A Nuclear Network Geared Towards Coupling with Hydrodynamics Simulations

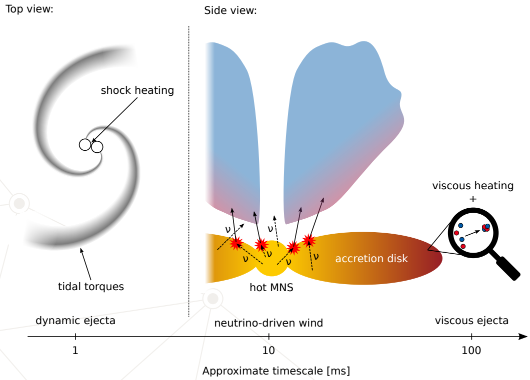
Federico Maria Guercilena (University of Trento)

with Albino Perego, Luca Maggioni, Li Shifang

Nuclear Physics in Astrophysics XI, Dresden - 18/09/2024

R-PROCESS IN BNS MERGERS

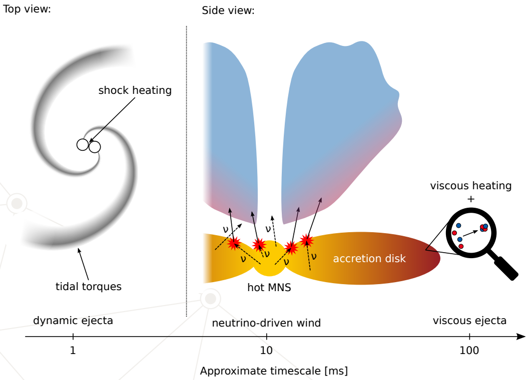
Matter is ejected via a variety of channels:



Ejecta of BNS mergers are hot, fast expanding and very neutron rich.

r-process in BNS Mergers

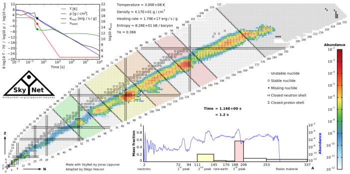
Matter is ejected via a variety of channels:



Ejecta of BNS mergers are hot, fast expanding and very neutron rich.

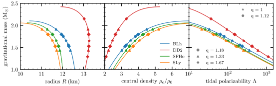
↓

Onset of (strong) r-process nucleosynthesis



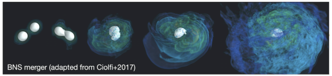
Numerical simulations and observables

EOS of dense matter

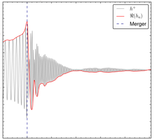


+

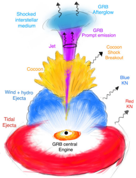
Hydrodynamical simulations



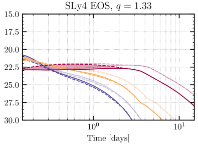
Gravitational waves



sGRB

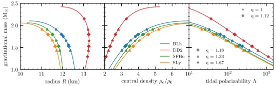


Kilonovae



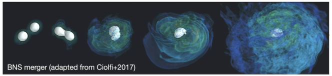
Numerical simulations and observables

EOS of dense matter

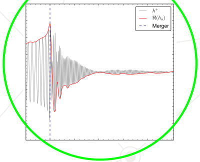


+

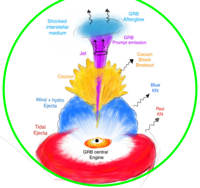
Hydrodynamical simulations



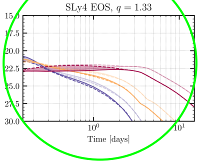
Gravitational waves



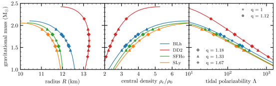
sGRB



Kilonovae

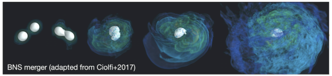


EOS of dense matter

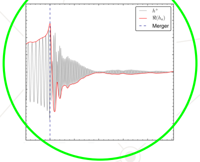


+

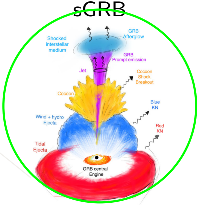
Hydrodynamical simulations



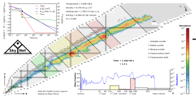
Gravitational waves



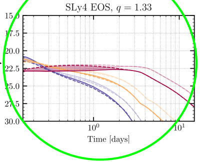
sGRB



r-process nucleosynthesis



Kilonovae



Nuclear networks: post-processing vs. in situ

A nuclear reaction network:

$$\frac{dY_i}{dt} = \sum_j \lambda_j Y_j + \sum_{jk} \lambda_{jk} Y_j Y_k + \cdots$$

Usual coupling to hydro simulations:

$\downarrow$

Extract initial Y_e, s, T along with history of ρ + homologous expansion. Assume NSE at start.

$\downarrow$

Post-process with nuclear network.

Nuclear networks: post-processing vs. in situ

A nuclear reaction network:

$$\frac{dY_i}{dt} = \sum_j \lambda_j Y_j + \sum_{jk} \lambda_{jk} Y_j Y_k + \cdots$$

Usual coupling to hydro simulations:

$\downarrow$

Extract initial Y_e, s, T along with history of ρ + homologous expansion. Assume NSE at start.

$\downarrow$

Post-process with nuclear network.

This method overly simplifies the density evolution and neglects the influence of the nuclear heating on the dynamics.

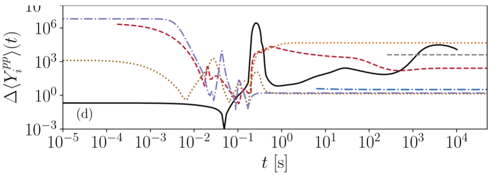


Image from *[Magistrelli et al., 2024]*

Proper coupling *in situ* to a long-lived simulation reveals significant discrepancies with the post processing approach.

Reduced networks

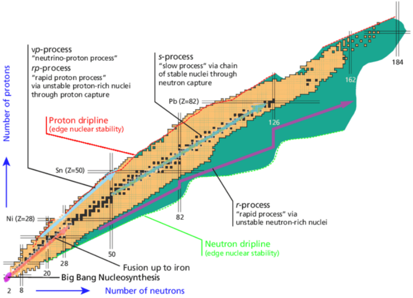


Image adapted from Martinez-Pinedo

The (strong) r-process runs through all nuclei between the valley of stability and the neutron drip line, for a total of $\sim 7000/8000$ DoF.

A typical hydrodynamics simulation has (several) 10^7 DoF. Coupling to a nuclear network would result in 10^{11} DoF.

Infeasible!

Either simplify the hydro simulation (cf. previous slide) or *simplify the nuclear network*, reducing the number of DoF necessary.

$\downarrow$

Reduced networks

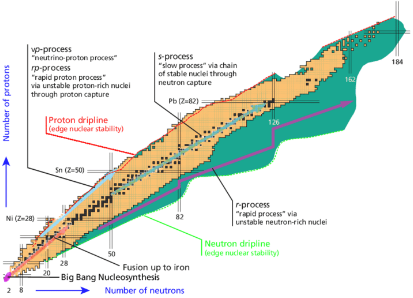


Image adapted from Martinez-Pinedo

The (strong) r-process runs through all nuclei between the valley of stability and the neutron drip line, for a total of $\sim 7000/8000$ DoF.

A typical hydrodynamics simulation has (several) 10^7 DoF. Coupling to a nuclear network would result in 10^{11} DoF.

Infeasible!

Either simplify the hydro simulation (cf. previous slide) or *simplify the nuclear network*, reducing the number of DoF necessary.

$\downarrow$

The **BARONET** code
(BetA flow ReactiOn NETwork)

$$(\mathrm{A},\mathrm{Z}) + \mathrm{n} \longleftrightarrow (\mathrm{A}+1,\mathrm{Z}) + \gamma$$

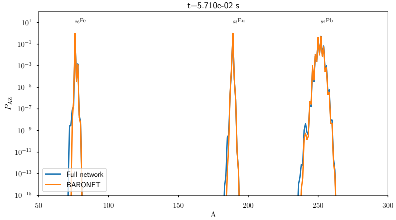
Valid until n_n is high enough, i.e. up to *neutron freeze out* (NFO).

Rewrite the abundances as $Y_{A,Z} = Y_Z P_{A,Z}$
where $Y_Z = \sum_A Y_{A,Z}$ and $P_{A,Z} = Y_{A,Z}/Y_Z$.

(n,γ)$\leftrightarrow$(γ, n) equilibrium implies that

$$\frac{P_{A+1,Z}}{P_{A,Z}} = \frac{1}{2} n_n \frac{G(T)_{A+1,Z}}{G(T)_{A,Z}} \left(\frac{2\pi\hbar^2}{m_b k_B T}\frac{A+1}{A}\right)^{3/2} \exp\left(\frac{S_{n,A+1,Z}}{k_B T}\right)$$

the $P_{A,Z}$ are known analytically, only the Y_Z must be evolved.



BETA FLOW

Y_Z evolve by reactions that change Z, but not A

$\downarrow$

β^- **decays**

$$\frac{dY_Z}{dt} = -Y_Z \sum_A P_{A,Z} \sum_{i=0}^{3} \lambda^i_{A,Z} + Y_{Z-1} \sum_{i=0}^{3} \sum_A P_{A+i,Z-1} \lambda^i_{A+i,Z}$$

Need to sum over the $P_{A,Z}$, which can be computed analytically.

Evolution of the neutron fraction:

$$\frac{dY_n}{dt} = -Y_n \lambda^0_n + Y_Z \sum_{i=1}^{3} \sum_A i P_{A,Z} \lambda^i_{A,Z} - \frac{1}{\tau}(\chi_{tot} - 1) Y_n$$

where $\chi_{tot} = \sum_{A,Z} A Y_Z P_{A,Z} \equiv 1$ and $\tau \simeq 1^{-6}$ seconds.

Y_Z evolve by reactions that change Z, but not A

$\downarrow$

β^- **decays**

$$\frac{dY_Z}{dt} = -Y_Z \sum_A P_{A,Z} \sum_{i=0}^{3} \lambda^i_{A,Z} + Y_{Z-1} \sum_{i=0}^{3} \sum_A P_{A+i,Z-1} \lambda^i_{A+i,Z}$$

Need to sum over the $P_{A,Z}$, which can be computed analytically.

Evolution of the neutron fraction:

$$\frac{dY_n}{dt} = -Y_n \lambda^0_n + Y_Z \sum_{i=1}^{3} \sum_A i P_{A,Z} \lambda^i_{A,Z} - \frac{1}{\tau}(\chi_{tot} - 1) Y_n$$

where $\chi_{tot} = \sum_{A,Z} A Y_Z P_{A,Z} = 1$ and $\tau \simeq 1^{-6}$ seconds.

The damping term is an effective way to recover missing reactions and ensure mass conservation.

Post-NFO phase

(n,γ)$\leftrightarrow$(γ, n) equilibrium valid until NFO, e.g. $Y_\mathrm{n}/Y_\mathrm{seed} \sim 1$ ($Y_\mathrm{seed} = \sum_{i\neq \mathrm{n}} Y_i$). What to do beyond this point?

Keeping only β^- decays, one can write:

$$\frac{\mathrm{d}Y_{\mathrm{A,Z}}}{\mathrm{d}t} = \mathbf{M}Y_{\mathrm{A,Z}}$$

with explicit solution

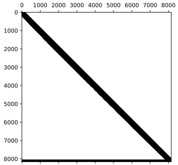
$$Y_{\mathrm{A,Z}}(t) = \exp(t\mathbf{M})Y_{\mathrm{A,Z}}|_{\mathrm{initial}}$$

since $\mathbf{M}$ is time-independent.

"Initial data" for this formula is easily expressed as

$$Y_{\mathrm{A,Z}}|_{\mathrm{initial}} = Y_{\mathrm{Z}}|_{\mathrm{NFO}} P_{\mathrm{A,Z}}|_{\mathrm{NFO}}$$

but the $P_{\mathrm{A,Z}}|_{\mathrm{NFO}}$ are easily computed on the fly by storing T_{NFO} and n_{n} **only**.



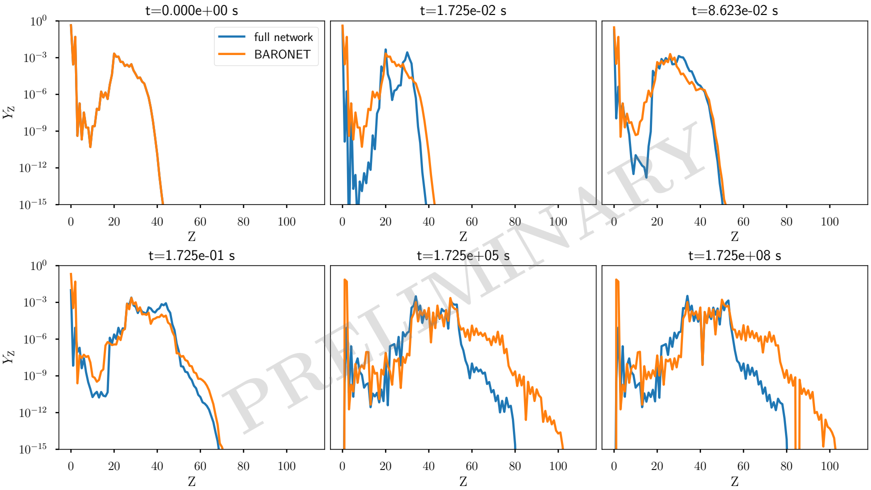
Sparsity pattern of $\mathbf{M}$

$\exp(t\mathbf{M})$ is not trivial to compute.

It is currently implemented as

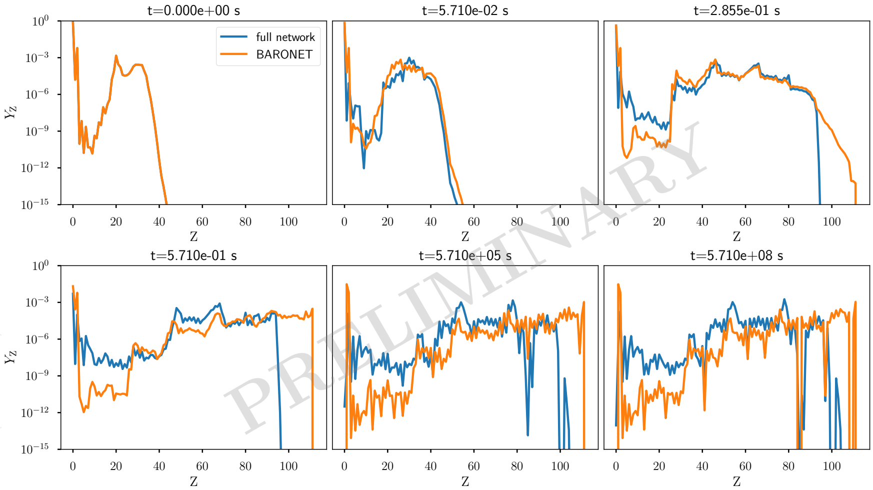
$$\mathbf{M} = \mathbf{V}\Lambda\mathbf{V}^{-1} \rightarrow \exp(t\mathbf{M}) = \mathbf{V}\exp(t\Lambda)\mathbf{V}^{-1}$$

Results: elemental abundances for "weak" r-process



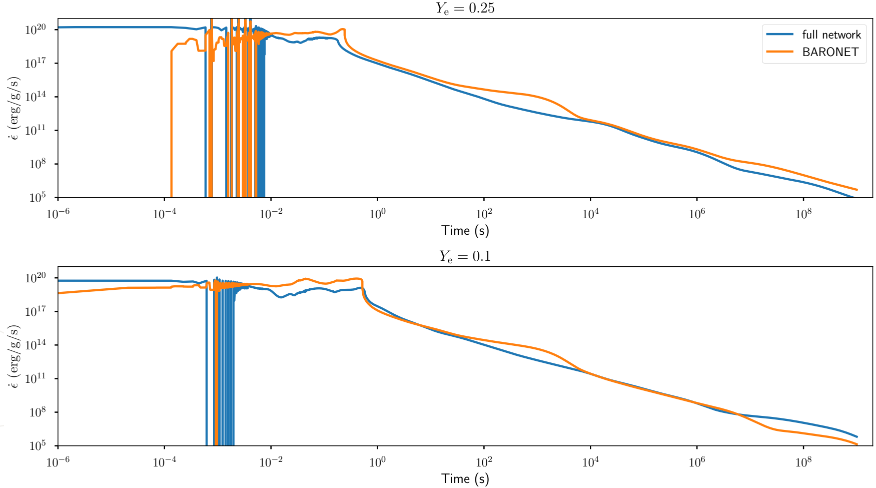
$Y_e = 0.25$. Comparison data generated with SkyNet *[Lippuner and Roberts, 2017]*

Results: elemental abundances for "strong" r-process



$Y_e = 0.1$. Comparison data generated with SkyNet *[Lippuner and Roberts, 2017]*

Results: nuclear heating rate



Heating rate as a function of time. Comparison data generated with SkyNet *[Lippuner and Roberts, 2017]*

Conclusions

- BARONET relies on dominant reactions to reduce the number of DoF to a few hundred pre-NFO
- post-NFO evolution coupled to hydro needs further simplification (impose functional form of $P_{A,Z}$)

Ongoing work:

- include neutron captures for Y_n
- include fission for heavy elements
- develop a "reduced" NSE solver
- better characterization of neutron freeze out
- extensive testing
- coupling to hydro simulations

Conclusions

- BARONET relies on dominant reactions to reduce the number of DoF to a few hundred pre-NFO
- post-NFO evolution coupled to hydro needs further simplification (impose functional form of $P_{A,Z}$)

Ongoing work:

- include neutron captures for Y_n
- include fission for heavy elements
- develop a "reduced" NSE solver
- better characterization of neutron freeze out
- extensive testing
- coupling to hydro simulations

Stay tuned... Thank you

References

References I

[Lippuner and Roberts, 2017] Lippuner, J. and Roberts, L. F. (2017).
SkyNet: A modular nuclear reaction network library.
Astrophys. J. Suppl., 233(2):18.

[Magistrelli et al., 2024] Magistrelli, F., Bernuzzi, S., Perego, A., and Radice, D. (2024).
Elements formation in radiation-hydrodynamics simulations of kilonovae.
ArXiv.