Challenges in non-equilibrium many-body dynamics

Capability versus Capacity computing

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Capability versus Capacity

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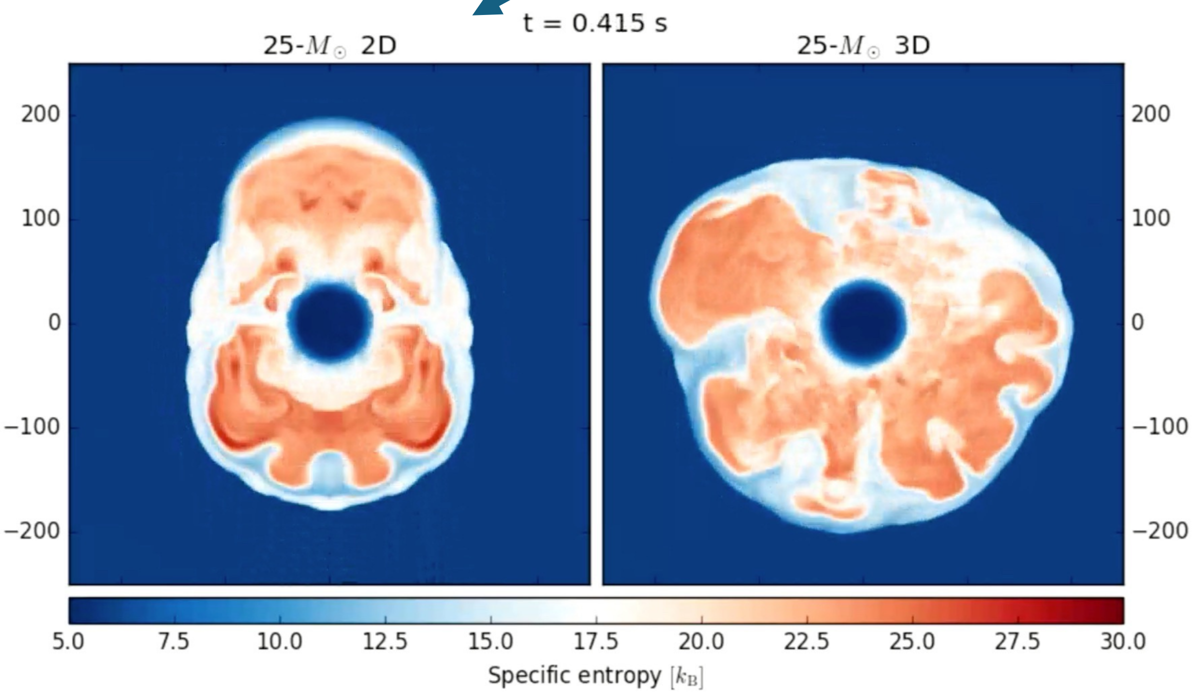


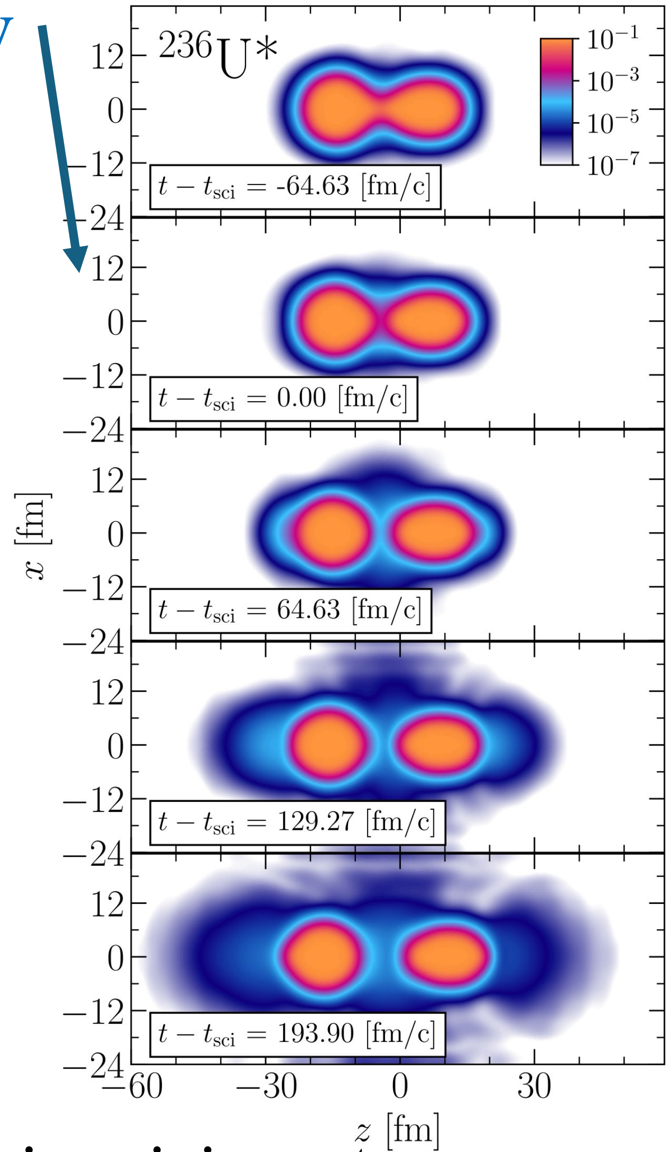
2D versus 3D

The emerging theory of three-dimensional core collapse supernova explosions

Adam Borrows, Princeton, UW Colloquium, 2023

Simulations performed on Polaris, ANL

About 1,000,000 node-hours on 400-500 nodes.



Nuclear fission, scission neutrons

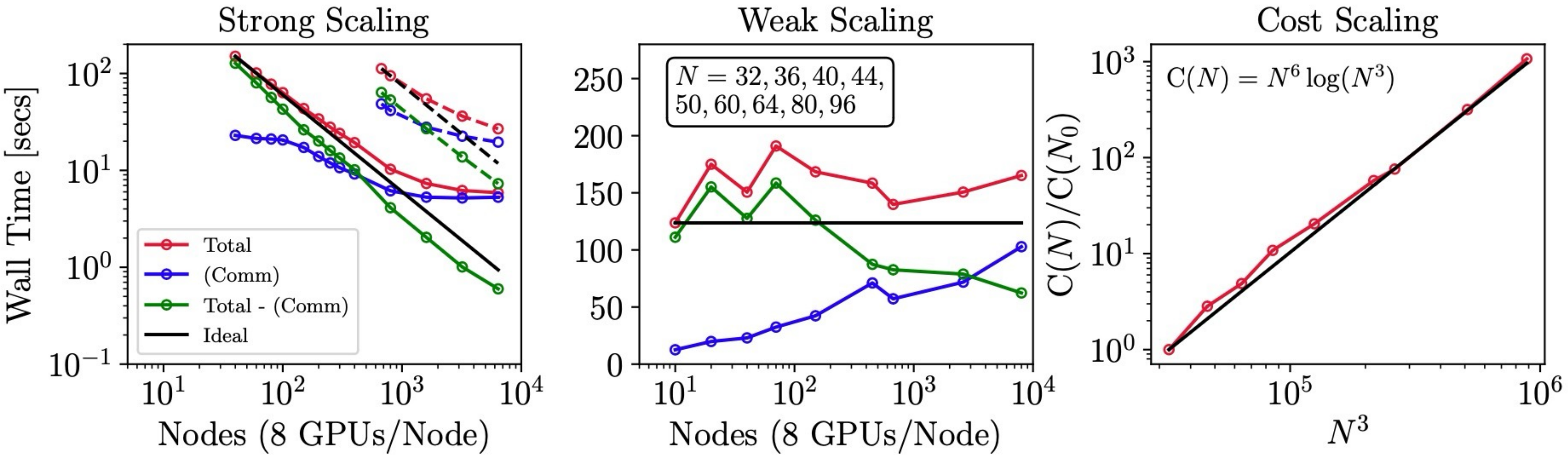
Abdurrahman, Kafker, Bulgac, Stetcu, PRL (2024)

Simulations performed on Summit, ORNL

About 1,000,000 node-hours on all available 4608 nodes.

89 TB new data generated at each time step

N is the number of spatial lattice points on one side of a cubic simulation box, with a total N^3 lattice points.



Scaling properties of the numerical codes used so far in simulations on Summit, Frontier, and Lumi (Finland), using in all cases almost the entire machine. Simulations were performed on GPUs, for 50,000 and almost 4,000,000 time steps, with very high numerical accuracy, and using numerical implementations, which required only two evaluations of the RHS of the PDEs per time step. 911 TB of new data generated at each time step. Number of time step =30,000-60,000.

For N = 96 we used 64,000 GPUs (out of 8×9408 = 75264 allowed) on Frontier! That is about the maximum size we can simulate on Frontier. Number of 3D+time nonlinear, complex, coupled PDEs = $16xN^3$, which for N=96 is **14,155,776 PDEs**, each PDE in a 3D spatial box with 96^3 = **884,736 lattice points**.

New data generated at each times–step $80\times N^6$ complex numbers.

Total GPU memory required at each time step $12\times16\times N^6$ complex numbers.

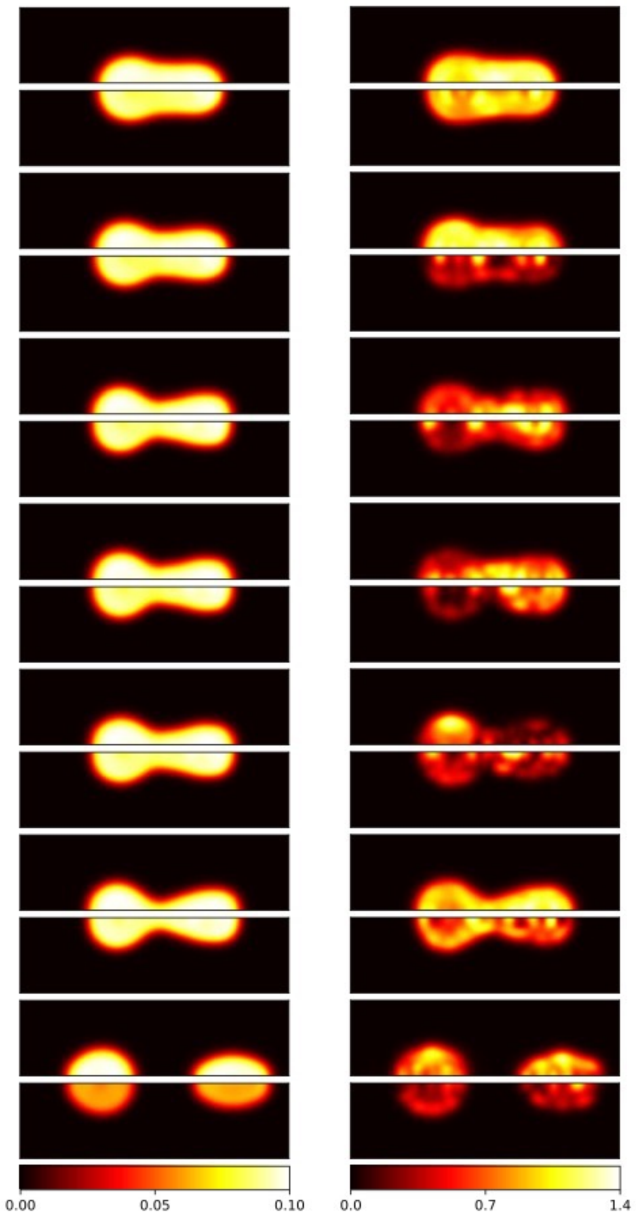
Non-equilibrium Time-Dependent Many-Fermion Problems

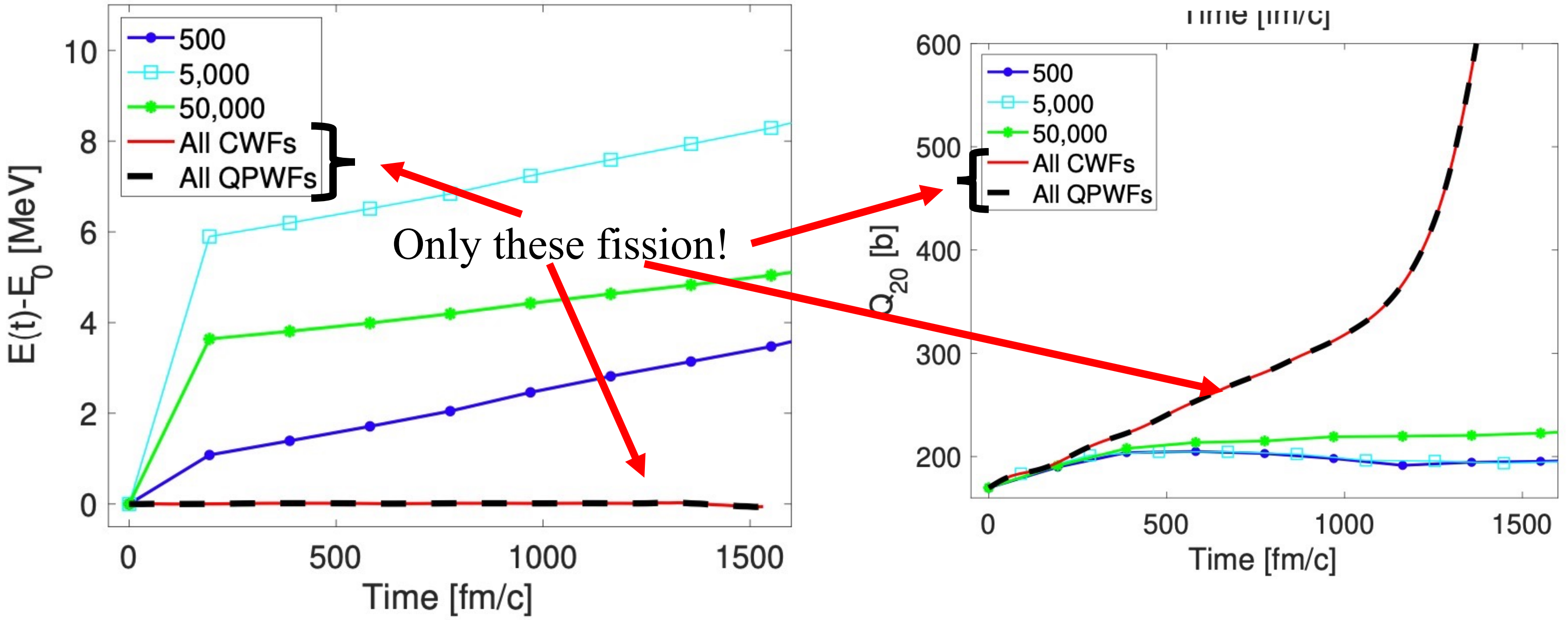
- Fission dynamics, heavy-ion collisions
- Schwinger mechanism for fermion-antifermion production in strong fields
- Quantum (and classical) turbulence
- Dynamics of neutron and proton quantized vortices in the neutron star crust
- Excitation of the Anderson-Bogoliubov-Higgs mode (order parameter) in superfluid nuclear systems
- Collective neutrino oscillations
- Schwinger-Keldysh, Baym-Kadanoff , and other truly quantum kinetic equations, which treat correctly superposition, entanglement, interference, and quantized vortices.

In the Boltzmann-Nordheim or Boltzmann-Uehling-Uhlenbeck "semiclassical" framework interference and entanglement are absent.

- Wave function thermalization, non-Markovian behavior, role of memory effects

Challenges in non-equilibrium many-body dynamics





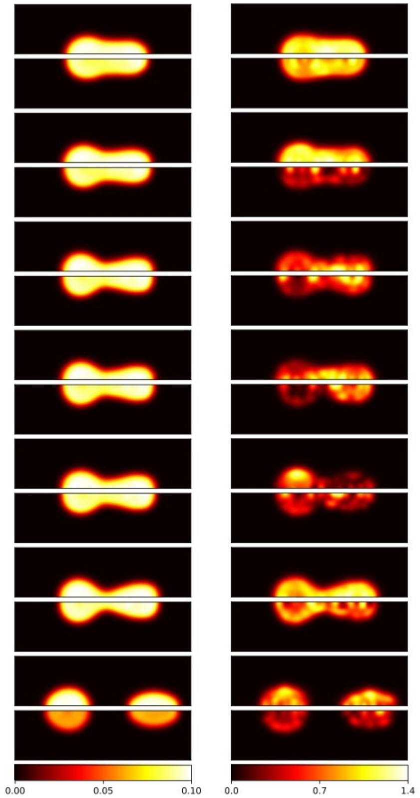
- In static calculations less than ≈600 orbitals are sufficient to describe properties of all nuclei with very high accuracy.
- In non-equilibrium simulations the inclusion of practically the entire set of single-particle orbitals determined by the spatial and phase-space volume are required to describe correctly the final state ($\approx 16\times N^3$orbitals)

Simulating fission with a reduced set of orbitals (canonical wave functions or natural orbitals) does not lead to fission!

One cannot use a small basis set!

Why time-dependent non-equilibrium processes are so different from static properties?

$^{235}U(n_{th},f)$



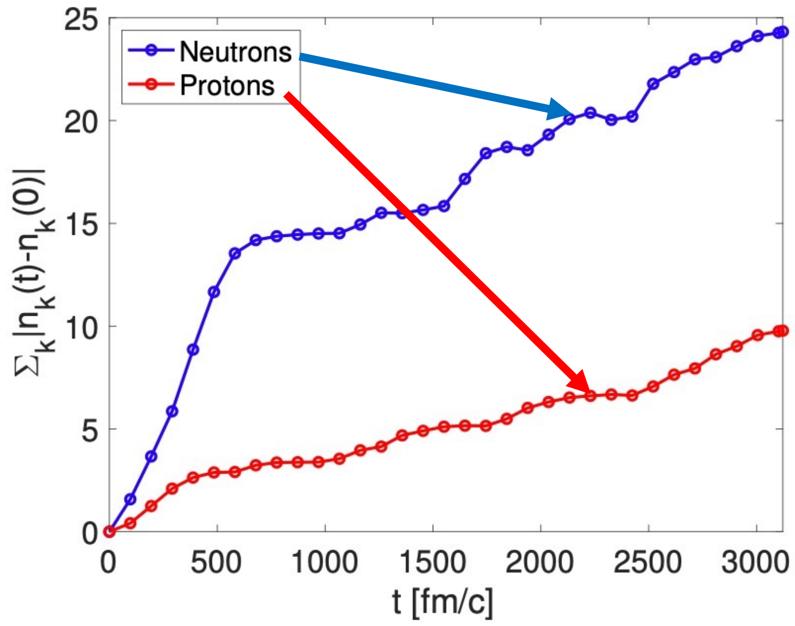
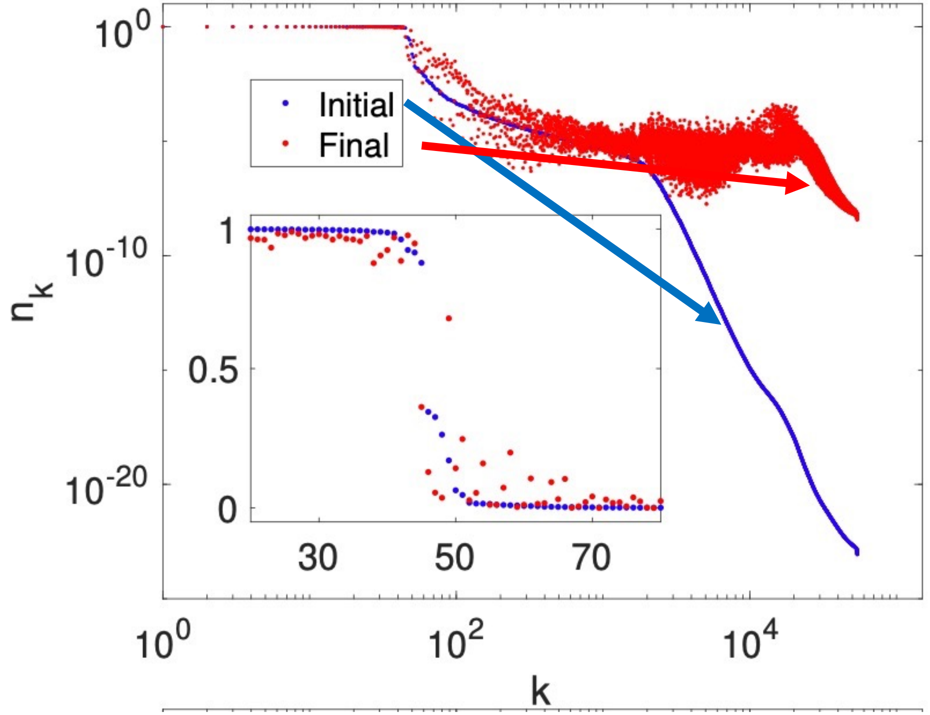


FIG. 3. The sum of the absolute differences between the single-particle occupation probabilities at the initial time and at time t. Initial conditions are the same as in Fig. 1.

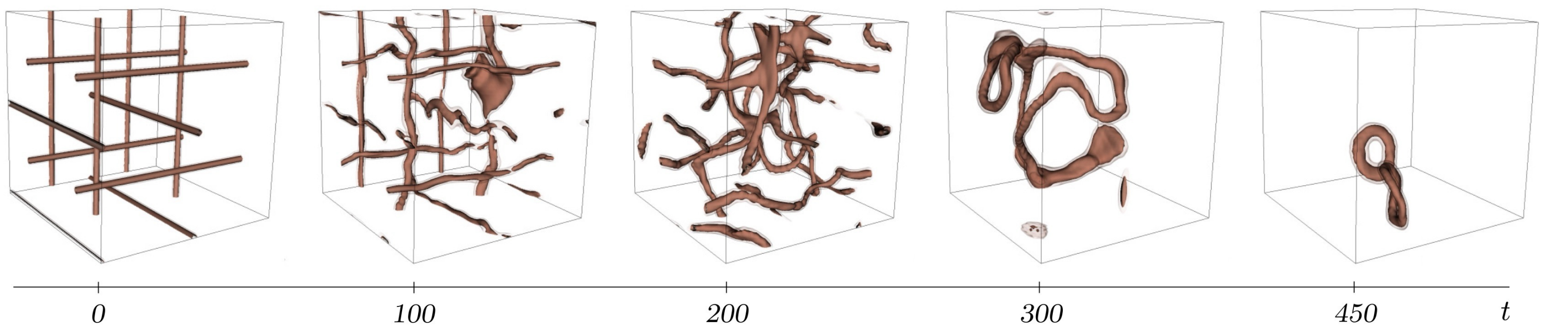


# States	Z_i	Z_f	ΔZ	N_i	N_f	ΔN
500	91.97	91.61	0.36	143.96	139.74	4.21
1000	91.98	91.64	0.34	144.00	139.92	4.07
2000	91.99	91.66	0.33	144.02	140.06	3.96
5000	91.99	91.69	0.30	144.03	140.33	3.70
50,000	91.99	91.97	0.017	144.03	143.23	0.80
108,000	91.99	91.99	6.5×10^{-6}	144.03	144.03	1.1×10^{-4}

Time-dependent orbitals with initial "negligible" occupation probabilities are populated with significant probabilities in the "final" state.

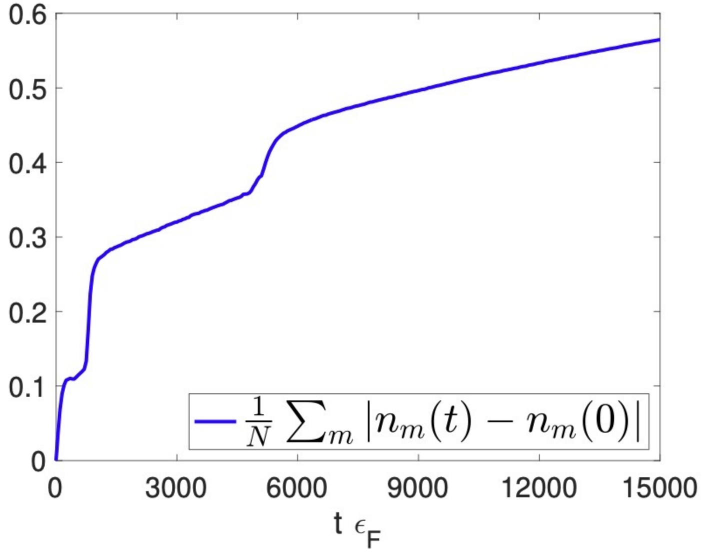
Unless the "entire set" of orbitals is included in the time-dependent simulation the properties of the final products are predicted with very large errors. **One cannot use a small basis set!**

Quantum turbulence, superfluidity, non-Markovian dynamics, and wave function thermalization

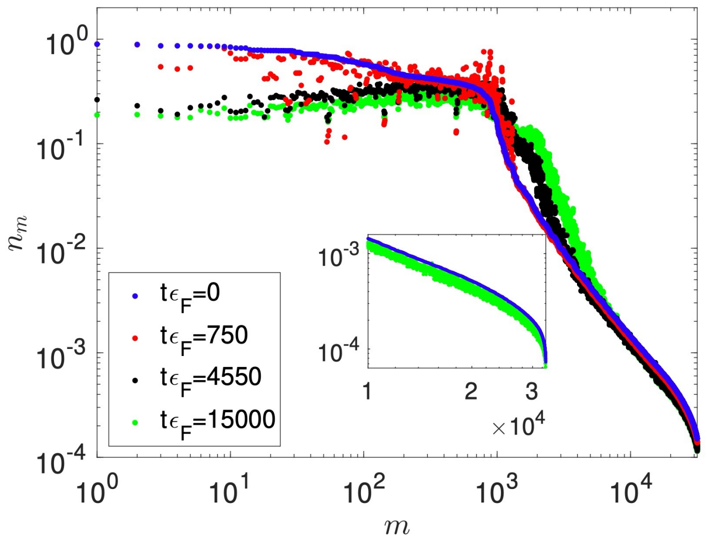


Time evolution of 12 quantized vortices

Crossing and reconnections
(similar to DNA chains), Feynman 1955

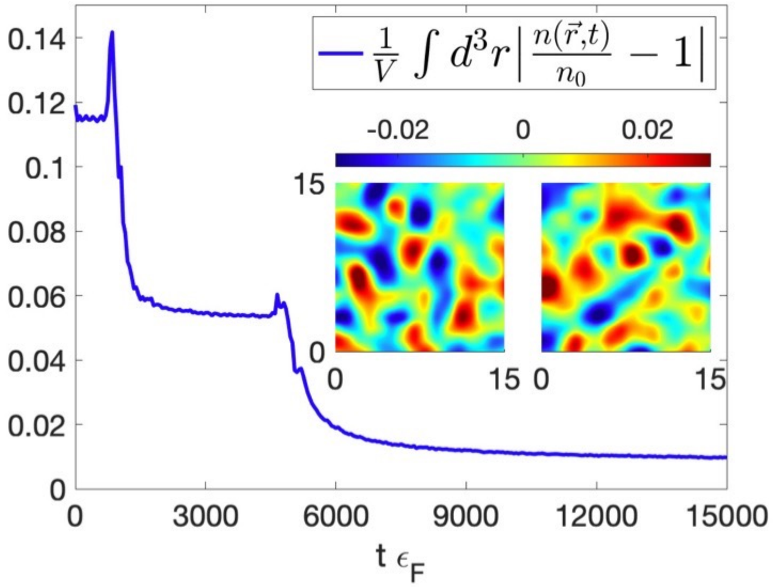


The massive total fractional change of the single-particle occupation probabilities.



Time-dependent single-particle occupation probabilities.

Notice power law behavior for large momenta $n(k,t) \approx \frac{C(t)}{k^4}$.



The average fluctuation of the number density as a function of time.

Initially: 12 quantized vortices.
Finally: homogeneous "thermal" fluctuations.

Conclusions

- There is a large class of physical phenomena, typically non-equilibrium long-term dynamics, which requires a qualitative new approach for generating reliable predictions:

nuclear fission, heavy-ion collisions, quantum turbulence, many-body entanglement, interference, fermion-antifermion production is strong fields, neutrino collective oscillations, excitation of the Higgs modes in fermionic superfluid systems, genuinely quantum transport and non-Markovian processes.

- The traditional methods devised to describe typical stationary or quasi-stationary processes are totally inadequate and there is the need to used capability computing at the largest scale accessible now and in the next decade or two.

- Quantum computing is not likely to be of use in this calendar time frame and neither AI tools (which require large training sets) will be adequate for the treatment of such systems and processes.

- The size of these problems scale as $\mathbf{N_s^6 \times N_t}$, where $\mathbf{N_s}$ is the number of lattice points in one space direction and $\mathbf{N_t}$ is the number of time-steps.

- New software tools are needed to overcome bottlenecks, mainly due to communications and to efficiently use the available hardware.

- These are truly capability problems, using the largest available supercomputers (Frontiers, Summit, Numi, …) for long periods of time (15 or more non-interrupted wall-hours) and essentially all the the available GPUs on a given supercomputer.