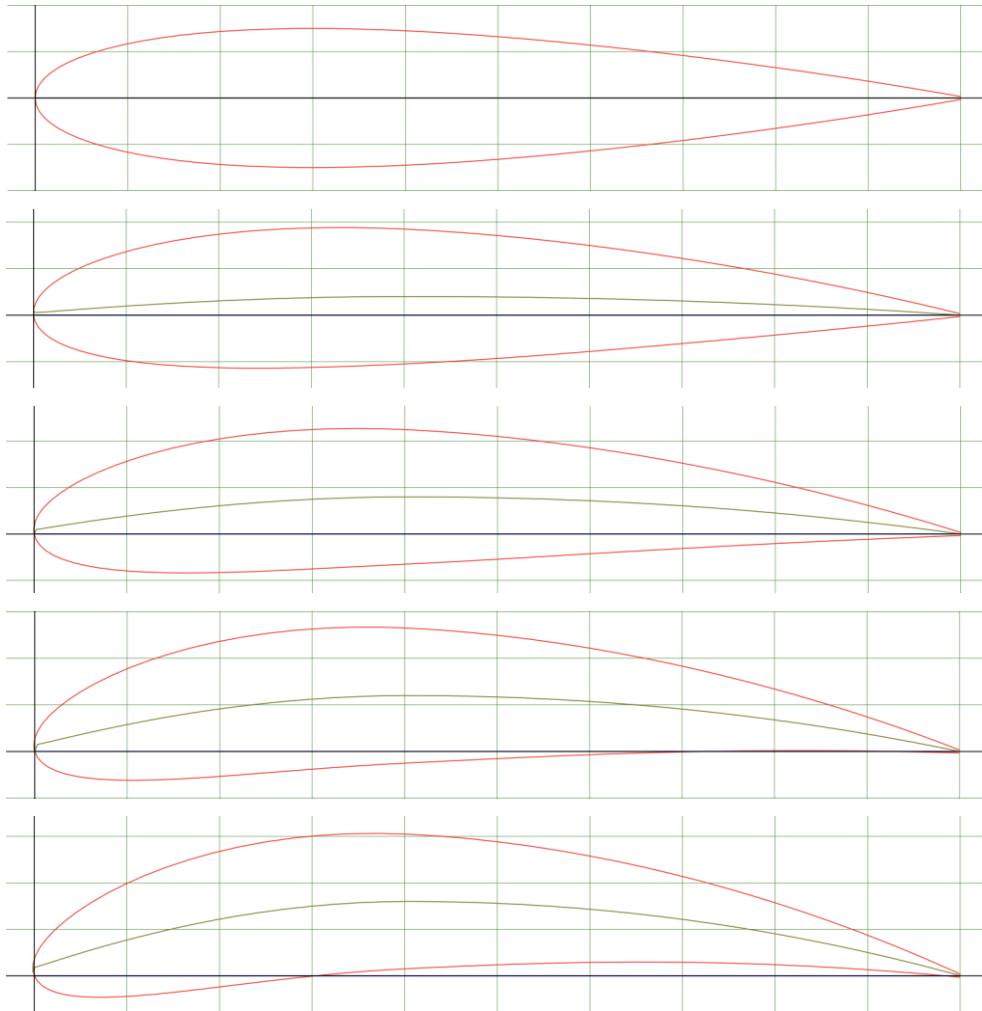
Application #1: Computational fluid dynamics



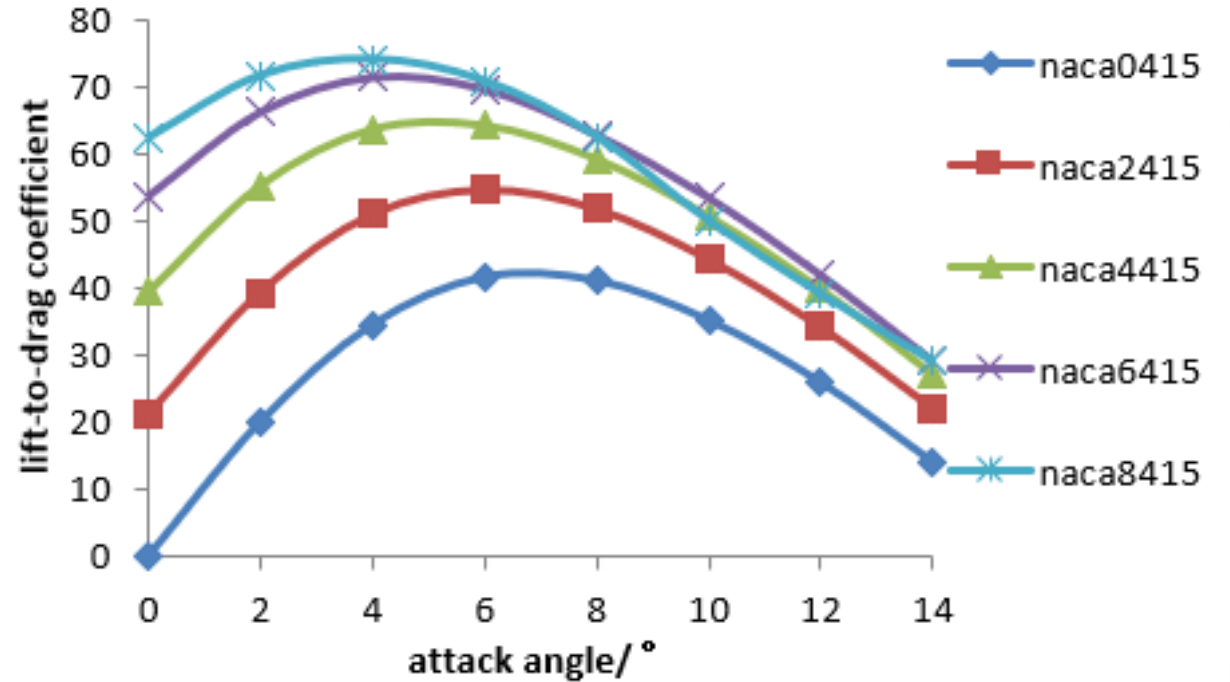
Application #1: Computational fluid dynamics



Application #2: Design optimization (not just for CFD)



Generated with airfoiltools.com



[DOI: 10.1088/1742-6596/1519/1/012020](https://doi.org/10.1088/1742-6596/1519/1/012020)

Exploit **quadratic speedup of quantum search algorithms** in design optimization

Boltzmann equation (BE)

$$\rho(\mathbf{x}, t) = \int f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$$
$$\rho \mathbf{u}(\mathbf{x}, t) = \int \mathbf{v} f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v}$$

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \mathbf{a} \cdot \nabla_{\mathbf{v}} f = -\frac{1}{\tau} (f - f^{\text{eq}})$$

effect of external forces

free streaming

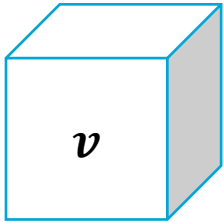
redistribution by collision

distribution function

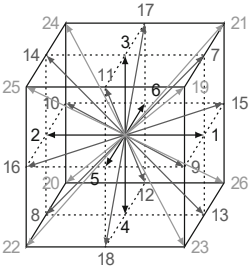
$$f(\mathbf{x}, \mathbf{v}, t) \quad \left[\frac{\text{kg s}^3}{\text{m}^6} \right]$$

From BE to the lattice Boltzmann method (LBM)

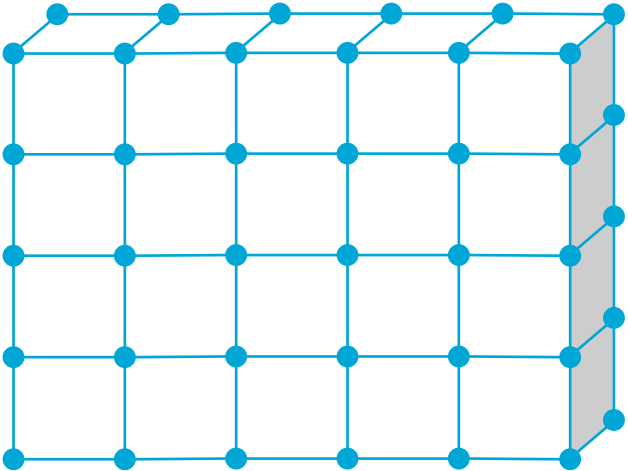
$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \Omega$$



$$f(\mathbf{x}, \mathbf{v}, t)$$



$$f_\alpha(\mathbf{x}, t) = f(\mathbf{x}, \mathbf{e}_\alpha, t)$$

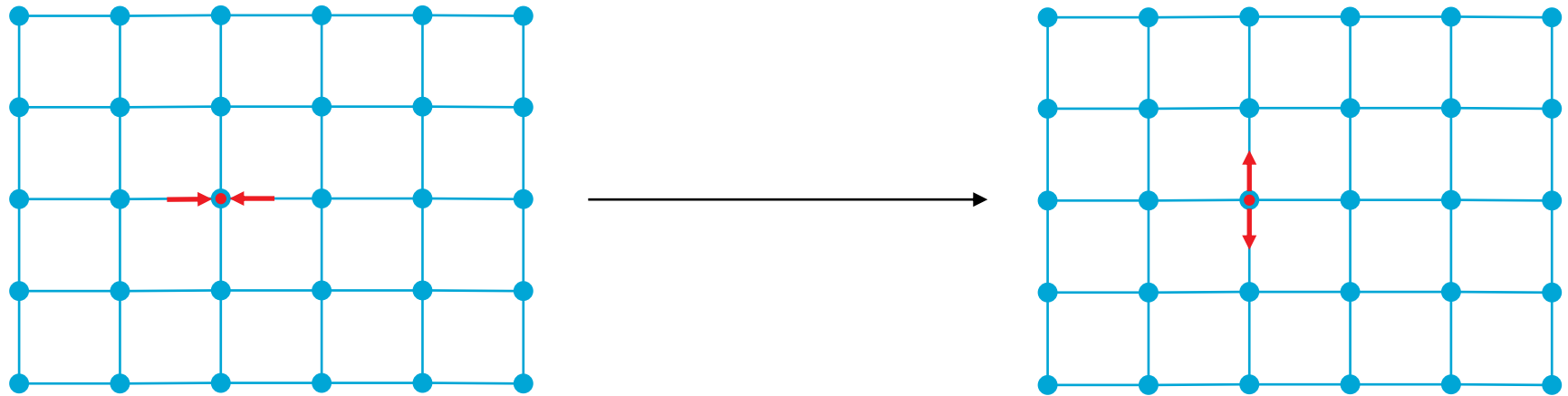


$$f_\alpha(\mathbf{x}_i, t^n)$$

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla f_\alpha = \Omega_\alpha$$

$$f_\alpha^*(\mathbf{x}_i, t^n) = f_\alpha(\mathbf{x}_i, t^n) + \Delta t \Omega_\alpha(\mathbf{x}_i, t^n)$$

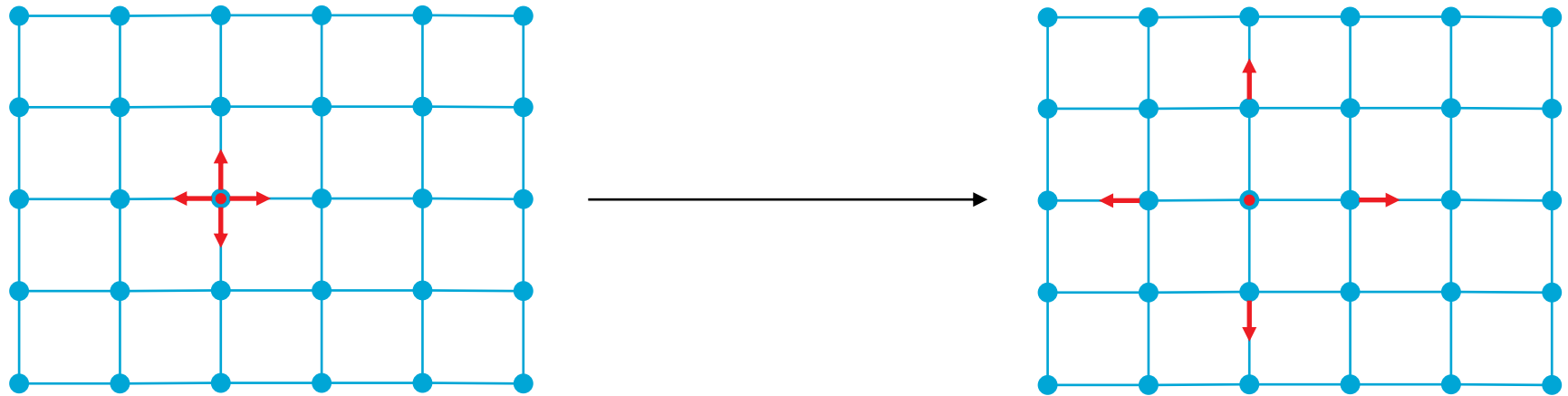
→ collision of all f_α at grid point \mathbf{x}_i



$$\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla f_\alpha = \Omega_\alpha$$

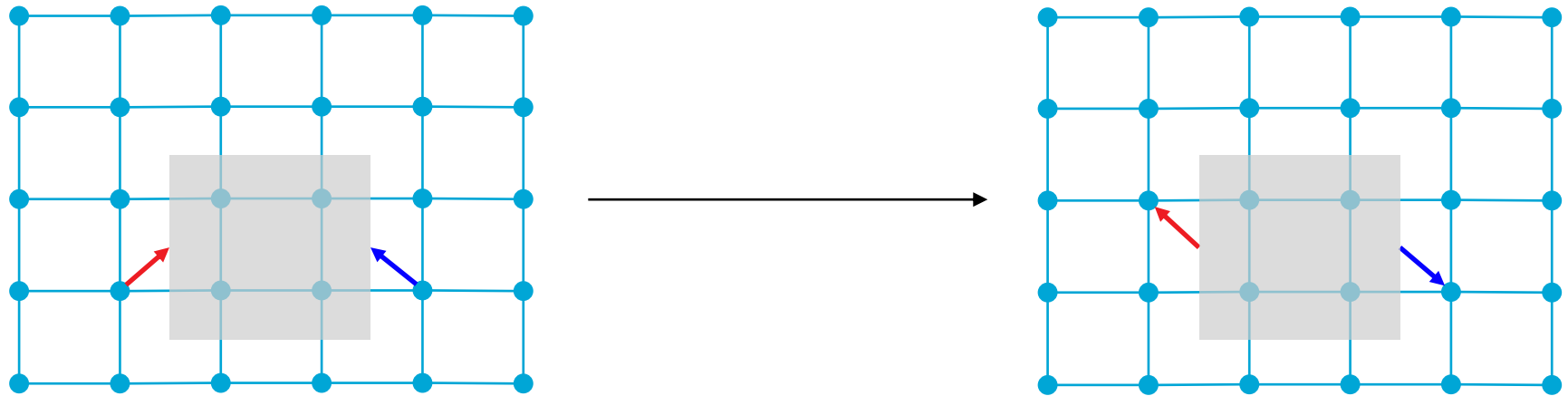
$$f_\alpha(\mathbf{x}_i + \mathbf{e}_\alpha \Delta t, t^n + \Delta t) = f_\alpha^*(\mathbf{x}_i, t^n)$$

streaming of all f_α along direction \mathbf{e}_α

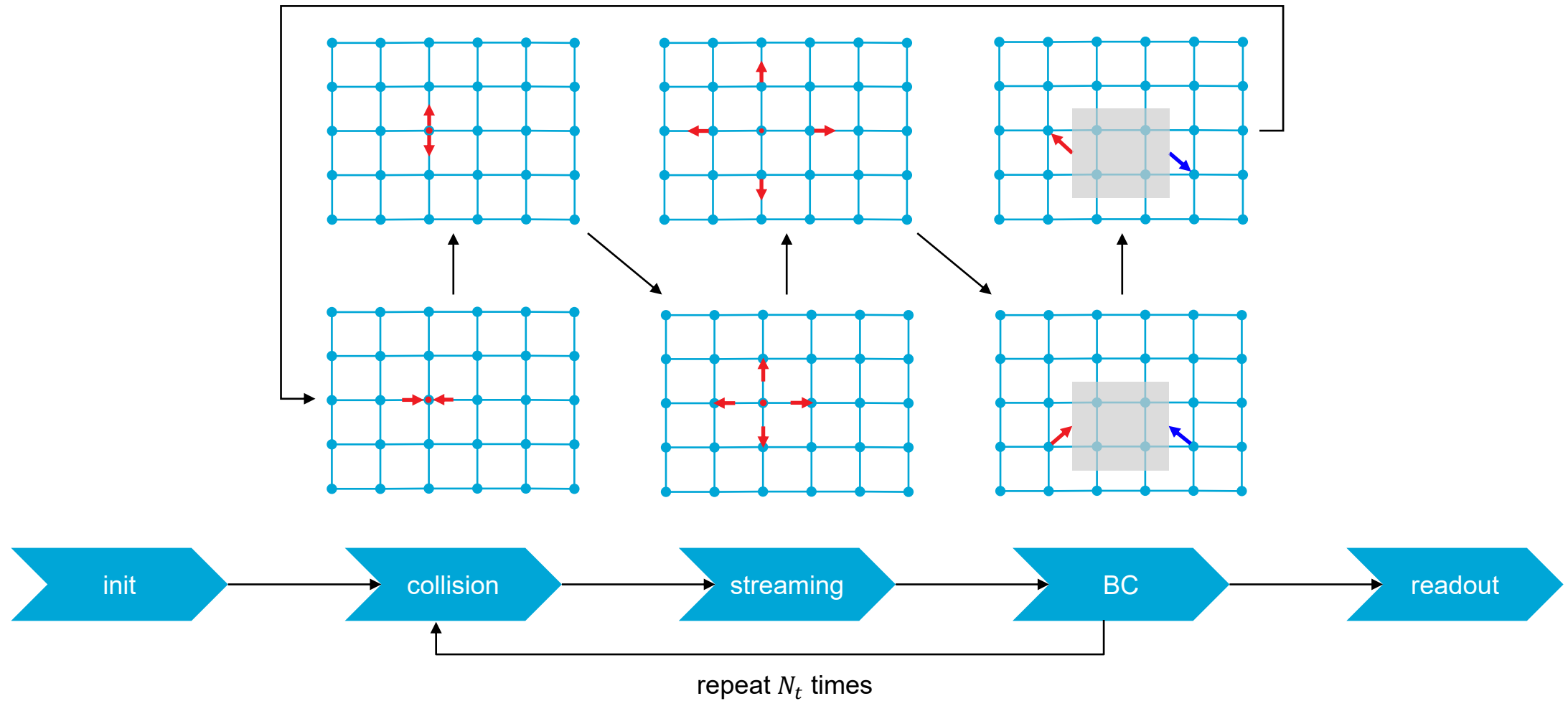


$$\frac{\partial f_\alpha}{\partial t} + \mathbf{e}_\alpha \cdot \nabla f_\alpha = \Omega_\alpha$$

→ reflection or bounce-back boundary



LBM



Advantages of LBM over other flow models

1. Update **moments** and **equilibrium distribution functions**

$$\rho = \sum_{\alpha} f_{\alpha}, \quad \mathbf{u} = \frac{1}{\rho} \sum_{\alpha} f_{\alpha} \mathbf{e}_{\alpha}, \quad f_{\alpha}^{\text{eq}} = w_{\alpha} \rho \left(1 + \frac{\mathbf{u} \cdot \mathbf{e}_{\alpha}}{c_s^2} + \frac{(\mathbf{u} \cdot \mathbf{e}_{\alpha})^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^4} \right)$$

2. Collide

$$f_{\alpha}^*(\mathbf{x}_i, t^n) = f_{\alpha}(\mathbf{x}_i, t^n) - \frac{\Delta t}{\tau} \left(f_{\alpha}(\mathbf{x}_i, t^n) - f_{\alpha}^{\text{eq}}(\mathbf{x}_i, t^n) \right) \quad \text{nonlinear \& local } \otimes$$

3. Stream

↕ decoupled ✓

$$f_{\alpha}(\mathbf{x}_i + \mathbf{c}_{\alpha} \Delta t, t^n + \Delta t) = f_{\alpha}^*(\mathbf{x}_i, t^n) \quad \text{linear \& global } \checkmark$$

4. Apply **boundary conditions**

5. Repeat

Data encoding

Classical register

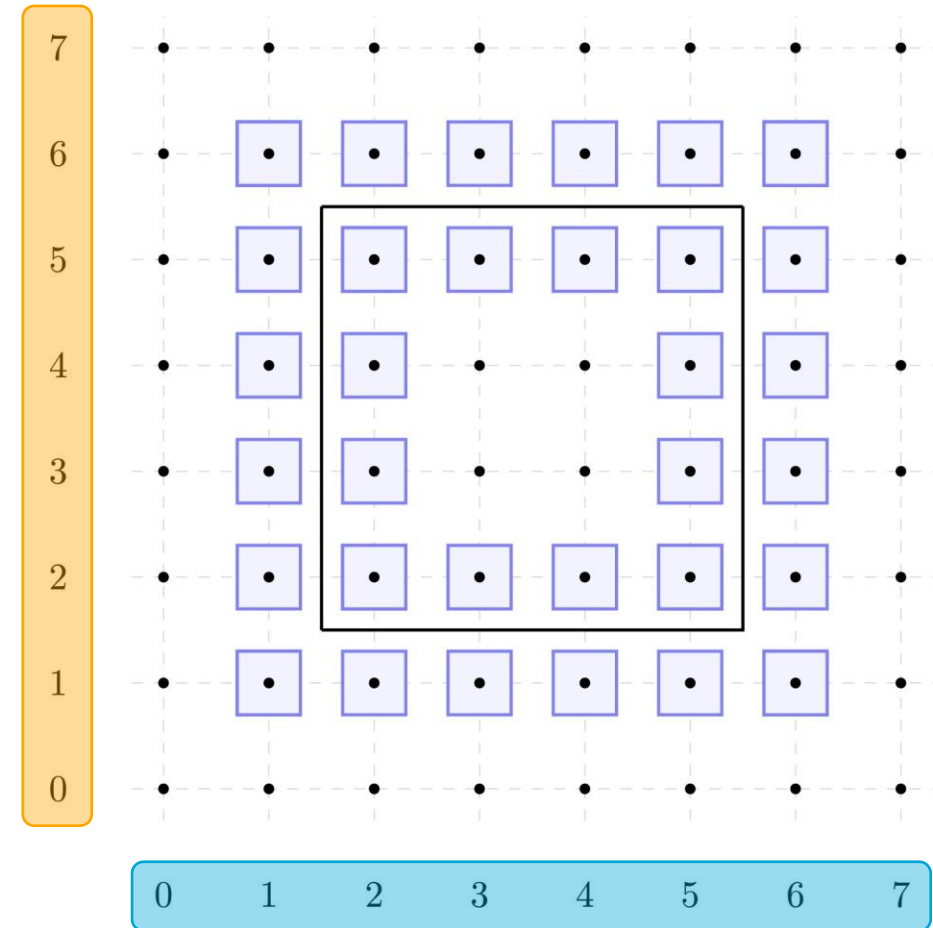
$$f[N_v][N_x][N_y] \quad N_v = 9, N_x = N_y = 8$$

$$f[\alpha][i][j] \mapsto f_\alpha(x_i, y_j)$$

Quantum register

$$|v\rangle \otimes |x\rangle \otimes |y\rangle, \quad n_v = \lceil \log_2 9 \rceil = 4, n_x = n_y = 3$$

$$|\psi\rangle = \sum_{\alpha, i, j} \gamma_{\alpha i j} |e_\alpha\rangle |i\rangle |j\rangle, \quad \gamma_{\alpha i j} \propto \sqrt{f_\alpha(x_i, y_j)}$$



Data encoding

Classical register

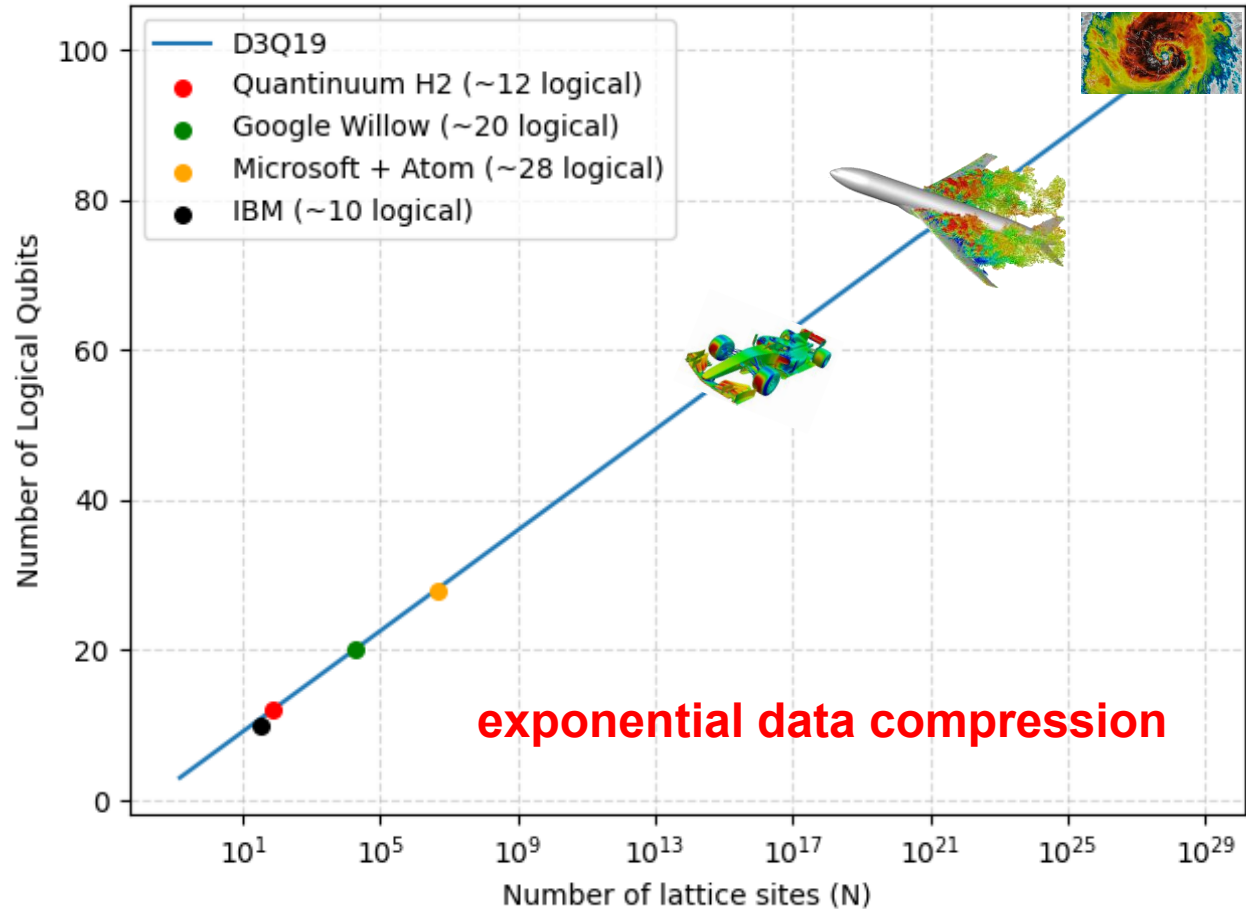
$$f[N_v][N_x][N_y] \quad N_v = 9, N_x = N_y = 8$$

$$f[\alpha][i][j] \mapsto f_\alpha(x_i, y_j)$$

Quantum register

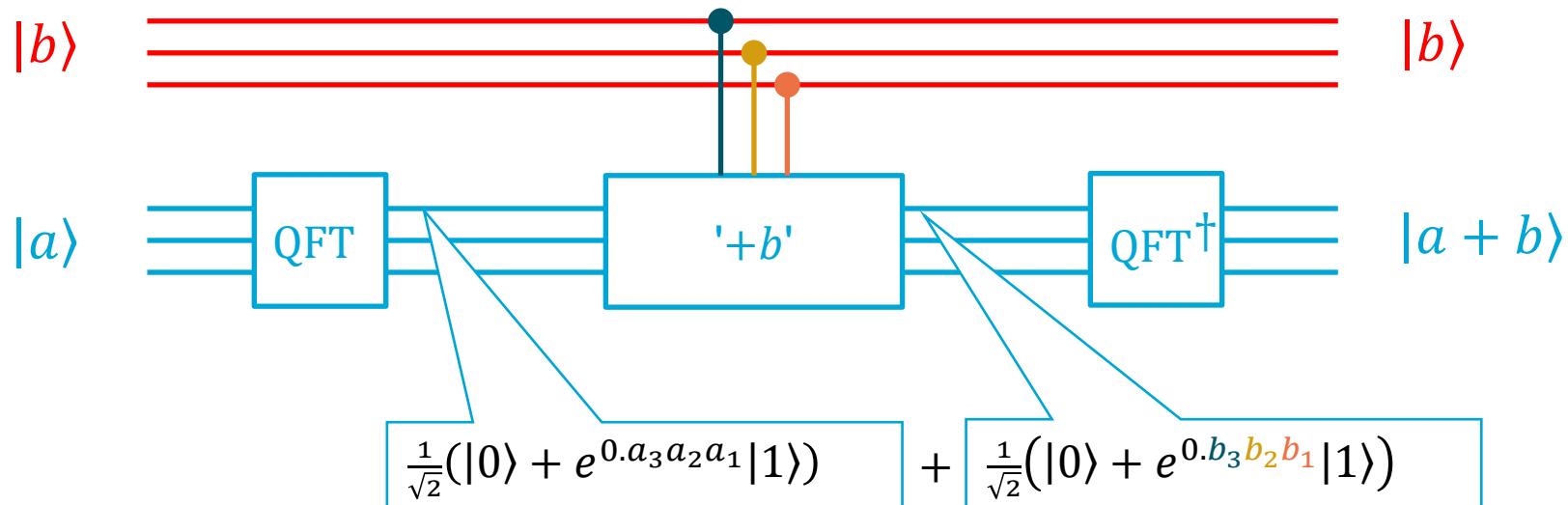
$$|v\rangle \otimes |x\rangle \otimes |y\rangle, \quad n_v = \lceil \log_2 9 \rceil = 4, n_x = n_y = 3$$

$$|\psi\rangle = \sum_{\alpha, i, j} \gamma_{\alpha ij} |e_\alpha\rangle |i\rangle |j\rangle, \quad \gamma_{\alpha ij} \propto \sqrt{f_\alpha(x_i, y_j)}$$

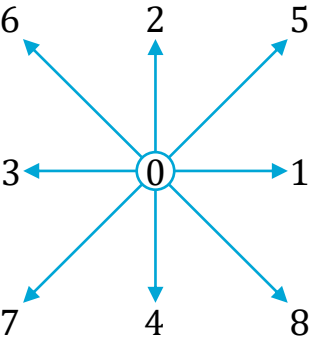


Sketch of the streaming operation

Our streaming primitive is based on **Draper's quantum adder** ("Addition on a Quantum Computer" '98) which is an in-place quantum adder for two integer values that works without auxiliary qubits

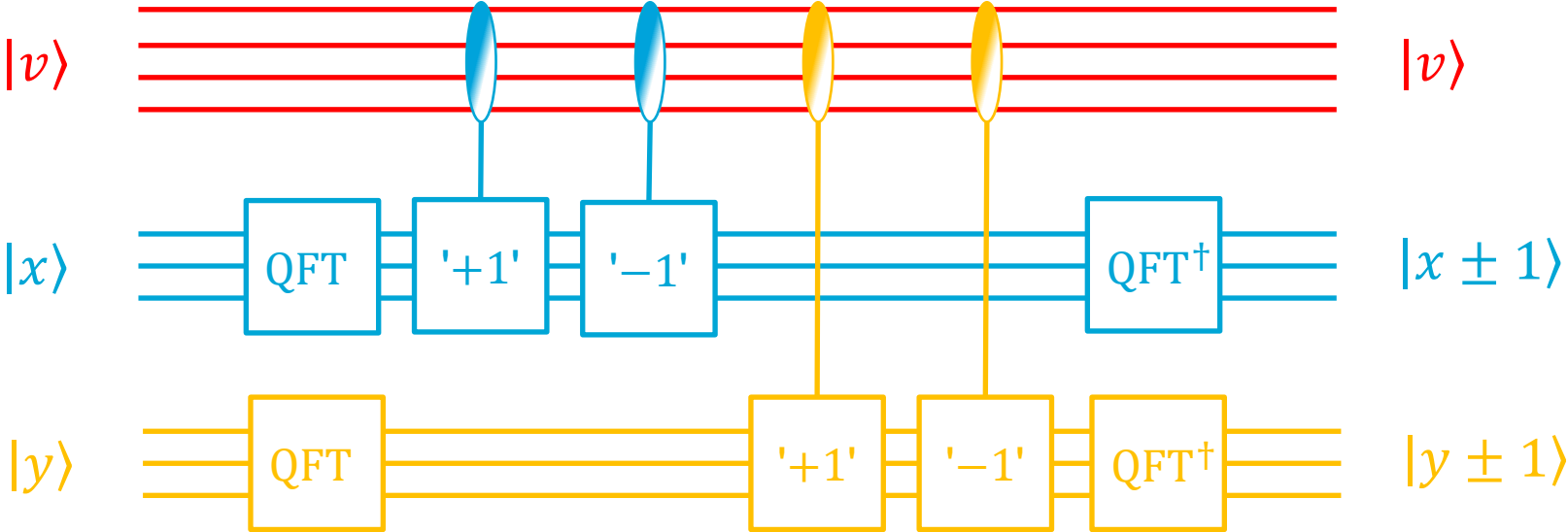


Sketch of the streaming operation



If $v \in \{1,5,8\}$ then $|x\rangle \rightarrow |x + 1\rangle$

$C\bar{C}\bar{C}\bar{C}[+1]|v\rangle|\tilde{x}\rangle$
 $C\bar{C}\bar{C}\bar{C}[+1]|v\rangle|\tilde{x}\rangle$
 $\bar{C}\bar{C}\bar{C}\bar{C}[+1]|v\rangle|\tilde{x}\rangle$



M. Schalkers, MM, *Efficient and fail-safe quantum algorithm for the transport equation*. JCP 502, 2024

Specular reflection / bounce back boundary conditions

For all quantum states $|x\ y\ ???? \rangle$ in the first inner layer of an obstacle

1. Place data back into flow domain

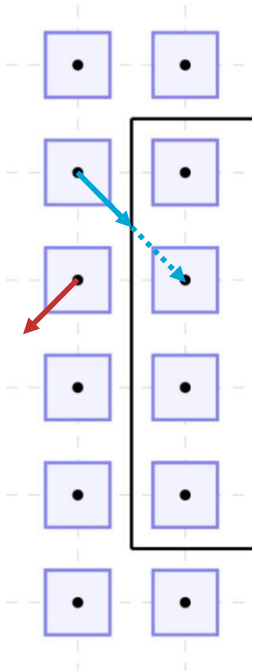
$$|x\ y\ ???? \rangle \xrightarrow{\text{CCCC}[\pm 1]} |x \pm 1\ y \pm 1\ ???? \rangle$$

2. Change velocity direction

$$|x \pm 1\ y \pm 1\ ???? \rangle \xrightarrow{\text{Perm}} |x \pm 1\ y \pm 1\ '?'?'?''\rangle$$

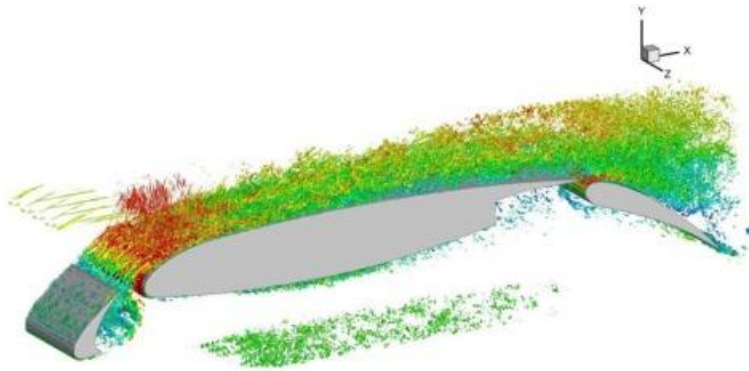
Obstacle detection

- *Quantum comparator*

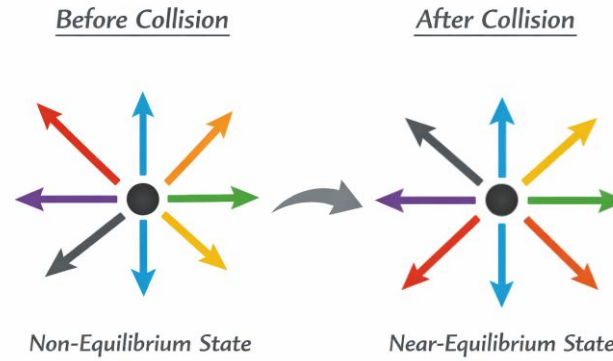


M. Schalkers, MM, *Efficient and fail-safe quantum algorithm for the transport equation*. JCP 502, 2024

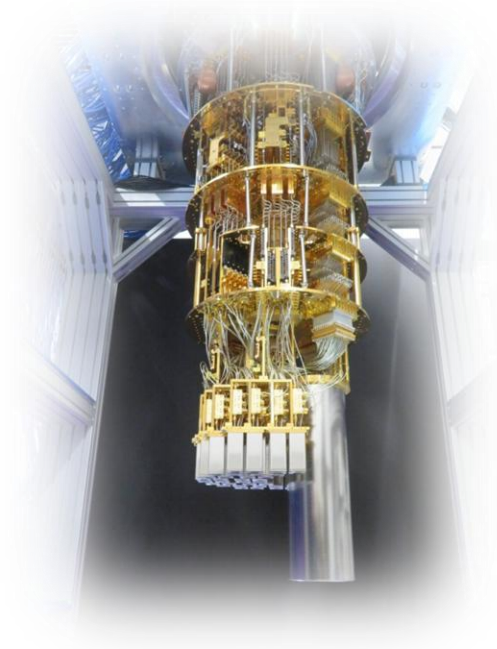
Three grand challenges in quantum LBM



Complex geometries

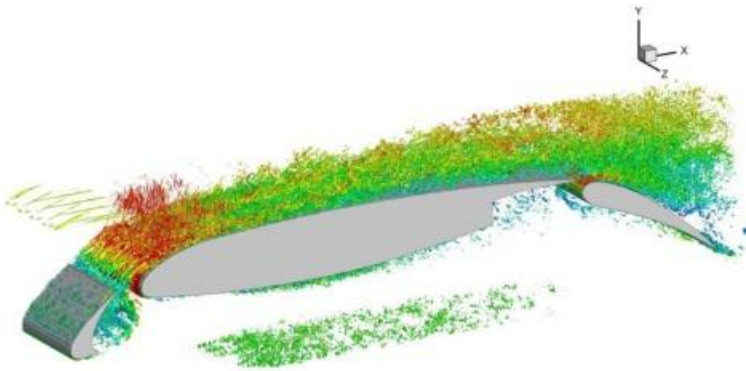


Nonlinear dynamics



Running on NISQ hardware

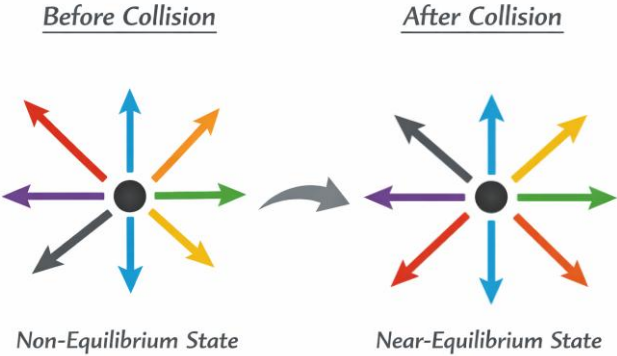
Zone-agnostic boundary conditions



Complex geometries

C. Georgescu, MM, *Efficient implementation of complex geometries in quantum lattice Boltzmann methods*. In preparation

Collision à la Bhatnagar-Gross-Krook (BGK)



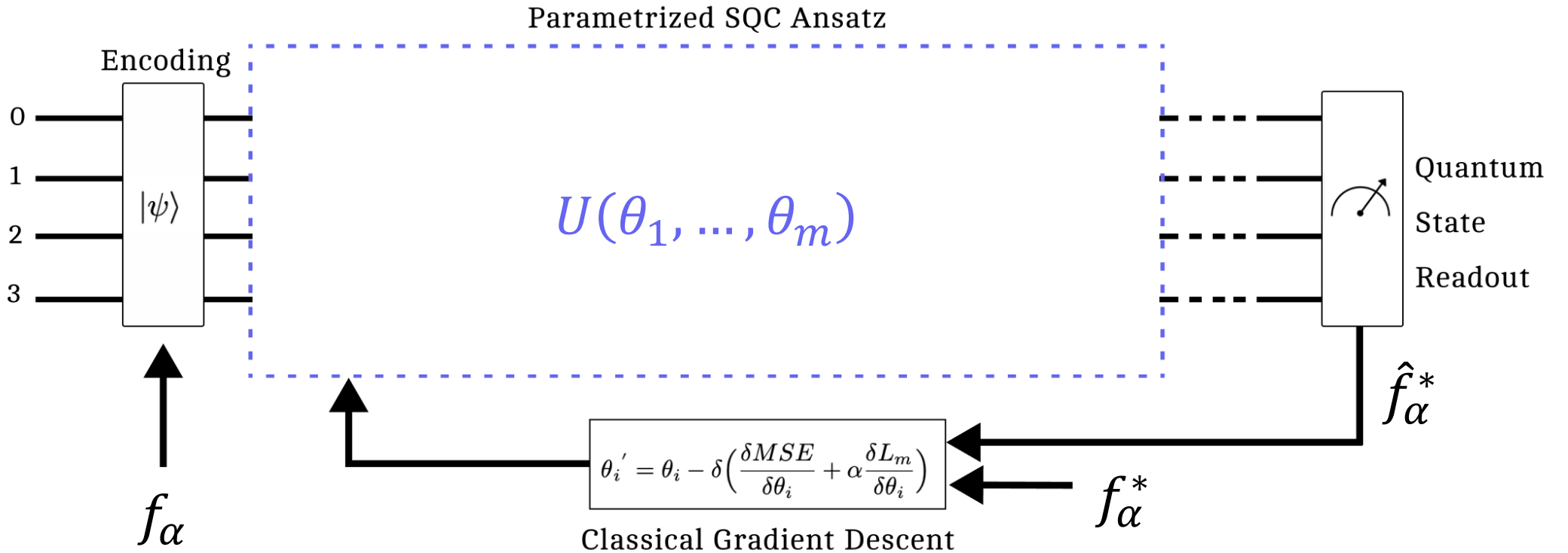
Nonlinear dynamics

$$f_{\alpha}^* = (1 - \omega)f_{\alpha} + \omega w_{\alpha} \rho \left(\overset{\text{linear}}{\underbrace{1 + \frac{u \cdot e_{\alpha}}{c_S^2}}_{\text{green}}} + \overset{\text{nonlinear}}{\underbrace{\frac{(u \cdot e_{\alpha})^2}{2c_S^4} - \frac{u \cdot u}{2c_S^4}}_{\text{red}}}} \right)$$

- ignore collision → collisionless QLBM
- ignore nonlinear term → linearized QLBM
- approximate nonlinear term → QLBM

Surrogate quantum circuits

Learn a low-depth, unitary **approximation** of the BGK operator that mimics its physical properties



M. Lacatus, MM, [Surrogate quantum circuit design for the lattice Boltzmann collision operator](#), *IJNME* 127(4):e70286, 2026

Physical properties of the BGK operator for D_2Q_9

Mass conservation

$$|\psi\rangle = \frac{1}{\sqrt{\rho}} \sum_{\alpha} \sqrt{f_{\alpha}} |\mathbf{e}_{\alpha}\rangle, \quad \rho = \sum_{\alpha} f_{\alpha}$$

Momentum conservation

Enforced weakly in the loss function

Scale invariance

$$\Omega(\lambda \cdot f_{\alpha}) = \lambda \cdot \Omega(f_{\alpha}), \quad \lambda > 0$$

	Discrete velocity	Velocity basis state
f_0	(0,0)	0000⟩
f_1	(1,0)	0001⟩
f_2	(0,1)	0010⟩
f_3	(-1,0)	0100⟩
f_4	(0,-1)	1000⟩
f_5	(1,1)	0011⟩
f_6	(-1,1)	0110⟩
f_7	(-1,-1)	1100⟩
f_8	(1,-1)	1001⟩

The remaining 7 basis states are unused and are assigned to the (0,0) velocity state, effectively contributing to the population f_0 , to ensure mass conservation

Physical properties of the BGK operator for D_2Q_9

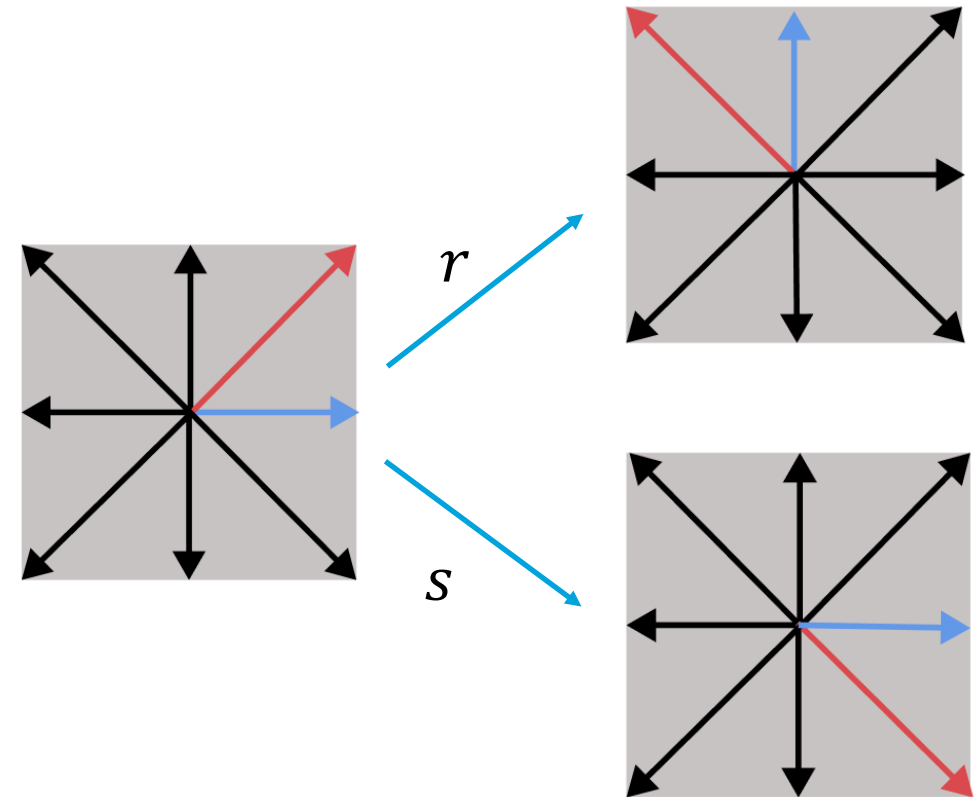
D_8 equivariance

D_2Q_9 lattice is invariant under the dihedral group D_8 , i.e., the full symmetry group of a square ($r = 90^\circ$ **rotation** and s is a **reflection**):

$$D_8 = [I, r, r^2, r^3, s, rs, r^2s, r^3s]$$

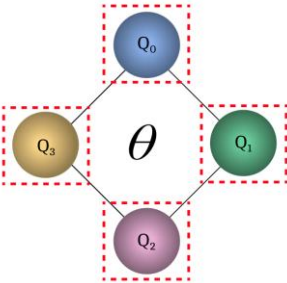
BGK operator **commutes** with all group elements:

$$\Omega(\sigma \circ f_\alpha) = \sigma \circ \Omega(f_\alpha) \quad \forall \sigma \in D_8$$

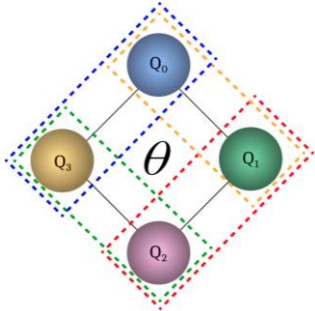


Construction of the SQC

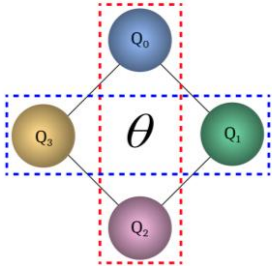
No entanglement



Axial entanglement



Diagonal entanglement



Single-qubit rotation layers

$$R_x(\theta)^{\otimes 4}$$

$$R_z(\theta)^{\otimes 4}$$

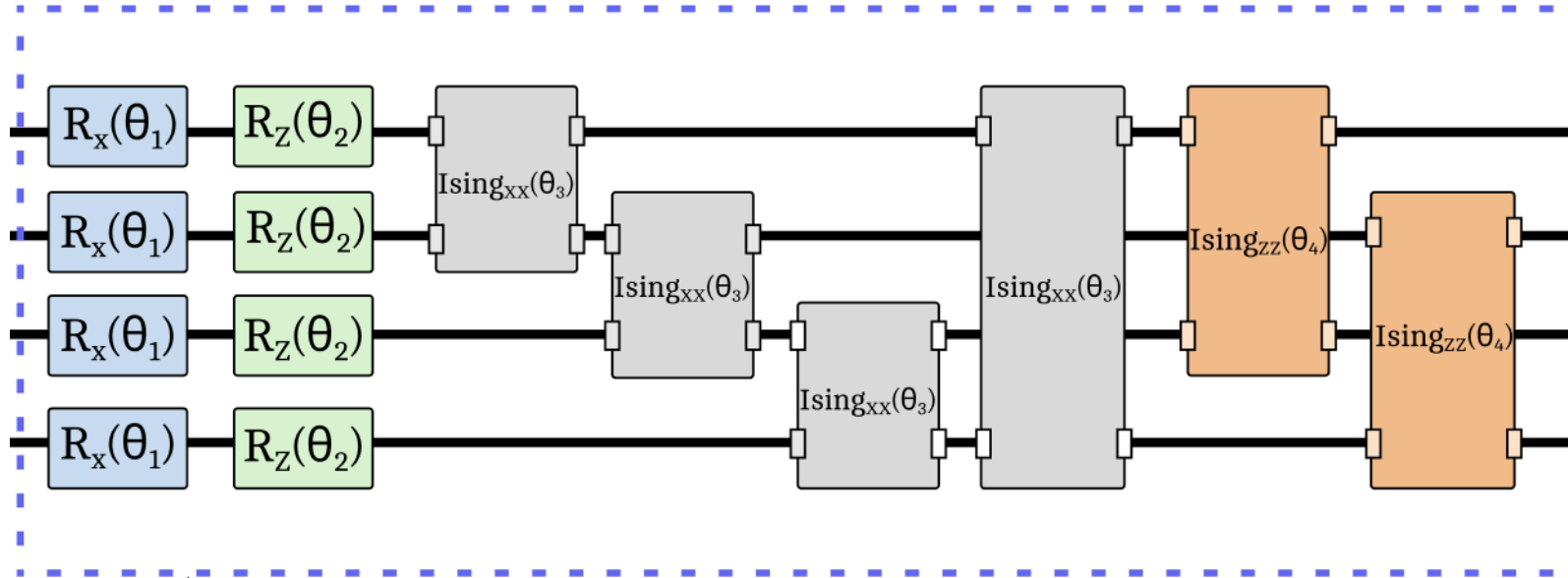
Ising XX & ZZ entangling layers

$$\text{Ising}_{xx} = \exp\left(-\frac{i\theta}{2} \sigma_x \otimes \sigma_x\right)$$

$$\text{Ising}_{zz} = \exp\left(-\frac{i\theta}{2} \sigma_z \otimes \sigma_z\right)$$

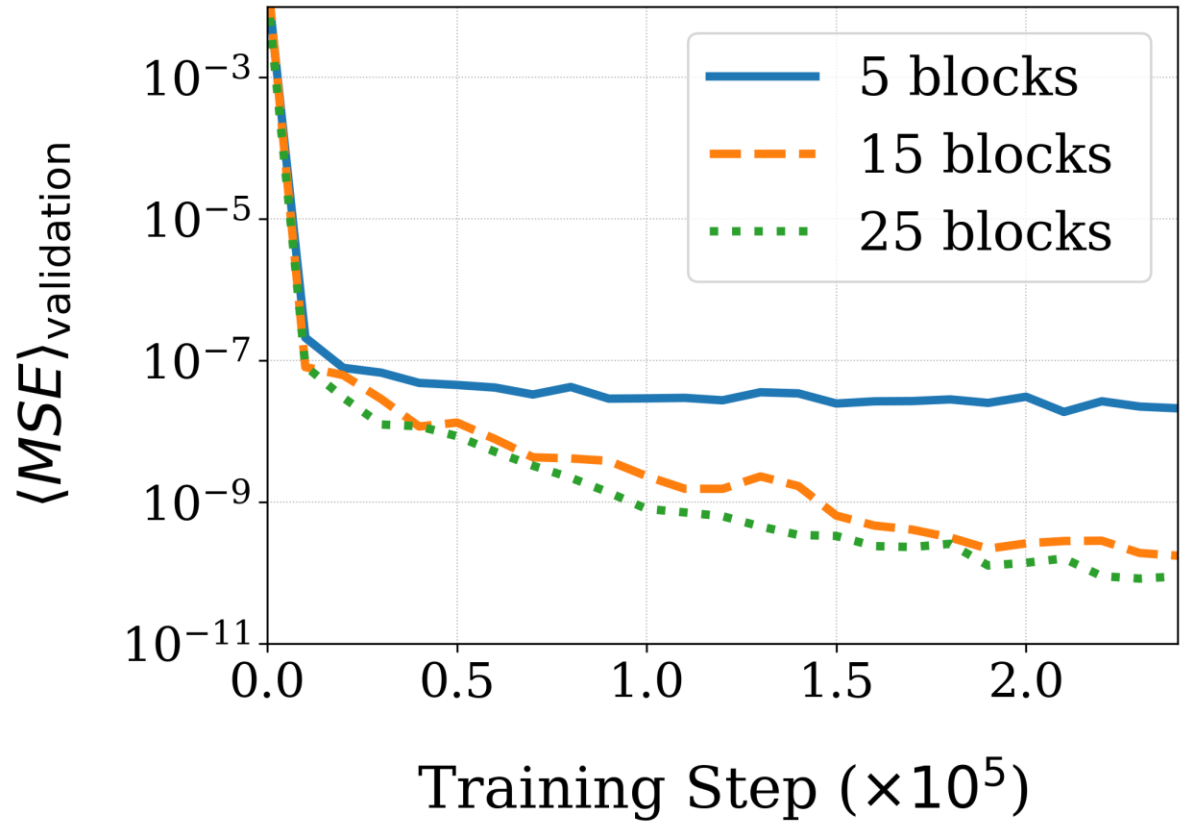
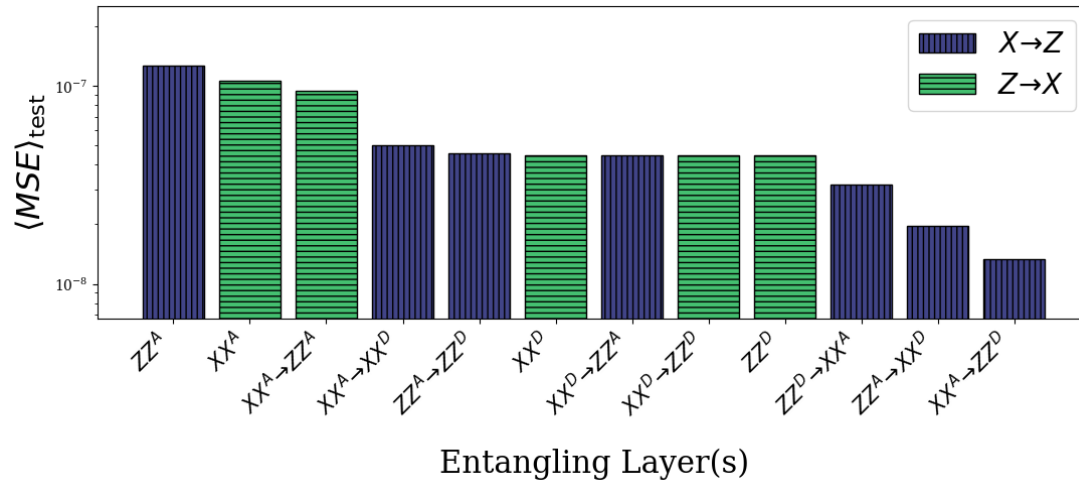
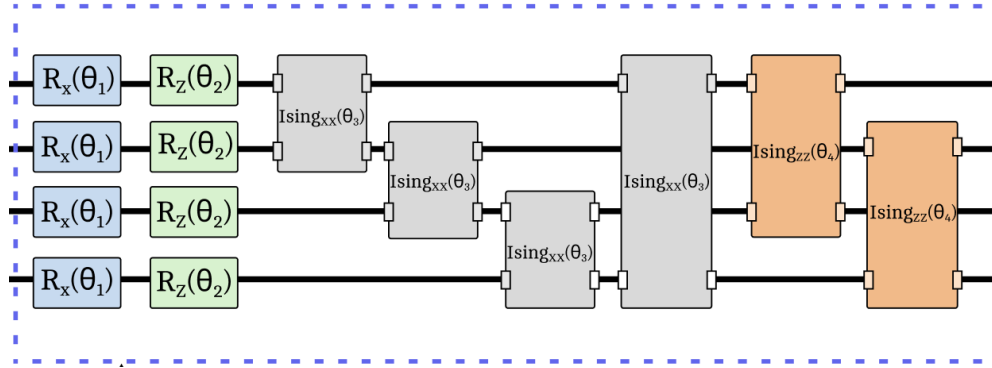
M. Lacatus, MM, Surrogate quantum circuit design for the lattice Boltzmann collision operator, IJNME 127(4):e70286, 2026

Training of the SQC



M. Lacatus, MM, [Surrogate quantum circuit design for the lattice Boltzmann collision operator](#), *IJNME* 127(4):e70286, 2026

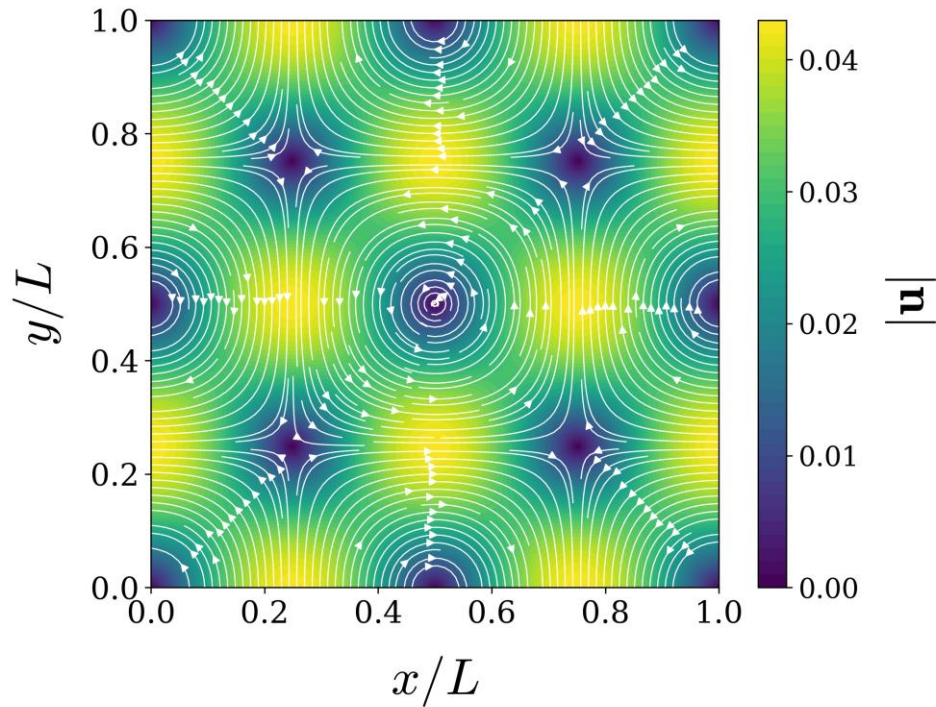
Training of the SQC



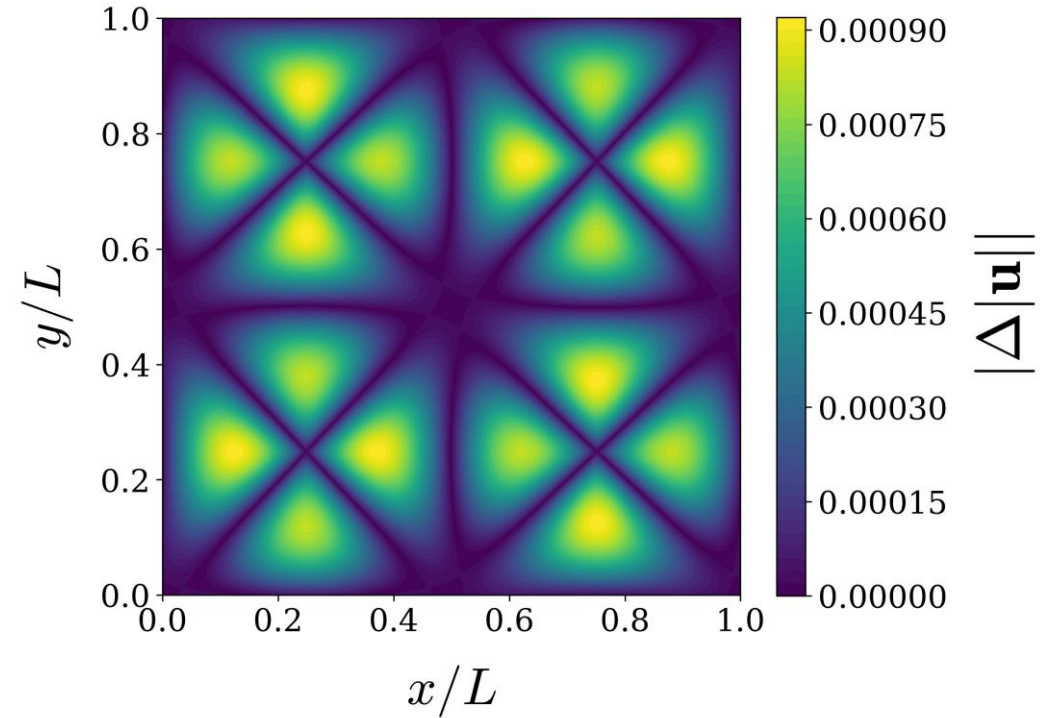
M. Lacatus, MM, [Surrogate quantum circuit design for the lattice Boltzmann collision operator](#), *IJNME* 127(4):e70286, 2026

Application of the SQC

Velocity magnitude



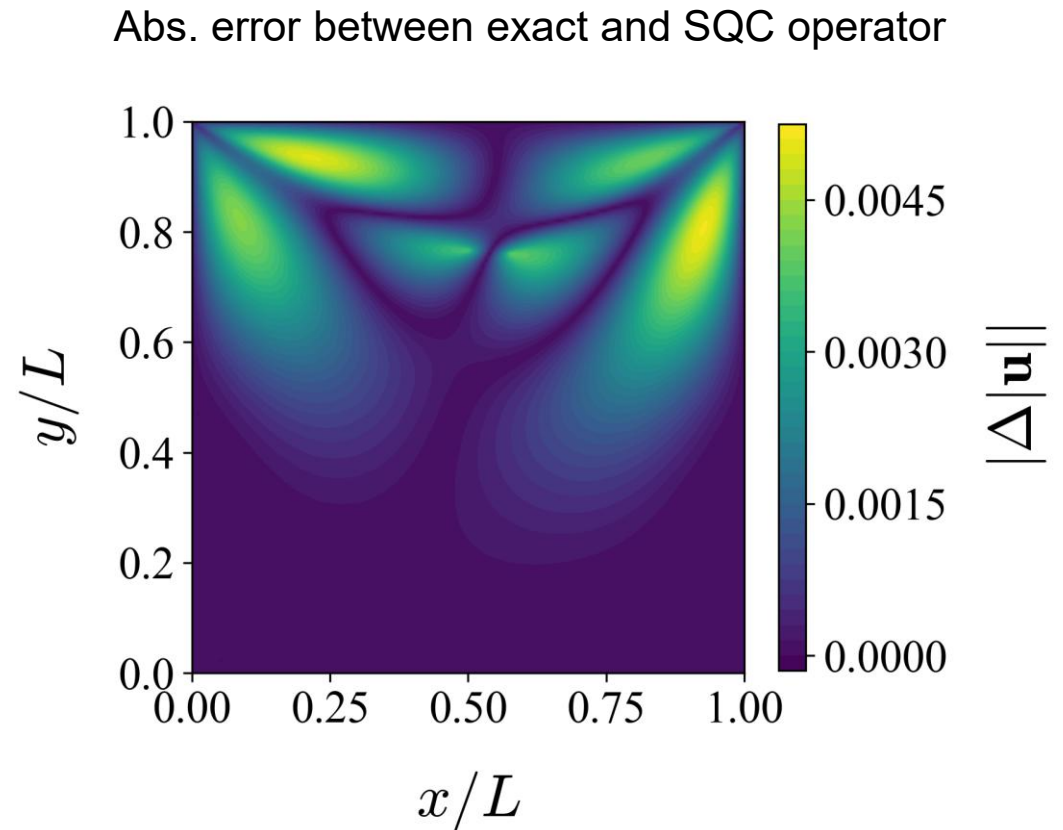
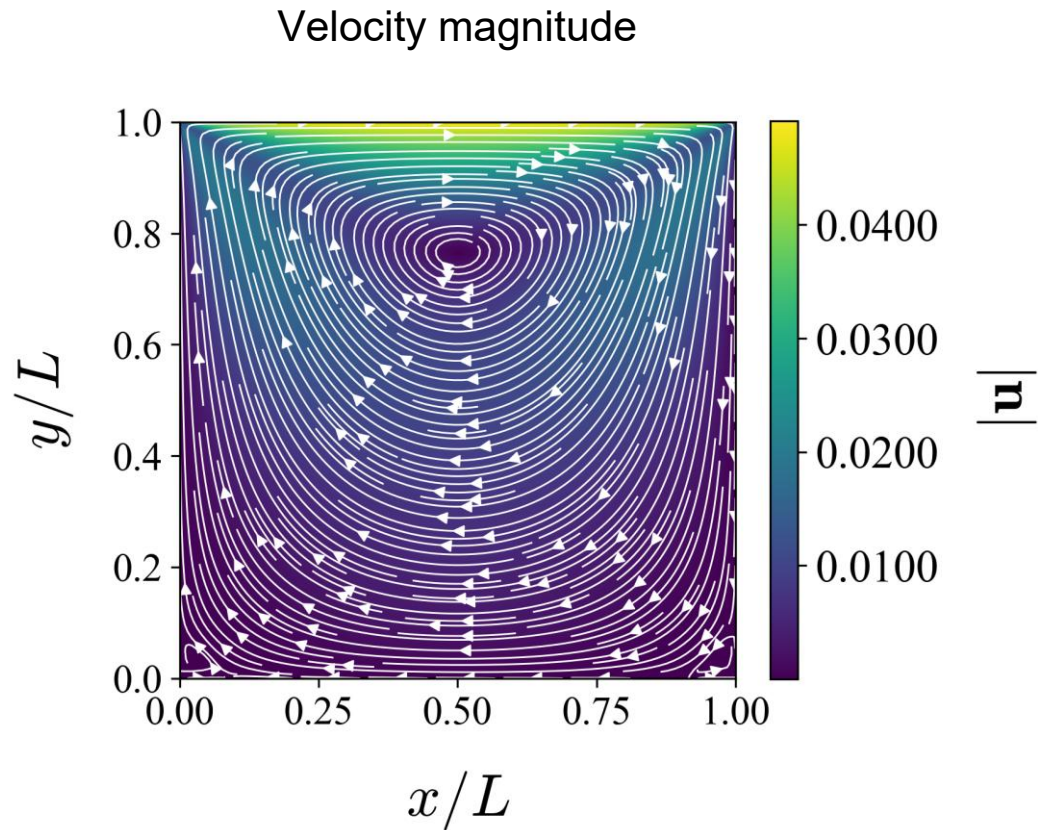
Abs. error between exact and SQC operator



Taylor-Green vortex decay: 64x64 grid, Re=50

M. Lacatus, MM, [Surrogate quantum circuit design for the lattice Boltzmann collision operator](#), *IJNME* 127(4):e70286, 2026

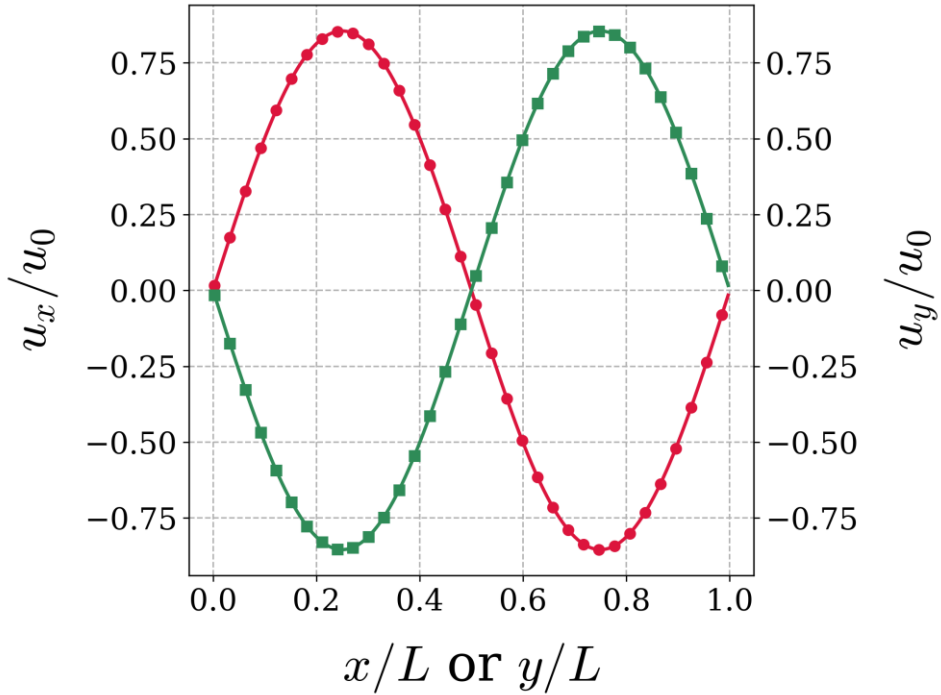
Application of the SQC



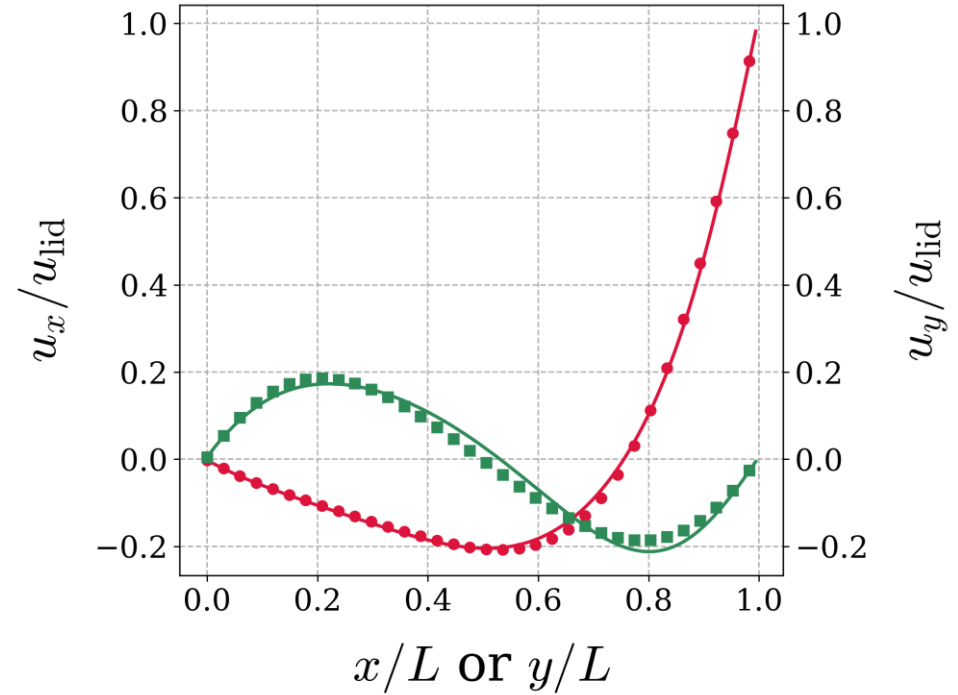
Lid-driven cavity: 64x64 grid, Re=50

M. Lacatus, MM, [Surrogate quantum circuit design for the lattice Boltzmann collision operator](#), *IJNME* 127(4):e70286, 2026

Application of the SQC



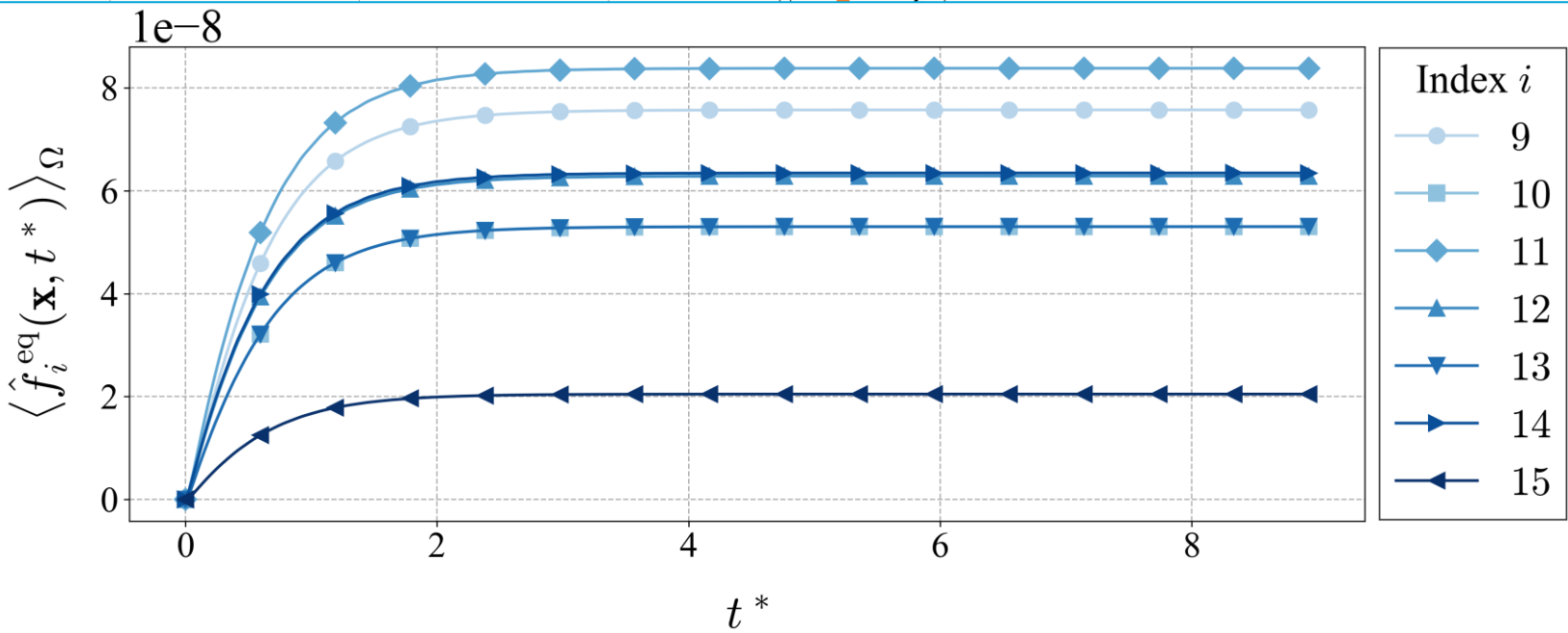
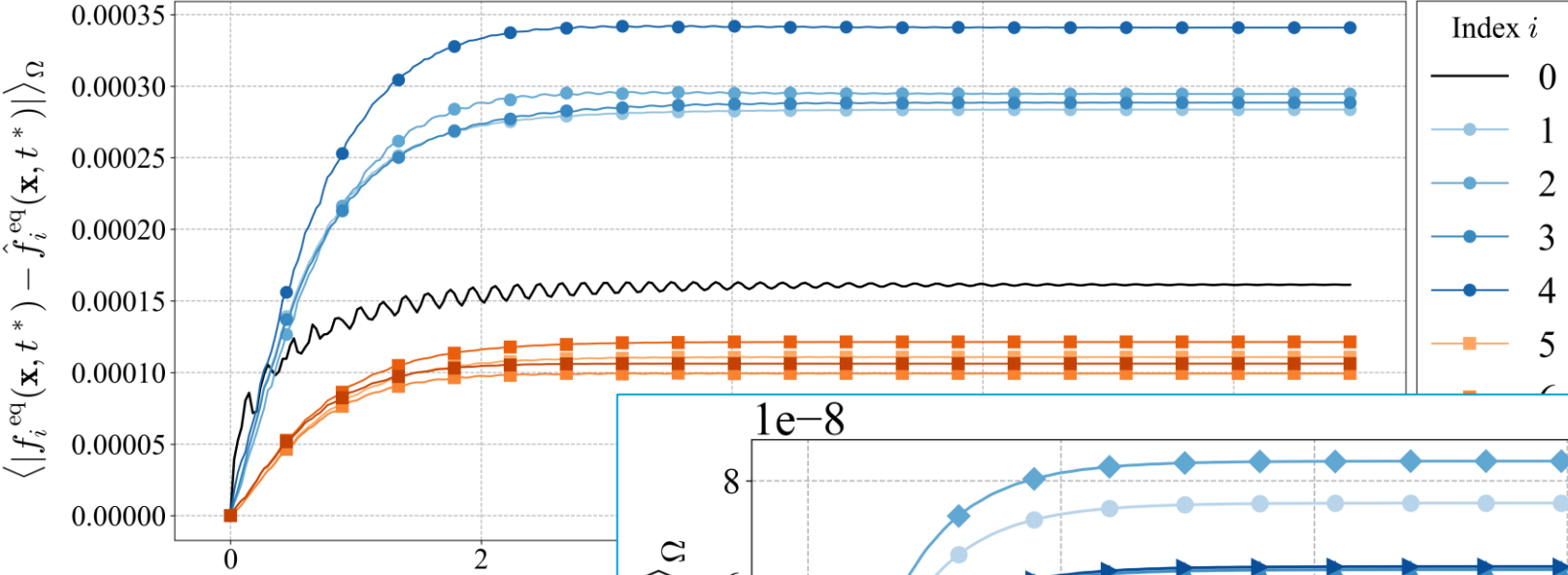
Taylor-Green vortex decay



Lid driven cavity

M. Lacatus, MM, [Surrogate quantum circuit design for the lattice Boltzmann collision operator](#), *IJNME* 127(4):e70286, 2026

Application of the SQC



Lid driven cavity: Time evolution

M. Lacatus, MM, Surrogate quant

Nonlinearity through measurement

- f_α^{eq} is **nonlinear** in \mathbf{u}

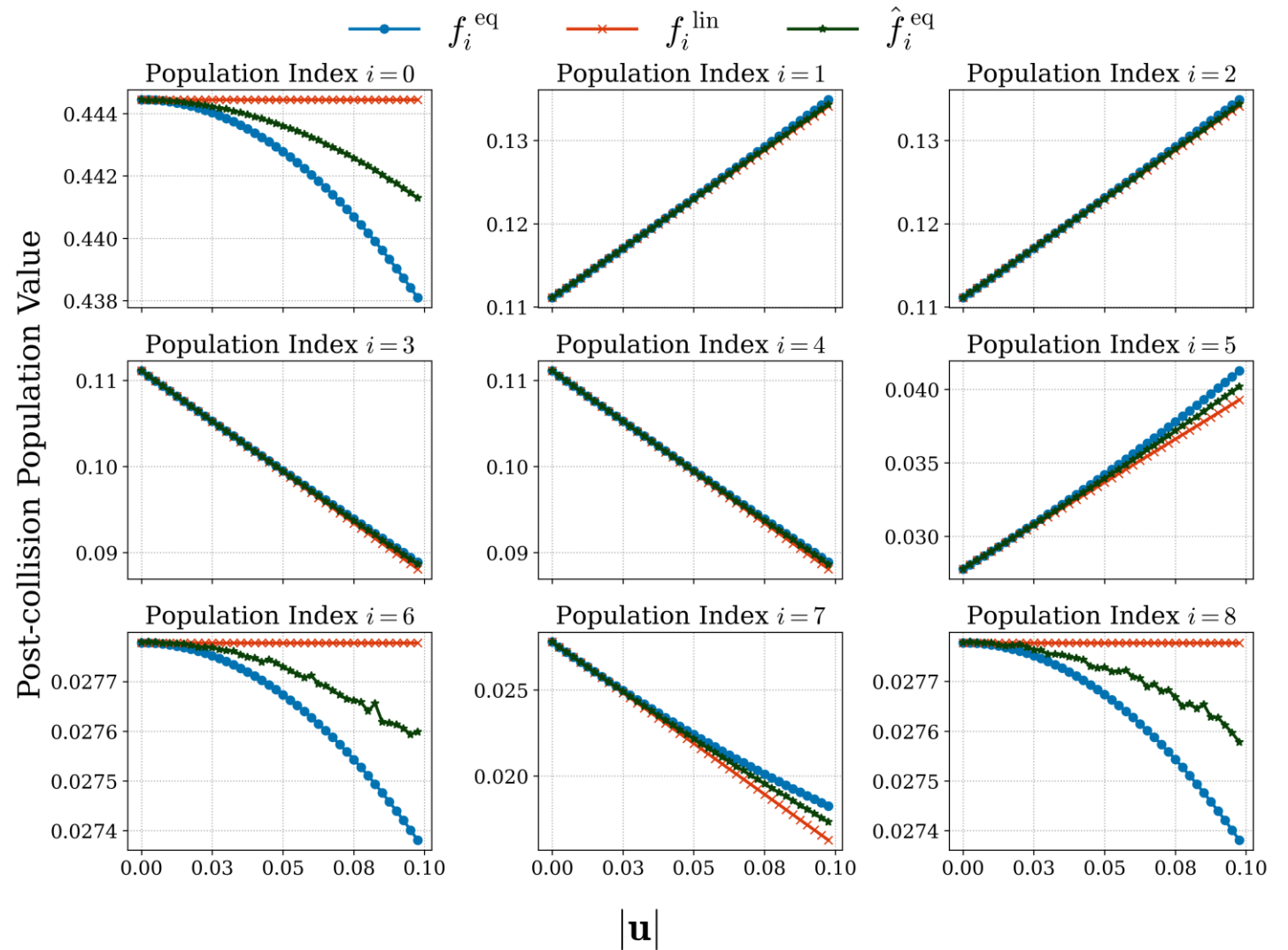
$$w_\alpha \varrho \left(1 + \frac{\mathbf{u} \cdot \mathbf{e}_\alpha}{c_s^2} + \frac{(\mathbf{u} \cdot \mathbf{e}_\alpha)^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^4} \right)$$

- f_α^{lin} is **linear** in \mathbf{u}

$$w_\alpha \varrho \left(1 + \frac{\mathbf{u} \cdot \mathbf{e}_\alpha}{c_s^2} \right)$$

- $\hat{f}_\alpha^{\text{eq}}$ is computed by a unitary

$$U(\Theta) \frac{1}{\sqrt{\rho}} \sum_\alpha \sqrt{f_\alpha} |\mathbf{e}_\alpha\rangle$$



M. Lacatus, MM, [Surrogate quantum circuit design for the lattice Boltzmann collision operator](#), *IJNME* 127(4):e70286, 2026

Nonlinearity through measurement

- f_α^{eq} is **nonlinear** in \mathbf{u}

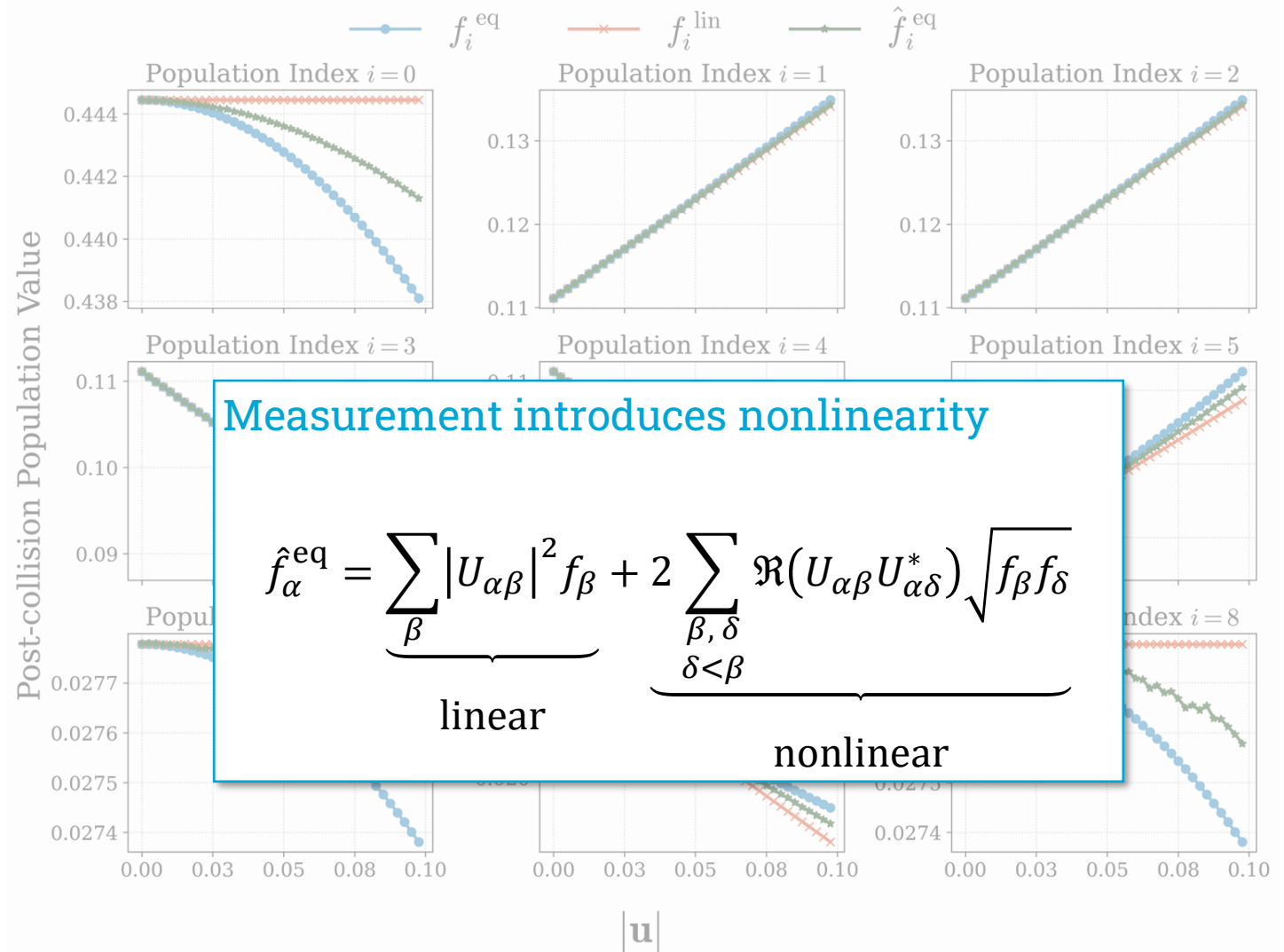
$$w_\alpha \varrho \left(1 + \frac{\mathbf{u} \cdot \mathbf{e}_\alpha}{c_s^2} + \frac{(\mathbf{u} \cdot \mathbf{e}_\alpha)^2}{2c_s^4} - \frac{\mathbf{u} \cdot \mathbf{u}}{2c_s^4} \right)$$

- f_α^{lin} is **linear** in \mathbf{u}

$$w_\alpha \varrho \left(1 + \frac{\mathbf{u} \cdot \mathbf{e}_\alpha}{c_s^2} \right)$$

- $\hat{f}_\alpha^{\text{eq}}$ is computed by a unitary

$$U(\Theta) \frac{1}{\sqrt{\rho}} \sum_\alpha \sqrt{f_\alpha} |\mathbf{e}_\alpha\rangle$$



M. Lacatus, MM, [Surrogate quantum circuit design for the lattice Boltzmann collision operator](#), *IJNME* 127(4):e70286, 2026

Running on NISQ hardware



QPU	IQM Crystal 20	IQM Crystal 54
Qubit count	20	54
1Q fidelity	99.92%	99.93%
2Q fidelity	99.51%	99.5%
Q-volume	32	64
CLOPS	2600	2550
Q-score	15	24

Sim



initialization

IQM20



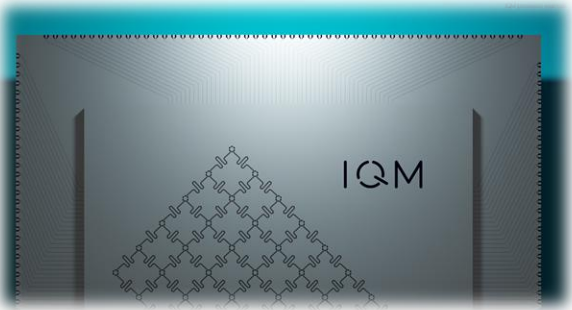
R: 1, CZ: 0, shots: 100.000, trials: 6

IQM54



R: 1, CZ: 0, shots: 100.000, trials: 6

Running on NISQ hardware



QPU	IQM Crystal 20	IQM Crystal 54
Qubit count	20	54
1Q fidelity	99.92%	99.93%
2Q fidelity	99.51%	99.5%
Q-volume	32	64
CLOPS	2600	2550
Q-score	15	24

Sim



1 timestep

IQM20



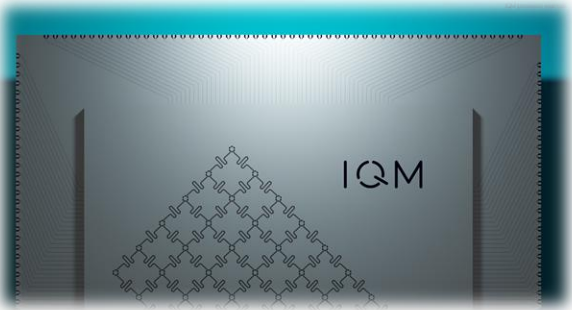
→ R: 227, CZ: 87

IQM54



→ R: 228, CZ: 85

Running on NISQ hardware



QPU	IQM Crystal 20	IQM Crystal 54
Qubit count	20	54
1Q fidelity	99.92%	99.93%
2Q fidelity	99.51%	99.5%
Q-volume	32	64
CLOPS	2600	2550
Q-score	15	24

Sim



2 timesteps

IQM20



R: 444, CZ: 176

IQM54



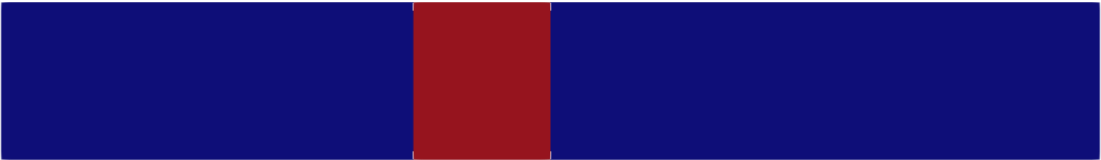
R: 441, CZ: 179

Running on NISQ hardware



QPU	IQM Crystal 20	IQM Crystal 54
Qubit count	20	54
1Q fidelity	99.92%	99.93%
2Q fidelity	99.51%	99.5%
Q-volume	32	64
CLOPS	2600	2550
Q-score	15	24

Sim



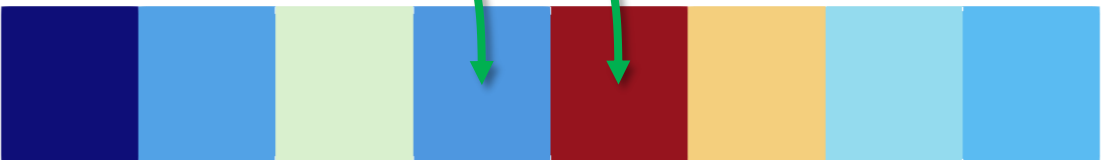
3 timesteps

IQM20



R: 655, CZ: 270
011 100

IQM54



R: 647, CZ: 260

Running on NISQ hardware



QPU	IQM Crystal 20	IQM Crystal 54
Qubit count	20	54
1Q fidelity	99.92%	99.93%
2Q fidelity	99.51%	99.5%
Q-volume	32	64
CLOPS	2600	2550
Q-score	15	24

Sim



5 timesteps

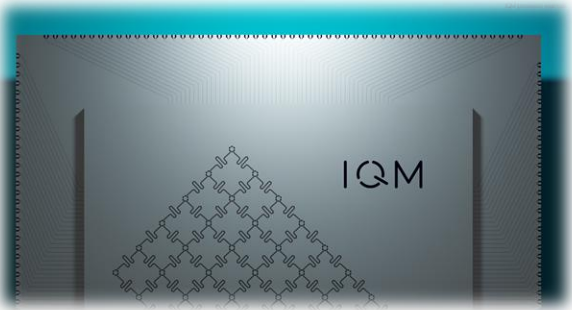
IQM20



IQM54

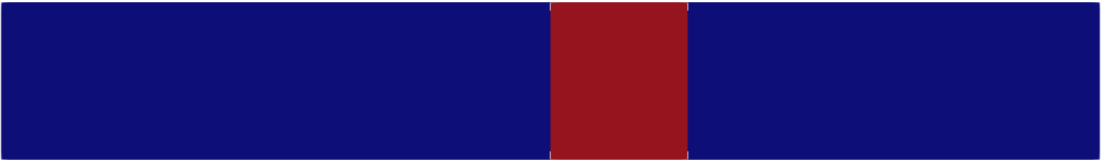


Running on NISQ hardware



QPU	IQM Crystal 20	IQM Crystal 54
Qubit count	20	54
1Q fidelity	99.92%	99.93%
2Q fidelity	99.51%	99.5%
Q-volume	32	64
CLOPS	2600	2550
Q-score	15	24

Sim



4 timesteps

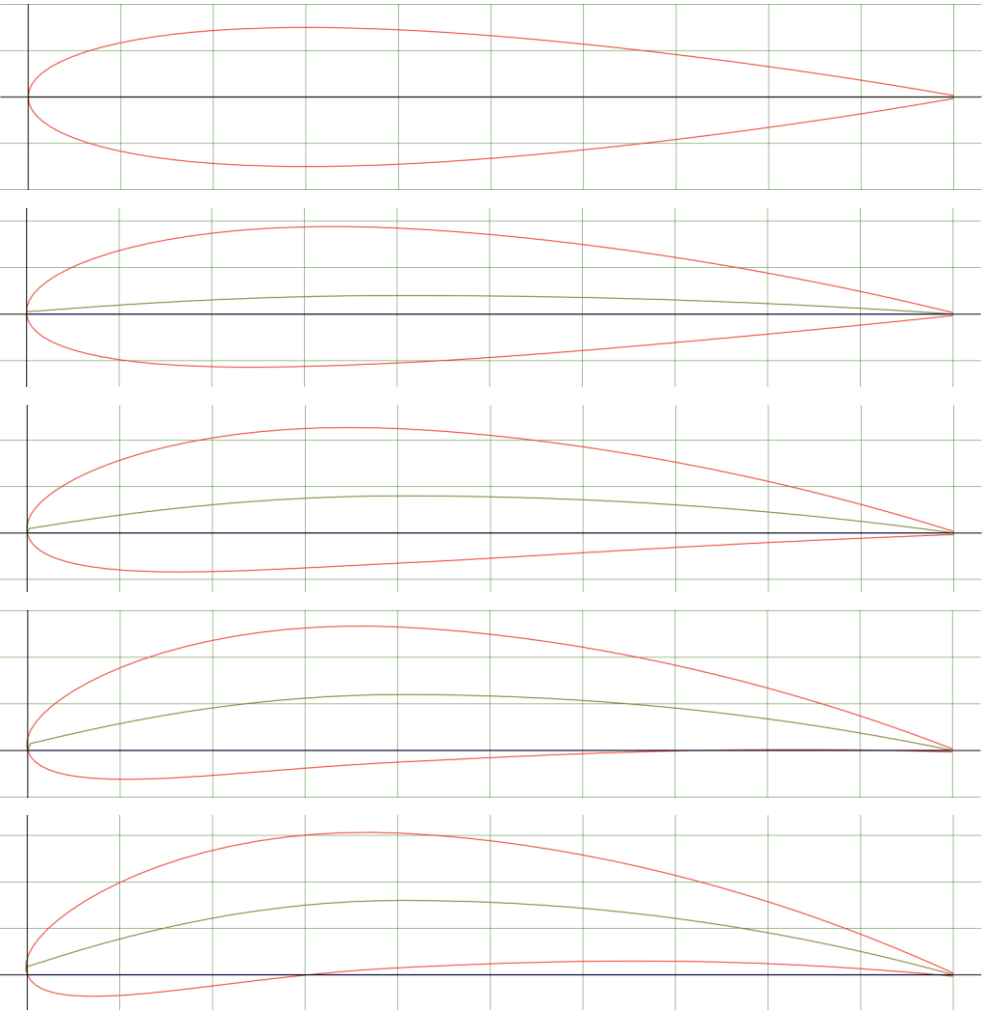
IQM20



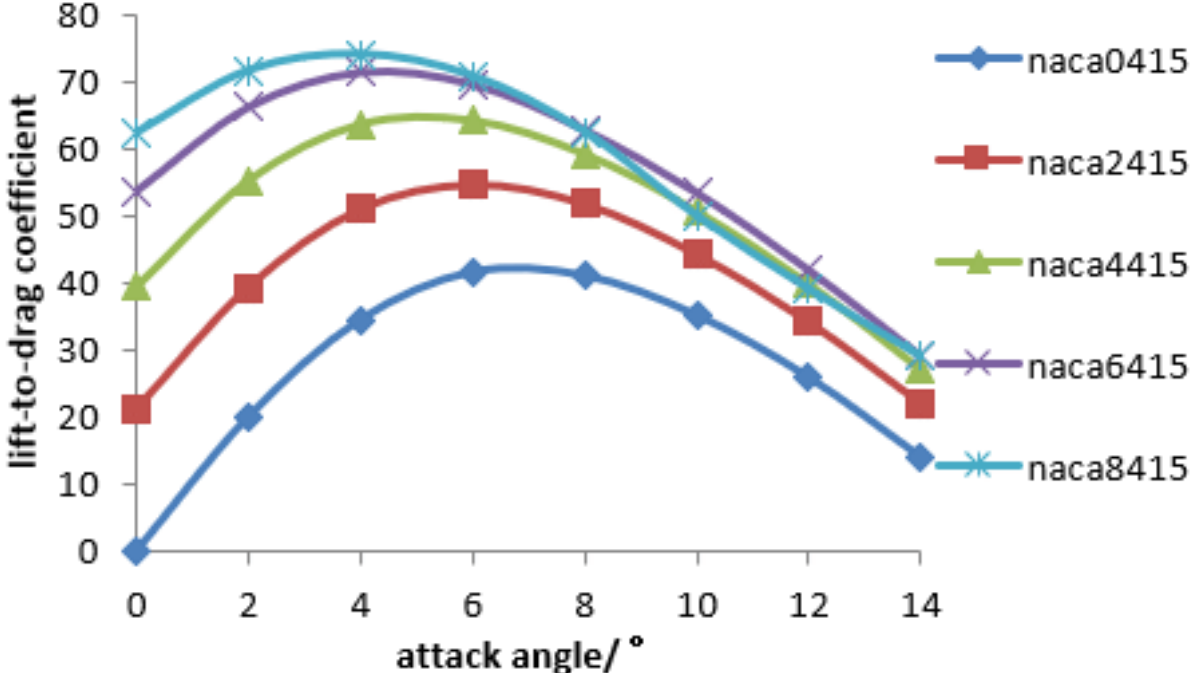
IQM54



Quantum-enhanced design optimization



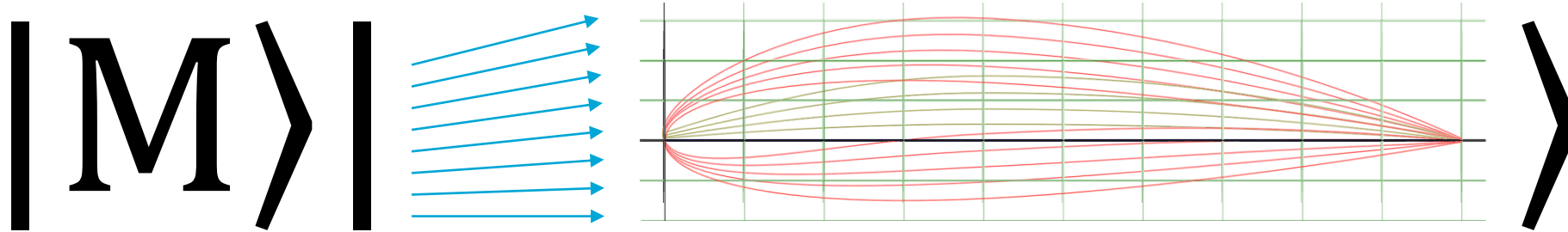
Generated with airfoiltools.com



[DOI: 10.1088/1742-6596/1519/1/012020](https://doi.org/10.1088/1742-6596/1519/1/012020)

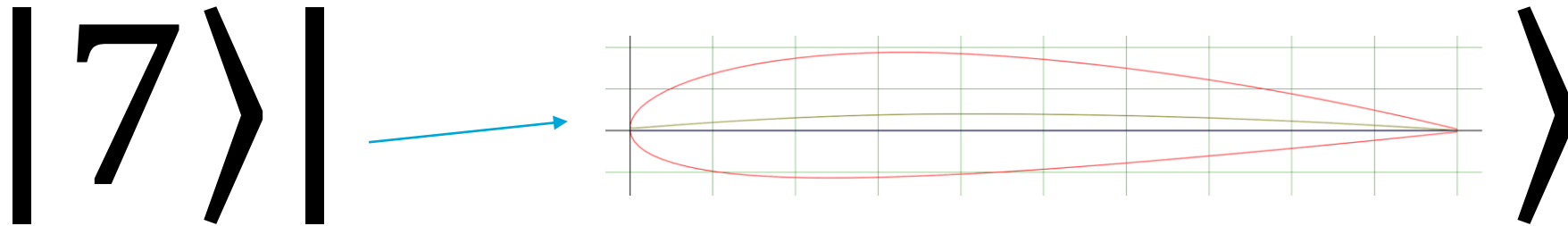
Exploit **quadratic speedup of quantum search algorithms** in design optimization

Quantum-enhanced design optimization



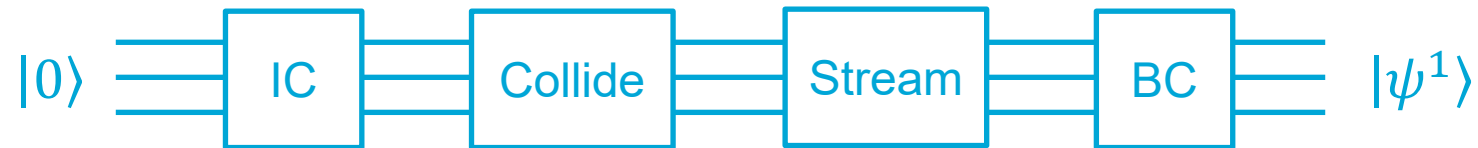
C. Georgescu, MM, [Quantum Search in Superposed Quantum Lattice Gas Automata and Lattice Boltzmann Systems](#), *arXiv: 2510.14062*

Quantum-enhanced design optimization



C. Georgescu, MM, [Quantum Search in Superposed Quantum Lattice Gas Automata and Lattice Boltzmann Systems](#), *arXiv: 2510.14062*

Quantum-enhanced design optimization

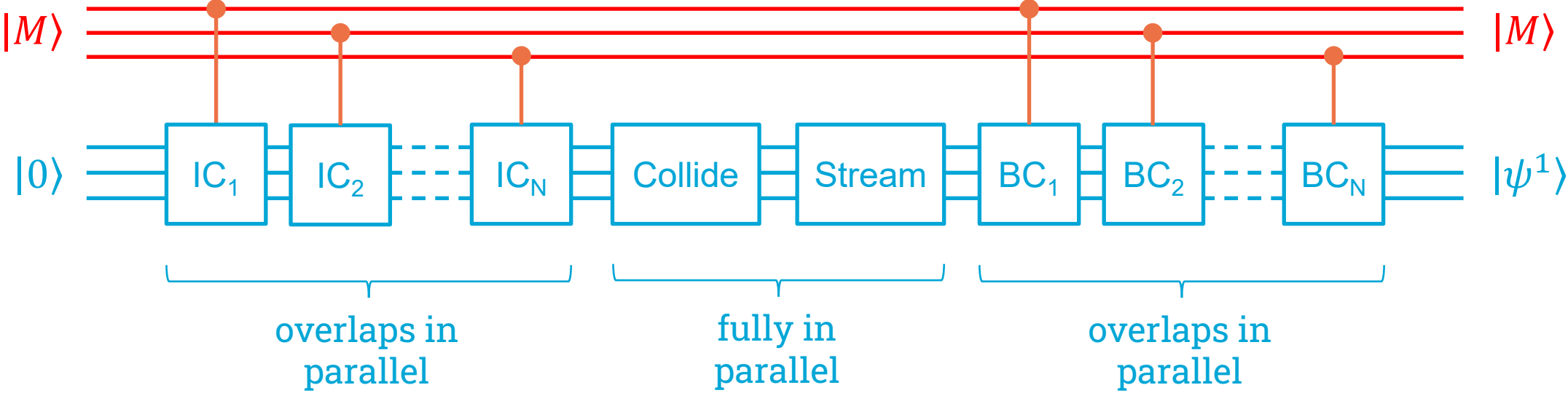


C. Georgescu, MM, Quantum Search in Superposed Quantum Lattice Gas Automata and Lattice Boltzmann Systems, *arXiv: 2510.14062*

Quantum-enhanced design optimization

Dürr-Høyer minimum-finding algorithm

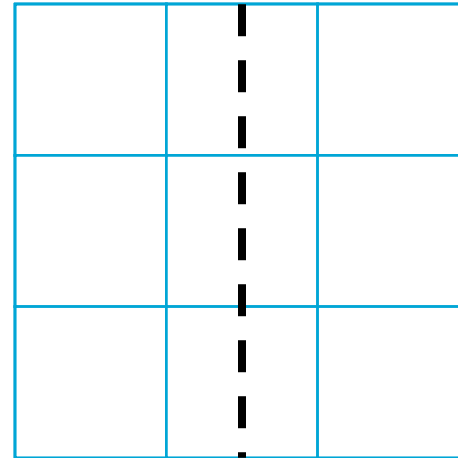
Finds optimal configuration with \sqrt{N} queries (N queries classically) → **quadratic speedup**



C. Georgescu, MM, Quantum Search in Superposed Quantum Lattice Gas Automata and Lattice Boltzmann Systems, arXiv: 2510.14062

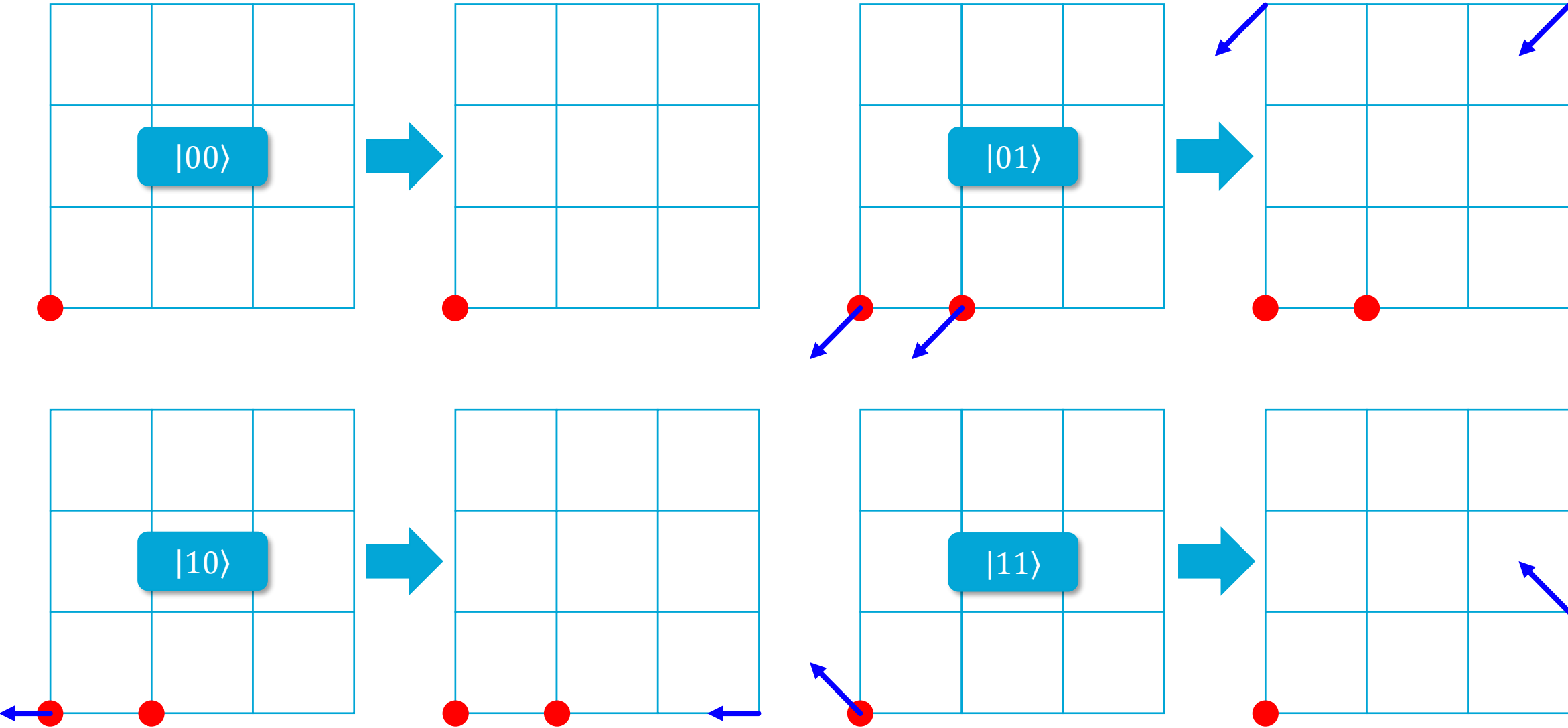
End-to-end implementation

Goal: Find the initial configuration for which the relative density in the right half-plane is largest

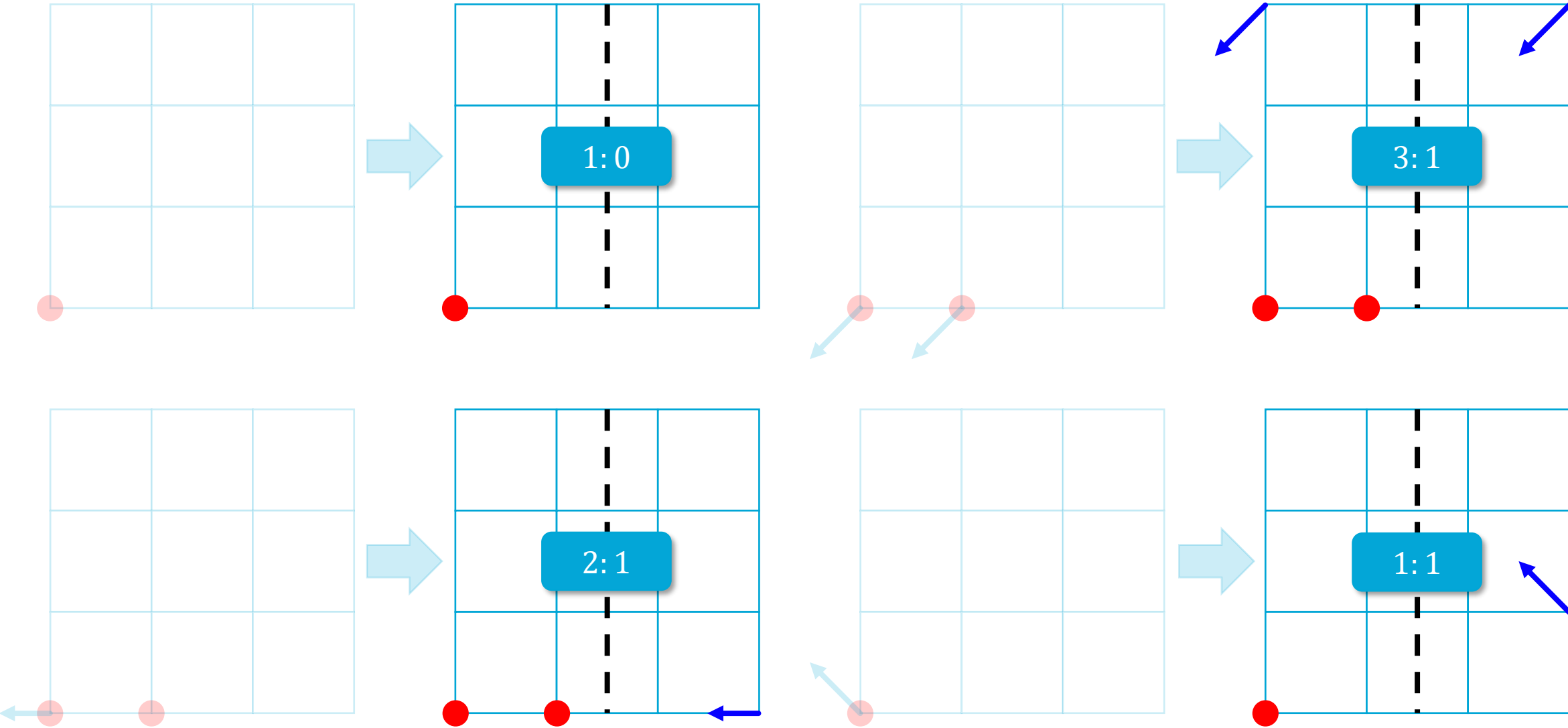


$$x > 0.5$$

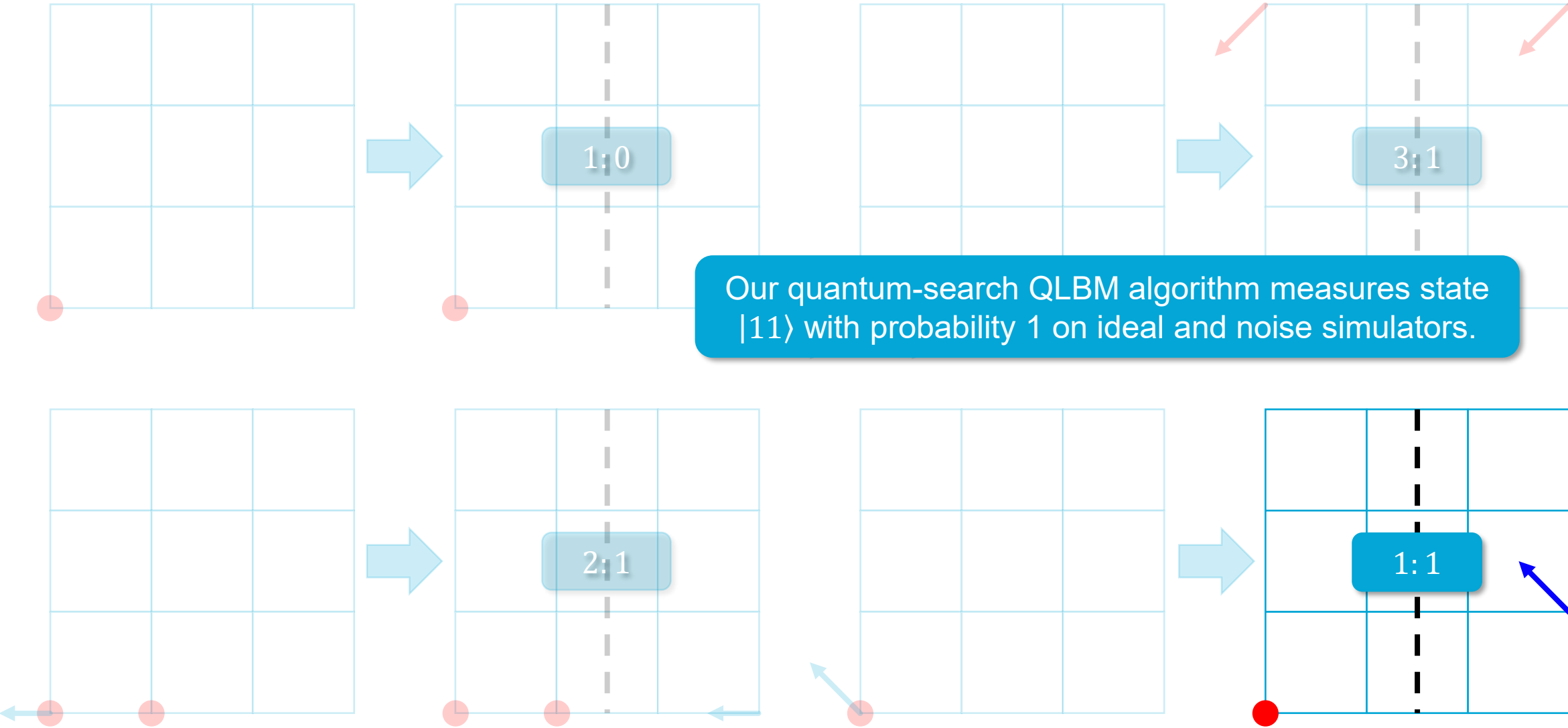
End-to-end implementation



End-to-end implementation



End-to-end implementation



Take-home lessons, continued

If quantum computing shall become the future of HPCSE we need to ...

- ... identify **applications** that cannot be solved efficiently with classical computers
- ... develop **algorithms** that exploit the strengths of quantum computers (and avoid their limitations)
- ... (most probably) change the **workflows** that were designed for classical computers



Application: large-scale direct numerical simulation of fluid dynamics

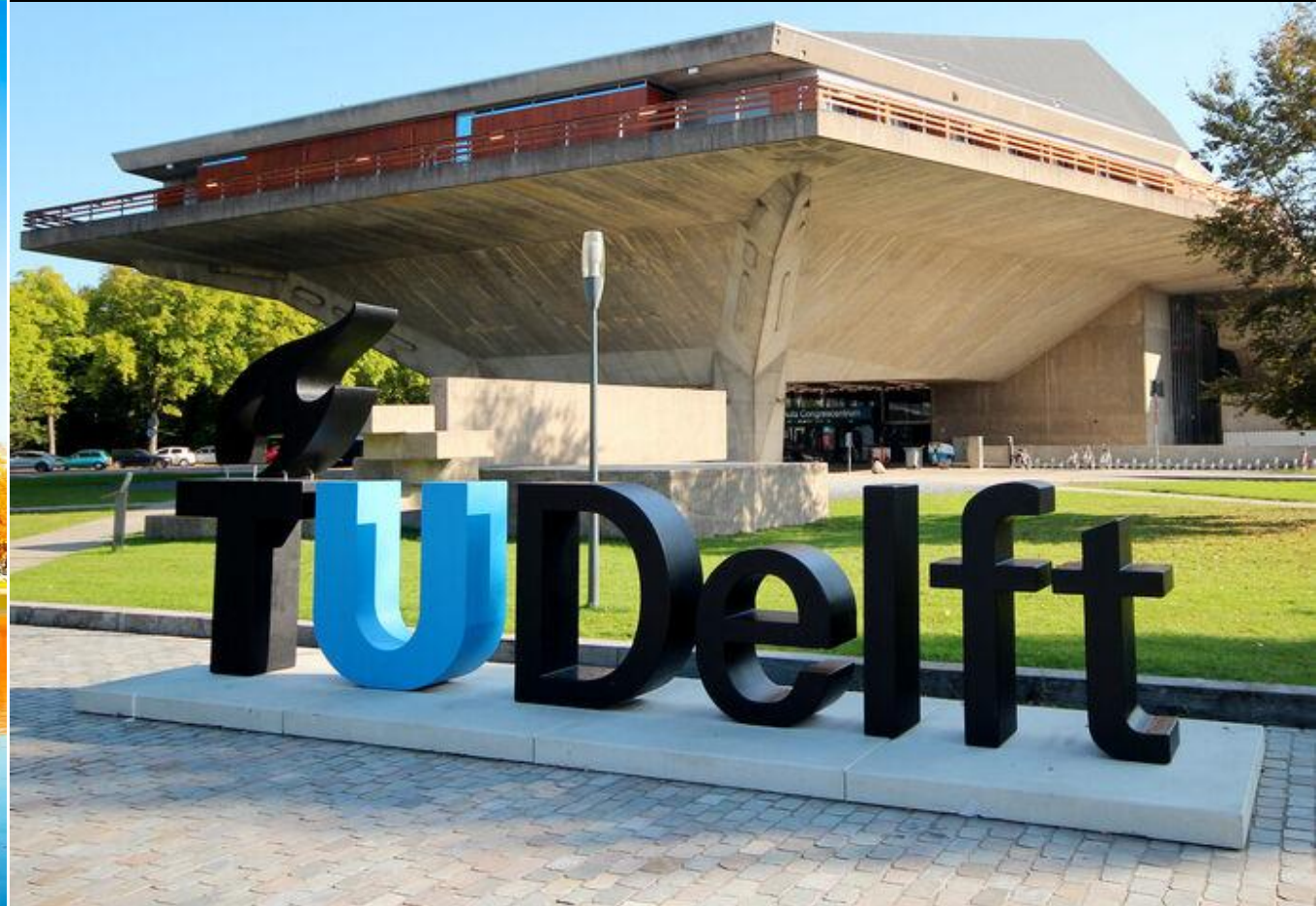
Algorithm: quantum lattice Boltzmann method

Workflow: quantum-accelerated design optimization workflow

Is this enough to make quantum the future of HPCSE? We will see ...

Applied Quantum Methods in Computational Science and Engineering

September 14-17, 2026 Delft, NL



Applied Quantum Methods in Computational Science and Engineering

September 14-17, 2026 Delft, NL



We have open positions,
please contact me

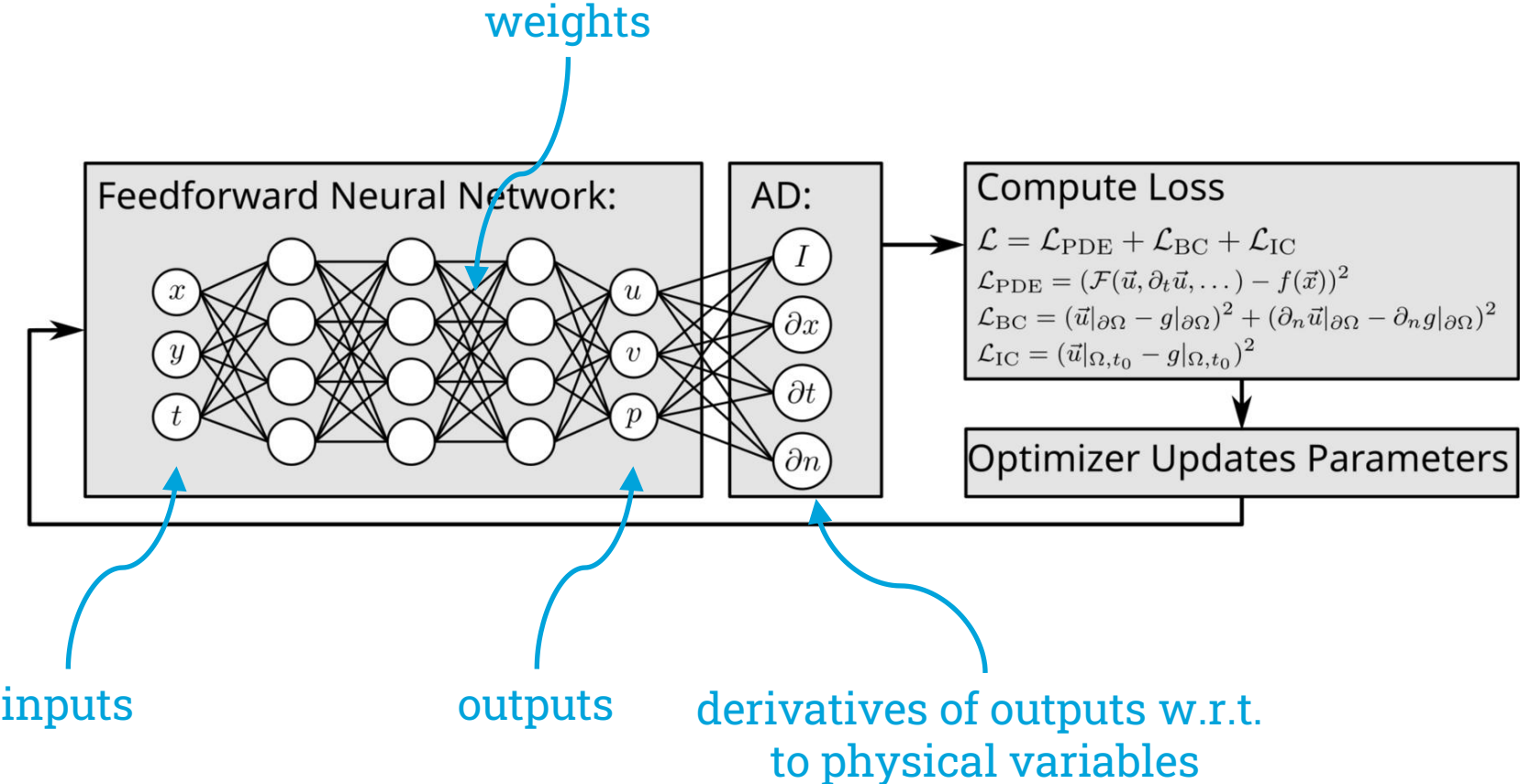
M.Moller@tudelft.nl

Acknowledgement

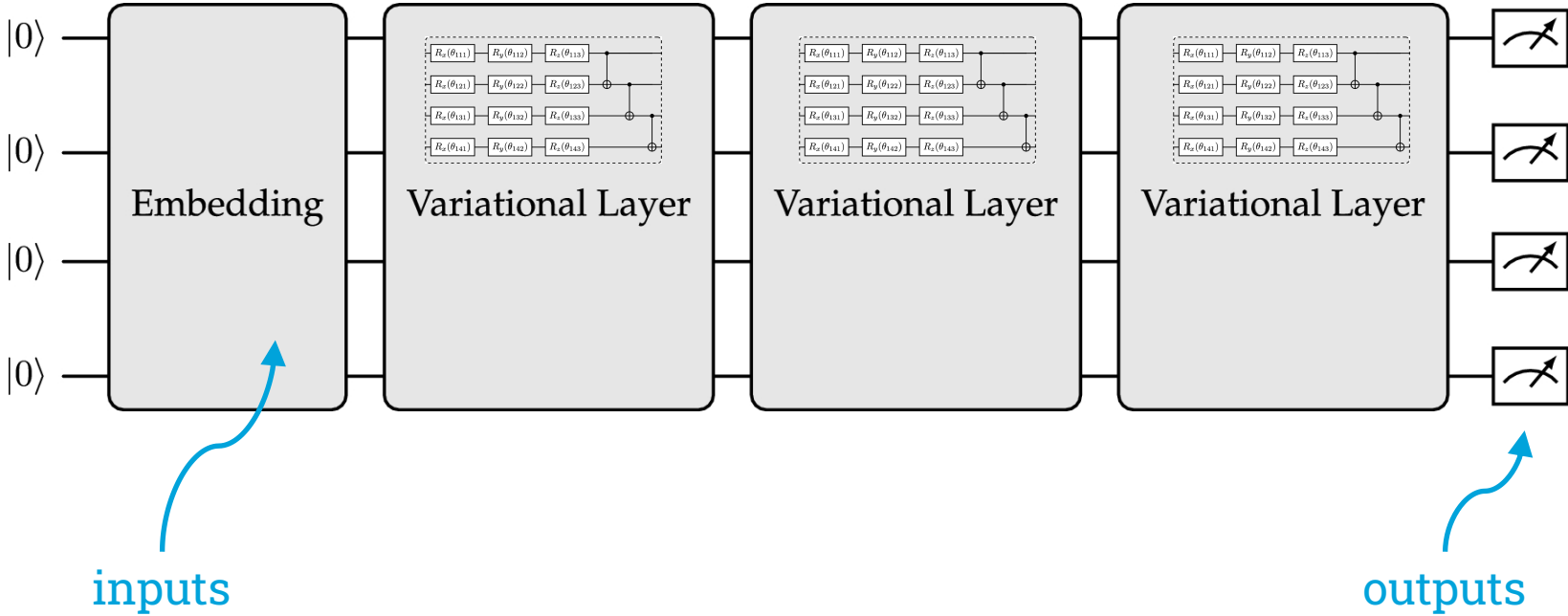
C. Georgescu, M. Lacatus,
M. Schalkers, N. Hosters,
S. Berger, E. Duong, ...

Fujitsu Limited, RVO NL

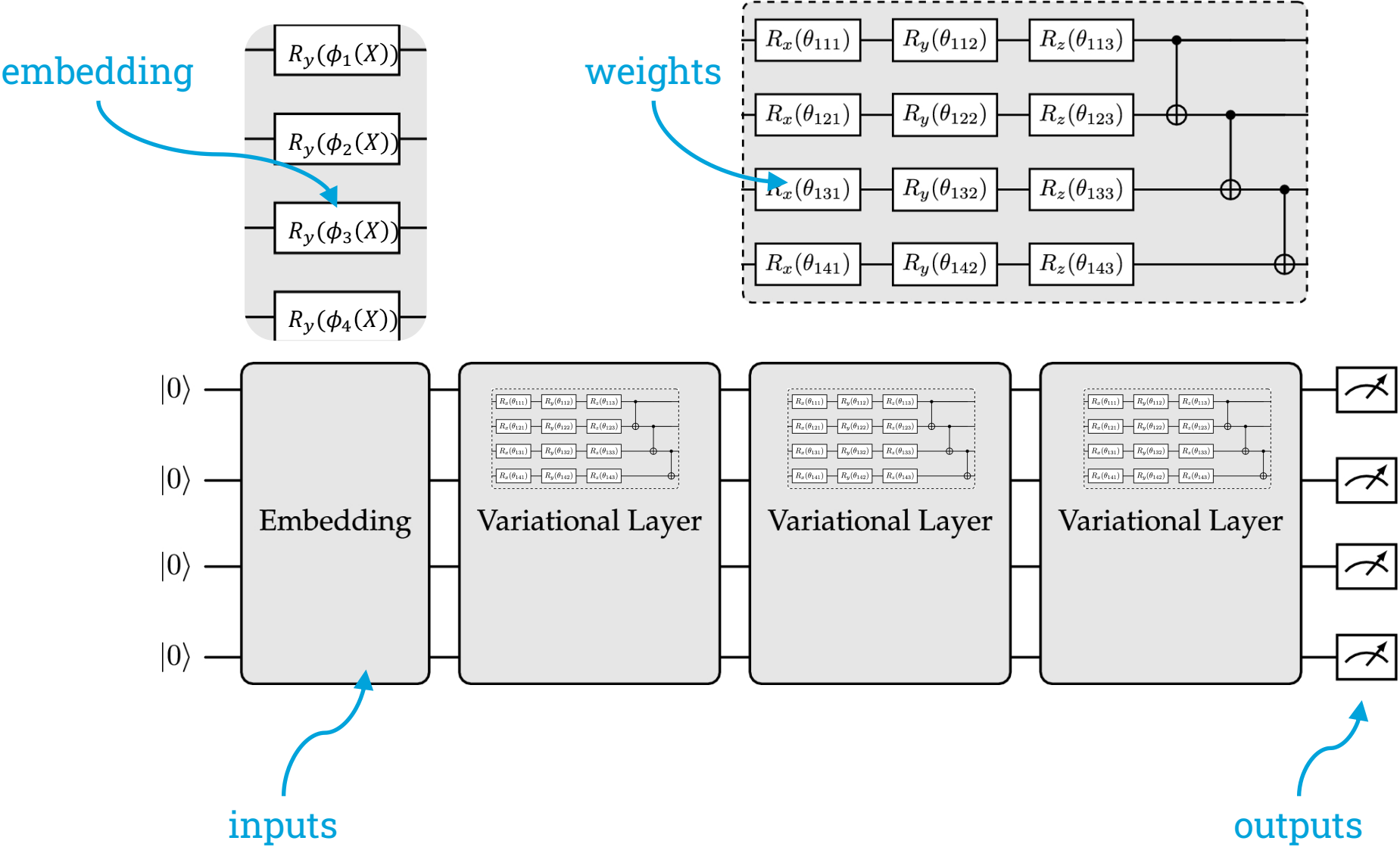
Physics-informed neural networks (PINNs)



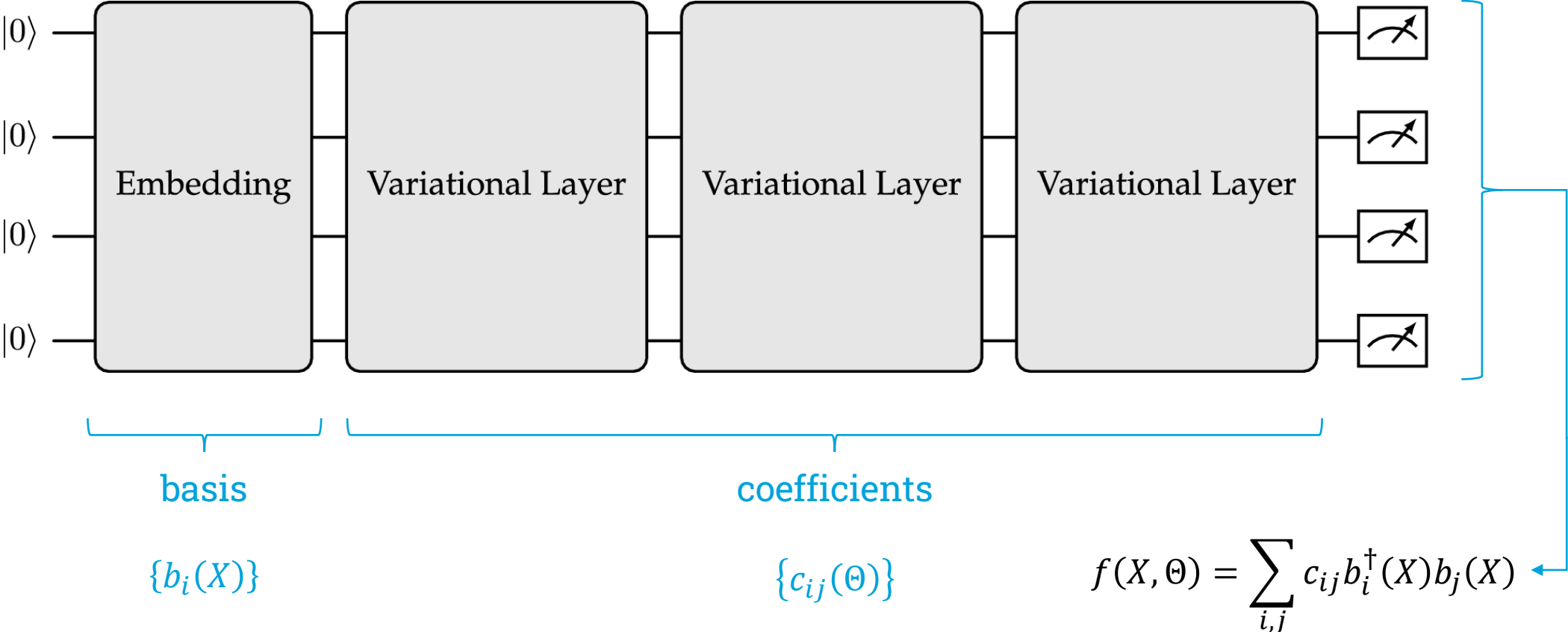
Quantum physics-informed neural networks (QPINNs)



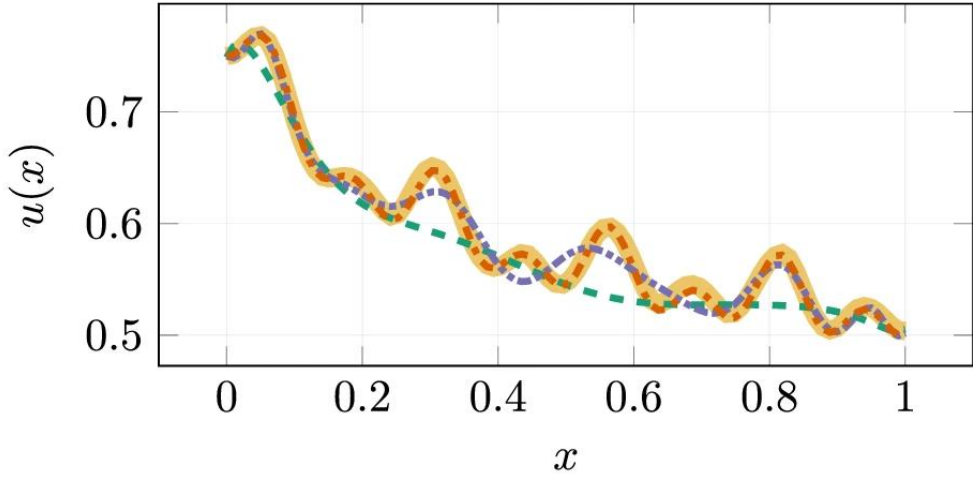
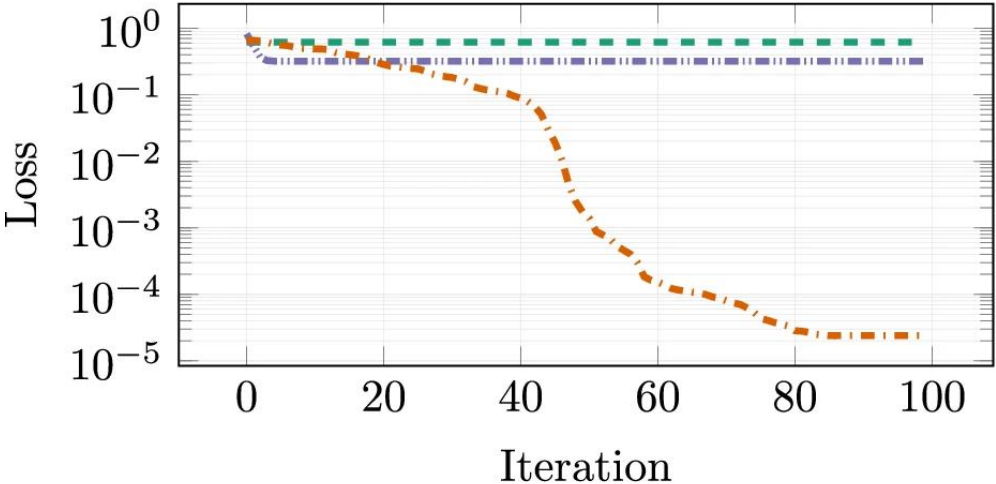
Quantum physics-informed neural networks (QPINNs)



Quantum physics-informed neural networks (QPINNs)



Our approach: Trainable embedding (TE-QPINNs)



█ Reference
 - - - Chebyshev
 ⋯ Tower-Chebyshev
 - · - · TE-QPINN

$\phi_i(X) = 2 \arccos(X_i)$

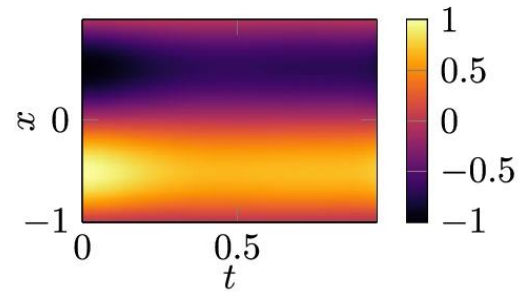
$\phi_i(X) = 2i \arccos(X_i)$

$\phi_i(X) = \text{FNN}_i(X) \tilde{X}_i$

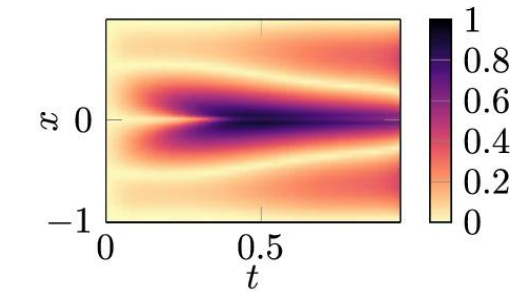
S. Berger et al., Trainable embedding quantum physics informed neural networks for solving nonlinear PDEs, *Sci. Rep.* 15 (2025)

TE-QPINNs applied to Burger's equation

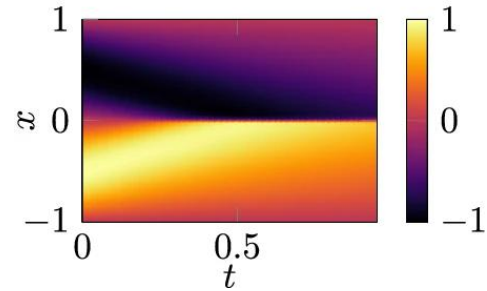
Tower Chebyshev 4 Qubits



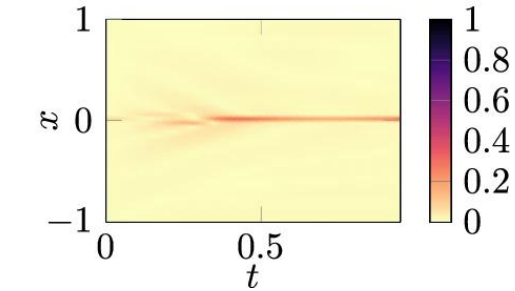
$|u(t, x)_{\text{ref.}} - u_{\text{Tower Cheb.}}(t, x)|$



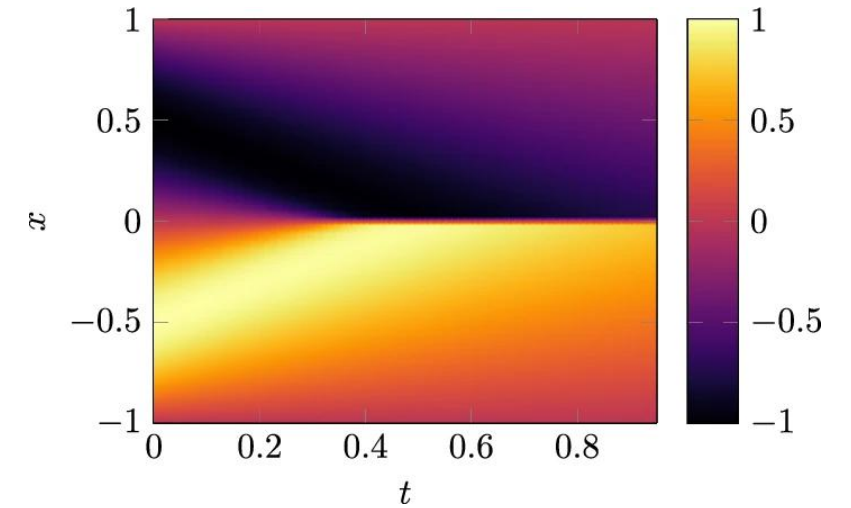
TE-QPINN 4 Qubits



$|u(t, x)_{\text{ref.}} - u_{\text{TE-QPINN}}(t, x)|$

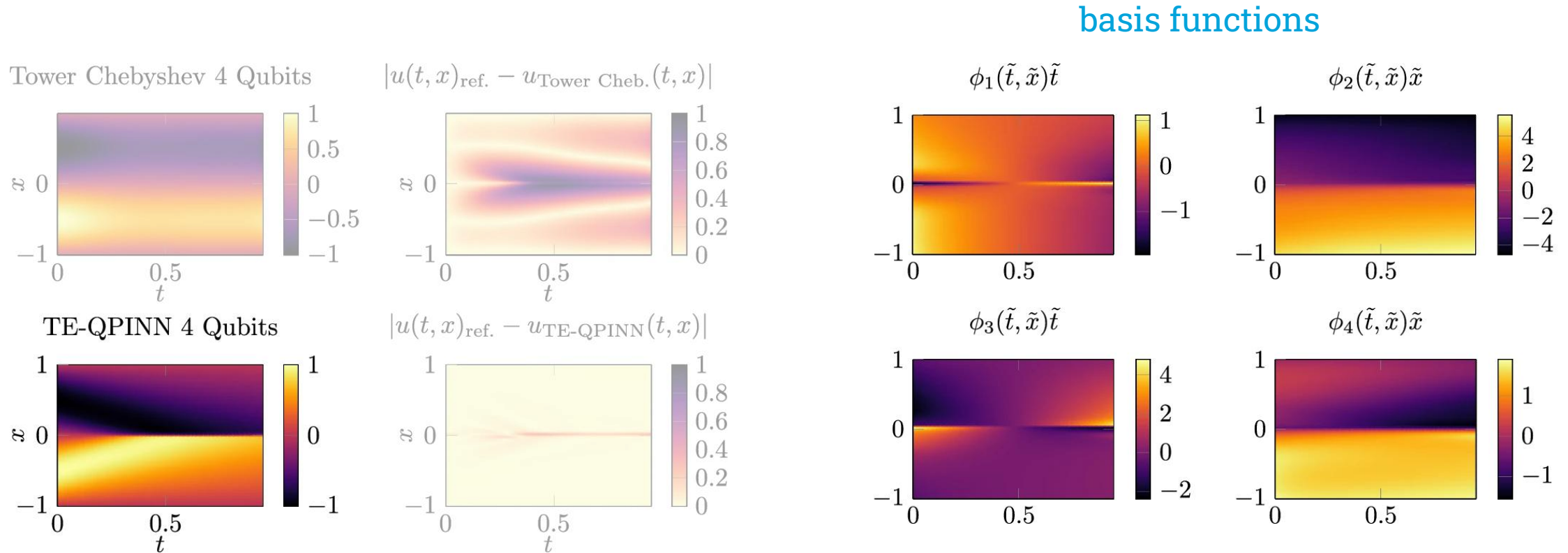


exact solution



S. Berger et al., Trainable embedding quantum physics informed neural networks for solving nonlinear PDEs, *Sci. Rep.* 15 (2025)

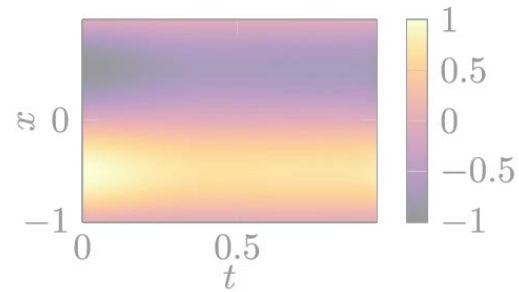
TE-QPINNs applied to Burger's equation



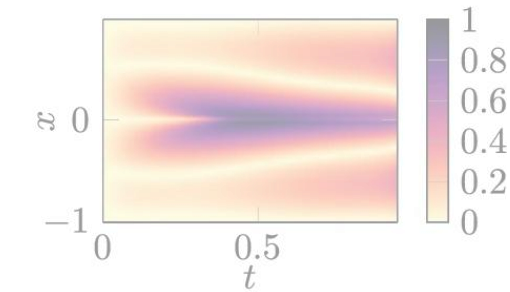
S. Berger et al., Trainable embedding quantum physics informed neural networks for solving nonlinear PDEs, *Sci. Rep.* 15 (2025)

TE-QPINNs applied to Burger's equation

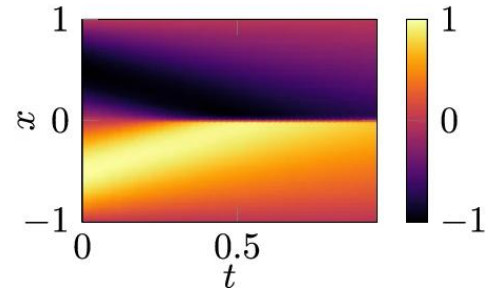
Tower Chebyshev 4 Qubits



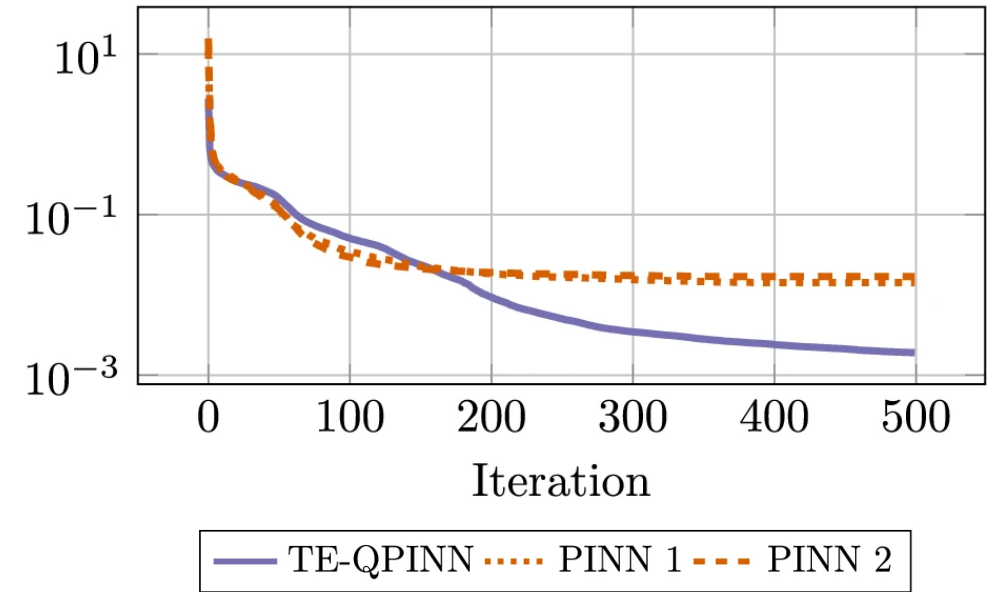
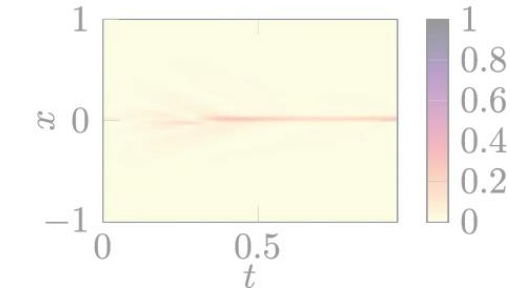
$|u(t, x)_{\text{ref.}} - u_{\text{Tower Cheb.}}(t, x)|$



TE-QPINN 4 Qubits

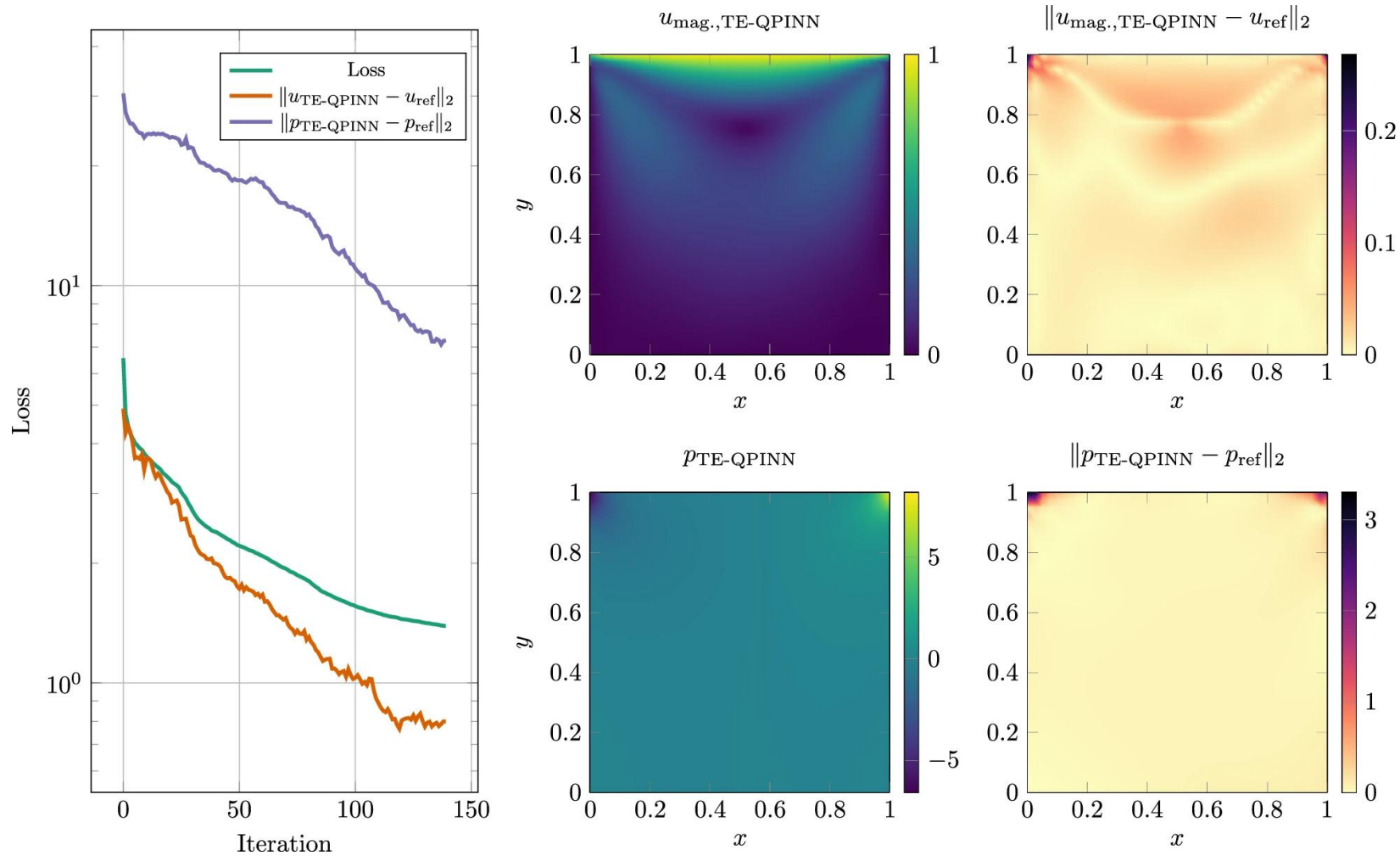


$|u(t, x)_{\text{ref.}} - u_{\text{TE-QPINN}}(t, x)|$



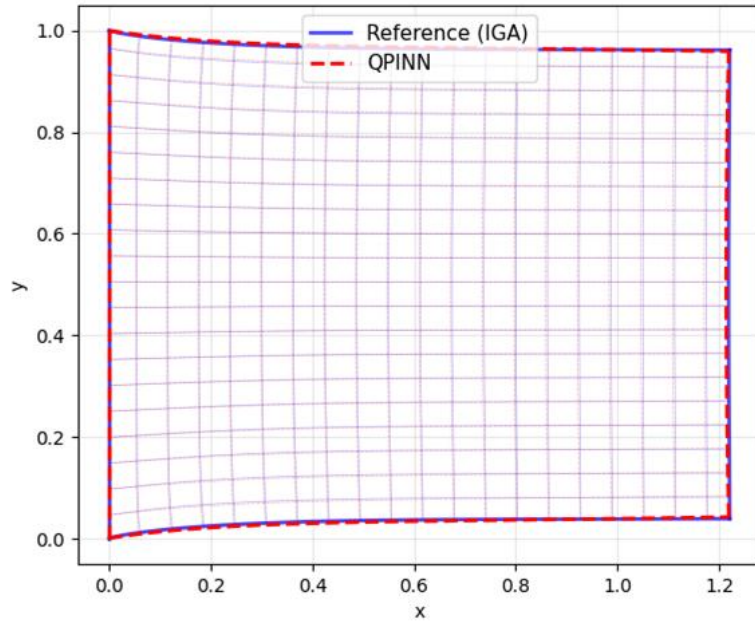
S. Berger et al., Trainable embedding quantum physics informed neural networks for solving nonlinear PDEs, *Sci. Rep.* 15 (2025)

TE-QPINNs applied to incompressible NSE

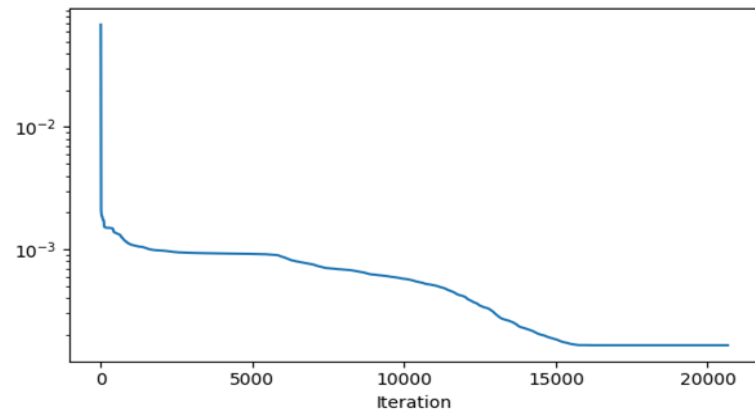
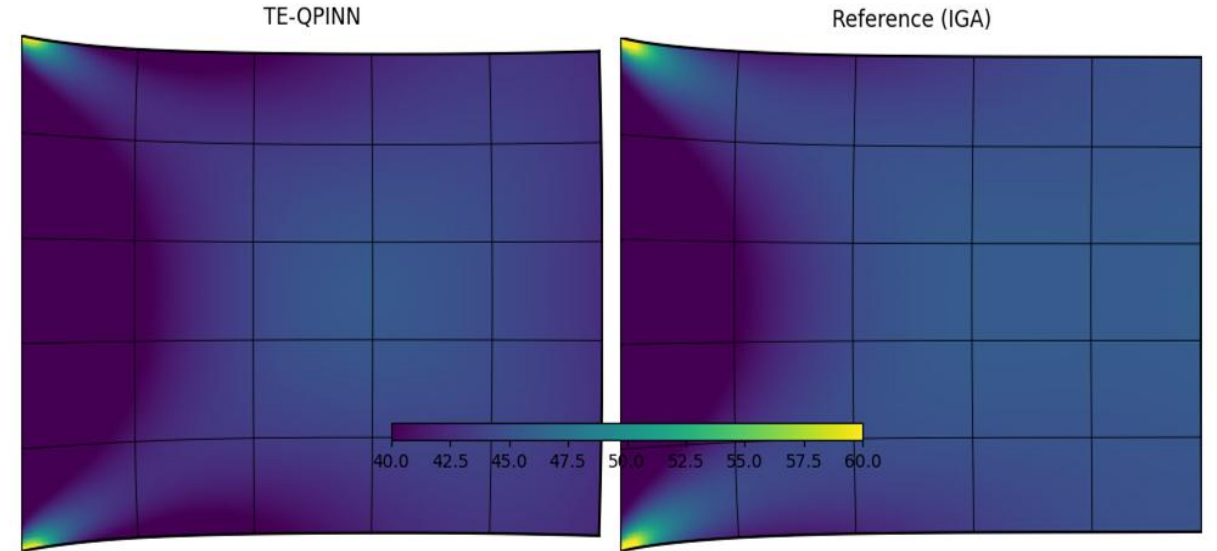


S. Berger et al., Trainable embedding quantum physics informed neural networks for solving nonlinear PDEs, *Sci. Rep.* 15 (2025)

TE-QPINNs applied to linear elasticity



van Mises stress \Rightarrow



Error in u and $v \Rightarrow$
 \Leftarrow Loss function

