QCE guest lecture on

Opportunities of Quantum Computing for CFD Applications

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Mission: Develop efficient and implementable end-to-end quantum methods for CFD applications

efficient = with provable advantage in terms of computational speed and/or memory requirement
implementable = worked out as quantum circuits in terms of (native) quantum gates, no c-U tricks
end-to-end = no oracles, no wishful thinking, no idealizing assumptions, demonstrated on simulators!

Motivation

Challenges in grid-based CFD

- Large memory requirements for high-resolution simulations $\sim N_x N_y N_z$
- Long compute times for time-dependent flows $\sim N_t$

$\Big\}$ $\sim N_t N_x N_y N_z$ ops

Possible solution: quantum computers

- Can encode N different states in $n = \log_2 N$ qubits via superposition of states
- Can operate on all $N = 2^n$ different states simultaneously (quantum parallelism)

Common pitfalls of quantum computing

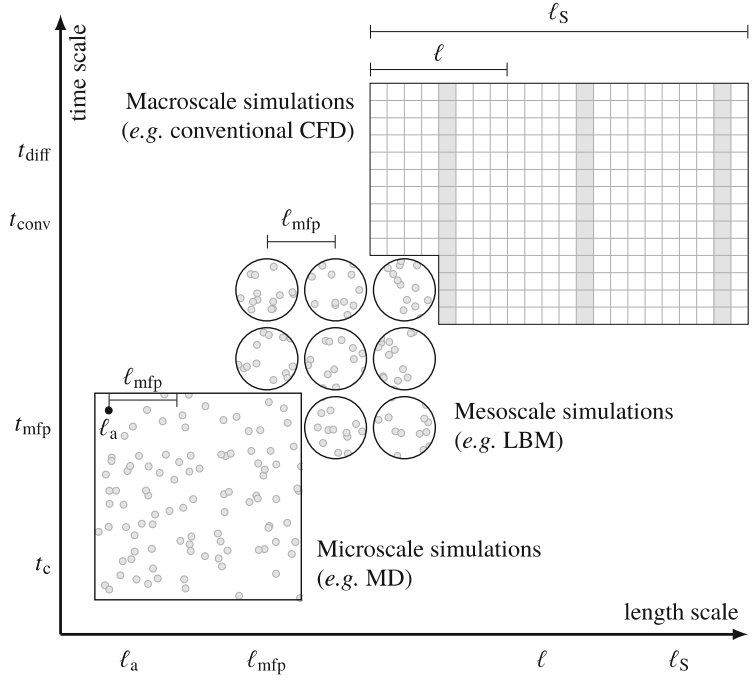
- How to encode data efficiently in the quantum register?
- How to load data efficiently into the quantum register (state preparation)?
- How to design the quantum algorithm as efficient quantum circuit?
- How to extract the algorithm's outcome efficiently via measurement?
- How to implement and test the algorithm on a quantum simulator/computer?

Outline

- Introduction into the lattice Boltzmann method (LBM)

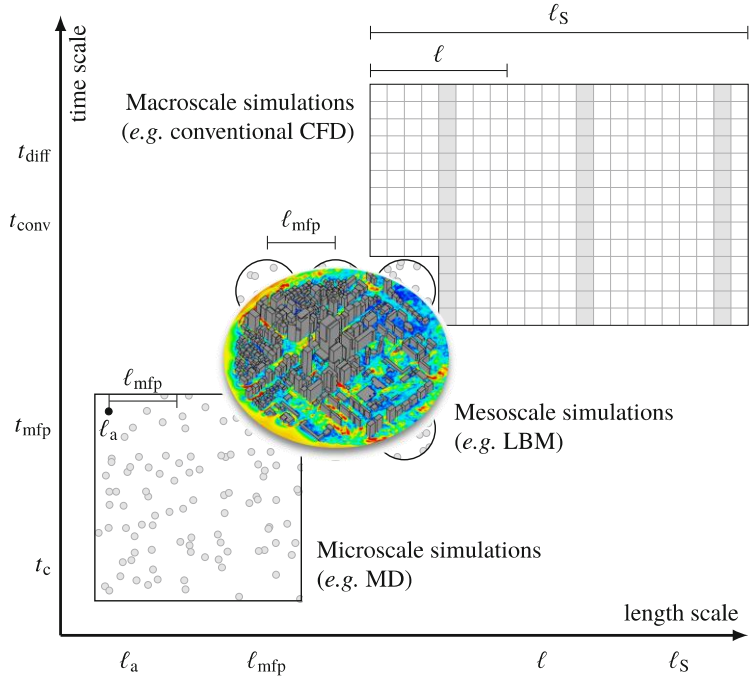
- Quantum LBM
  - Data encoding
  - Streaming & collision operators
  - Momentum exchange method

Hierarchy of length and time scales



DOI: 10.1007/978-3-319-44649-3

Hierarchy of length and time scales – the mesoscale



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- Kinetic theory based on **distribution function**

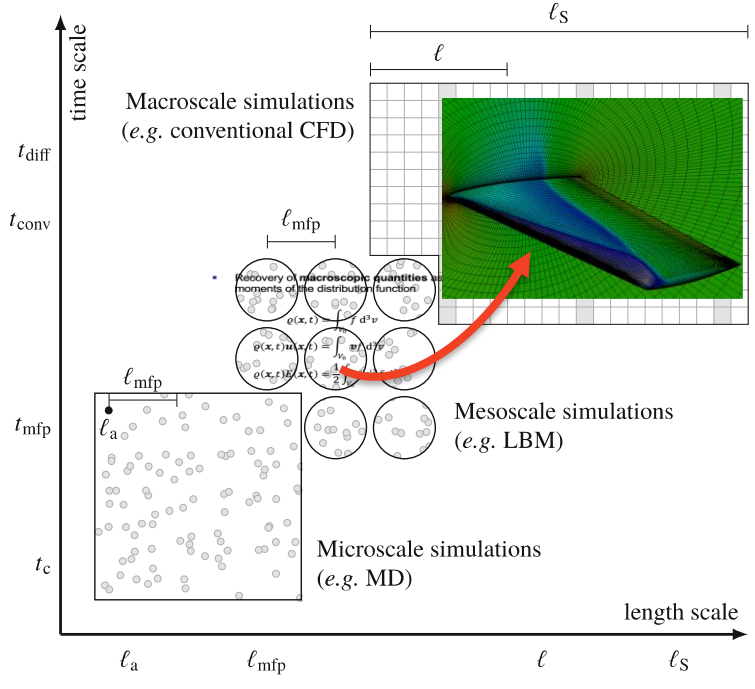
$$f(\boldsymbol{x}, \boldsymbol{v}, t) \qquad \left[\frac{\mathrm{kg\ s^3}}{\mathrm{m^6}}\right]$$

- **Interpretation**: $f(\boldsymbol{x}, \boldsymbol{v}, t)$ represents the density of mass in the physical space ($\boldsymbol{x}$) and the velocity space ($\boldsymbol{v}$) at time t

- When left alone for sufficiently long the distribution function will reach equilibrium

$$f^{\mathrm{eq}}(\boldsymbol{x}, \boldsymbol{v}, t)$$

Hierarchy of length and time scales – the mesoscale



- Recovery of **macroscopic quantities** as the moments of the distribution function

$$\varrho(\boldsymbol{x},t) = \int_{V_0} f \, \mathrm{d}^3 v$$

$$\varrho(\boldsymbol{x},t)\boldsymbol{u}(\boldsymbol{x},t) = \int_{V_0} \boldsymbol{v} f \, \mathrm{d}^3 v$$

$$\varrho(\boldsymbol{x},t)E(\boldsymbol{x},t) = \frac{1}{2}\int_{V_0} |\boldsymbol{v}|^2 f \, \mathrm{d}^3 v$$

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Boltzmann equation

- Total derivative of f with respect to time yields

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \left(\frac{\partial f}{\partial t}\right)\underbrace{\frac{\mathrm{d}t}{\mathrm{d}t}}_{=1} + \left(\frac{\partial f}{\partial x_\beta}\right)\underbrace{\frac{\mathrm{d}x_\beta}{\mathrm{d}t}}_{=v_\beta} + \left(\frac{\partial f}{\partial v_\beta}\right)\underbrace{\frac{\mathrm{d}v_\beta}{\mathrm{d}t}}_{=\frac{\mathrm{d}^2 x_\beta}{\mathrm{d}^2 t}=\frac{F_\beta}{\varrho}}$$

- The **Boltzmann equation**

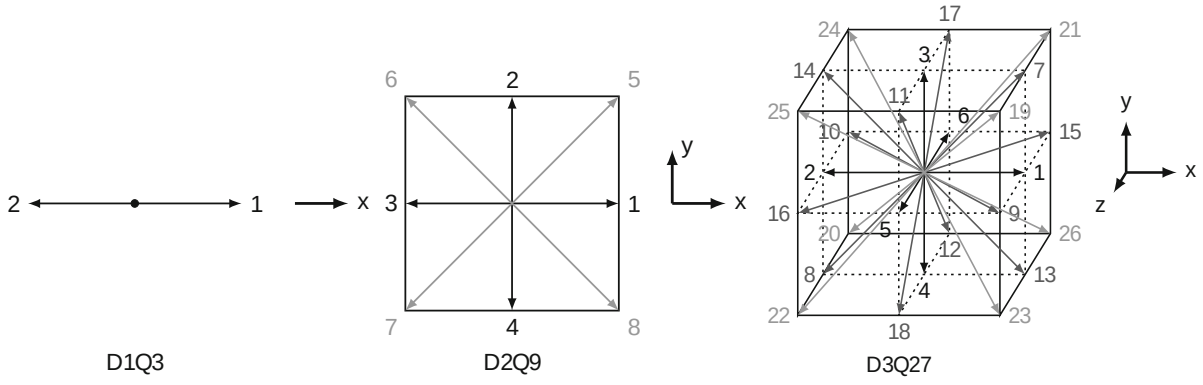
$$\frac{\partial f}{\partial t} + v_\beta \frac{\partial f}{\partial x_\beta} + \frac{F_\beta}{\varrho}\frac{\partial f}{\partial v_\beta} = \Omega(t)$$

with the **collision operator** $\Omega(t)$ representing the local redistribution of f due to collisions, e.g.,

$$\Omega^{\mathrm{BGK}}(t) = -\frac{1}{\tau}(f - f^{\mathrm{eq}})$$

Lattice Boltzmann method (LBM)

- Discretize the continuous velocity space into a set of **discrete velocities** $\boldsymbol{c}_\alpha = (c_{\alpha x}, c_{\alpha y}, c_{\alpha z})$, e.g.,



$|\boldsymbol{c}_\alpha| \in \{0, 1\}$ $|\boldsymbol{c}_\alpha| \in \{0, 1, \sqrt{2}\}$ $|\boldsymbol{c}_\alpha| \in \{0, 1, \sqrt{2}, \sqrt{3}\}$

- **Notation**: $\mathrm{D}d\mathrm{Q}N_v$ with spatial dimension d and number of discrete velocities N_v

Lattice Boltzmann method (LBM)

- Then $f(\boldsymbol{x}, \boldsymbol{v}, t)$ becomes a **discrete-velocity distribution function**

$$f_\alpha(\boldsymbol{x}, t) = f(\boldsymbol{x}, \boldsymbol{c}_\alpha, t)$$

- Discretization in space and time yields

$$f_\alpha(\boldsymbol{x}_i + \boldsymbol{c}_\alpha \Delta t, t^n + \Delta t) = f_\alpha(\boldsymbol{x}_i, t^n) + \Omega_\alpha(\boldsymbol{x}_i, t^n)$$

for all discrete velocities $\alpha = 1, \dots, N_v$,
for all grid points $i = 1, \dots, N_x N_y N_z$ and
for all time steps $n = 0, \dots, N_t$

Lattice Boltzmann method (LBM)

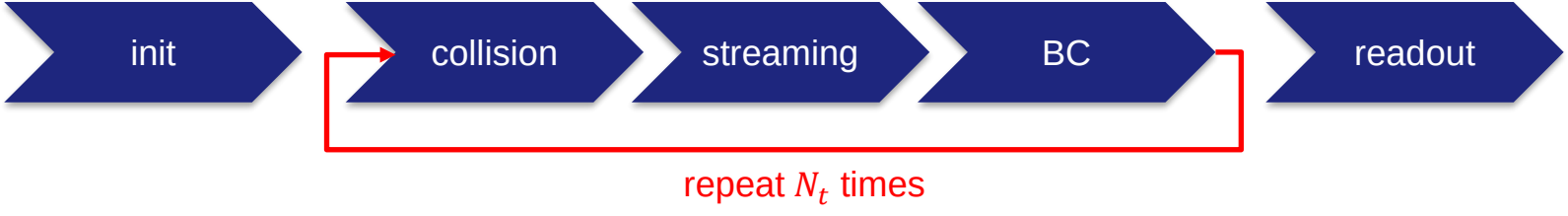
1. Update the moments and the equilibrium $f_i \rightarrow \varrho, \boldsymbol{u} \rightarrow f_i^{\mathrm{eq}}$
2. Compute the **collision** (or relaxation)

$$f_i^*(\boldsymbol{x}_j, t^n) = f_i(\boldsymbol{x}_j, t^n)\left(1 - \frac{\Delta t}{\tau}\right) + f_i^{\mathrm{eq}}(\boldsymbol{x}_j, t^n)\frac{\Delta t}{\tau}$$

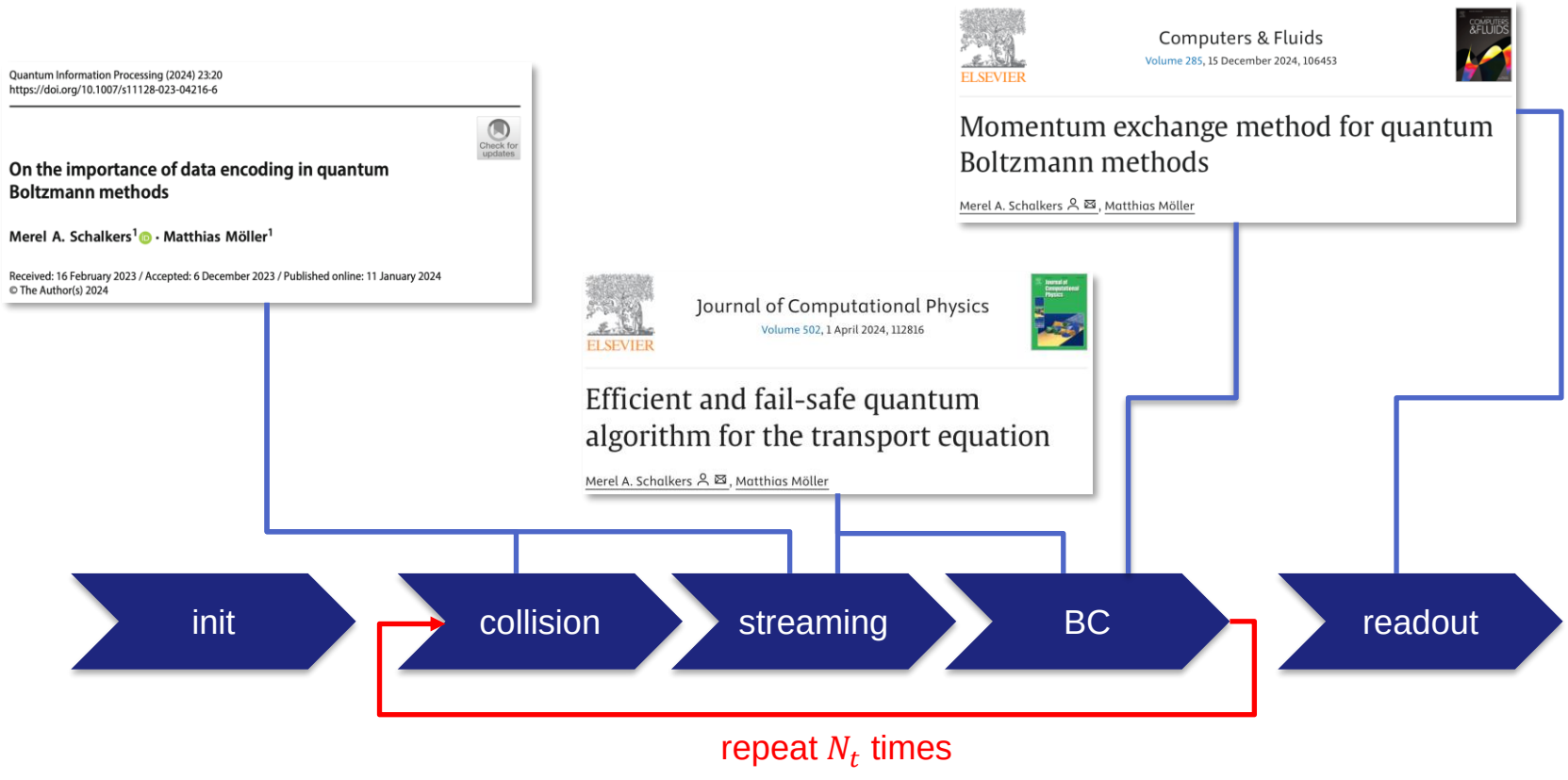
3. Compute the **streaming** (or propagation)

$$f_i(\boldsymbol{x}_j + \boldsymbol{c}_i \Delta t, t^n + \Delta t) = f_i^*(\boldsymbol{x}_j, t^n)$$

4. Apply **boundary conditions**
5. Set $t^{n+1} = t^n + \Delta t$ and go back to step 1



Quantum lattice Boltzmann method (LBM)



Collisionless quantum lattice Boltzmann method (CQLBM)

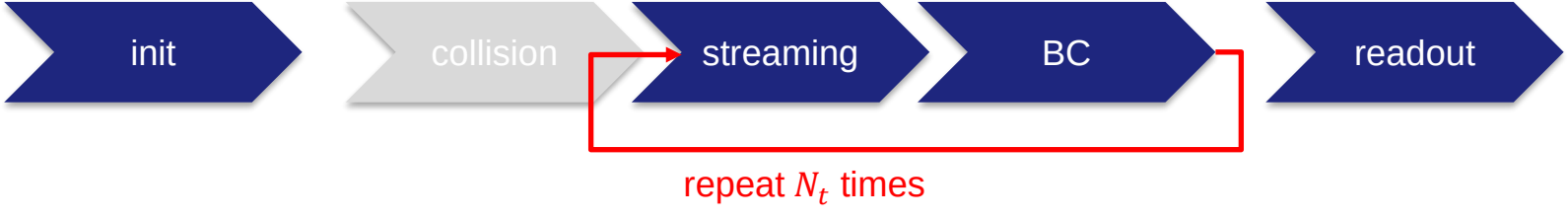
- Then $f(\boldsymbol{x}, \boldsymbol{v}, t)$ becomes a **discrete-velocity distribution function**

$$f_\alpha(\boldsymbol{x}, t) = f(\boldsymbol{x}, \boldsymbol{c}_\alpha, t)$$

- Discretization in space and time and ignoring the collision term yields

$$f_\alpha(\boldsymbol{x}_i + \boldsymbol{c}_\alpha \Delta t, t^n + \Delta t) = f_\alpha(\boldsymbol{x}_i, t^n) + \Omega_\alpha(x_i, t^n)$$

for all discrete velocities $\alpha = 1, \dots, N_v$, grid points $i = 1, \dots, N_x N_y N_z$ and time steps $n = 0, \dots, N_t$



Data encoding of the grid

Classical register of size $N_x N_y N_v$

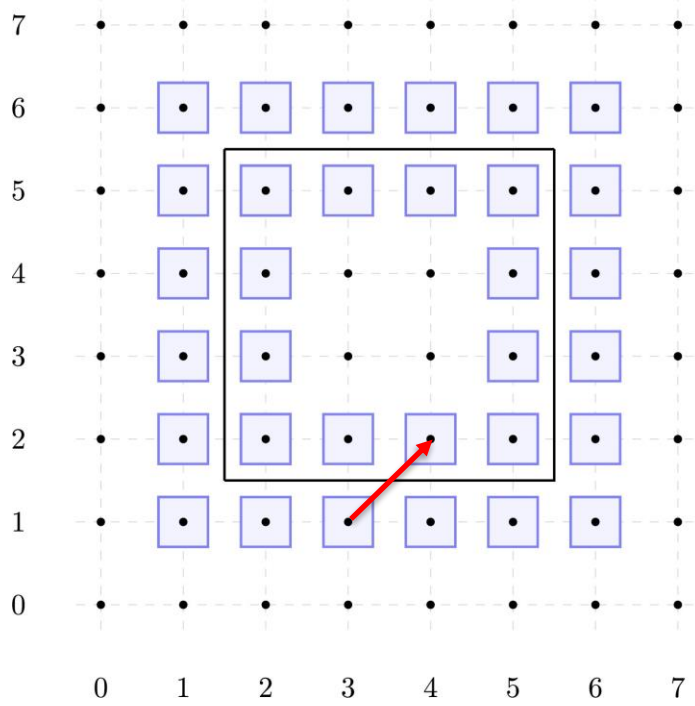
$$f[N_x][N_y][N_v]$$

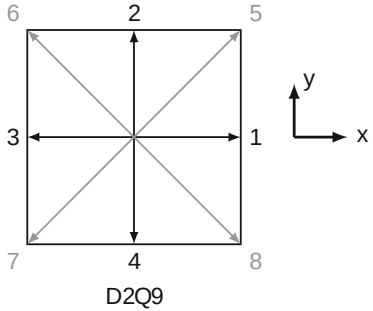
$$f[ix][iy][\alpha] \;\mapsto\; f_\alpha(x_{ix}, y_{iy})$$

Example for D2Q9

$$\text{size } 8 \cdot 8 \cdot 9 = 576$$

$$f[3][1][5] \;\mapsto\; f_5(x_3, y_1)$$





Data encoding of the grid

Quantum register of size $n_x + n_y + 2n_v$ $(n = \log_2 N)$

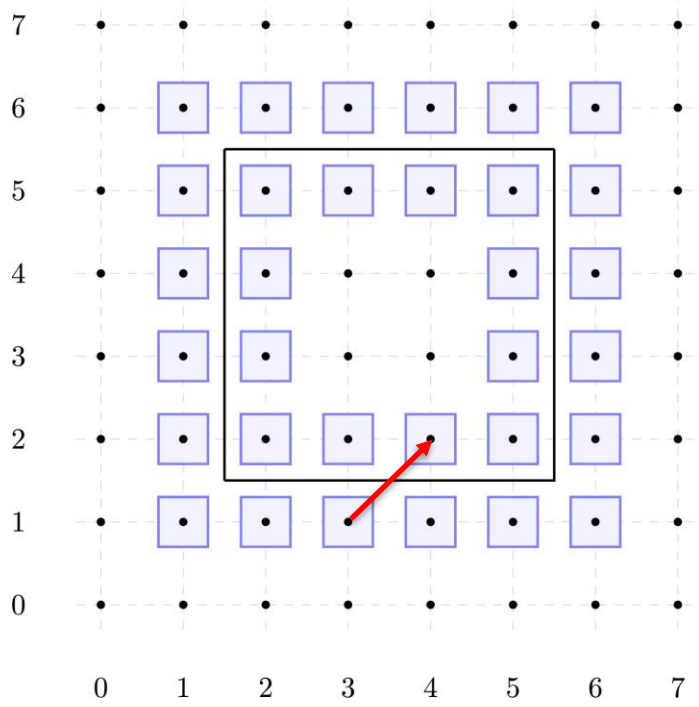
$$|n_x\rangle \otimes |n_y\rangle \otimes |n_v\rangle \otimes |n_v\rangle = \sum_{\ell=0}^{2^{n_x+n_y+2n_v-1}} \rho_\ell |\ell\rangle$$

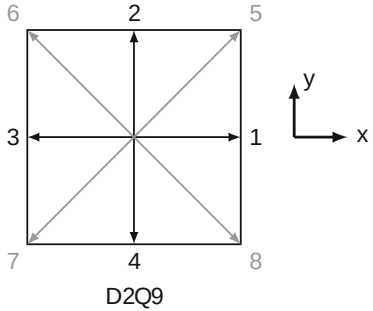
$$\rho_{ix\ iy\ \alpha x\ \alpha y} \mapsto \sim f_{\alpha x,\alpha y}(x_{ix}, y_{iy})$$

Example for D2Q9

$$\text{size } 3 + 3 + 2 \cdot 2 = 10$$

$$\rho_{011\ 001\ 01\ 01} \mapsto \sim f_5(x_3, y_1)$$





D2Q9

Data encoding of the velocity

$$\left|v_{\mathrm{dir}} v_{n_v-1} \dots v_1\right\rangle = \begin{bmatrix} -v_{\min} \\ -v_{\min} - \Delta v \\ \vdots \\ -v_{\max} \\ v_{\min} \\ v_{\min} + \Delta v \\ \vdots \\ v_{\max} \end{bmatrix}$$

- **Example**: Let $v_{\min} = 1$ and $\Delta v = 0.5$ then
  - $|v\rangle = |\ \ 1.5\rangle = |101\rangle$
  - $|v\rangle = |-1.5\rangle = |001\rangle$

Remark:
All standard $DdQN_v$ velocity stencils can be realized with two qubits per direction, i.e.

$$|u_{\mathrm{dir}} u_1\rangle \otimes |v_{\mathrm{dir}} v_1\rangle \otimes |w_{\mathrm{dir}} w_1\rangle = \{\cdot = |00\rangle = |10\rangle, \quad \leftarrow = |01\rangle, \quad \rightarrow = |11\rangle\}^{\otimes d}$$

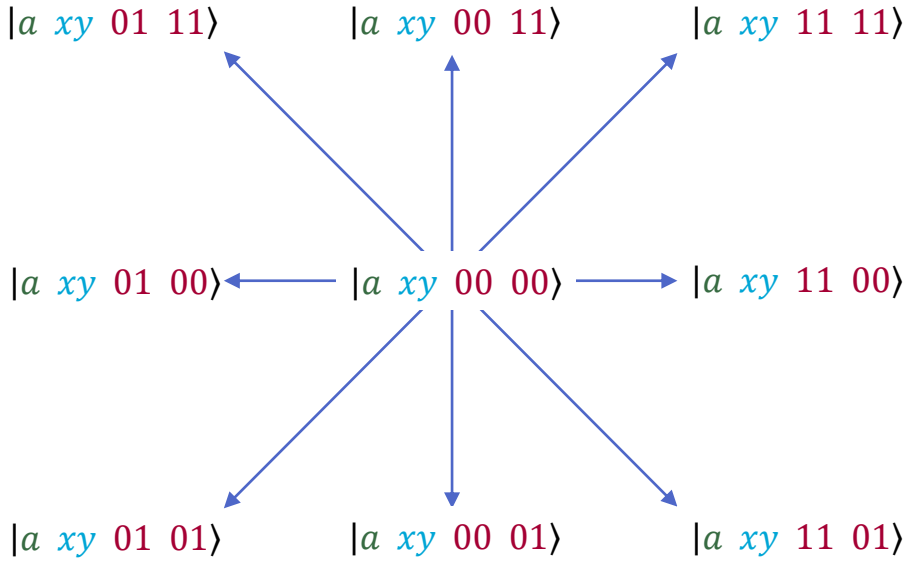
A variant of the LBM is the discrete-velocity method with many more discrete velocities which can be realized with the above data encoding at the cost of more qubits per direction.

Amplitude-based data encoding

$$|\psi\rangle = \sum_{\ell=0}^{2^{4d-2+n_x+n_y+n_z+3n_v}-1} \rho_\ell \left| \underbrace{a_{4d-2} \dots a_1}_{4d-2 \text{ ancillas}} \; \underbrace{x_{n_x} \dots x_1 \; y_{n_y} \dots y_1 \; z_{n_z} \dots z_1}_{n_x+n_y+n_z \text{ grid qubits}} \; \underbrace{u_{n_v} \dots u_1 \; v_{n_v} \dots v_1 \; w_{n_v} \dots w_1}_{3n_v \text{ velocity qubits}} \right\rangle$$

- Ancillas are used to hold decision variables, e.g., to detect objects, etc.
- Example of **memory savings** for D3Q27 on 1024^3 grid using **superposition of states**
  - classical: $27 \cdot 1024^3 =$ ~29 billion floating-point numbers (~232 GB FP64)
  - quantum: $4 \cdot 3 - 2 + 3 \cdot 10 + 3 \cdot 2 =$ 46 qubits
- Can we also reduce the **'compute time'** (compute complexity) using **quantum parallelism**?

A closer look at the encoding of the discrete velocities for D2Q9

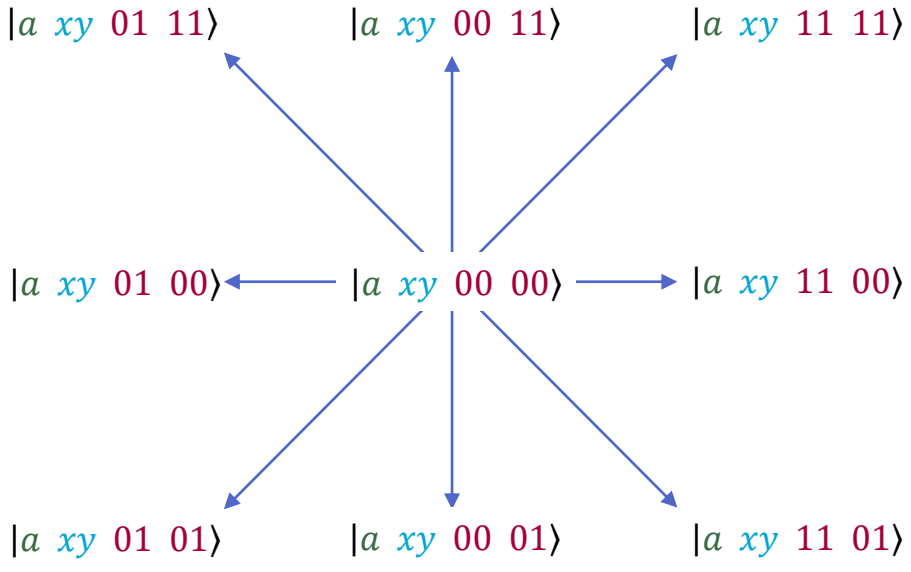


A closer look at the encoding of the discrete velocities for D2Q9

Since particle densities are encoded in the amplitudes, **streaming** amounts to shifting them between grid positions depending on their velocities, e.g.

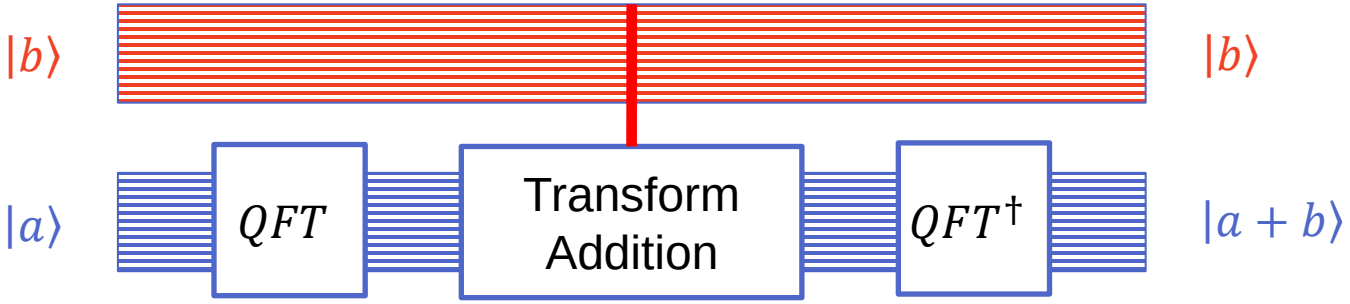
$$
\begin{aligned}
\rho_{a\ x.y\ 00\ 00} &\mapsto \rho_{a\ x.y\ 00\ 00} \\
\rho_{a\ x.y\ 11\ 00} &\mapsto \rho_{a\ x+1.y\ 11\ 00} \\
\rho_{a\ x.y\ 01\ 00} &\mapsto \rho_{a\ x-1.y\ 01\ 00} \\
\rho_{a\ x.y\ 00\ 11} &\mapsto \rho_{a\ x.y+1\ 00\ 11} \\
\rho_{a\ x.y\ 00\ 01} &\mapsto \rho_{a\ x.y-1\ 00\ 01} \\
\rho_{a\ x.y\ 11\ 11} &\mapsto \rho_{a\ x+1.y+1\ 11\ 11} \\
&\dots
\end{aligned}
$$

Apply streaming primitive to all grid positions simultaneously controlled on the value of the velocity qubits

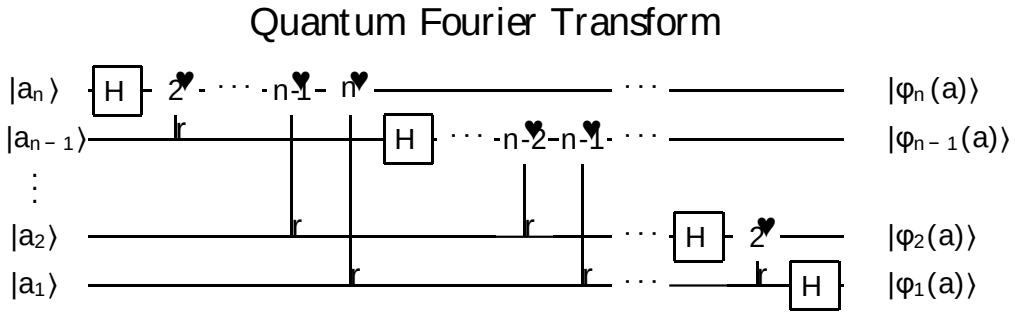


Sketch of the streaming operation

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 any ancillas



Intermezzo: Draper's quantum adder



$$|a_n\rangle \longrightarrow \tfrac{1}{\sqrt{2}}(|0\rangle + e(0.a_n)|1\rangle) \qquad \text{Hadamard transform}$$

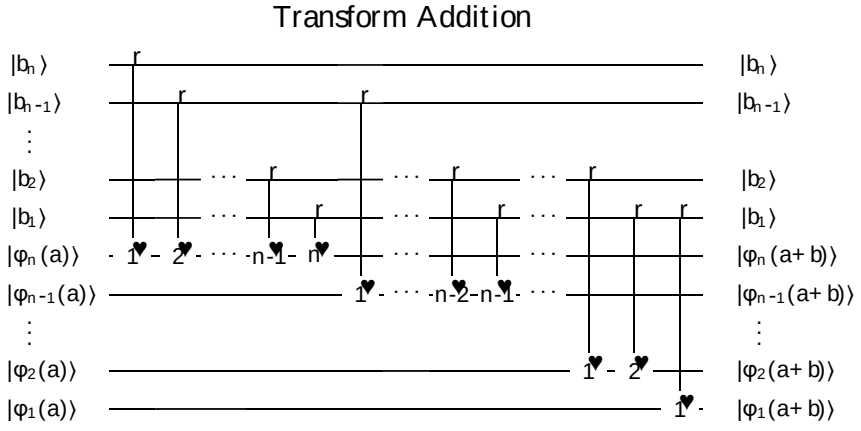
$$\longrightarrow \tfrac{1}{\sqrt{2}}(|0\rangle + e(0.a_n a_{n-1})|1\rangle) \qquad R_2 \text{ rotation conditioned on } a_{n-1}$$

$$\vdots \qquad\qquad \vdots$$

$$\longrightarrow \tfrac{1}{\sqrt{2}}(|0\rangle + e(0.a_n a_{n-1} \ldots a_1)|1\rangle) \qquad R_n \text{ rotation conditioned on } a_1$$

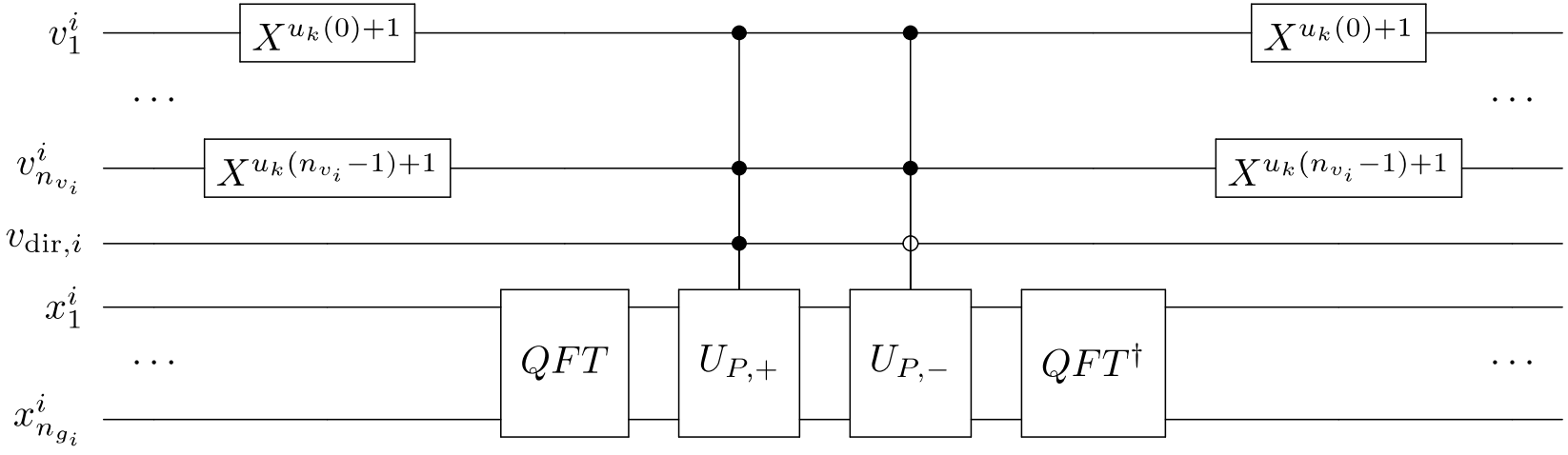
$$= |\varphi_n(a)\rangle$$

Intermezzo: Draper's quantum adder



$$
\begin{aligned}
|\varphi_n(a)\rangle &\longrightarrow \tfrac{1}{\sqrt{2}}(|0\rangle + e(0.a_n a_{n-1}\ldots a_1 + 0.b_n)|1\rangle) && R_1 \text{ rotation from } b_n \\
&\longrightarrow \tfrac{1}{\sqrt{2}}(|0\rangle + e(0.a_n a_{n-1}\ldots a_1 + 0.b_n b_{n-1})|1\rangle) && R_2 \text{ rotation from } b_{n-1} \\
&\qquad\vdots && \vdots \\
&\longrightarrow \tfrac{1}{\sqrt{2}}(|0\rangle + e(0.a_n a_{n-1}\ldots a_1 + 0.b_n b_{n-1}\ldots b_1)|1\rangle) && R_n \text{ rotation from } b_1 \\
&= |\varphi_n(a+b)\rangle
\end{aligned}
$$

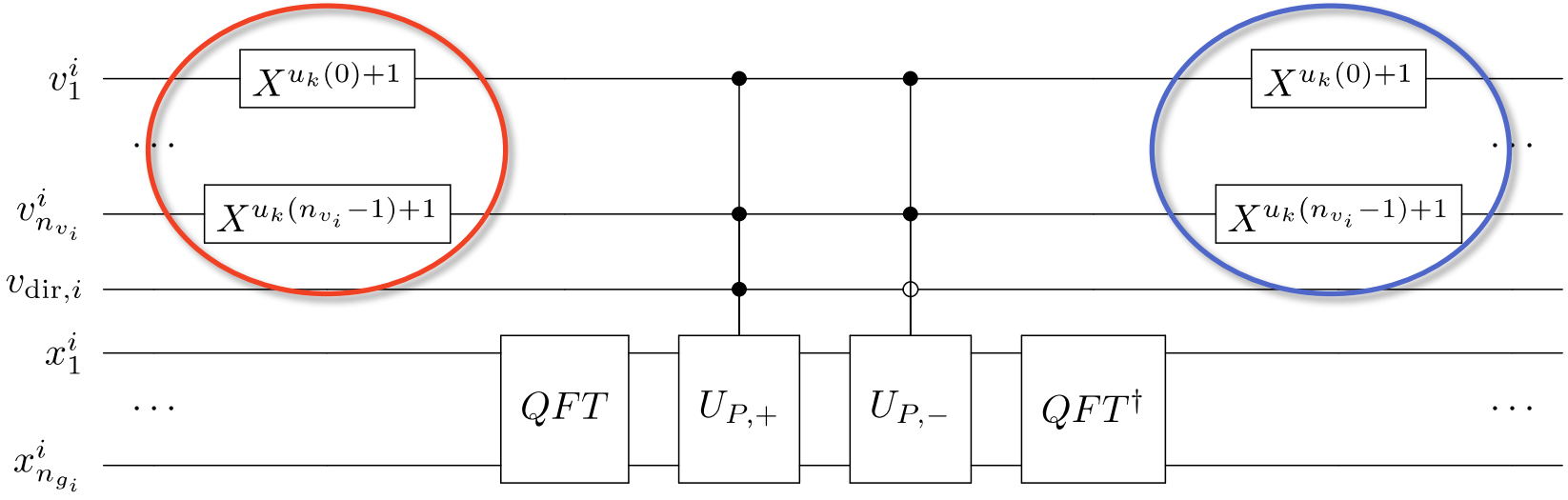
Streaming in Fourier space (schematic view)



Streaming in Fourier space (schematic view)

Set all velocity qubits that we want to stream in the i-th direction "on"

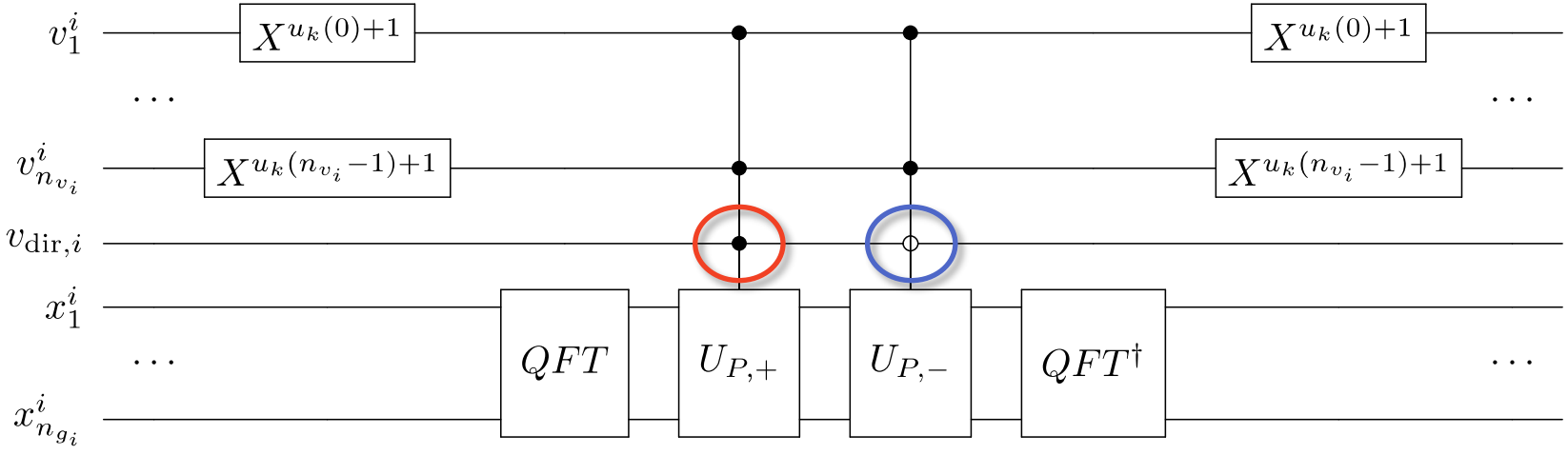
Reset the velocity qubits



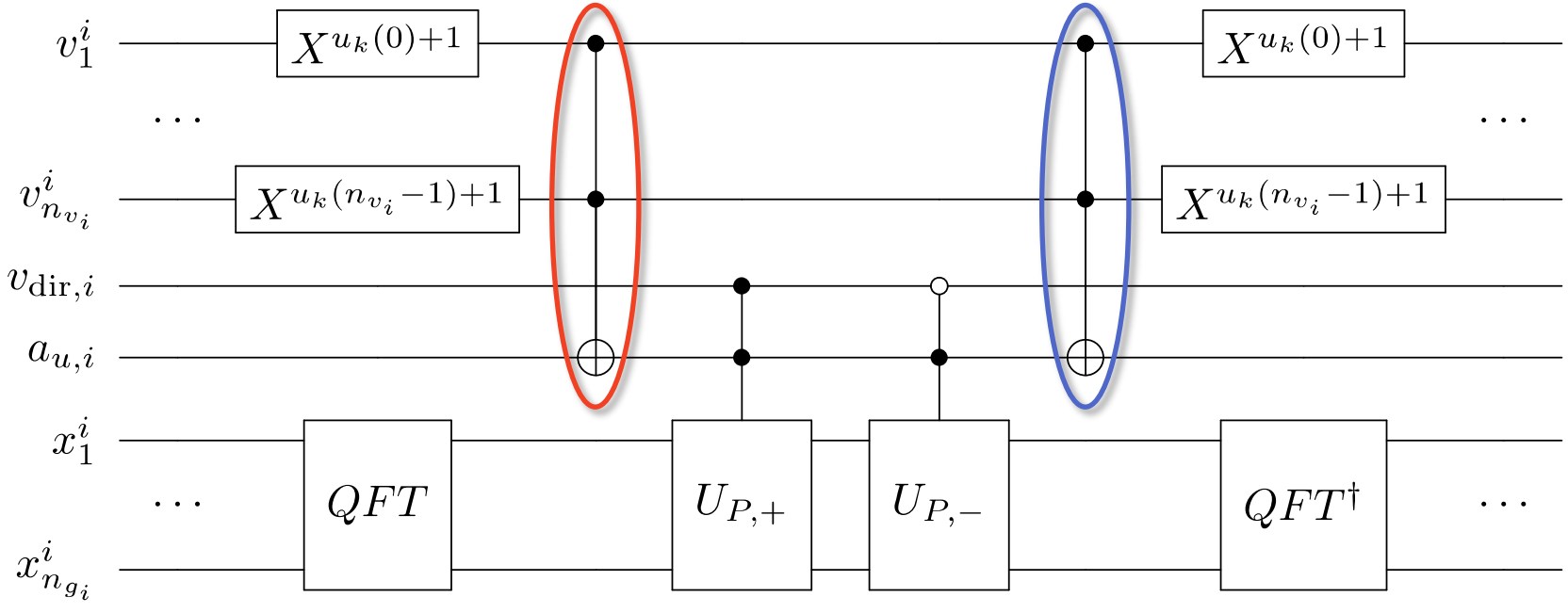
Example: want to stream $c_5 = 101$, set $\tilde{c}_5 = 111$ so that the multi-controlled $U_{P,+}$ (incrementer) or the multi-controlled $U_{P,-}$ (decrementer) get activated

Streaming in Fourier space (schematic view)

If $v_{\mathrm{dir},i}$ is "on" we stream in the positive direction otherwise ("off") we stream in the negative direction



Streaming in Fourier space (schematic view)



The ancillary qubit $a_{u,i}$ reduces the amount of multi-controlled $U_{P,*}$ operations

Streaming in Fourier space (the math)

- **Claim**: $|j+1\rangle = QFT^{\dagger}\, U_{P,+}\, QFT\, |j\rangle$
- QFT in a nutshell

$$QFT\,|j\rangle = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}\omega_N^{kj}|k\rangle = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}e^{\frac{2i\pi kj}{N}}|k\rangle$$

- Since

$$\theta_j \coloneqq \frac{\pi}{2^{N-1-j}} = \frac{\pi 2^{j+1}}{N}$$

- Then

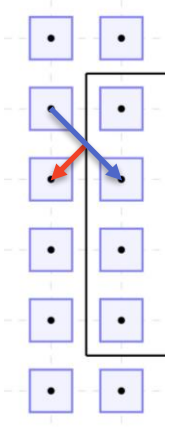
$$U_{P,+}\, QFT\,|j\rangle = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}e^{\frac{2i\pi kj}{N}}e^{\theta_j}|k\rangle = \frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}e^{\frac{2i\pi k(j+1)}{N}}|k\rangle$$

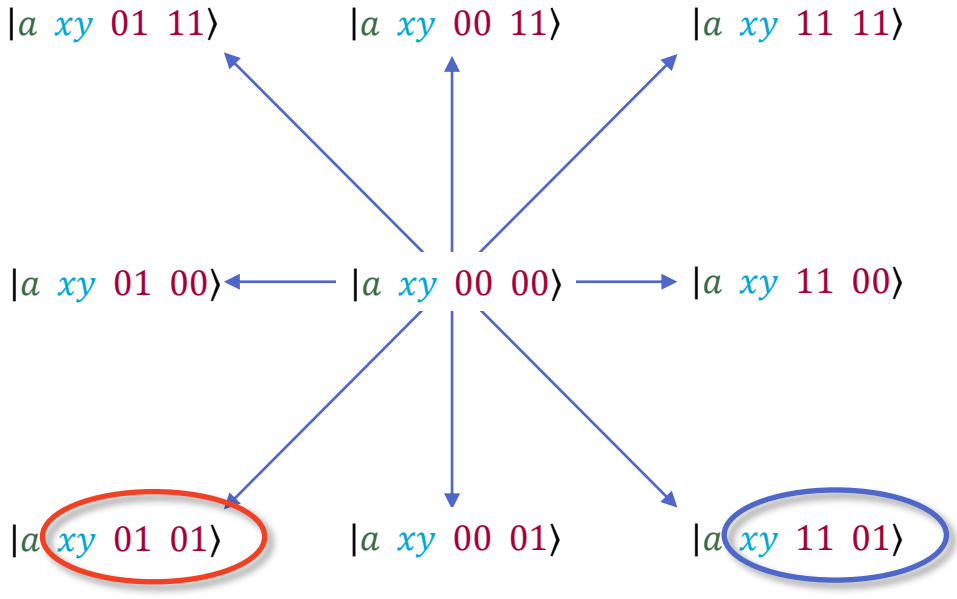
- Finally

$$QFT^{\dagger}\, U_{P,+}\, QFT\,|j\rangle = QFT^{\dagger}\,\frac{1}{\sqrt{N}}\sum_{k=0}^{N-1}e^{\frac{2i\pi k(j+1)}{N}}|k\rangle = |j+1\rangle$$

Specular reflection boundary condition

If a particle needs to change its flow direction because of a reflection at the boundary it suffices to flip a single qubit and update the particle's grid position





Specular reflection boundary condition

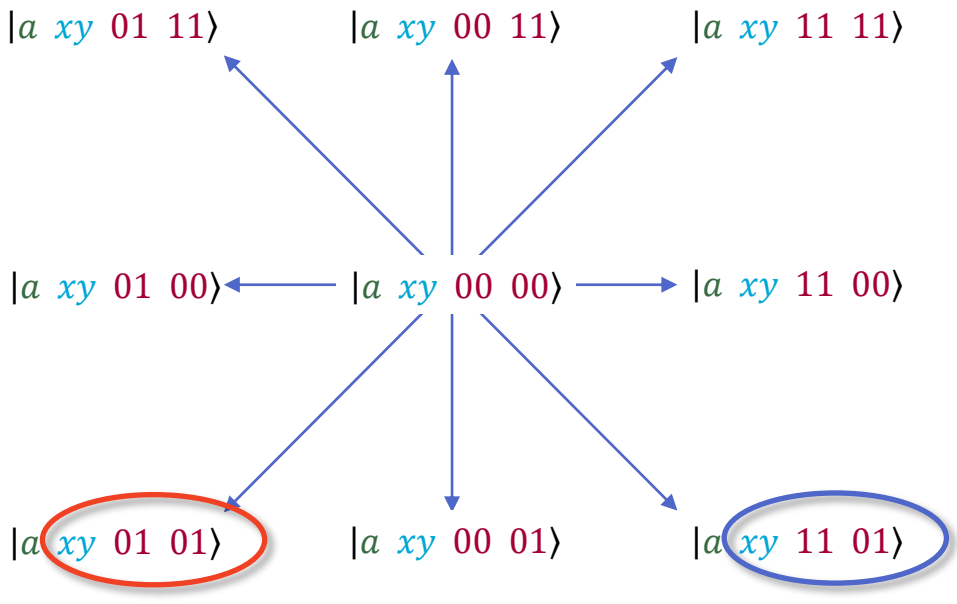
For all quantum states $|a\ x\ y\ 11\ 01\rangle$ with (x, y) *outside* and $(x+1, y)$ *inside* any obstacle with a vertical wall do

$$|a\ x\ y\ 11\ 01\rangle \rightarrow |a\ x\ y-1\ 01\ 01\rangle$$

- C^m-NOT for the bitflip
- ±1 Draper-type adder for the shift

Same shift-logic as for streaming

How do we detect that we are at a boundary, i.e. (x, y) is *outside* and $(x+1, y)$ is *inside* an obstacle?



Quantum comparator operator

- **Goal**: check $i \geq k$
- Start from $|0\rangle \otimes |i\rangle$ and
- subtract k from the state
  - if $i \geq k$

    $$|0\rangle \otimes |i-k\rangle$$

  - else $i < k$

    $$|2^{n+1} - 1 - k + i\rangle = |1\rangle \otimes |2^n - 1 - k + i\rangle$$

- add k to the last n qubits
  - if $i \geq k$

    $$|0\rangle \otimes |i\rangle$$

  - else $i < k$

    $$|1\rangle \otimes |i\rangle$$

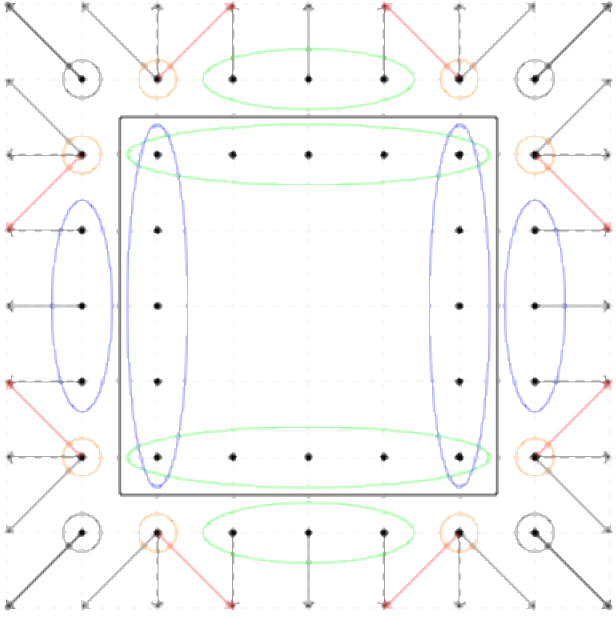
- use ancilla qubit as control

Exploiting quantum parallelism

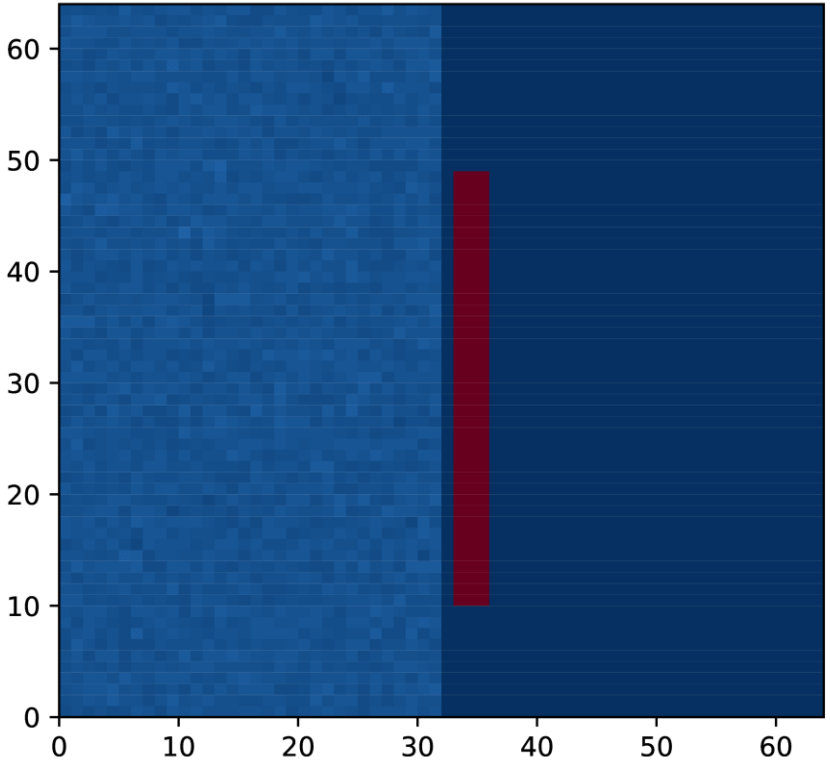
SeqFor 00, 01, 11
  QParFor "stream" along x direction
  QParFor "stream" along y direction

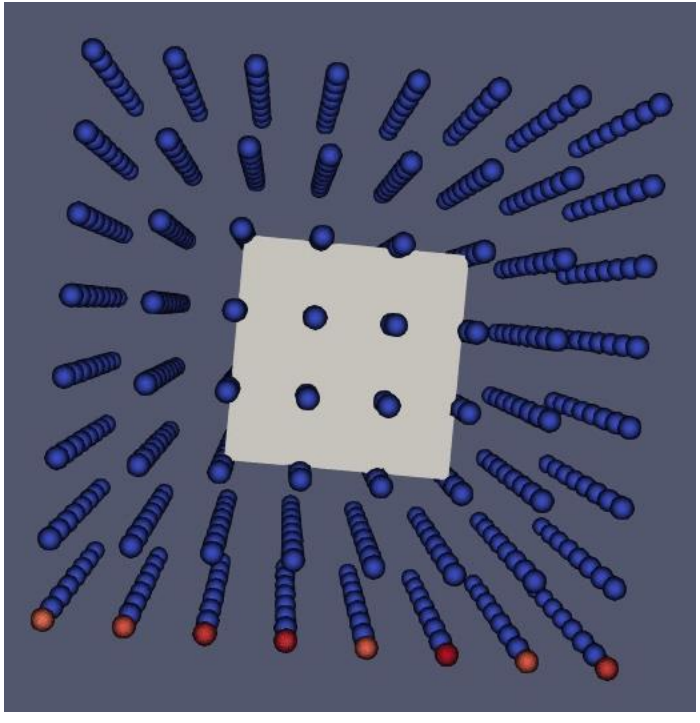
SeqFor ◯, ◯, ◯,…
  SeqFor 00, 01, 11
    QParFor "reflect" along x direction
    QParFor "reflect" along y direction

Sequential loops are "blocks" in the quantum circuit that can potentially be parallelized by adding more ancillas

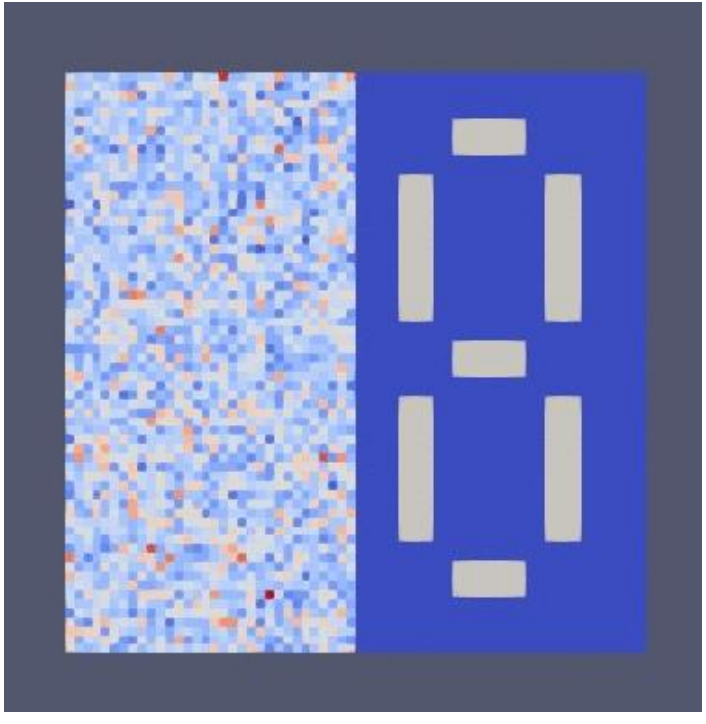


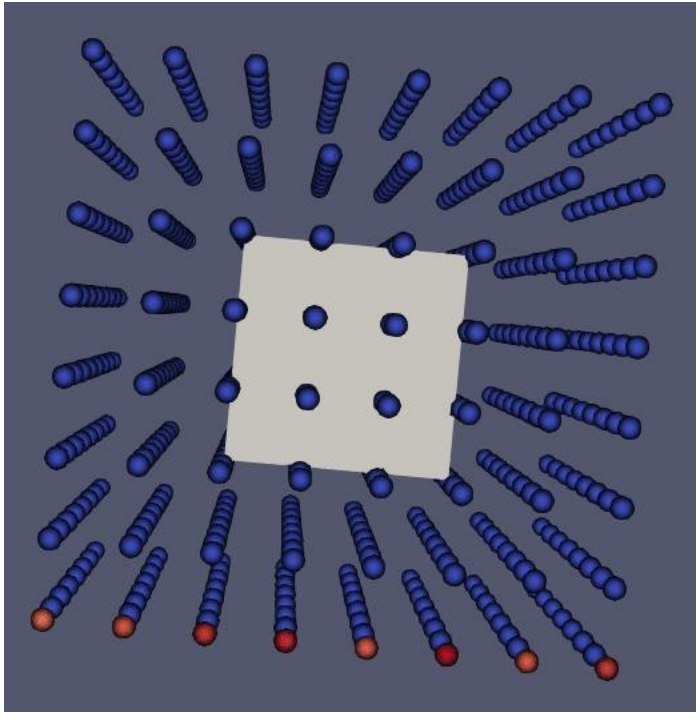
Results: D2Q9 on a 64x64 grid (left) and D3Q27 on an 8x8x8 grid (right)





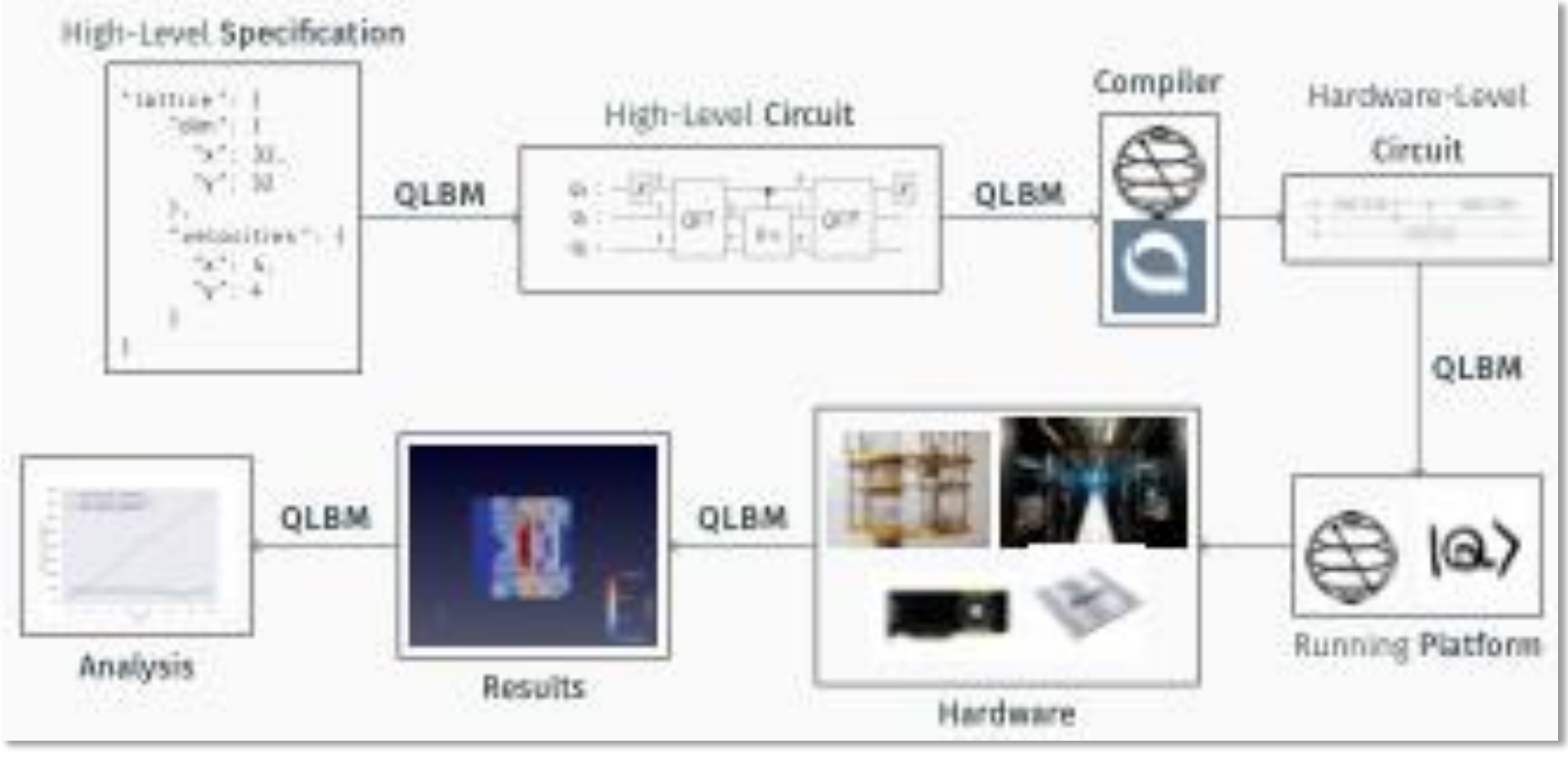
Results: D2Q9 on a 64x64 grid (left) and D3Q27 on an 8x8x8 grid (right)





QLBM software framework

https://github.com/qcfd-lab/qlbm



QLBM software framework

```
"dim": {
    "x": 16,
    "y": 16
},
"velocities": {
    "x": 4,
    "y": 4
}
},
"geometry": [[
    "x": [9, 12],
    "y": [3, 6],
    "boundary": "specular"
},
{
    "x": [9, 12],
    "y": [9, 12],
    "boundary": "bounceback"
}]
```

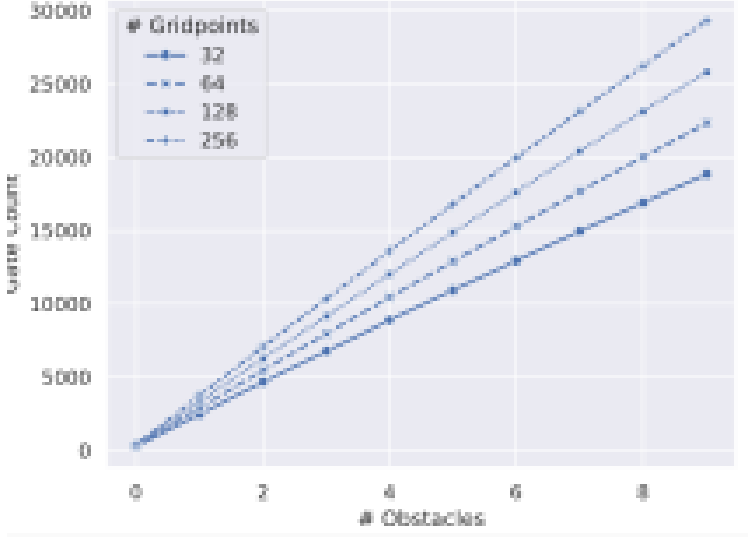
QLBM software framework

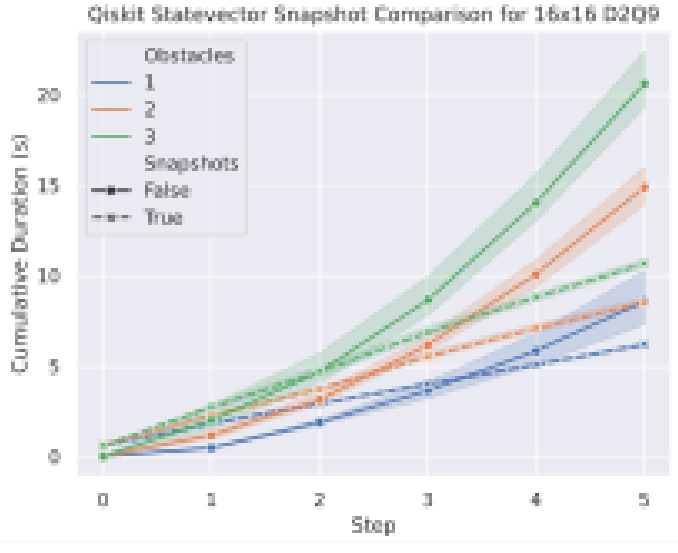
```
# Load the system specification
lattice = CollisionlessLattice("lattice.json")

# Define all parameters
cfg = SimulationConfig(
    initial_conditions=CollisionlessInitialConditions(lattice),
    algorithm=CQLBM(lattice),
    postprocessing=EmptyPrimitive(lattice),
    measurement=GridMeasurement(lattice),
    target_platform="QISKIT",
    compiler_platform="QISKIT",
    optimization_level=0,
    statevector_sampling=True,
    execution_backend=AerSimulator(method="statevector"),
    sampling_backend=AerSimulator(method="statevector"),
)
```

QLBM software framework

```
cfg.prepare_for_simulation()
# Create a runner object to simulate the circuit
runner = QiskitRunner(
    cfg,
    lattice,
)

# Simulate the circuits using both snapshots and sampling
runner.run(
    100,  # Number of time steps
    2**12,  # Number of shots per time step
    "output_dir/sim", # Output directory
    statevector_snapshots=True, # Performance opt.
)
```

QLBM software framework





Momentum exchange method

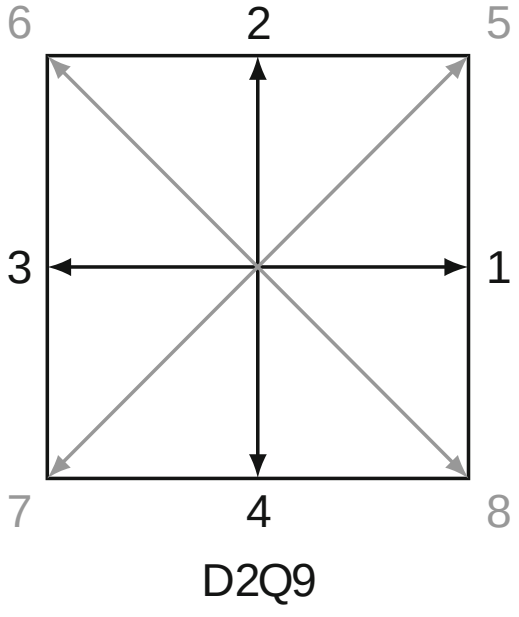
Force exerted on objects

$$\boldsymbol{F} = \sum_{\alpha=1}^{N_v} \boldsymbol{c}_\alpha f_\alpha(\boldsymbol{x}_{\text{fluid}}, t) - \boldsymbol{c}_{\bar{\alpha}} f_{\bar{\alpha}}(\boldsymbol{x}_{\text{fluid}}, t)$$

with $\boldsymbol{x}_{\text{fluid}}$ denoting the location in the fluid domain next to the obstacle, $\boldsymbol{c}_\alpha$ the discrete velocities, e.g.,

$$\boldsymbol{c}_\alpha = \begin{cases} (0,0) & \alpha = 0 \\ (1,0), (0,1), (-1,0), (0,-1) & \alpha = 1, \dots, 4 \\ (1,1), (-1,1), (-1,-1), (1,-1) & \alpha = 5, \dots, 8 \end{cases}$$

and $\boldsymbol{c}_{\bar{\alpha}}$ referring to the α-th velocity direction after contact with the obstacle



Momentum exchange method

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and $\boldsymbol{c}_{\bar{\alpha}}$ referring to the α-th velocity direction after contact with the obstacle

Bounce back boundary conditions yield

$$\boldsymbol{c}_{\bar{\alpha}} = -\boldsymbol{c}_\alpha$$

$$f_\alpha(\boldsymbol{x}_{\text{fluid}}, t) = f_{\bar{\alpha}}(\boldsymbol{x}_{\text{fluid}}, t)$$

Hence

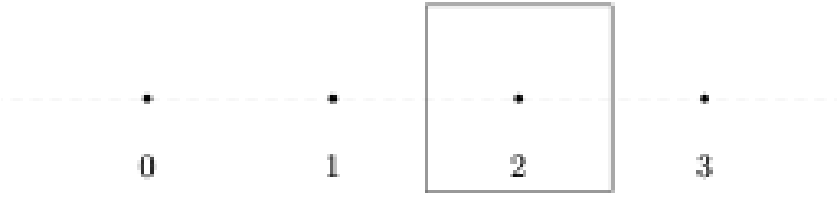
$$\boldsymbol{F} = \sum_{\alpha=1}^{N_v} 2\boldsymbol{c}_\alpha f_\alpha(\boldsymbol{x}_{\text{fluid}}, t)$$

Sketch of the *quantum* momentum exchange method

Change the amplitude-based data encoding

$$f_\alpha(\boldsymbol{x}, t) \;\rightarrow\; \sqrt{f_\alpha(\boldsymbol{x}, t)}$$

Example: D1Q3

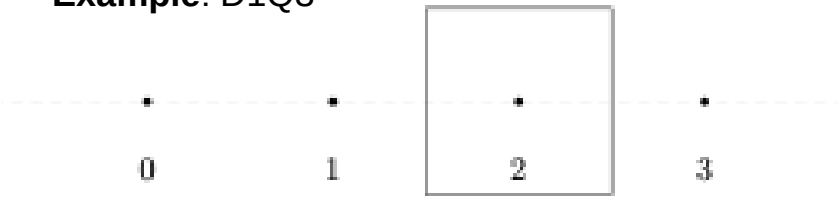


$$|\psi\rangle = \frac{1}{\sqrt{\sum_{x,\alpha} f_\alpha(x,t)}} \sum_{x,\alpha} \sqrt{f_\alpha(x,t)} |x_2 x_1 \; v_{\mathrm{dir}} v_1\rangle$$

$$|\psi\rangle = \frac{1}{\sqrt{\sum_{x,\alpha} f_\alpha(x,t)}} \begin{bmatrix} 0 \\ \sqrt{f_0(0,t)} \\ \sqrt{f_1(0,t)} \\ \sqrt{f_2(0,t)} \\ 0 \\ \sqrt{f_0(1,t)} \\ \sqrt{f_1(1,t)} \\ \sqrt{f_2(1,t)} \\ 0 \\ \sqrt{f_0(2,t)} \\ \sqrt{f_1(2,t)} \\ \sqrt{f_2(2,t)} \\ 0 \\ \sqrt{f_0(3,t)} \\ \sqrt{f_1(3,t)} \\ \sqrt{f_2(3,t)} \end{bmatrix}$$

Sketch of the *quantum* momentum exchange method

Example: D1Q3



$$\langle\psi|?\,|\psi\rangle = \frac{2f_1(1,t)}{\sqrt{\sum_{x,\alpha} f_\alpha(x,t)}}$$

$$|\psi\rangle = \frac{1}{\sqrt{\sum_{x,\alpha} f_\alpha(x,t)}} \begin{bmatrix} 0 \\ \sqrt{f_0(0,t)} \\ \sqrt{f_1(0,t)} \\ \sqrt{f_2(0,t)} \\ 0 \\ \sqrt{f_0(1,t)} \\ \sqrt{f_1(1,t)} \\ \sqrt{f_2(1,t)} \\ 0 \\ \sqrt{f_0(2,t)} \\ \sqrt{f_1(2,t)} \\ \sqrt{f_2(2,t)} \\ 0 \\ \sqrt{f_0(3,t)} \\ \sqrt{f_1(3,t)} \\ \sqrt{f_2(3,t)} \end{bmatrix}$$

Observable

$$\mathcal{O} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & B & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Intermediate summary

Quantum-LBM has the potential to overcome two of the grand challenges of CFD – high memory consumption and long compute times – by using superposition of states and quantum parallelism

- amplitude-based encoding of LBM data with $\#\text{qubits} = 4d - 2 + n_x + n_y + n_z + 3n_v$
- quantum primitives for streaming, specular reflection/bounce back BC treatment, object detection
- efficient read-out of body forces via quantum momentum exchange method

WAIT! What about collision?

We showed that amplitude-based encoding cannot work for the collision operator and computational basis state encoding cannot work for the streaming operator.

Sketch of the proof – part 1

- Consider two admissible states in **amplitude encoding**

$$|\psi_1\rangle = |x\rangle(\alpha_0|v_0\rangle + \alpha_1|v_1\rangle) \quad \text{and} \quad |\psi_2\rangle = |x\rangle|v_2\rangle$$

- Let U_{col} be a hypothetical collision operator then

$$|\psi_1{}'\rangle = I \otimes U_{\text{col}}|\psi_1\rangle = |x\rangle \otimes U_{\text{col}}(\alpha_0|v_0\rangle + \alpha_1|v_1\rangle) = |x\rangle\big(\gamma_0(\alpha_0|v_0\rangle + \alpha_1|v_1\rangle) + \gamma_1(\beta_2|v_2\rangle + \beta_3|v_3\rangle)\big)$$

$$|\psi_2{}'\rangle = I \otimes U_{\text{col}}|\psi_2\rangle = |x\rangle \otimes U_{\text{col}}|v_2\rangle = \mathrm{e}^{i\theta}|x\rangle|v_2\rangle$$

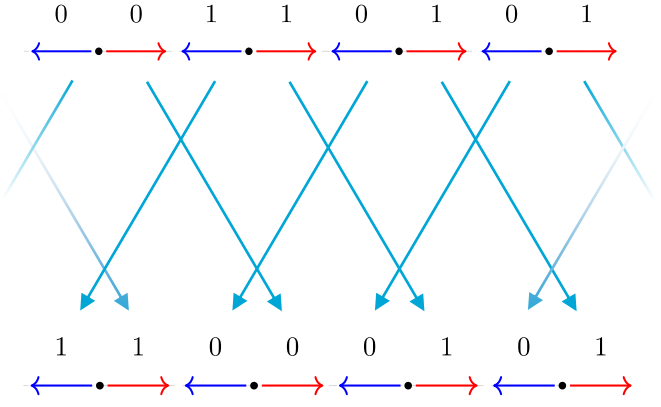
- For U_{col} to be unitary we must have that $\langle\psi_1|\psi_2\rangle = \langle\psi_1|U_{\text{col}}^{\dagger}U_{\text{col}}|\psi_2\rangle$. However

$$0 = \langle\psi_1|\psi_2\rangle = \cdots = e^{i\theta}\langle\gamma_0(\alpha_0\langle v_0| + \alpha_1\langle v_1|) + \gamma_1(\beta_2\langle v_2| + \beta_3\langle v_3|)|\langle x||x\rangle|v_2\rangle = e^{i\theta}\gamma_1\beta_2$$

Sketch of the proof – part 2

- Encoding of velocities in the **computational basis**

$$|\psi_1\rangle = \frac{1}{2}(|00\rangle|00\rangle + |01\rangle|11\rangle + |10\rangle|01\rangle + |11\rangle|01\rangle)$$



- After streaming

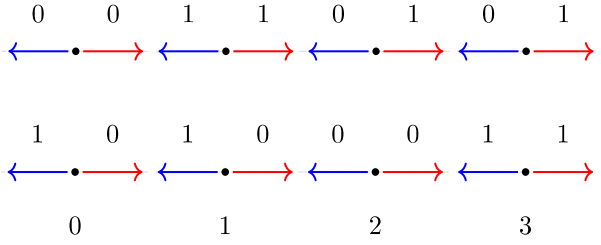
$$|\psi_1'\rangle = \frac{1}{2}(|00\rangle|11\rangle + |01\rangle|00\rangle + |10\rangle|10\rangle + |11\rangle|10\rangle)$$

Sketch of the proof – part 2

- Encoding of velocities in the **computational basis**

$$|\psi_1\rangle = \tfrac{1}{2}(|00\rangle|00\rangle + |01\rangle|11\rangle + |10\rangle|01\rangle + |11\rangle|01\rangle)$$

$$|\psi_2\rangle = \tfrac{1}{2}(|00\rangle|10\rangle + |01\rangle|10\rangle + |10\rangle|00\rangle + |11\rangle|11\rangle)$$



- After streaming

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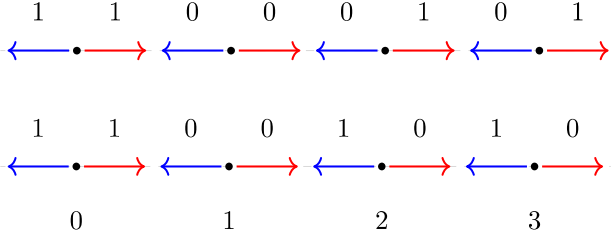


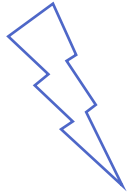
Sketch of the proof – part 2

- Encoding of velocities in the **computational basis**

$$|\psi_1\rangle = \tfrac{1}{2}(|00\rangle|00\rangle + |01\rangle|11\rangle + |10\rangle|01\rangle + |11\rangle|01\rangle)$$

$$|\psi_2\rangle = \tfrac{1}{2}(|00\rangle|10\rangle + |01\rangle|10\rangle + |10\rangle|00\rangle + |11\rangle|11\rangle)$$

$$\langle\psi_1|\psi_2\rangle = 0$$



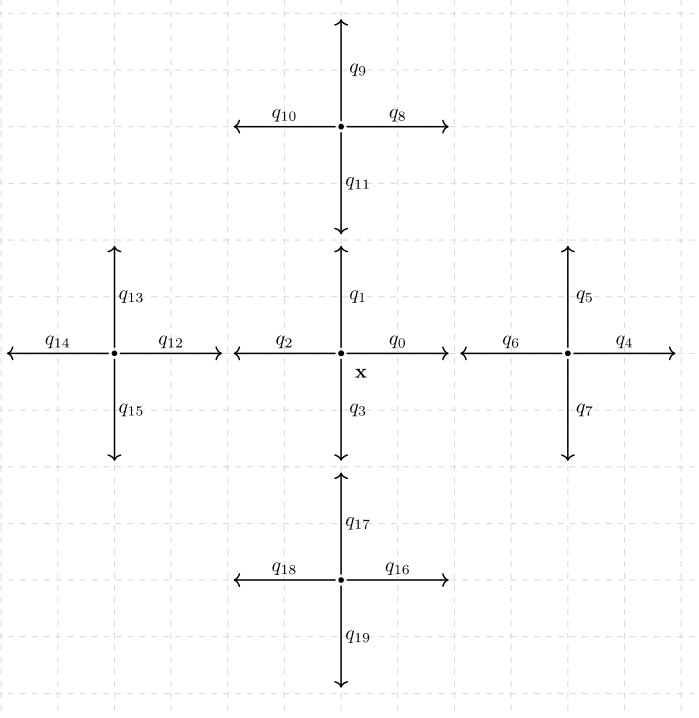
- After streaming

$$|\psi_1'\rangle = \tfrac{1}{2}(|00\rangle|11\rangle + |01\rangle|00\rangle + |10\rangle|10\rangle + |11\rangle|10\rangle)$$

$$|\psi_2'\rangle = \tfrac{1}{2}(|00\rangle|11\rangle + |01\rangle|00\rangle + |10\rangle|01\rangle + |11\rangle|01\rangle)$$

$$\langle\psi_1'|\psi_2'\rangle = \tfrac{1}{2}$$

Space-time encoding



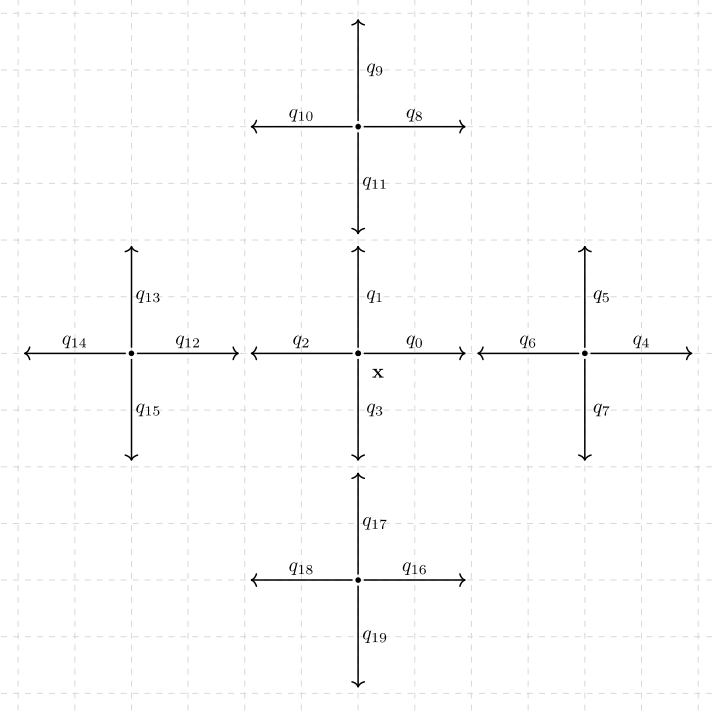
- **Idea**: Basis encoding taking into account "all" lattices from which particles can reach $\boldsymbol{x}$ within N_t time steps

$$|x\rangle|q_0 \dots q_{19}\rangle$$

- Number of qubits for N_t time steps of D2Q4

$$n_v = 4 + \sum_{i=1}^{N_t} 16i = 8N_t^2 + 8N_t + 4$$

Space-time encoding



- **Pros**
  - streaming *and* collision as unitary operators
  - streaming is just a sequence of swaps with less and less swaps for later time steps
  - collision operator can be constructed by inspecting equivalent classes
- **Cons**
  - Resource requirements (#qubits and #swaps) grow with N_t

Further reading

- Merel A. Schalkers and Matthias Möller. Efficient and fail-safe quantum algorithm for the transport equation. Journal of Computational Physics, 502:112816, April 2024. DOI: 10.1016/j.jcp.2024.112816
- Merel A. Schalkers and Matthias Möller. On the importance of data encoding in quantum Boltzmann methods. Quantum Information Processing, 23(1), January 2024. DOI: 10.1007/s11128-023-04216-6
- Merel A. Schalkers and Matthias Möller. Momentum exchange method for quantum Boltzmann methods. Computers & Fluids, 285:106453, December 2024. DOI: 10.1016/j.compfluid.2024.106453
- Calin A. Georgescu, Merel A. Schalkers, and Matthias Möller. QLBM - a quantum lattice Boltzmann software framework, 2024. arXiv:2411.19439
- https://github.com/qcfd-lab/qlbm

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Save the date

- CISM Advanced Course: Opportunities and Challenges of Quantum Computing in Computational Mechanics, May 5-9, 2025, Udine
- 1st ECCOMAS Thematic Conference Applied Quantum Methods in Computational Science and Engineering (AQMCSE), Oct 8-10, 2025, Aachen

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