Monte Carlo Radiative Transfer for Neutron Star Merger Simulations

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ARTIS radiative transfer code

- ARTIS is a 3D-capable Monte Carlo radiative transfer code (method of Lucy 2002)
- Radioactive decay energy release over simulation period is discretised into packets at simulation start
- Pellets of radioactive energy co-move with the ejecta until a decay, then can make several state transitions according to energy flows until a photon packet exits the simulation volume (contributing to the synthetic spectra and light curve).
- Simulations always follow a time evolution with light travel time accounted for (no single-time snapshots like CMFGEN, TARDIS).

Kromer & Sim (2009)

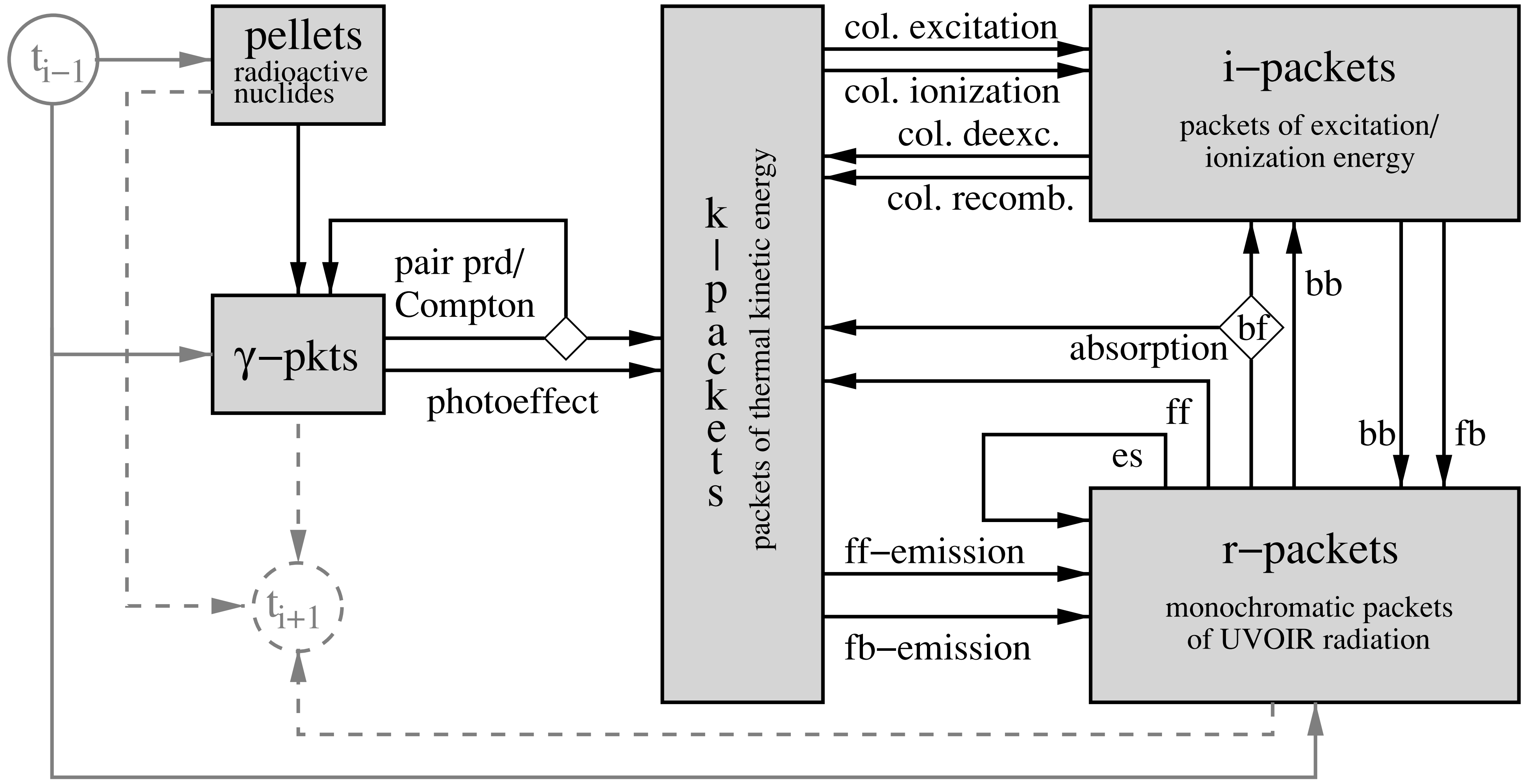
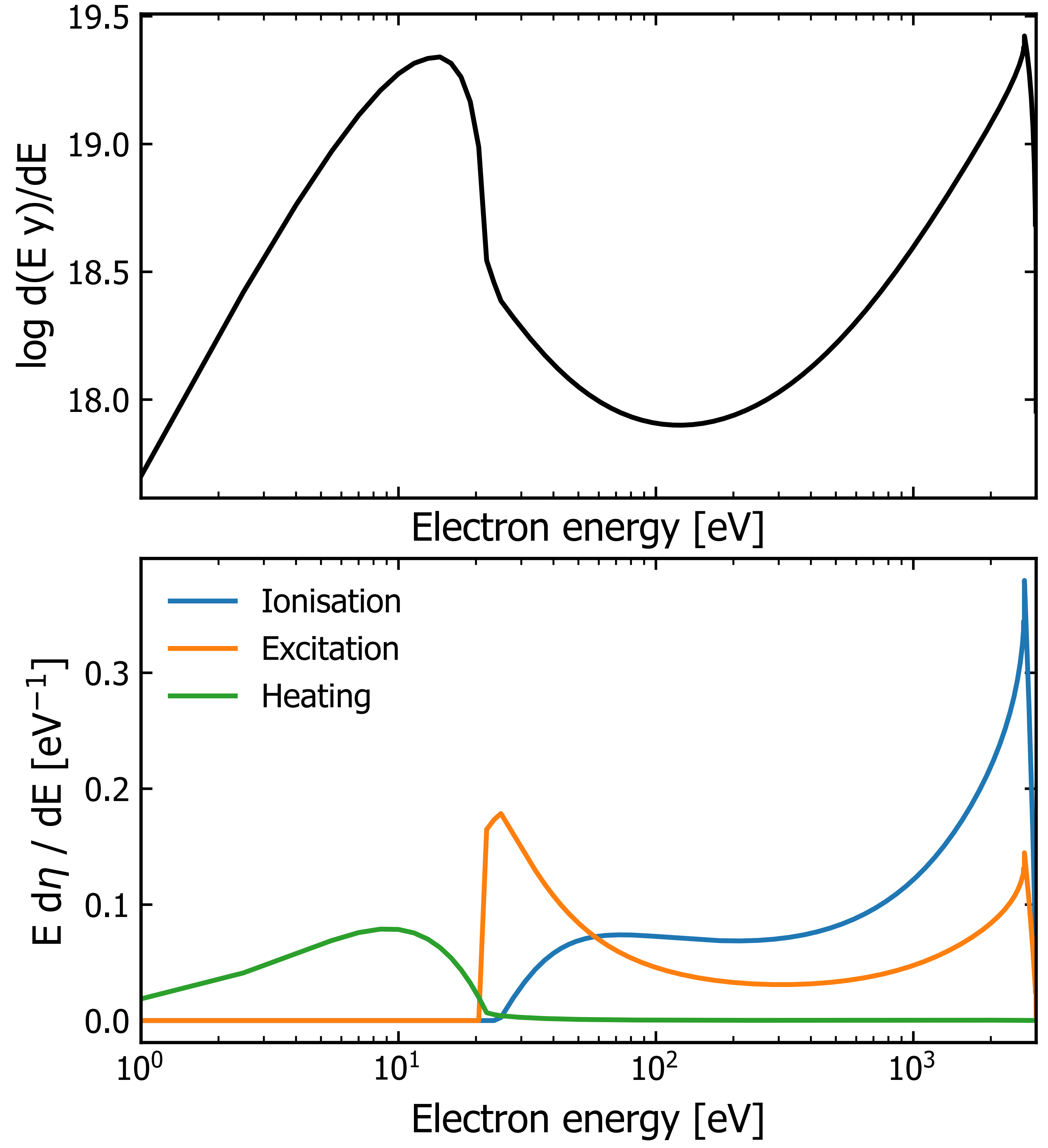


Figure 1. Flow chart outlining the mode of operation of the code. For discussion, see the text.

Non-thermal particle deposition

- With a continuous source of high-energy decay particles that don't thermalise efficiently, the energy distribution stays non-Maxwellian
- e.g., Type Ia supernovae at late times: positrons from Co56 decay and electrons Compton-scattered by gamma rays
- We obtain the non-thermal electron distribution by numerically solving the Spencer & Fano (1954) equation using the method of Kozma & Fransson (1992)
- SF equation accounts for sources and sinks due to energy deposition, heating (Coulomb scattering), excitation, and ionisation.
- Similar to Li, Hillier, & Dessart (2012) for CMFGEN, using impact ionisation cross sections from Arnaud & Rothenflug (1985) and Arnaud & Raymond (1992).
- Rates for non-thermal ionisation, excitation, and heating obtain by integrating over the energy distribution

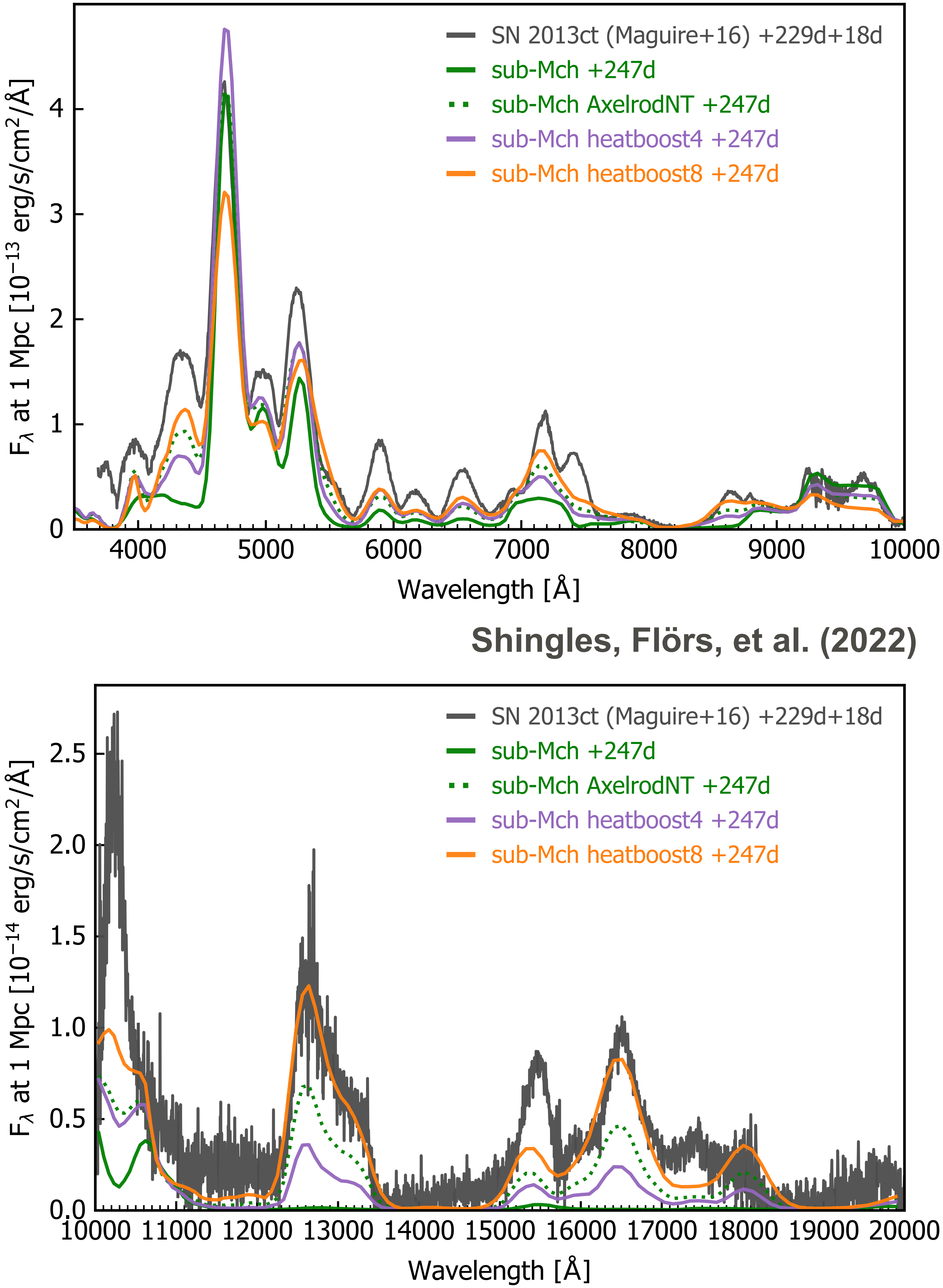
Test with 99% O^0, 1% O^+



$$\sum_j n_j \sum_k \int_E^{E+E_{j\to k}} y(E')\sigma_{\mathrm{exc},j\to k}(E')dE' + y(E)L_e(E)$$
$$+ \sum_i N_i \sum_m \int_E^{E_{\max}} y(E') \int_{E'-E}^{(E'+E)/2} \sigma_{\mathrm{ion},m}(E',\epsilon)d\epsilon dE'$$
$$= \sum_i N_i \sum_m \int_{2E+I_m}^{E_{\max}} y(E') \int_{E+I_m}^{(E'+I_m)/2} \sigma_{\mathrm{ion},m}(E',\epsilon)d\epsilon dE'$$
$$+ \sum_i N_i \sum_m \int_E^{E_{\max}} \delta(E' - \bar{E}_{\mathrm{Auger},m})dE' \int_E^{E_{\max}} y(E')\sigma_{\mathrm{ion},m}(E')dE'$$
$$+ \int_E^{E_{\max}} S(E')dE',$$

Importance of non-thermal ionisation

- Matching observed ionisation state is a major challenge for Type Ia supernovae models > ~100 days
- Sub-Chandrasekhar-mass models are too highly ionised with detailed non-thermal ionisation (Wilk+ 2018, Shingles+ 2020)
- Wilk et al. (2018, 2020) suggest ejecta clumping boosts recombination rate
- We tested reduction of non-thermal ionisation rates by boosting thermal losses (Shingles+ 2022)
- Relevance to kilonovae: Pognan+ 2022 estimate that as early at three days after merger, non-thermal ionisation > collisional and photoionisation for non-neutral species.
  - Used a similar Spencer-Fano solver and approximate cross sections (no impact ion. data available for Lanthanides?)

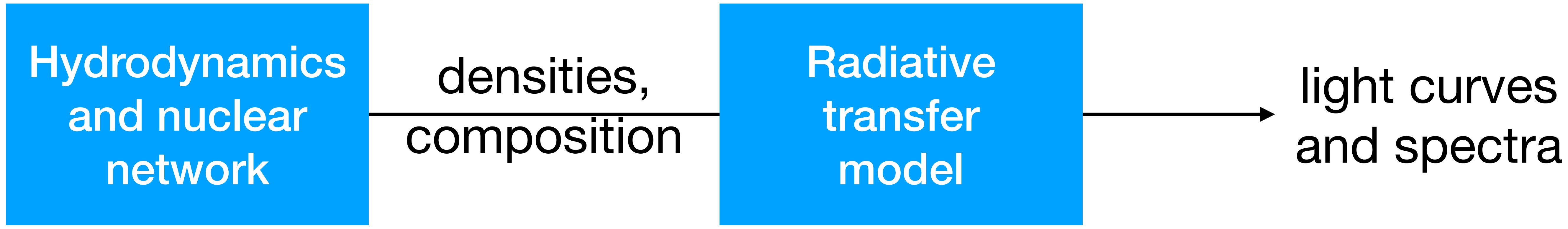


Shingles, Flörs, et al. (2022)

ARTIS developments

- ARTIS now has a non-thermal solver, non-LTE level populations, binned radiation field and detailed photoionisation rate estimators (Shingles et al. 2020)
- ARTIS originally followed just a few decay chains relevant to Type Ias (e.g., Ni56->Co56->Fe56) beta-plus and electron-capture only.
- Now includes decays in a more generalised way
  - Models here include 2591 nuclides with alpha and beta-minus decays from ENDF/B-VII.1 (Chadwick+ 2011 via Hotokezaka's data file public on GitHub)
  - Abundance calculation from Bateman equation summed over all ancestor paths. No loops allowed (e.g. no n or p-capture reactions)
  - Gamma-ray decay spectra from NNDC and full transport
  - Particle emission using average kinetic energy per decay
    - local but non-instantaneous deposition (assumed to be fully trapped)

Synthetic spectra and light curves from merger models



Hydrodynamics and nuclear network

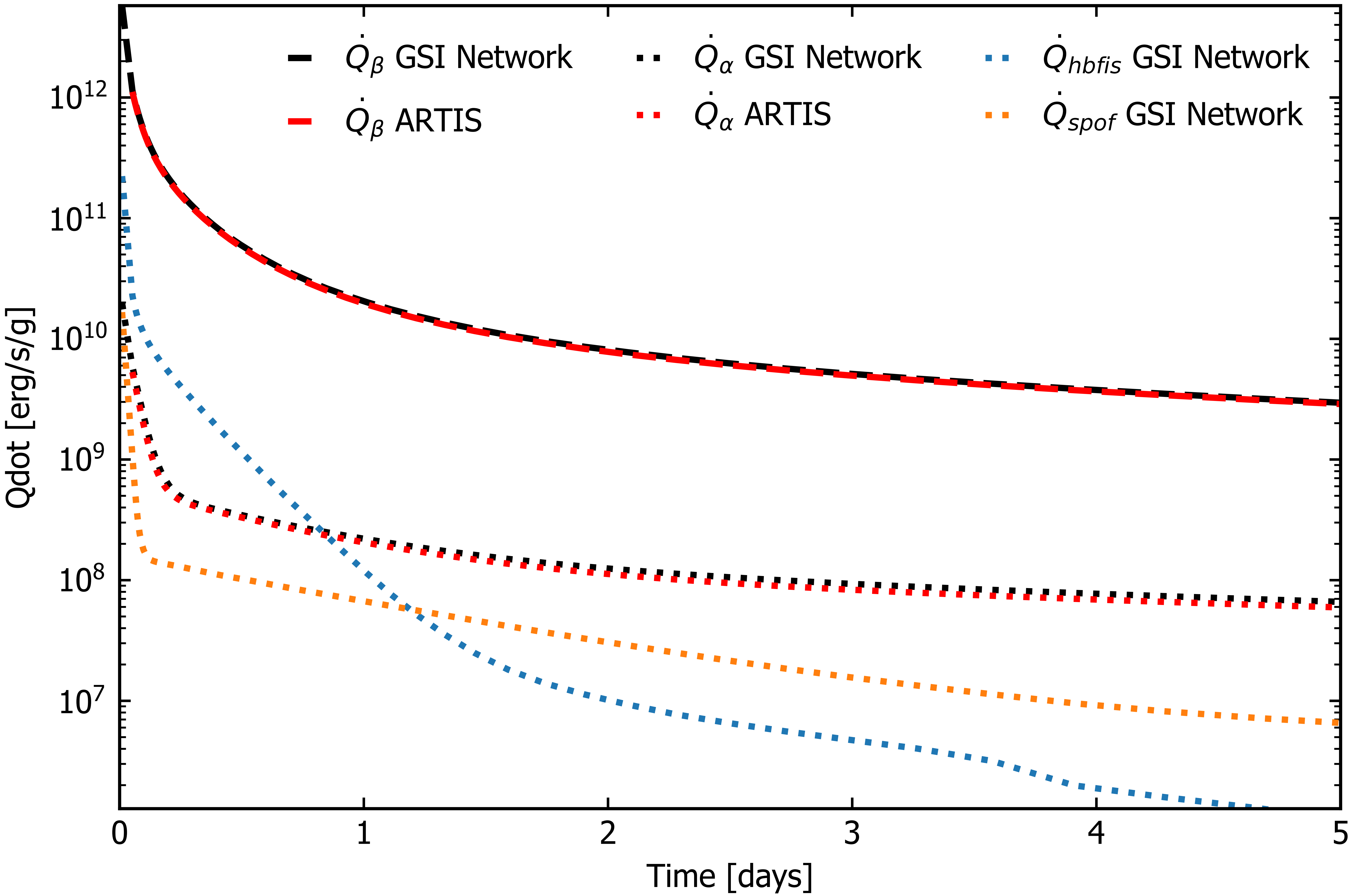
densities, composition

Radiative transfer model

light curves and spectra

- Model of dynamical ejecta density by Vimal Vijayan (SFHO EoS including neutrinos for the mass 1.35-1.35 Msun, ejecta mass: 0.004 Msun, see Vimal's talk)
- Density structure combined with r-process abundances from detailed nuclear network calculation at 0.01 days (Martínez-Pinedo)
- Currently, 1D spherical average is used for fast prototyping (but 2D/3D is planned)
- ARTIS follows simple density (homologous) and abundance evolution (decays) while calculating radiative transfer
- For now, I test with Tanaka+ 2020 grey opacity vs Ye (same as Collins model)
  - Future: line-by-line Sobolev opacity with element/ion composition and NLTE level populations

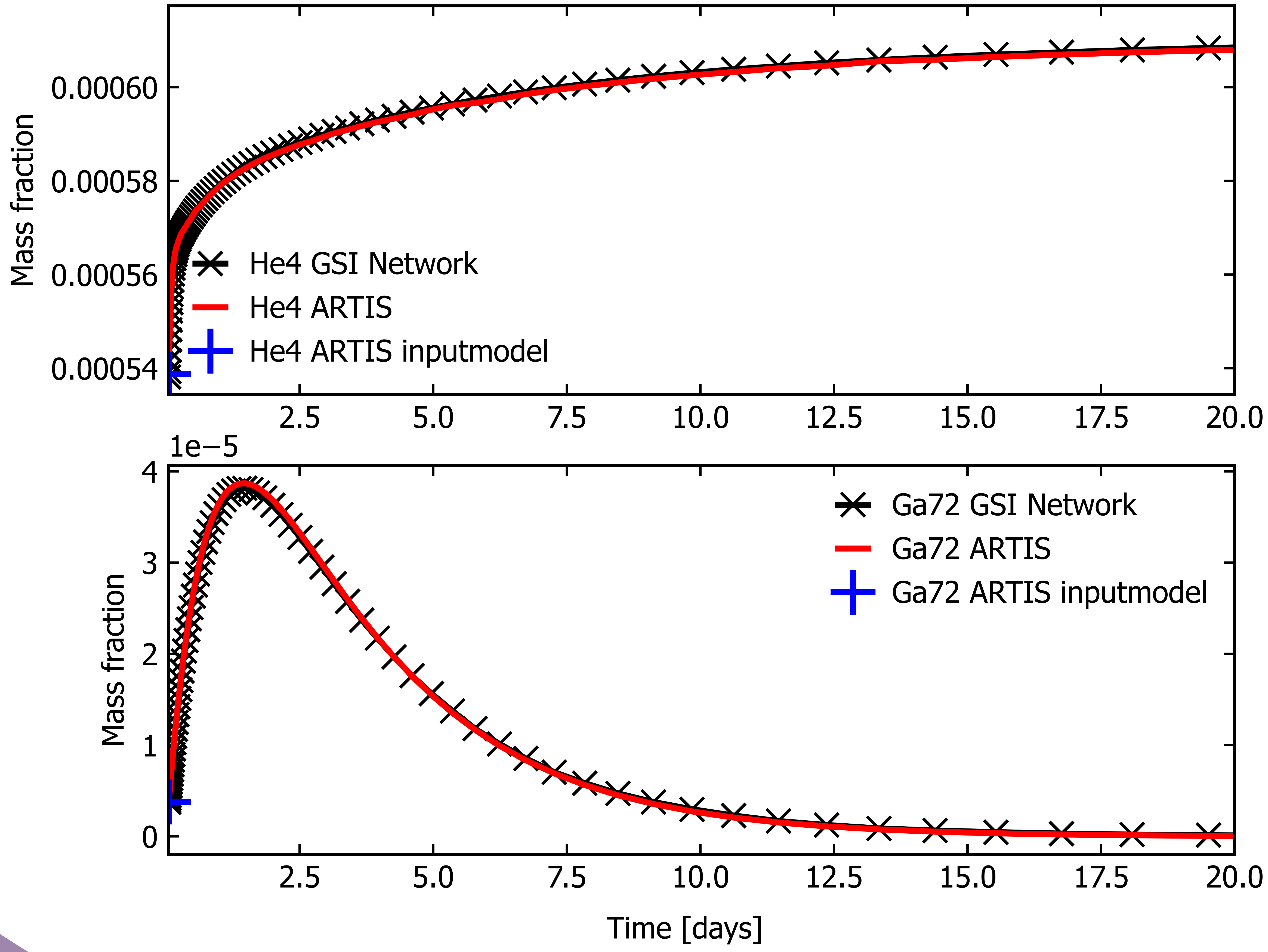
Radioactive decay power ARTIS vs full network

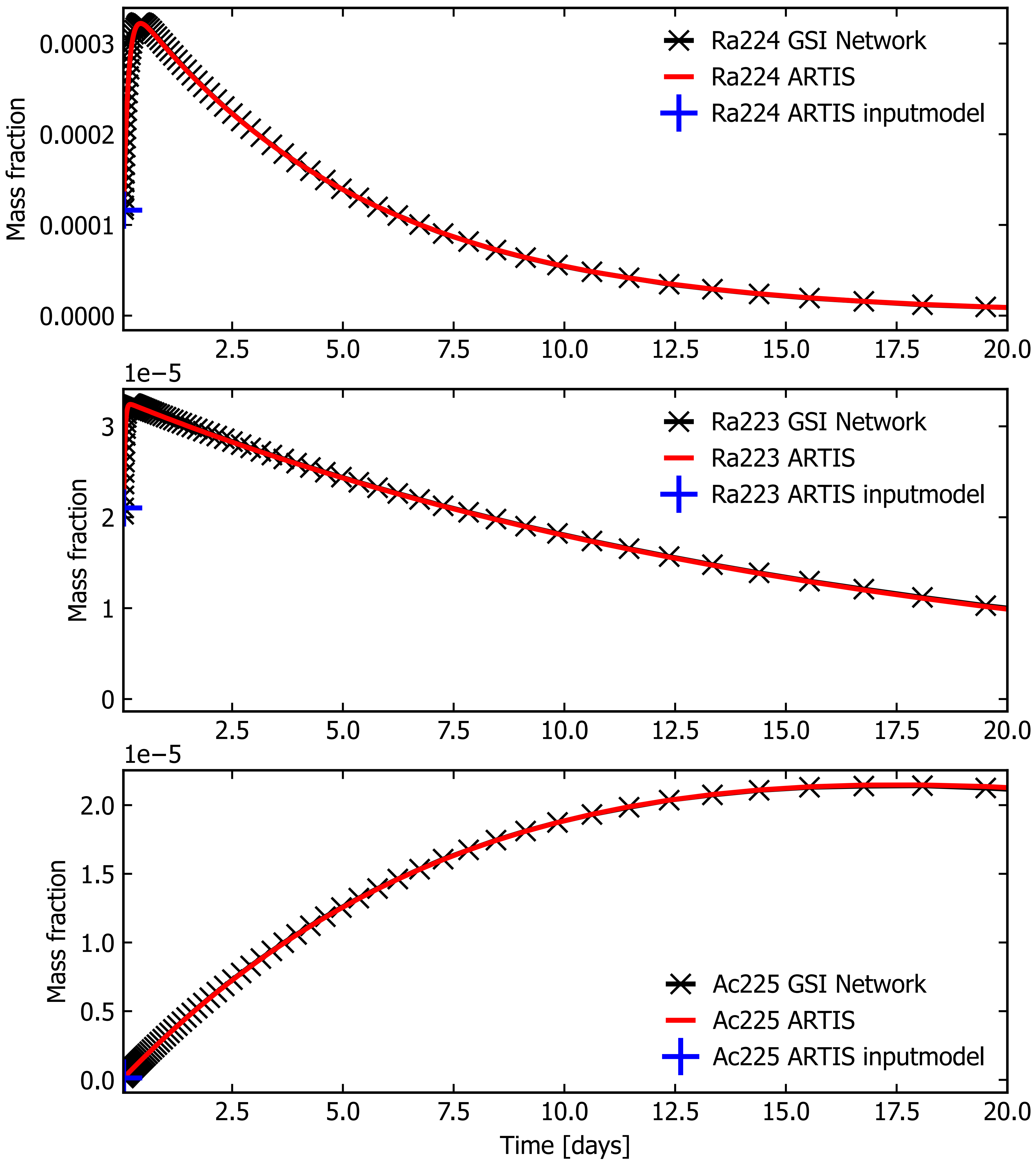


Good tracking of decay power

Fission not included, but contribution is small

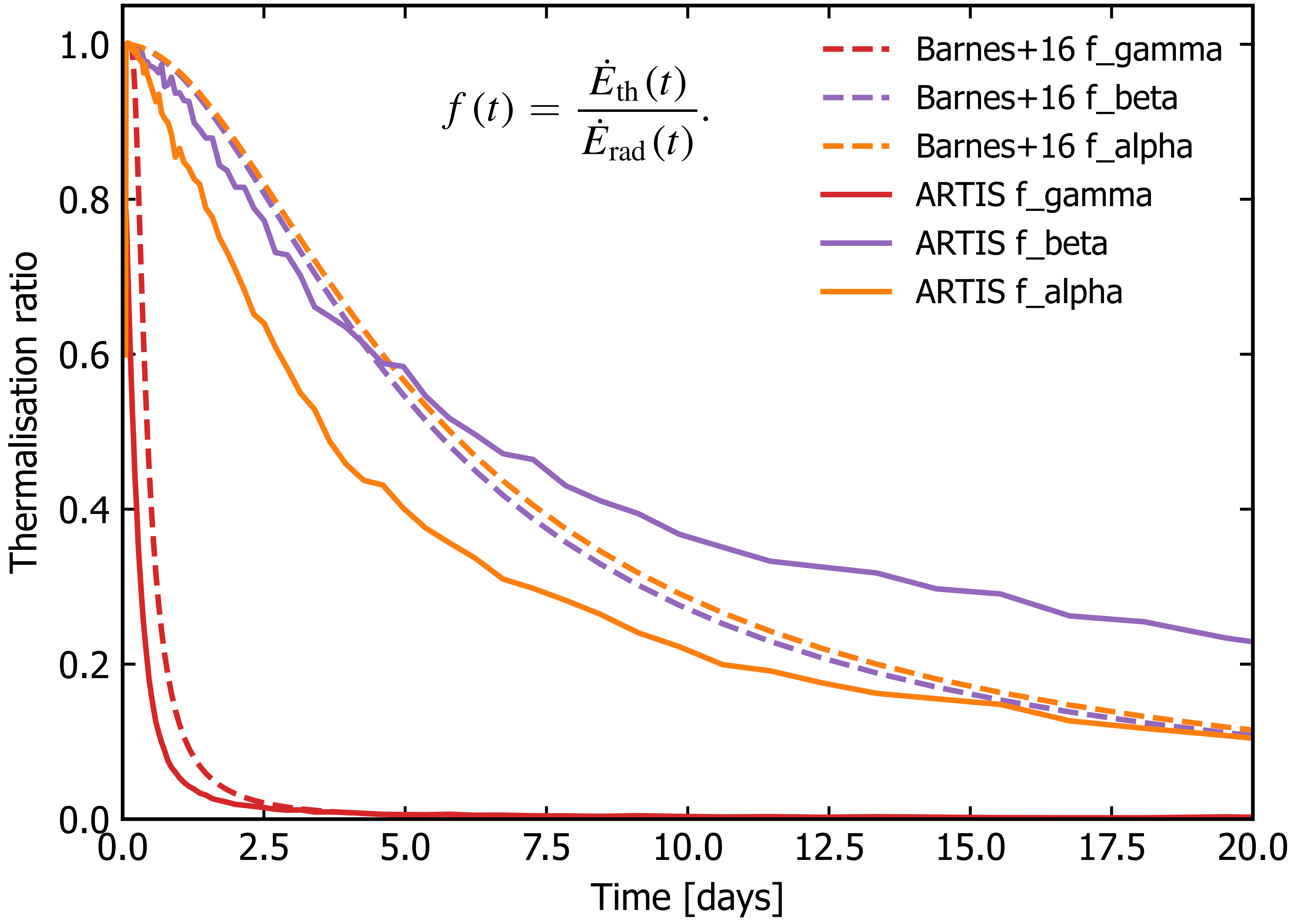
Abundance evolution ARTIS vs full network





Thermalisation results and Barnes+ (2016) approximation

- Deposition time from average particle energy per nuclear decay and approximate loss rate (4e10*ρ/(g cm^{-3}) [MeV/s] for beta, 5e11*ρ/(g cm^{-3}) for alpha) particle deposition occurs after emission, but in the same location.
- Deposition is local (no escape). Assumed to be trapped by magnetic fields.
- (preliminary) Right: compare this to the Barnes+16 analytical approximation (one-zone sphere and typical beta, alpha energy of 1, 5 MeV/decay)



$$t_{\rm ineff} \approx 7.4 \left(\frac{E_{\beta,0}}{0.5\ {\rm MeV}}\right)^{-1/2} M_5^{1/2}\ v_2^{-3/2}\ {\rm days}.$$

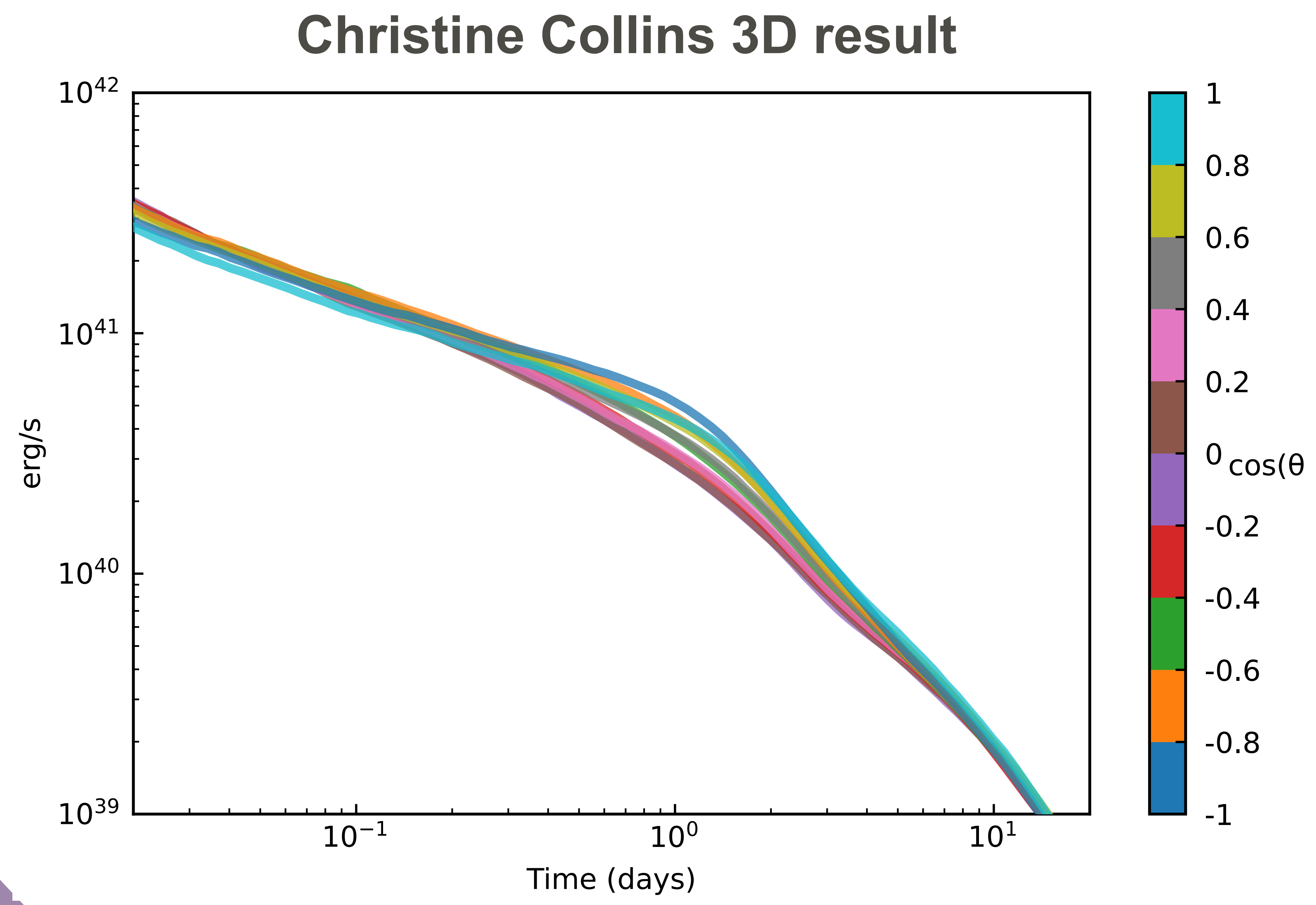
$$f_{\rm p}(t) = \frac{\dot{E}_{\rm th}}{\dot{E}_{\rm rad}} = \frac{\ln\left[1 + 2\left(\frac{t}{t_{\rm ineff,p}}\right)^2\right]}{2\left(\frac{t}{t_{\rm ineff,p}}\right)^2}.$$

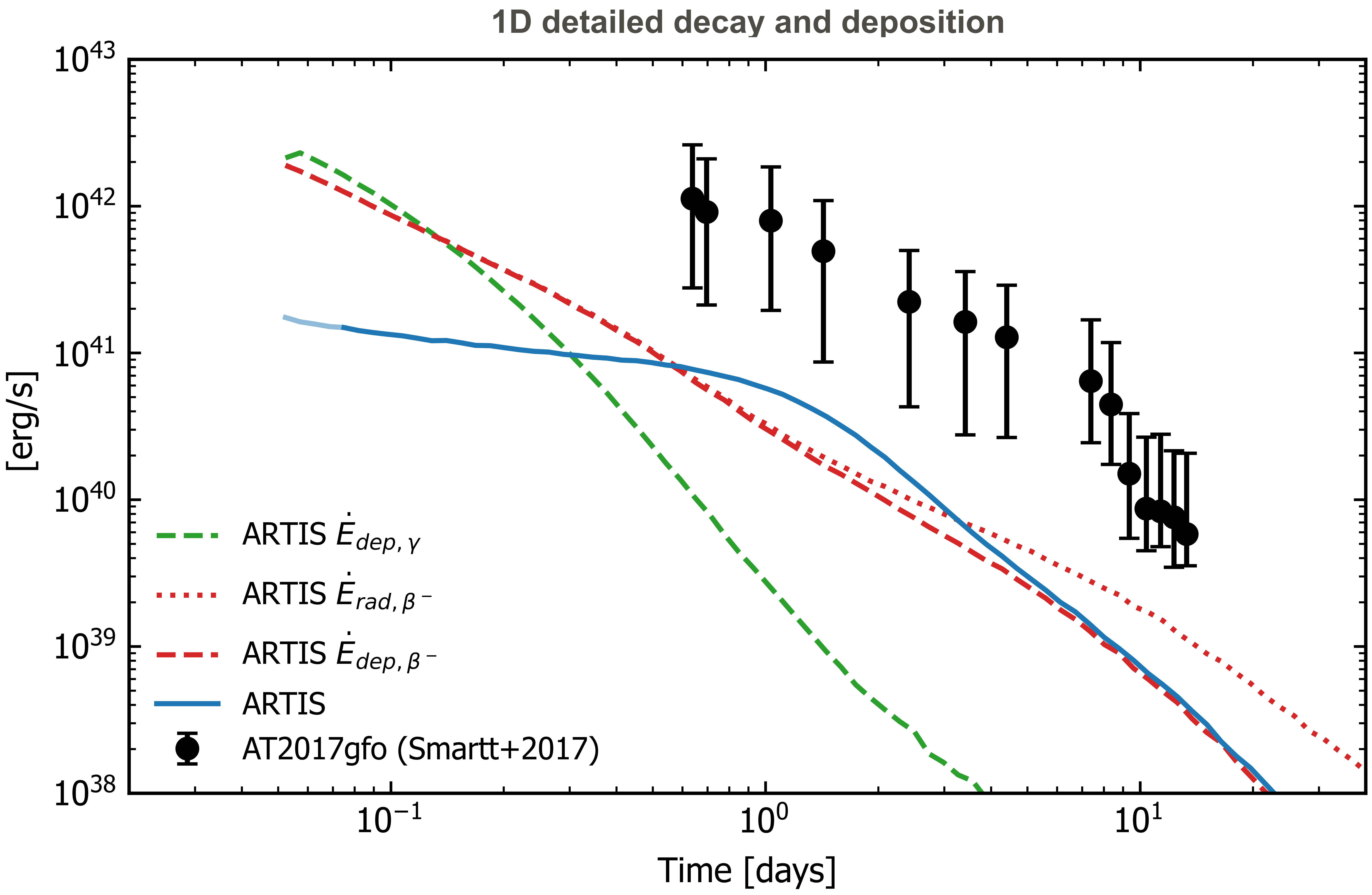
⇦ **Barnes+16 analytical result**

$$t_{\rm th} \approx \frac{E_{\beta,0}}{\dot{E}_{\beta,0}} = \frac{E_{\beta,0}}{4 \times 10^{10}\ \rho\ {\rm MeV\ s^{-1}}}$$

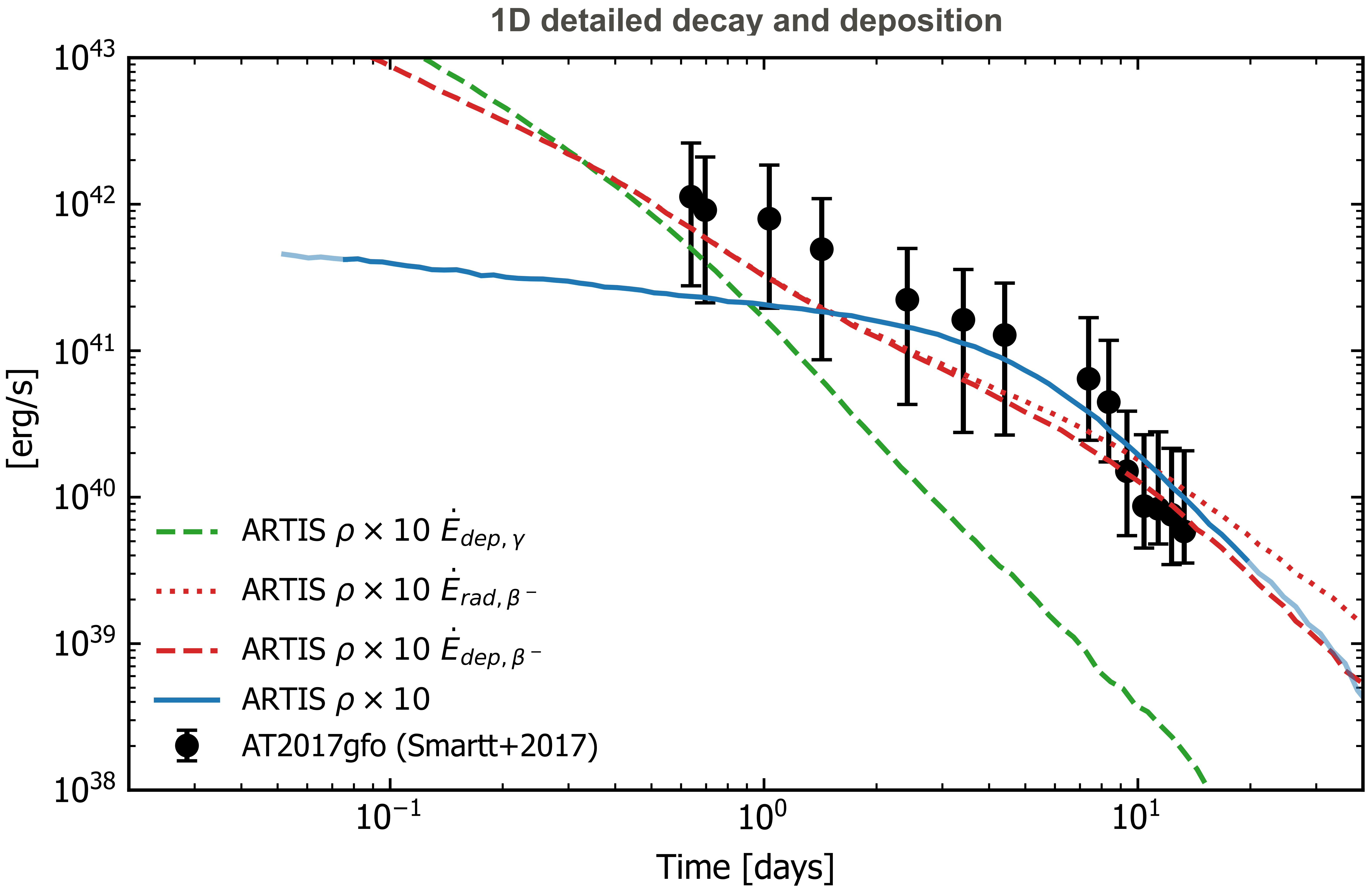
⇦ **used by ARTIS**

1D grey-opacity light curve





10x density test (0.04 Msun) vs AT2017gfo



Conclusions and future work

- We have modelled radioactive emission, thermalisation, and luminosity for simulated merger ejecta
- Change in slope is due to optical depth transition rather than thermalisation efficiency drop (agreement with Hotokezaka & Nakar 2020)
- Soon: use new atomic data set for lanthanides and actinides for detailed line-by-line opacities and synthetic spectra (see talks of Andreas Flörs and Gerrit Leck on atomic data)
- 2D/3D is possible, just expensive (see Christine's 3D results with simplified deposition)
  - Memory limit: 50^3 grid with ~70,000 non-empty cells means 1GB RAM holds 1900 FP64/cell
  - Number of levels treated in full NLTE will be need to be selected (but node shared memory)
  - Per level photoionisation rate estimators not practical (not node sharable without atomic access)
  - Christine showed some angle-dependence of luminosity with a grey opacity model
    - Spectra with an asymmetric ionisation/temperature structure might show more variation