Towards a predictive modelling capability for projectile-driven ICF

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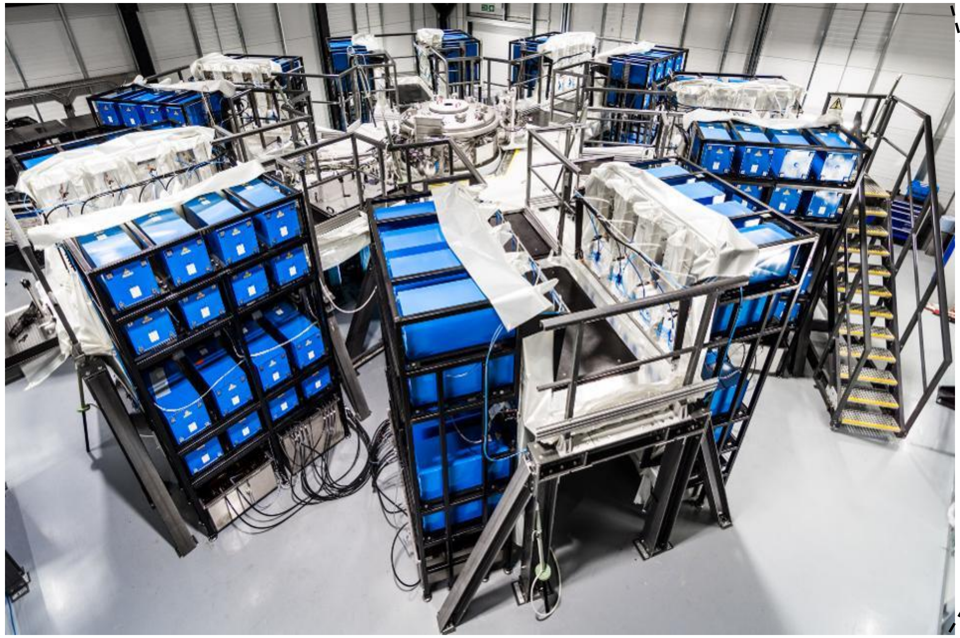
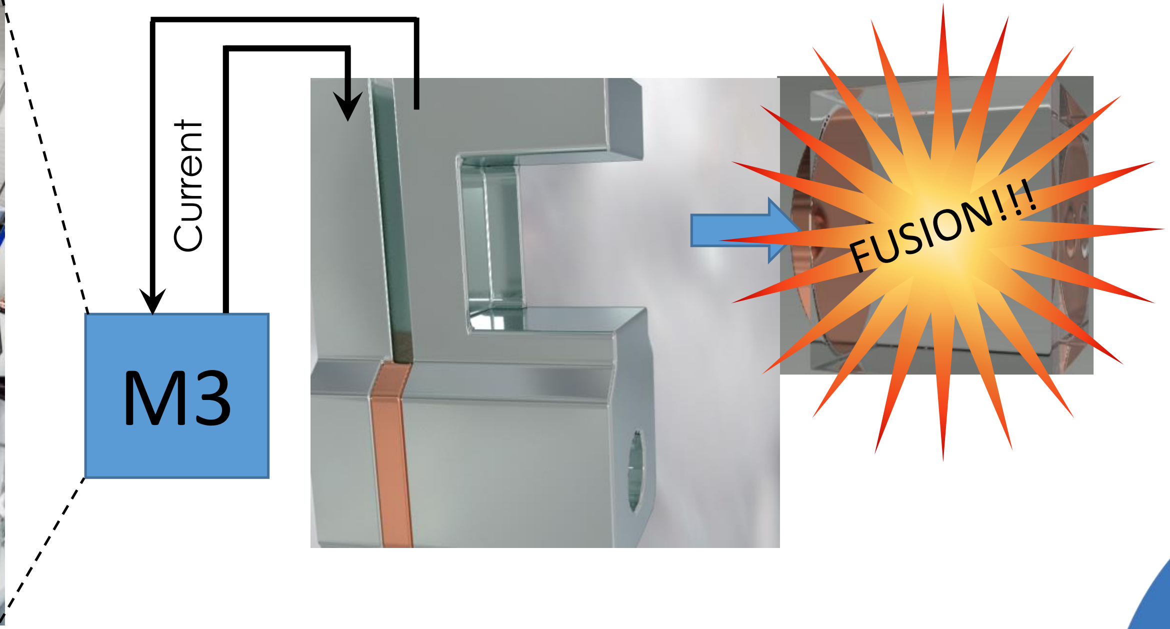
Outline of talk

- About FLF: what are we trying to achieve?
- FLF simulation tools
- Validation results for Hytrac and Code B
- Equation of State (EoS) and microphysics modelling
- Code-to-code comparison with HELIOS-CR and sensitivity study
- Prioritisation for direction of future development
- Summary

What are we trying to achieve?

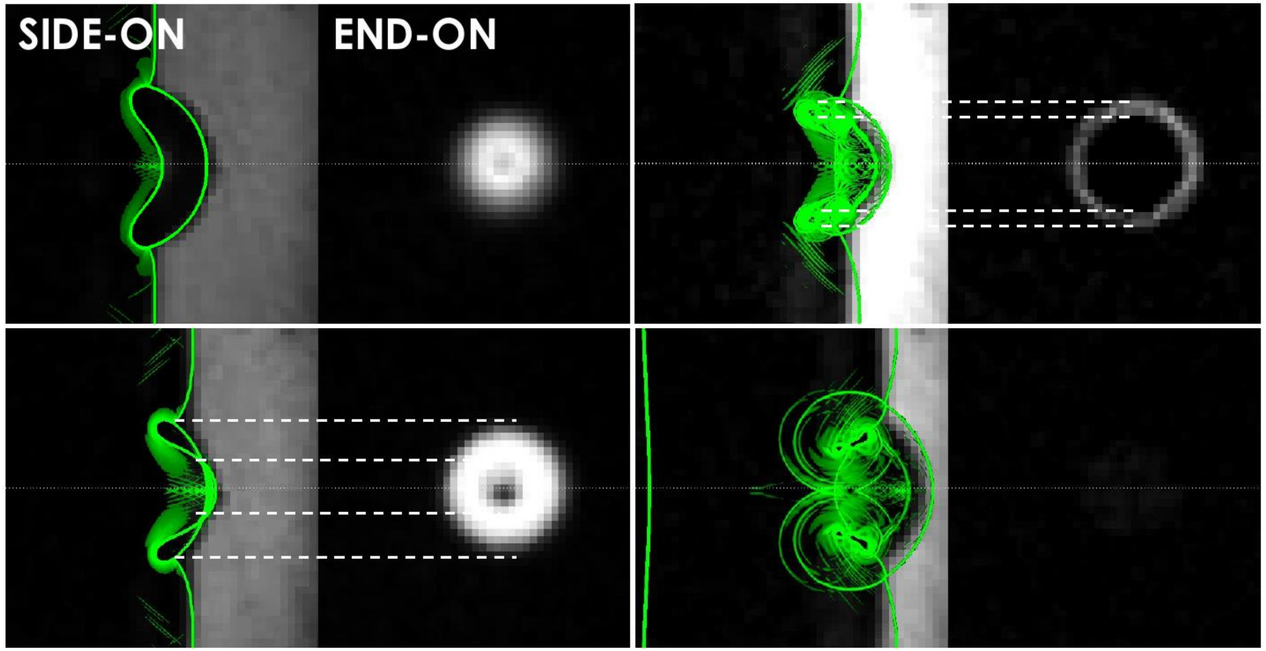
- FLF aims to design, demonstrate and commercialise fusion energy
  - As [**soon**, **simply**, **cheaply**] as possible
- **M3 machine now operational - See N. Hawker (2C05) and M. Betney (3P59)**
- **Combine with novel (proprietary) target designs to maximise shock coupling**





FLF simulation tools

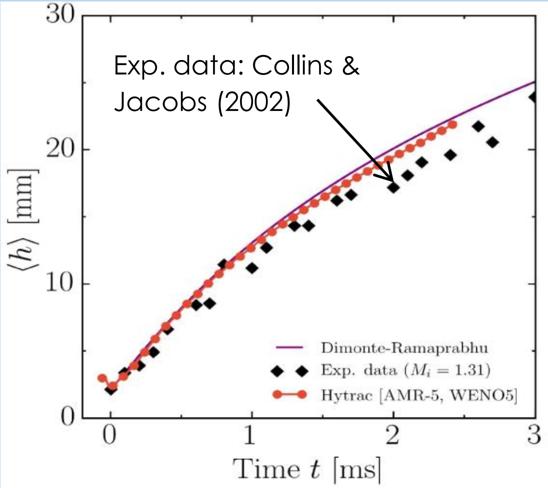
- **Hytrac (right):** Highly configurable 2D-axisymmetric AMR-Eulerian
  - High-fidelity shock physics utilising N-fluid front tracking for target modelling

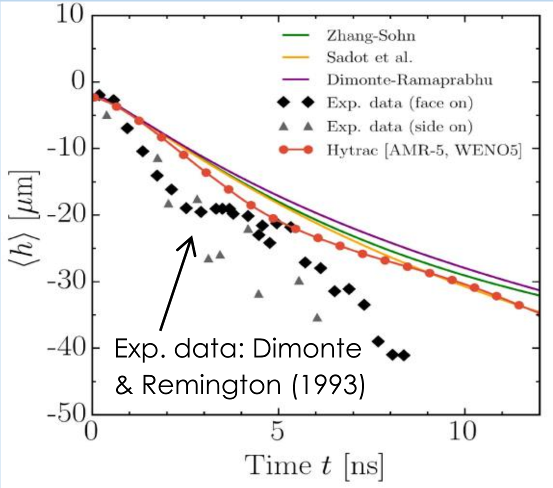


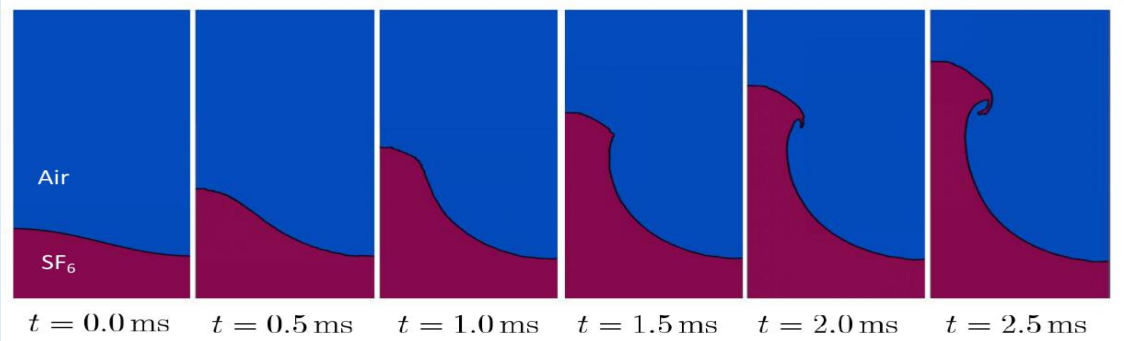
- **'Code B' (left):** 3D Lagrangian-remap massively parallel RMHD
  - Fully-integrated, dynamic launcher-flyer-target simulation capability
- **Rigourously validated, tabulated EoS support, multi-material, 2T, conduction and radiation loss**

Selection of Hytrac/Code B validation results

Hytrac validation vs RM instability growth data

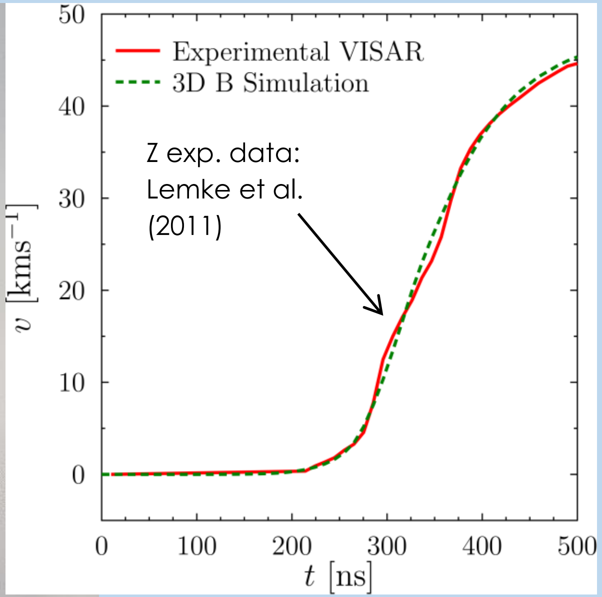






- Close agreement with amplitude growth and spike roll-up
- **See poster: M. Read (5P25)**

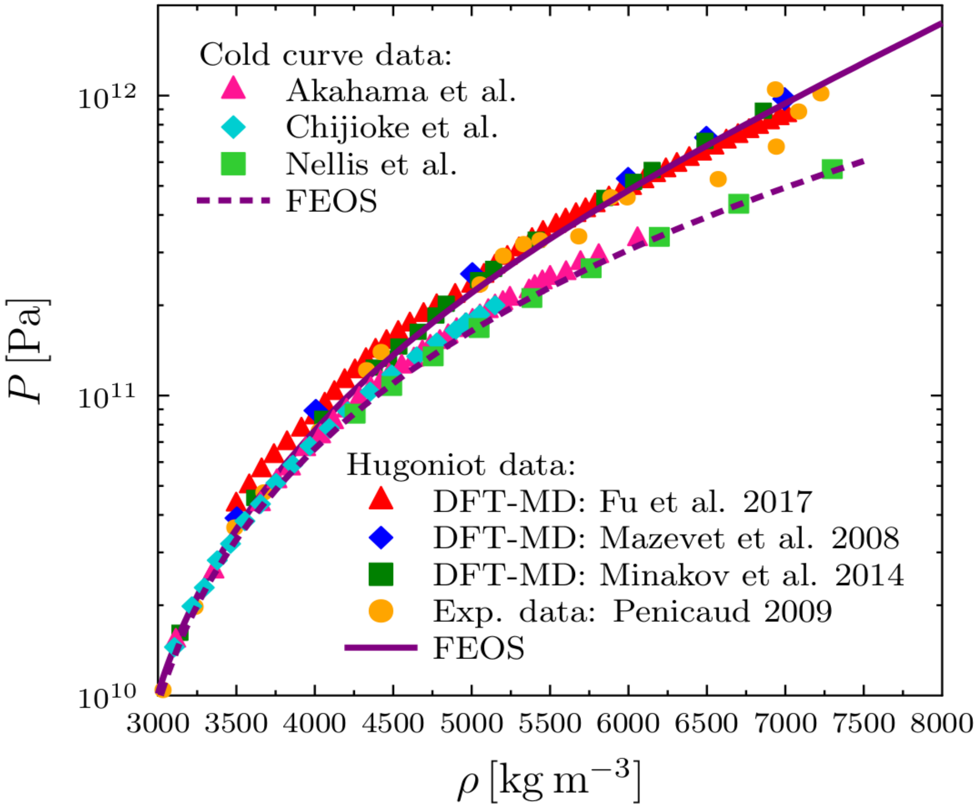
Code B validation vs Z experimental data

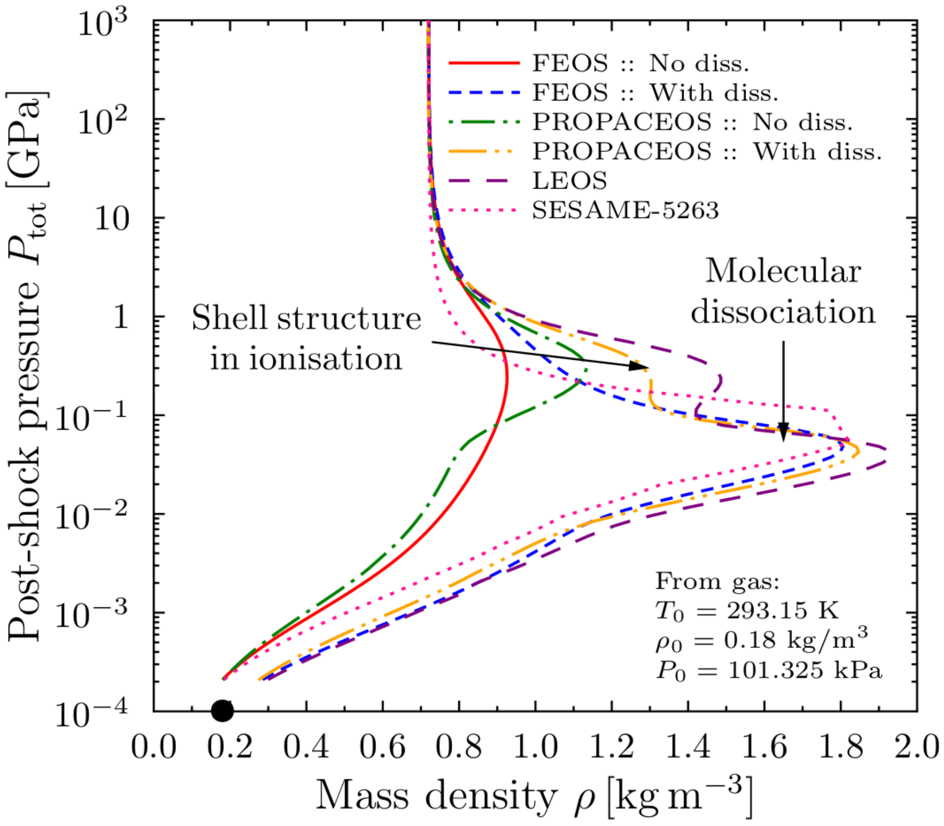


3D Code B simulation rendered using OSPRay Paraview package

- Excellent agreement
- No need for ad hoc geometrical correction factor
- **See poster: J. Pecover (5P27)**

Equation of State modelling

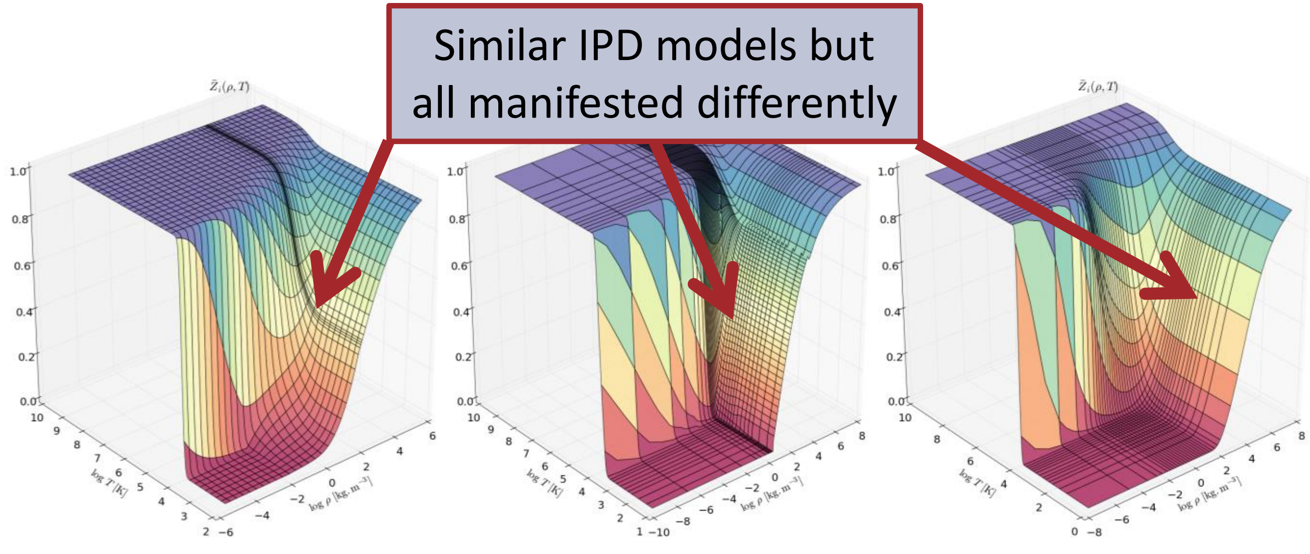




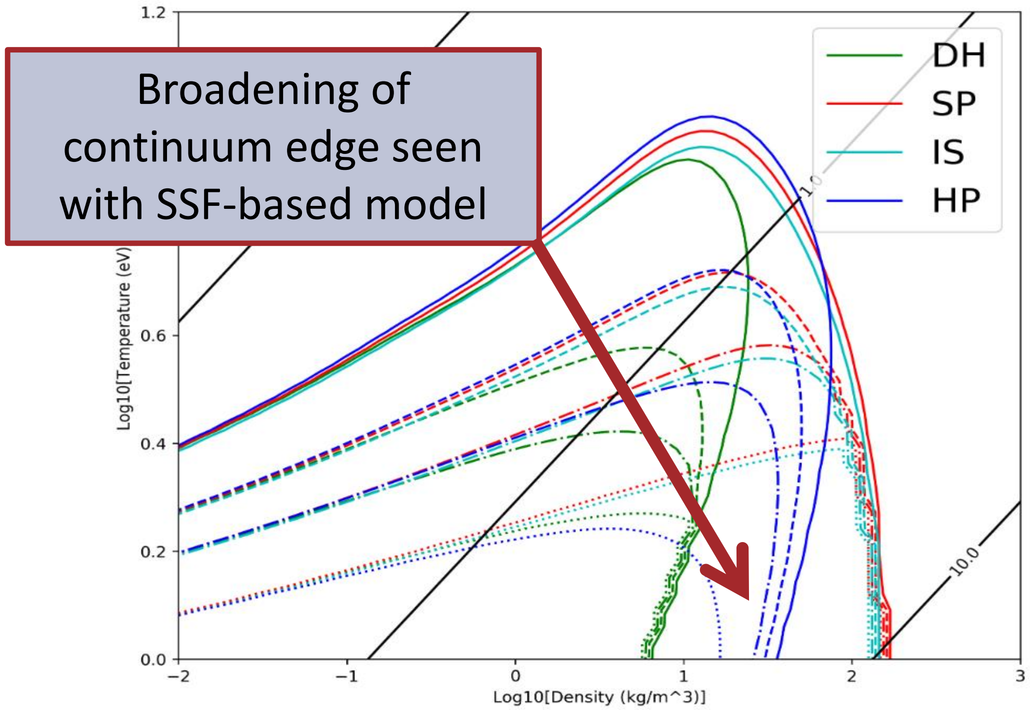
- FEOS code [Faik et al. (2012)] used for solid materials - poor results for deuterium fuel
- PROPACEOS [MacFarlane et al. (2006)] captures shell structure
- Simple linear mixing model [Ross et al. (1995)] gives correction for molecular dissociation

- **Dissociation-corrected PROPACEOS principal hugoniot for initially ambient deuterium gas reproduces LEOS and SESAME EoS**

Future work on EoS model development



PROPACEOS   SHM-ℓ [Faussurier et al. (2008)]   SpK [Niasse (2012)]

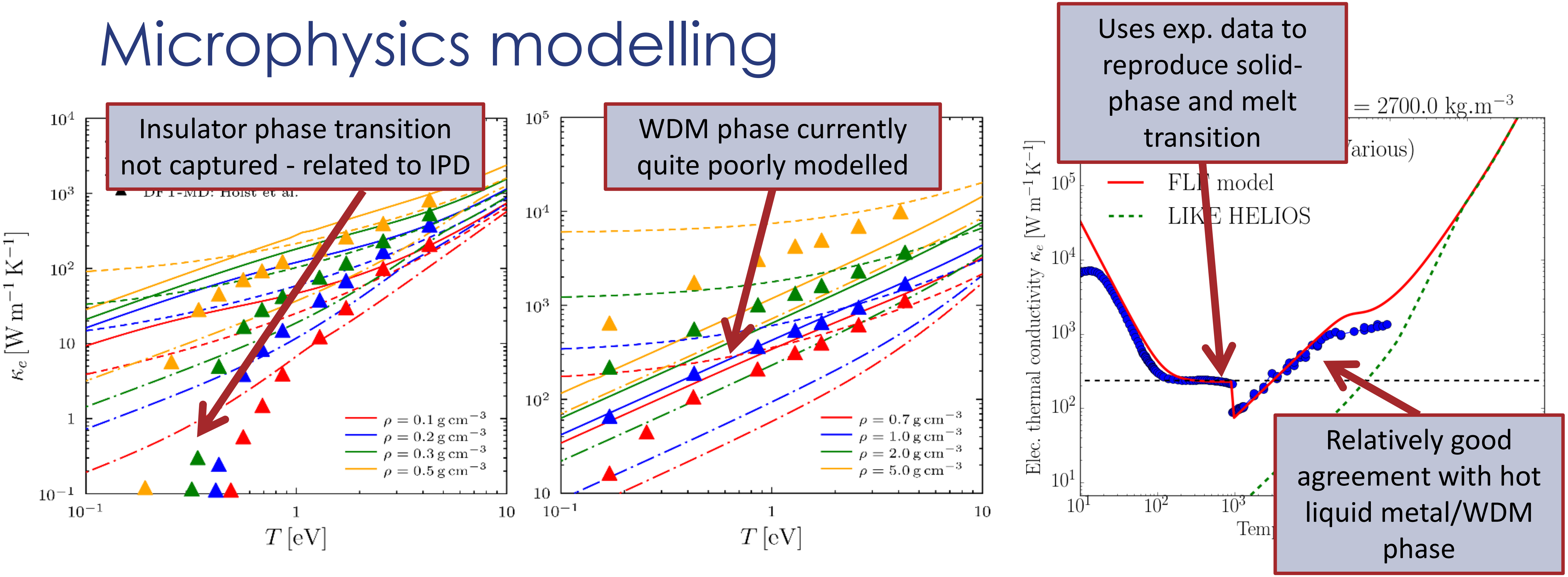


- Main differences in fuel EoS due to IPD
- **Developing structure factor-based model [Lin et al. (2017)] - self-consistently used within SpK code [Niasse PhD thesis (2012)]**
- **FLF-sponsored PhD student at Imperial College developing full EoS driven by SpK**

$$\Delta_{\mathrm{IPD}}^{\mathrm{ion}} = -\frac{(\bar{Z}_i+1)^2 e^2}{2\pi^2\varepsilon_0}\frac{\kappa_i^2(\Gamma_{ii})}{k_{\mathrm{F}i}}\int_0^\infty \frac{\mathrm{d}k}{k} S_{ii}(k)\left[1-\frac{q_i(k)}{\bar{Z}_i}\right]^2$$

Hypernetted-chain (HNC) → $S_{ii}(k)$
Hayter-Penfold (HP) → $S_{ii}(k)$
Hard-core screened OCP (SOCP) → $S_{ii}(k)$

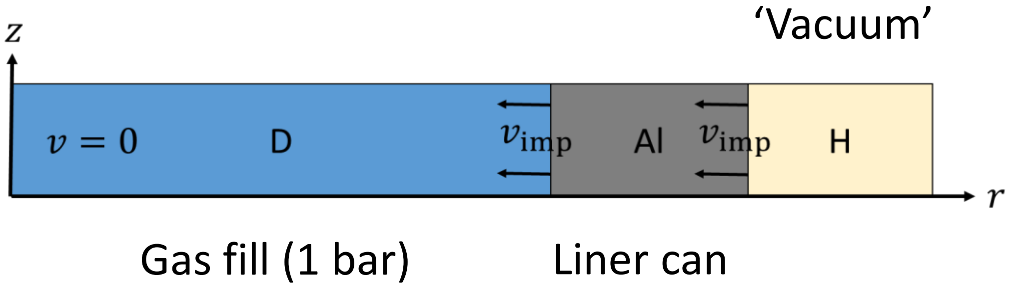
Microphysics modelling



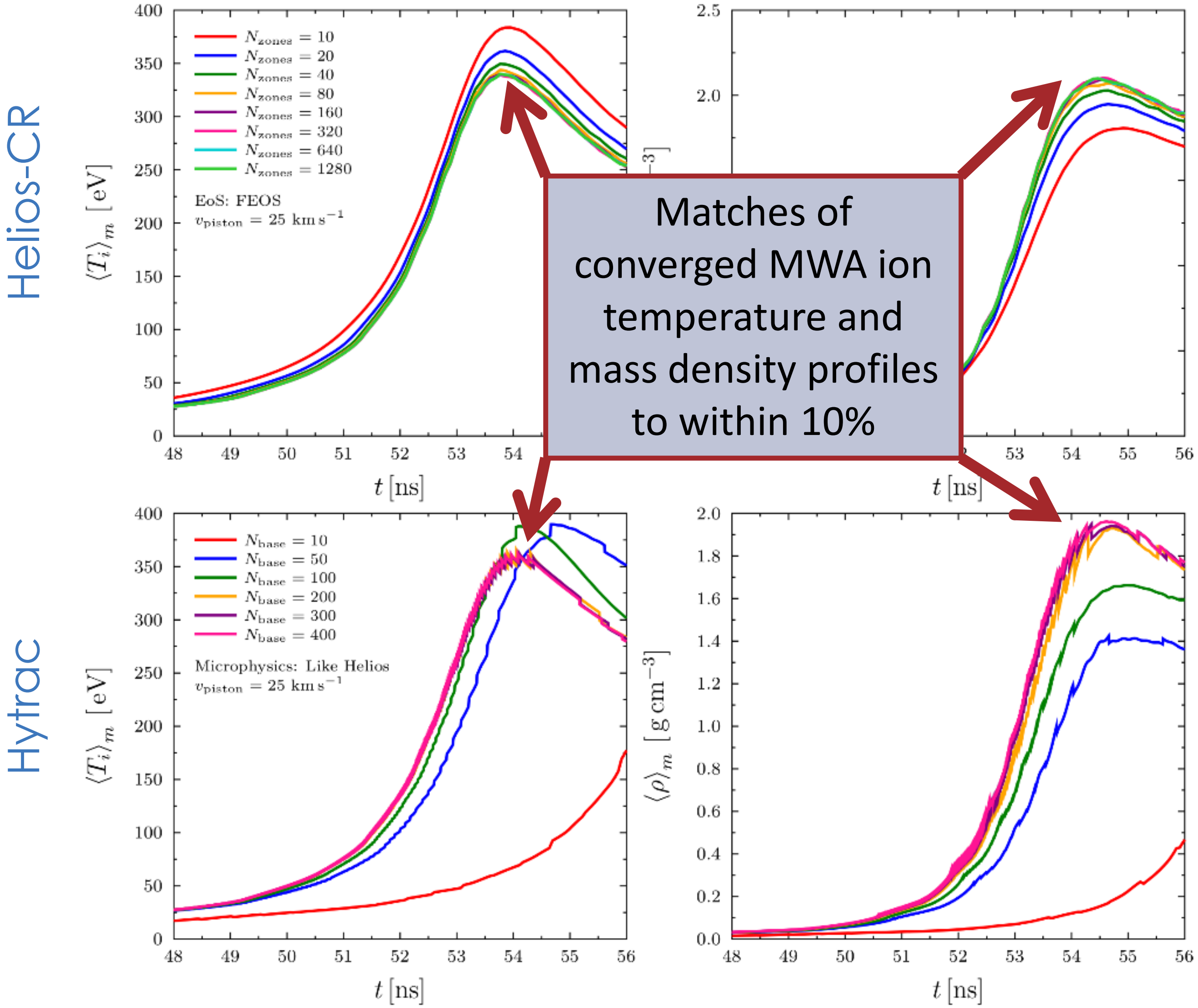
- Large discrepancies for H/D for low T – some uncertainty in fuel energetics
- Good agreement for CH and Al – lower uncertainty in launch modelling
- **Working on improved transport model and coupling to DCA ionisation equilibrium for fully consistent EoS, opacity and microphysics tables**

Code-to-code benchmarking vs HELIOS-CR

- Limit to simple geometry and materials
- Liner-like configuration (1D axial) relevant to pulsed power machines such as M3
- High convergence ratio - good test of AMR

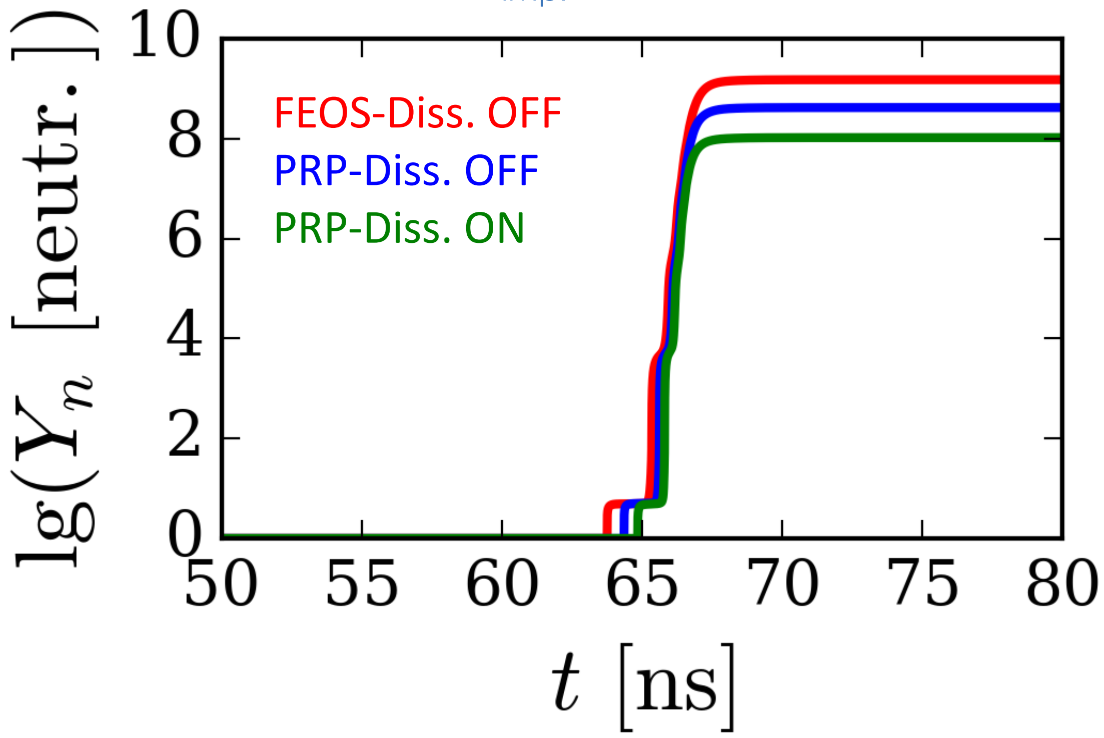


- **Compare to well-established and widely-used code HELIOS-CR [MacFarlane et al. (2006)]**

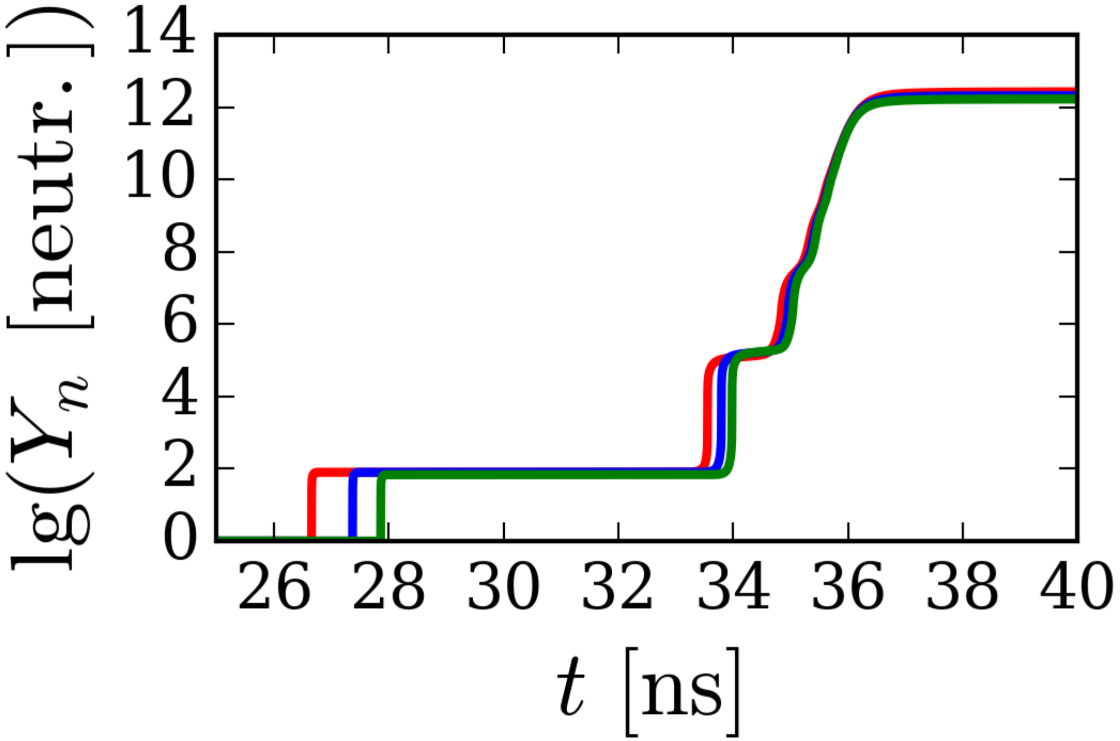


Sensitivity study - EoS model

v_{impl} = 25 km/s

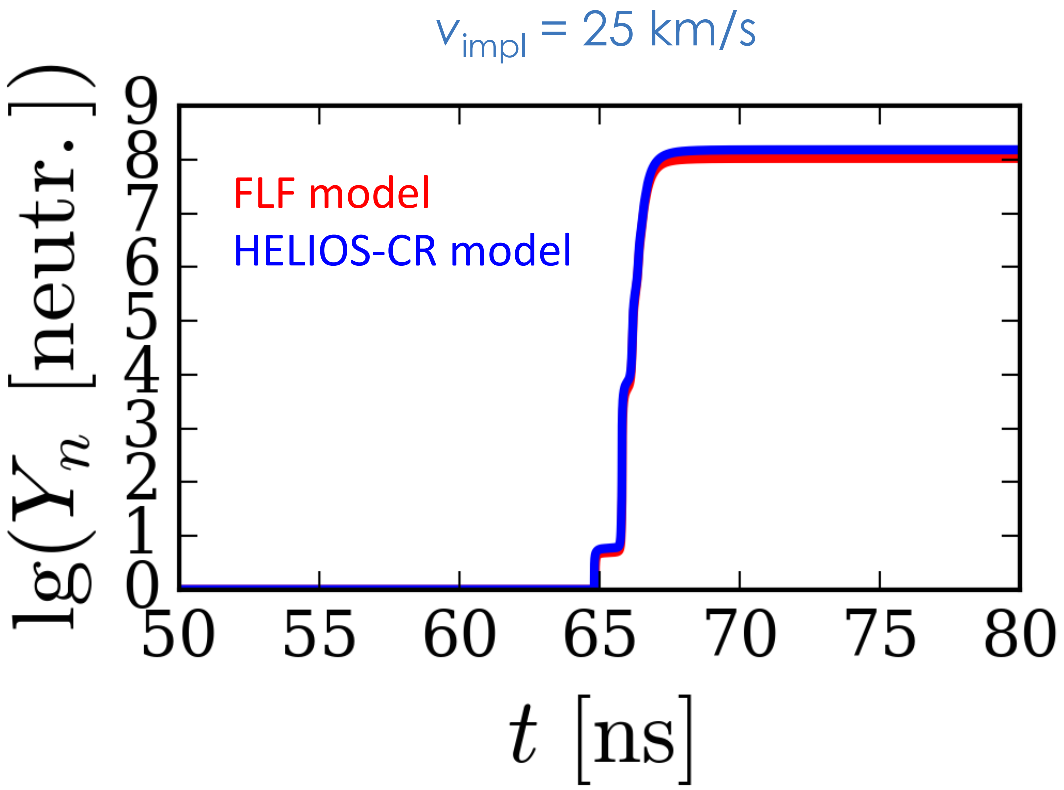


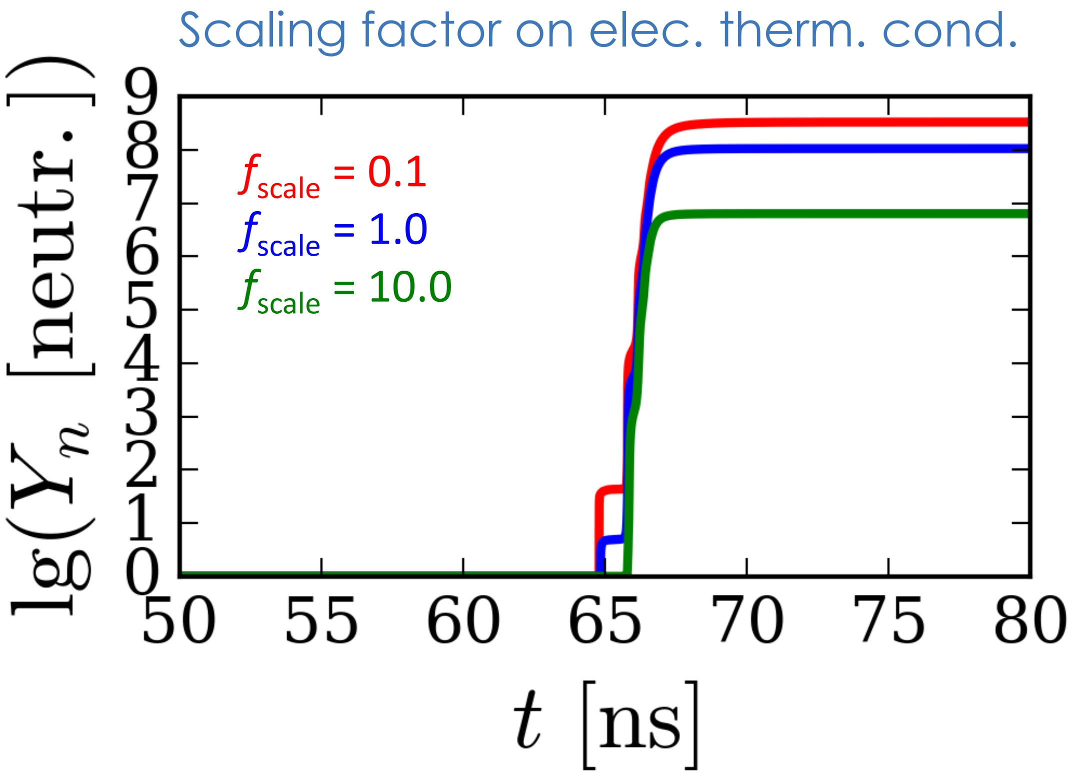
v_{impl} = 50 km/s



- Yield degradation of ~10x due to fuel EoS for low-speed implosion
- **Sensitivity decreases with faster implosions - strong shock limit of Hugoniot**

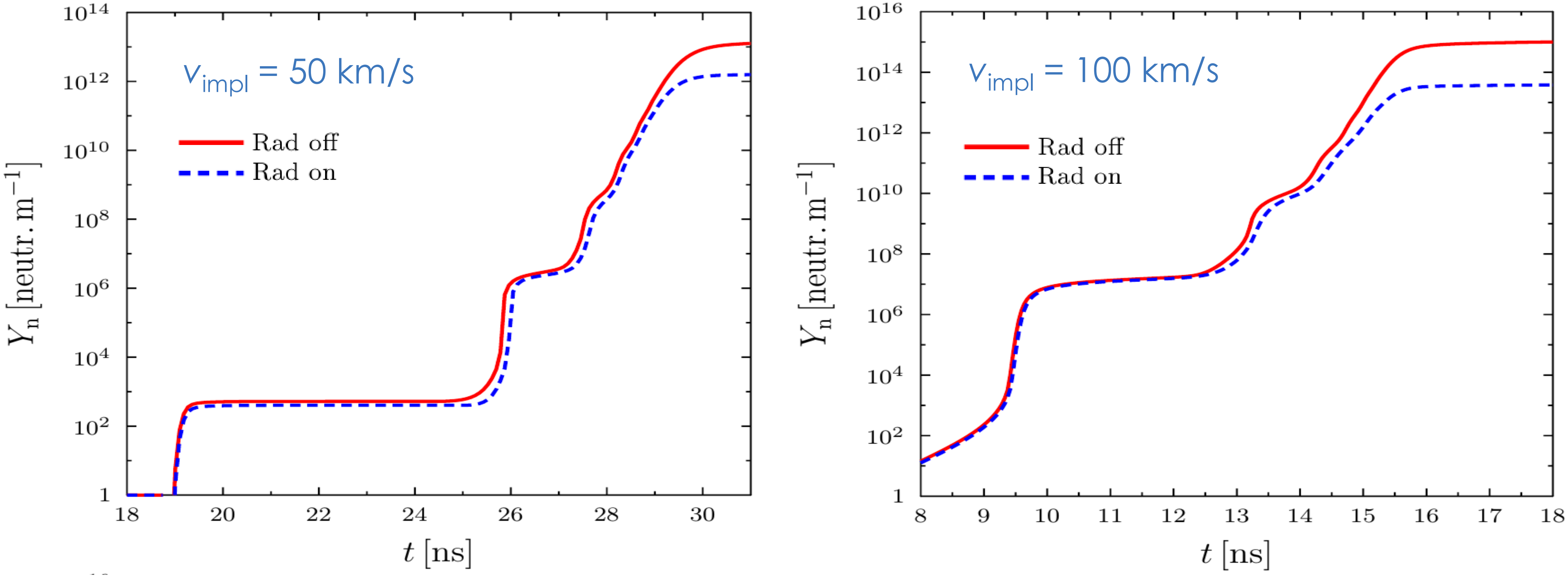
Sensitivity study - Transport model





- Simple (ideal plasma only) thermal conductivity gives small yield increase
- **Model should be OK at conditions where large uncertainities matter**

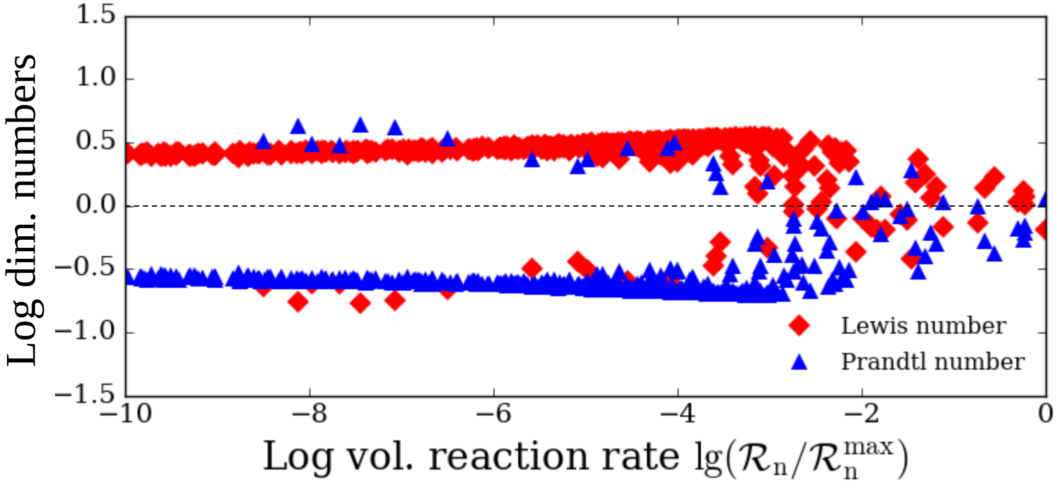
Sensitivity study - Radiation model



- Local escape factor (LEF) radiative loss predicts ~10^4 fold reduction in yield!
- **LEF grossly over-estimates loss - using HELIOS-CR multi-group diffusion model predicts yield reduction of ~10-20 for moderate-fast implosions**

Sensitivity study - Missing hydro physics

v_{impl} = 25 km/s

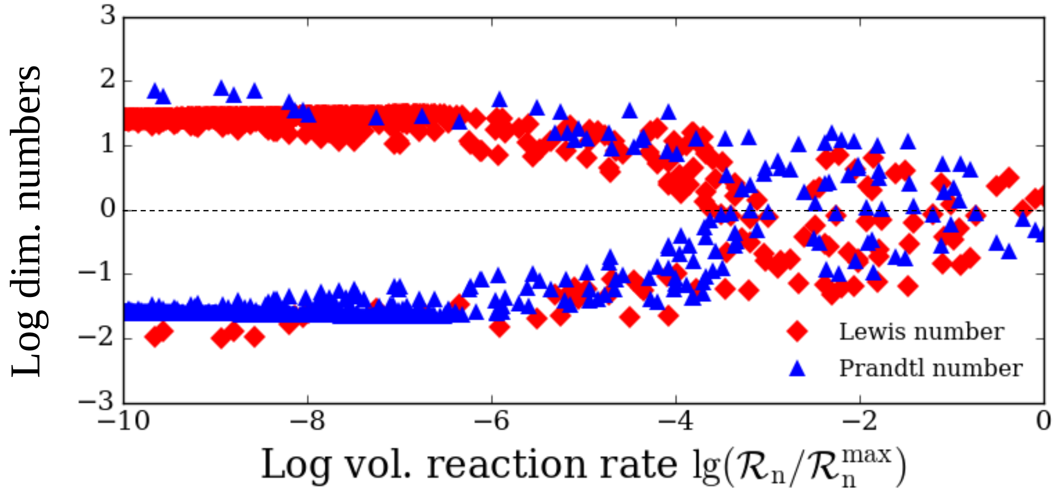


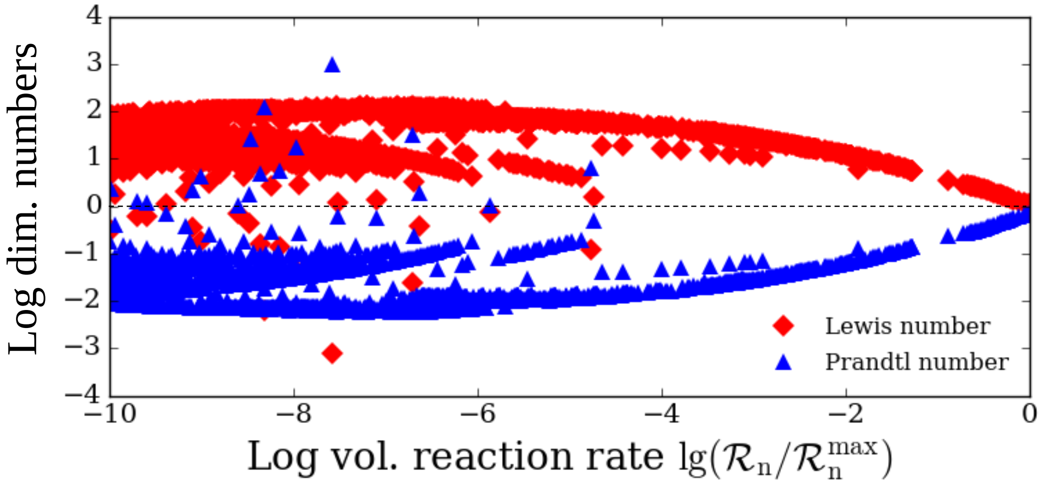
- Assessed through Prandtl/Lewis numbers

$$\mathrm{Pr} = \frac{\nu}{\alpha} \quad \mathrm{Le} = \frac{\alpha}{D}$$

- **Thermal conduction geneally more important than viscosity/mass-driven diffusion until peak neutron emission**

v_{impl} = 50 km/s





v_{impl} = 100 km/s

Prioritisation of future work - towards a predictive capability

Multi-physics improvements required

1. **Multi-group radiation transport (Automatic Flux Limiter method?)**
2. Self-consistent EoS/opacity/microphysics tables
3. Extended hydrodynamics terms and non-local heat transport

Things to do for Hytrac:

1. **Improvements to existing AMR (wavelet transform method?) and HPC scalability**
2. Conservative front-tracking
3. Extension to 3D geometry

Things to do for Code B:

1. **Implement AMR (PhD student started at Imperial College)**
2. Improved interface tracking
3. Magnetised transport

Summary

- FLF has developed an in-house code suite specifically tailored to our research
- Growing capabilities for supplementary physics including EoS, microphysics and radiation transport
- First significant code-to-code comparison against commercially available software (HELIOS-CR) shows good agreement
- Sensitivity studies help guide path for code development:
  - **Radiation transport and fuel EoS must be prioritised for development**
  - **Some evidence that extended hydrodynamics (additional energy transport mechanisms - viscosity and mass diffusion) may be important**
  - **Similar studies are guiding our understanding of launch on M3**
- We welcome collaboration on all areas; numerical, theoretical and experimental, and are actively involved with UK government and academia, as well as international institutions at the forefront of IFE research

THANK YOU FOR YOUR ATTENTION,
AND PLEASE GET IN TOUCH!

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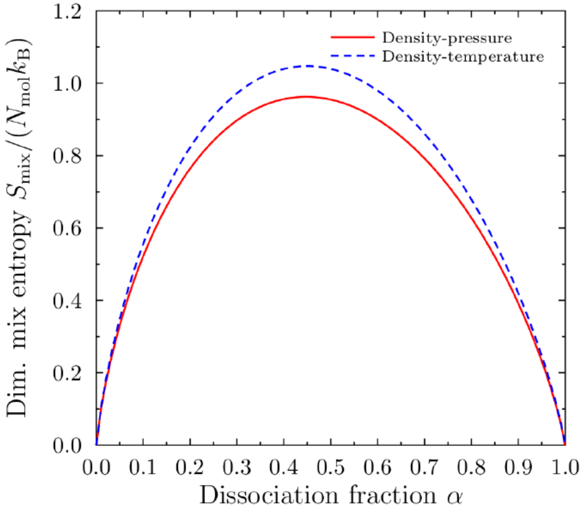
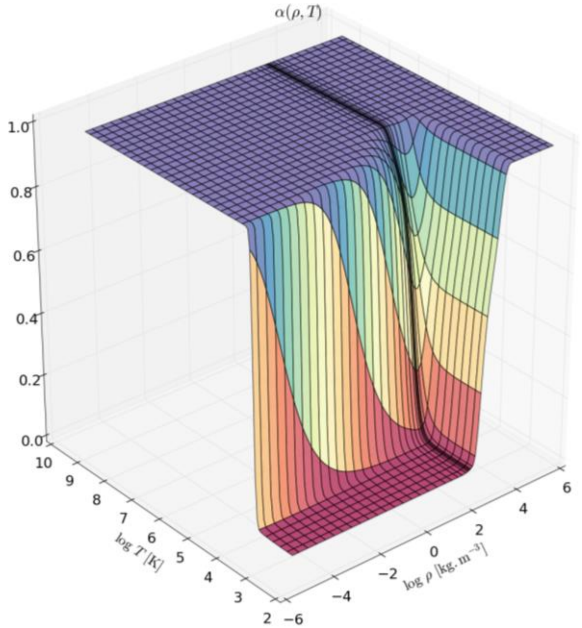
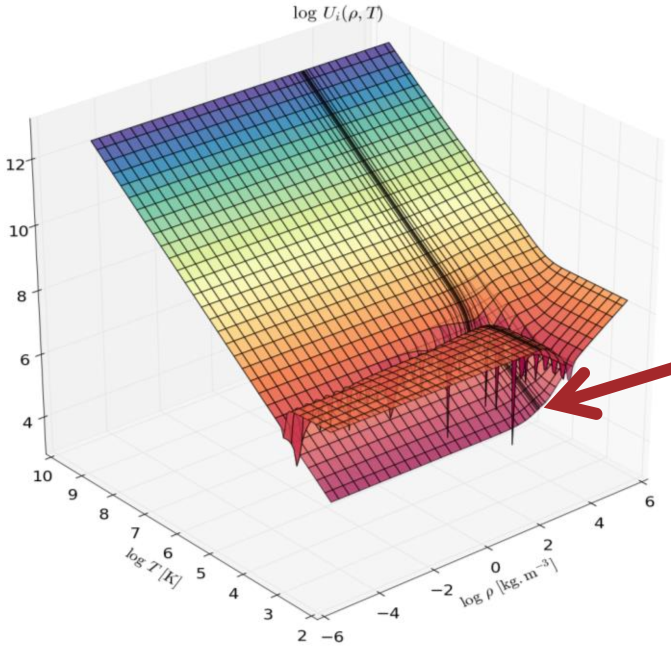
ADDITIONAL SLIDES

Additional: Dissociation model for PROPACEOS







Divergence of tables due to internal energy from molecular bond energy and rotational/vibrational modes of D_2

- Linear mixing model of Ross et al. (1995)
  - Consider chemical equilibrium of atoms and molecules through partition functions
  - Existing EoS table values taken for atomic phase

$$F = (1-\alpha)F_{\mathrm{mol}}(\alpha=0) + \alpha F_{\mathrm{table}} - TS_{\mathrm{mix}}$$

$$U = (1-\alpha)U_{\mathrm{mol}}(\alpha=0) + \alpha U_{\mathrm{table}}$$

$$P = (1-\alpha)P_{\mathrm{mol}}(\alpha=0) + \alpha P_{\mathrm{table}}$$

$$S = (1-\alpha)S_{\mathrm{mol}}(\alpha=0) + \alpha S_{\mathrm{table}} - S_{\mathrm{mix}}$$

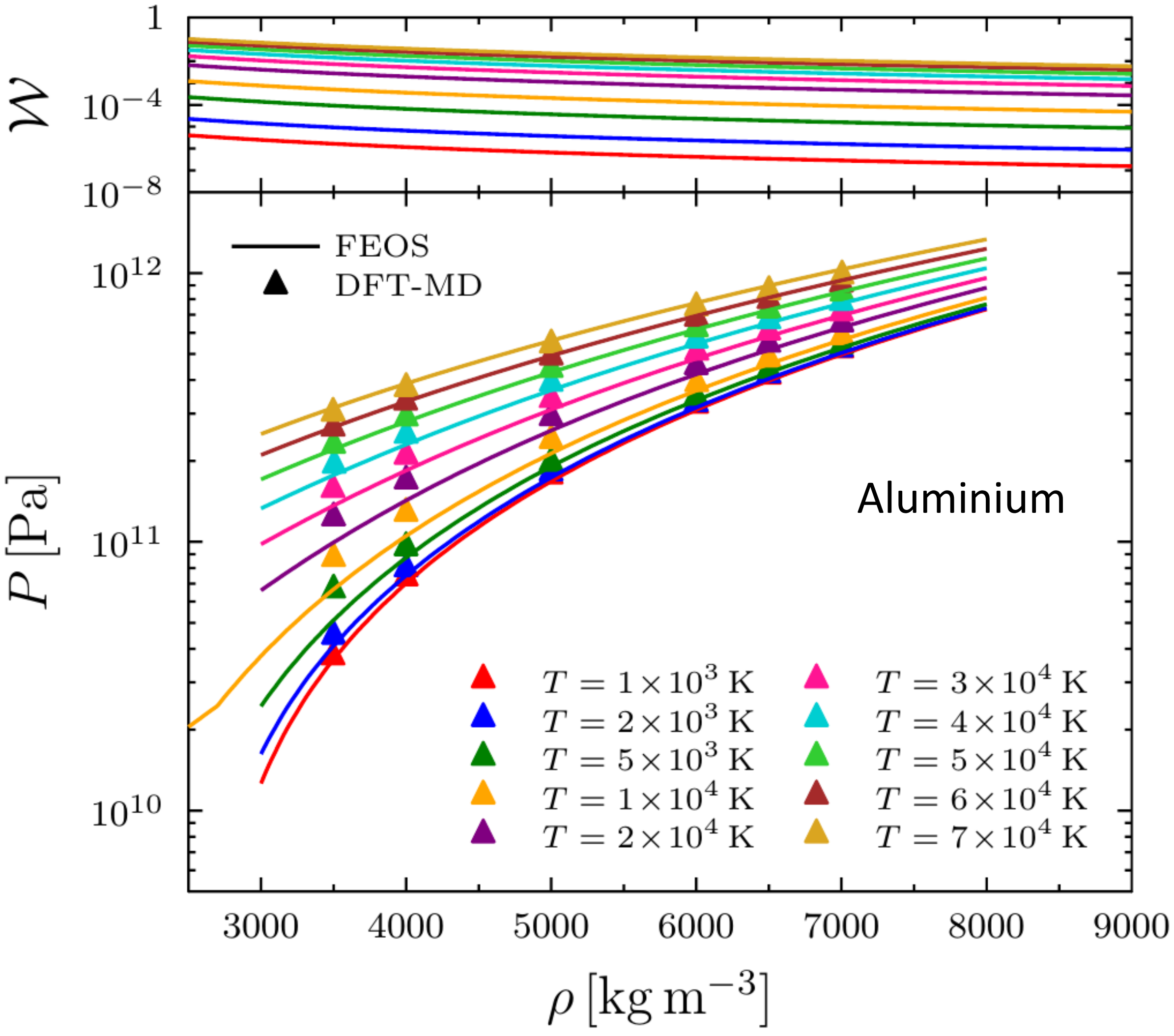
- Dissociation fraction calculated using atomic phase model featuring fitted metallic hydrogen results (LDA/EG/OCP)

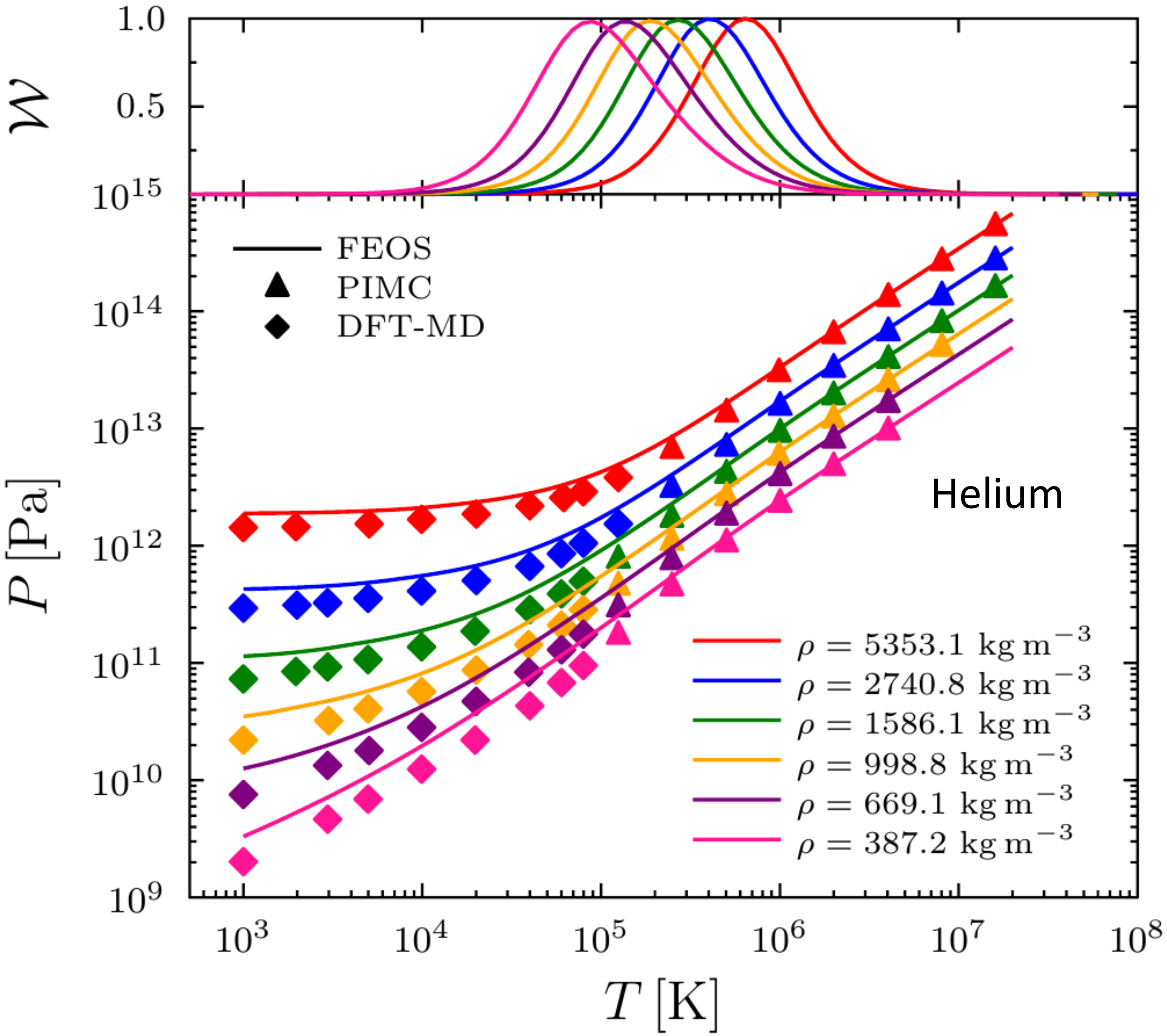
$$\frac{\alpha^2}{1-\alpha} = \exp\left(-\frac{F_{\mathrm{atom}} - F_{\mathrm{mol}}}{N_{\mathrm{mol}}k_{\mathrm{B}}T}\right)$$

- Molecular phase contributions:

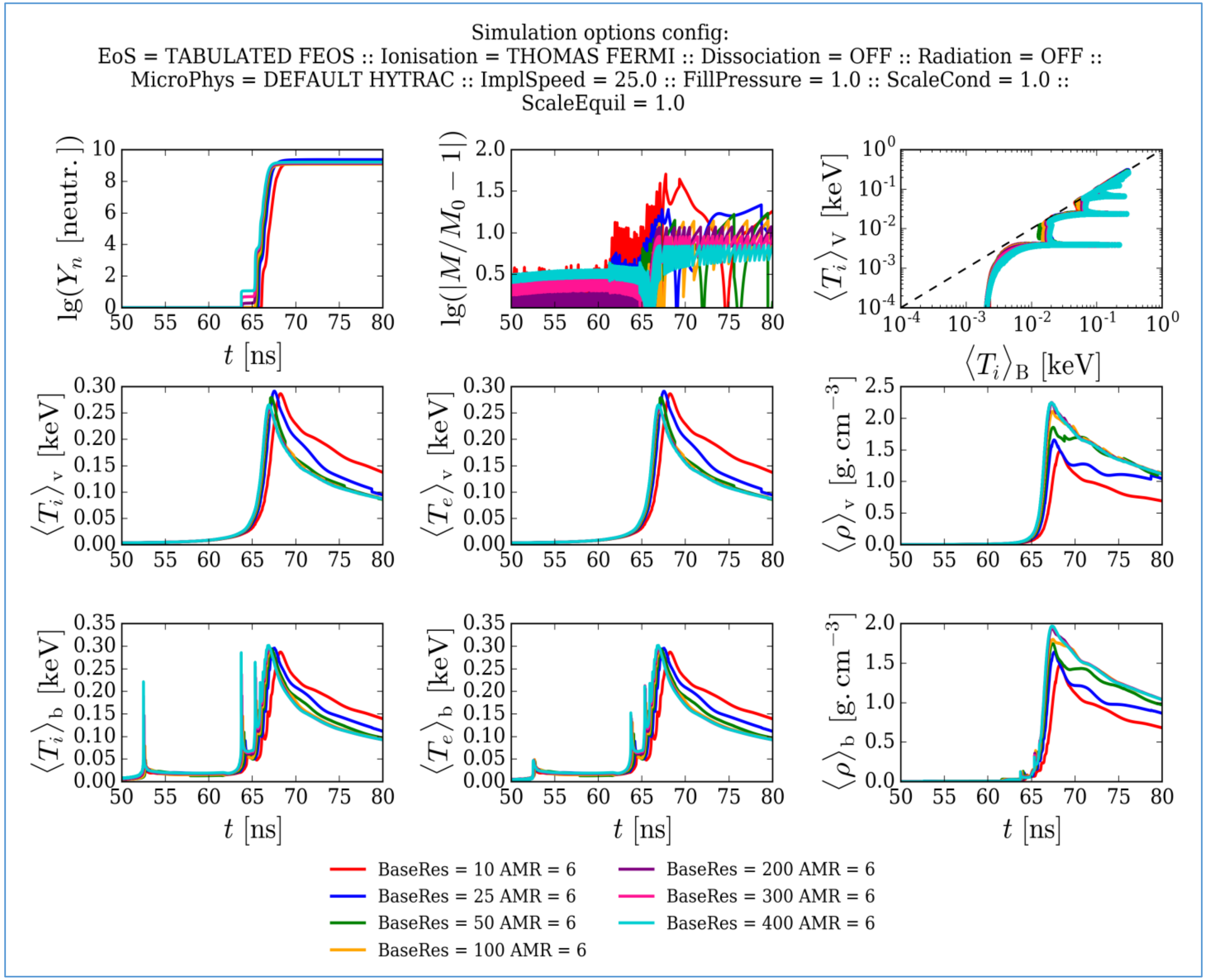
$$F_{\mathrm{mol}} = F_{\mathrm{trans}} + F_{\mathrm{int}} + F_{\mathrm{conf}} - E_{\mathrm{bond}}$$

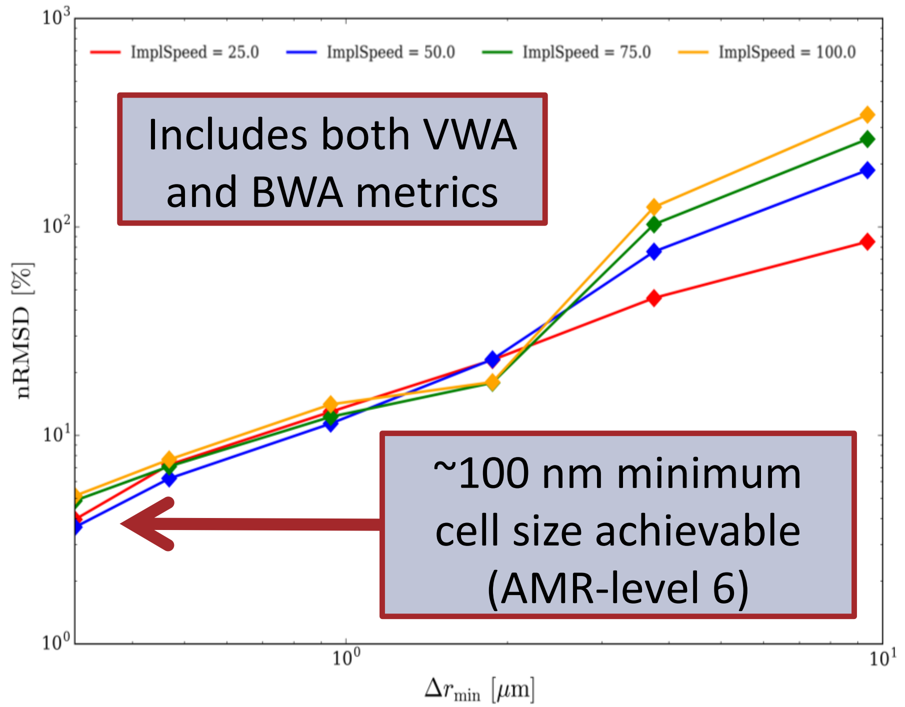
Additional: Benchmarking of FEOS against DFT-MD





Additional: Hytrac EGrid convergence study



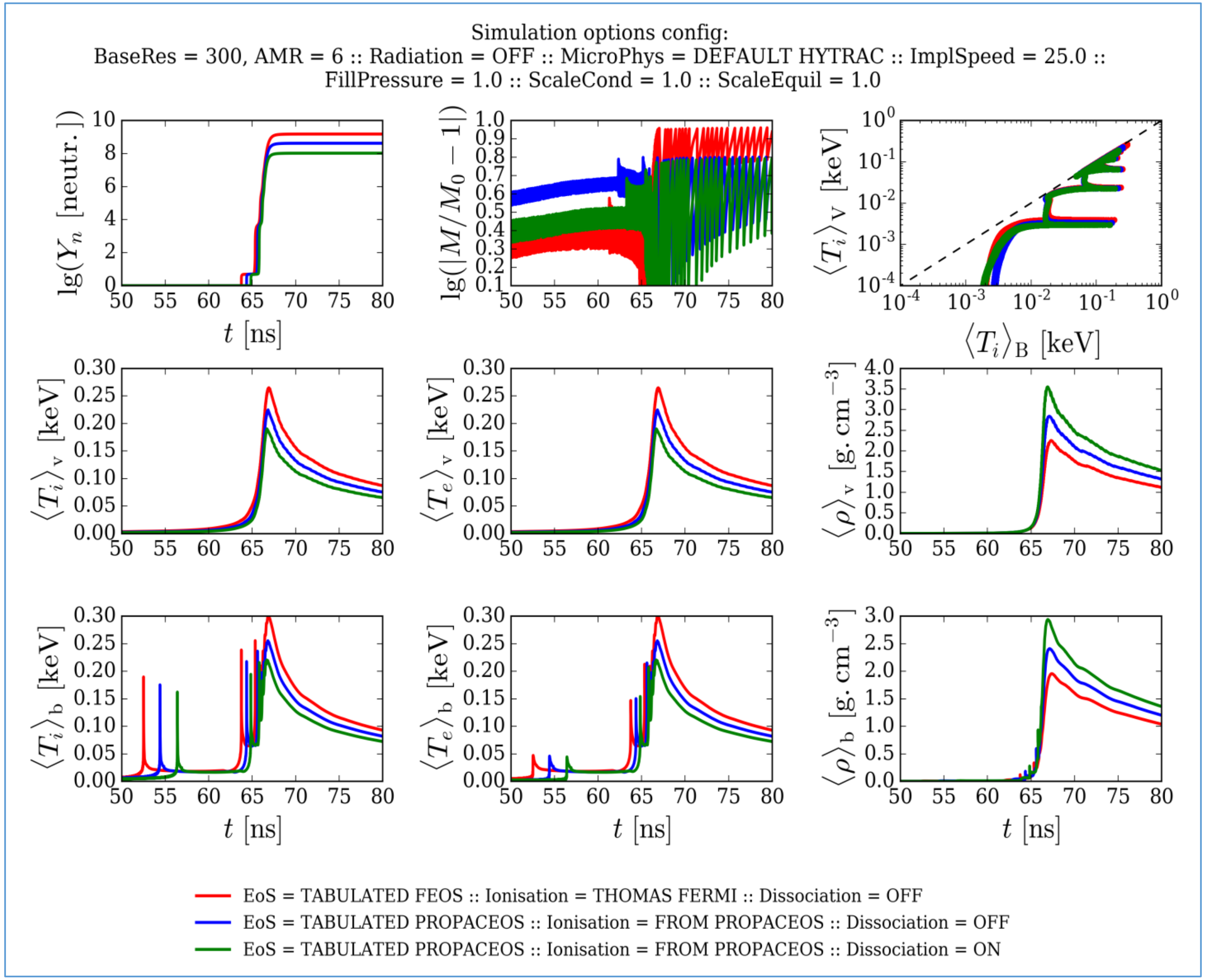


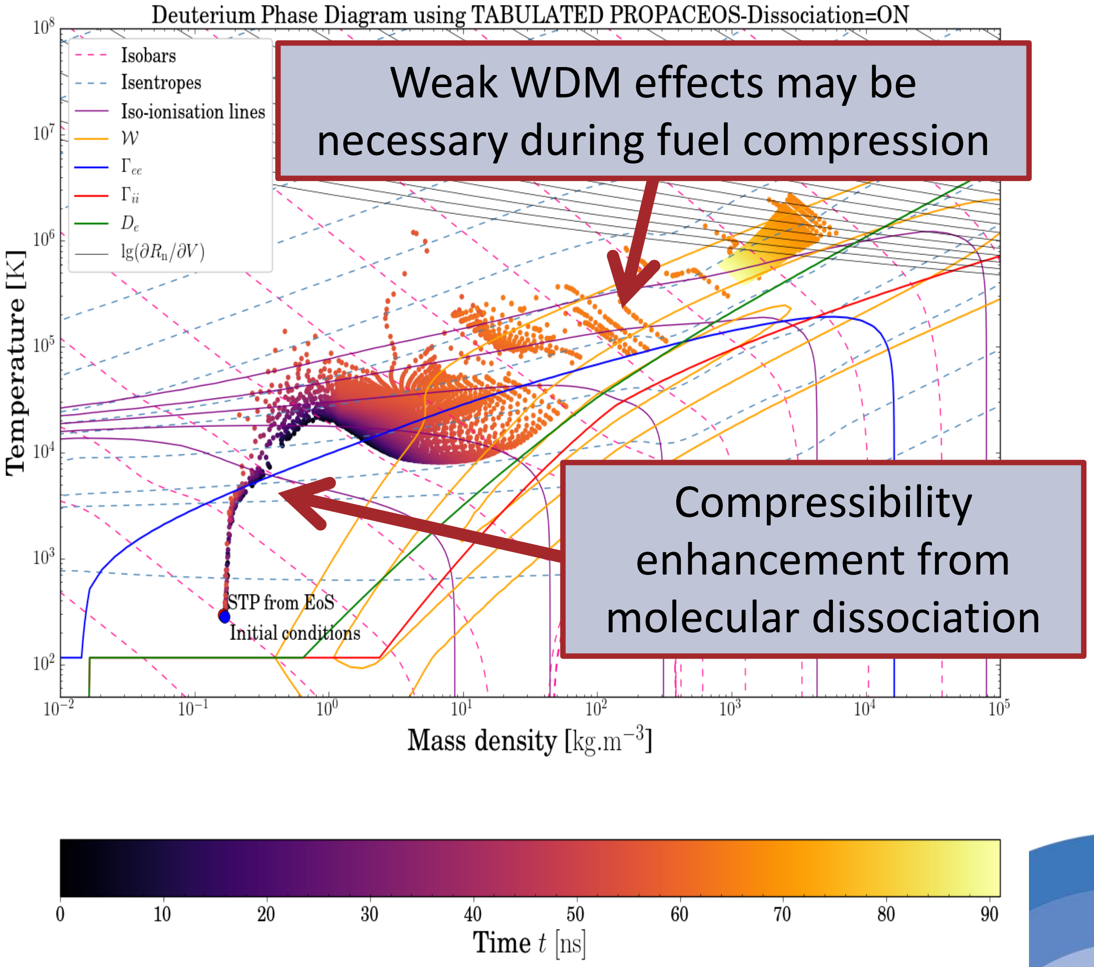
$$\mathrm{RMSD}_{X,y}(R) = \sqrt{\frac{1}{N_t}\sum_{i=1}^{N_t}\left(\langle X(t_i;R)\rangle_y - \langle X(t_i;R_{\max})\rangle_y\right)^2}$$

$$\langle X(t)\rangle_{\mathrm{b}} = \frac{1}{\partial Y_{\mathrm{n}}/\partial t}\int_{\mathrm{Fuel}} \mathrm{d}V\, \frac{\partial^2 Y_{\mathrm{n}}}{\partial V \partial t} X(\mathbf{r},t)$$

$$\langle X(t)\rangle_{\mathrm{v}} = \frac{1}{V(t)}\int_{\mathrm{Fuel}} \mathrm{d}V\, X(\mathbf{r},t)$$

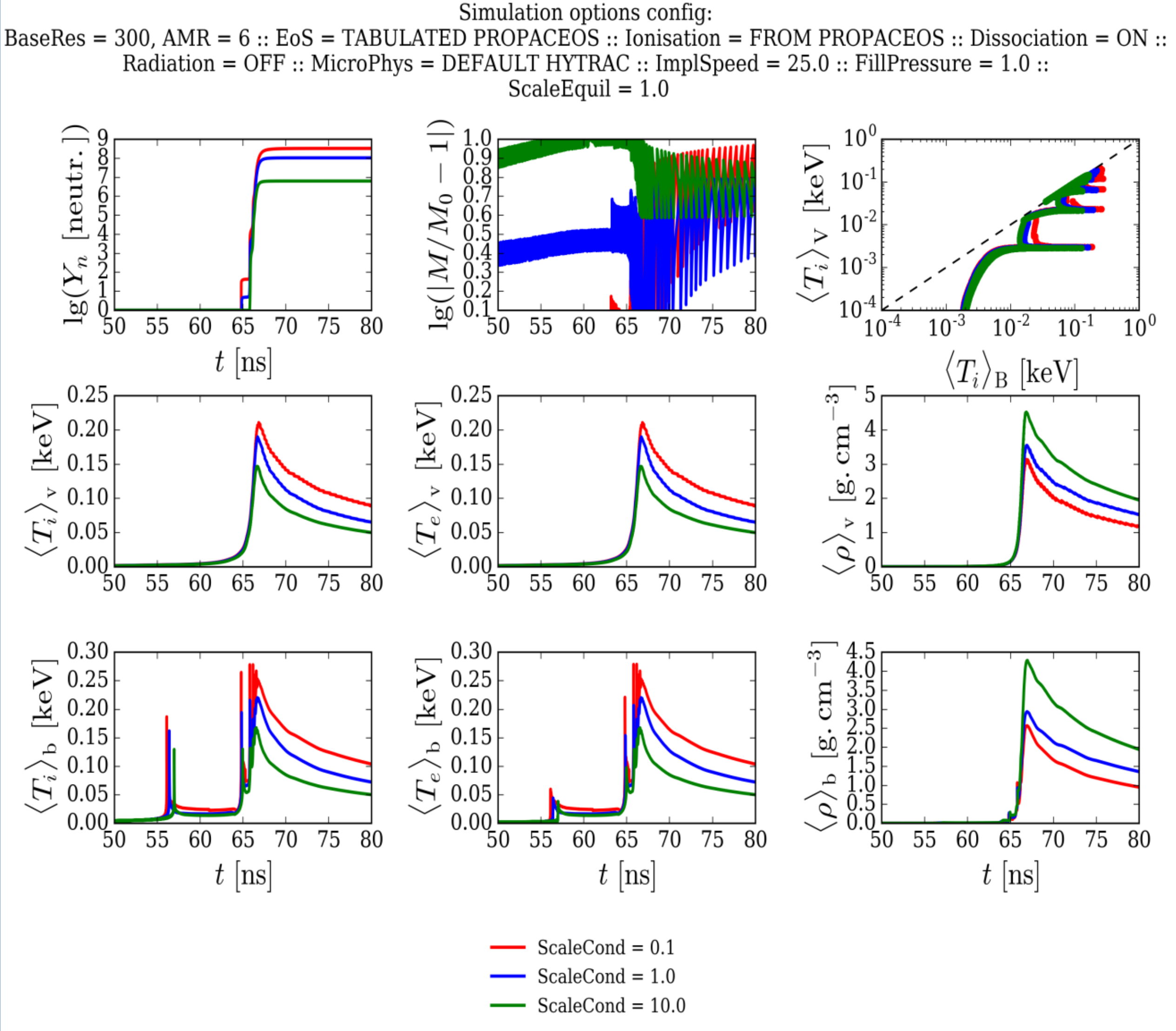
Additional: EoS model sensitivity



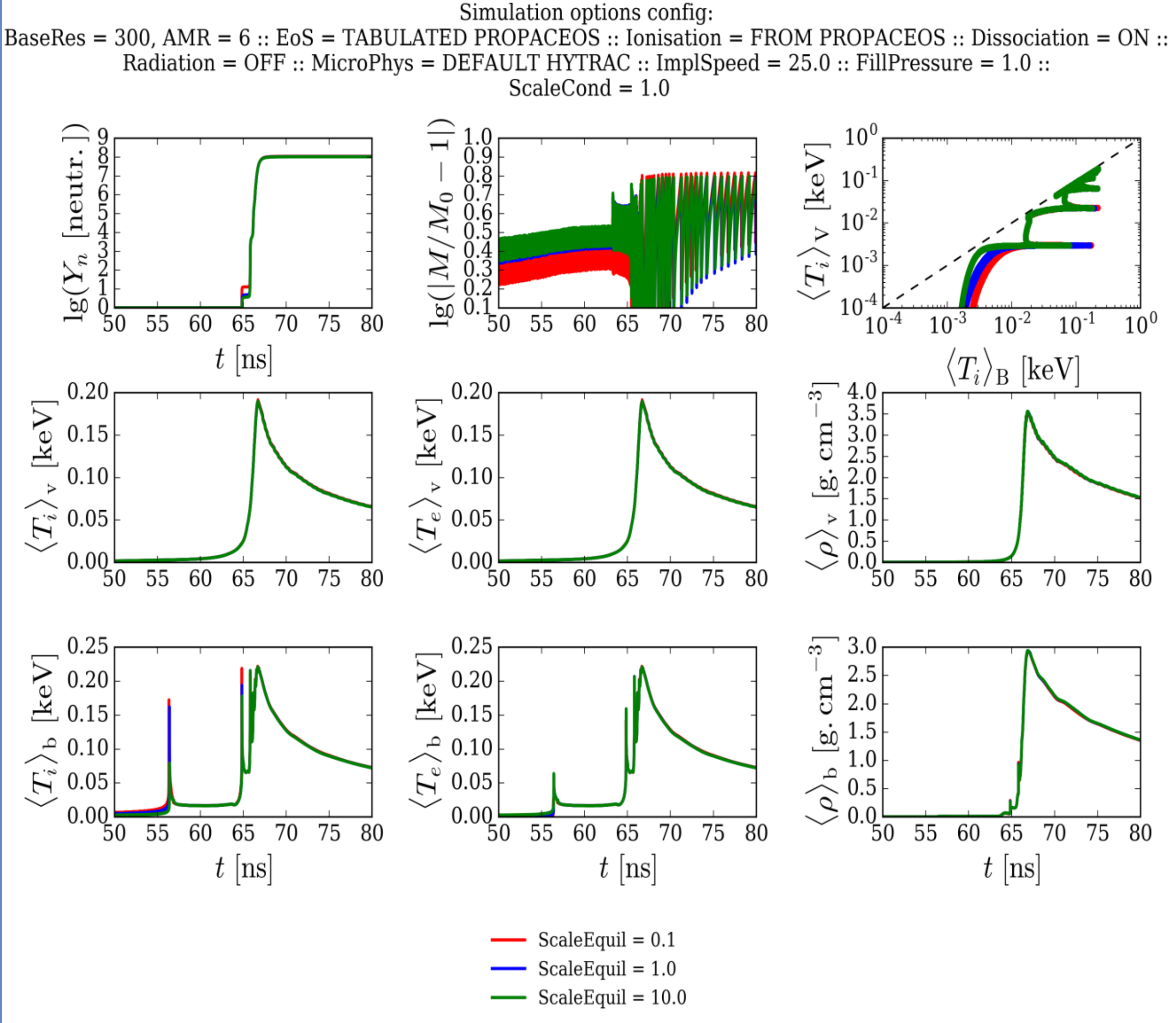


Additional: Transport model sensitivity

Scaling factor on electron thermal conductivity

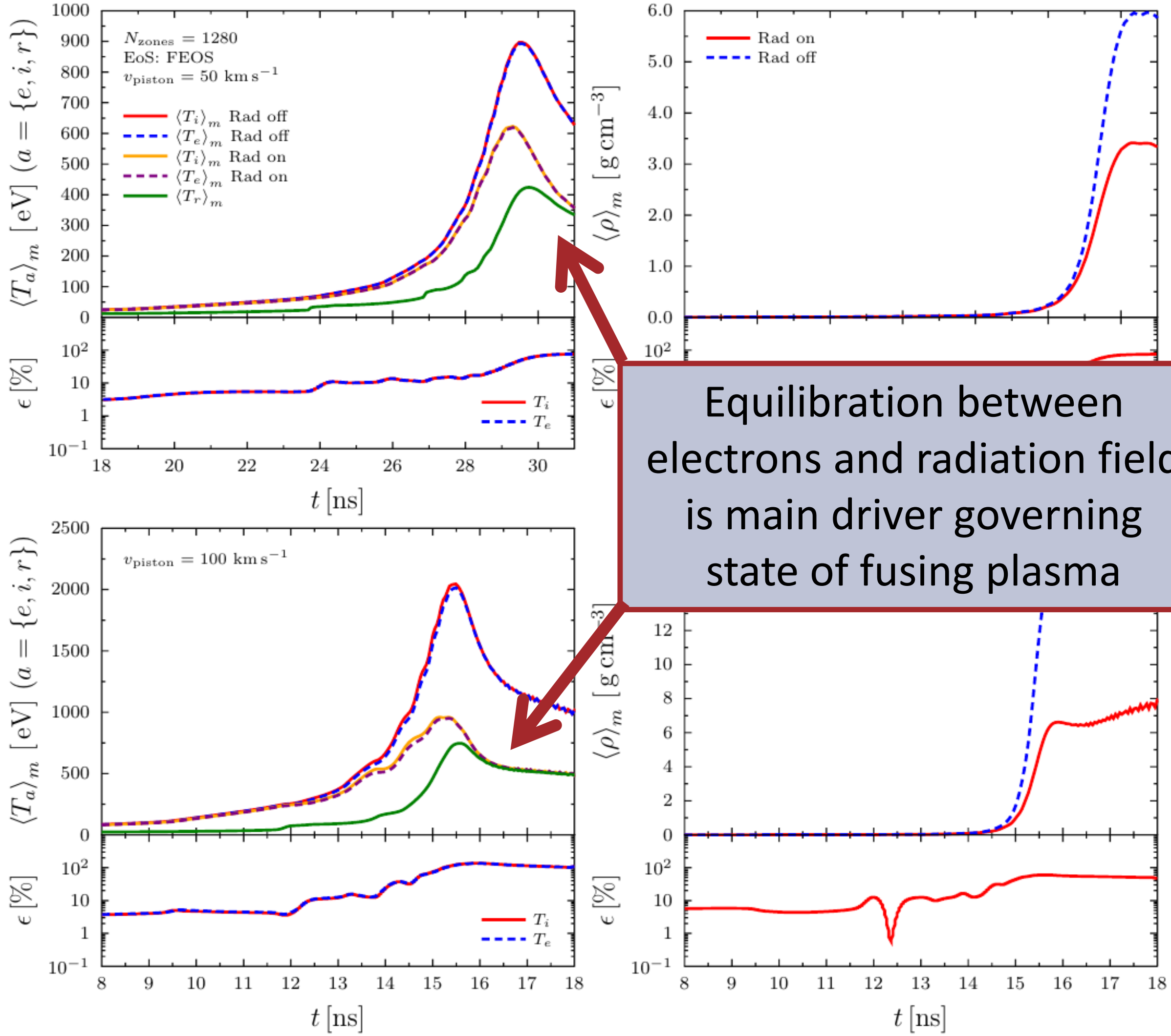


Scaling factor on electron-ion equilibration rate

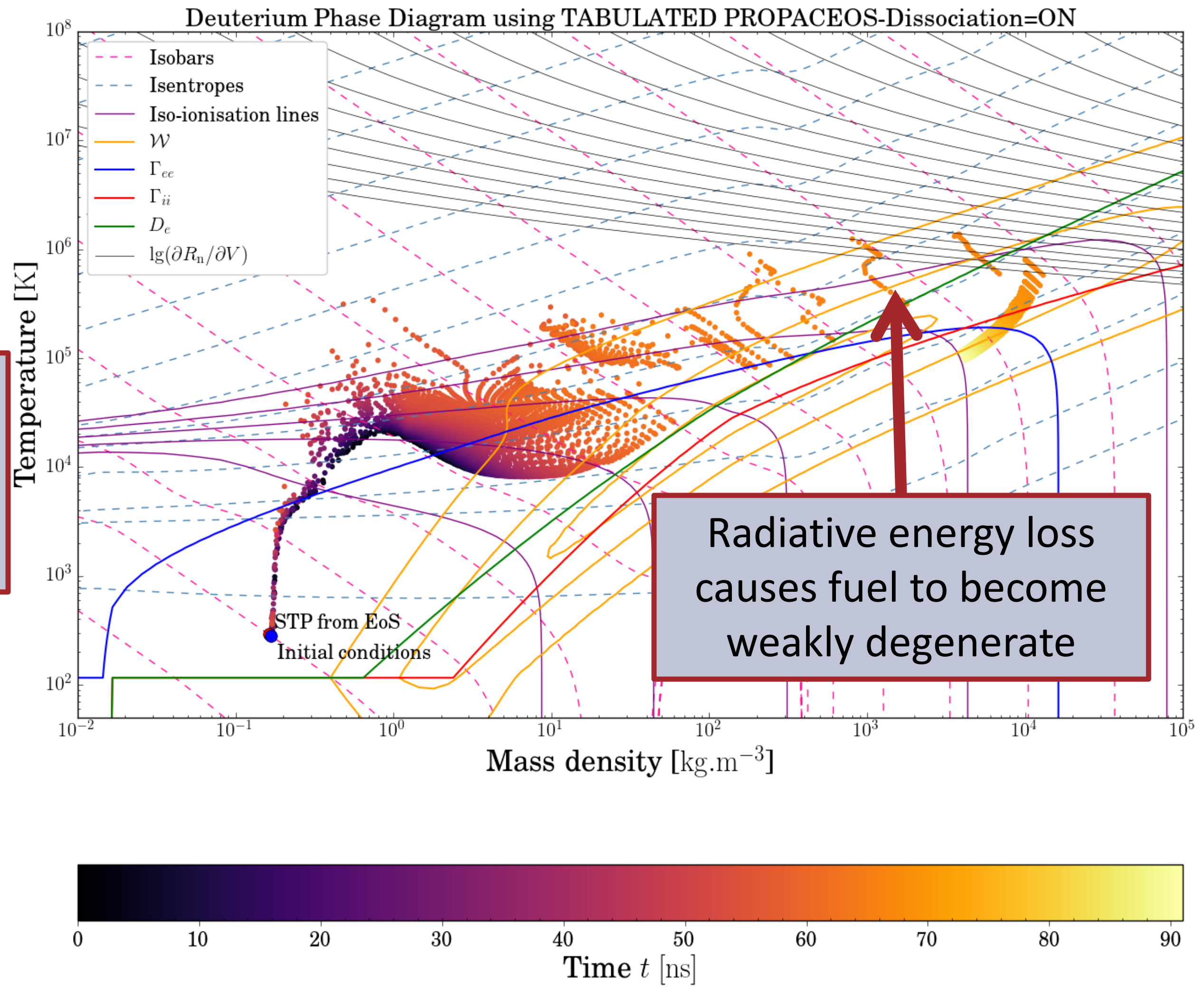


Additional: Radiation model sensitivity

Multi-group rad. transport modelling in HELIOS-CR



Equilibration between electrons and radiation field is main driver governing state of fusing plasma



Radiative energy loss causes fuel to become weakly degenerate