BENCHMARKS FROM PLASMA PHYSICS AND CFD

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Quantum Computing Requires Linearity and Unitarity

Plasma Physics, CFD
- Nonlinear
- Nonunitary

MHD
Two-fluids
Vlasov

Quantum Computing
- Linear
- Unitary

$$\frac{d|\psi\rangle}{dt} = -iH|\psi\rangle$$

Quantum algorithms need to linearize and embed into a larger Hilbert space to be able to simulate.

Quantum encoding

- Building blocks are qubits (not considering analog encodings in this talk).
- Single-qubit state:

Linear combination

$$|\psi\rangle = \overbrace{a|0\rangle + b|1\rangle} = \begin{pmatrix} a \\ b \end{pmatrix}$$

Amplitudes can encode information.

- Encoding of initial states into amplitudes and extraction of classical information from the amplitudes can lead to additional computational complexity.
- Embedding into a larger Hilbert space (block encoding) also leads to added complexity and typically needs sparsity.

From verifiable to intractable benchmarks

Can classical computers verify plasma physics simulations?

Verifiable benchmark plasma physics problems? → **Computationally expensive plasma physics problems**

- Solutions could be analytically known.
- Classical algorithms for efficient verification
- Quantum algorithm has only a polynomial speed-up

Initial benchmarks

- Analytically or computationally intractable classically.
- Solutions not necessarily known.
- Can only be tested through experiments in the plasma physics.

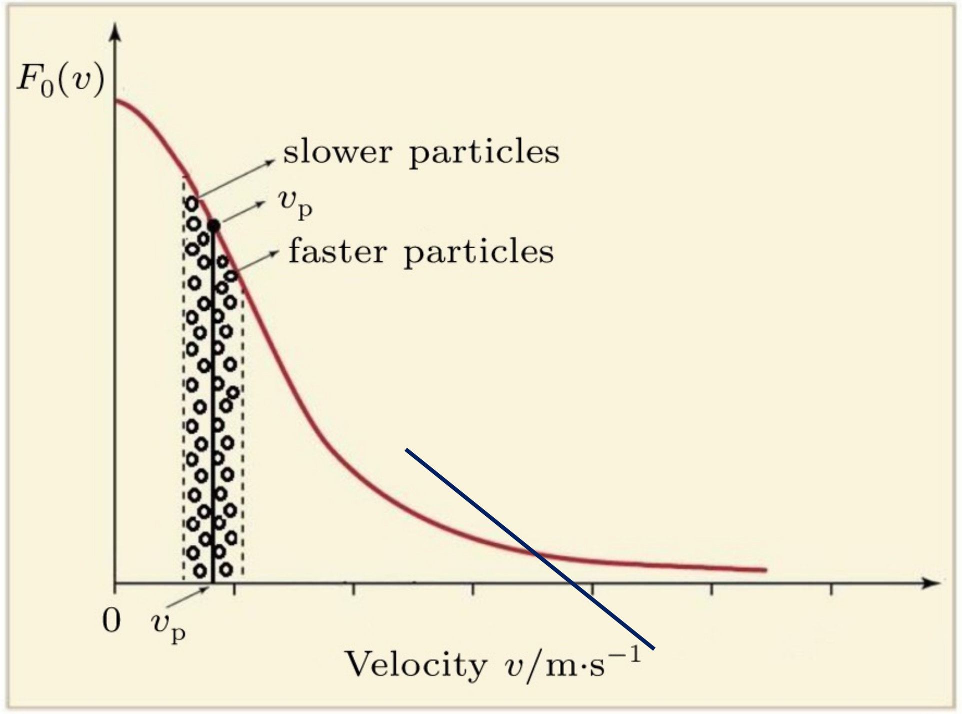
Final benchmarks

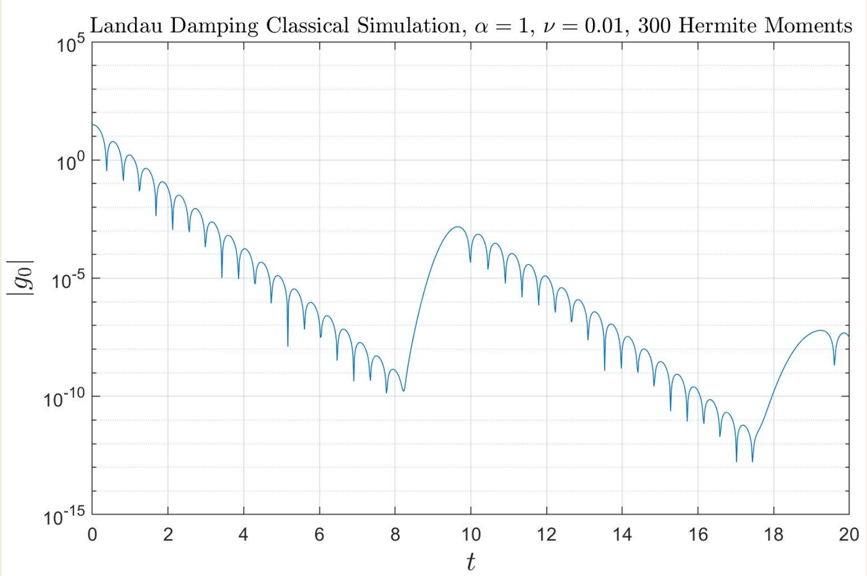
Solving Benchmark Problems for resource estimation

Can we solve benchmark plasma physics problems on quantum computers?

Can we recreate linear Landau damping on quantum computers?

- Well-known result in plasma physics.
- Nontrivial to solve in general.
- Linearize to solve on quantum computers.





Linearized Vlasov equation

Transform the linearized Vlasov-Poisson system to one that is easier to work with on a quantum computer.

↓ Hermite transform

Linear differential equation in the Hermite basis with a stable matrix.

↓ Quantum ODE solver

Determine the spectral abscissa to extract the Landau damping rate.

Collisional Vlasov-Poisson System

Transform the linearized Vlasov-Poisson system to a system that is easier to work with on a quantum computer.

Distribution function | Species (ion/electron) | Mass | Charge | Electric field | Collision operator

$$\frac{\partial f_s}{\partial t} + \boldsymbol{v} \cdot \nabla f_s + \frac{q_s}{m_s} \boldsymbol{E} \cdot \frac{\partial f_s}{\partial \boldsymbol{v}} = C[f_s]$$

$$\epsilon_0 \nabla \cdot \boldsymbol{E} = \sum_{s=i,e} q_s \int f_s d^3\boldsymbol{v}$$

- Solves for the time evolution of the distribution functions $f_s(\boldsymbol{x}, \boldsymbol{v}, t)$ as well as the electric field $\boldsymbol{E}(\boldsymbol{x}, t)$.

From Nonlinear PDEs to Linear ODEs

Transform the linearized Vlasov-Poisson system to a system that is easier to work with on a quantum computer.

$$\frac{\partial f_s}{\partial t} + \boldsymbol{v} \cdot \nabla f_s + \frac{q_s}{m_s} \boldsymbol{E} \cdot \frac{\partial f_s}{\partial \boldsymbol{v}} = C[f_s]$$

	Solves for
1D in space and 1D in velocity	$f(z, v, t)$
Linearize about a Maxwellian background	$g(z, v, t)$
Hermite Transform in v	$g_m(z, t)$
Fourier transform in z	$g_{m,k}(t)$
Rescale Variables	$\tilde{g}_{m,k}(t)$

$$\frac{d\tilde{\boldsymbol{g}}_k}{dt} = \tilde{A}\tilde{\boldsymbol{g}}_k$$

$$\tilde{A} = -\begin{pmatrix} 0 & ik\sqrt{\frac{1+\alpha}{2}} & 0 & 0 & 0 & 0 \\ ik\sqrt{\frac{1+\alpha}{2}} & 0 & ik & 0 & 0 & 0 \\ 0 & ik & 2\nu & ik\sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & ik\sqrt{\frac{m_{max-1}}{2}} & \nu m_{max-1} & ik\sqrt{\frac{m_{max-1}+1}{2}} \\ 0 & 0 & 0 & 0 & ik\sqrt{\frac{m_{max}}{2}} & \nu m_{max} \end{pmatrix}$$

α captures the physics of the problem.

ν is the collision frequency.

Collisionless Case

$$\tilde{A} = -\begin{pmatrix} 0 & ik\sqrt{\frac{1+\alpha}{2}} & 0 & 0 & 0 & 0 \\ ik\sqrt{\frac{1+\alpha}{2}} & 0 & ik & 0 & 0 & 0 \\ 0 & ik & 0 & ik\sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & ik\sqrt{\frac{m_{max-1}}{2}} & 0 & ik\sqrt{\frac{m_{max-1}+1}{2}} \\ 0 & 0 & 0 & 0 & ik\sqrt{\frac{m_{max}}{2}} & 0 \end{pmatrix}$$

Collisionless Case

$$\tilde{A} = -\begin{pmatrix} 0 & ik\sqrt{\frac{1+\alpha}{2}} & 0 & 0 & 0 & 0 \\ ik\sqrt{\frac{1+\alpha}{2}} & 0 & ik & 0 & 0 & 0 \\ 0 & ik & 0 & ik\sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & ik\sqrt{\frac{m_{max-1}}{2}} & 0 & ik\sqrt{\frac{m_{max-1}+1}{2}} \\ 0 & 0 & 0 & 0 & ik\sqrt{\frac{m_{max}}{2}} & 0 \end{pmatrix}$$

$\tilde{A}$ can be written as iH, where H is a Hermitian matrix ($H^\dagger = H$).

The equation becomes:

$$\frac{d\tilde{\boldsymbol{g}}_k}{dt} = iH\tilde{\boldsymbol{g}}_k$$

$$\tilde{\boldsymbol{g}}_k = e^{iHt}\tilde{\boldsymbol{g}}_k(t=0)$$

Schrodinger's equation:

$$\frac{d|\psi\rangle}{dt} = -iH|\psi\rangle$$

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

Can use Hamiltonian simulation algorithms to solve this problem.

Collisional Case

- $\nu \neq 0, A \neq iH.$
  - *Cannot use Hamiltonian simulation.*

$$\tilde{A} = -\begin{pmatrix} 0 & ik\sqrt{\frac{1+\alpha}{2}} & 0 & 0 & 0 & 0 \\ ik\sqrt{\frac{1+\alpha}{2}} & 0 & ik & 0 & 0 & 0 \\ 0 & ik & 2\nu & ik\sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & ik\sqrt{\frac{m_{max-1}}{2}} & \nu m_{max-1} & ik\sqrt{\frac{m_{max-1}+1}{2}} \\ 0 & 0 & 0 & 0 & ik\sqrt{\frac{m_{max}}{2}} & \nu m_{max} \end{pmatrix}$$

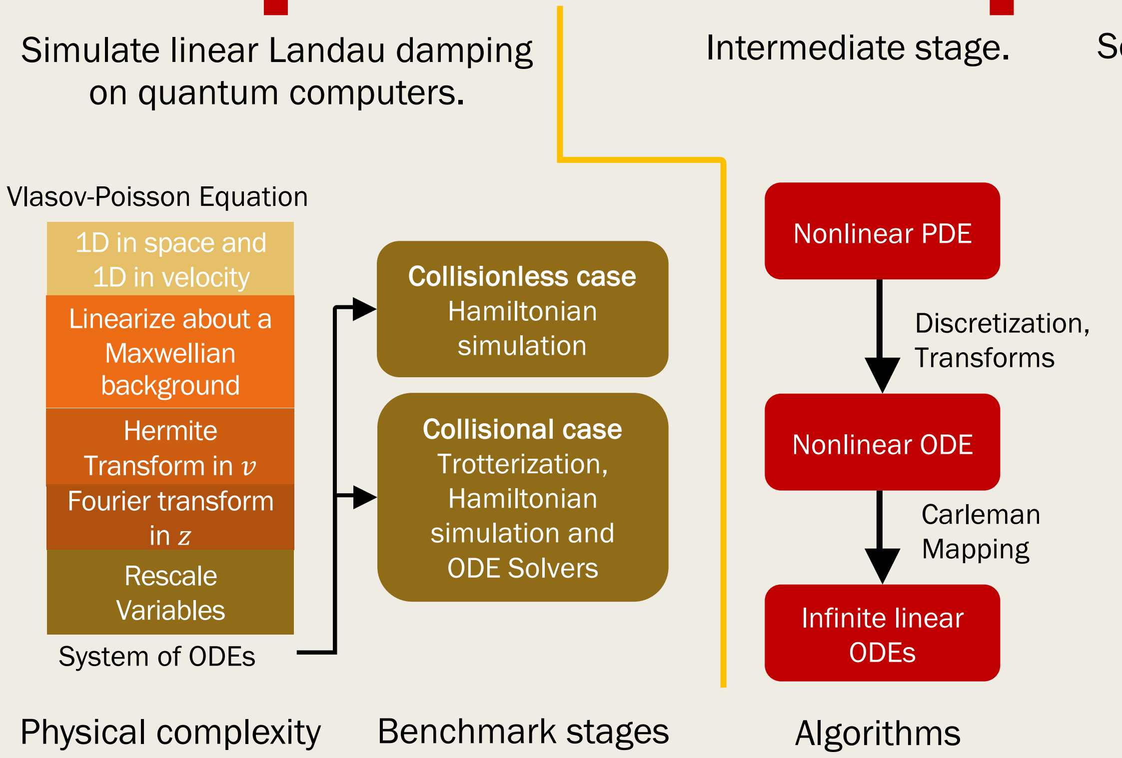
Phys Rev A 107, 062412

Vlasov equation

Impact

- Plasma Physics
- Inertial confinement
- Other fields (e.g., galactic dynamics)

Can quantum computers speed up plasma physics simulations?



Representation	Gate Complexity Classical	Gate Complexity Quantum
ESP [34]	$\mathcal{O}(N_v/\epsilon^{\theta})$	$\mathcal{O}(\mathrm{polylog}(N_v)/\epsilon)$
Hermite	$\mathcal{O}(N/\epsilon^{\theta})$	$\mathcal{O}(\sqrt{N}\log(N)/\epsilon)$

TABLE I. Gate complexities of the algorithms to estimate Landau damping discussed in this paper. Here N is the Hermite system size, N_v is the ESP system size, ϵ is the absolute error in amplitude estimation, and $\theta \leq 1$ is the order of the classical ODE solver, with smaller values corresponding to higher-order solvers. The simulation time T is a constant and is omitted from the complexity analysis.

Phys Rev A 107, 062412

Inertial confinement Fusion

VLASOV EQUATION IS IMPORTANT TO UNDERSTAND FOR INERTIAL CONFINEMENT FUSION

COLLISIONLESS ELECTROSTATIC,

COLLISIONLESS ELECTROMAGNETIC

COLLISIONAL VLASOV EQUATIONS

$$\frac{\partial f(x,v,t)}{\partial t} + v \cdot \nabla_x f(x,v,t) - E(x,t) \cdot \nabla_v f(x,v,t) = 0$$

$$-\Delta\phi(x,t) = 1 - \rho(x,t) \quad , \quad E(x,t) = -\nabla\phi(x,t)$$

$$\nabla \cdot E = \frac{\rho}{\epsilon} \quad , \quad \rho = \int f(x,v,t)\,.$$

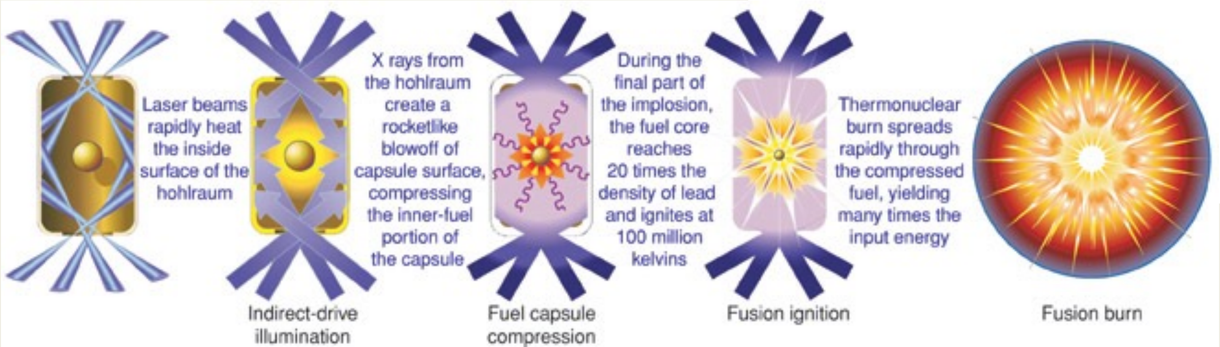
$$\frac{\partial c_\ell^k}{\partial t} + \frac{1}{\epsilon\gamma\sqrt{2}}\frac{2\pi k i}{L_x}\left(\sqrt{\ell+1}\,c_\ell^k + \sqrt{\ell}\,c_{\ell-1}^k\right)$$

$$-\frac{\sqrt{2}\epsilon}{\gamma}\left((\gamma^2-1)\sqrt{\ell+1}[E(t)*c_{\ell+1}][k] - \sqrt{\ell}[E(t)*c_{\ell-1}][k]\right) = 0\,,$$

$$[E(t)*c_{\ell+1}][k] = \sum_{j=-N_x}^{N_x} E_{k-j}c_\ell^j\,.$$

$$E_k(t) = \frac{iL_x}{2\pi k}\sum_{\ell=0}^{N_v-1} c_\ell^k(t) I_\ell \text{ for } k \neq 0\,.$$

BIT Numer. Math 61, 881-909 (2021)



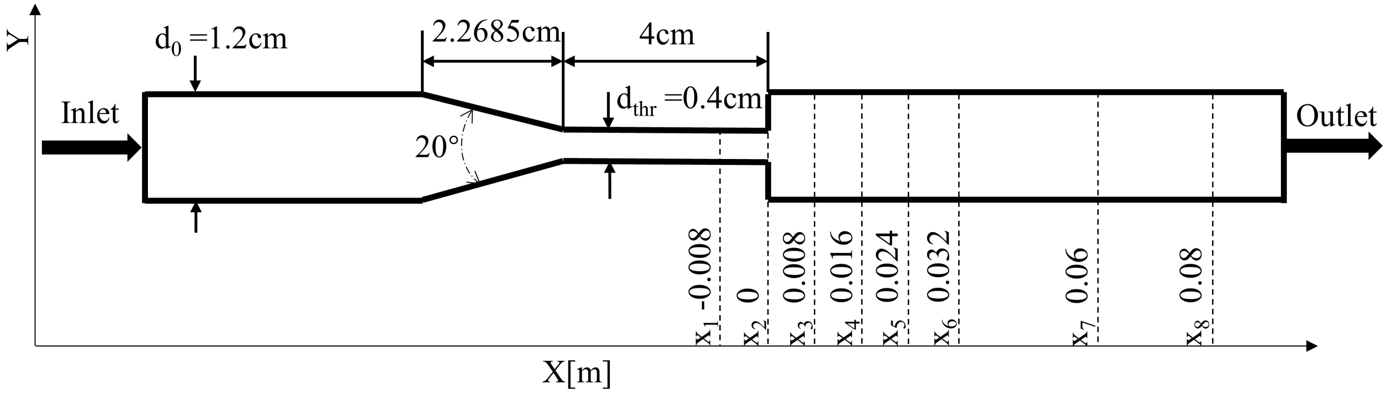
FDA Nozzle

FDA BENCHMARK NOZZLE FLOW

CORE PROBLEM IS A NAVIER-STOKES EQUATION

MAPPED TO A LATTICE BOLTZMANN EQUATION WITH LOW MACH NUMBER

REYNOLDS NUMBER CAN BE HIGH



$$\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta) + \partial_\beta \mathcal{T}_{\alpha\beta} = 0,$$

$$\mathcal{T}_{\alpha\beta} = p\delta_{\alpha\beta} - \mu\left(\partial_\beta u_\alpha + \partial_\alpha u_\beta - \frac{2}{D}\partial_\gamma u_\gamma \delta_{\alpha\beta}\right) - \eta\partial_\gamma u_\gamma \delta_{\alpha\beta}$$

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i\delta t, t + \delta t) - f_i(\boldsymbol{x}, t) = \frac{\delta t}{\bar{\tau}}\left(f_i^{\text{eq}}(\rho, \boldsymbol{u}) - f_i(\boldsymbol{x}, t)\right)$$

$$f_i^{\text{eq}}(\rho, \boldsymbol{u}) = \sum_{n=0}^{N} \frac{w_i}{i!\theta_0^i} \boldsymbol{a}_n^{\text{eq}}(\rho, \boldsymbol{u}) : \mathcal{H}_n(\boldsymbol{c}_i)$$

Hermite basis

Comput Methods Programs Biomed (2022)

Quantum lattice Boltzmann

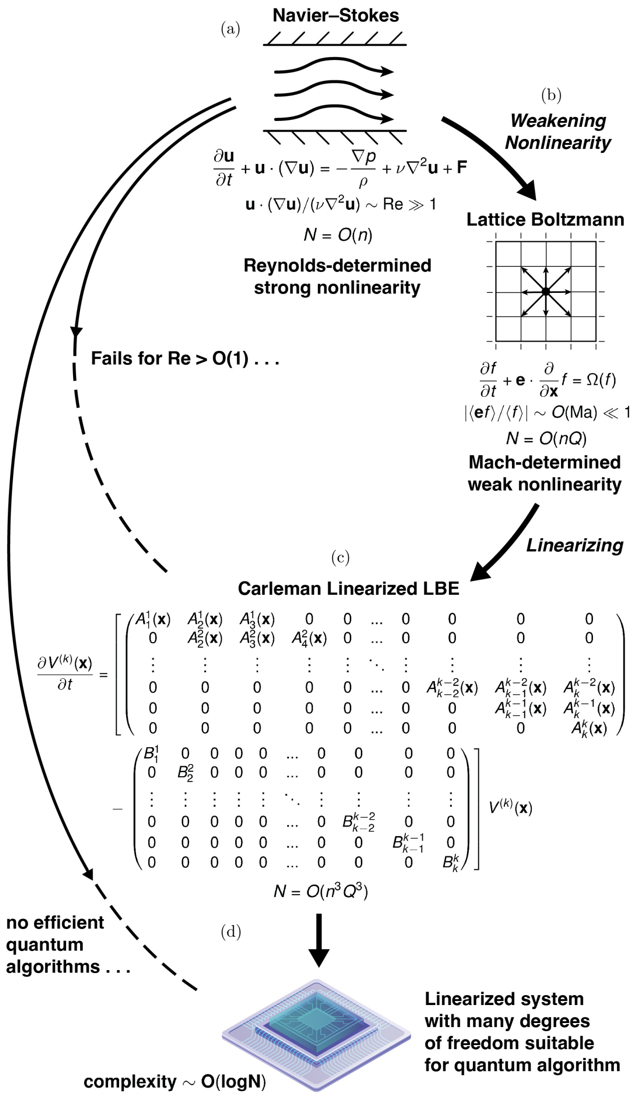
BECOMES NAVIER-STOKES IN THE LOW MACH NUMBER APPROXIMATION

THE COMPLEXITY OF THE ALGORITHM DEPENDS ON THE KNUDSEN NUMBER

KN = O(MACH/REYNOLDS)

CAN GO TO HIGHER REYNOLDS NUMBERS THAN CLASSICAL COMPUTERS IN THIS REGIME.

RECENT WORK (ARXIV:2303:16550) HAS LOOKED AT USING QUANTUM CARLEMAN LINEARIZATION (PNAS 118, E2026805118 (2021)).



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

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho \mathbf{u}) = 0,$$

$$\frac{\partial \tilde{f}_m}{\partial \tilde{t}} + \tilde{\mathbf{e}}_m \cdot \tilde{\nabla} \tilde{f}_m = -\frac{1}{\tilde{\tau}}\left(\tilde{f}_m - \tilde{f}_m^{\mathrm{eq}}\right)$$

$$\partial_t f_m + \mathbf{e}_m \cdot \nabla f_m = -\frac{1}{\tau\,\mathrm{Kn}}(f_m - f_m^{\mathrm{eq}})$$

$$m \in 1, \ldots, Q$$

From arxiv: 2303:16550

Summary

- Plasma physics is difficult to simulate.
  - *Time-and length-scales have an extraordinary range.*
  - *Need massive amounts of computational resources.*
- Limits the rate at which our understanding of the subject expands.
- Many problems in CFD need a large Reynolds number.
- This translates to large nonlinearities in differential equations.
- It would be useful to increase the applicability of quantum algorithms such as quantum Carleman linearization more into the nonlinear regime.
- Also need to find good lower bounds to problems in CFD.