rans(eXtreme)

Analysis framework for multi-fluid compressible hydrodynamic simulations

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Physics motivation

- Limitations of the current 1D modelling of turbulence in stars
- Closures for approximated or neglected physics
  - what do we actually neglect?
- Hydrodynamic stellar structure equations (time-dependent, non-local)
  - (no rotation, no magnetic fields)

Computational motivation

- Comprehensive analysis of hydrodynamic simulations done at runtime and user-friendly post-processing

Structure

- Theory: Reynolds and Favrian decomposition

$$A(r,\theta,\phi) = \overline{A}(r) + A'(r,\theta,\phi) \qquad \overline{A(r)} = \frac{1}{\Delta T \Delta\Omega}\int_{\Delta T}\int_{\Delta\Omega} A(r,\theta,\phi)\, dt\, d\Omega$$

$$F(r,\theta,\phi) = \widetilde{F}(r) + F''(r,\theta,\phi) \qquad \widetilde{F} = \overline{\rho F}/\overline{\rho}$$

$$\underbrace{\overline{u}_r}_{\text{mean velocity}} = \underbrace{\widetilde{u}_r}_{\text{expansion velocity } \partial_t M/4\pi r^2\overline{\rho}} - \underbrace{\overline{u''}_r}_{\text{turbulent mass flux } -\overline{\rho' u'_r}/\overline{\rho}}$$

  - https://github.com/mmicromegas/ransX/tree/master/DOCS

- Hydrodynamic Code Implementation: calculation of mean-fields at runtime of simulation
  - https://github.com/mmicromegas/ransX/tree/master/UTILS/FOR_YOUR_HYDRO
- Post-Processing in Python
  - https://github.com/mmicromegas/ransX

Results

- Transport/Flux/Variance equations for evolution of mass, momenta, kinetic/internal/total energy, temperature, enthalpy, pressure
- Transport/Flux/Variance equations for evolution of chemical composition
- Eulerian diffusivities (to guide us towards new composition mixing models)
- Hydrodynamic stellar structure equations (3 versions)

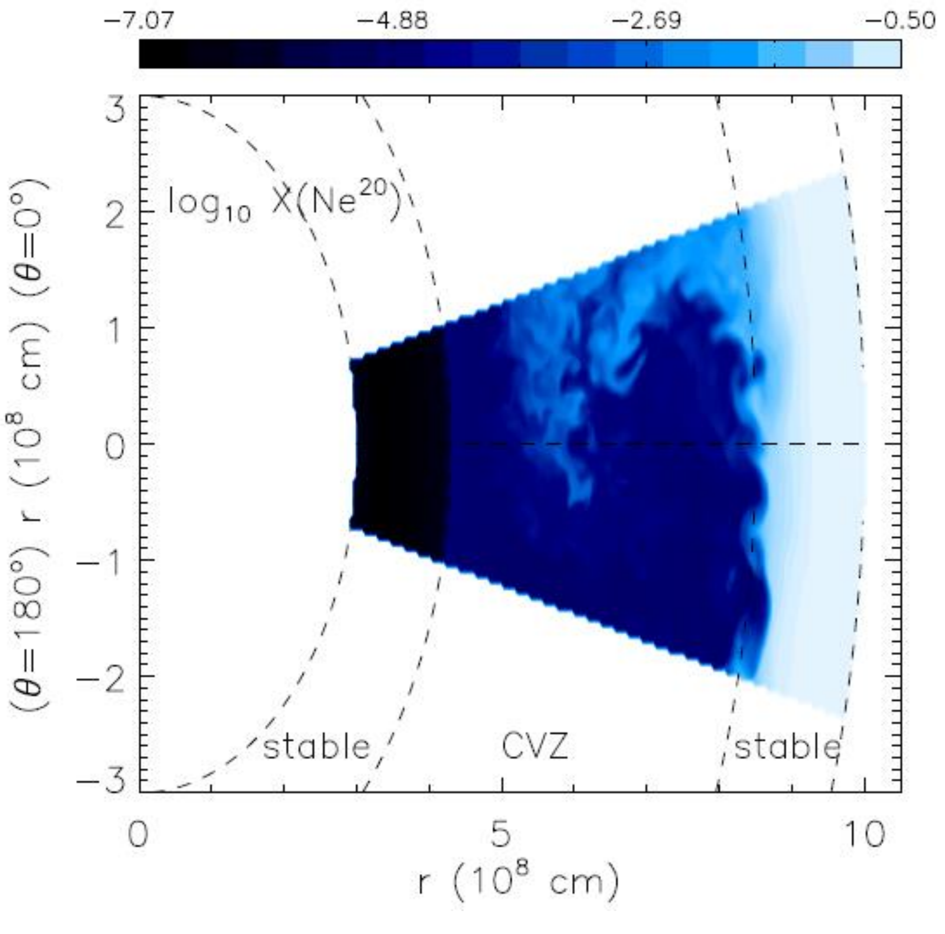
  - general
  - simplified (based on flux evolution equations)
  - simplified (for adiabatic flow in HSE)

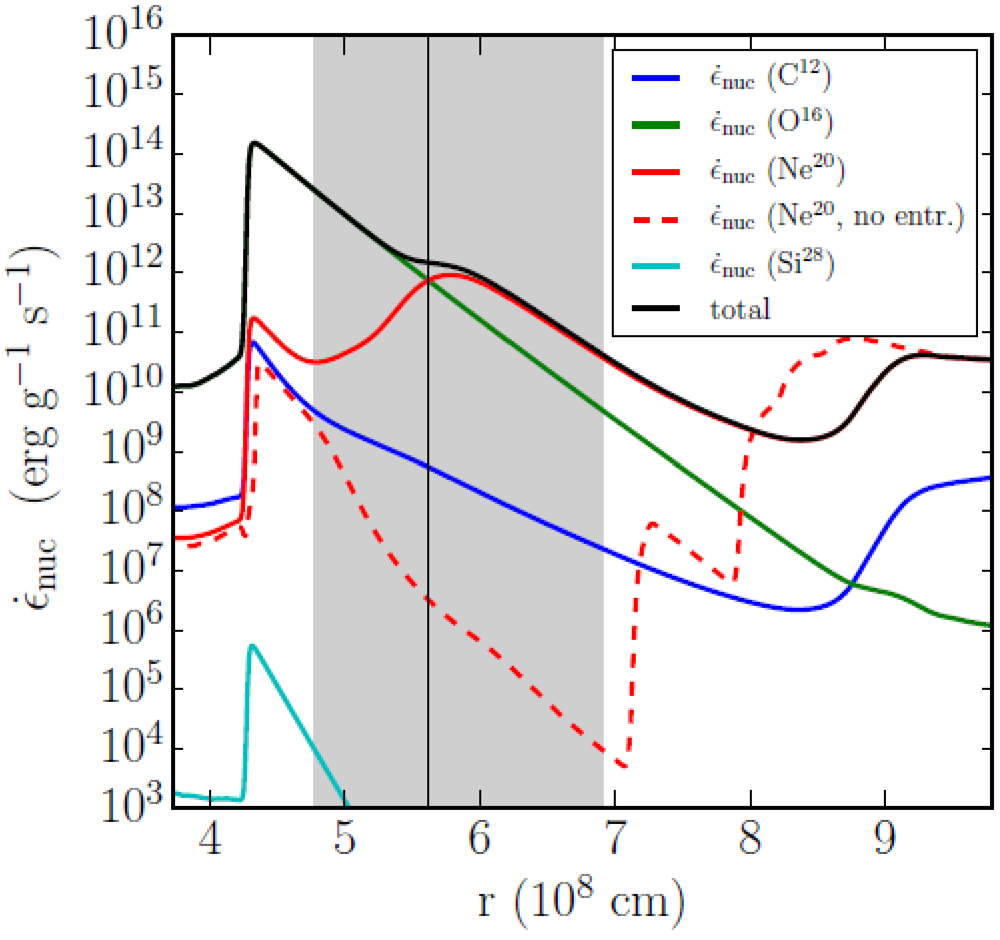
  * all of them well validated with our oxygen-neon burning simulation
  * for more details see https://github.com/mmicromegas/ransX/tree/master/DOCS/RANDOM

Oxygen-Neon burning convective shell

2018MNRAS.481.2918M Mocák et al, 2018

- multiple burning zones within single convection zone





Hydrodynamic stellar structure equations

- Below is a complete set of hydrodynamic stellar structure equations derived from RANS equations (viscosity explicitly neglected), where red terms are the ones used in classical approach:

$$\partial_r \overline{m} = 4\pi r^2 \overline{\rho} + (4\pi r^3/3\widetilde{u}_r)\left[-\nabla_r f_\rho + (f_\rho/\overline{\rho})\partial_r\overline{\rho} - \overline{\rho}\overline{d} - \partial_t\overline{\rho}\right]$$

$$\partial_r \overline{P} = \overline{\rho}\widetilde{g} - \overline{\rho}\partial_t\widetilde{u}_r - \nabla_r \widetilde{R}_{rr} - \overline{G}^M_r - \overline{\rho}\widetilde{u}_r\partial_r\widetilde{u}_r$$

$$\partial_r \widetilde{L} = 4\pi r^2\overline{\rho}\widetilde{\epsilon}_{nuc} + 4\pi r^2\left[-\nabla_r(f_i + f_{th} + f_K + f_p) - \overline{P}\overline{d} - \widetilde{R}_{ir}\partial_r\widetilde{u}_i + W_b + \overline{\rho}\widetilde{D}_t\widetilde{u}_i\widetilde{u}_i/2 - \overline{\rho}\partial_t\widetilde{\epsilon}_t\right] + \widetilde{\epsilon}_t\partial_r 4\pi r^2\overline{\rho}\widetilde{u}_r$$

$$\partial_r \overline{T} = (1/\overline{u}_r)\left[-\nabla_r f_T + (1-\Gamma_3)\overline{T}\,\overline{d} + (2-\Gamma_3)\overline{T'd'} + \epsilon_{nuc}/c_v + \nabla\cdot f_{th}/(\rho c_v) - \partial_t T\right]$$

$$\partial_t \widetilde{X}_i = \widetilde{\dot{X}}_i^{nuc} - (1/\overline{\rho})\nabla_r f_i - \widetilde{u}_r\partial_r\widetilde{X}_i$$

https://github.com/mmicromegas/ransX/blob/master/DOCS/RANDOM/hsse.pdf

https://github.com/mmicromegas/ransX/blob/master/DOCS/RANDOM/hsse_alternative.pdf

Hydrodynamic stellar structure equations

- Stellar gradients and dilatation flux $\widetilde{R}_{rr}\partial_r\overline{Q} \sim -\overline{\rho}\ \overline{Q}\ \overline{u'_r d''}$ (inferred from flux equations)
- Below is a set of alternative hydrodynamic stellar structure equations derived from the relation between stellar gradients and dilatation flux, where the Q was replaced by density (ρ), pressure (P), total energy (e_t) and temperature (T) [composition X equation is standard continuity equation]

$$
\begin{aligned}
\partial_r\overline{m} &= -\overline{\rho}\ \overline{m}\ \overline{u'_r d''}/\widetilde{R}_{rr} + 4\pi r^2\overline{\rho} \\
\partial_r\overline{P} &= -\Gamma_1\ \overline{\rho}\ \overline{P}\ \overline{u'_r d''}/\widetilde{R}_{rr} \\
\partial_r\widetilde{L} &= +\widetilde{\epsilon}_t\partial_r 4\pi r^2\overline{\rho}\widetilde{u}_r - 4\pi r^2\overline{\rho}\ \widetilde{u}_r\ \overline{P}\ \overline{u'_r d''}/\widetilde{R}_{rr} \\
\partial_r\overline{T} &= -(\Gamma_3 - 1)\ \overline{\rho}\ \overline{T}\ \overline{u'_r d''}/\widetilde{R}_{rr} \\
\partial_t\widetilde{X}_i &= \dot{\widetilde{X}}_i^{nuc} - (1/\overline{\rho})\nabla_r f_i - \widetilde{u}_r\partial_r\widetilde{X}_i \\
\widetilde{u}_r &= -\partial_t\overline{M}/4\pi r^2\overline{\rho}
\end{aligned}
$$

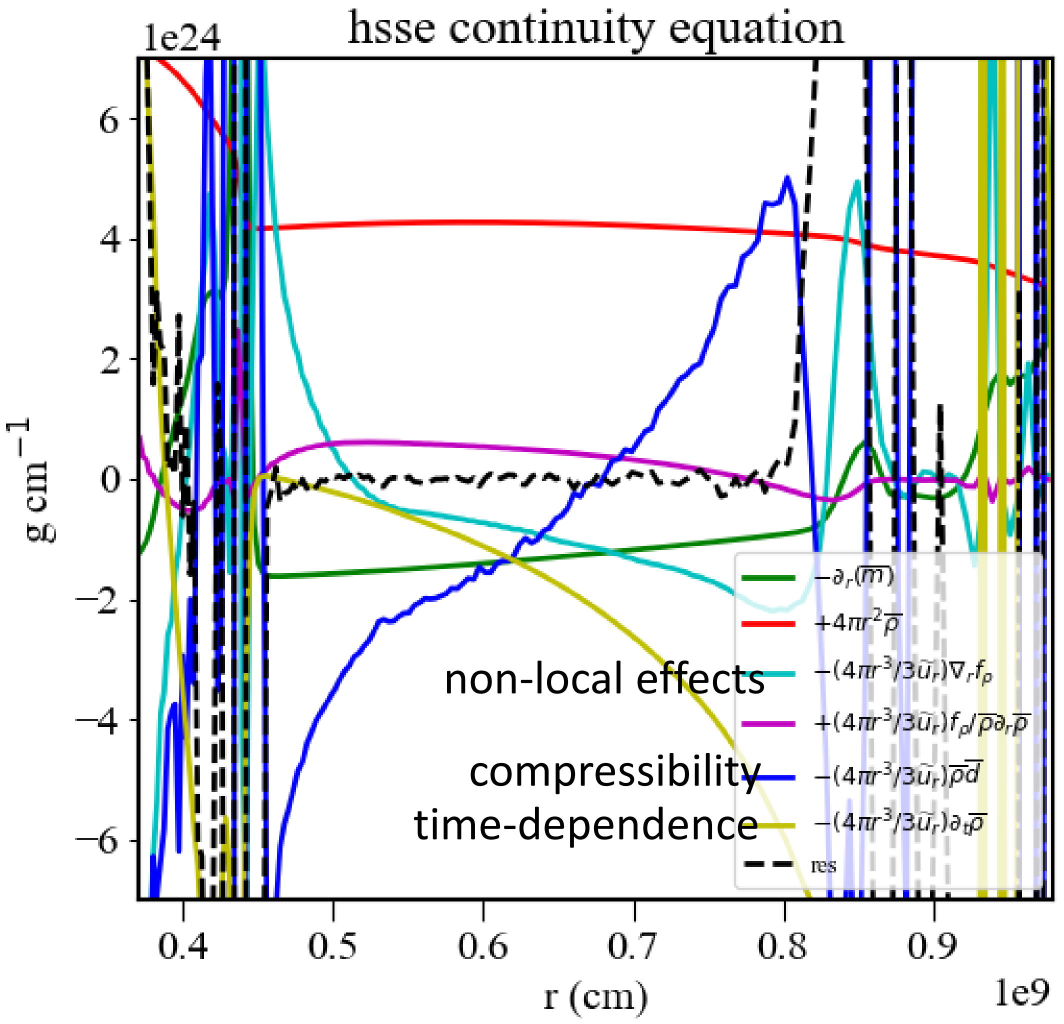
$$
\xrightarrow[\overline{u'_r d''} \sim \frac{\widetilde{R}_{rr}\ \overline{g}_r}{\Gamma_1\ \overline{P}}]{\partial_r\overline{P} \sim -\overline{\rho}\ \overline{g}_r}
$$

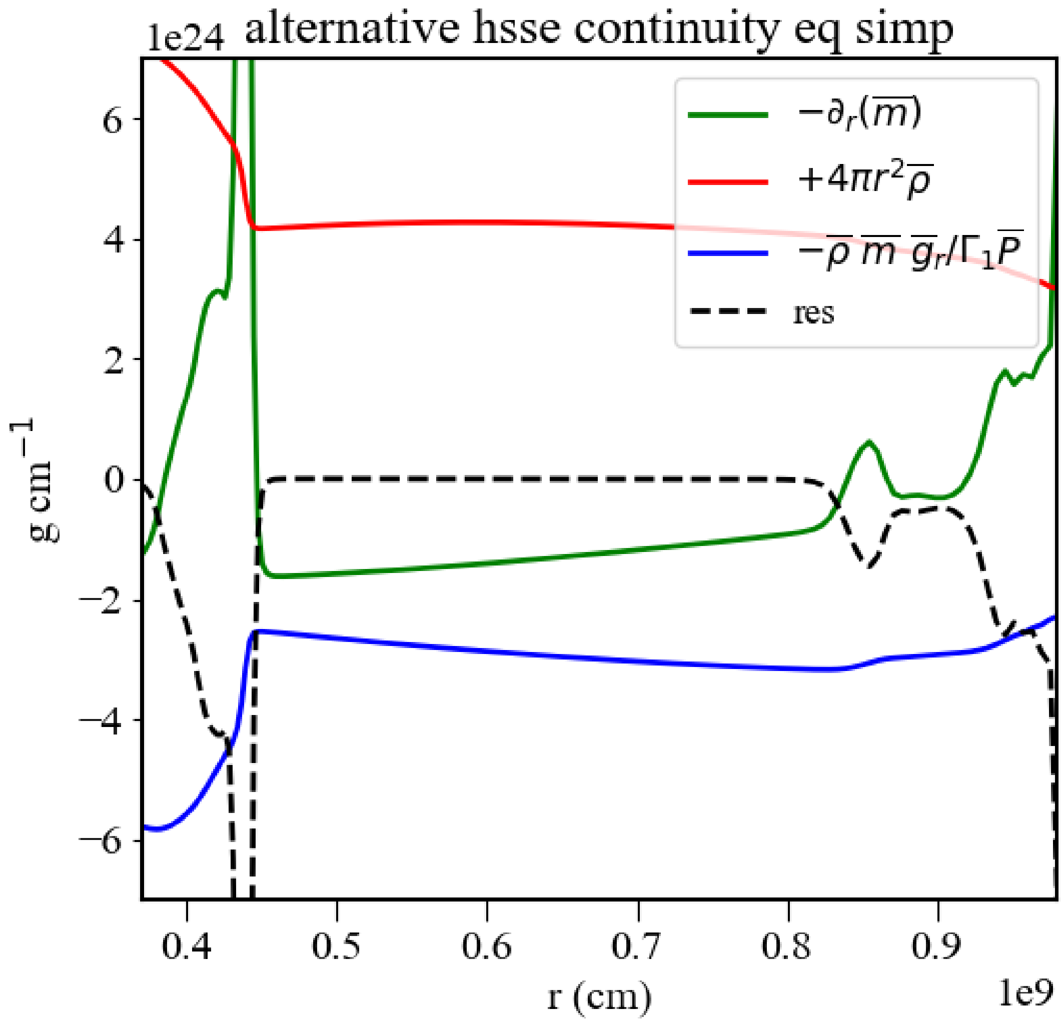
$$
\begin{aligned}
\partial_r\overline{m} &= -\overline{\rho}\ \overline{m}\ \overline{g}_r/\Gamma_1\overline{P} + 4\pi r^2\overline{\rho} \\
\partial_r\overline{P} &= -\overline{\rho}\ \overline{g}_r \\
\partial_r\widetilde{L} &= -4\pi r^2\widetilde{u}_r\ \overline{\rho}\ \overline{g}_r/\Gamma_1 + \widetilde{\epsilon}_t\partial_r 4\pi r^2\overline{\rho}\widetilde{u}_r \\
\partial_r\overline{T} &= -(\Gamma_3 - 1)\ \overline{\rho}\ \overline{T}\ \overline{g}_r/\Gamma_1\overline{P} \\
\partial_t\widetilde{X}_i &= \dot{\widetilde{X}}_i^{nuc} - (1/\overline{\rho})\nabla_r f_i - \widetilde{u}_r\partial_r\widetilde{X}_i
\end{aligned}
$$

$$m = \rho V = \rho\frac{4}{3}\pi r^3 \qquad M = \int \rho(r)dV$$

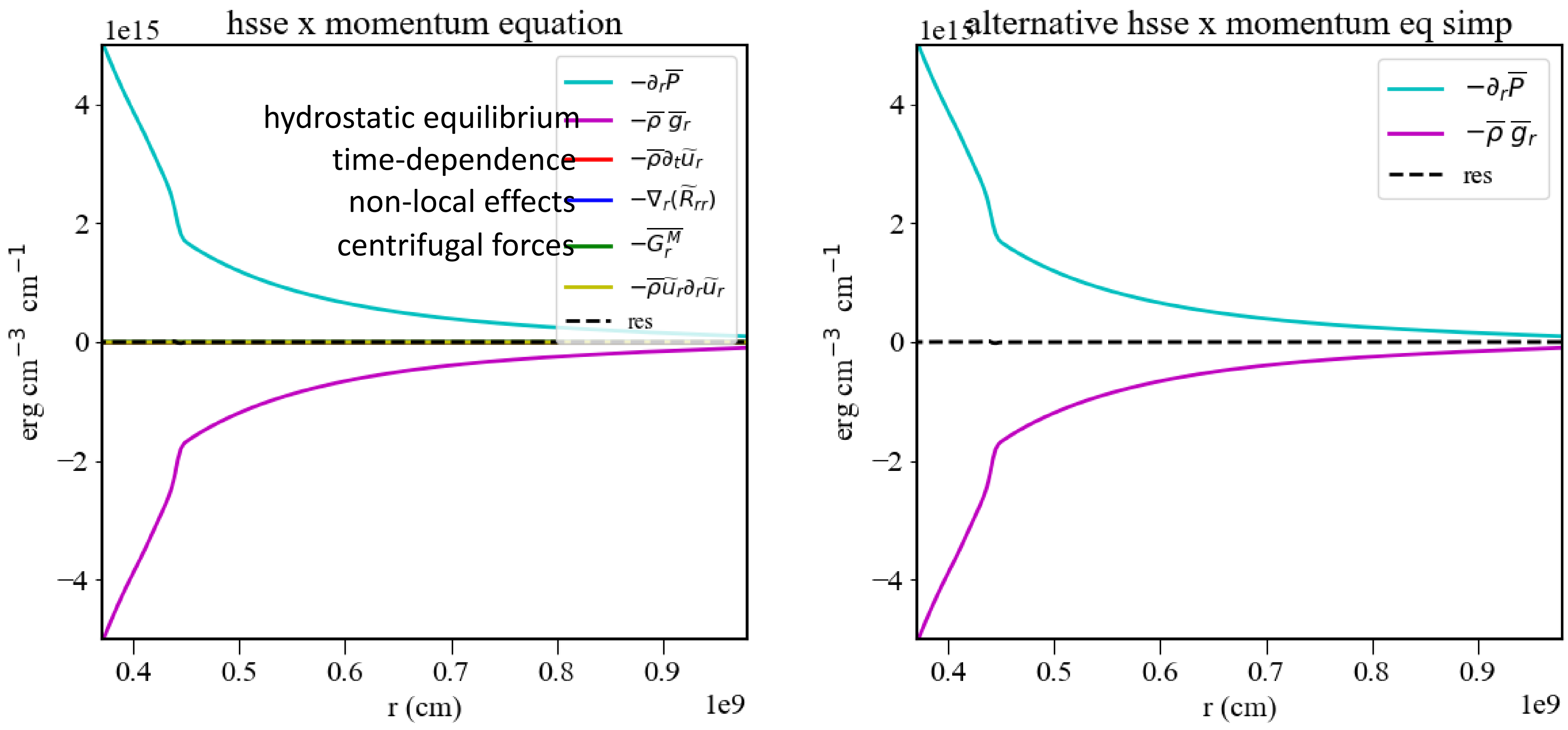
https://github.com/mmicromegas/ransX/blob/master/DOCS/RANDOM/hsse_explained.pdf

Hydrodynamic stellar structure equations

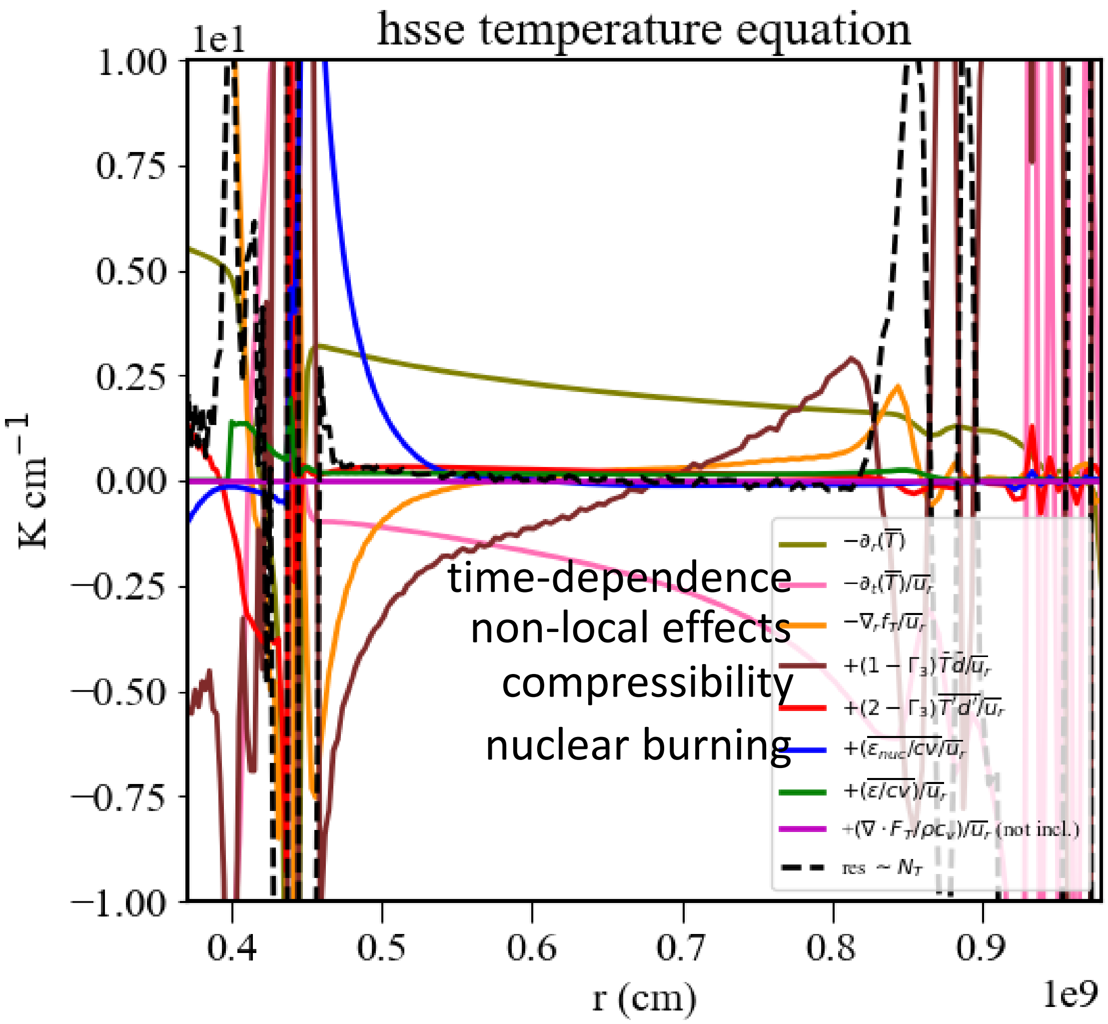


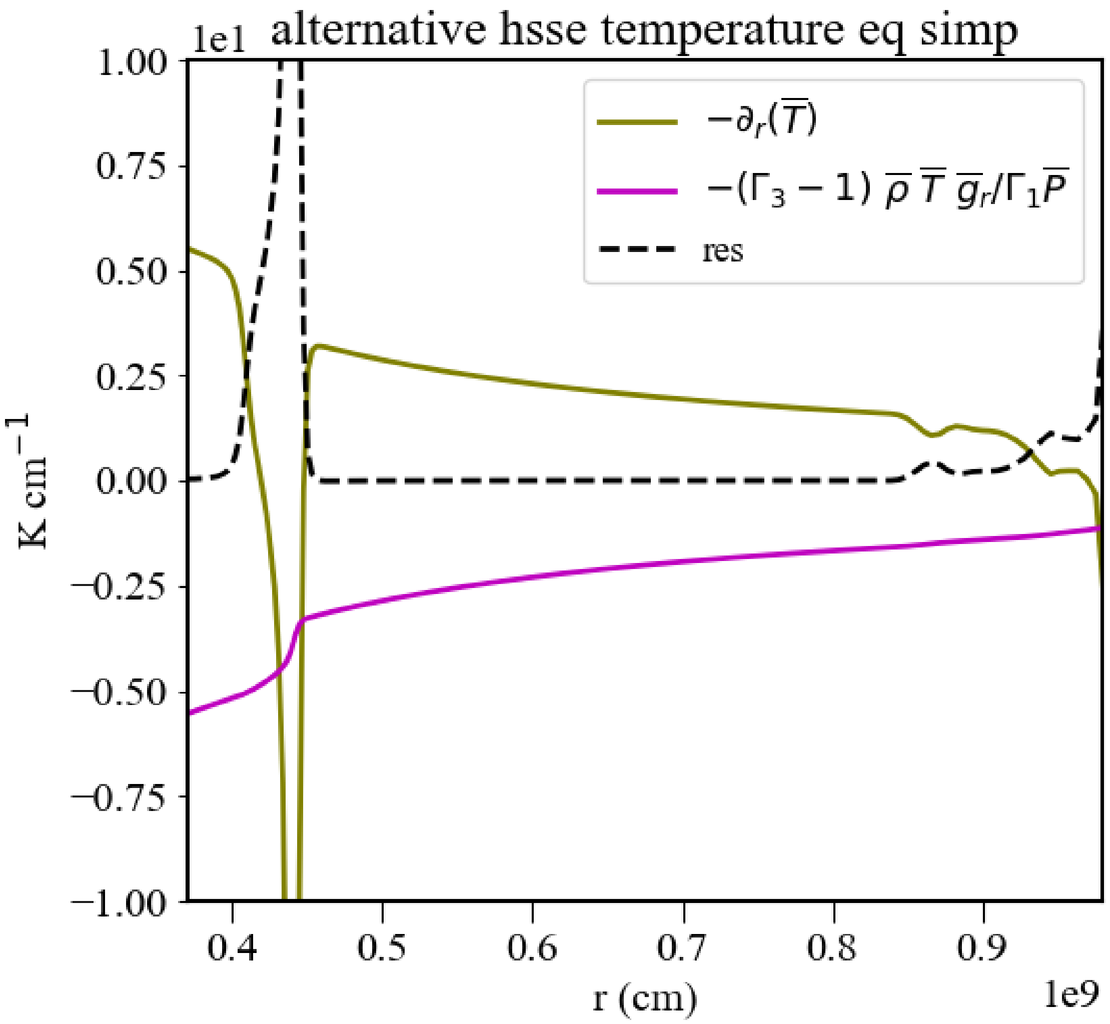


Hydrodynamic stellar structure equations

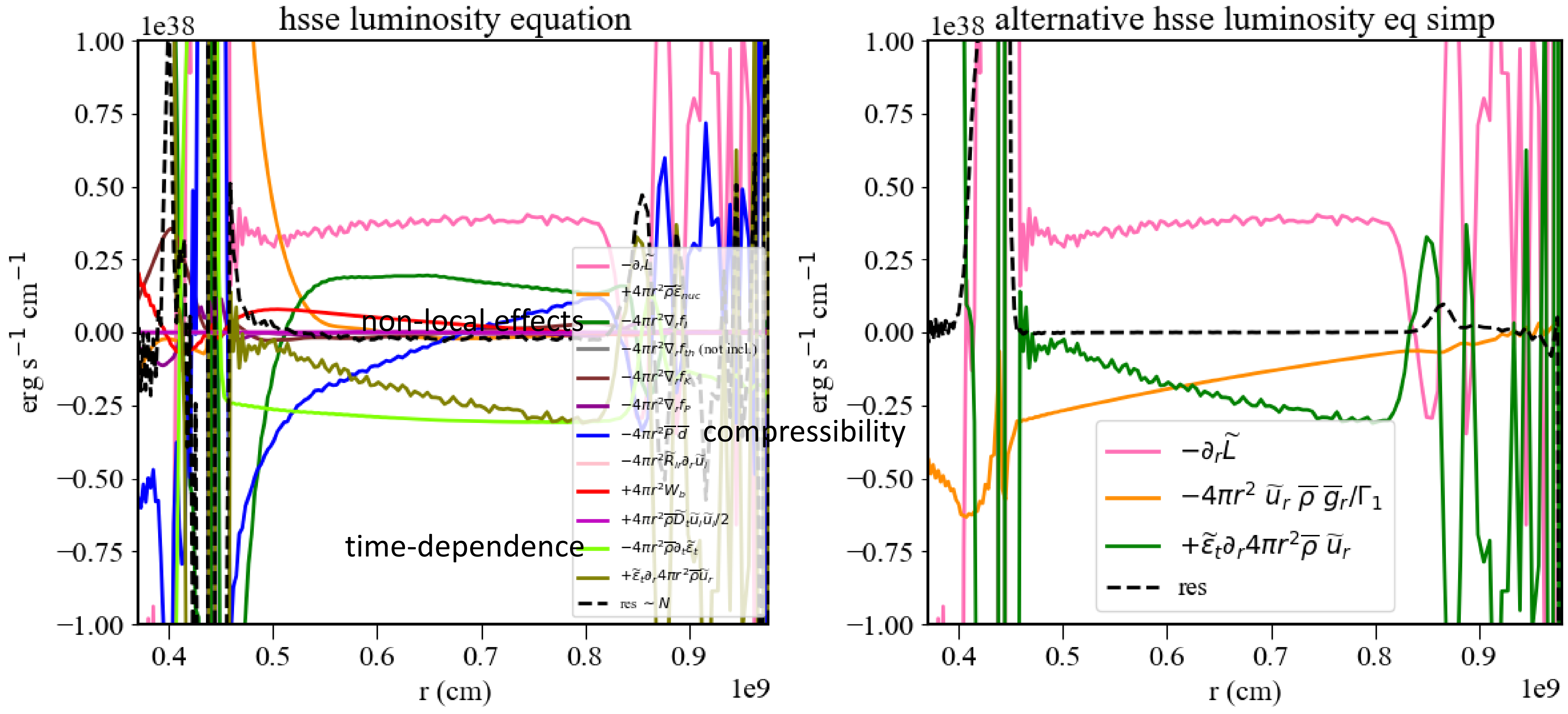


Hydrodynamic stellar structure equations

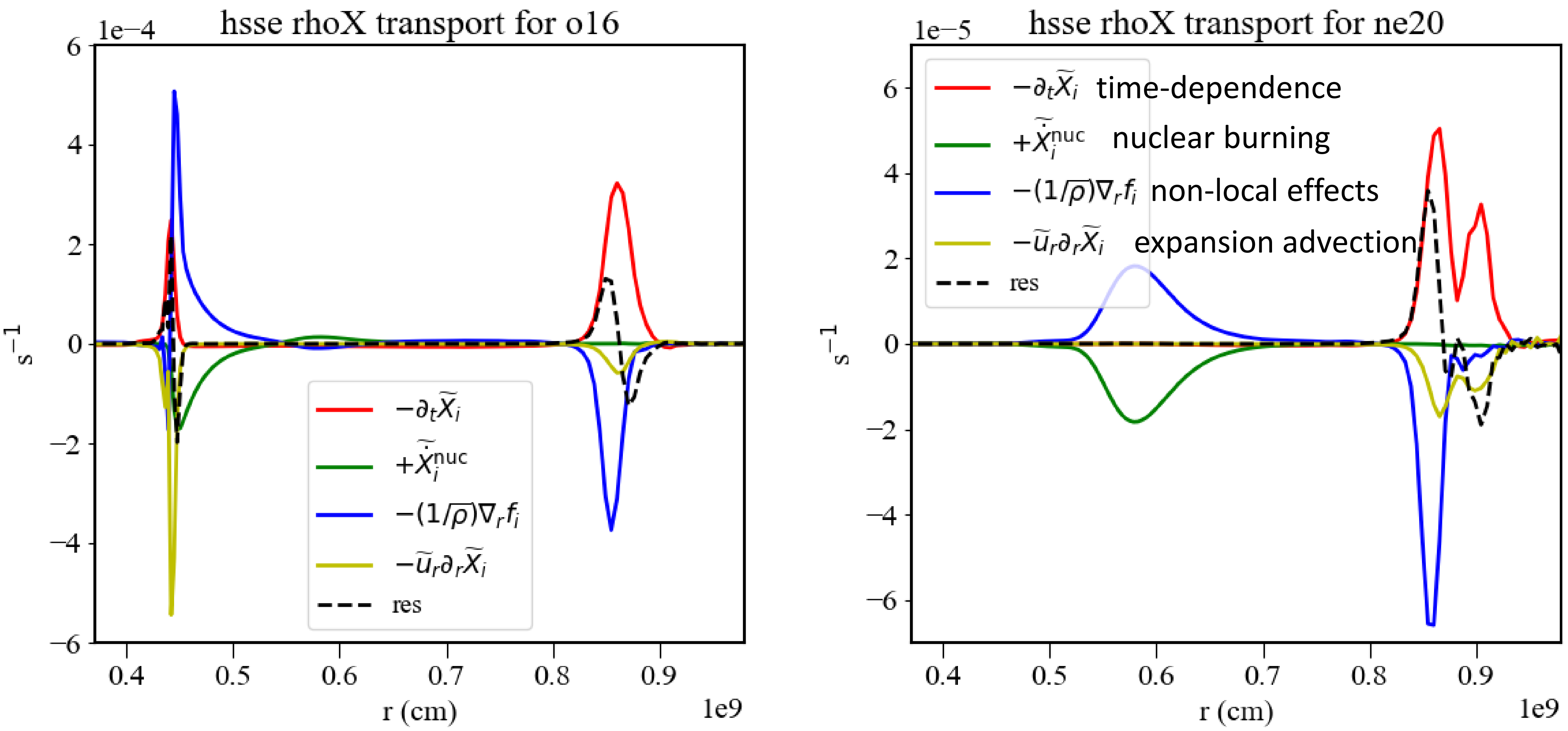




Hydrodynamic stellar structure equations



Hydrodynamic stellar structure equations



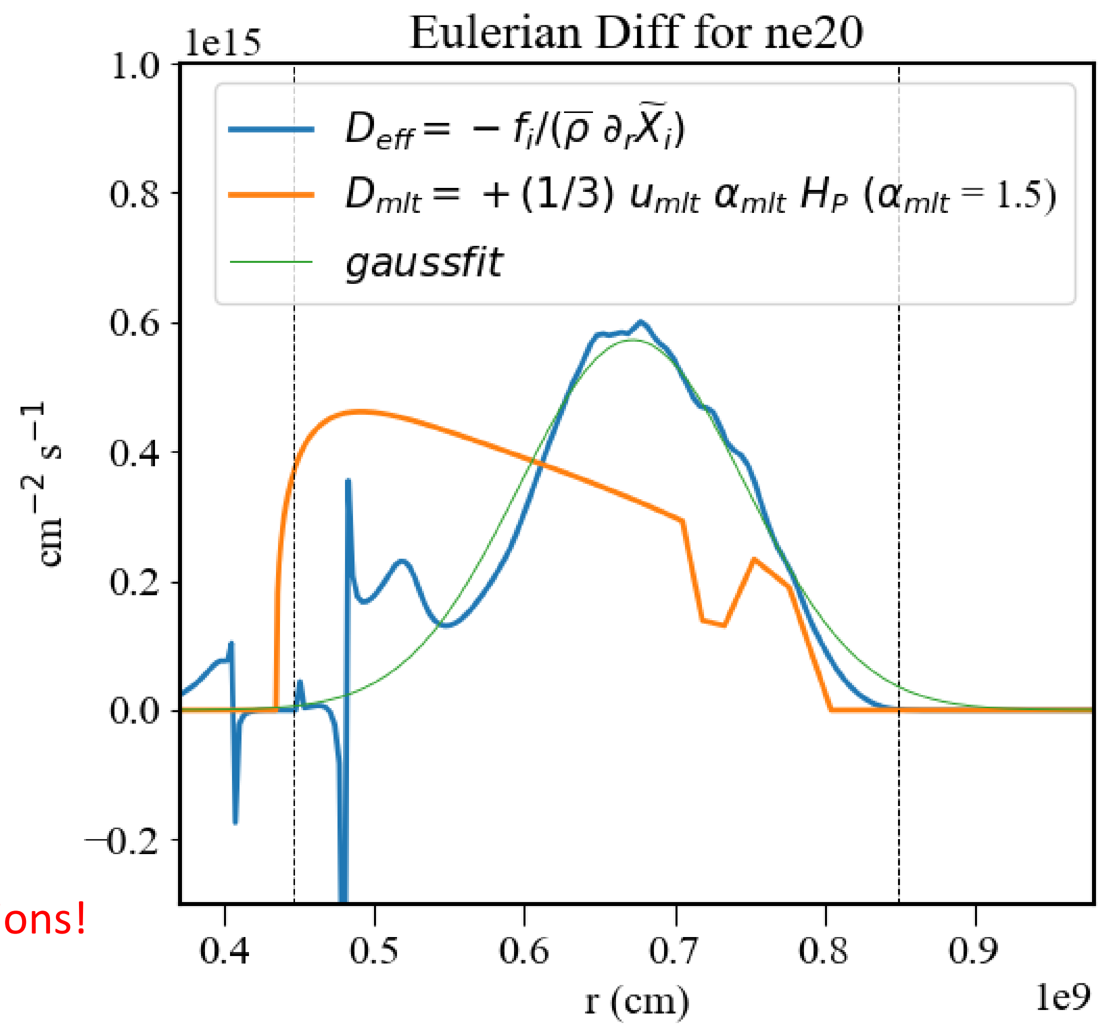
Composition flux model with Gaussian eddy diffusivity

$$f_i = -D\ \overline{\rho}\ \partial_r \widetilde{X}_i$$

$$D_{mlt} = \frac{1}{3}\ u_{mlt}\ (\alpha H_P)$$

$$D_{eff} = -f_i/(\overline{\rho}\partial_r \widetilde{X}_i)$$

$$D_{gauss} = max(D_{mlt})\ e^{-\frac{(r-r_c^{middle})^2}{2\ width_c{}^2}}$$



To get this right is essential, because in reactive flows, mixing controls rate of nuclear reactions!

Summary and results

- Analysis framework for multi-fluid compressible hydrodynamic simulations completed https://github.com/mmicromegas/ransX (for cartesian and spherical geometry only, no rotation, no magnetic fields)
- Time-dependence, non-locality and compressibility effects play important roles during life of stars
- Transport-diffusion model for composition flux requires Gaussian-like eddy- diffusivity (fluxes of some active elements, where nuclear burning significantly affects their mean gradients are even more complicated) - MLT based diffusivities have limitations
- ransx@googlegroups.com (if interested, please send an email to miroslav.mocak@gmail.com to be added to our group)

Future plans (to science the shit of out this 🙂)

- Look for potential closures of unknowns in general hydrodynamic stellar structure equations in engineering literature and atmospheric sciences for turbulent regions, their boundaries and stable layers
- Help ransX to become standard for all stellar hydrodynamic simulations including core, envelope and atmospheric convection
- Extend library of our ransX hydrodynamic simulations with core helium flash, dual core flash, core carbon flash, O-Ne-C burning with two distinct convection shells – all setups prepared in PROMPI already
- Incorporate the Gaussian eddy-diffusivity mixing model to 1D stellar code (e.g. MESA)
- **Compete for 3+ years full-time position in astrophysics (please advise) – research proposal here** https://github.com/mmicromegas/ransX/blob/master/DOCS/RANDOM/ransXproposal2019.pdf
- **CV** https://github.com/mmicromegas/ransX/blob/master/DOCS/RANDOM/cvmmocak2019.pdf

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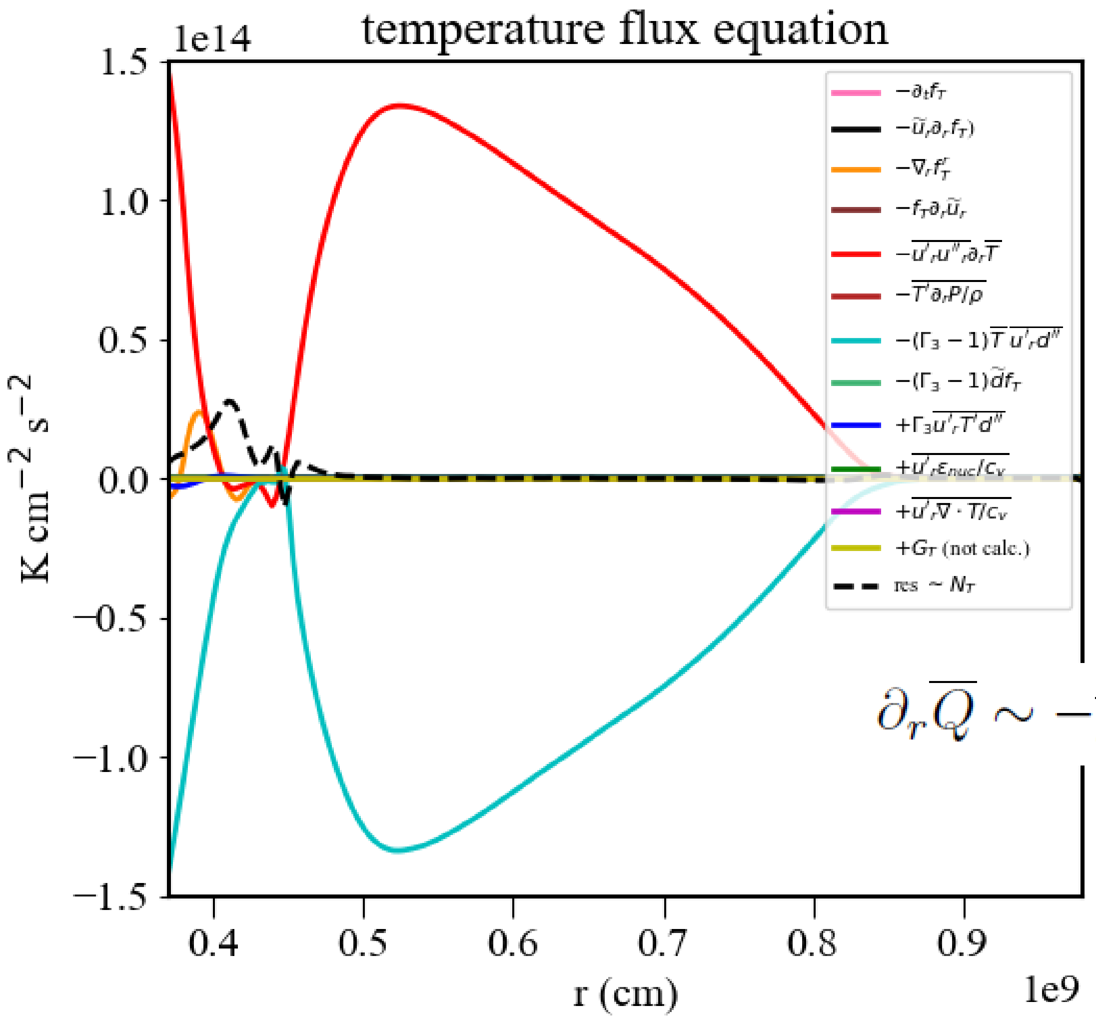
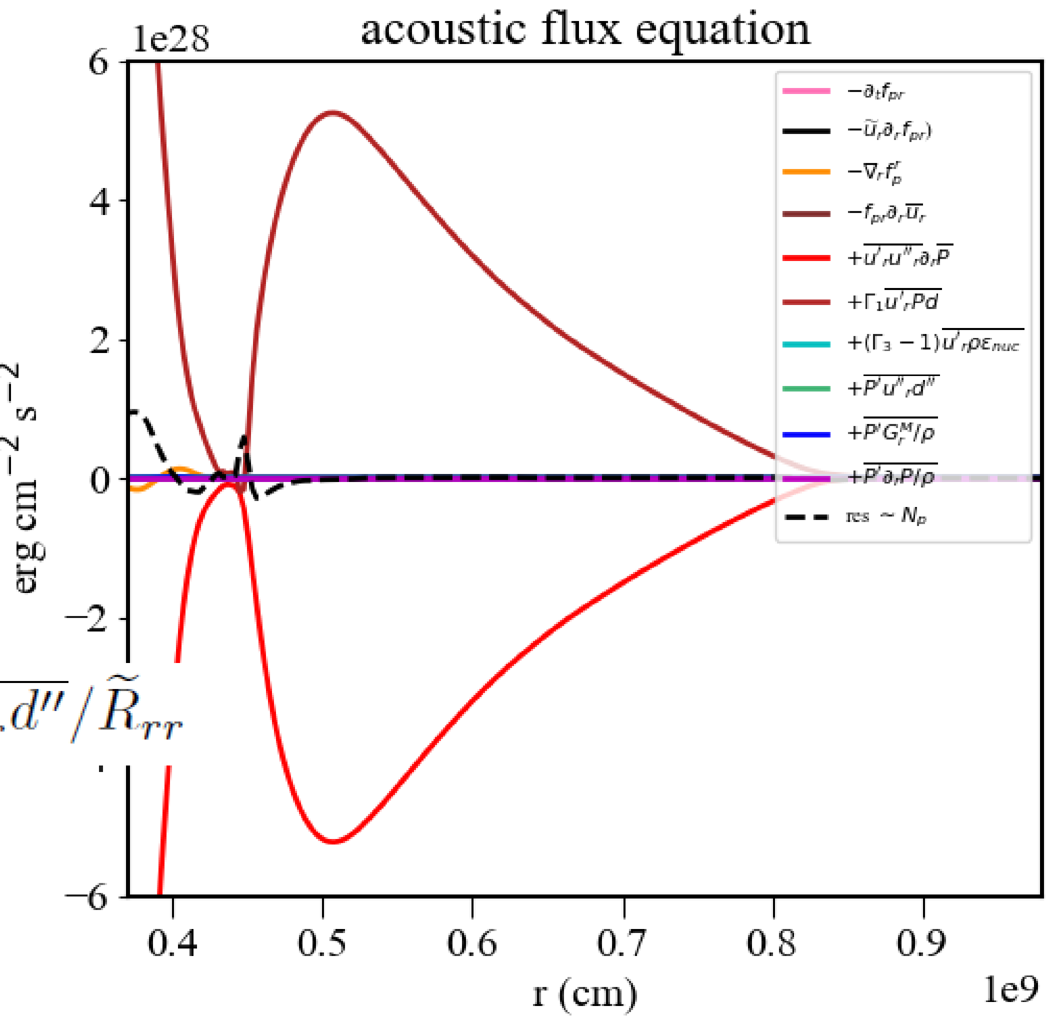
THANKS

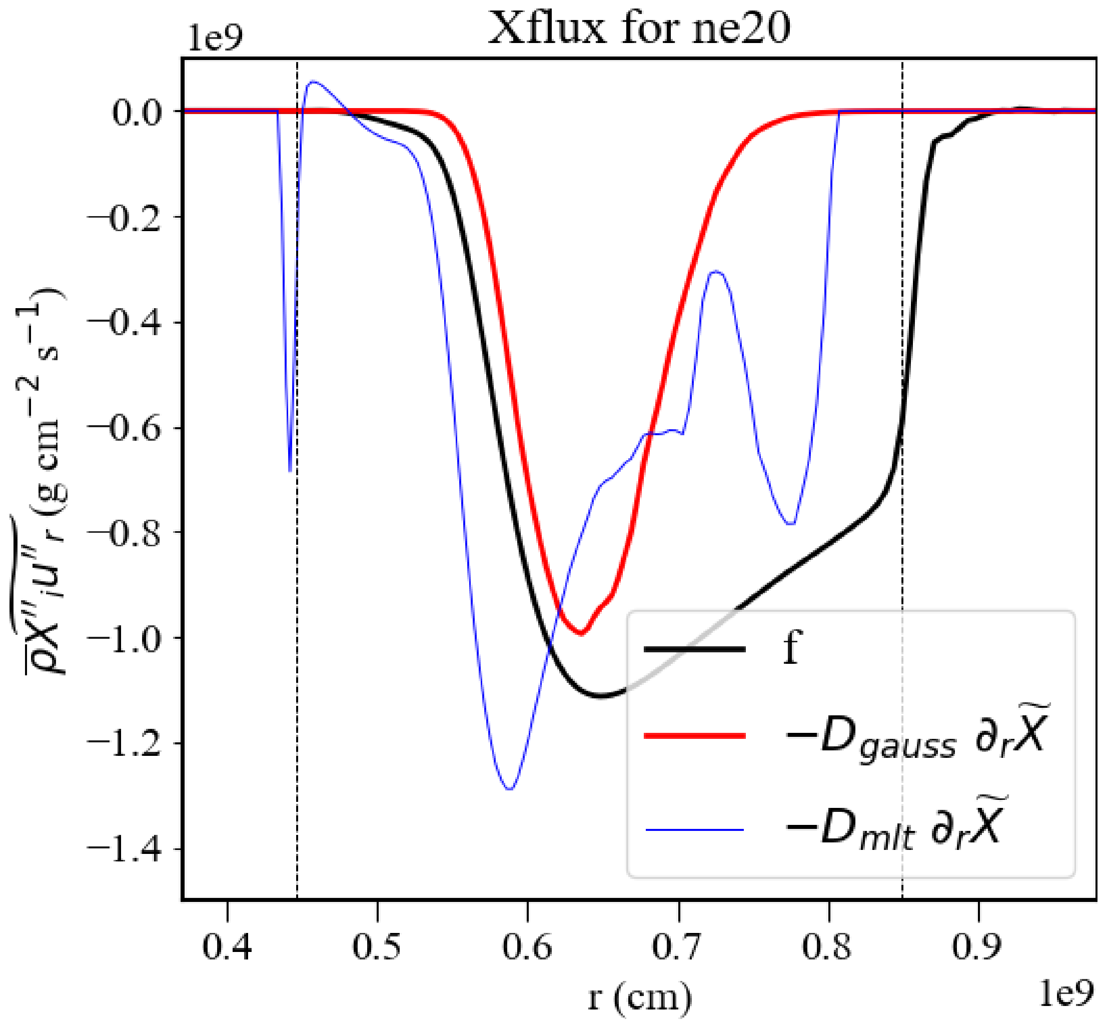
Flux evolution equations and stellar gradients

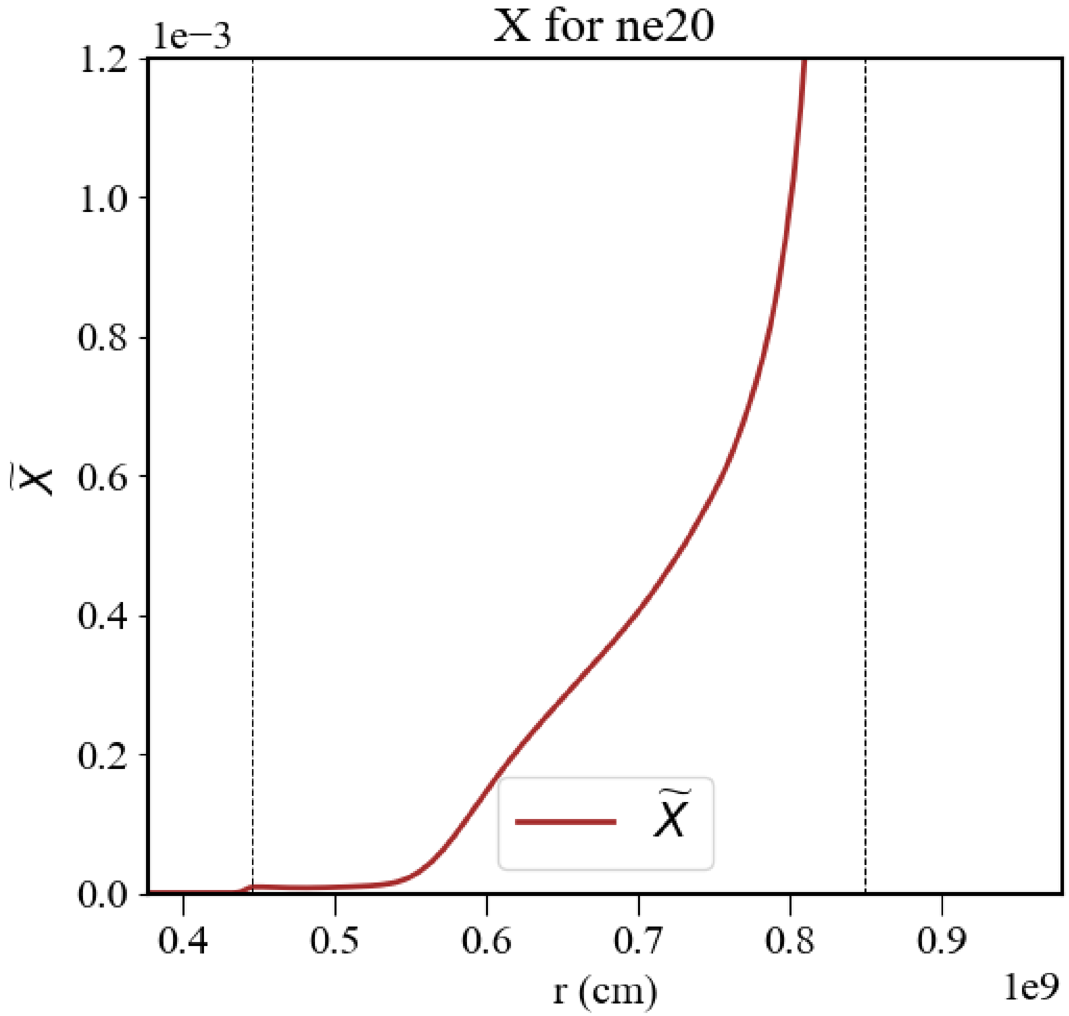




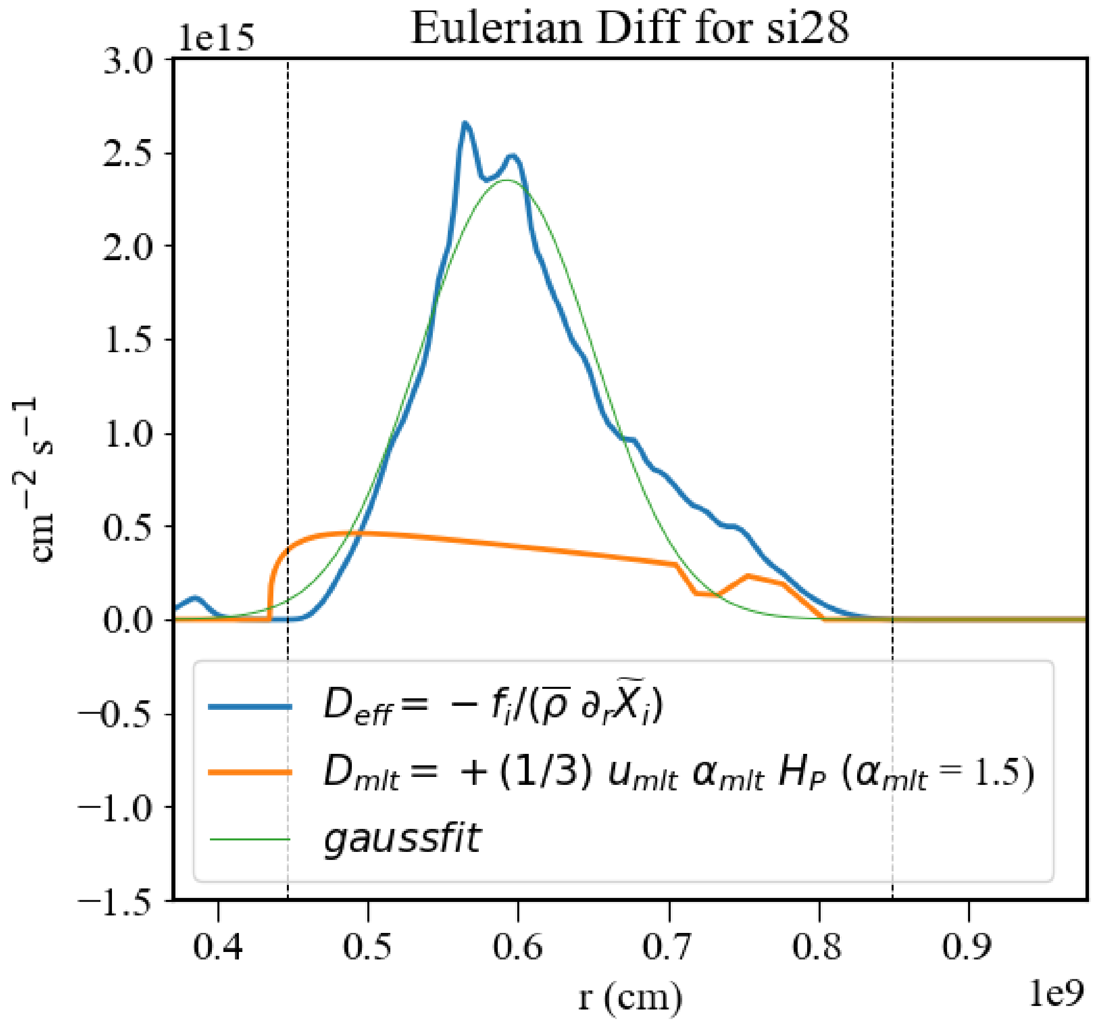
$$\partial_r \overline{Q} \sim -\overline{\rho}\ \overline{Q}\ \overline{u'_r d''} / \widetilde{R}_{rr}$$

Composition flux model

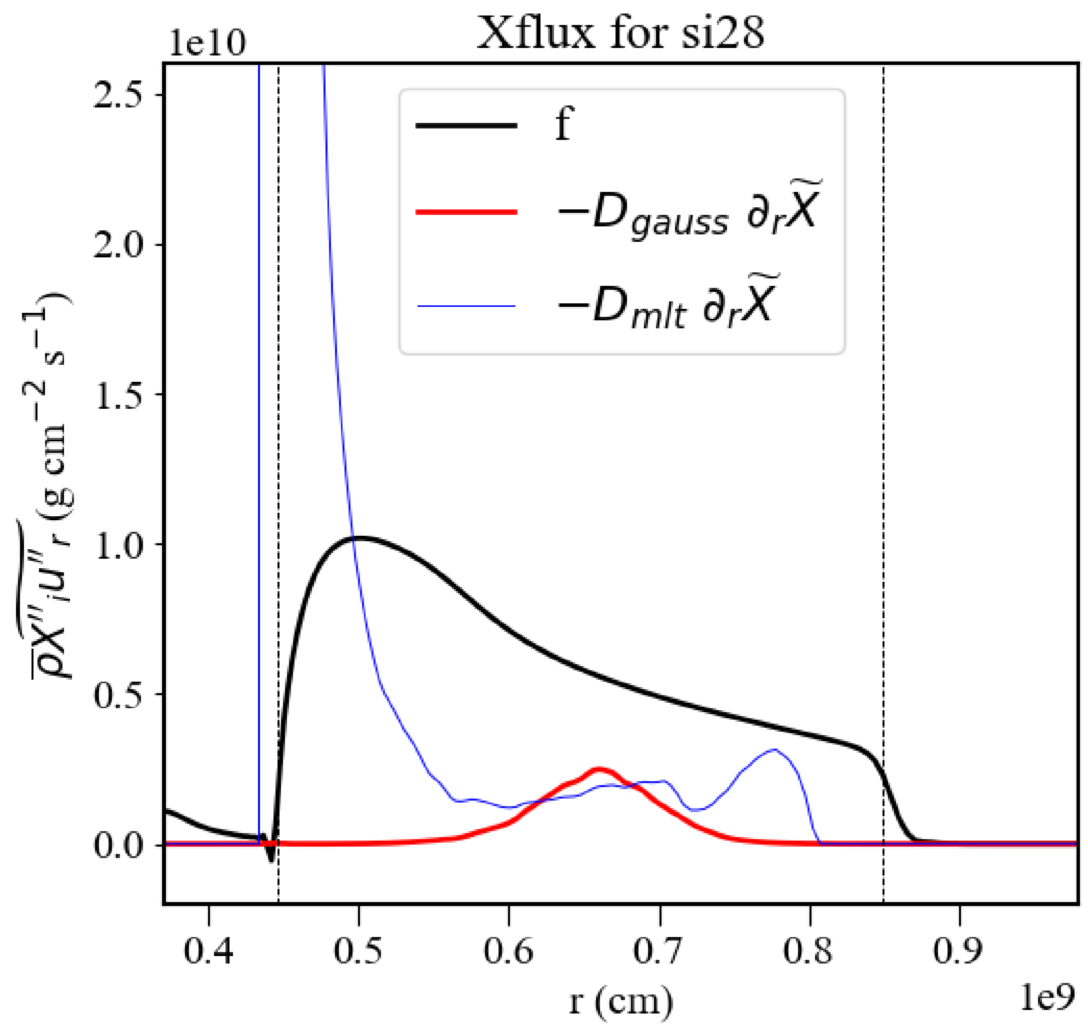


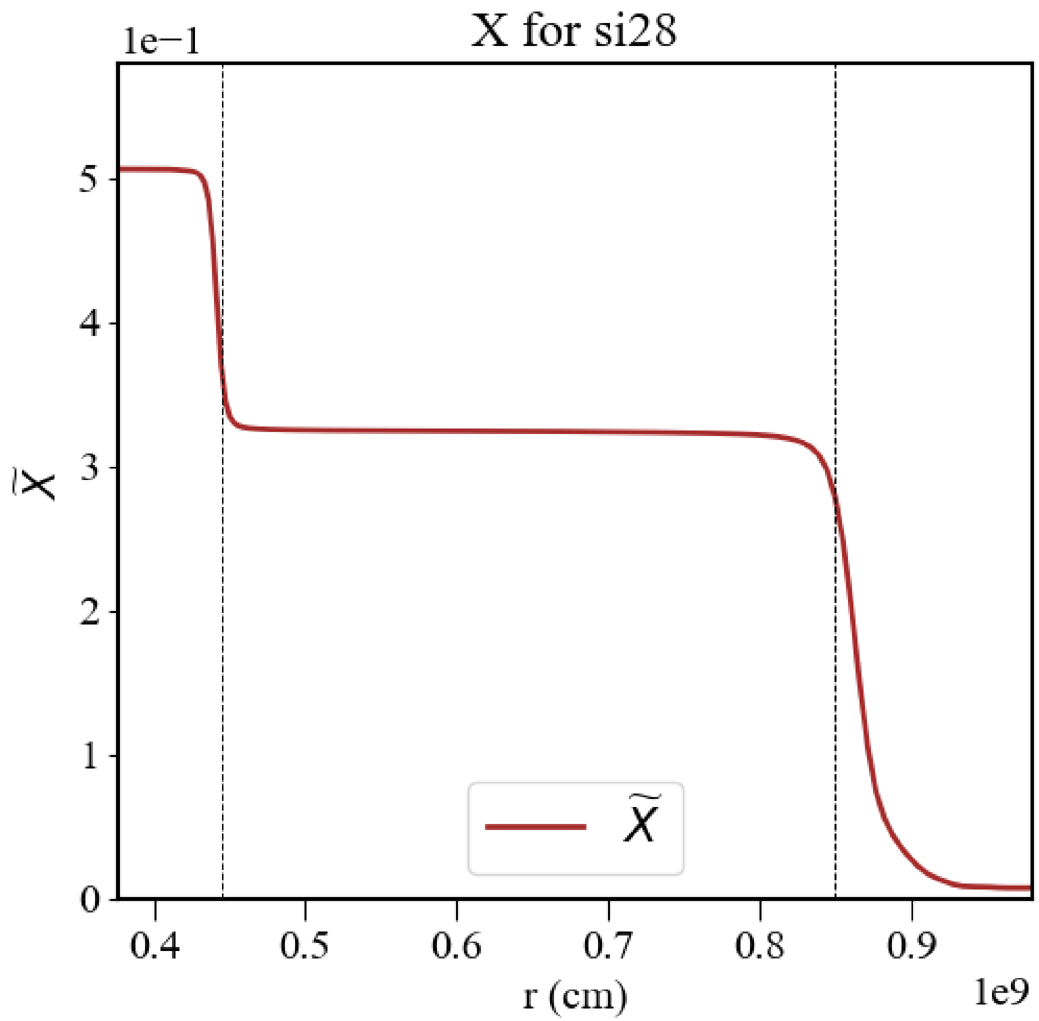


Composition flux model

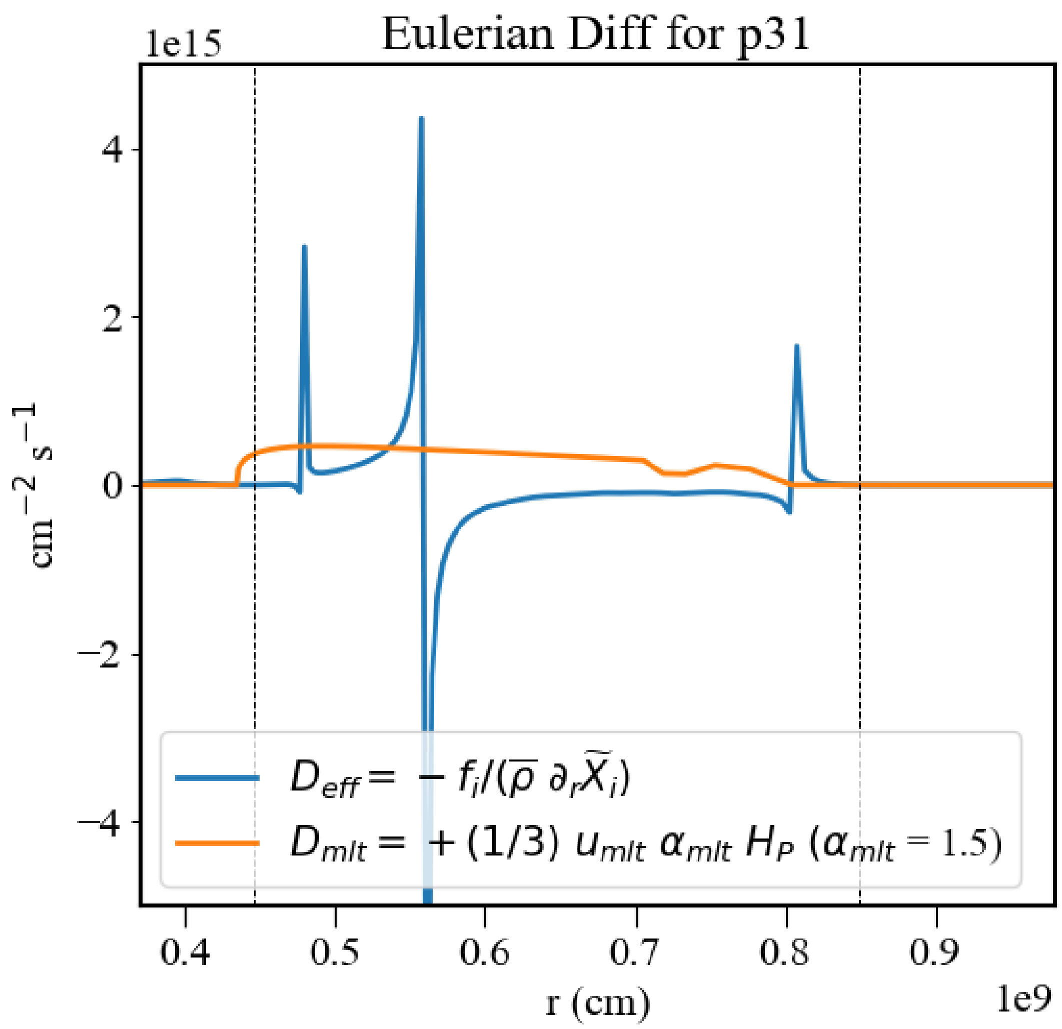


Composition flux model

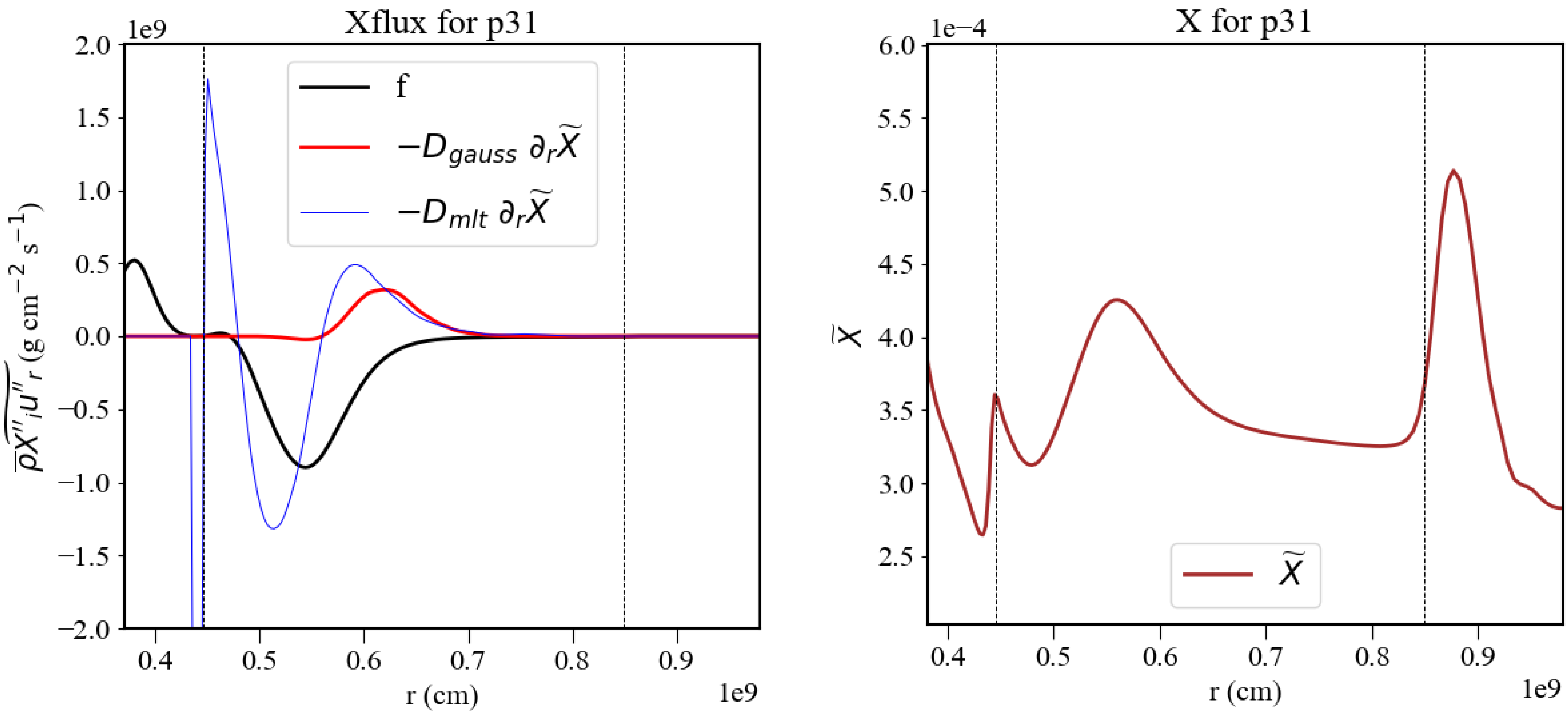




Composition flux model



Composition flux model



Downgradient approximation

$$\widetilde{F}_i^q \sim -\Gamma_t \frac{\partial \widetilde{q}}{\partial x_i} \quad (\Gamma_t \text{ is turbulence diffusivity and } \widetilde{F}_i^q = \overline{\rho q'' u_i''} \text{ is a flux of } q)$$

- can be derived from a transport equation of a diffusive passive scalar (Harlow & Hirt, 1969; Daly & Harlow, 1970):

$$\partial_t \widetilde{F}_i^q - \overline{u_i'' q'' \partial_t \rho} - \widetilde{R}_{in} \partial_n \widetilde{q} + \widetilde{u}_n \overline{\rho \partial_n u_i'' q''} + \widetilde{F}_n^q \partial_n \widetilde{u}_i + \partial_n \overline{\rho u_n'' u_i'' q''} - \overline{u_i'' q'' \partial_n \rho u_n''} = -\overline{q''} \partial_i \overline{P} - \overline{q'' \partial_i P'} + \partial_n (\overline{\lambda \rho u_i'' \partial_n q''}) + f \widetilde{F}_i^q$$

where q is the passive scalar governed by a diffusion equation $D_t q = \lambda \nabla^2 q$

It implies, that the downgradient approximation holds only for:

- a transport of a diffusive passive scalar
- a flow in steady state ($\partial_t \widetilde{F}_i^q = 0$)
- an incompressible flow ($\partial_t \rho = 0$)
- a flow with no background velocities ($\widetilde{u}_i = 0$)
- a flow with no pressure-scalar correlations ($\overline{q''} \partial_i \overline{P} = \overline{q'' \partial_i P'} = 0$)
- a homogeneous flow ($\partial_n \overline{\rho u_n'' u_i'' q''} = 0$)
- an isotropic flow (decay-rate assumption: $\overline{\partial_n q'' \partial_n \rho u_i''} \sim f \widetilde{F}_i^q$)

But, stellar turbulent convection is:

- stratified (not homogeneous)
- anisotropic
- compressible on expanding/contracting background

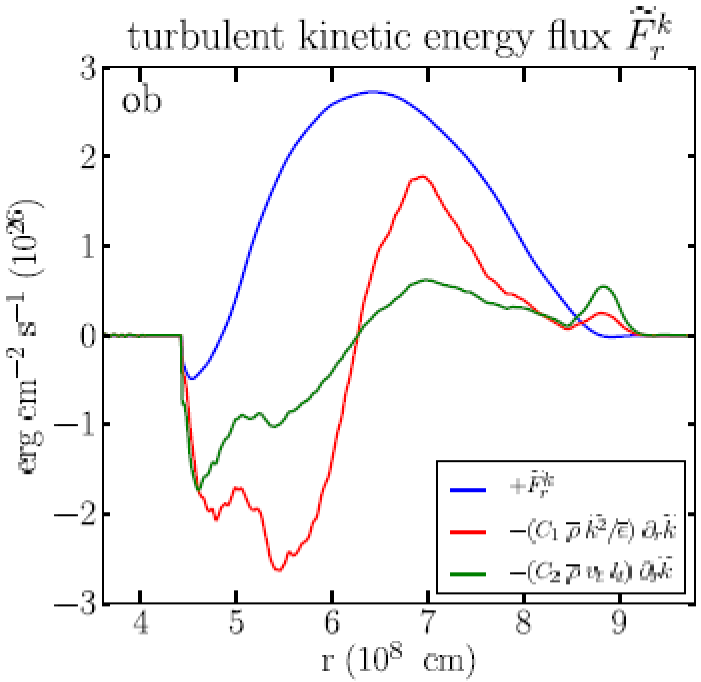


Figure 1: Downgradient approximations to the turbulent kinetic energy flux $\widetilde{F}_r^k = \overline{\rho u_r'' k''}$ derived from 3D oxygen burning shell model.

- **downgradient approximation is not suitable for modelling stellar processes**