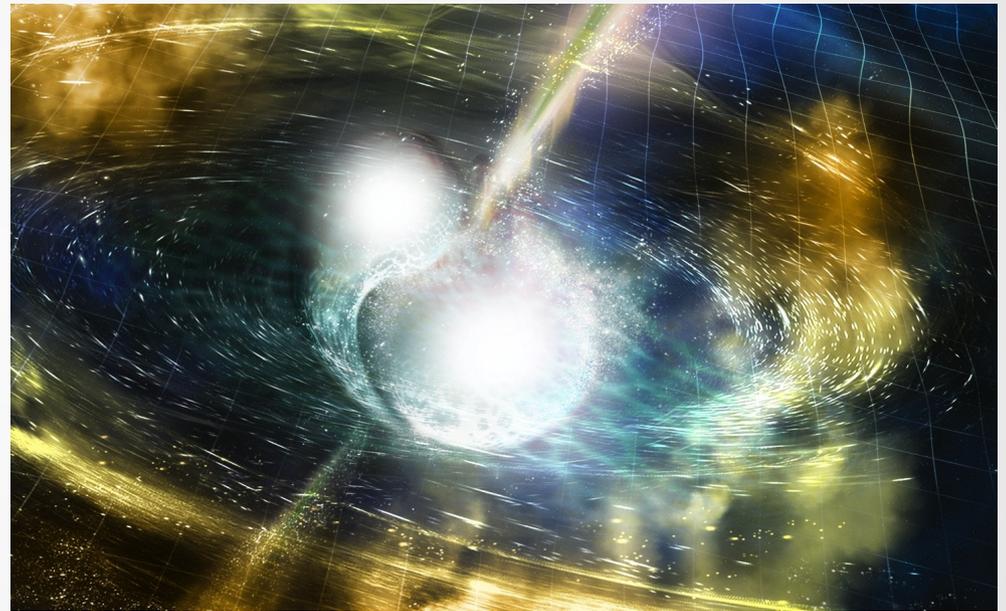


# Stellar Modeling for R-Process Nucleosynthesis

-Amber Lauer: Triangle Universities Nuclear Laboratory, Duke University, Durham, NC 27708

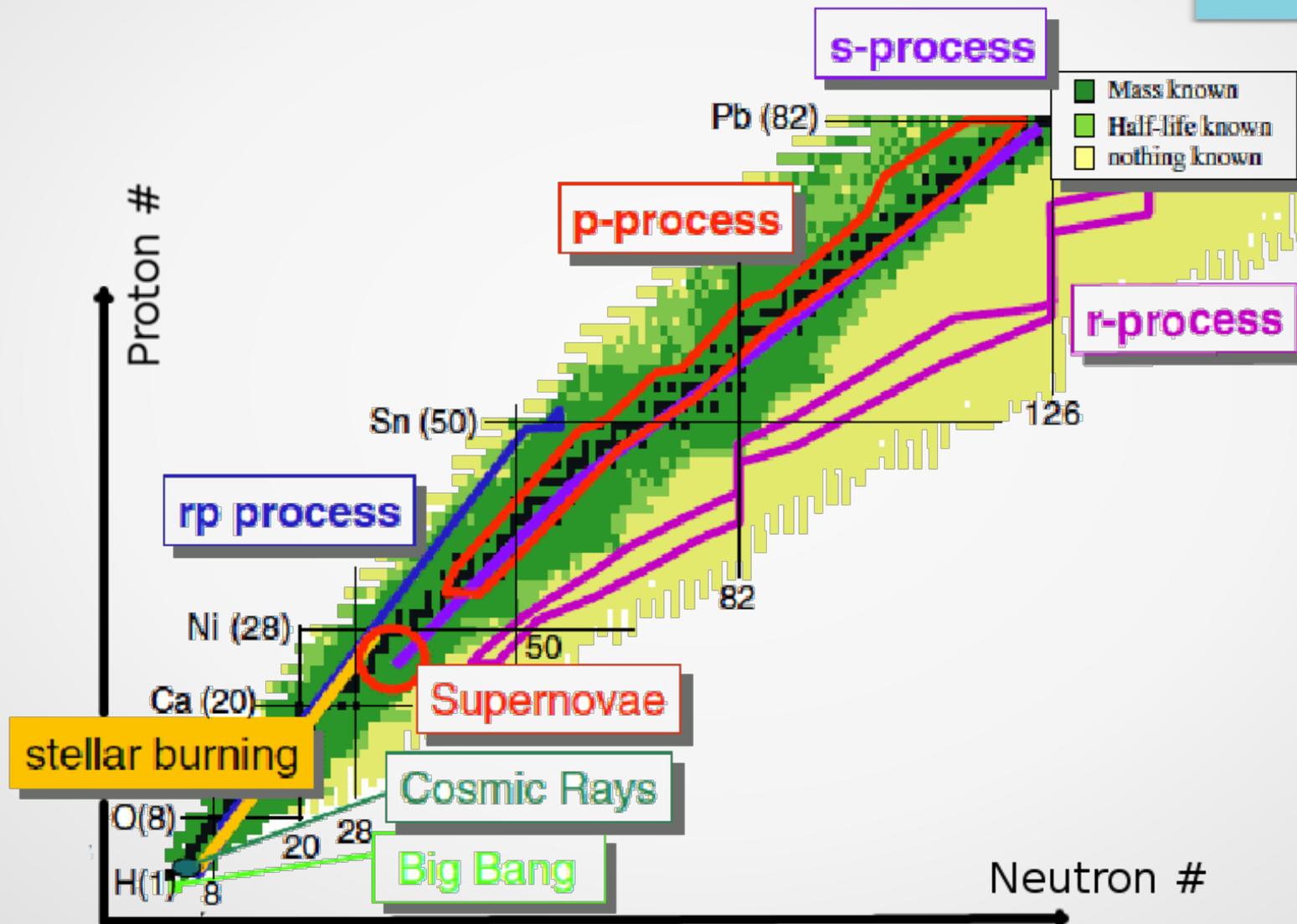
*Abstract:* One of the primary mechanisms for guiding experimental research in nuclear astrophysics is the sensitivity study. In a broad sense, these studies involve a stellar model in which quantities related to nuclear reactions are varied to examine the effects. These variables can include a single, or multiple, reaction rates, Q-values, nuclear masses, and others. Subsequently, various aspects of the model are examined, such as elemental abundances, thermodynamics, and astronomical observables, and compared with theory and observations. This talk will examine the underlying stellar models, their strengths and limitations both broadly and as it applies to R-process, and discuss the findings of the most recent works, as well as improvements that must be made in the future in order to improve the accuracy of the results of the sensitivity study.



# Stellar Modeling for R-Process Nucleosynthesis: 2010- present

- 1) Why do we need stellar models?
- 2) Networks for Nuclear-astrophysics (nucaastro):
- 3) Stellar Models: Theory and limitations
- 4) Stellar Models for R-process nucleosynthesis

# Stellar Modeling for R-Process Nucleosynthesis Sites



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Create and experiment with environments and time scales we will never visit or recreate otherwise\*

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Test theories for physics and the relationships between quantities

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How do test stellar models?

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# Stellar Modeling for R-Process Nucleosynthesis Sites

Why do we need stellar modeling?

Create and experiment with environments and time scales we will never visit or recreate otherwise\*

Test theories for physics and the relationships between quantities

How do test stellar models?

Comparison with theory

Comparison with observables

\*probably

# Networks for Nuclear Astrophysics

•Realistic nucleosynthesis 3 levels of complexity:

1) Nuclear Network Only

2) Network & Stellar Model- post-processed

3) Network & Stellar Model (3D)- co-processed

# Networks for Nuclear Astrophysics

- Nuclear network only

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- Nuclear network only
  - Solve: diff eq's, NSE
  - Use: Linear algebra, matrix & stiff ODE solvers
  - Input
    - Initial  $X_i$ 's
    - Rxn rates
    - $T$  &  $\rho$  (constant or  $T(t)/\rho(t)$ ) , from sim. or obs.\*\*\*

# Networks for Nuclear Astrophysics

- Nuclear network only
- Network & stellar model- post-processed net
  - 1<sup>st</sup> model: 3D Hydro or 1D SE w/Hydro
  - Small (or no), de-coupled Net (5-20  $NZ$ )
  - More physical (coupled hydro, mixing, EOS,  $\kappa$ )
  - 2<sup>nd</sup> model: Full/Large net
  - 1 or multi-zone/multi-particle
  - Input
    - $T$  &  $\rho$  from 1<sup>st</sup>, sometimes mixing

# Networks for Nuclear Astrophysics

- Nuclear network only
- Network & stellar model- post-processed net
- Network & stellar model (3D)- co-processed net
  - All physics fully coupled in single time step (hydro, SE, & Net)
  - Large (but not necessarily complete) net: 20-500 species

# Networks for Nuclear Astrophysics

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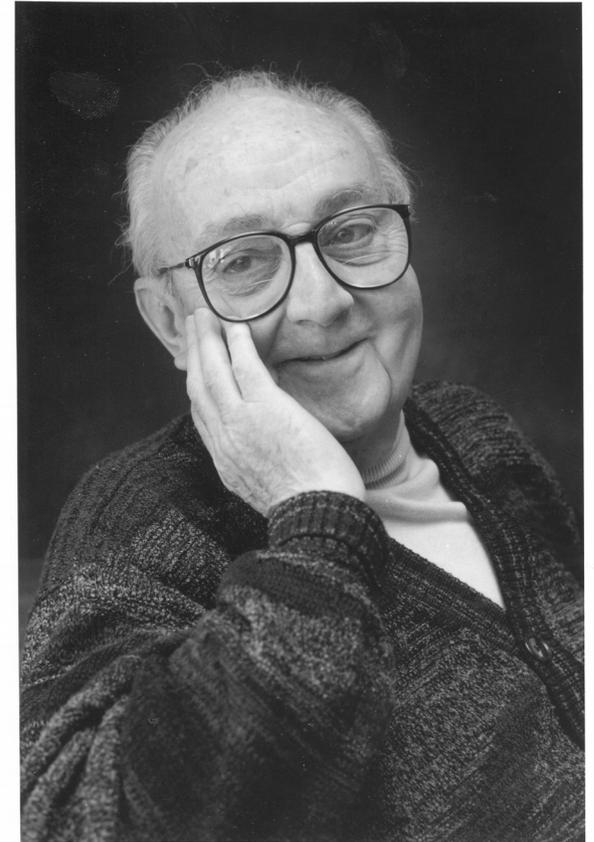
3) Network & stellar model (3D)- co-processed

# Stellar Models: Theory and limitations

“All models are wrong, some are useful”

-G. E. P. Box

- Full 3D coupled physics not yet possible
- Why?
  - C. A. Meakin<sup>1</sup>
    - Need:  $\Theta(10^{22})$  computational cells
    - Moore's law:  $\log_2(\text{flops}/\$) = \text{time} / (18 \text{ months})$
    - Horizon Run 2/3 on Tachyon ii<sup>2</sup>
      - 2011
      - $3.74 \times 10^{11}$  particles



<https://commons.wikimedia.org/w/index.php?curid=14941622>

1. <https://arxiv.org/pdf/0806.4542.pdf> - (2008)

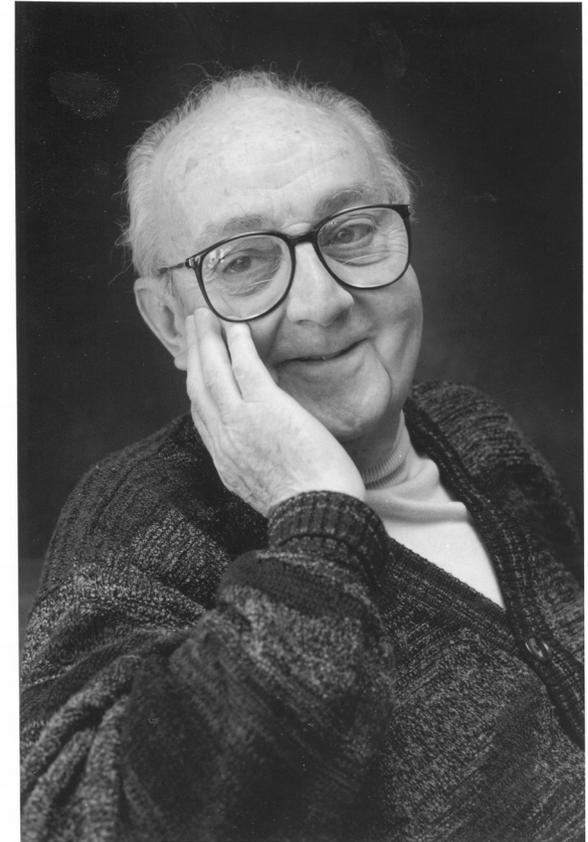
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      - $3.74 \times 10^{11}$  particles
  - $\implies$  ~50 years



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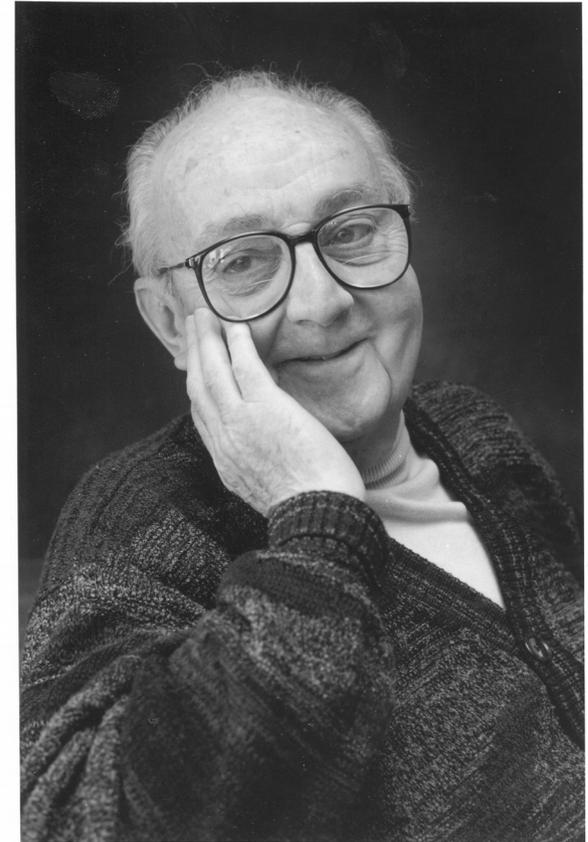
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  - ==> ~50 years



Stellar models characterized by how they make use of resources: Resolution or evolution?

<https://commons.wikimedia.org/w/index.php?curid=14941622>

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# Stellar Models: Theory and limitations

- **Stellar Evolution (SE)**

Conservation of momentum

$$\frac{\partial P}{\partial M_r} = -\frac{GM_r}{4\pi r^4} - \frac{1}{4\pi r^2} \frac{\partial^2 r}{\partial t^2},$$

Conservation of mass

$$\frac{\partial r}{\partial M_r} = \frac{1}{4\pi r^2 \rho},$$

Energy Transport

$$\frac{\partial T}{\partial M_r} = -\frac{3\kappa L_r}{64\pi^2 acT^3 r^4},$$

Conservation of energy

$$\frac{\partial L_r}{\partial M_r} = \epsilon - T \frac{\partial S}{\partial t}.$$

- **Fluid/Hydro Dynamics**

Conservation of momentum

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \vec{v}$$

Conservation of mass

$$\frac{d\vec{v}}{dt} = -\frac{\nabla P}{\rho} + \vec{g}$$

Conservation of energy  
(heating- $\Gamma$ , cooling- $\Lambda$ )

$$\frac{du}{dt} = -\frac{P}{\rho} \nabla \cdot \vec{v} + \Gamma - \Lambda,$$

EOS (eg)

$$P = (\gamma - 1)\rho u$$

[4],[5]

# Stellar Evolution (SE) & Hydrodynamics

Hydrodynamic:



Eulerian:  $M(r)$ - AMR (FLASH)

3D



LaGrangian:  $R(m)$ - SPH (PHANTOM)

# Stellar Models: Theory and limitations

Hydrodynamic:



Eulerian:  $M(r)$ - AMR (FLASH)

3D



LaGrangian:  $R(m)$ - SPH (PHANTOM)

Common issues:

- Advection errors
- Excessive Diffusion
- Angular Momentum errors
- Containment of experimental volume

- Viscosity issues
- Mesh Deformation

# Stellar Models: Theory and limitations

Hydrodynamic:



Eulerian:  $M(r)$ - AMR

3D



LaGrangian:  $R(m)$ - SPH (PHANTOM)

Hydrodynamics + SE: MESA, KEPLER, GENECA, GARSTEC:

1D

# Stellar Models: Theory and limitations

Hydrodynamic:



Eulerian:  $M(r)$ - AMR

3D



LaGrangian:  $R(m)$ - SPH (PHANTOM)

Hydrodynamics + SE: MESA, KEPLER, GENEC, GARSTEC:

Pre-MS-  $\rightarrow$  WD & other long term evol



EOS, Mixing (simple 1D), Large nets (co-processed), mass loss, opacity, diffusion

Images courtesy Jordi Jose: <http://www.fen.upc.edu/users/jjose/images/CRC/>, ESO/L. Calçada., NASA/STScI

# Stellar Models: Theory and limitations

Hydrodynamic:



3D  
short timescales  
high spatial resolution

Eulerian:  $M(r)$ - AMR (FLASH)

LaGrangian:  $R(m)$ - SPH

Hydrodynamics + SE: MESA, KEPLER, GENE, GARSTEC:

long timescales  
NO 3D

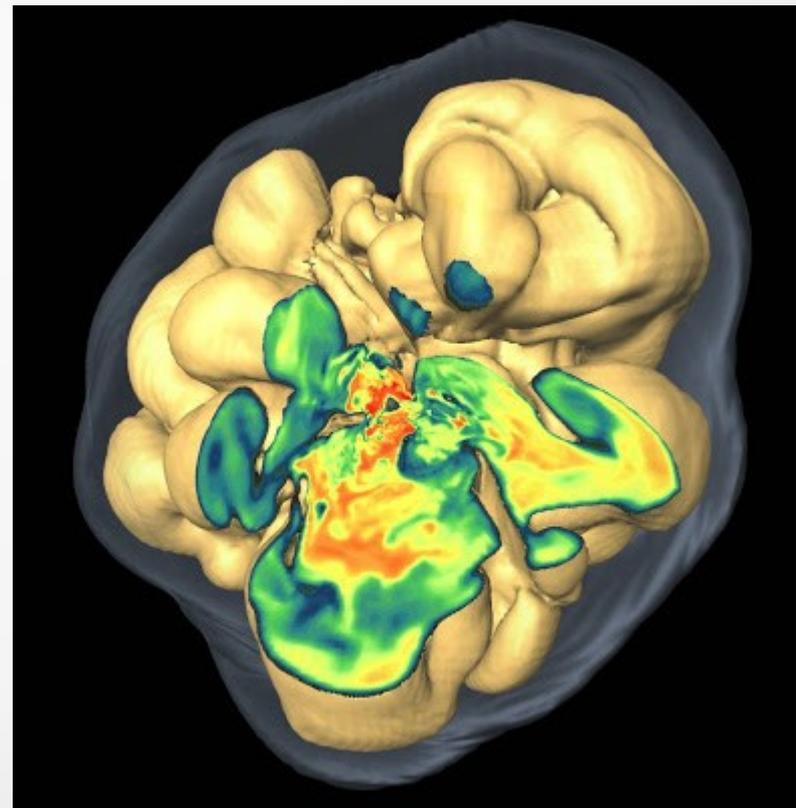


# Stellar Models for R-process nucleosynthesis

R-Process:  $n$  rich, high  $T$ , seed  $X_i$

$$\rightarrow t_{n\_cap} < t_{\beta^-} < \sim 1 \text{ s}$$

- Compact object merger
- Ejecta- LIGO 2017 [1] ✓
- Gamma Ray Burst [2]
- Supernovae, CCSN [2]
- Neutrino-driven wind [2]
- Relativistic/MHD Jets [2]



[3]

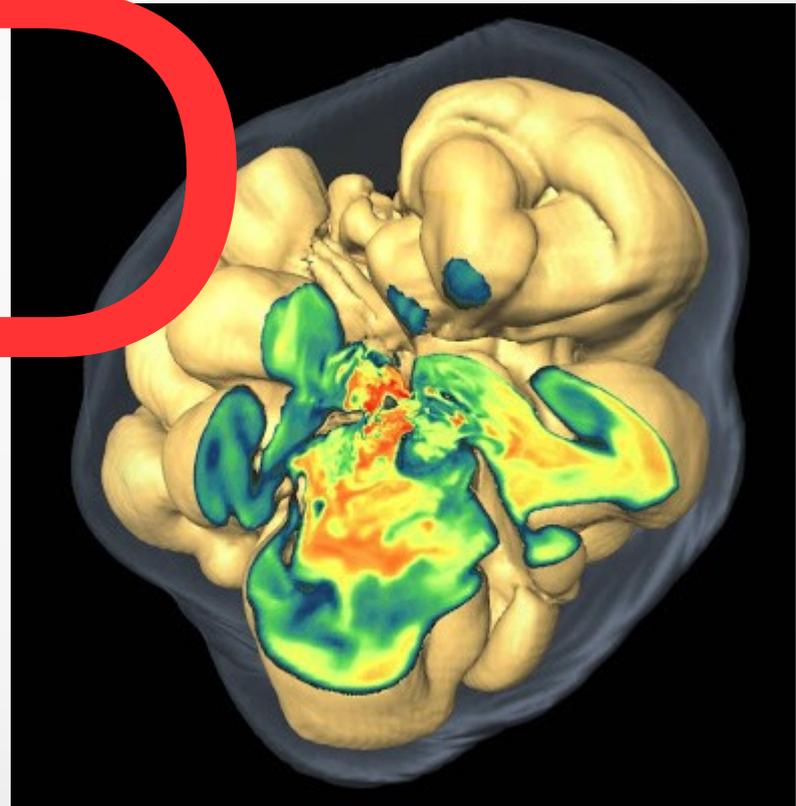
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3D



[3]

# Stellar Models for R-process nucleosynthesis

- Nuclear network only
  - Solve: diff eq's, NSE
  - Use: Linear algebra, matrix & stiff ODE solvers
  - Input
    - Initial  $X_i$ 's
    - Rxn rates
    - $T$  &  $\rho$  (constant or  $T(t)/\rho(t)$ ) , from sim. or obs.\*\*\*

R-process:  $S$ ,  $Y_e = \frac{n_p}{n_p + n_n}$ ,  $\tau_{dyn}$  in order to calculate  $T$  &  $\rho$  profile & set  $X_n$

Physics: MHD, Neutrino transport, GR

Authors	Scenario	Simulation	Tested quantity	year
Beun, Blackmon, Hix McLaughlin, Smith, Surman[6]	$\eta$ wind	param	$n$ capture	2008
Surman,Beun, McLaughlin, Hix[7]	$\eta$ wind	param	$n$ capture	2009
Arcones, Martinez-Pinedo[8]	$\eta$ wind	PPM	$m, S_n$	2011
Mumpower, McLaughlin, Surman[9]	Hot, cold	param	$m$	2012
Brett, Bentley, Paul, Aprahamian, Surman[10]	$\eta$ winds	param	$m, S_n$	2012
Surman, Mumpower, Cass, Aprahamian[11]	Early universe?	param	$m, S_n$	2013
Surman, Mumpower, Cass, Bentley, Aprahamian, McLaughlin[12]	$\eta$ winds, NSM,	param, PPM, R-SPH	$m, n$ capture, $\beta^-$ rates	2013
Surman, Mumpower, Sinclair, Jones, Hix, McLaughlin[13]	CCSN	param	$n$ capture	2014
Aprahmian, Bentley, Mumpower, Surman[14]	CCSN	param	$m, S_n$	2014
Mumpower, Cass, Passuci, Surman, Aprahamian[15]	$\eta$ winds, NSM, GRB	Param, PPM	$\beta^-$ rates	2014
Mumpower, Surman,Fang, Beard, Moller, Kawano, Aprahamian [16]	$\eta$ winds, NSM	param, PPM, R-SPH	$m \rightarrow n$ capture, $(\gamma, p), \beta^-$	2015

Abbreviations:

PPM: Piecewise Parabolic Method (Eulerian)

R-SPH: Relativistic Smoothed Particle Hydrodynamics (LaGrangian)

Param: Parameterized: Equation or constant

# Stellar Models for R-process nucleosynthesis

## Is 3D necessary for r-process nucleosynthesis?

- Ideally, yes.
- But 2D will probably suffice
- Problems with level 2:
  - 1D uses approximations for 3D effects
  - Hydro timescales (dynamical) vs Myrs for SE
    - (either-or)
  - ★ Hydro → some physics issues due to mesh or smoothing
  - ★ Post-processed → Harder to test astron observables
    - Little/No feed back with net in 3D

# Stellar modelling for nuc-astro

- What can we improve:
  - Physics: eg EOS, Neutrino treatment
  - Extending Models:
    - SE equations to 2D-3D hydro & vice versa\*
    - Adaptive Hydro 1D, 2D → 3D\*
    - 2D Nuclear nets w/ mixing &/or Monte Carlo  $X_i$
    - Eulerian smoothing
    - Hybrid Eulerian & Lagrangian\*
  - Computing power:
    - This will motivate advancement
  - Algorithms & Solvers:
    - Probably have to rely on CS
  - Access model:

\*already under way

## Pros:

Deriving from first principles is useful exercise  
Encourages variation of solutions

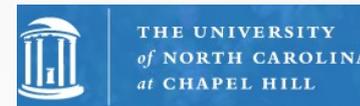
## Cons:

Closed source contrary to spirit of scientific method  
"black box", irreproducible  
Encourages replication & abandonware  
Slows advancement

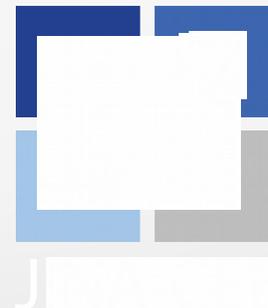
Take cues from FOSS: "All bugs are shallow" or "Sunlight is the best disinfectant"

# Thank You- Collaborators

- Manos Chatzopoulos- LSU
- Zach Meisel- Ohio U
- Carl Fields- MSU
- Art Champagne- TUNL/ UNC
- Modules for Experiments With Astrophysics (MESA)



## MESA



# References

- [1] K. Hotokezaka, P. Beniamini, and T. Piran, (2018).
- [2] S. Brett, I. Bentley, N. Paul, R. Surman, and A. Aprahamian, Eur. Phys. J. A (2012).]
- [3] L. Scheck, H.-T. Janka, T. Foglizzo, and K. Kifonidis, Multidimensional Supernova Simulations with Approximative Neutrino Transport II. Convection and the Advective-Acoustic Cycle in the Supernova Core (2007).
- [4][http://flash.uchicago.edu/site/flashcode/user\\_support/tutorial\\_talks/May2004/PR\\_tutorial\\_talk.pdf](http://flash.uchicago.edu/site/flashcode/user_support/tutorial_talks/May2004/PR_tutorial_talk.pdf)
- [5]Wadsley, J. W., Keller, B. W., & Quinn, T. R. (2017). Gasoline2: A Modern SPH Code. In MNRAS (Vol. 000). Retrieved from <http://gasoline-code.com>
- [6]Arcones, A., & Martínez-Pinedo, G. (2011). Dynamical r-process studies within the neutrino-driven wind scenario and its sensitivity to the nuclear physics input. PHYSICAL REVIEW C, 83, 45809. <https://doi.org/10.1103/PhysRevC.83.045809>
- [7]Arcones, A., & Martínez-Pinedo, G. (2011). Dynamical r-process studies within the neutrino-driven wind scenario and its sensitivity to the nuclear physics input. PHYSICAL REVIEW C, 83, 45809. <https://doi.org/10.1103/PhysRevC.83.045809>
- [8]Mumpower, M. R., McLaughlin, G. C., & Surman, R. (2012). Formation of the rare-earth peak: Gaining insight into late-time r-process dynamics. PHYSICAL REVIEW C, 85, 45801. <https://doi.org/10.1103/PhysRevC.85.045801>
- [9]Brett, S., Bentley, I., Paul, N., Surman, R., & Aprahamian, A. (2012). Sensitivity of the r-process to nuclear masses. Eur. Phys. J. A. <https://doi.org/10.1140/epja/i2012-12184-4>
- [10]Surman, R., Mumpower, M., Cass, J., Bentley, I., Aprahamian, A., & McLaughlin, G. C. (2013). Sensitivity studies for r-process nucleosynthesis in three astro-physical scenarios. Retrieved from <https://arxiv.org/pdf/1309.0059.pdf>
- [11]Surman, R., Mumpower, M., Cass, J., Bentley, I., Aprahamian, A., & McLaughlin, G. C. (2013). Sensitivity studies for r-process nucleosynthesis in three astro-physical scenarios. Retrieved from <https://arxiv.org/pdf/1309.0059.pdf>
- [12]Surman, R., Mumpower, M., Sinclair, R., Jones, K. L., Hix, W. R., & McLaughlin, G. C. (2014). Sensitivity studies for the weak r process: neutron capture rates. AIP Advances, 4(4), 041008. <https://doi.org/10.1063/1.4867191>
- [13]Mumpower, M. R., Surman, R., Fang, D.-L., Beard, M., Möller, P., Kawano, T., & Aprahamian, A. (2015). Impact of individual nuclear masses on r-process abundances. PHYSICAL REVIEW C, 92, 35807. <https://doi.org/10.1103/PhysRevC.92.035807>
- [14]Mumpower, M. R., Surman, R., Fang, D.-L., Beard, M., Möller, P., Kawano, T., & Aprahamian, A. (2015). Impact of individual nuclear masses on r-process abundances. PHYSICAL REVIEW C, 92, 35807. <https://doi.org/10.1103/PhysRevC.92.035807>
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# Finite Difference & Related Methods

Finite differences are simple and effective, although their applicability is restricted to structured meshes. In this technique, variables are assigned to individual grid points (either located at the edges, corners, or centers of each computational cell), and the corresponding derivatives are evaluated as differences of variables in neighboring cells, in a Taylor series expansion.

Finite elements and finite volumes are particularly suited for arbitrary meshes (unstructured grids, in particular).

Finite elements operate by splitting the domain of the problem into a number of subdomains, called finite elements, each represented by a set of equations. But in contrast to the direct (strong-form) approach adopted in finite difference techniques (also in SPH), by which the partial differential equations are directly discretized and solved, finite element methods rely on an indirect or weak-form approach, in which the original equations are transformed, often in integral form, on the basis of trial solutions and weighting functions. The collection of local equations is then reassembled into a global system of equations through a transformation of coordinates.

Finite-volume methods [507, 1855] are gaining popularity as a suitable form of discretization in multidimensional codes. They are somewhat similar to finite-difference and finite-element methods, since they rely on the discretization of a system of partial differential equations onto a discrete set of points of a grid-based geometry. To this end, the computational domain is divided into a set of discrete, nonoverlapping discretization cells or control volumes, with physical variables assigned to the centroid of each control volume. The set of partial differential equations is then integrated over each control volume, resulting in balance equations that are subsequently discretized. The cornerstone of finite-volume methods is the discretization of the fluxes at the boundaries of each control volume. This discretization technique guarantees conservation of physical magnitudes for any control volume as well as for the overall computational domain. Note that discretization is again performed on local balance equations rather than on the original partial differential equations (as in finite-differences). For more information on these and other methods used in computational fluid dynamics, the reader is referred to LeVeque et al. [1083] and Toro [1812].

# Nuclear Net Theory

Differential equation of species change:

$$\frac{\partial n_i}{\partial t} + \frac{\partial n_1 u}{\partial x} = -n_1 n_2 \langle \sigma v \rangle \quad n_i = \rho N_A Y_i$$

nuc ↑ term      mix ↑ term      number density      ↑      avg cross section

• Reactions

$$\frac{dY_i}{dt} = -\lambda_i Y_i$$

$$\frac{dY_i}{dt} = -\rho N_A Y_i Y_j \langle \sigma v \rangle$$

$$\frac{dY_i}{dt} = -\rho^2 N_A^2 Y_i Y_j Y_l \langle \sigma v \rangle_{j,k,l}$$

• Total differential equation

$$\dot{Y}_i = \sum_j N_j^i \lambda_j Y_j + \sum_{j,k} N_{j,k}^i \rho N_A \langle \sigma v \rangle_{j,k} Y_j Y_k + \sum_{j,k,l} N_{j,k,l}^i \rho^2 N_A^2 \langle \sigma v \rangle_{j,k,l} Y_j Y_k Y_l$$

• Euler's method

$$\frac{\vec{Y}(t+\Delta t) - \vec{Y}(t)}{\Delta t} = (1 - \Theta) \dot{\vec{Y}}(t+\Delta t) + \Theta \dot{\vec{Y}}(t)$$

# Stellar Evolution & Hydrodynamics

- SE- Conservation of momentum

$$\frac{\partial P}{\partial M_r} = -\frac{GM_r}{4\pi r^4} - \frac{1}{4\pi r^2} \frac{\partial^2 r}{\partial t^2},$$

Hydrostatic equilibrium

Conservation of mass

$$\frac{\partial r}{\partial M_r} = \frac{1}{4\pi r^2 \rho},$$

Energy Transport

$$\frac{\partial T}{\partial M_r} = -\frac{3\kappa L_r}{64\pi^2 acT^3 r^4},$$

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Thermal  
Equilibrium

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Conservation of energy

$$\frac{\partial L_r}{\partial M_r} = \epsilon - T \frac{\partial S}{\partial t}.$$

Thermal  
Equilibrium

- Fluid dynamics (Eulerian)-

# R-process Reaction Rates:

- Rate Types:
  - Fast Neutron Captures
  - Photodisintegration
  - $\beta$ - decay
- What do we know about these rates:
  - For R-process: Nothing\*.

WE RELY ON THEORETICAL RATE CALCULATIONS  
Mass models

\*Almost

# Nuclear Net Theory

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nuc ↑ term    mix ↑ term    no. density & avg ↑ cross section

- Mixing term handled by hydrodynamic code

- Reactions

$$\frac{dY_i}{dt} = -\lambda_i Y_i \quad \frac{dY_i}{dt} = -\rho N_A Y_i Y_j \langle \sigma v \rangle \quad \frac{dY_i}{dt} = -\rho^2 N_A^2 Y_i Y_j Y_l \langle \sigma v \rangle_{j,k,l}$$

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