

Performance and architectural improvements in Hermes-3

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Task

Make Hermes-3 faster, easier to use, and easier to develop.

New normalisation scheme for SNES solver

Problem

Variables differ by many orders of magnitude across domain, SNES solver error evaluation dominated by largest. Need very tight tolerance to ensure smaller variables solved adequately.

Solution

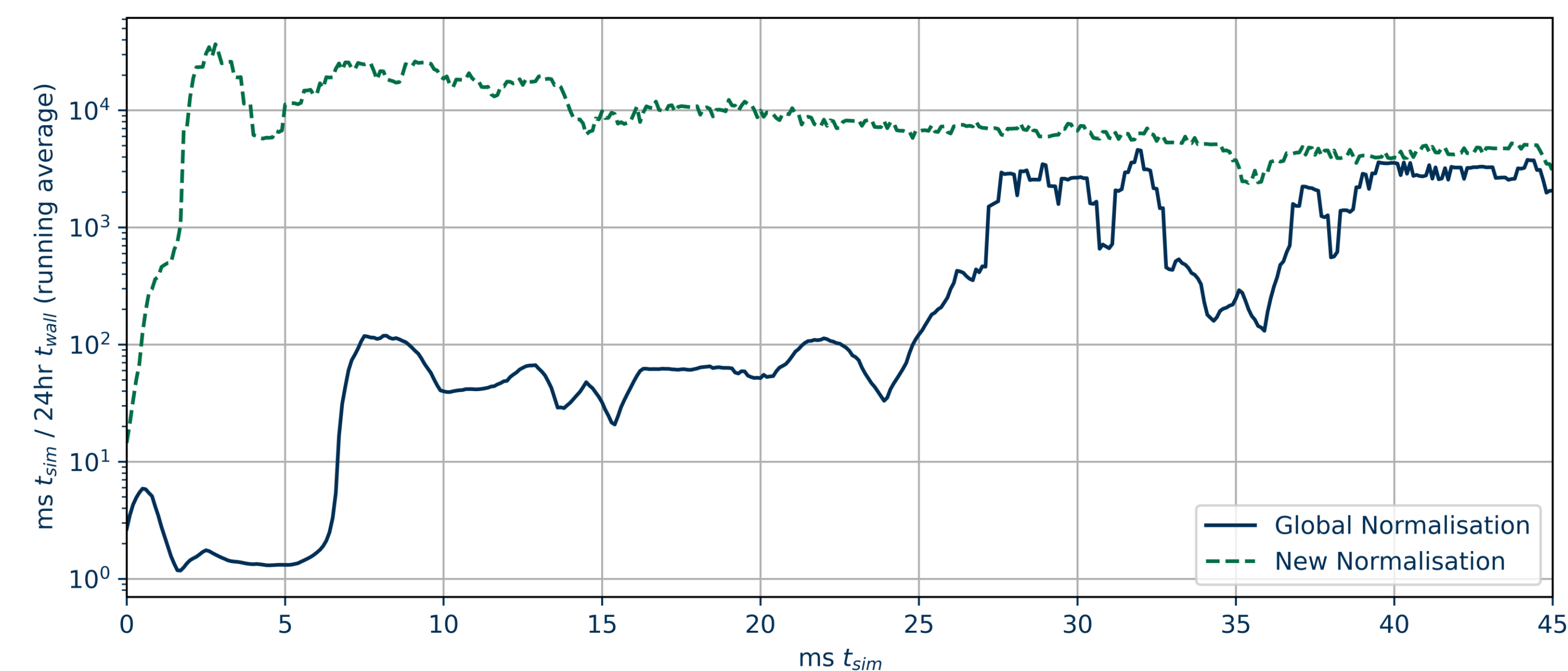
Rescale all variable component be ~ 1 , transforming backwards Euler equation being solved:

$$\mathbf{F}(\mathbf{x}_{n+1}) = \frac{\mathbf{x}_n - \mathbf{x}_{n+1}}{\Delta t} + \mathbf{f}(\mathbf{x}_{n+1}) = 0 \Rightarrow \tilde{\mathbf{F}}(\tilde{\mathbf{x}}_{n+1}) = \frac{\tilde{\mathbf{x}}_n - \tilde{\mathbf{x}}_{n+1}}{\Delta t} + \mathbf{S}\mathbf{f}(\mathbf{S}^{-1}\tilde{\mathbf{x}}_{n+1}) = 0$$

where $\frac{\partial \mathbf{x}}{\partial t} = \mathbf{f}(\mathbf{x})$, $\tilde{\mathbf{x}} = \mathbf{S}\mathbf{x}$, and $S_{ij} = \frac{\delta_{ij}}{x_{i,prev}}$. Allows looser tolerances.

Example: ST40 simulation

Full resolution simulation, run from flat profiles to steady state, for 45ms. Comparison of traditional simulation with one using new normalisation.



	Global Normalisation	New Normalisation
Jacobian Lag	1 iteration	3 iterations
Rel. Tolerance	10^{-6}	10^{-5}
Abs. Tolerance	10^{-7}	10^{-4}
Runtime	111h 21m	59m

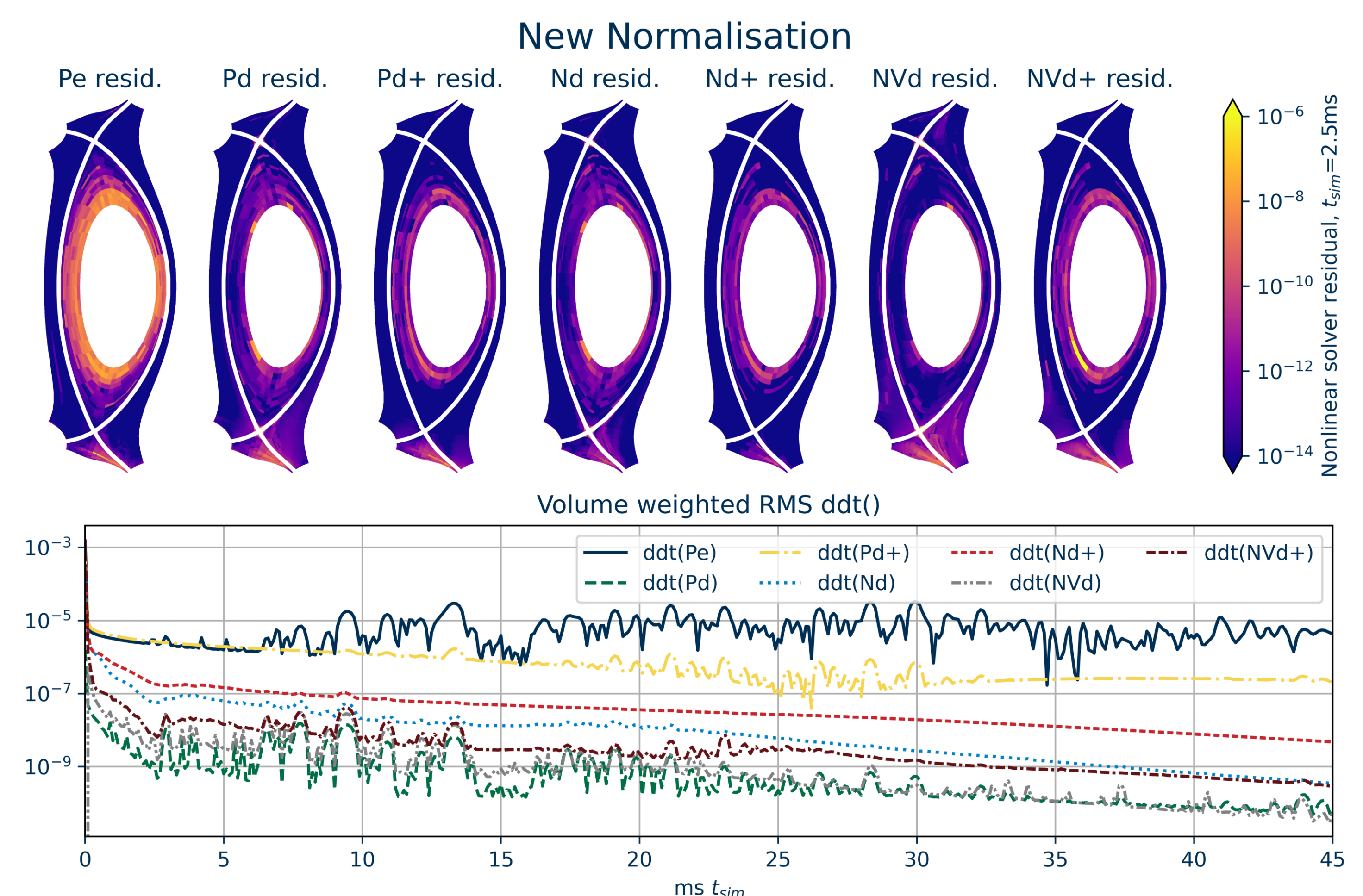
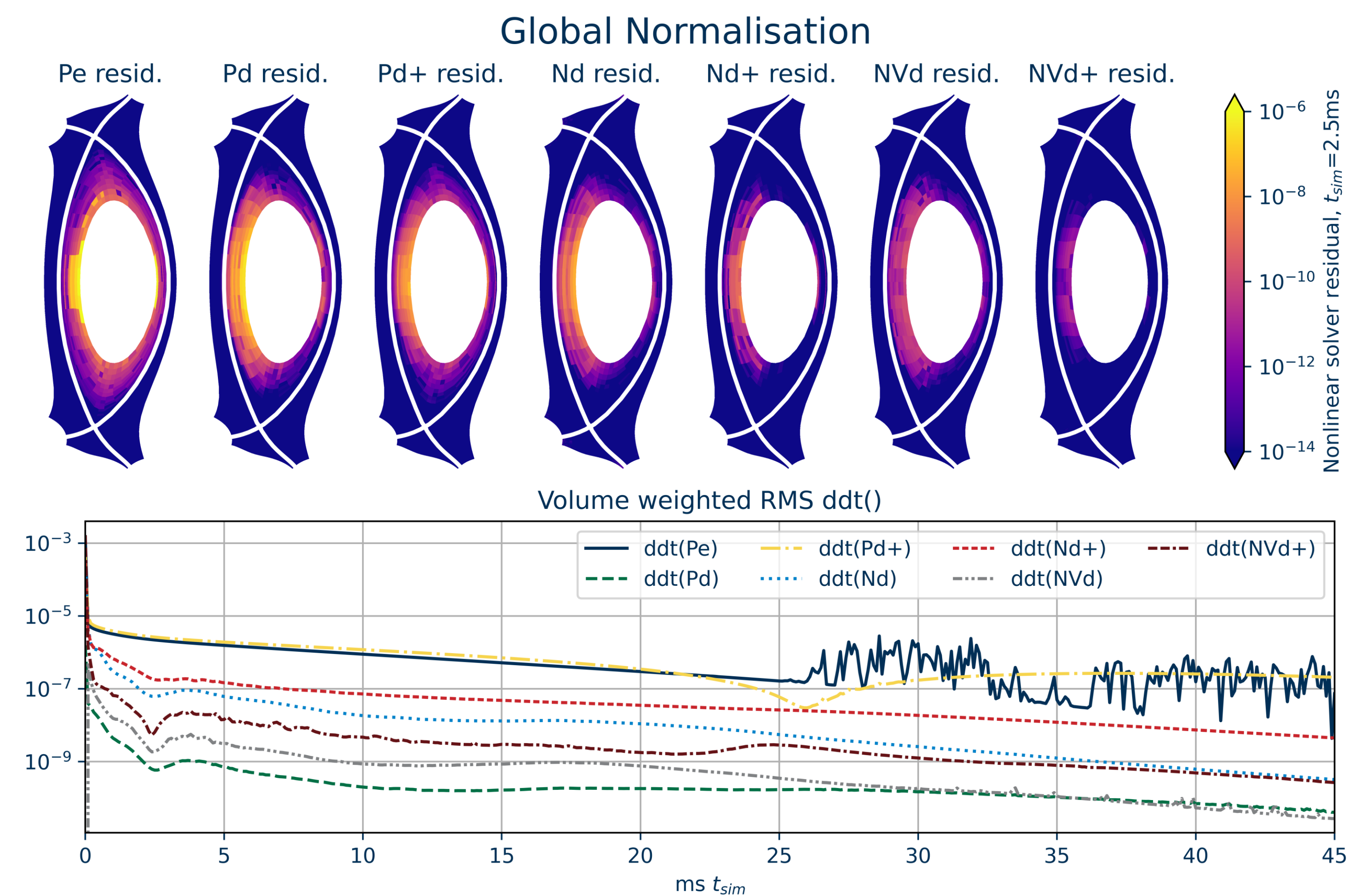
Result: 113× speedup!

New Feature

SNES solver can output residual of nonlinear solve for each variable/cell.

What is Hermes-3?

- Plasma simulation model built on BOUT++
- Mainly used to simulate edge of magnetically confined plasmas
- Multi-species, multi-fidelity simulation of fusion reactors
- Modular/reusable components, configurable at run-time



Automatic benchmarking in CI

Problem

Must ensure changes to Hermes-3 and BOUT++ do not introduce performance regressions.

Solution

Use Airspeed Velocity (ASV) to run benchmarks in CI, for code before and after changes. If PR causes performance to fall, CI fails and PR won't be merged.

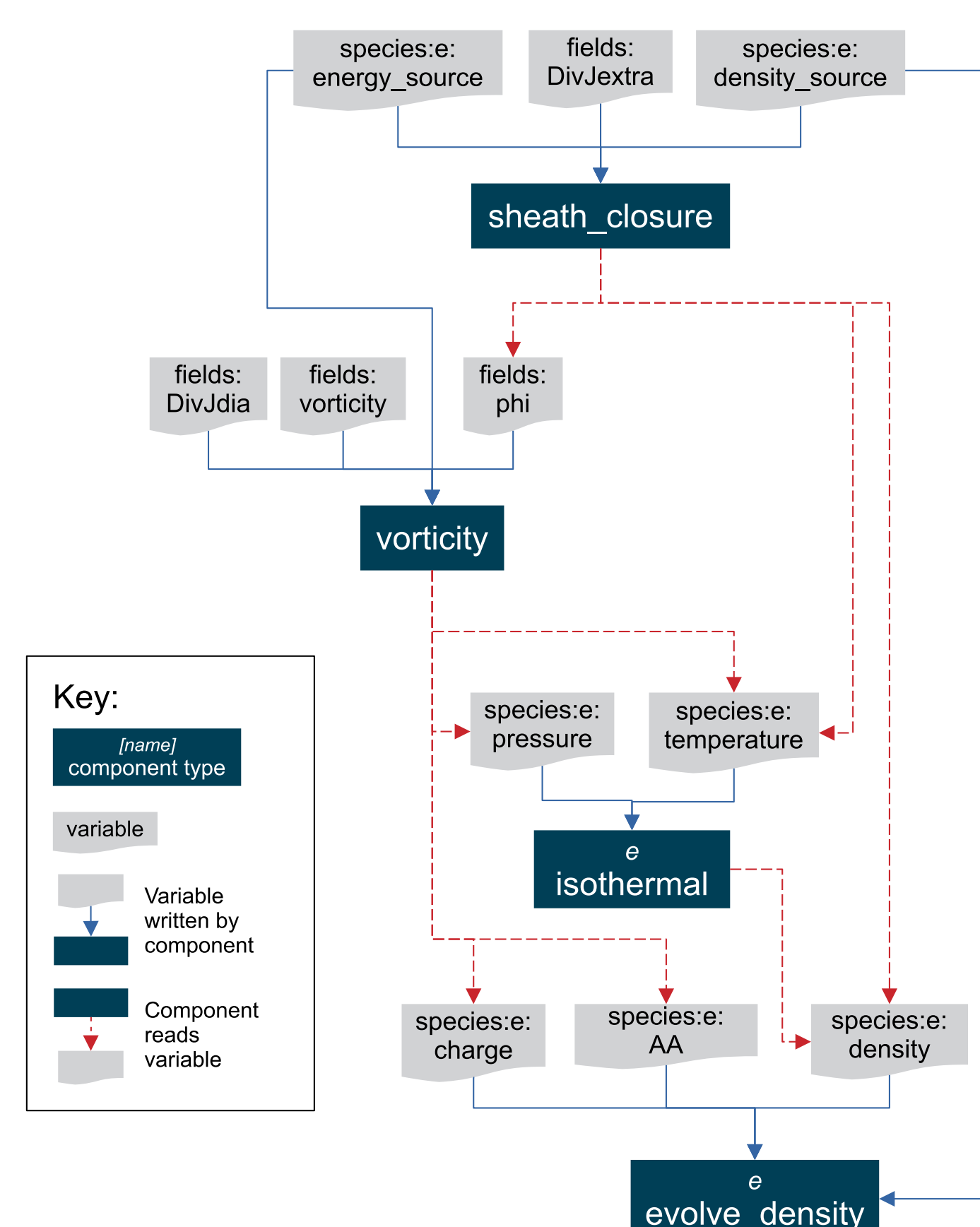
Example ASV output

Before	After	Ratio	Benchmark
[c69f8d32]	[62aa7e4d]		
37.7±0.1s	37.5±0.2s	0.99	1D-recycling-dthe
2.21±0m	2.15±0m	0.97	2D-production
1.34±0m	1.34±0m	1	tokamak-2D-driftplane

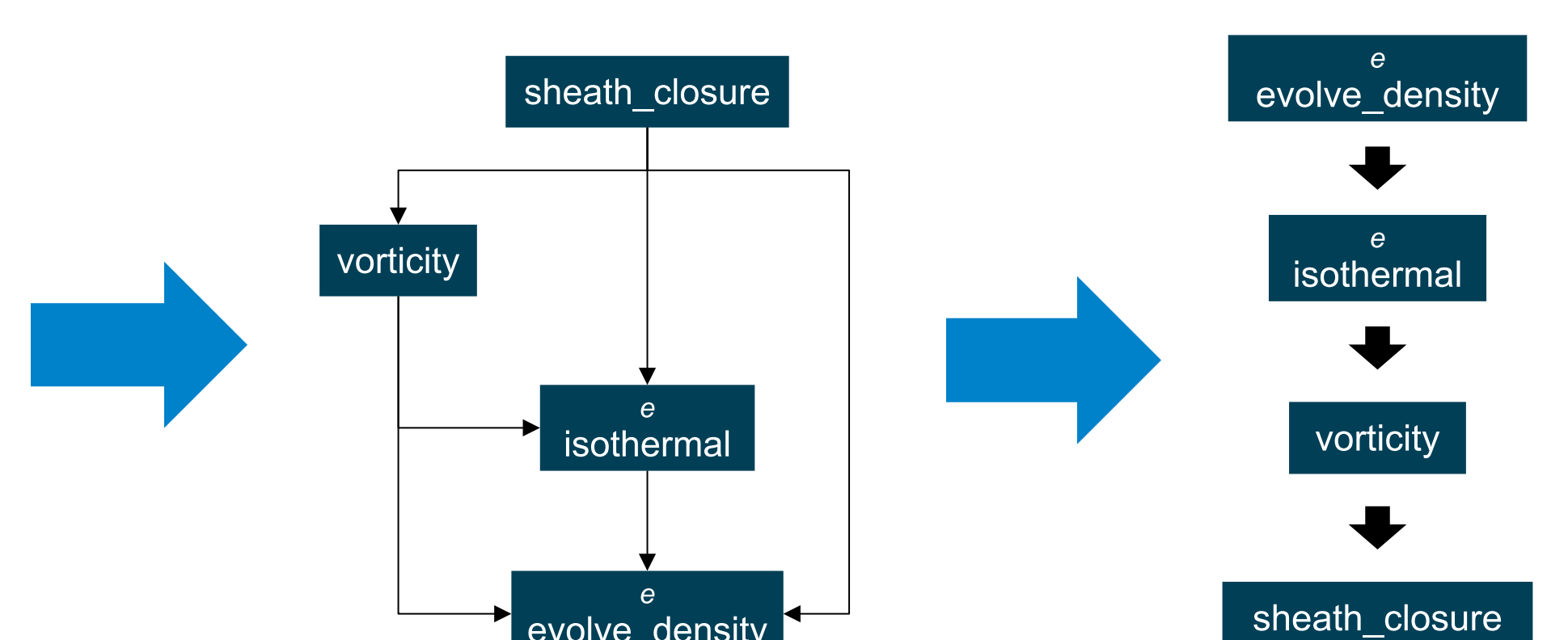
Automatic component ordering

Problem

Users must list components in right order to ensure all inputs are available when needed. Difficult for new users.



Sorting algorithm applied to example Blob2D-Te



Solution

Introduce access permission system to track variables read/written by each component. Construct DAG and perform topological sort to place components in correct order. Print error message if that is impossible.