Dynamics of atomic nuclei with SUNDIALS

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SUNDIALS VIRTUAL BIRDS-OF-A-FEATHER EVENT

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Computing nuclear response functions with time-dependent coupled-cluster theory

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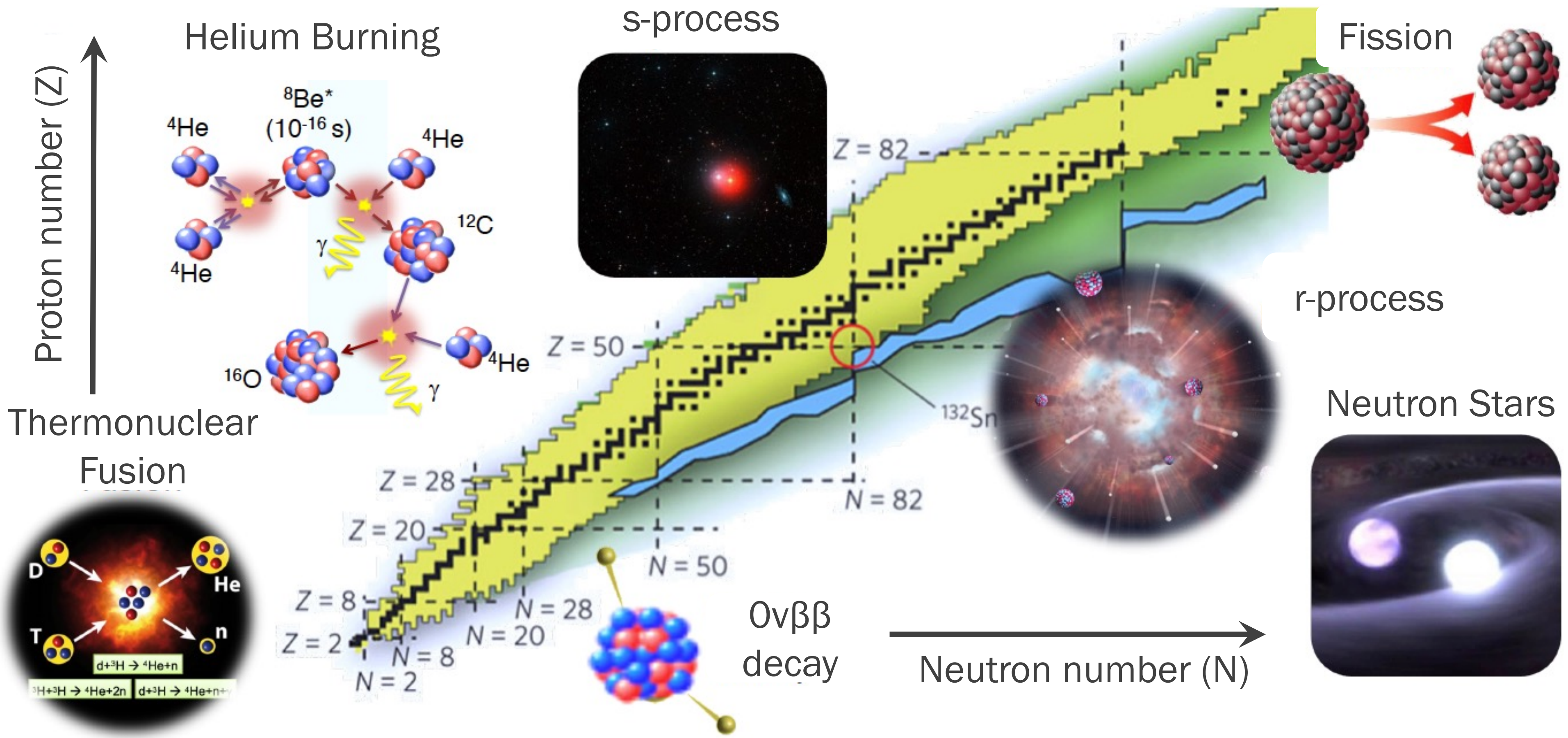
We compute nuclear response functions by solving the time-dependent A-body Schrödinger equation, recording the time-dependent transition moment and extracting spectral information via Fourier transforms. The solution of the time-dependent many-body problem accounts for correlations on top of the mean field by taking advantage of a time-dependent formulation of coupled-cluster theory. As a validation, we focus on electric dipole transitions in ^{4}He and ^{16}O and compare moments of the response function distribution to the results of an equivalent static framework, finding negligible discrepancies. We investigate how proton and neutron densities evolve in time, and we see the traditional picture of soft and giant dipole resonances as collective oscillations of protons and neutrons emerging from our calculations in ^{16}O and ^{24}O. This method also allows us to investigate the behavior of the nucleus in the presence of a strong electric field. In that regime, the behavior of the system becomes chaotic. Qualitatively, the spectral information obtained in this limit is in line with previous time-dependent mean-field results.

The physics case

Goal: predictive understanding of structure and reactions in atomic nuclei



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How to solve the time-dependent Schrödinger equation for nuclear dynamics?

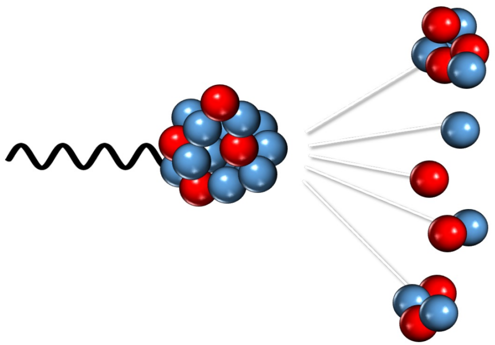
$$i\hbar\frac{d}{dt}\left|\Psi(t)\right\rangle = \hat{H}(t)\left|\Psi(t)\right\rangle$$

Nuclear response function

- A simpler test case to start: nuclear electromagnetic responses in a time-dependent approach.

- Contain information on all the possible final states $|\Psi_f>$ the nucleus can reach by interacting with a photon of energy ω, starting from its ground state $|\Psi_0>$.

$^{16}O + \gamma \rightarrow X$



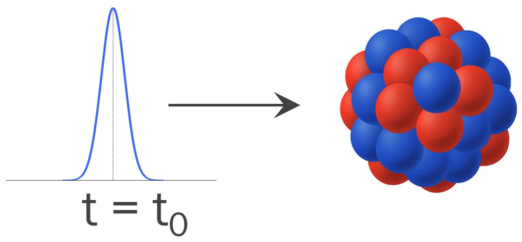
$$R(\omega) = \sum\!\!\!\!\!\!\!\int_f |\langle \Psi_f | \hat{D} | \Psi_0 \rangle|^2 \delta(E_f - E_0 - \omega)$$

transition operator

Responses in a time-dependent approach

- **Goal:** solving

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H}(t)\, |\Psi(t)\rangle$$



with

gaussian pulse

$$\hat{H}(t) = \hat{H}_0 + \epsilon f(t) \hat{D}$$

nuclear Hamiltonian

transition operator

- We record expectation value of the transition operator $\langle \Psi(t) | \hat{D} | \Psi(t) \rangle$
- Build response from Fourier transform.
- How to calculate $|\Psi(t) >$? We use time-dependent coupled-cluster theory (TDCC).

Time-dependent coupled-cluster equations

- In TDCC, $|\Psi(t)>$ is connected to the reference state $|\Phi_0>$ via

$$|\Psi(t)\rangle = e^{T(t)}|\Phi_0\rangle \qquad T(t) = t_0(t) + \sum_{ia} t_i^a(t) a_a^\dagger a_i + \sum_{ijab} t_{ij}^{ab}(t) a_a^\dagger a_b^\dagger a_j a_i$$

D.A. Pigg, G. Hagen, H. Nam, T. Papenbrock, PRC 86, 014308 (2012).

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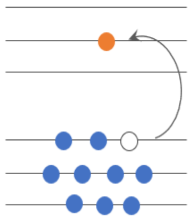

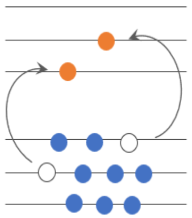

- The TDCC amplitudes evolve in time according to:

$$i\hbar \dot{t}_0(t) = \langle \Phi_0 | \overline{H} | \Phi_0 \rangle$$
$$i\hbar \dot{t}_i^a(t) = \langle \Phi_i^a | \overline{H} | \Phi_0 \rangle \qquad \overline{H} = e^{-T(t)} H(t) e^{T(t)}$$
$$i\hbar \dot{t}_{ij}^{ab}(t) = \langle \Phi_{ij}^{ab} | \overline{H} | \Phi_0 \rangle$$

D.A. Pigg, G. Hagen, H. Nam, T. Papenbrock, PRC 86, 014308 (2012).

What drives the computational cost?

The TDCC equations are in the form

$$\dot{y} = f(t, y),\ \ y(t_0) = y_0$$

where *y* vector of amplitudes → we use time integration solvers from CVODE package of SUNDIALS.

The TDCC amplitudes are complex-valued → required implementation of SUNDIALS vector data structure working with complex datatype.

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Using the diagnostics tools available in SUNDIALS, we saw that the equations become stiffer:

- ❑ when increasing the model space size,
- ❑ when increasing the mass number (e.g. going from ^{4}He to ^{16}O).

How to solve this?

We took advantage of the wide suite of solvers available in the CVODE package of SUNDIALS.

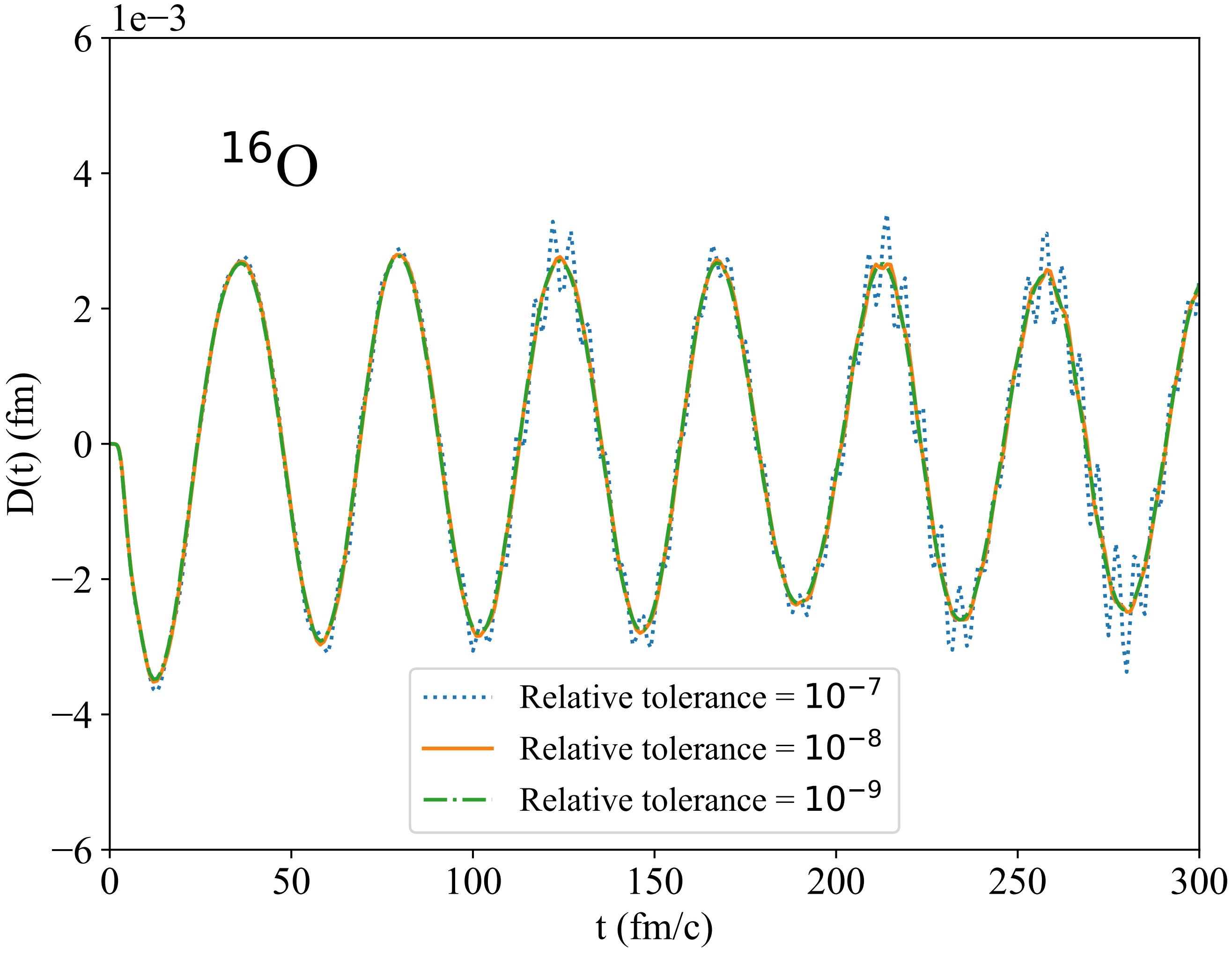
In non-stiff scenarios (e.g. ^{4}He, model space small):

- We use Adams-Moulton methods in CVODE, combined with the SUNDIALS fixed-point iterative nonlinear solver.

In stiff scenarios (e.g. ^{16}O):

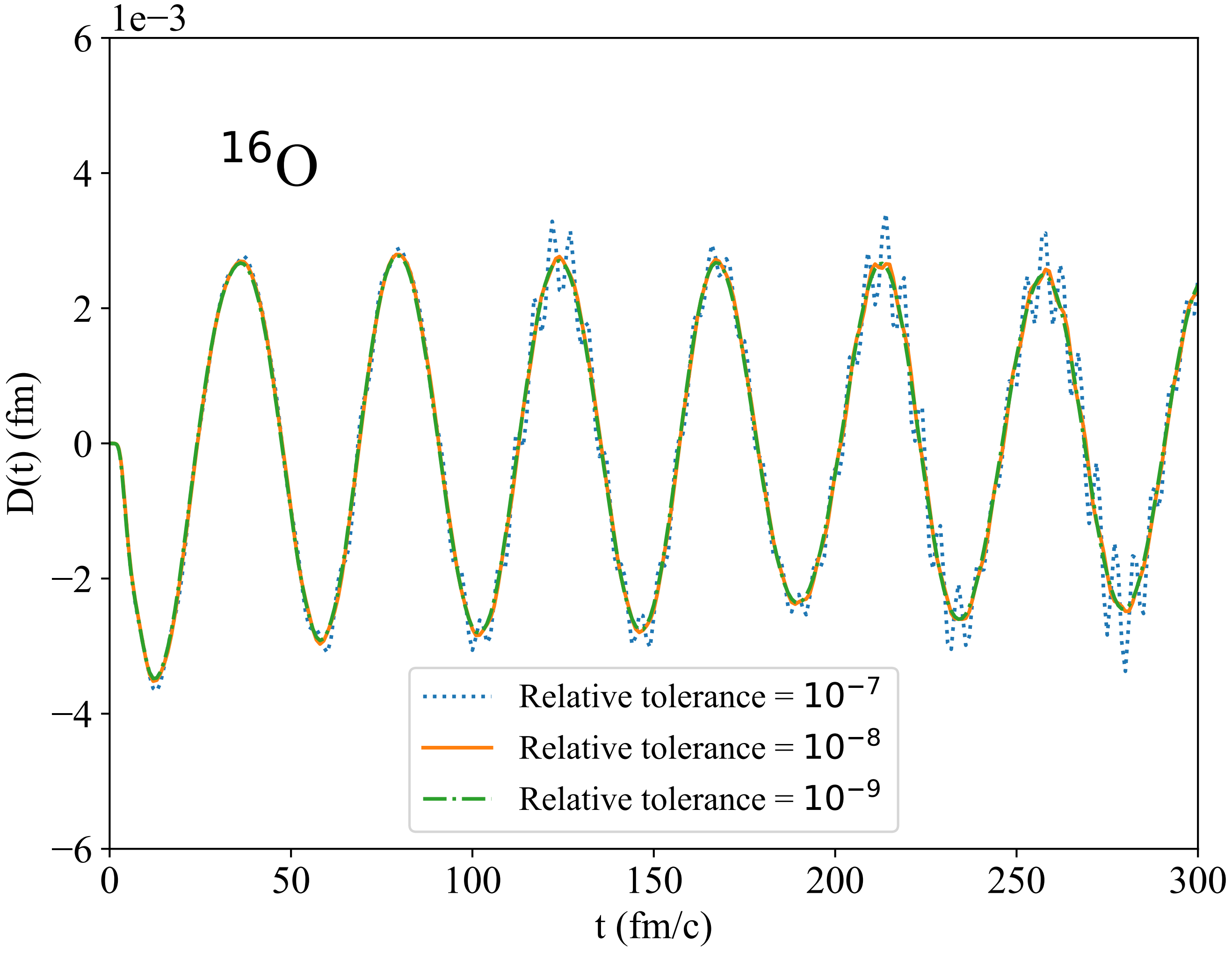
- We use BDF methods in CVODE, paired with the SUNDIALS modified Newton's method solver.
- The resulting linear system at each Newton step is solved using a scaled, unpreconditioned, GMRES Krylov method.
- Jacobian estimated through finite differences.

Tuning the relative tolerance



FB, C. Balos, ..., C. S. Woodward, PRC 113, 024312 (2026).

Tuning the relative tolerance

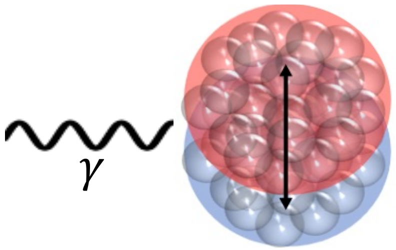


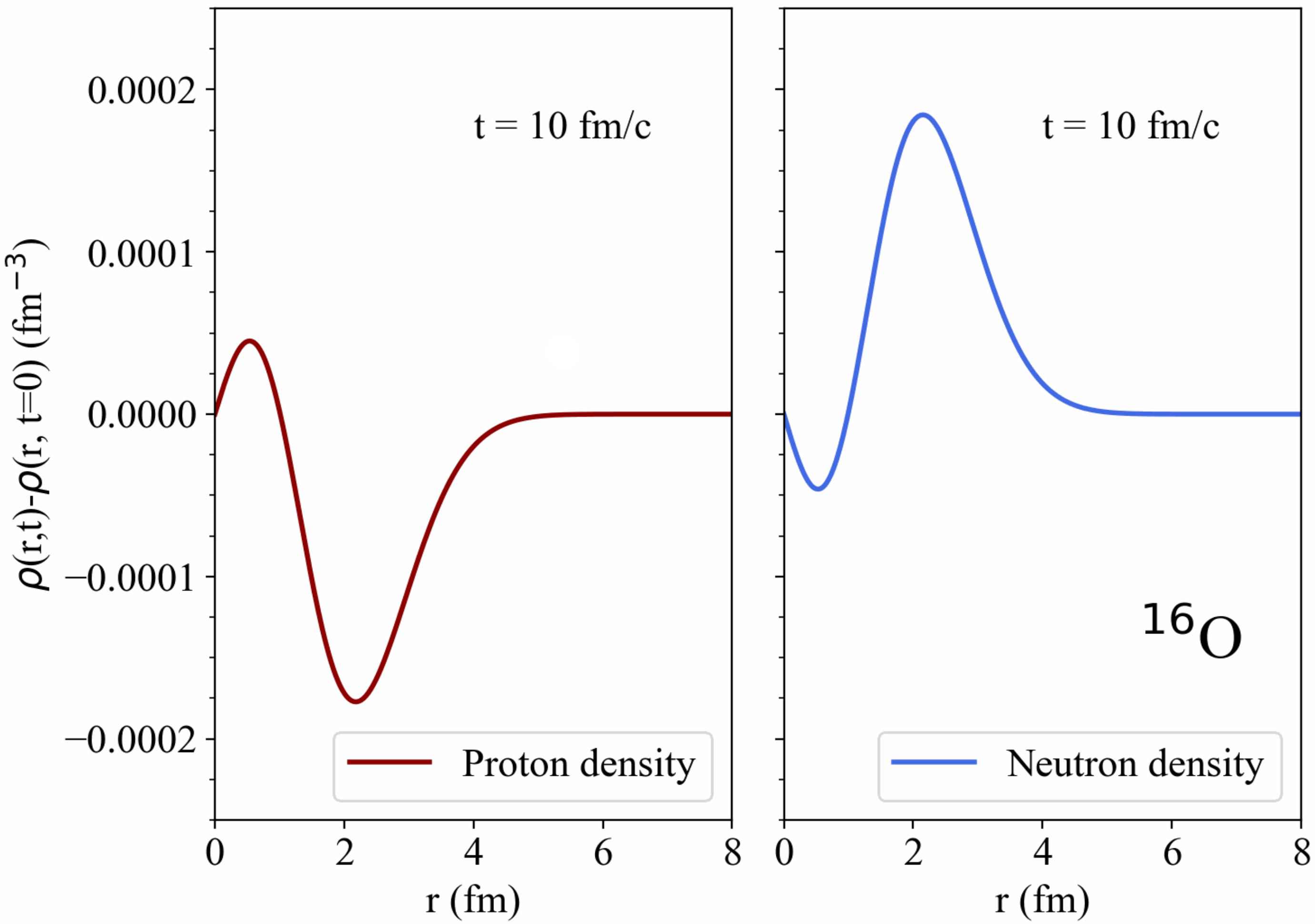
- When the perturbation is different from 0, we introduce a **cap on the CVODE internal step size** to prevent the solver to step over the more rapid dynamics in this time interval.

FB, C. Balos, …, C. S. Woodward, PRC 113, 024312 (2026).

Collective nuclear motion in real time

$^{16}O + \gamma \rightarrow X$





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SUNDIALS wishlist

- Possibility of implementing **checkpoints** (stop time integration at t_{stop} and restart from t_{stop} onwards in a subsequent run).
- We are also interested in a **complex Python implementation**.
- Integrating solvers with **AI** for **time interpolation/extrapolation**?

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@FRIB/MSU: Kyle Godbey

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