Quantum Computing for Continuum Mechanics

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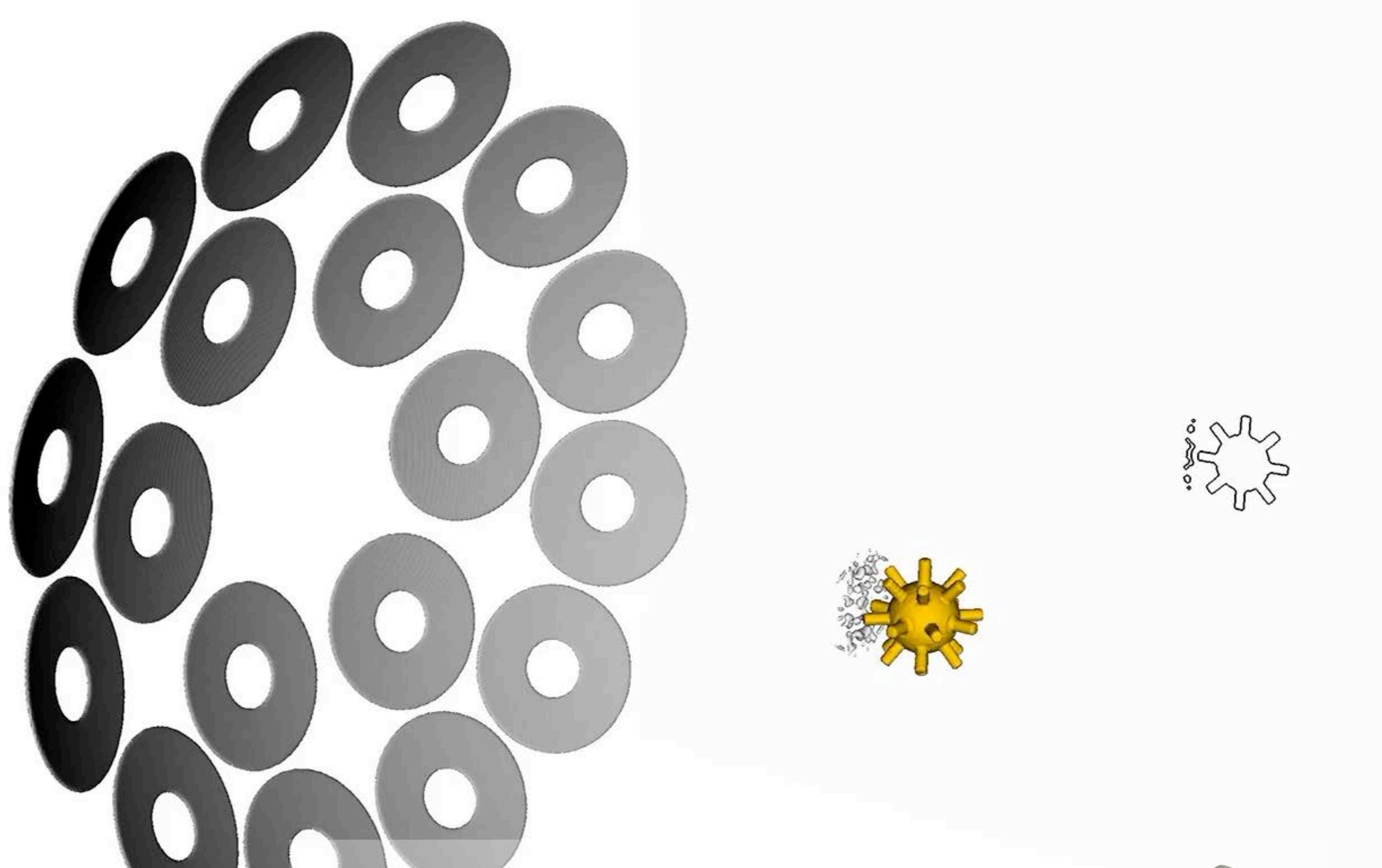
CRNCH Summit 2022

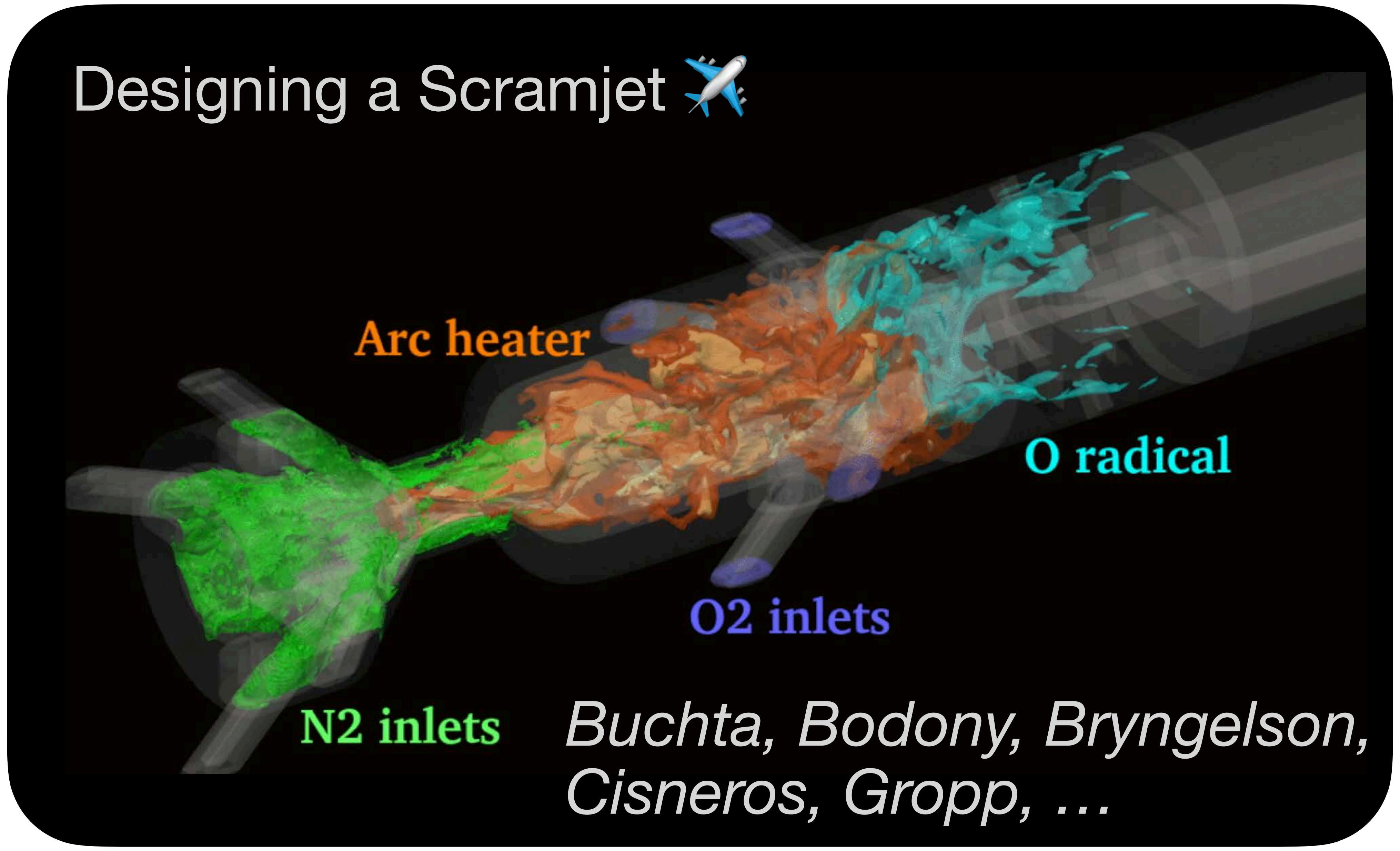
https://comp-physics.group

We do computational mechanics!

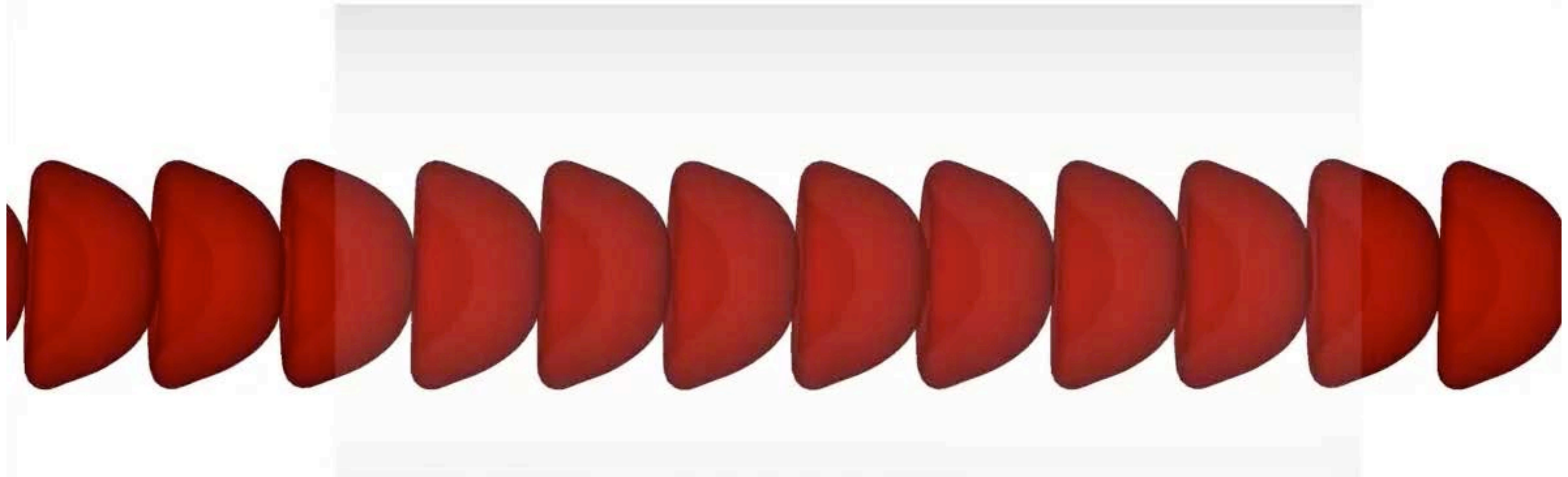
Droplet Atomization 😮‍💨
Schmidmayer, Dorschner, Bryngelson



Treating Kidney Stones 🪨
Maeda, Bryngelson, Colonius



Designing a Scramjet ✈️
Buchta, Bodony, Bryngelson, Cisneros, Gropp, …



Creating a Bio-microfluidic Device 🩸
Bryngelson, Freund, Zhao

Typical CFD

- Grid + connectivity
- PDE model

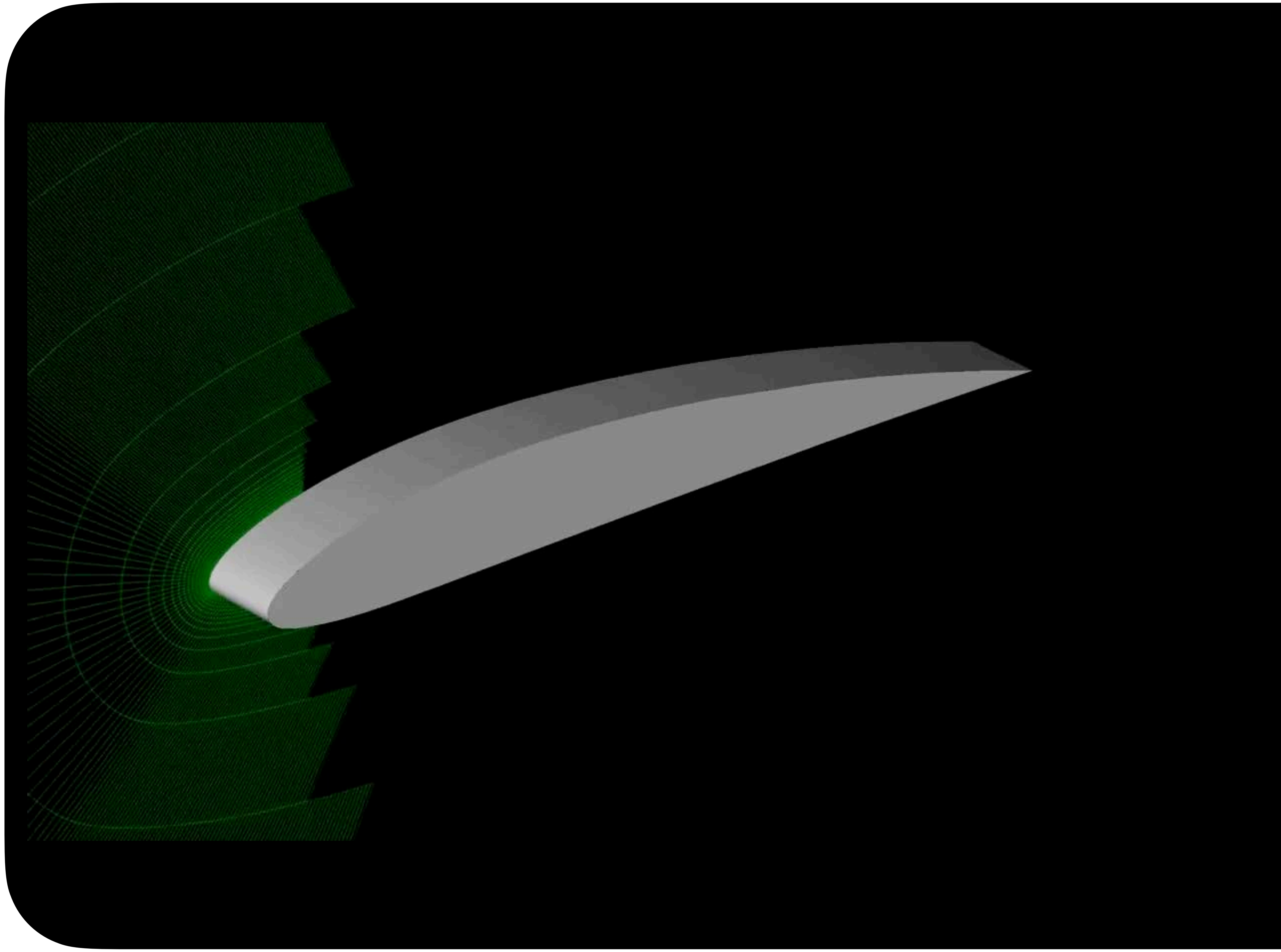
$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = - \nabla p + \mu \nabla^2 \mathbf{u}$$

- Numerics

$$\frac{\partial u_{i,j}}{\partial x_i} \approx \frac{u_{i,j+1} - u_{i,j-1}}{2\Delta x_{i,j}}$$

- Loop through space $N \sim 10^{12}$ and time



Dan Henningson *et al.*, SeRC, KTH (2015)

The problem

OLCF Summit: 10 MW

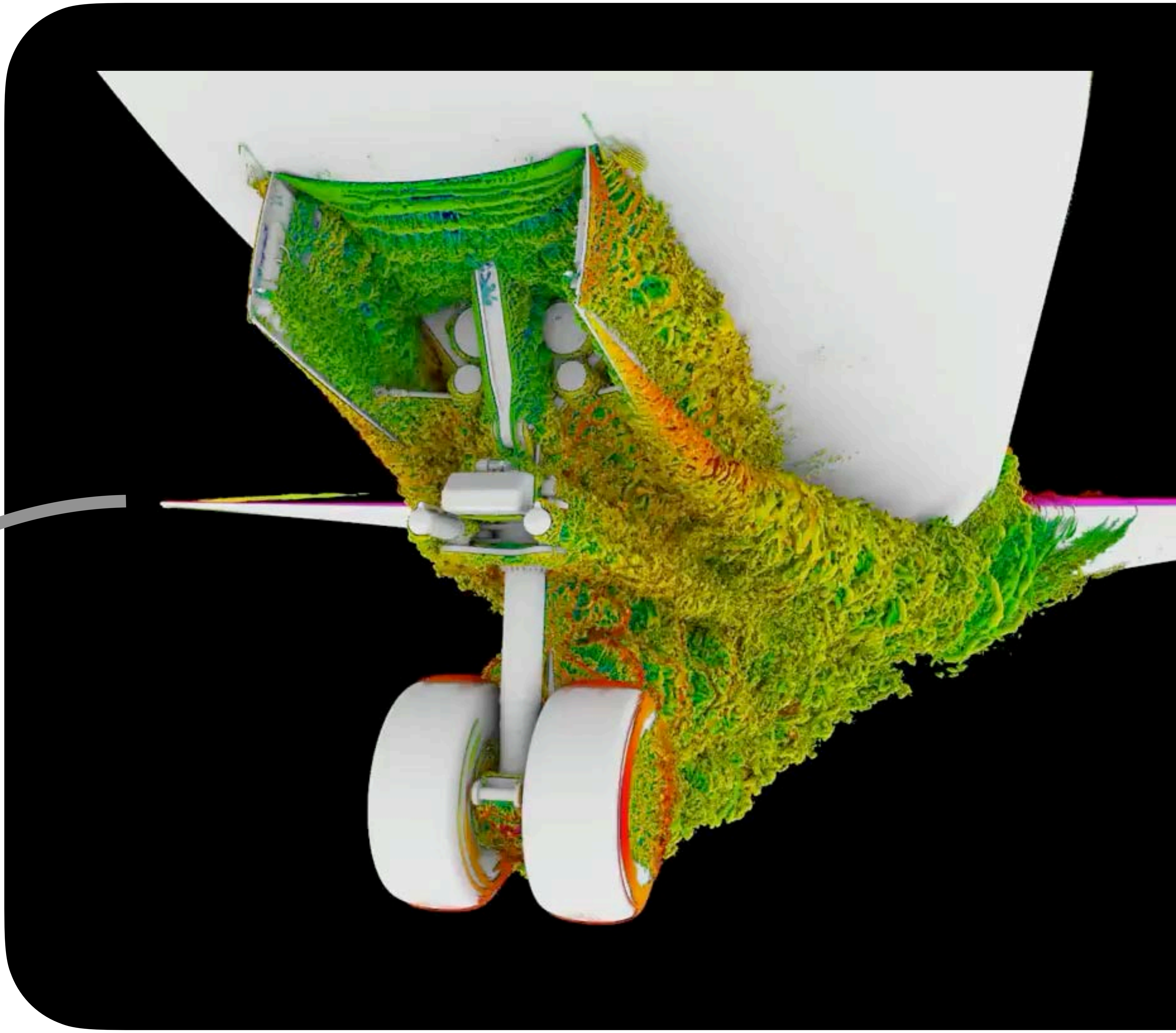
Coal Power Plant: 10 MW

→ 22,000 lb of CO_2 per hour

EPA eGRID (2018)
ZBG Energy (2021)

An experiment

- Boeing 737, LA ↔ NYC: 1,000 lb CO_2
- Simulation of flow over landing gear
  - 25,000 lb CO_2



C_D

Drag Coefficient
(Scalar!)

This is unsustainable

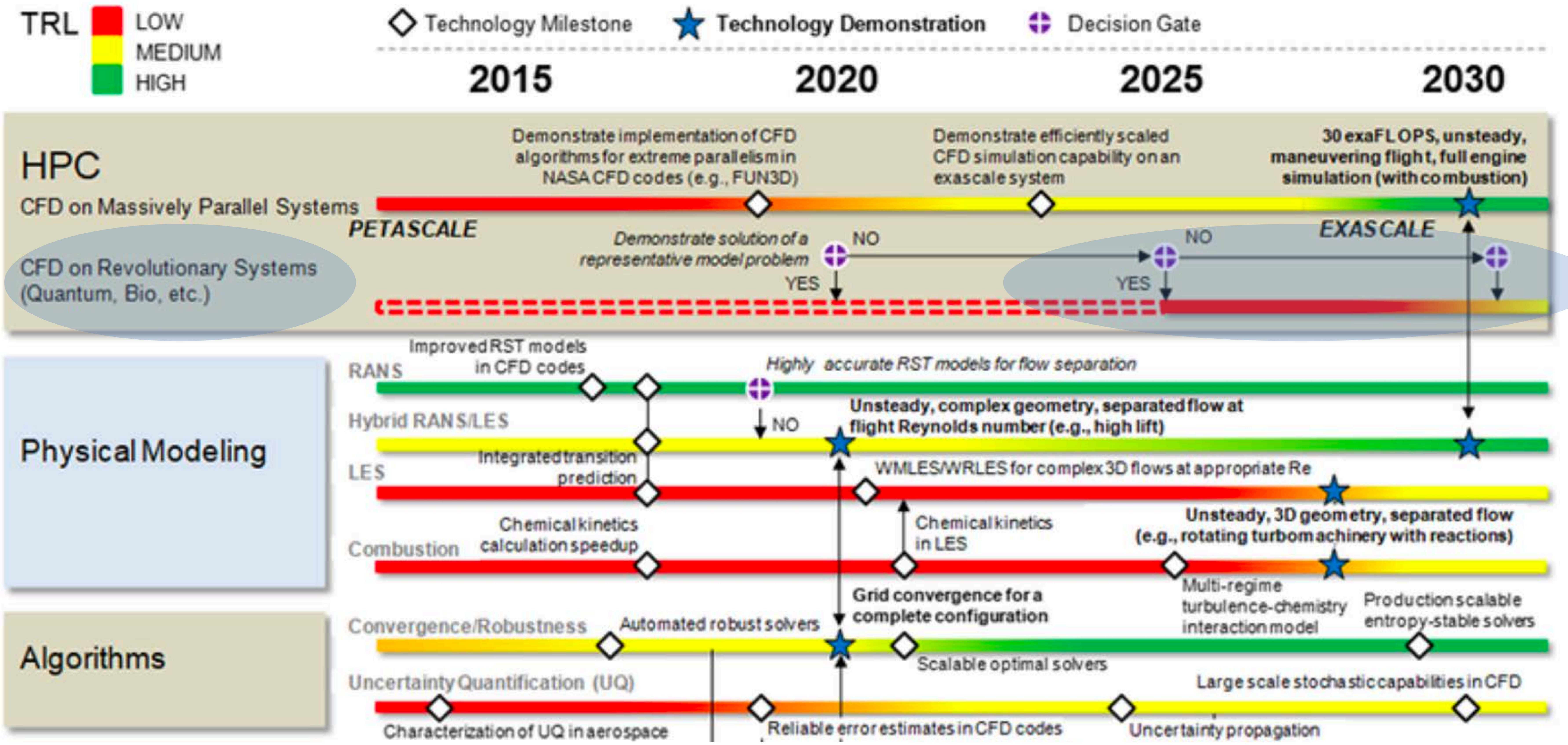
Moran *et al.*, SC17

1.6B Grid Points, NASA Pleiades, 1 Week

Why quantum?

- Classical CFD inefficient
- Few key observables
- N is large (~10^{12}) and growing
- We *need* to explore alternatives

The CFD Vision 2030 Roadmap (NASA)



Cary et al. (2020)
cfd2030.com

Help!

*“...we need to generate more interaction between **aerospace scientists and engineers and quantum computing researchers**. We have reached a point in the development of quantum computing and other quantum technologies where **collaboration beyond a specific scientific field is going to be key to further developments**…”*

—P. Givi, A. Daley, D. Mavriplis and M. Malik (2020)

Our effort (est. Oct 2021)

- A. Alexeev (ME)
- S. Bryngelson (CSE)
- J. Young (CS)

- F. Chrit (ME/CSE)
- S. Kocherla (CS)
- A. Adams (CS)
- … and more!

- B. Gard (CIPHER)

- R. Bennink (QCSG)
- E. Dumitrescu (QCSG)
- C. Hauck (CSM)

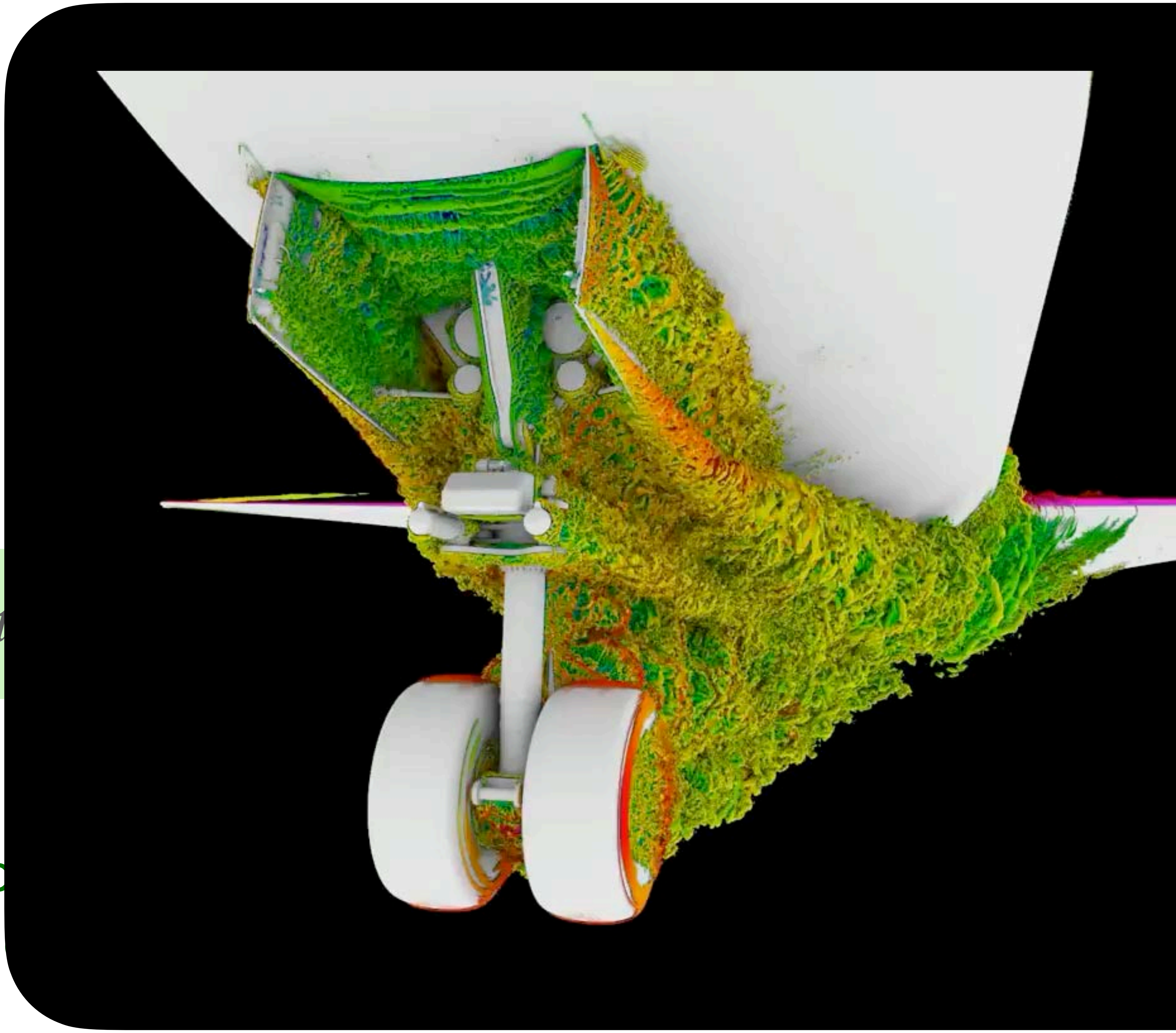
Lattice Boltzmann

- Model fluid as fictive particles
- Undergo processes on a lattice
- Distribution evolves in time and space

$$f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_{ij} \left(f_j^{(\mathrm{eq})}(\mathbf{x}, t \right.$$

Streaming
(model for advection)

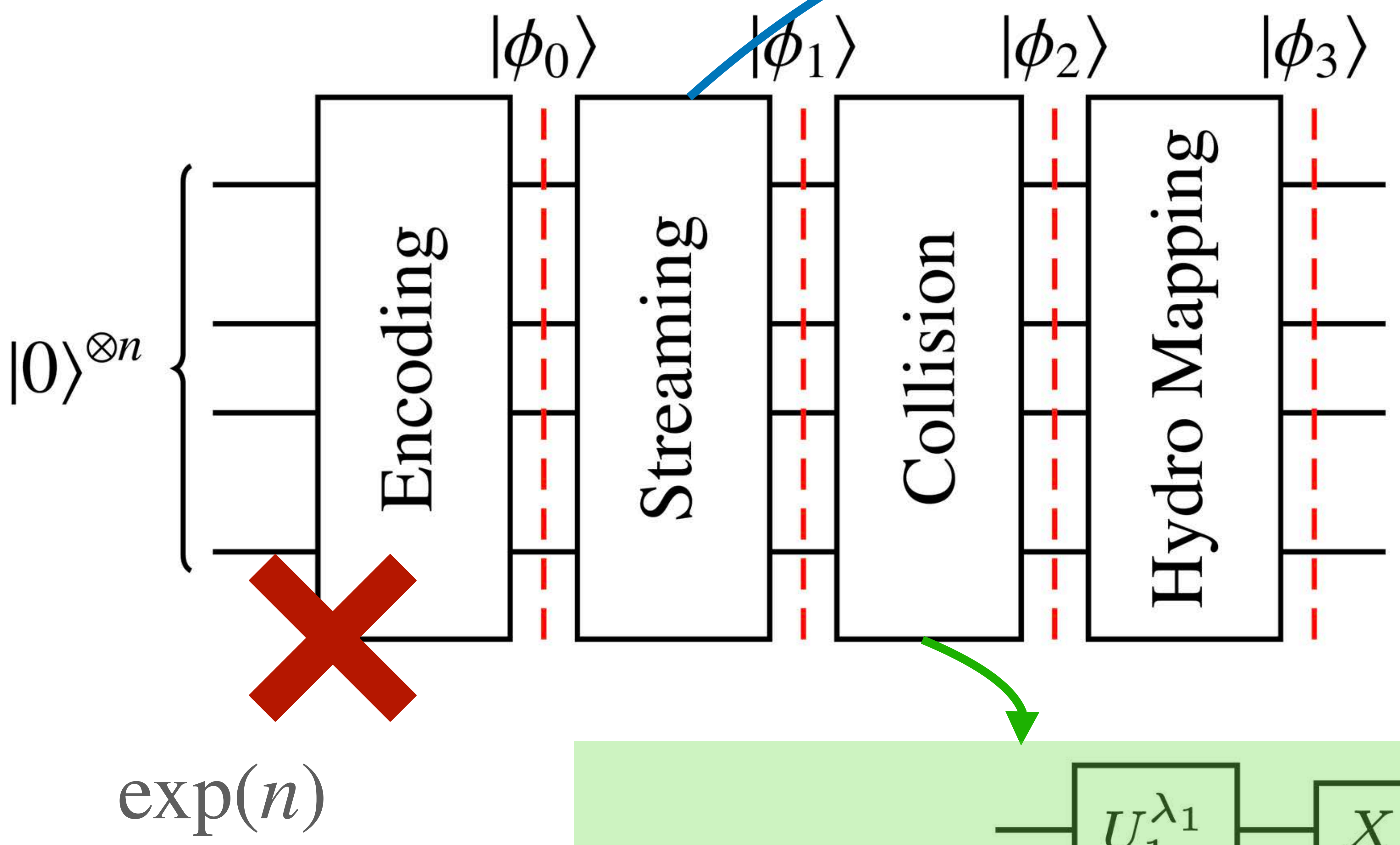
Co
(m



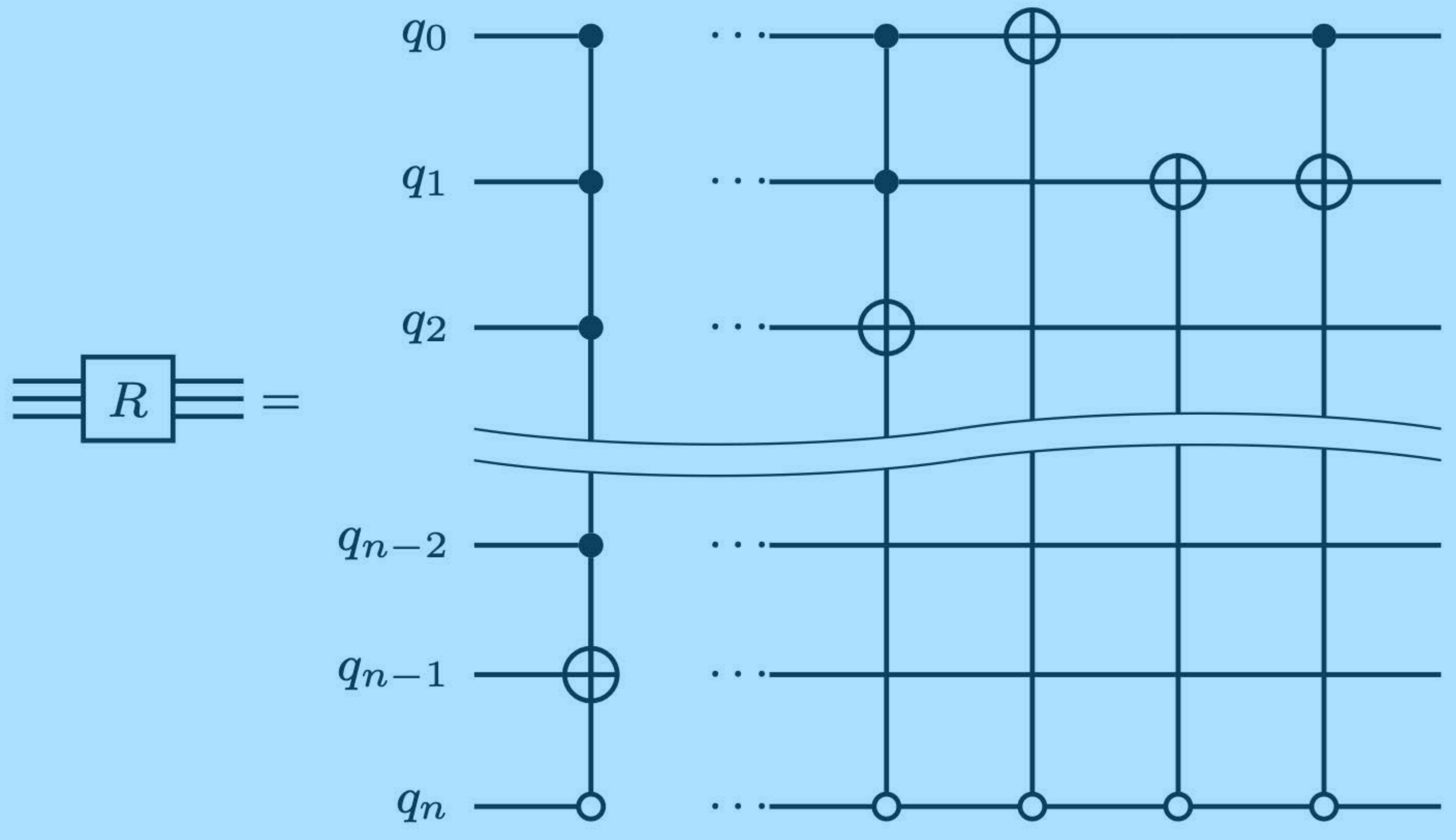
- Recover macroscopic quantities from fictive ones

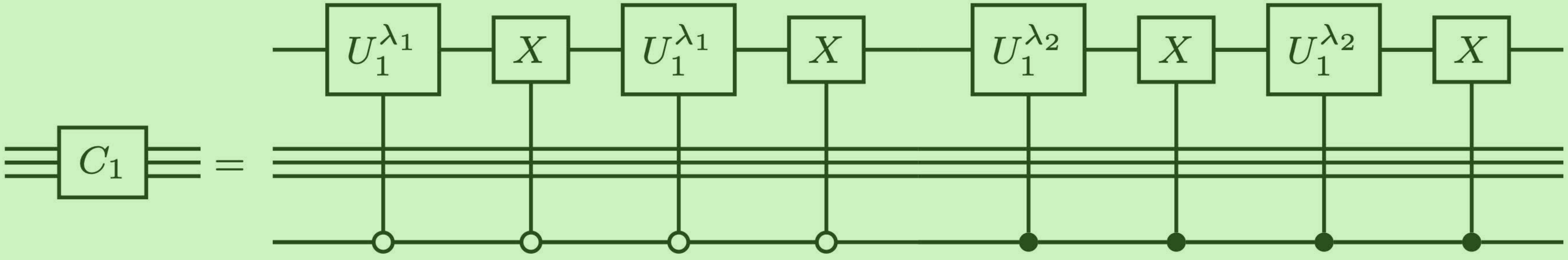
Chen and Doolen (1998)

A quantum lattice Boltzmann



Streaming: quantum random walk $\mathcal{O}(\log_2 \alpha)$



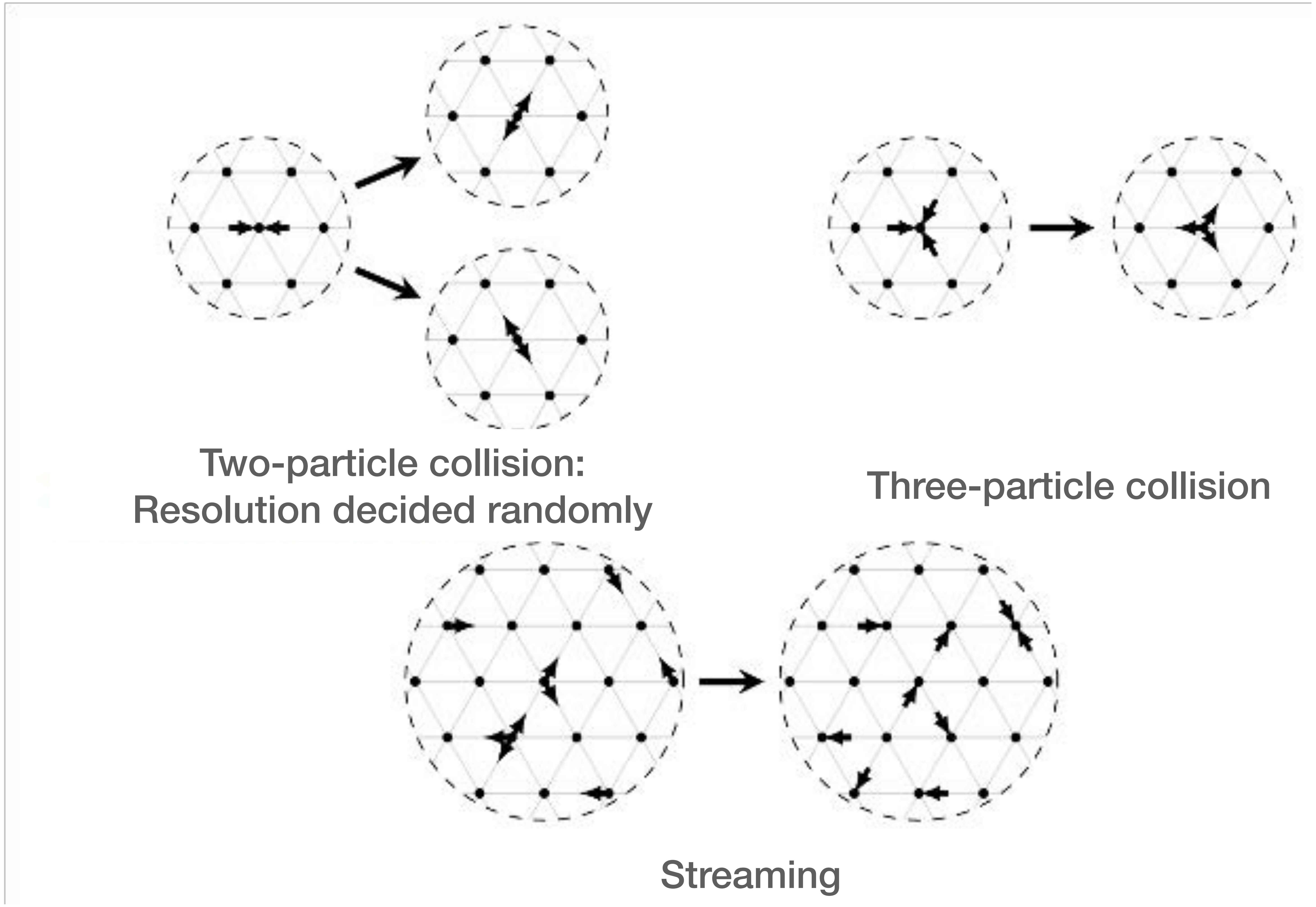


Collision: linear combination of unitaries $\mathcal{O}(\alpha)$

Aharonov *et al.* (1993)
Meyer (1999)
Shende *et al.* (2006)
Budinski (2021)

A quantum lattice gas

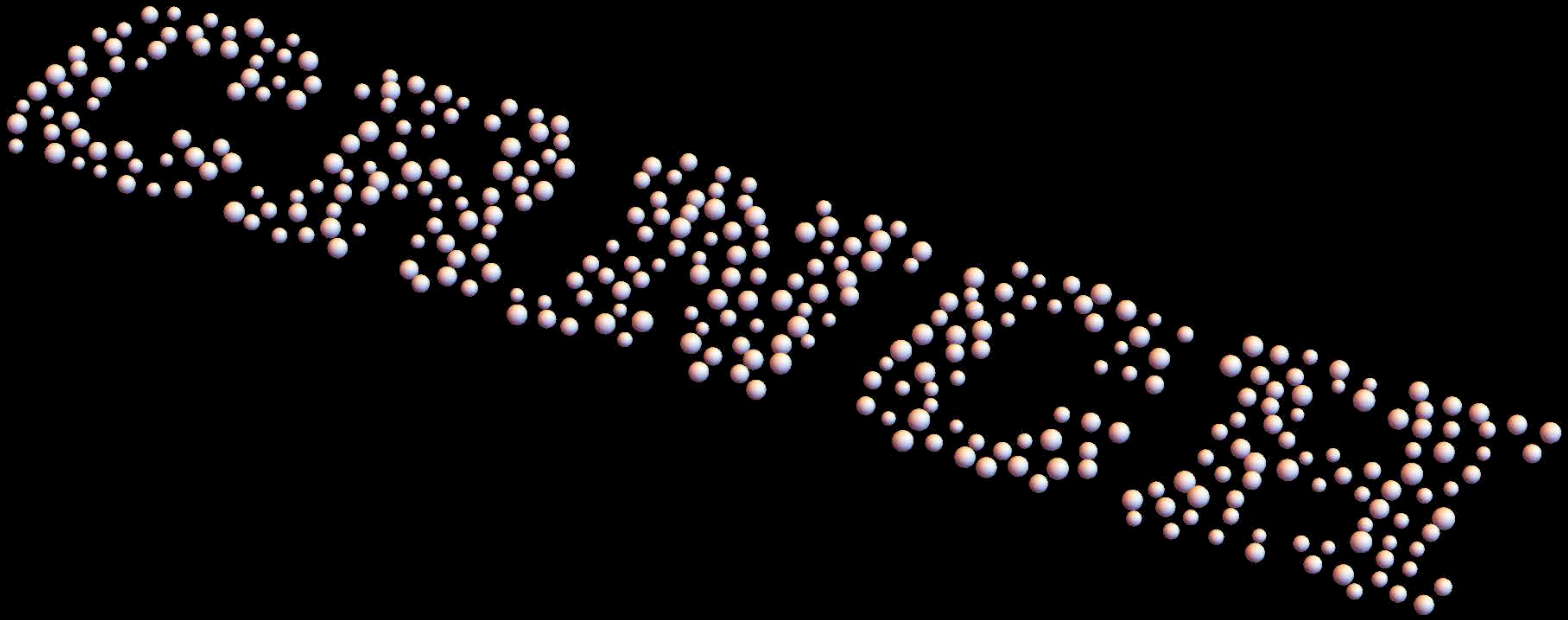
- Lattice gas fallen out of favor to LB in classic computing
- QLG special case of quant. cellular automata (QCA)
- Could recover missing classic properties
- Fewer collision gates



Grössing and Zeilinger (1988)
Lent, Tougaw, *et al.* (1993)
Yepez (1998–2002)

Onward

- Alternative encoding required for large N
  - Leverage low-dimensionality of observables?
- QLG resurrection for CFD
  - Can it cure the classical lattice gas method?
  - Integrate streaming and hydrodynamic operators



Thank you!

Animation shows bubbles cavitating in response to a shock wave