Action Dark Energy, October 29, 2024

Quantum algorithm for collisionless Boltzmann simulation

Naoki Yoshida (University of Tokyo)

Please find the technical details in
Yoshikawa, Tanaka, Yoshida 2021, arxiv:2110.15867
Miyamoto, Yamazaki, Uchida, Fujisawa, Yoshida, 2024, PRD, 6, 013200

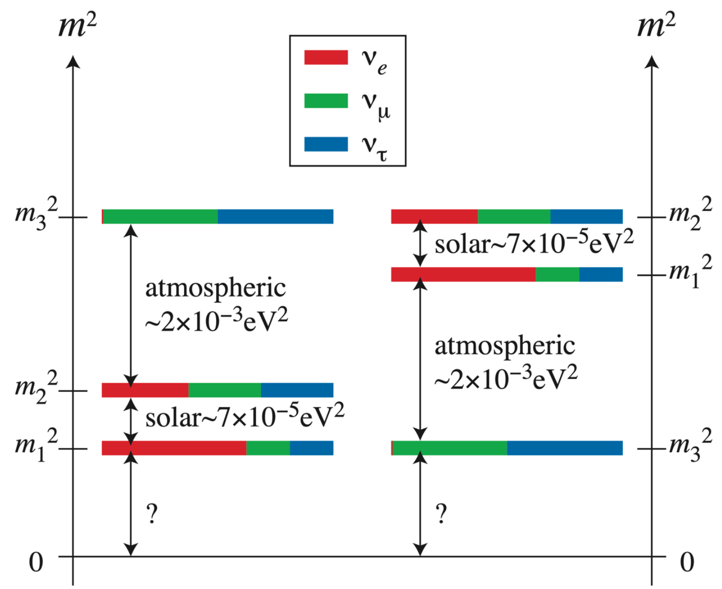
The “minimalist” particle

Neutrinos … they have zero charge, zero size, and possibly zero mass.

Neutrino oscillations have been discovered for atmospheric *ν* and solar *ν*. (2015 Nobel Prize in Physics)

The absolute mass scale is extremely important, but remains largely unknown.

$$\Omega_\nu h^2 = \frac{\sum m_\nu}{94.12\,\mathrm{eV}/c^2}$$

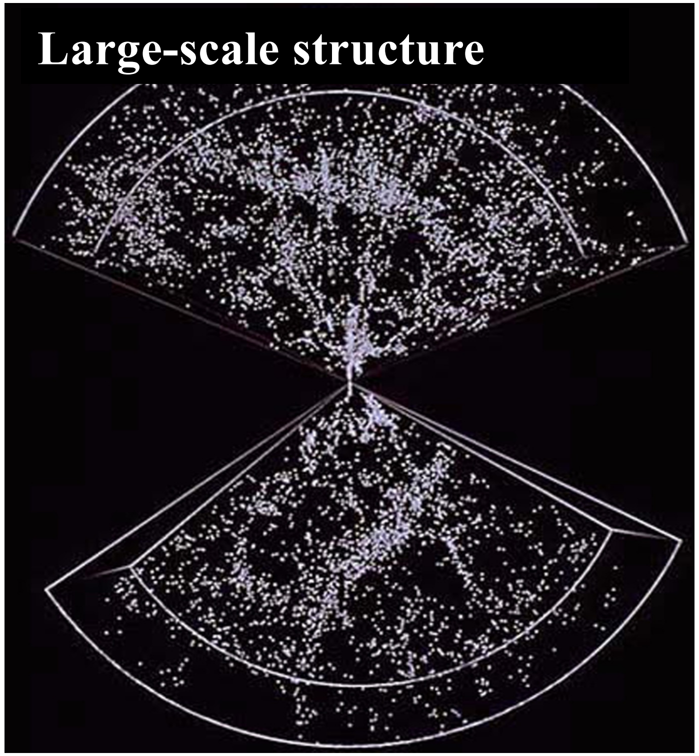


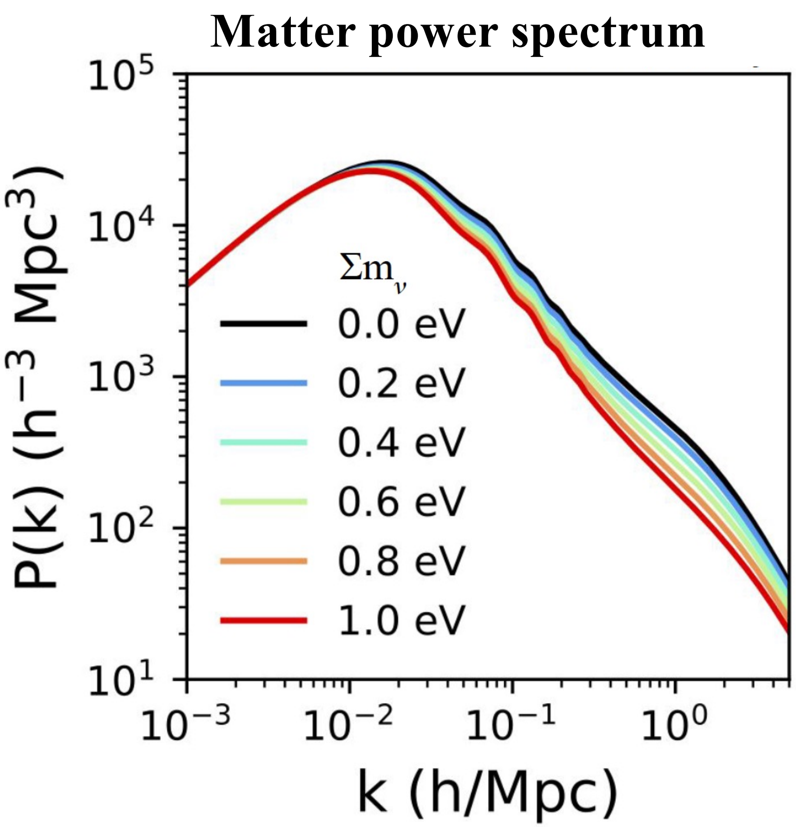
Normal hierarchy
m3 > m2 ∼ m1

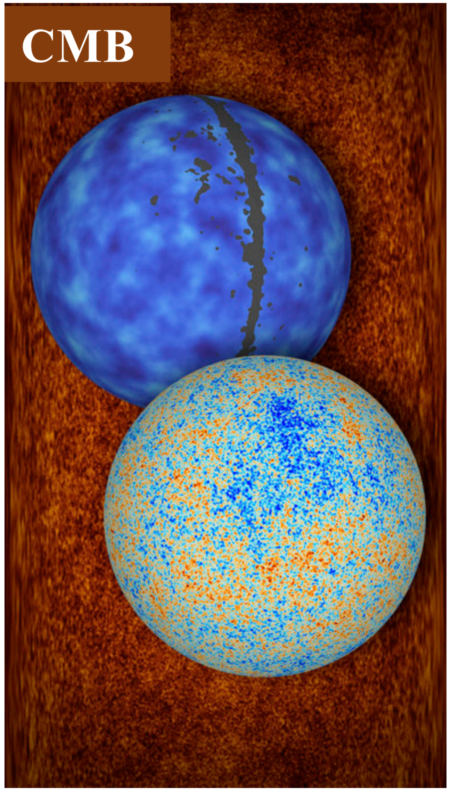
Inverted hierarchy
m2 ∼ m1 > m3

Cosmological probe of fundamental quantities

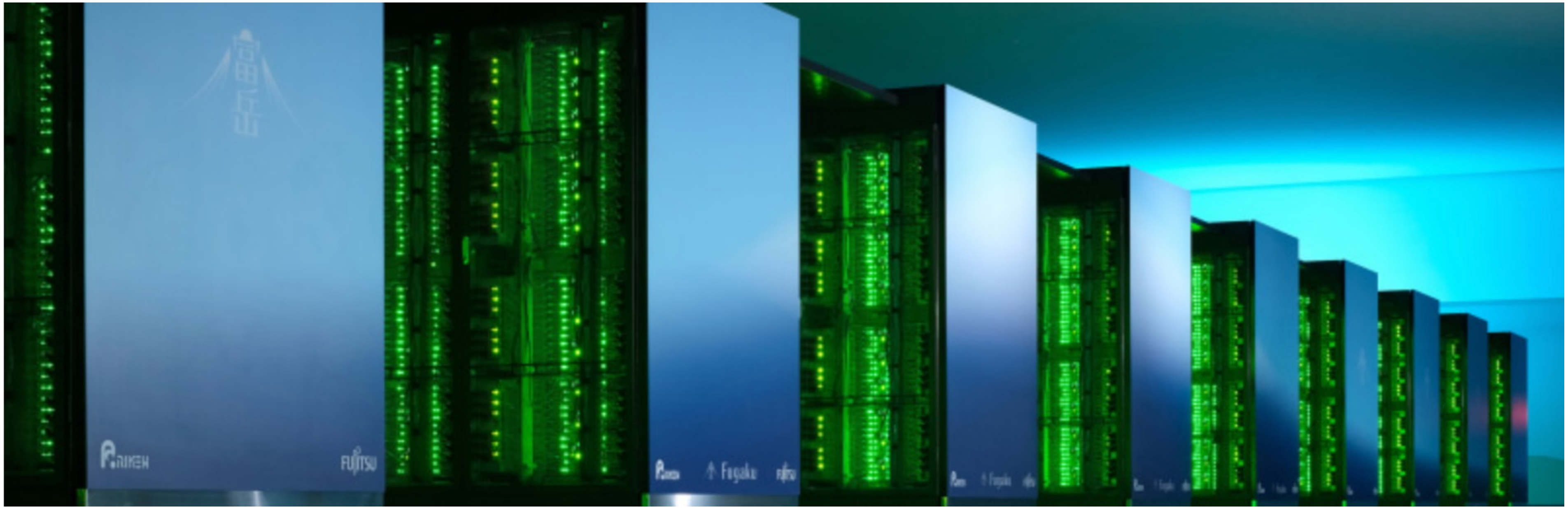
Measuring the effect of the relic neutrinos on structure formation







Fugaku (富岳) with its full power

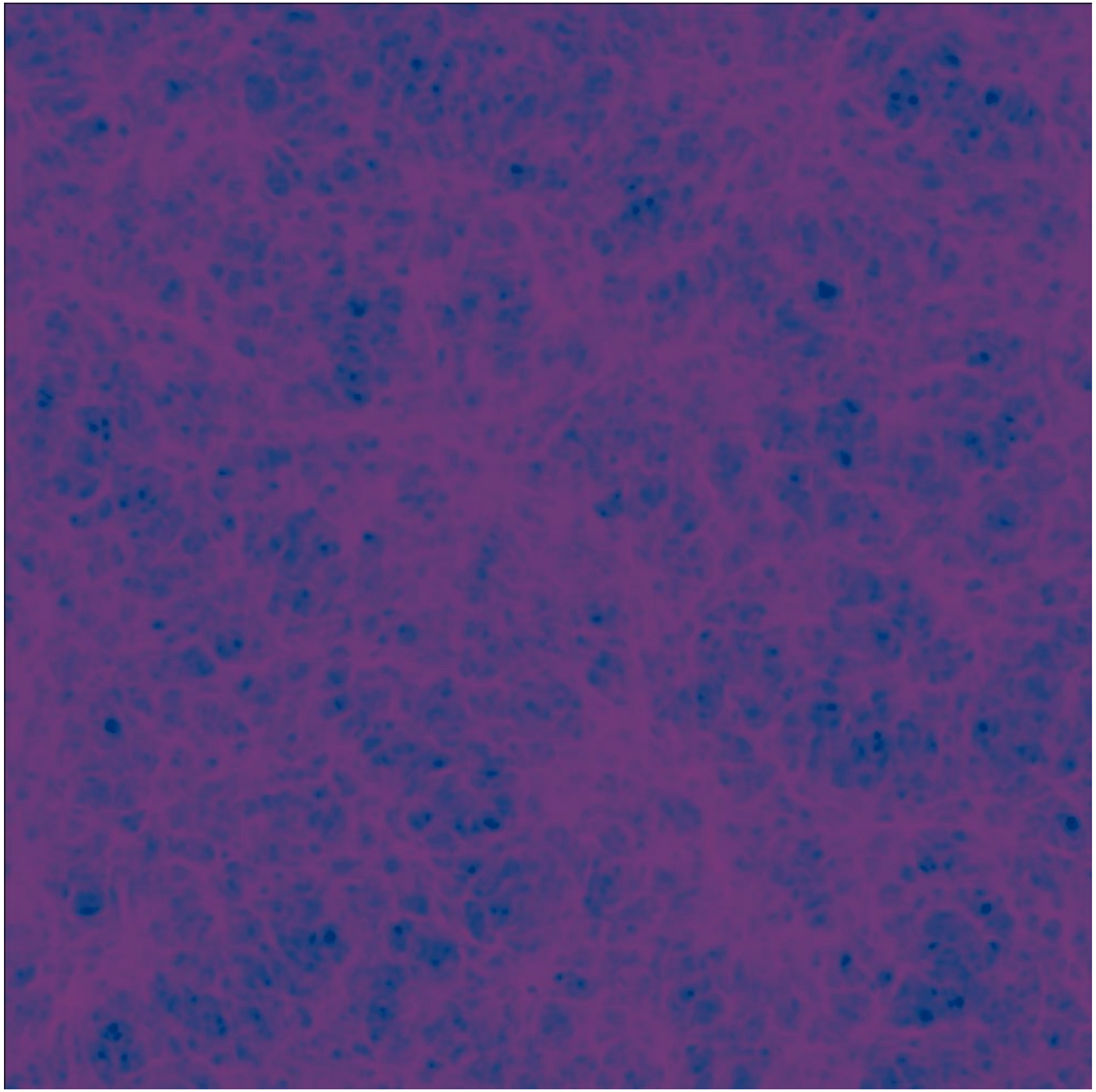


158,976 nodes (52 cores per node)

32 giga byte memory *per node*, 160 peta byte + cloud storage

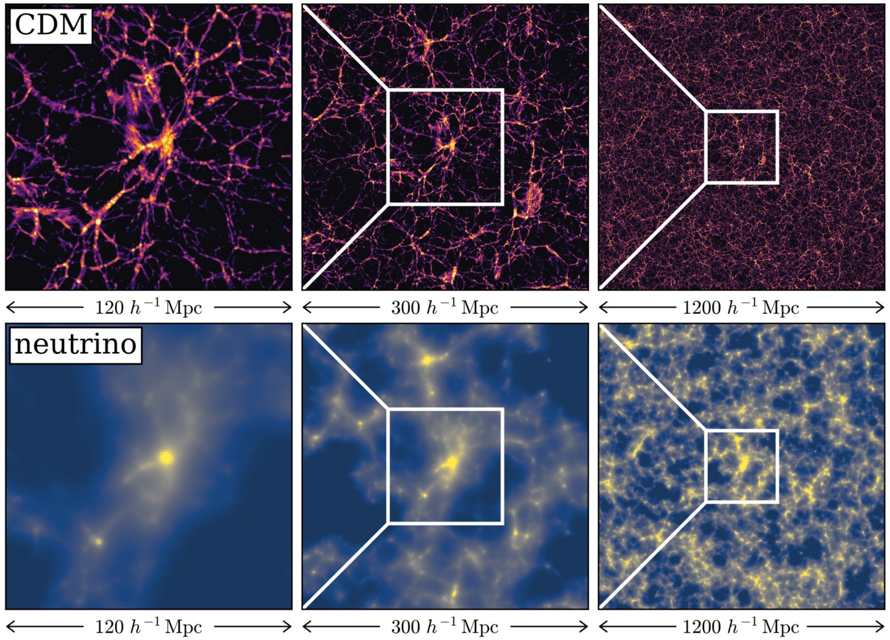
Peak performance 415 peta-flops

2020-2021 No. 1 in TOP500, HPCG, HPL-AI, Graph500



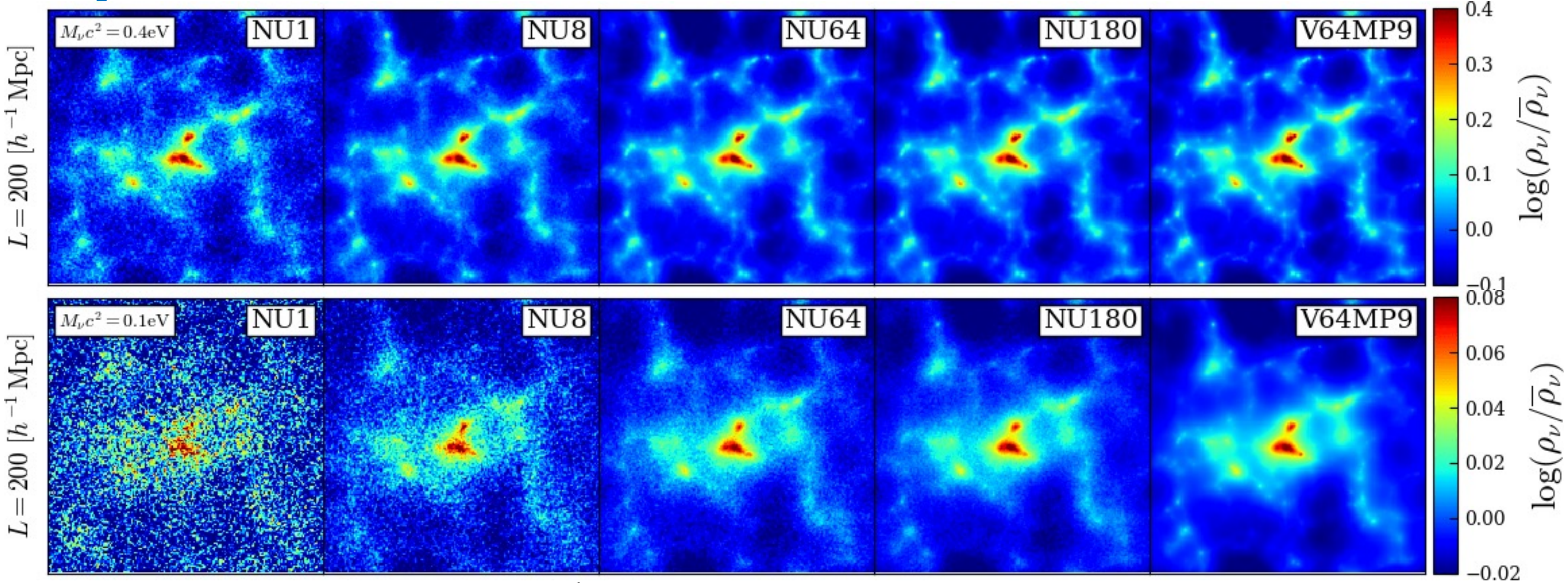
A 400 trillion-grid Vlasov simulation + 330 billion(!) CDM particles

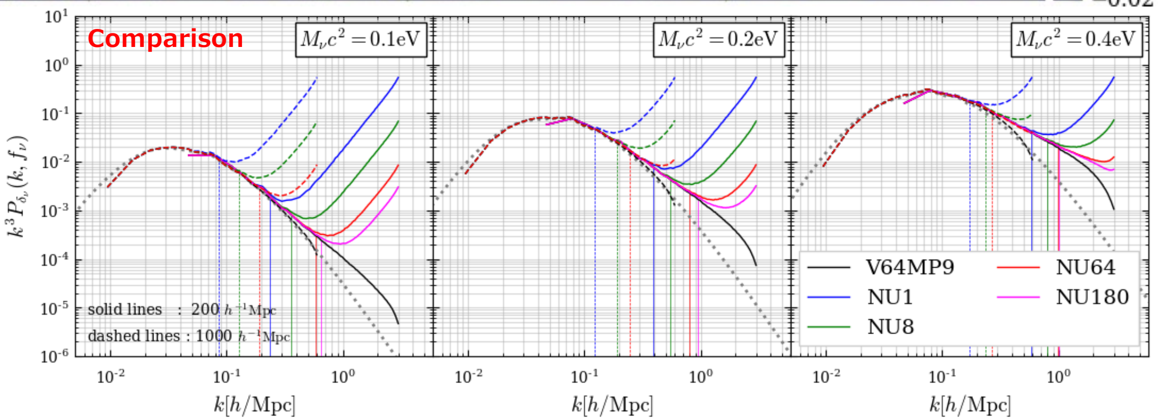
Nonlinear clustering and neutrino "halos"



2021 Gordon Bell Finalist

ν Density Fields

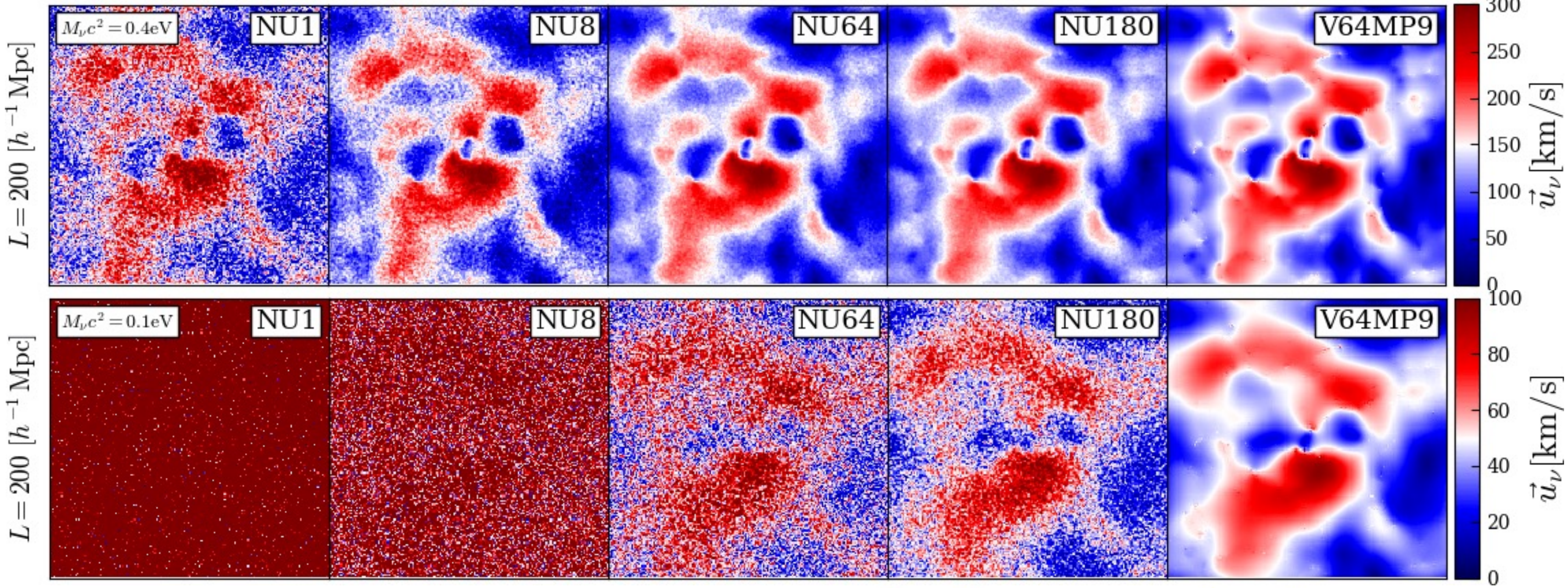


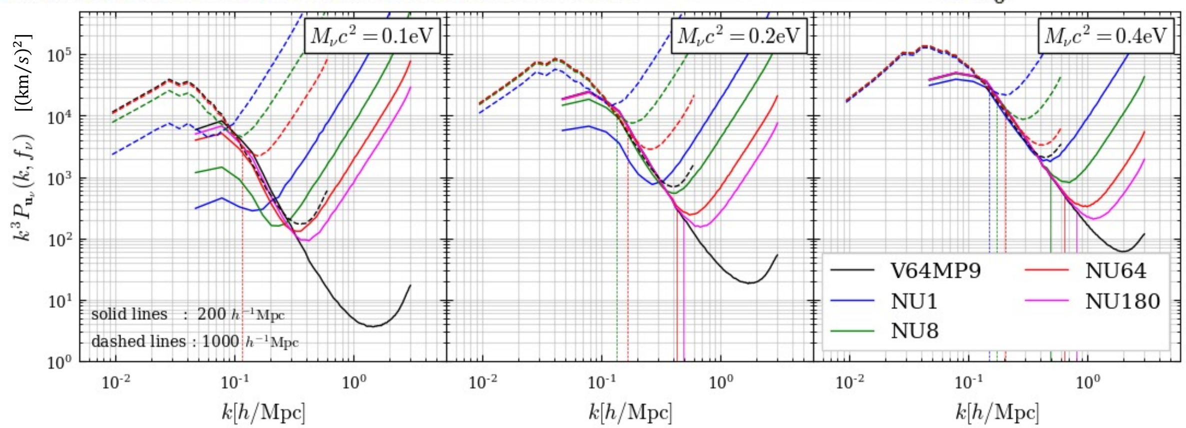


- ✓ *Neutrino velocity distribution function*
- ✓ *Large N reduces the noise in N-body*
- ✓ Small ν mass → large velocity dispersion

  Effective resolution gets worse

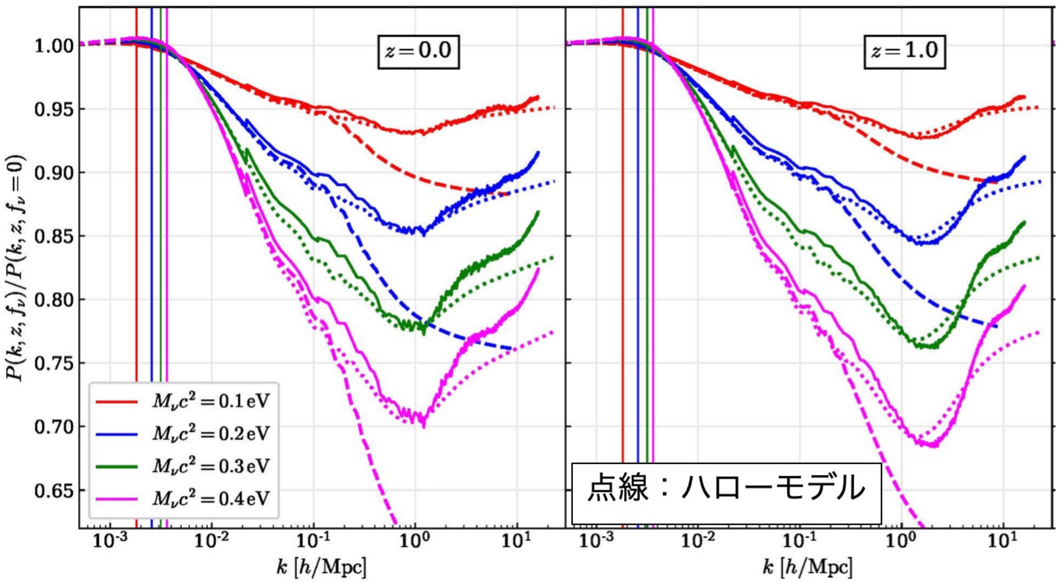
ν Velocity Fields



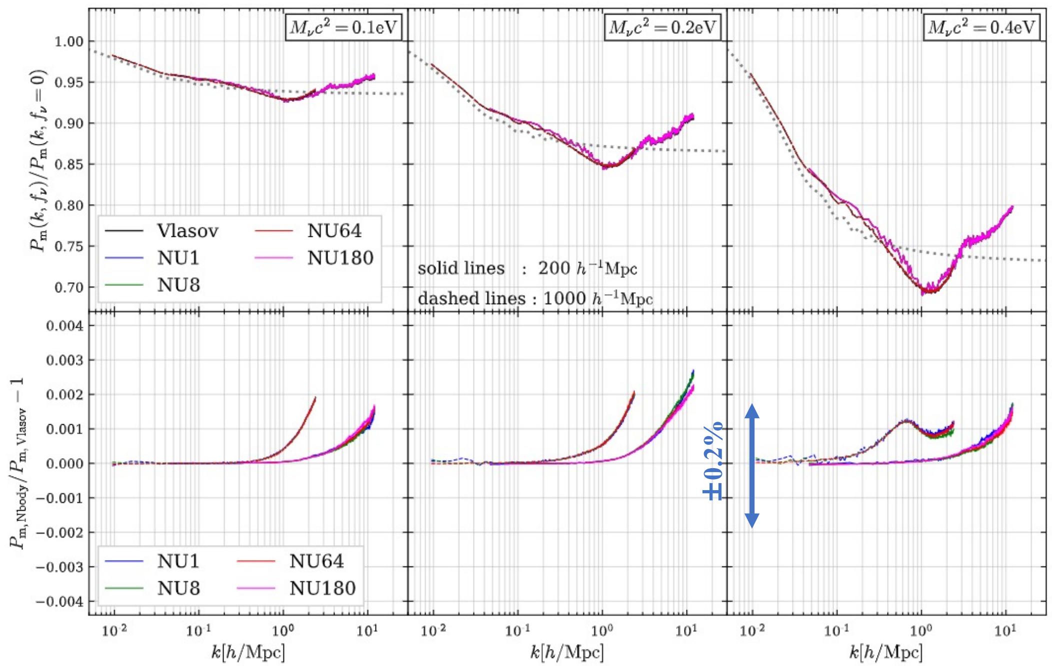


- ✓ *Velocity 1st moment*
- ✓ Impossible to infer the bulk motion for low m_ν
- ✓ Vlasov shows no/little shot noise

Total Matter Power Spectrum: Vlasov vs *N*-body



Power spectrum damping owing to (nearly) free-streaming neutrinos as a function of m_ν



Comparison of our Vlasov sim and *N*-body

- There are residual shot-noise, but can be made small enough using a large number of particles
- ***It is safe! to use N-body simulations to calculate the total matter power spectrum***

Putting the universe on a quantum computer

Boltzmann solver on a quantum computer

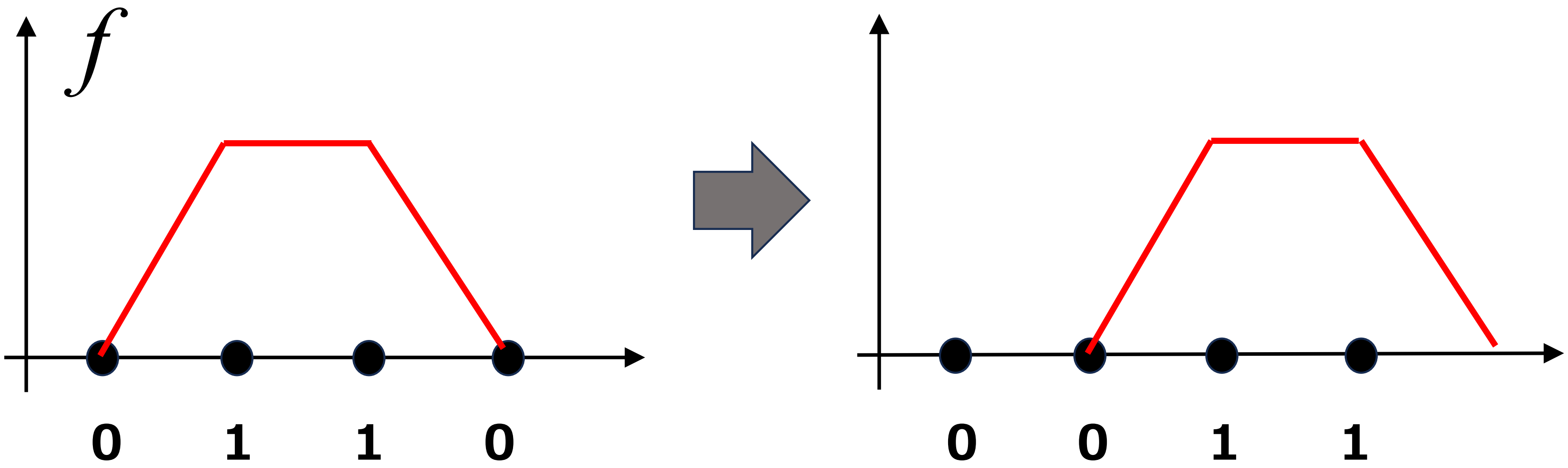
- Time evolution of the velocity distribution function $\underline{f(\boldsymbol{x}, \boldsymbol{v}, t)}$

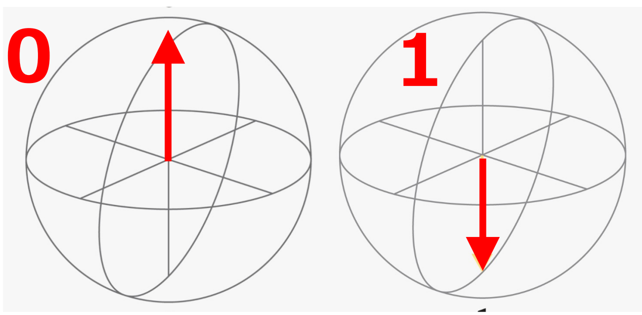
$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{x}} + F \cdot \frac{\partial f}{\partial \boldsymbol{v}} = 0$$

- Both memory- and CPU-demanding (Curse of dimension!)
- Quantum computing may offer a good solution

Essentially a transport equation (but in 6-dimension):

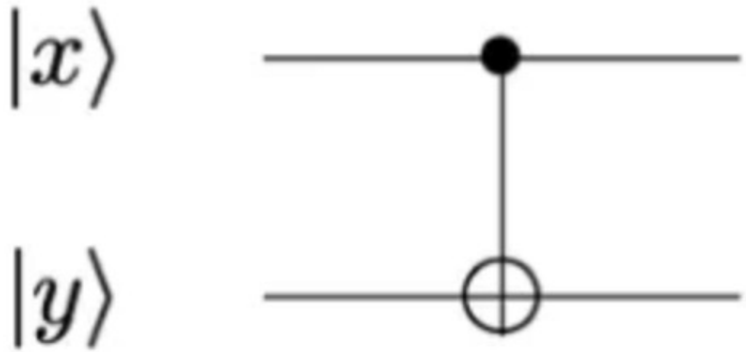
$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{x}} = 0$$





Quantum gate operation

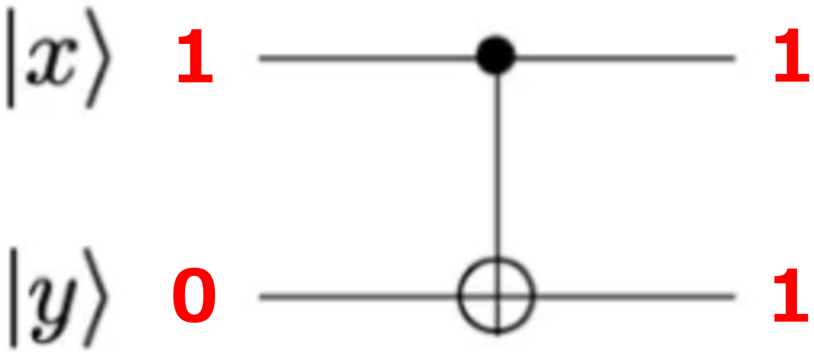
An example: Controlled NOT gate



$$CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Quantum gate operation

An example: Controlled NOT gate



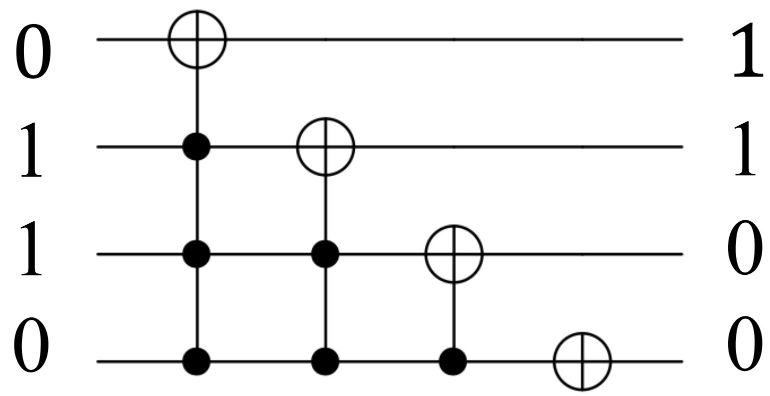
$$CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Increment operator and decrement operator

$$\sum_{i=0}^{2^n-1} a_i|i\rangle \rightarrow \sum_{i=0}^{2^n-1} a_i|i \pm 1\rangle$$

We use the convention $|2^n\rangle = |0\rangle$, $|-1\rangle = |2^n - 1\rangle$

Increment with 4 qubits



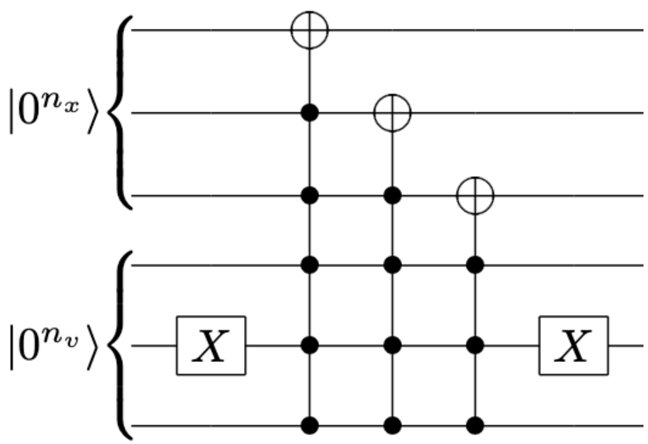
Recall binary numerics: $1 + 1 \rightarrow 0$

Essentially a transport equation: $\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{x}}$

- Streaming operation can be done by using simple circuits

An example with $n_x = n_v = 3$

$v_k > 0$

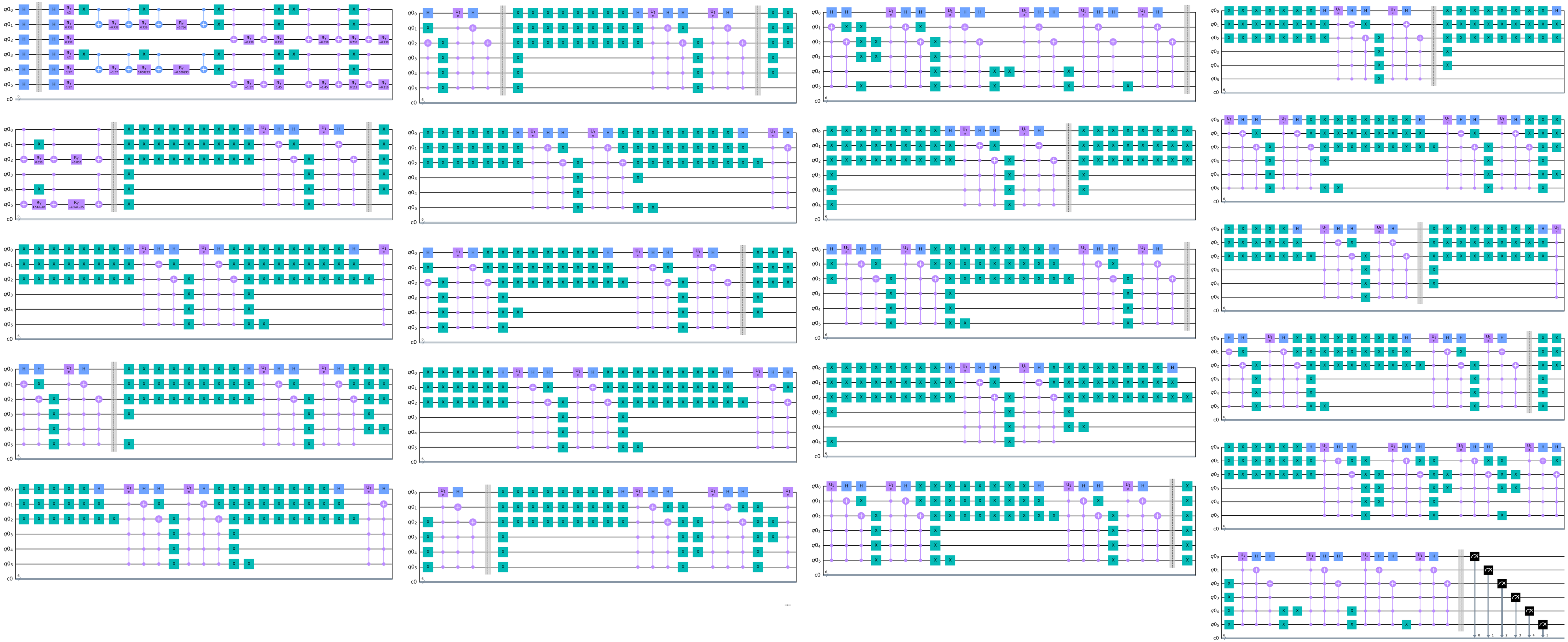


A unitary matrix

$$U^{(3)}|\psi\rangle \rightarrow \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} C_{000} \\ C_{111} \\ C_{010} \\ C_{001} \\ C_{100} \\ C_{011} \\ C_{110} \\ C_{101} \end{pmatrix} = \begin{pmatrix} C_{111} \\ C_{000} \\ C_{001} \\ C_{010} \\ C_{011} \\ C_{100} \\ C_{101} \\ C_{110} \end{pmatrix}$$

Yamazaki, Uchida, Fujisawa, NY arXiv:2303.16490

In reality, with $n_x = n_v = 3$

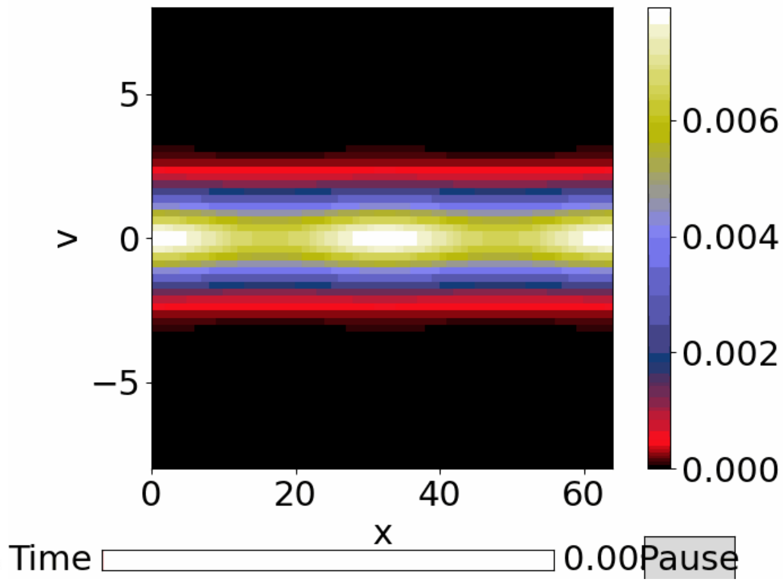


A self-gravitating system

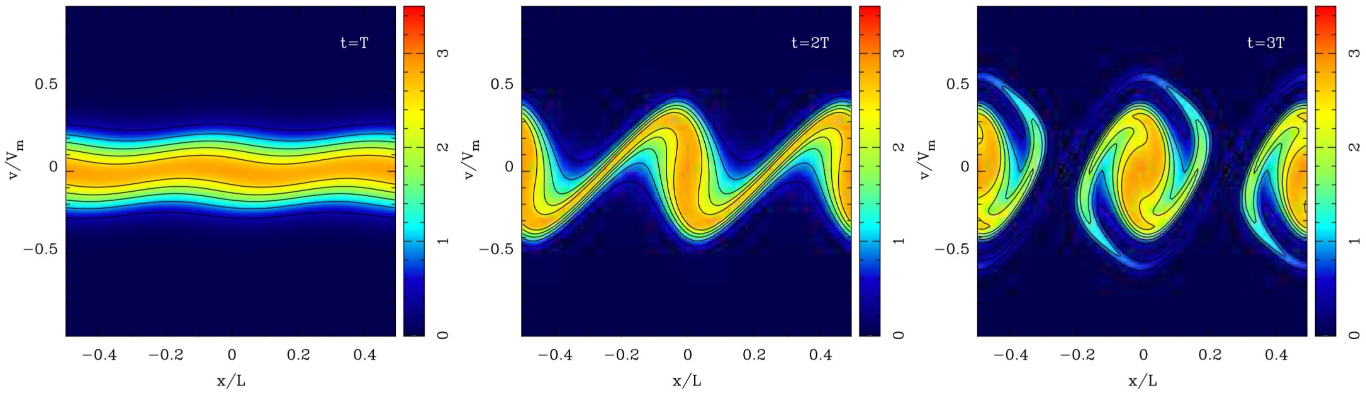
- $n_x = n_v = 6$ (Mere 12qubits)
- *Jeans instability*

$A = 0.1, k = 0.5$

$$f(x,v) = \frac{\rho_{ref}}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{v^2}{2\sigma^2}\right)(1 + A\cos kx)$$



Quantum simulation



←Supercomputer
(Yoshikawa et al. 2013)

Yamazaki, Uchida, Fujisawa, NY arXiv:2303.16490

See also Miyamoto et al. arXiv:2310.01832

How fast, and how efficient ?

	Time complexity	Space complexity
Quantum	$\tilde{\mathcal{O}}\left((N_v + N_x^3)N_t^2 2^{6S}\right)$	$\tilde{\mathcal{O}}\left({N_x}^3 N_t\right)$
Classical	$\mathcal{O}\left({N_x}^3 {N_v}^3 N_t\right)$	$\mathcal{O}\left({N_x}^3 {N_v}^3\right)$

N_x : Number of grids per dimension
N_v : Number of velocity grids per dimension
N_t : Number of timesteps
S : The order of approximation

Hamiltonian simulation

For an ODE $\frac{\mathrm{d}}{\mathrm{d}t}\vec{x}(t) = A\,\vec{x}(t)$, the formal solution is $\vec{x}(t) = e^{At}\,\vec{x}(0)$

So, the whole point is to calculate the exponential matrix e^{At}

For a particular Schrödinger form $\frac{\mathrm{d}}{\mathrm{d}t}|\phi(t)\rangle = -iH|\phi(t)\rangle$, the Hermitian operator H is the system's Hamiltonian, and calculating $|\phi(t)\rangle = e^{-iHt}|\phi(0)\rangle$

is called Hamiltonian simulation.

Unfortunately, calculating e^{At} for a large $N \times N$ matrix is extremely hard on a classical

computer. But, a quantum computer can make the miracle (we hope).

Hamiltonian simulation as a Vlasov solver

Partial derivatives are approximated as $\frac{\partial f}{\partial x} \sim \frac{f(x_{i+1}, v_j) - f(x_{i-1}, v_j)}{2\Delta x}$, simple!

This transforms the original partial differential equation to an ODE $\frac{\mathrm{d}}{\mathrm{d}t} f = A f$

Here, $\vec{f} = \left(f(t, x_1, v_1), \ldots, f(t, x_{\mathrm{ngr}}, v_{\mathrm{ngr}}) \right)$

We linearize the Vlasov equation by assuming (approximating) gravity is dominated by CDM:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \mathbf{F}_{\mathrm{CDM}} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0$$

Note that $\rho_\nu / \rho = 7.6 \times 10^{-3} (M_\nu / 0.1\mathrm{eV})$

In reality, the huge matrix would look like

$$\frac{\mathrm{d}}{\mathrm{d}t} f = A f$$

$$A = A_x + A_y + A_z + A_{v_x} + A_{v_y} + A_z :$$

$$A_x = -\begin{pmatrix} 0 & 1/2\Delta_x & & & -1/2\Delta_x \\ -1/2\Delta_x & 0 & 1/2\Delta_x & & \\ & \ddots & \ddots & \ddots & \\ & & -1/2\Delta_x & 0 & 1/2\Delta_x \\ 1/2\Delta_x & & & -1/2\Delta_x & 0 \end{pmatrix} \otimes \mathrm{diag}(v_{x,1}, \ldots, v_{x,n_{\mathrm{gr}}})$$

$$A_{v_x} = -\mathrm{diag}\left(F_{\mathrm{CDM},x}(t, x_1), \ldots, F_{\mathrm{CDM},x}(t, x_{n_{\mathrm{gr}}})\right) \otimes \begin{pmatrix} 0 & 1/2\Delta_v & & & \\ -1/2\Delta_v & 0 & 1/2\Delta_v & & \\ & \ddots & \ddots & \ddots & \\ & & -1/2\Delta_v & 0 & 1/2\Delta_v \\ & & & -1/2\Delta_v & 0 \end{pmatrix}$$

Note that A is anti-Hermitian: $A = -A^{\dagger}$

So we write $\frac{\mathrm{d}}{\mathrm{d}t}|f\rangle = -iH|f\rangle$ with $H = -iA$ This is Schrödinger equation!

Neutrino power spectrum

We can solve the Schrödinger equation on a quantum computer,

to obtain a quantum state $|f\rangle = \sum_{i,j} f(t, x_i, v_j)\,|i\rangle\,|j\rangle$ Excellent!

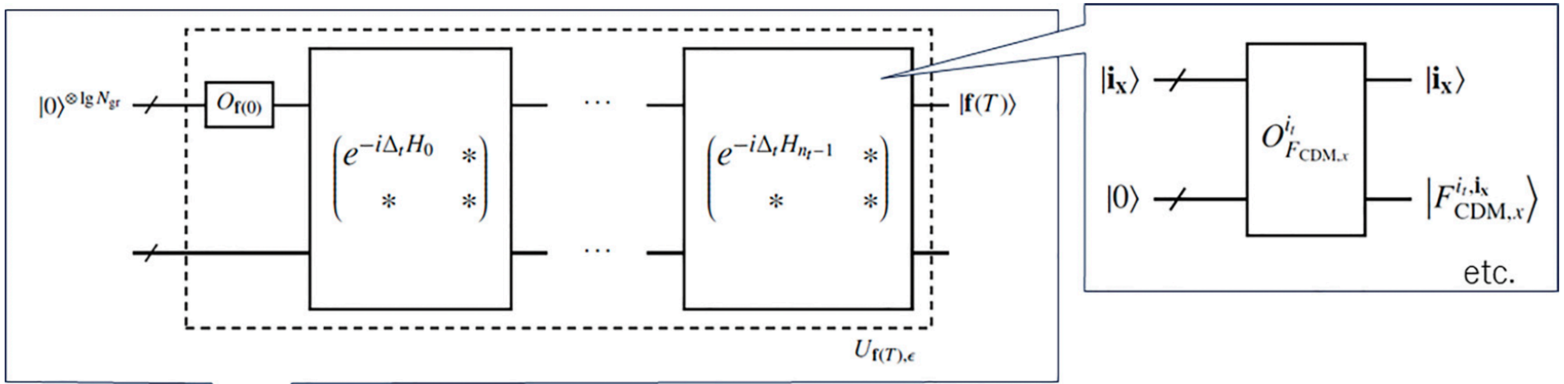
However, maybe we are not very much interested in the final quantum state itself.

Often we are interested in summary statistics such as $P(k)$.

We apply quantum Fourier-transform (QFT) to $|f\rangle$ via summation to obtain

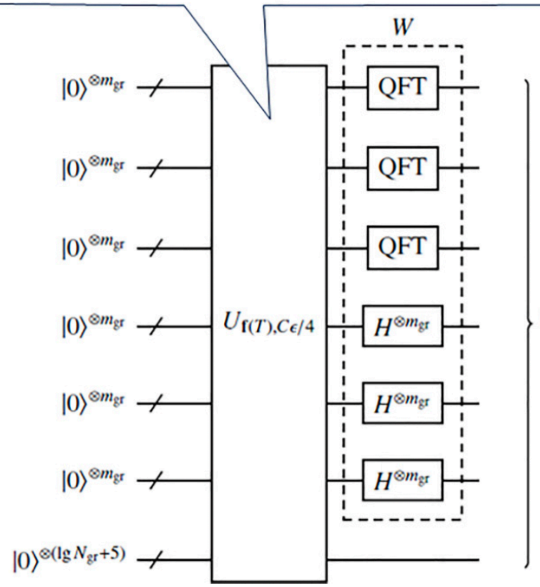
$\left|\langle \Omega_{i_k} | W | f \rangle\right|^2 = C\,|\tilde{\delta}_{i_k}|^2$ with proper normalization.

A quantum circuit that calculates P(k)



inputs F_CDM
(as QRAM)

Hamiltonian simulation



Estimate the amplitude of a basis state $|i\rangle|0\rangle$ of $|\tilde{\delta}\rangle$ using QAE, which is $P(k) = |\tilde{\delta}|^2$

Algorithm 1. Estimation of $|\tilde{\delta}^{\nu}_{\mathbf{i_k}}|^2$.

Input: Accuracy $\epsilon \in (0, 1/2)$, success probability $1-\delta \in (0,1)$, the value of C.

1: Construct the unitary quantum circuit $U_{\mathbf{f}(T),C\epsilon/4}$ on a $(2\lg N_{gr}+5)$-qubit system following Theorem 1.

2: Construct $W' := I_{32N_{gr}} \otimes W$ the unitary on the same system, where $I_{32N_{gr}}$ is the identity operator on the first $\lg N_{gr}+5$ qubits and W is the operator in Eq. (46) that acts on the other $\lg N_{gr}$ qubits.

3: Estimate the squared amplitude of $|\Omega'_{\mathbf{i_k}}\rangle := |0\rangle^{\otimes(\lg N_{gr}+5)}|\Omega_{\mathbf{i_k}}\rangle$ in the state $W'U_{\mathbf{f}(T),C\epsilon/4}|0\rangle$ by QAE with accuracy $C\epsilon/4$ and success probability $1-\delta$, and let the estimate be $\tilde{p}$.

4: Output $\tilde{p}/C$.

Quantum Amplitude Estimation

There are efficient algorithms that yields a good estimate of the amplitude of

a target basis state $|\psi\rangle$ in $|\Psi\rangle$. To be specific,

given a quantum circuit that generates $|\Psi\rangle$ by $A|0\rangle = a|\psi\rangle + \sqrt{1-|a|^2}\,|\psi'\rangle|0\rangle$,

QAE estimates the amplitude $|a|^2$ with accuracy ε.

The algorithm is used to extract the solution embedded in the amplitude

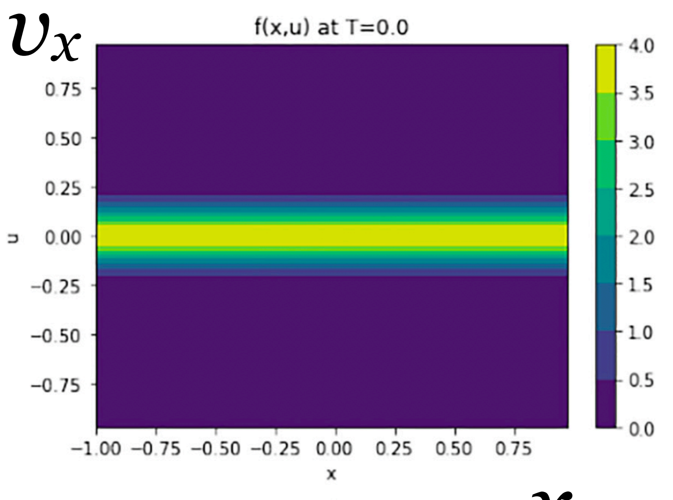
of $|x(t)\rangle = \dfrac{1}{\|x(t)\|}\sum x_i|i\rangle$

Brassard et al., Contemporary Mathematics, 305, 53 (2002)

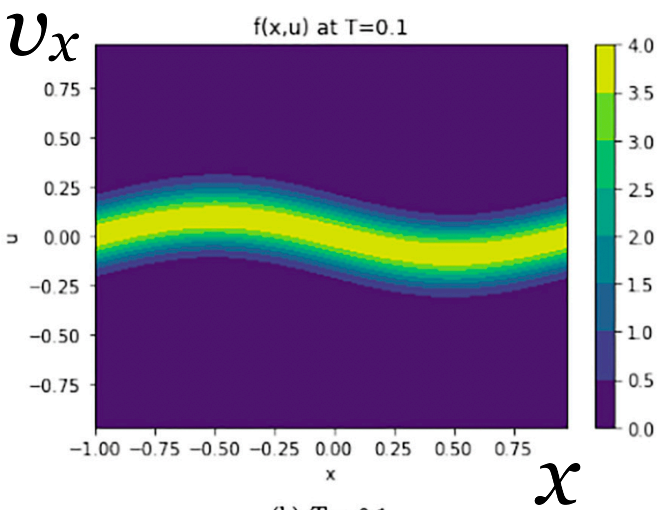
Proof of concept

A simulation of quantum simulation with 6 + 6 qubits ($N_{\rm grid}$ = 64)

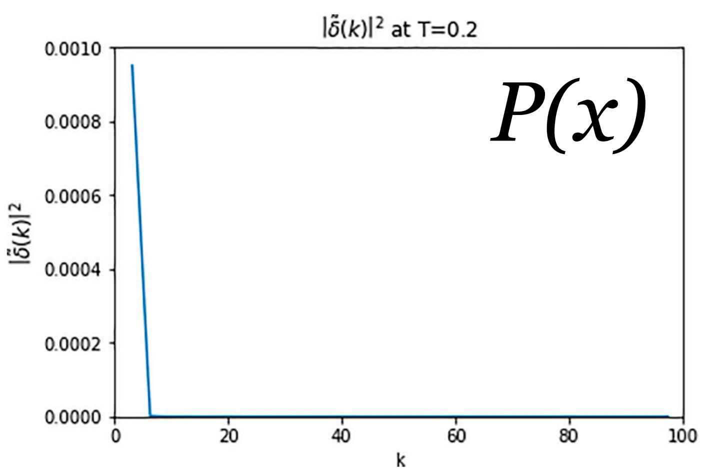
1-dimensional gravitational instability



(a) $T = 0$



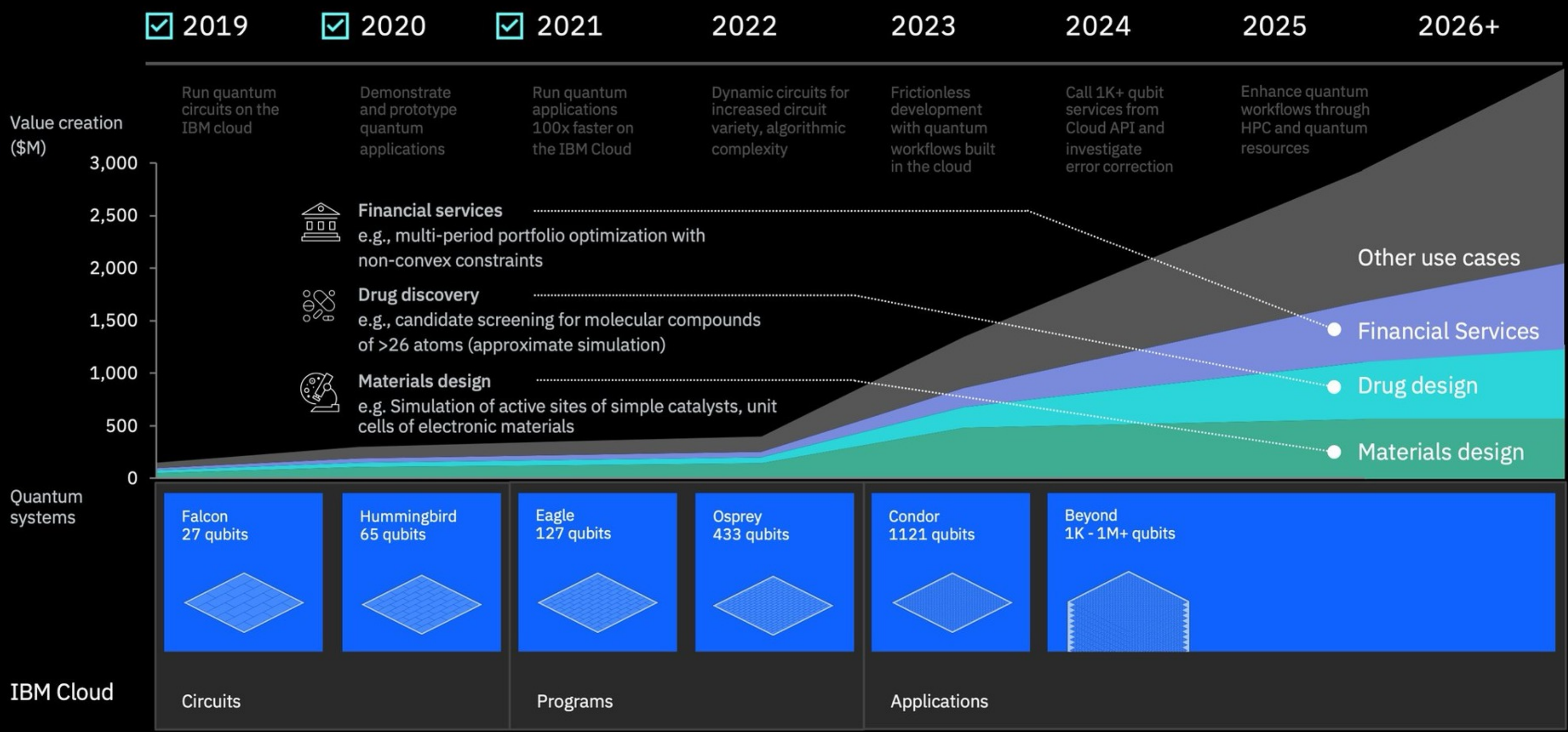
(b) $T = 0.1$



$3B+ in near-term value creation based on IBM roadmap, with inflection points starting in 2023

IBM Quantum

BCG BOSTON CONSULTING GROUP



Summary

- Largest cosmological Vlasov-Poisson simulations have been performed. Extensive comparisons with N-body simulations have been done.
- Velocity moments are substantially affected by particle shot-noise.
- New observables are needed to discern the differences between neutrino mass hierarchies.
- The simulation method is applicable to non-standard DM models such as thermal/non-thermal warm dark matter models.
- Road ahead to cosmological quantum computing