ReMKiT1D – A novel framework for building 1D reactive multi-fluid models of the Scrape-Off Layer with kinetic electrons

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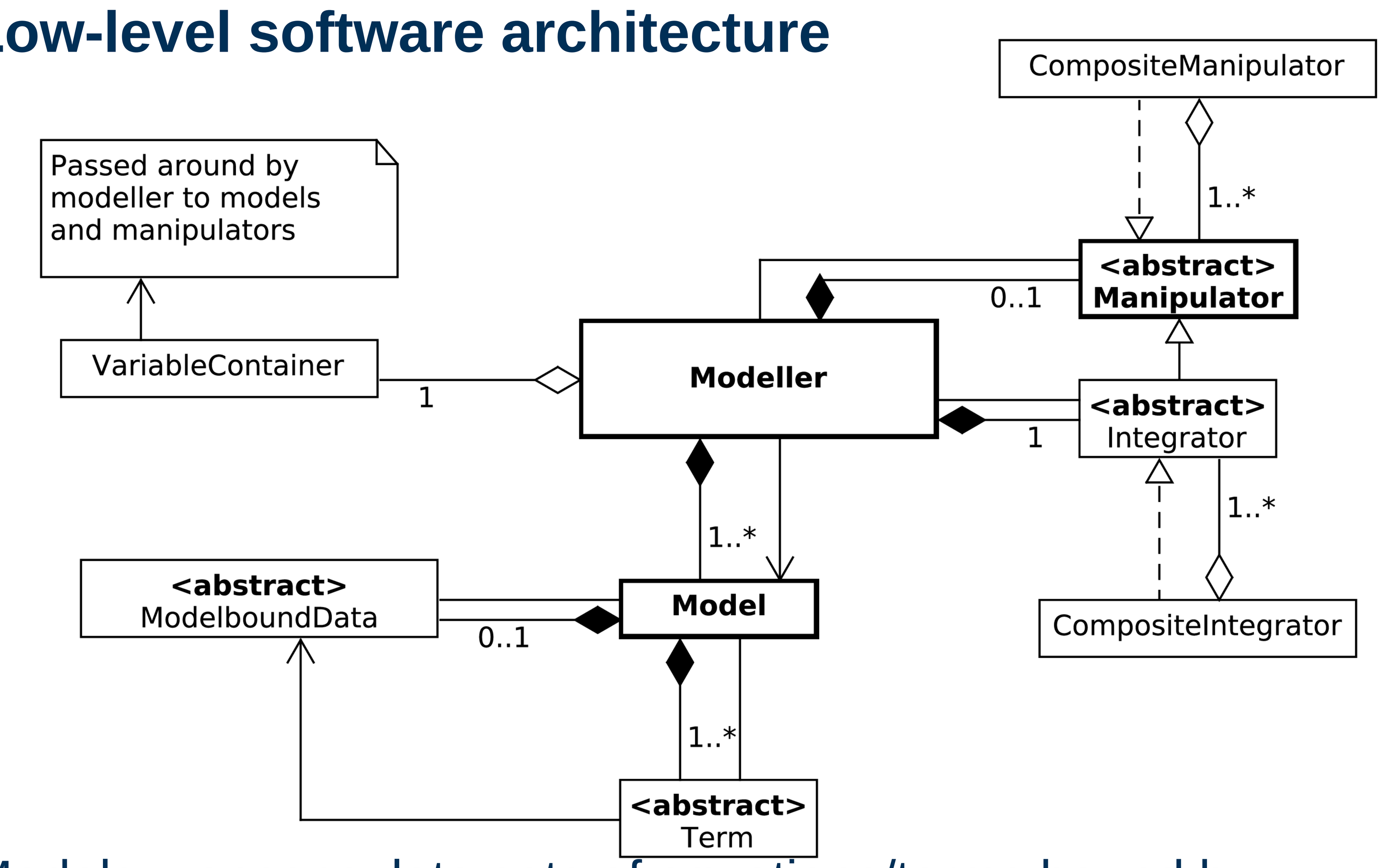
Background and Motivation

- Even 1D simulations of the Scrape-Off Layer can be rich in complex physics:
  - Plasma reactions/chemistry
  - Multi-species effects
  - Transient and kinetic effects
- Many different 1D codes and models exist, treating all sorts of physics [1,2,3,4]

Goals of this framework

- Flexibility – One framework that can handle:
  - 0D Collisional-Radiative Models $\frac{d\vec{v}}{dt}=\boldsymbol{M}\cdot\vec{v}+\vec{\Gamma}$
  - 1D fluid equations $\frac{\partial X(\vec{x})}{\partial t}+\nabla\cdot\vec{\Gamma}(\vec{x})=S_X$
  - Electron kinetic equations $\frac{\partial f}{\partial t}+v_x\frac{\partial f}{\partial x}-\frac{eE}{m_e}\frac{\partial f}{\partial v_x}=\left(\frac{\delta t}{\delta t}\right)_c, \quad \frac{\partial f_l}{\partial t}=A_l+E_l+C_l$
- User-friendliness – Main features accessible from Python
- Extensibility – Modern software design enabling easy addition of new features
- Performance – All of the above without massive performance sacrifices

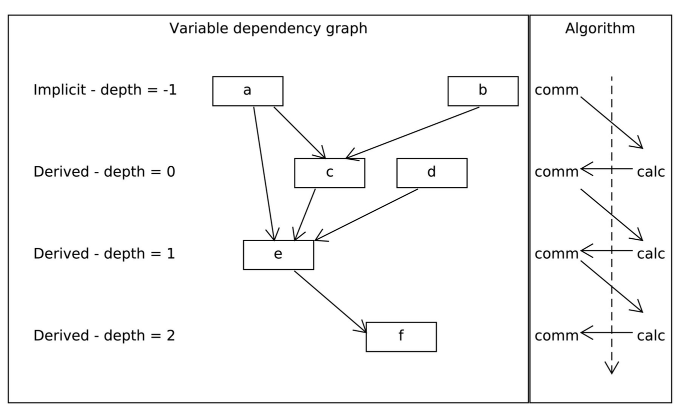
Low-level software architecture

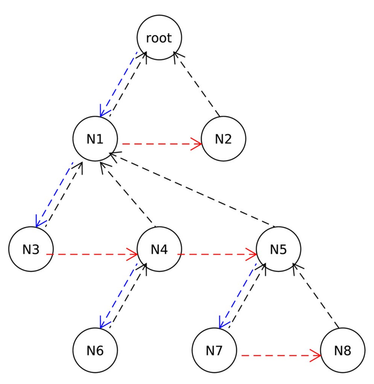


- Models – encapsulate sets of equations/terms bound by common physics
- Terms – additive (RHS) terms in various equations
- Modeller – central object handling communication between models and manipulators
- Manipulators – data manipulation objects (e.g. time integration or some diagnostics)

Variables

- Variables can be associated with calculation rules or can be used with PETSc for implicit solves
- Communication-safe calculation
- Calculation rules can be represented with simple Python expressions using an expression tree





Other features

- Terms and models definable at Python level with many pre-built examples
- Flexible integrator support (RK and Backwards Euler at the moment) with high degree of control over how the integration is done
- Data can be associated with models – particularly useful for Collisional-Radiative Models
- Manipulators allow for flexible data access (e.g. evaluating individual terms in equations etc.)

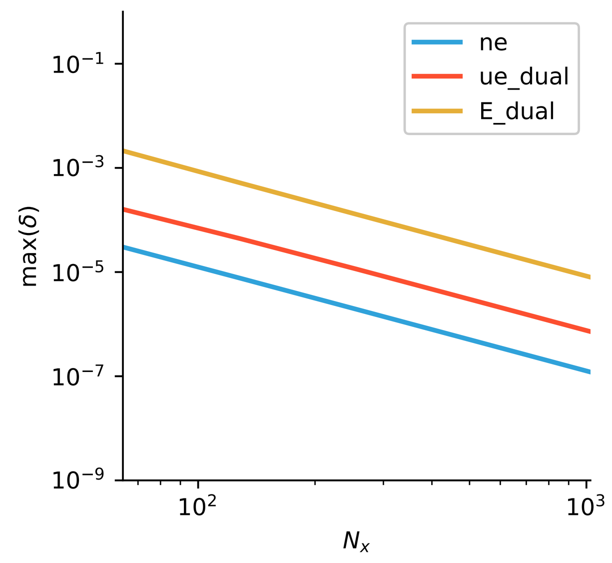
Verification

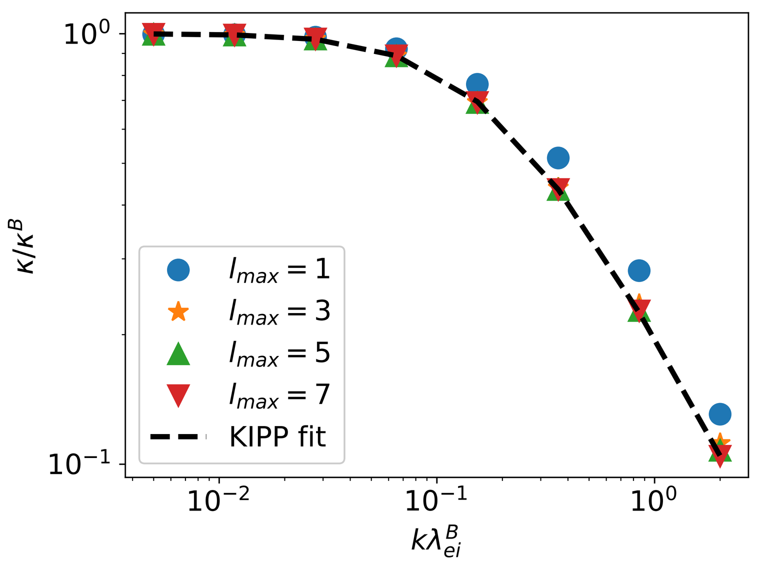
Simple fluid model test with the Method of Manufactured Solutions

$$\frac{\partial n_s}{\partial t}+\frac{\partial \Gamma_s}{\partial x}=0$$

$$m_s\partial\Gamma_s\partial t+\frac{\partial}{\partial x}\left(n_s k T_s+m_s\Gamma_s u_s\right)-Z_s e n_s E=0$$

$$\frac{\partial E}{\partial t}=-\frac{j}{\epsilon_0}$$

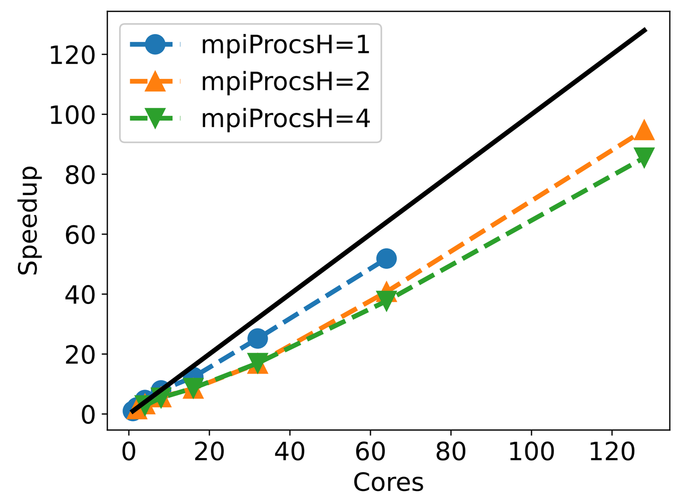




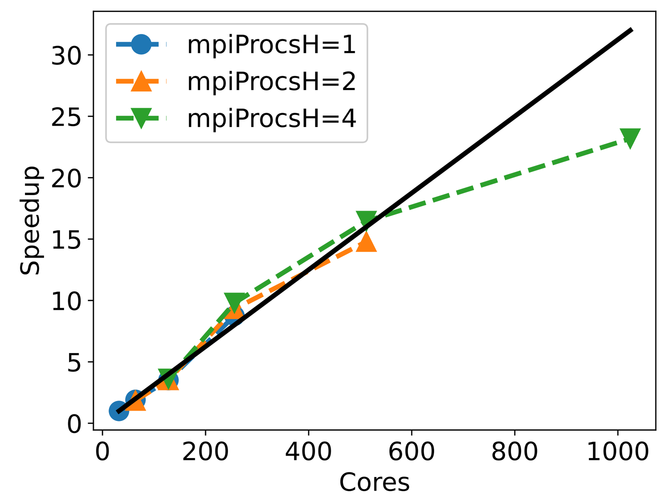
Epperlein-Short test electron heat conductivity comparison with fits of KIPP results [2,5]

Benchmarking

Scaling tested on ARCHER2



Epperlein-Short test



SOL-KiT-like model [5]

- Fluid runs scale poorly, as expected (not shown)
- Novel kinetic parallelisation in distribution function harmonics

Summary and Outlook

- New framework[6] publicly available on UKAEA GitHub https://github.com/ukaea/ReMKiT1D
- Ongoing code comparisons with other 1D codes [3,7]
- Planned model exploration for equilibria and transients in SOL (multi-fluid and kinetic effects)

References

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[6] Mijin, S. et al. ReMKiT1D - A framework for building reactive multi-fluid models of the tokamak Scrape-Off Layer with coupled electron kinetics in 1D – submitted to Computer Phys. Comm. - https://arxiv.org/abs/2307.15458

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