An EOS implementation for astrophyisical simulations

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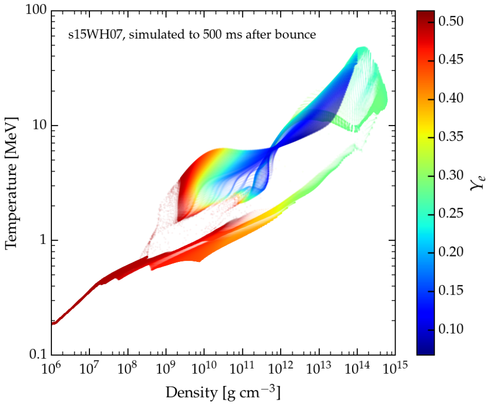
Nuclear EOS

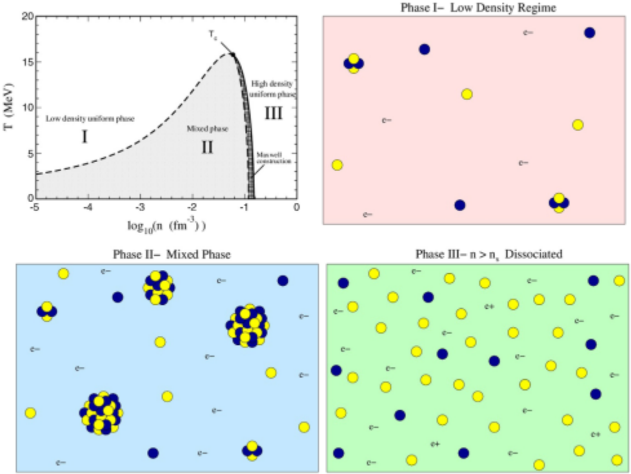
Equation of state (EOS):
$\Rightarrow \varepsilon(n, y, T), P(n, y, T), s(n, y, T), \ldots$

Astrophysical relevance

- Core-collapse supernovae;
- NS structure and evolution;
- Merger of compact stars;
- *r*-process nucleosynthesis;
- ...



Nuclear EOS



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Nuclear EOS

Long-standing problem in nuclear physics.
Combines efforts from:

- heavy ion collision experiments;
- nuclear reaction experiments;
- computer simulations of astrophysical phenomena;
- computer simulations of dense matter;
- theoretical many-body calculations;
- ...

Nuclear EOS

Nuclear forces are complicated $\Rightarrow$ combine different approaches!
Hot-dense EOS available:

1. Lattimer and Swesty
2. H. Shen *et al.*
3. G. Shen *et al.*
4. Hempel *et al.*
5. Steiner *et al.*
6. Banik *et al.*
7. ...

Classification:

1. Relativistic vs Non-relativistic
2. Realistic potentials vs Effective potentials
3. SNA vs NSE vs reaction networks
4. Muons? Hyperons? Quarks?

Nuclear EOS

Goals:

1. Write code to construct EOS tables for astrophysical simulations.
2. Easy to update EOS as new nuclear matter constraints become available.
3. Make the code open-source. (soon)

The Lattimer & Swesty EOS

The Lattimer & Swesty EOS [Nucl. Phys. A **535**, 331 (1991)]
Most used EOS for simulations of CCSNe and NS mergers.
Non-relativistic compressible liquid-drop description of nuclei.

Contains

1. Nucleons;
2. alpha particles;
3. electrons and positrons;
4. photons.

Nucleons may cluster to form nuclei.

LS EOS use the single nucleus approximation (SNA).

The Lattimer & Swesty EOS

Free energy $F(n, y, T) = F_o + F_h + F_\alpha + F_e + F_\gamma$

- $F_o \equiv$ nucleons outside heavy nuclei (nucleon gas)
- $F_h \equiv$ nucleons clustered into heavy nuclei

In this work, F depends on seven variables:

- u: volume fraction occupied by heavy nuclei
- r: generalized size of heavy nuclei
- n_{ni}: neutron density inside heavy nuclei
- n_{pi}: proton density inside heavy nuclei
- n_{no}: neutron density outside heavy nuclei
- n_{po}: proton density outside heavy nuclei
- n_α: alpha particle density

The Lattimer & Swesty EOS

Heavy nuclei free energy:

$$F_h = F_i + F_S + F_C + F_T$$

- $F_i \equiv$ nucleons inside heavy nuclei
- $F_S \equiv$ surface free energy
- $F_C \equiv$ coulomb free energy
- $F_T \equiv$ translational free energy

The EOS of each component:

- Nucleons $\Rightarrow$ local phenomenological Skyrme-type effective interaction.
- Alpha particles $\Rightarrow$ hard spheres.
- Electrons, positrons and photons $\Rightarrow$ background gas.

The Lattimer & Swesty EOS

Energy density of bulk nuclear matter with Skyrme-type interactions

$$E_B(n, y, T) = \frac{\hbar^2}{2m_n^*}\tau_n + \frac{\hbar^2}{2m_p^*}\tau_p + (a + 4by(1-y))\, n^2 + \sum_i (c_i + 4d_i y(1-y))\, n^{1+\delta_i} - yn(m_n - m_p).$$

Nucleon effective mass m_t^*

$$\frac{\hbar^2}{2m_t^*} = \frac{\hbar^2}{2m_t} + \alpha_1 n_t + \alpha_2 n_{-t}.$$

where $t = n \Rightarrow -t = p$ and vice versa, $n_n = (1-y)n$ and $n_p = yn$.
Nucleon kinetic energy density τ_t

$$\tau_t = \frac{1}{2\pi^2}\left(\frac{2m_t^* T}{\hbar^2}\right)^{\frac{5}{2}} F_{3/2}(\eta_t(n, y)),$$

The Lattimer & Swesty EOS

$$a = \frac{t_0}{4}(1 - x_0)\,,$$

$$b = \frac{t_0}{8}(2x_0 + 1)\,,$$

$$c_i = \frac{t_{3i}}{24}(1 - x_{3i})\,,$$

$$d_i = \frac{t_{3i}}{48}(2x_{3i} + 1)\,,$$

$$\delta_i = \sigma_i + 1\,,$$

$$\alpha_1 = \frac{1}{8}\left[t_1(1 - x_1) + 3t_2(1 + x_2)\right]\,,$$

$$\alpha_2 = \frac{1}{8}\left[t_1(2 + x_1) + t_2(2 + x_2)\right]\,.$$

Nuclear surface and Coulomb free energies

$$F_S = \frac{3s(u)}{r}\sigma(y_i, T) \qquad \text{and} \qquad F_C = \frac{4\pi\alpha}{5}(y_i n_i r)^2 c(u).$$

- $s(u)$: surface shape function
- $c(u)$: Coulomb shape function
- r: generalized nuclear size
- $\sigma(y_i, T)$: surface tension per unit area

Nuclear virial Theorem: $F_S = 2F_C$

$$r = \frac{9\sigma}{2\beta}\left[\frac{s(u)}{c(u)}\right]^{1/3} \qquad \text{where} \qquad \beta = 9\left[\frac{\pi\alpha}{15}\right]^{1/3}(y_i n_i \sigma)^{2/3}$$

$$F_S + F_C = \beta\left[c(u)s(u)^2\right]^{1/3} \equiv \beta\mathscr{D}(u).$$

Nuclear surface and Coulomb free energies

Lattimer & Swesty interpolate $\mathscr{D}(u)$ with

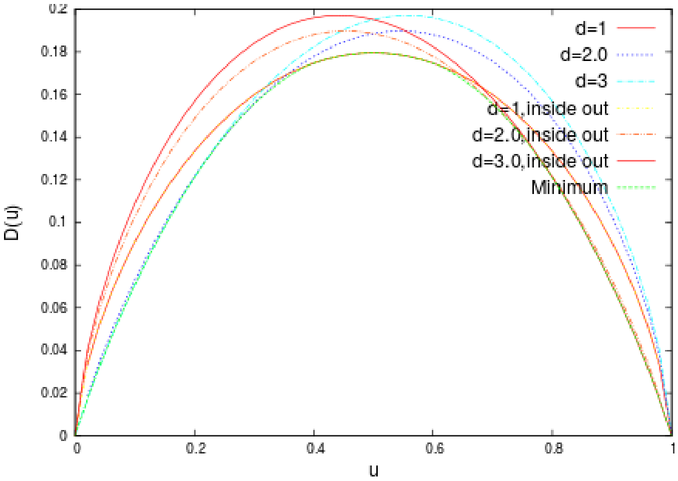
$$\mathscr{D}(u) = u(1-u)\frac{(1-u)D(u)^{1/3} + uD(1-u)^{1/3}}{u^2 + (1-u)^2 + 0.6u^2(1-u)^2}$$

where

$$D(u) = 1 - \frac{3}{2}u^{1/3} + \frac{1}{2}u$$

- as $u \to 0$ reproduces free energy of spherical nuclei
- as $u \to 1$ reproduces free energy of "bubble nuclei"
- intermediate u: reproduces free energy of pasta phases:
  - cylinders;
  - slabs;
  - cylindrical holes.

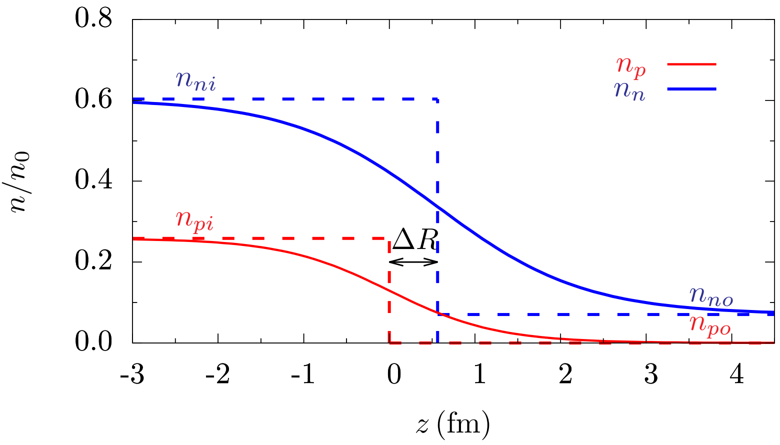
Nuclear surface and Coulomb free energies



Lim (2012)

Nuclear surface and Coulomb free energies

Surface Tension $\sigma(y, T)$.



Nuclear surface and Coulomb free energies

Set temperature T and proton fraction y_i.

Solve equilibrium equations:

$$P_i = P_o\,, \quad \mu_{ni} = \mu_{no}\,, \quad \text{and} \quad \mu_{pi} = \mu_{po}\,, \quad \text{and} \quad y_i = \frac{n_{pi}}{n_{ni} + n_{pi}}$$

Set density to

$$n_t(z) = n_{to} + \frac{n_{ti} - n_{to}}{1 + \exp\left((z - z_t)/a_t\right)}$$

$t = n, p$.

Nuclear surface and Coulomb free energies

Find z_t and a_t that minimizes

$$\sigma(y_i, T) = \int_{-\infty}^{+\infty} \left[F_B(z) + E_S(z) + P_o - \mu_{no} n_n(z) - \mu_{po} n_p(z) \right] dz \,.$$

where

$$E_S(z) = \frac{1}{2} \left[q_{nn} \left(\nabla n_n \right)^2 + q_{np} \nabla n_n \cdot \nabla n_p + q_{pn} \nabla n_p \cdot \nabla n_n + q_{pp} \left(\nabla n_p \right)^2 \right]$$

and

$$q_{nn} = q_{pp} = \frac{3}{16} \left[t_1 (1 - x_1) - t_2 (1 + x_2) \right] ,$$
$$q_{np} = q_{pn} = \frac{1}{16} \left[3 t_1 (2 + x_1) - t_2 (2 + x_2) \right] .$$

Solving the EOS

Minimize $F(n, y, T)$ w.r.t. u, r, n_{ni}, n_{pi}, n_{no}, n_{po}, and n_α.

$$
\begin{aligned}
A_1 &= P_i - B_1 - P_o - P_\alpha = 0\,, \\
A_2 &= \mu_{ni} - B_2 - \mu_{no} = 0\,, \\
A_3 &= \mu_{pi} - B_3 - \mu_{po} = 0\,.
\end{aligned}
$$

where

$$
\begin{aligned}
B_1 &= \frac{\partial \mathscr{F}}{\partial u} - \frac{n_i}{u}\frac{\mathscr{F}}{\partial n_i}\,, \\
B_2 &= \frac{1}{u}\left[\frac{y_i}{n_i}\frac{\partial \mathscr{F}}{\partial y_i} - \frac{\partial \mathscr{F}}{\partial n_i}\right]\,, \\
B_3 &= -\frac{1}{u}\left[\frac{1-y_i}{n_i}\frac{\partial \mathscr{F}}{\partial y_i} + \frac{\partial \mathscr{F}}{\partial n_i}\right]\,,
\end{aligned}
$$

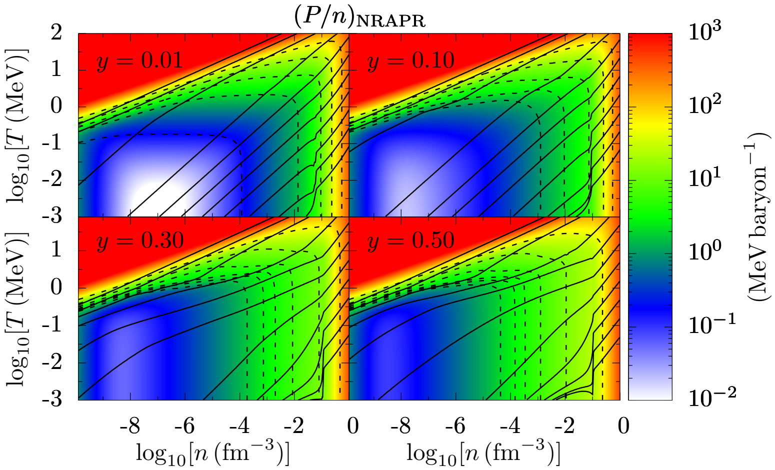
with $\mathscr{F} = F_S + F_C + F_T$.

Solving the EOS

Constraints

$$
\begin{aligned}
n &= un_i + (1-u)[4n_\alpha + n_o(1 - n_\alpha v_\alpha)]\,, \\
ny &= un_i y_i + (1-u)[2n_\alpha + n_o y_o(1 - n_\alpha v_\alpha)]\,. \\
\mu_\alpha &= 2(\mu_{no} + \mu_{po}) + B_\alpha - P_o v_\alpha\,, \\
r &= \frac{9\sigma}{2\beta}\left[\frac{s(u)}{c(u)}\right]^{1/3}\,,
\end{aligned}
$$

Solving the EOS



Solving the EOS

Nuclear Statistical Equilibrium

Consider ensemble of nuclei at low densities.
Given an ensemble of nuclei i, solve for μ_n and μ_p such that

$$\begin{aligned} \mu_i &= m_i + E_{c,i} + T\log\left[\frac{n_i}{g_i}\left(\frac{2\pi}{m_i T}\right)^{3/2}\right], \\ &= Z_i\mu_p + (A_i - Z_i)\mu_n \end{aligned}$$

that minimizes the free energy of the system.

Nuclear Statistical Equilibrium

L&S EOS is obtained in the single nucleus approximation (SNA). Properties in the SNA can differ significantly from observed properties of nuclei.

- No shell closure;
- No pairing;
- liquid drop model neglects many-body effects;
- ...

Conversely,

- NSE breaks down close to nuclear saturation density $n_0 \simeq 0.16\,\text{fm}^{-3}$;
- Needs very large and very neutron rich nuclei at low y and/or high $n \sim n_0$;
- No nuclear inversion (pasta phase).

Nuclear Statistical Equilibrium

Use ad-hoc procedure to mix NSE and SNA free energies:

$$F_{\rm MIX} = \chi(n) F_{\rm SNA} + [1 - \chi(n)] F_{\rm NSE} .$$

Chose $a(n)$ such that:

$$\chi(n) \to 0, \text{ if } n \ll n_0$$
$$\chi(n) \to 1, \text{ if } n \lesssim n_0/10$$

Corrections to thermodynamic quantities, *e.g.*

$$P_{\rm MIX} = n^2 \frac{\partial (F_{\rm MIX}/n)}{\partial n}\bigg|_{T,y} = \chi(n) P_{\rm SNA} + [1 - \chi(n)] P_{\rm NSE} + n^2 \frac{\partial \chi(n)}{\partial n} (F_{\rm SNA} - F_{\rm NSE}) .$$

EOS is self consistent!

High density extension

- Skyrme parametrizations only constrained up to $n \lesssim 3n_0$.
- NS maximum mass depend on EOS at $n \sim 10n_0$.
- Most Skyrme EOS unable to reproduce NS maximum mass, $M_{\max} \sim 2M_\odot$.

Add extra c_i, d_i, and δ_i terms to Skyrme interactions:

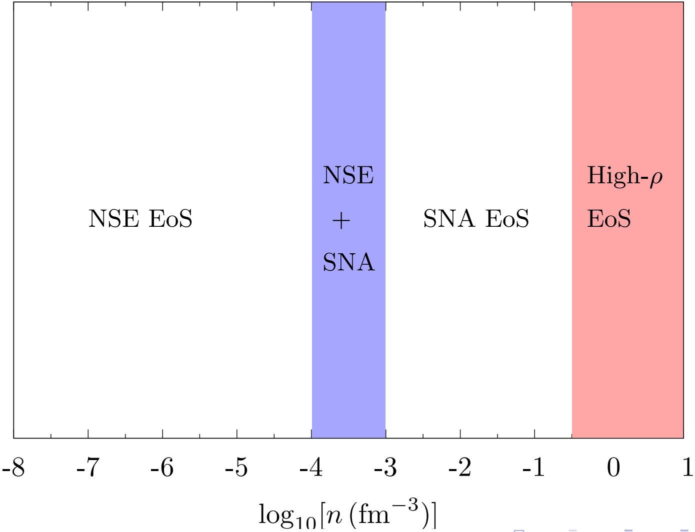
$$\varepsilon_B(n,y,T) = \frac{\hbar^2}{2m_n^*}\tau_n + \frac{\hbar^2}{2m_p^*}\tau_p + \left(a + 4by(1-y)\right)n^2 + \sum_i \left(c_i + 4d_i y(1-y)\right)n^{1+\delta_i} - yn(m_n - m_p).$$

Extra terms should:

- barely affect EOS for $n \lesssim 3n_0$;
- increase $M_{\max} \sim 2M_\odot$.

Problem: may imply in $(c_s/c) \gtrsim 1$ for $n \sim (6-10)n_0$.

Final EOS


NSE EoS
NSE
+
SNA
SNA EoS
High-ρ
EoS
-8
-7
-6
-5
-4
-3
-2
-1
0
1
$\log_{10}[n\ (\mathrm{fm}^{-3})]$

Skyrme parametrizations

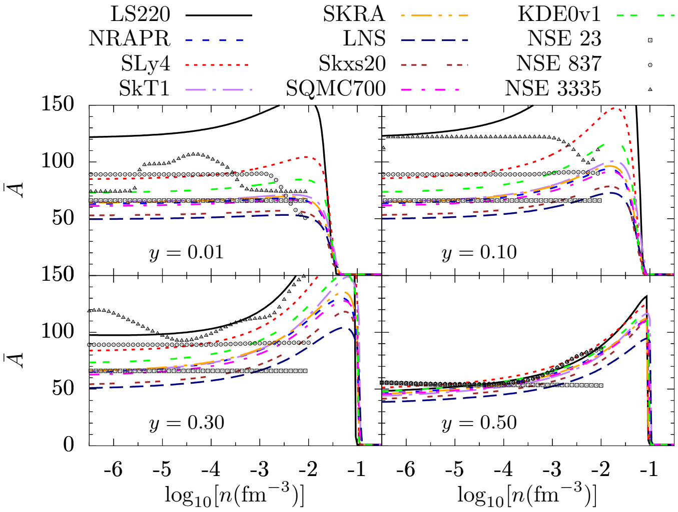
Dutra *et al.* [Phys. Rev. C **85** 035201 (2012)]

- Analyzed over 240 Skyrme parametrizations available in the literature.
- Only 11 fulfill all well established nuclear physics constraints!
- Not all 11 reproduce $M_{\rm max} \sim 2M_\odot$!

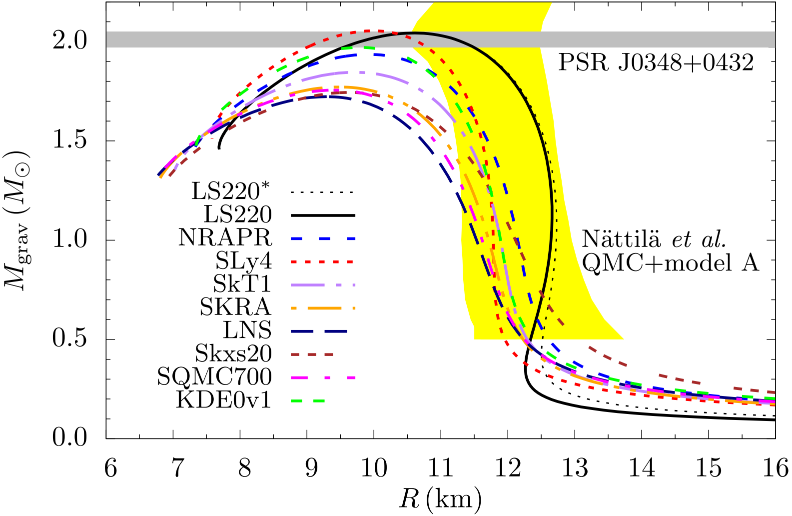
We produced hot-dense EOS tables for a few of these parametrizations.

Skyrme parametrizations

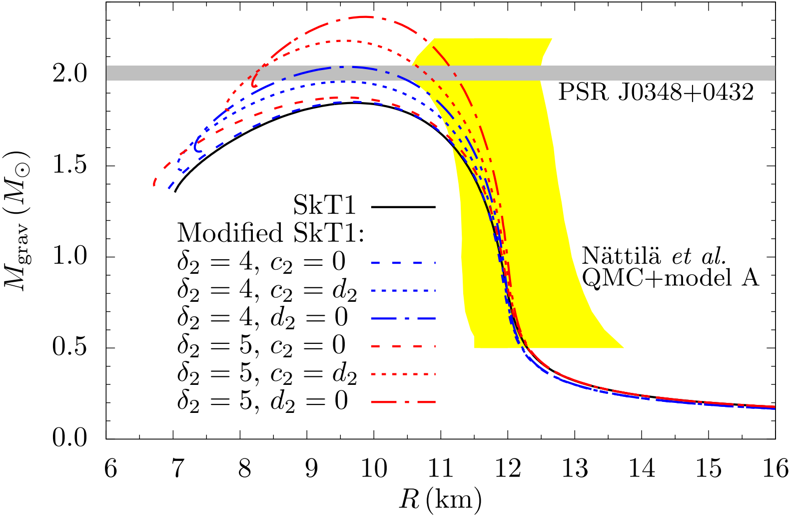
Average nuclear size $\bar{A}$ along $s = 1\, k_B \,\text{baryon}^{-1}$



NS mass-radius relationship

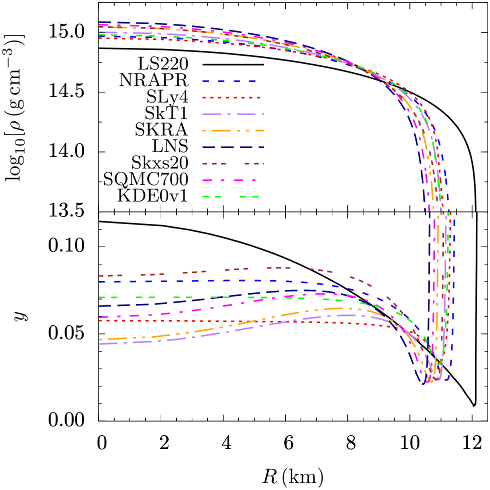


NS mass-radius relationship



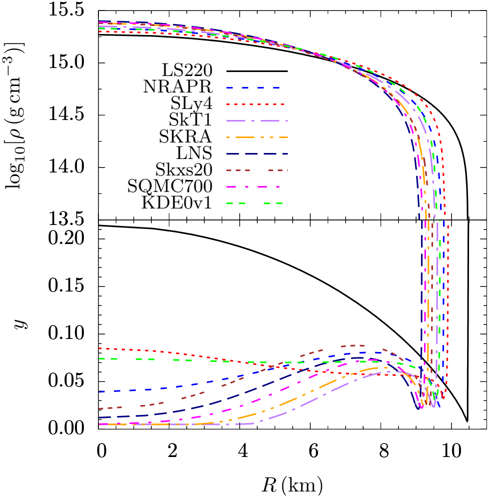
NS Structure

$1.4M_{\odot}$

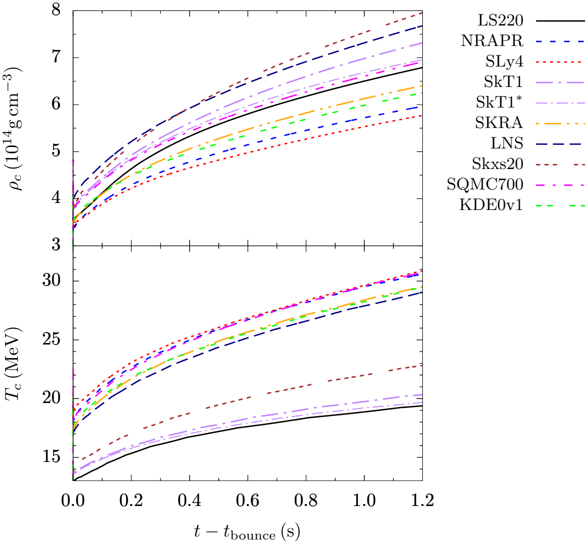


NS Structure

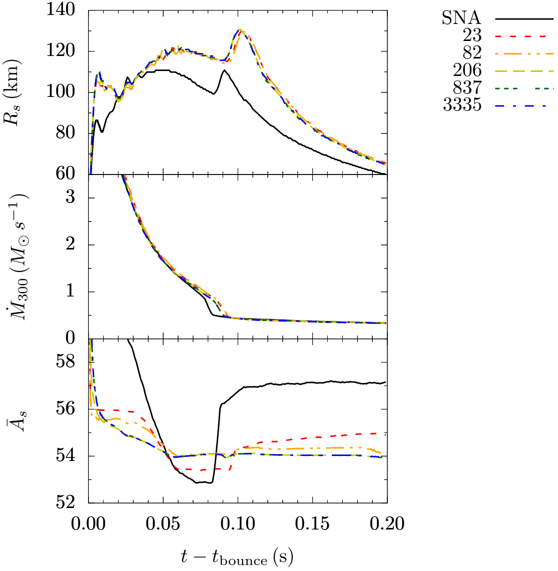
$M_{\max}$



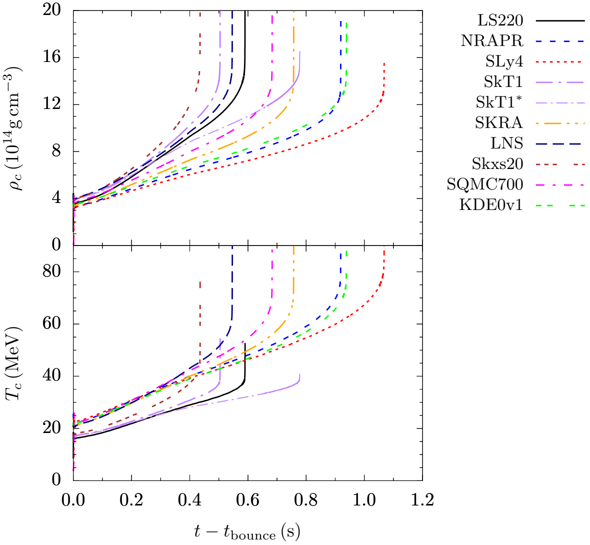
Spherically symmetric collapse of a $15M_{\odot}$ star



Spherically symmetric collapse of a $15M_\odot$ star



Spherically symmetric collapse of a $40M_\odot$ star



Summary

- Generalize L&S formalism to obtain hot dense EOS for most Skyrme parametrizations.
- Improved calculation of surface properties.
- Added smooth ad-hoc transition from SNA to NSE EOS.
- Extended formalism to allow stiffening of EOS for $n \gtrsim 3n_0$.
- Code converges for large region of parameter space.
  - Temperatures $10^{-4}\,\mathrm{MeV} \lesssim T \lesssim 10^{2.5}\,\mathrm{MeV}$;
  - Proton fractions $10^{-3} \lesssim y \lesssim 0.70$;
  - Densities $10^{-13}\,\mathrm{fm}^{-3} \lesssim n \lesssim 10\,\mathrm{fm}^{-3}$.
- Successfully generated many new EOS tables to study CCSNe, NS mergers, ...

Future

Near future:

- publish results and make code open source;
- study EOS effects on CCSN and NS mergers $\Rightarrow$ EOS may affect neutrino and GW emissions;
- perform 2D and 3D simulations;
- add an improvement treatment of neutron skins to the EOS;
- add reaction network treatment for low temperatures/densities;
- ...