PROCEEDINGS OF SCIENCE

Monte Carlo Radiative Transfer for Neutron Star Merger Simulations

Luke J. Shingles,[a,*] **Gabriel Martínez-Pinedo,**[a,b] **Vimal Vijayan,**[a,c] **Andreas Flörs,**[a] **Christine E. Collins**[a] **and Stuart A. Sim**[d]

[a] *GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany*
[b] *Institut für Kernphysik (Theoriezentrum), Fachbereich Physik, Technische Universität Darmstadt, Schlossgartenstraße 2, 64289 Darmstadt, Germany*
[c] *Department of Physics and Astronomy, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer feld 226, 69120 Heidelberg, Germany*
[d] *Astrophysics Research Centre, School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, Northern Ireland, UK*

E-mail: `luke.shingles@gmail.com`

The kilonova AT2017gfo that resulted from the merger of two neutron stars has provided new insights into the rapid neutron capture process that is responsible for producing many of the nuclei that are heavier than iron. As with supernovae, progress in understanding kilonova spectra can be achieved either by using simplified models to connect spectral features with particular elements, or by attempting to construct detailed simulations that capture all of the relevant physics. In the forward modelling approach, we require a theoretical simulations of the merger and ejection physics, r-process nucleosynthesis, radioactive energy deposition, and radiative transfer. We plan to calculate synthetic spectra for a three-dimensional merger and r-process nucleosynthesis simulation using the ARTIS Monte Carlo radiative transfer code. Here, we describe current progress in developing the code to handle energy deposition from β- and α-decay reactions and thermalisation of decay particles.

FAIR next generation scientists - 7th Edition Workshop
23-27 May 2022
Paralia, Greece

PoS(FAIRness2022)054

---

[*] Speaker

1. Introduction

The gravitational wave signal GW170817 from a merger of two neutron stars has been complemented by a rich dataset of electromagnetic signals from the associated kilonova, AT2017gfo[1,2]. Simple analysis of the luminosity decline rate of AT2017gfo indicates decaying material that has undergone rapid neutron captures, a regime responsible for producing many of the elements beyond Fe.

The time-series spectra of the kilonova in the first few days after the merger in principle provide a high level of detail about the ejecta composition and physical conditions, if we have the tools to interpret them. Detailed interpretation of these spectra requires knowledge of a large amount of relevant atomic and nuclear data, and numerical modelling tools to make the connections between the initial conditions, subsequent evolution, and the emitted spectra for comparison to observations.

2. NSM model and radiative transfer method

To produce synthetic light curves (in future, spectra), we compute radiative transfer for a neutron star merger (NSM) simulation of two 1.35 $M_\odot$ neutron stars. The NSM has been calculated with a 3D general relativistic smoothed-particle hydrodynamics code that includes an advanced neutrino treatment, ILEAS[3] and the nuclear abundances are calculated as a post-processing step with an advanced r-process network. Three-dimensional radiative transfer calculations for the same NSM simulation have been published[4]. Here, we also use the Planck-mean opacities as a function of electron fraction by Tanaka et al.[5], but we enforce spherical symmetry on the model to simplify the computational requirements while developing more advanced decay and thermalisation physics.

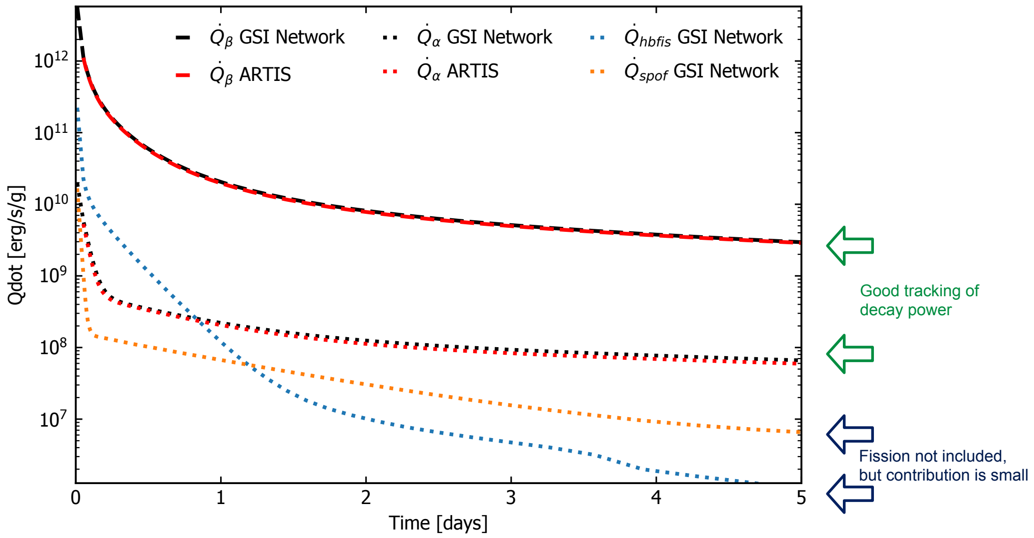
We use the Monte Carlo radiative transfer code ARTIS[6–8], with extended capabilities to handle kilonova ejecta. ARTIS handles energy deposition by tracking radioactive decay reactions that follow from an initial snapshot of the composition and density throughout the model (in this work, 0.05 days after merger). The snapshot abundances are taken from a calculation with a detailed nuclear network, as the complex nuclear reactions other than simple decays mostly take place within the first few minutes after the merger. The density profile is taken from the hydrodynamic model, after which which ejecta are assumed to evolve simply by homologous (ballistic) expansion. This avoids the need for expensive calculations of hydrodynamics to be performed simultaneously with the radiative transfer.

In contrast with thermonuclear supernovae, which require electron-capture and β^+ decays from just a few nuclei, treating the decays of the NSM material from 0.05 days requires thousands of α and β^- reactions. Models presented here use 2591 nuclides with α and β^- reaction data (gamma-decay spectra and mean emitted particle kinetic energy) from ENDV/B-VII.1[9*]. This set of decays (and the solution of the Bateman equation) series is able to maintain close tracking of the energy release rates from the full network calculation (see Figure 1).

We use α and β-particle loss rate approximations that are a constant factor of the density by Barnes et al.[10]. The initial kinetic energy of each emitted α and β-particle is set by the average particle energy for the particular decay reaction that emitted the particle. It is assumed that magnetic fields keep the particles from crossing significant fraction of the ejecta before losing their energy.

---

[*] conveniently redistributed via https://github.com/hotokezaka/HeatingRate



Good tracking of decay power

Fission not included, but contribution is small

Figure 1: Comparison of energy release rates of the ARTIS treatment versus the output of the full nuclear network calculation. The tracking error remains small, and although fission reactions are not included, this has a negligible effect on the total energy release rates during the simulation.

In our treatment, the β and α particles thermalise over time and deposit their energy locally at the same location as they were emitted.

3. Results

The time evolution of thermalisation ratios in Figure 2 show reasonable agreement between our model and the analytical approximation of Barnes et al[10]. One difference compared to the analytical prediction is that we find a larger variation between the α and β-particle thermalisation ratios, with β-particles being more efficiently thermalised in our model.

The bolometric light curve of the model is shown in Figure 3. The luminosity initially declines gradually in the optically-thick phase, followed by a change in slope near the transition to the free-streaming regime (virtually no gamma deposition or photon trapping). Beyond this transition point, the luminosity converges to the β-particle deposition rate.

The bolometric luminosity of our model is much lower than AT2017gfo, mainly because our total mass (with only dynamical ejecta) of 0.005 $M_\odot$ is about ten times lower than the estimated mass of AT2017gfo[1]. It is interesting to observe the changes when simply multiplying the densities by a factor of ten to obtain a total mass similar to that inferred for AT2017gfo. Figure 4 shows such a model, and the transition to free-streaming now takes place at a later time is quite similar to the change in slope of the AT2017gfo light curve.

4. Future work

The models presented here use a simple wavelength-independent (‘grey’) opacity as a function of the electron fraction. We will soon present models that use a Sobolev treatment for tens of

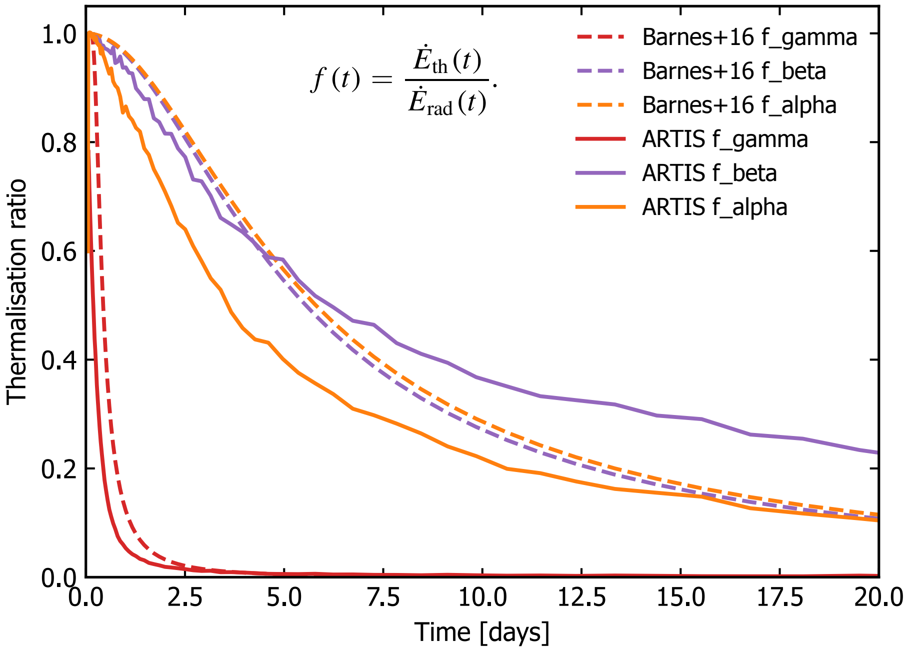


Figure 2: Thermalisation ratios over time for gamma-rays, β^-, and α particles in ARTIS versus the analytical approximation of Barnes[10].

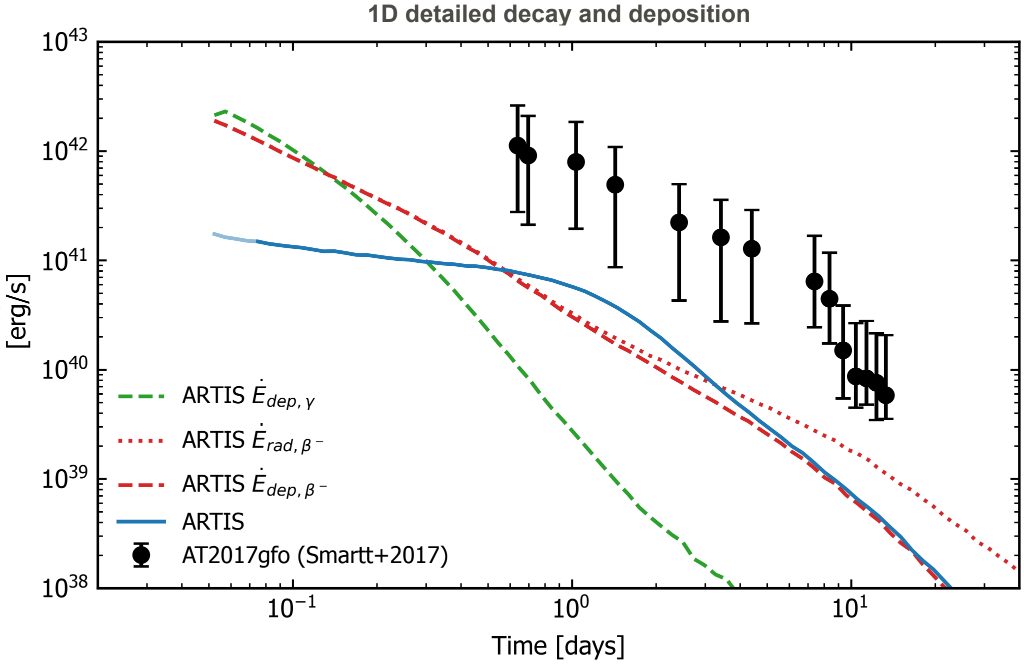


Figure 3: Bolometric (combined ultraviolet, optical, and infrared) luminosity, deposition rate from gamma rays, emission and deposition rates for β^- particle kinetic energy, and the inferred bolometric light curve for AT2107gfo[1]. The lighter blue parts of the ARTIS light curve may be underestimated due to light travel time effects and the simulation start and end time cutoffs.

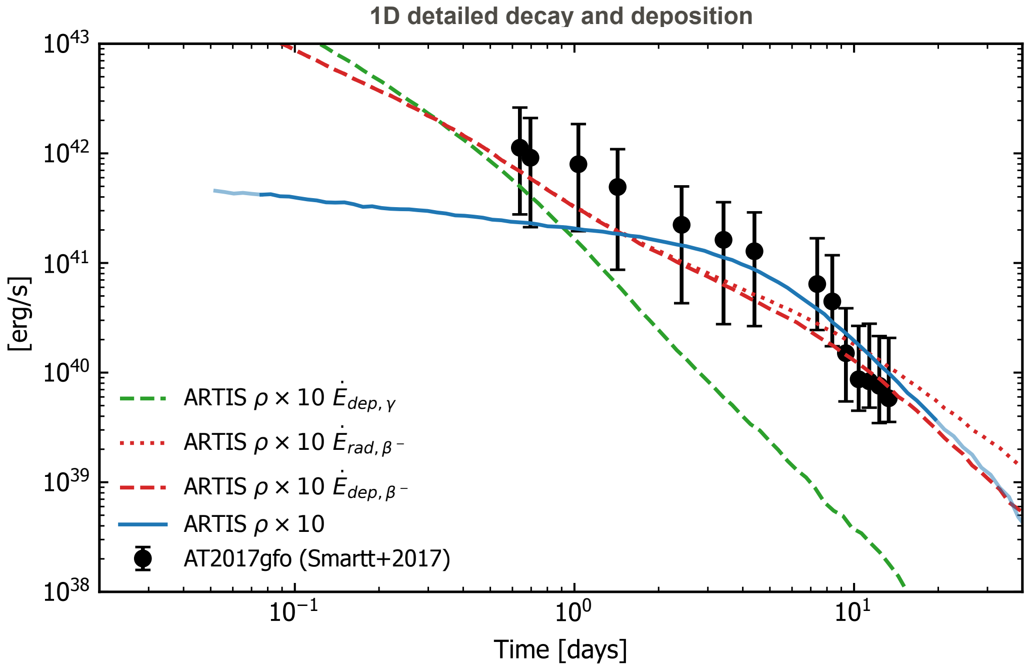


Figure 4: Similar to Figure 3 except for an ARTIS model in which the densities have been multiplied by ten. The total ejecta mass is 0.05 $M_\odot$.

millions of individual transition lines (with data from the Japan-Lithuania database[5] and new calculations from our collaborators). ARTIS can also compute the radiative transfer in three-dimensions, although this greatly increases the computing time and memory requirements. Through new performance optimisations and a large investment of computing resources, we have recently calculated angle-dependent spectra for a 3D LTE (local thermodynamic equilibrium) model of the dynamical NSM ejecta at around one day after the merger, which we intend to publish soon. It may eventually also be possible to extend these models to include non-LTE effects that become important at later times, although this might require us to work in only one or two dimensions, or limit the full non-LTE treatment to particular elements.

Acknowledgements

LJS, G.M.-P, and AF acknowledge support by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (ERC Advanced Grant KILONOVA No. 885281). CEC acknowledges support by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program under grant agreement No. 759253. G.M.-P acknowledges support by Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project-ID 279384907 - SFB 1245. VV acknowledges support by DFG - Project-ID 138713538 - SFB 881 ("The Milky Way System", subproject A10). G.M.-P acknowledges support by the State of Hesse within the Cluster Project ELEMENTS. The work of SAS was supported by the Science and Technology Facilities Council [grant numbers ST/P000312/1, ST/T000198/1]. LJS, CEC, and VV are grateful for computational support by the VIRGO cluster at GSI. Data analytics and plotting were done using NumPy, [11], Matplotlib [12], and ARTISTOOLS[†].

[†] https://github.com/artis-mcrt/artistools/

References

1. Smartt, S. J. *et al.* A kilonova as the electromagnetic counterpart to a gravitational-wave source. *Nature* **551**, 75–79 (2017).
2. Abbott, B. P. *et al.* Multi-messenger Observations of a Binary Neutron Star Merger. *ApJ* **848**, L12 (2017).
3. Ardevol-Pulpillo, R., Janka, H. T., Just, O. & Bauswein, A. Improved leakage-equilibration-absorption scheme (ILEAS) for neutrino physics in compact object mergers. *MNRAS* **485**, 4754–4789 (2019).
4. Collins, C. E. *et al.* 3D radiative transfer kilonova modelling for binary neutron star merger simulations. *arXiv e-prints* arXiv:2209.05246 (2022).
5. Tanaka, M., Kato, D., Gaigalas, G. & Kawaguchi, K. Systematic opacity calculations for kilonovae. *MNRAS* **496**, 1369–1392 (2020).
6. Sim, S. A. Multidimensional simulations of radiative transfer in Type Ia supernovae. *MNRAS* **375**, 154–162 (2007).
7. Kromer, M. & Sim, S. A. Time-dependent three-dimensional spectrum synthesis for Type Ia supernovae. *MNRAS* **398**, 1809–1826 (2009).
8. Shingles, L. J. *et al.* Monte Carlo radiative transfer for the nebular phase of Type Ia supernovae. *MNRAS* **492**, 2029–2043 (2020).
9. Chadwick, M. B. *et al.* ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data. *Nuclear Data Sheets* **112**, 2887–2996 (2011).
10. Barnes, J., Kasen, D., Wu, M.-R. & Martinez-Pinedo, G. Radioactivity and Thermalization in the Ejecta of Compact Object Mergers and Their Impact on Kilonova Light Curves. *The Astrophysical Journal* **829**, 110 (2016).
11. Oliphant, T. E. Python for Scientific Computing. *Computing in Science & Engineering* **9**, 10–20 (2007).
12. Hunter, J. D. Matplotlib: A 2D Graphics Environment. *Comput. Sci. Eng.* **9**, 90–95 (2007).