



Ab initio calculations of atomic nuclei

Recent progress and future challenges

Lecture 3: Equation of state & connections to astrophysics

Università di Padova
7-10 June 2021

Vittorio Somà
CEA Saclay



Contents

1. Inter-nucleon forces

- Brief introduction to the nuclear many-body problem
- Properties and modelling of nuclear forces
- The modern view: chiral effective field theory

2. Ab initio techniques for the nuclear many-body problem

- Configuration-interaction approaches
- Techniques to mitigate the “curse of dimensionality” (SRG, NO2B, IT)
- Mean field and correlations
- Expansion methods for closed-shell nuclei
- Symmetry breaking
- Expansion methods for open-shell nuclei
- State of the art and open problems

3. Equation of state of nuclear matter & connections to astrophysics

- Neutron stars & Tolman-Oppenheimer-Volkoff equations
- Equation of state of neutron-star matter
- Astrophysical constraints on the nuclear EoS

Contents

1. Inter-nucleon forces

- Brief introduction to the nuclear many-body problem
- Properties and modelling of nuclear forces
- The modern view: chiral effective field theory

2. Ab initio techniques for the nuclear many-body problem

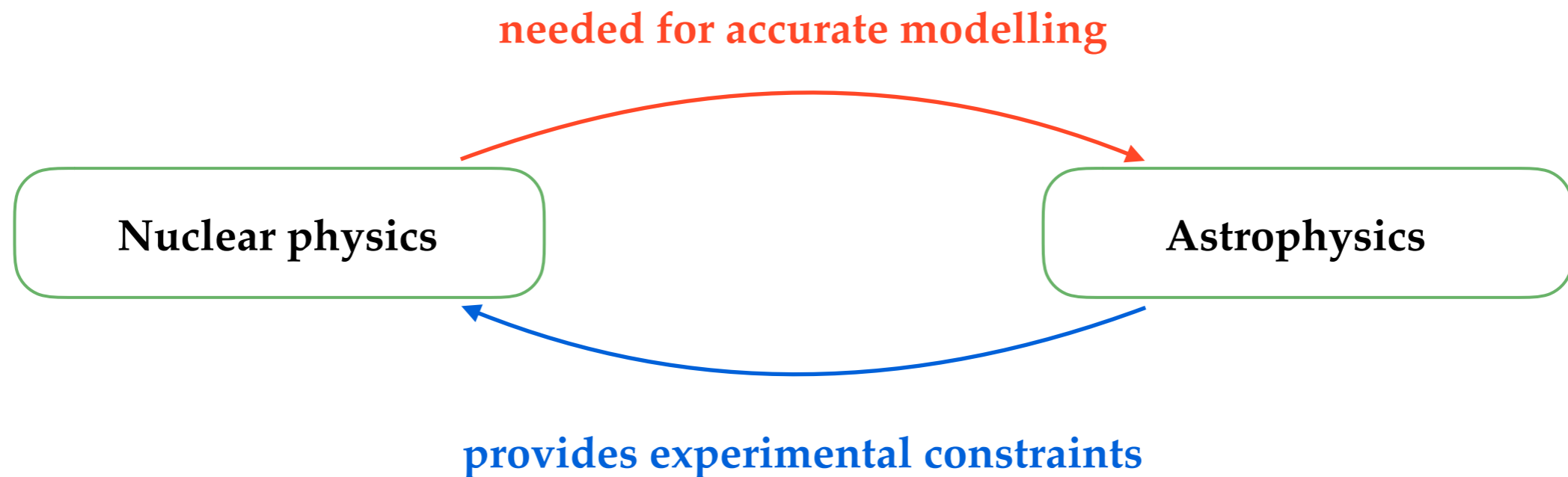
- Configuration-interaction approaches
- Techniques to mitigate the “curse of dimensionality” (SRG, NO2B, IT)
- Mean field and correlations
- Expansion methods for closed-shell nuclei
- Symmetry breaking
- Expansion methods for open-shell nuclei
- State of the art and open problems

3. Equation of state of nuclear matter & connections to astrophysics

- **Neutron stars & Tolman-Oppenheimer-Volkoff equations**
- Equation of state of neutron-star matter
- Astrophysical constraints on the nuclear EoS

Inputs and constraints

- Properties of **finite nuclei** (BE, spectra, decay rates, scattering cross sections, ...)
 - Many nuclei of interest are currently out of reach for ab initio calculations
- EoS of **nuclear matter** (P or E vs. density for different proton fractions and temperatures)
 - Ab initio calculations of nuclear matter available



- ⊙ Constraints on nuclear properties under **extreme conditions** (unattainable on Earth)
 - Very neutron-rich nuclei
 - Nuclear matter at high densities (and low temperatures)
 - Complementary to what accessed in high-energy experiments (low density- high T)

What are neutron stars?

◎ Neutron stars are different things for different people

[Credits: I. Vidaña]

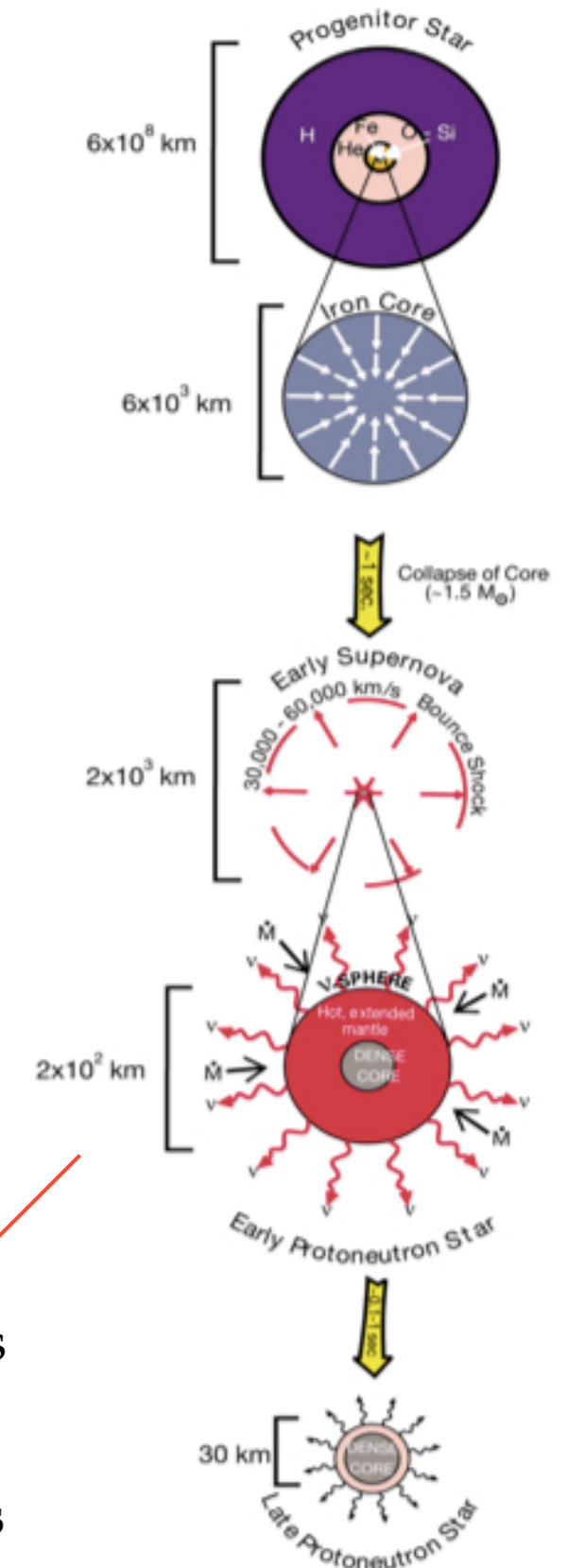
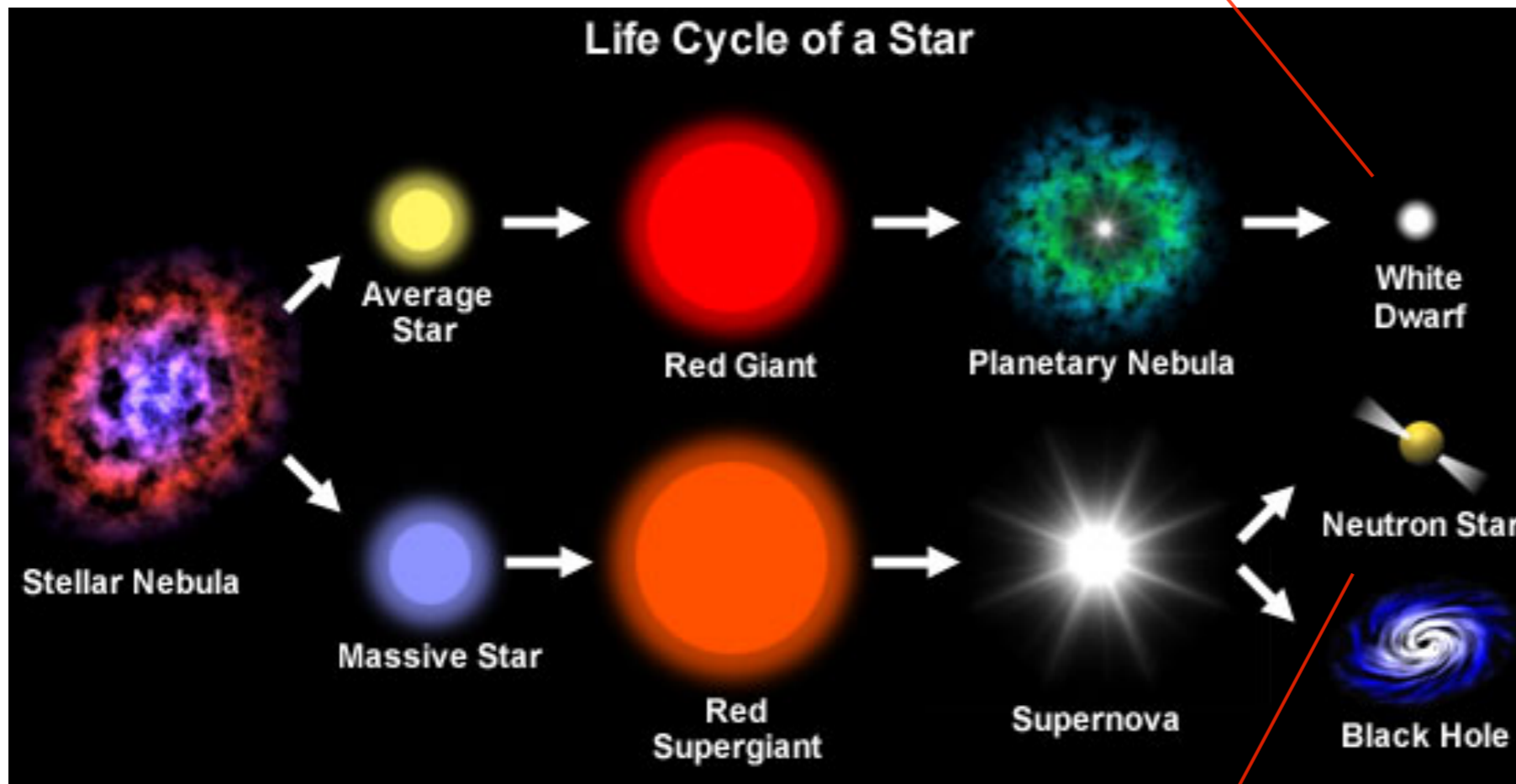
- For **astronomers**, they are tiny stars visible as radio pulsars or sources of X- or γ -rays
- For **particle physicists**, they are neutrino sources and probably the only place in the universe where deconfined quark matter may be abundant
- For **cosmologists**, they are almost black holes
- For **nuclear physicists**, they are the largest (neutron-rich) nuclei in the universe ($A = 10^{56}$ - 10^{57} ; $M \sim 1$ - $2 M_{\odot}$; $R \sim 10$ km)



◎ **However everybody agrees** on the fact that they are a type of stellar compact remnant originating from the gravitational collapse of a massive star ($8 - 25 M_{\odot}$) during a supernova event

Birth of a neutron star

White dwarf: stabilised by degeneracy pressure of electrons



Neutron star: stabilised by degeneracy pressure of neutrons

Modelling of **supernova explosions** involves nuclear physics ingredients (EoS across a large range of densities, proton fraction and temperatures)

→ Complex multi-scale modelling, hinders **feedback on nuclear physics**

From a minimal model...

◎ Minimal constituents

- **Neutrons** (to generate the needed degeneracy pressure stabilising the star)
- **Protons & electrons** (neutrons do decay → β -equilibrium needed)

◎ Three simple conditions must be satisfied

- **Charge neutrality** $n_p = n_e$

→ Even a small charge unbalance would make the star blow up

- **Beta equilibrium** $\mu_n = \mu_p + \mu_e$

→ Neutrinos fly out of the star shortly after they are produced

- **Conservation of total baryon number** $n_B = n_p + n_n$

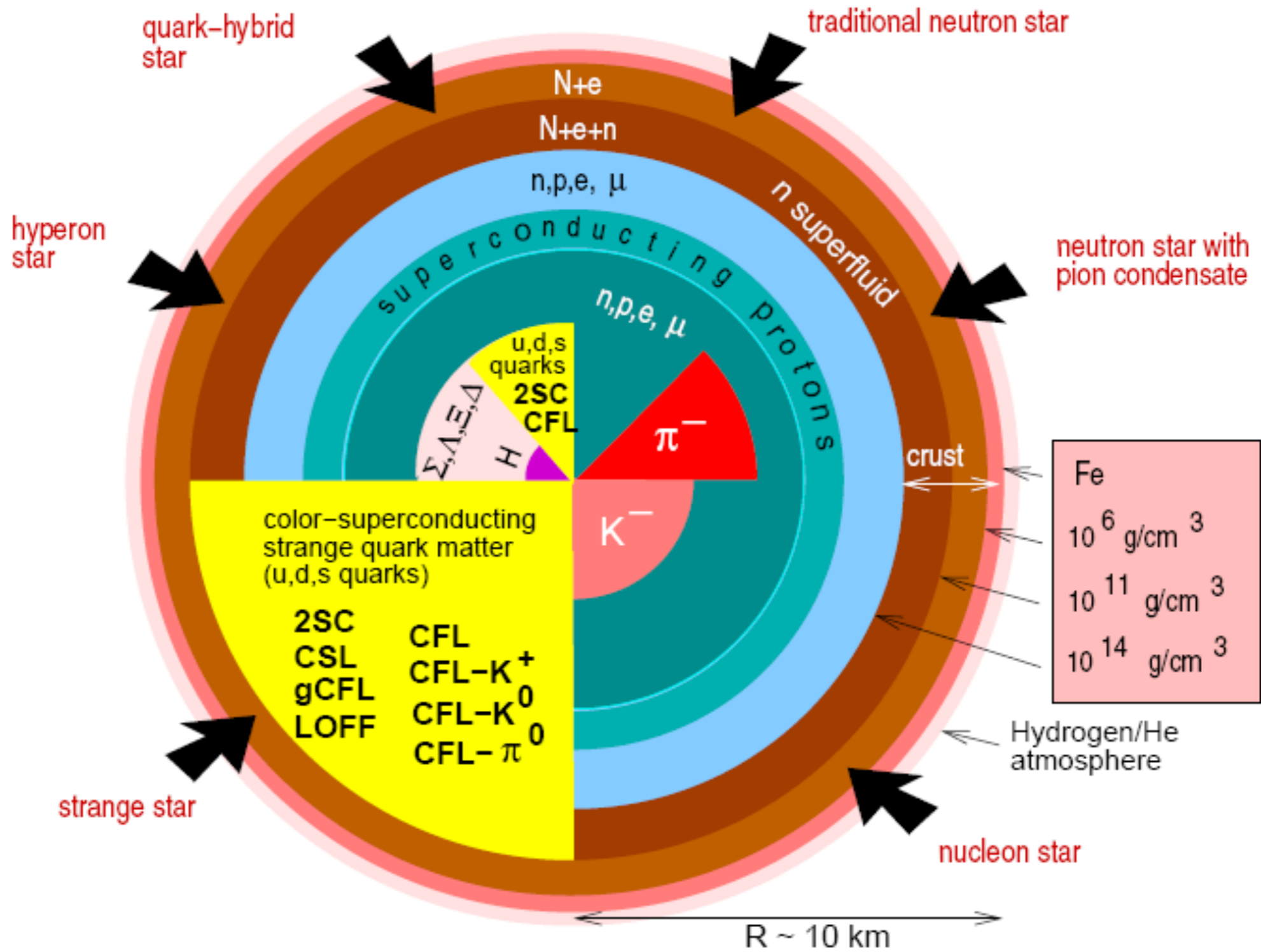


Charge-neutral β -equilibrium matter

→ **Proton fraction**

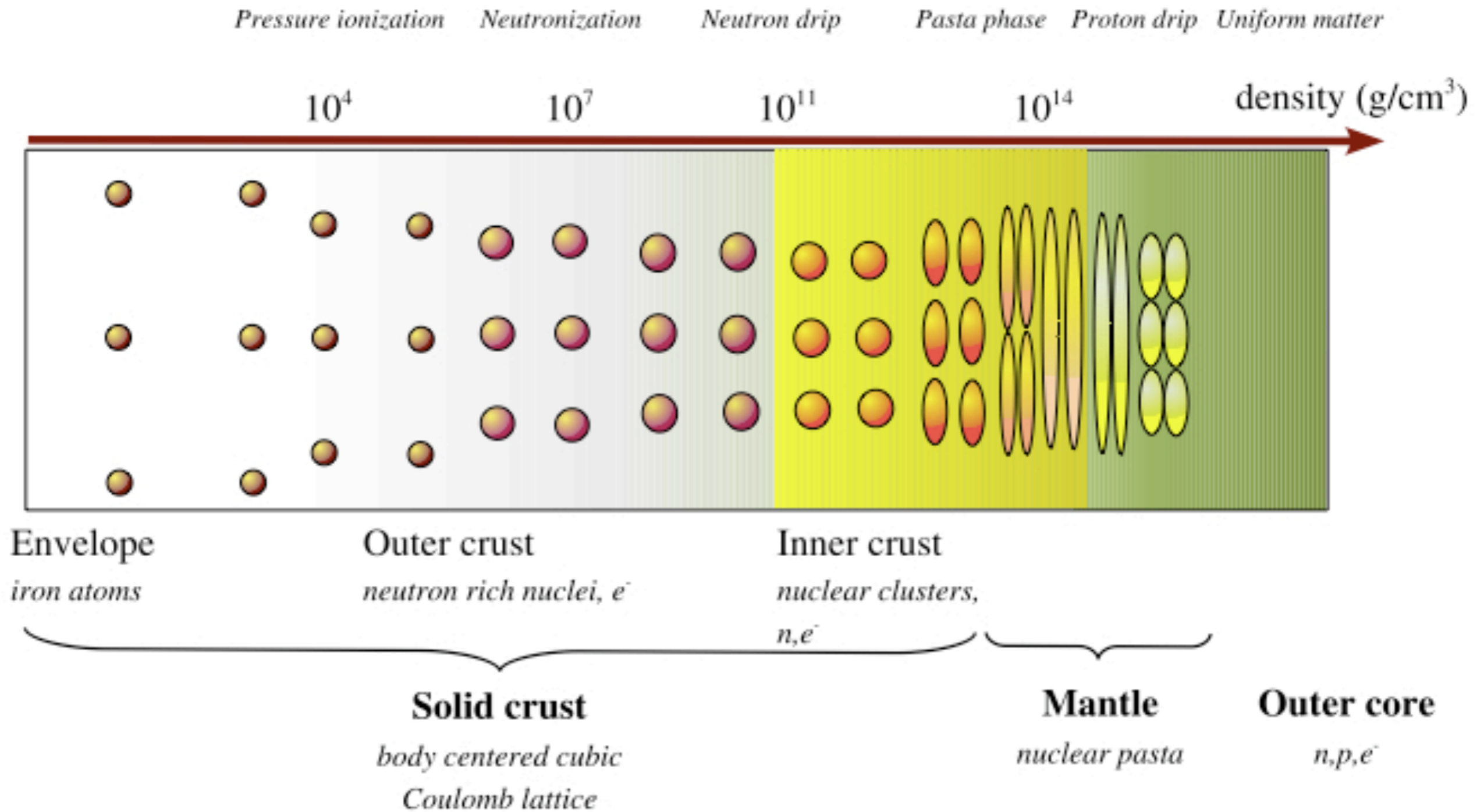
- Simple estimate (non-interacting nucleons) 3%
- More refined calculations 11%

...to, possibly, a very rich structure



[Figure: F. Weber]

Neutron star crust



[Figure: ...]

TOV equations

◎ Basic description of neutron-star structure

○ Hydrostatic equilibrium equations

+ General relativity corrections necessary given the compactness of these objects

Tolman-Oppenheimer-Volkoff (TOV) equations

pressure

$$\frac{dP}{dr} = -G \frac{m(r)\epsilon(r)}{r^2} \left(1 + \frac{4\pi r^3 P}{m(r)c^2}\right) \left(1 + \frac{P}{\epsilon(r)c^2}\right) \left(1 - \frac{2Gm(r)}{rc^2}\right)^{-1}$$

$$\frac{dm}{dr} = 4\pi \epsilon(r)r^2$$

mass

energy density

Boundary conditions

$$r=0 \rightarrow P = P_c \text{ and } m = 0$$

$$r=R \rightarrow P = 0 \text{ and } m(R) = M$$

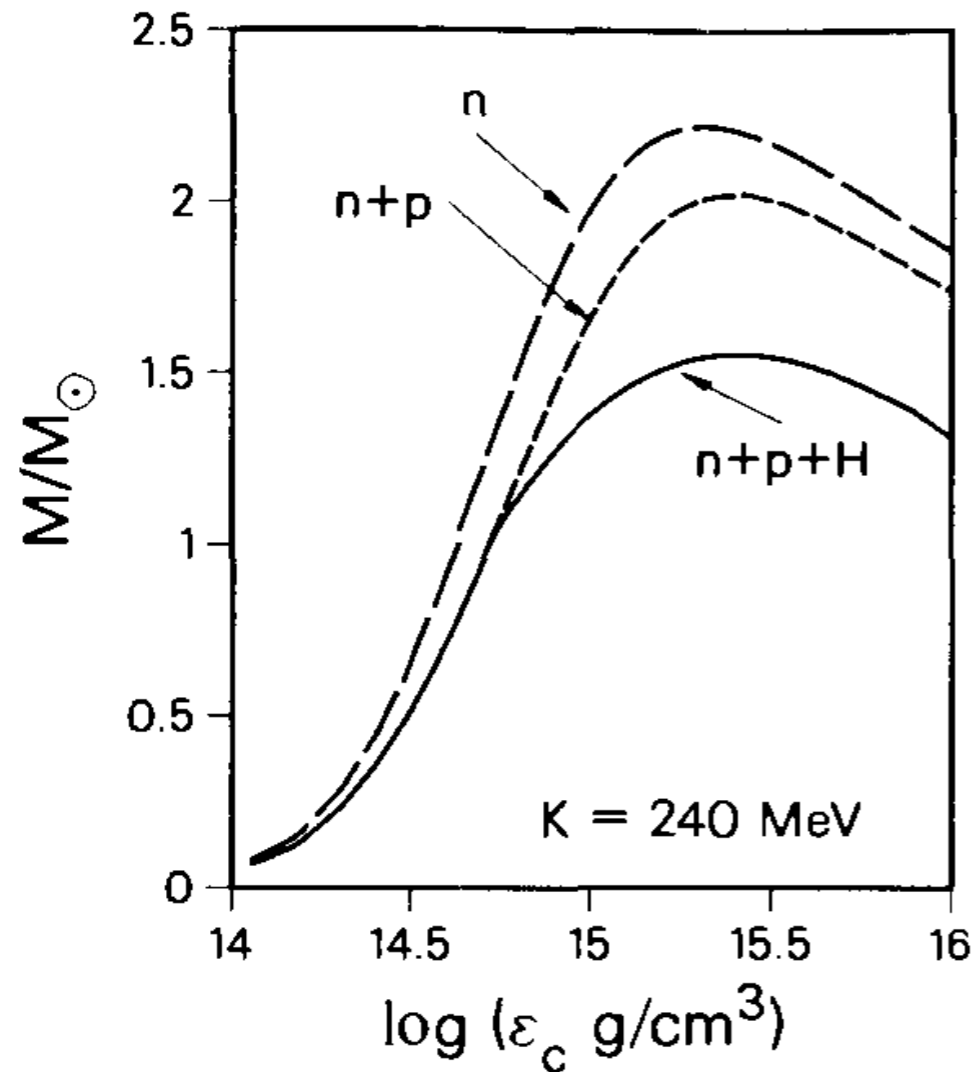
Relation between pressure and energy density required to close the system of equations

$$P = P(\epsilon) \rightarrow \text{Equation of state (EOS)}$$

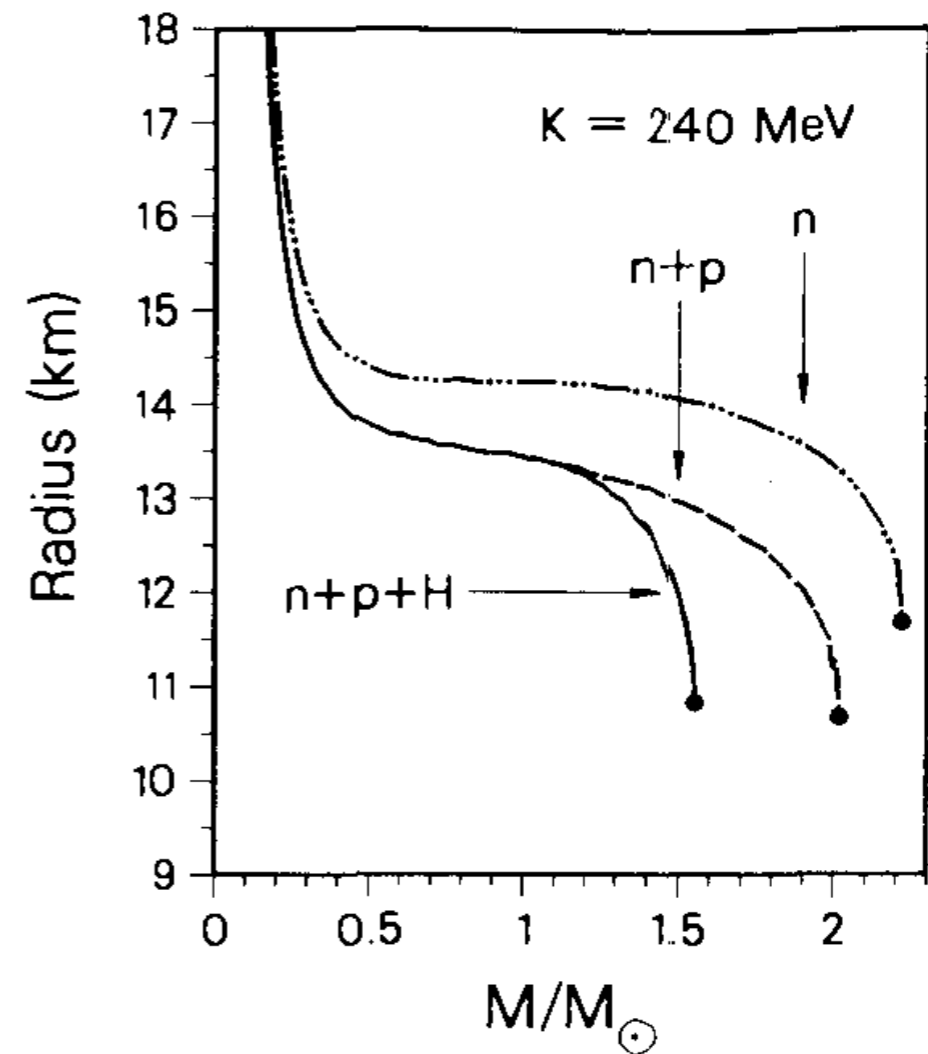
Mass-radius relation

- Solution determines **mass M** and **radius R** of the compact object
- **Central pressure** acts as a parameter

Mass vs. central energy density



Mass vs. radius



Equation of state of neutron-star matter

⊙ In the minimal model, equation of state of neutron-proton-electron matter needed

○ Electrons produce negligible pressure → proton-neutron (“neutron-star”) matter

○ Neutron stars have temperatures $T \sim 10^7\text{-}10^8$ K; $E_{\text{th}} = 8$ keV $\ll E_F$ → $T = 0$ good approximation

⊙ Equation of state of neutron-star matter

○ Baryon density $n = \frac{A}{V}$

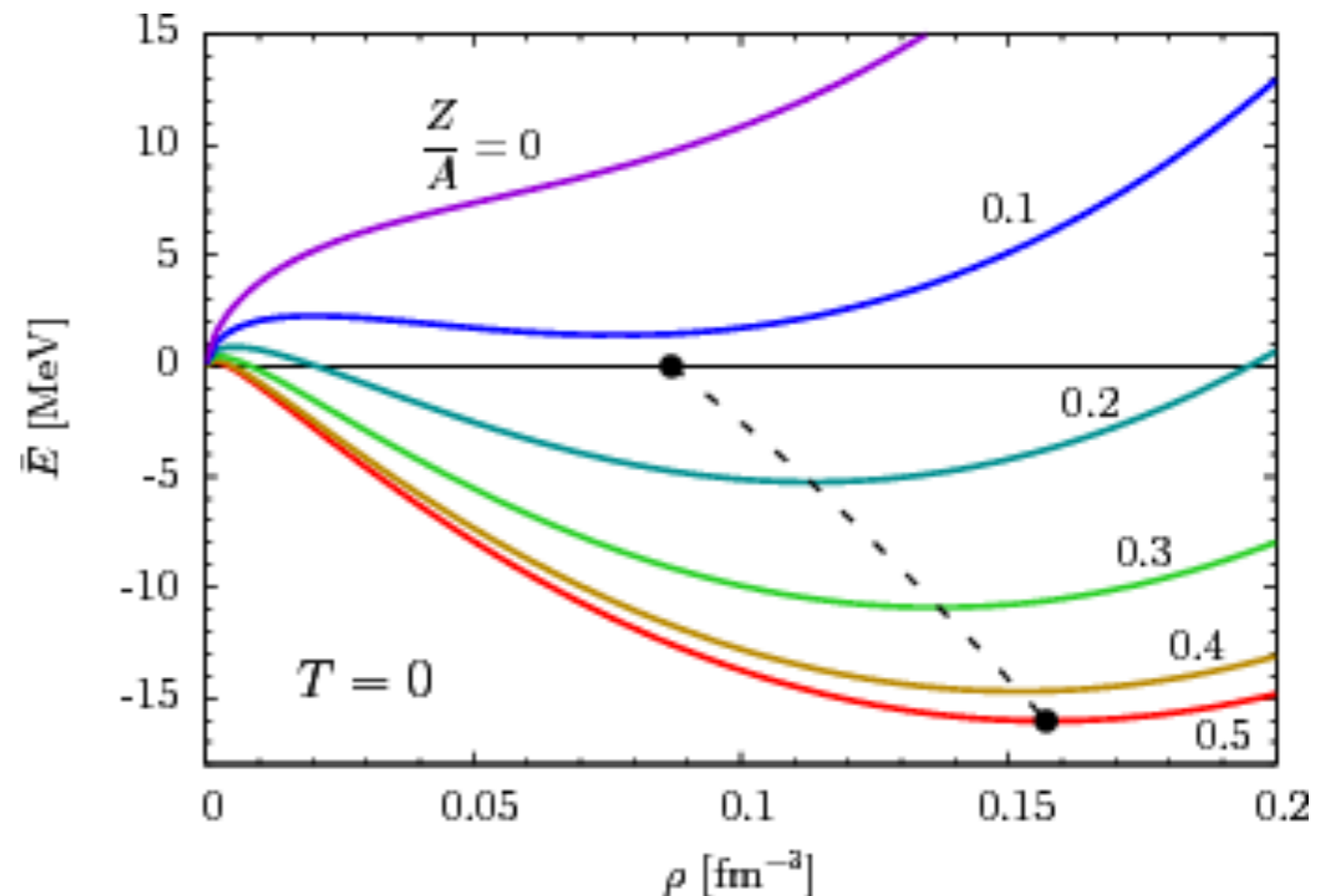
○ Energy density $\epsilon = \frac{E}{V} = n \frac{E}{A}$

○ Pressure $P = n^2 \frac{\partial E/A}{\partial n}$

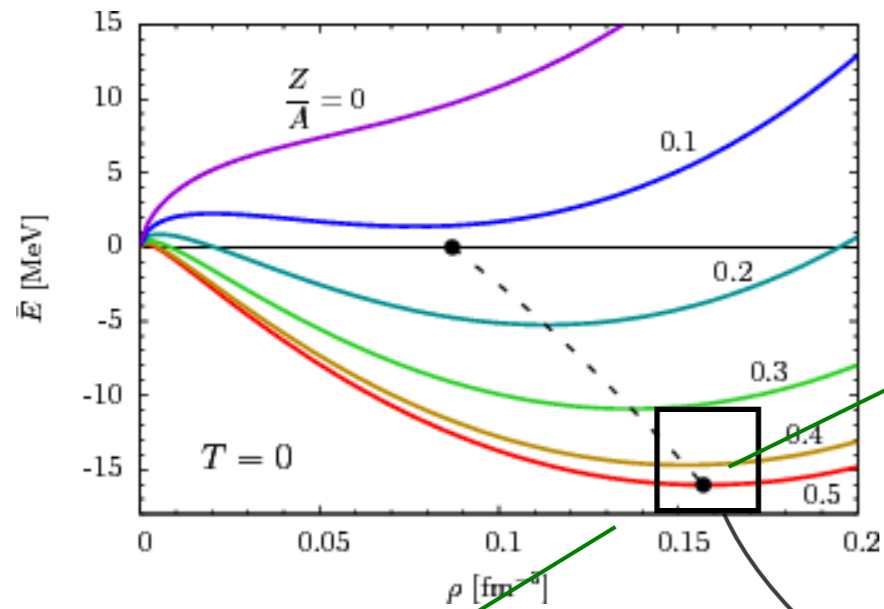


Equation of state $\frac{E}{A}(n, x)$

with proton fraction $x \equiv n_p/n$



Equation of state of neutron-star matter



1. Saturation density

2. Saturation energy

$$E_0 = E(n_0, 0)/A$$

3. Incompressibility

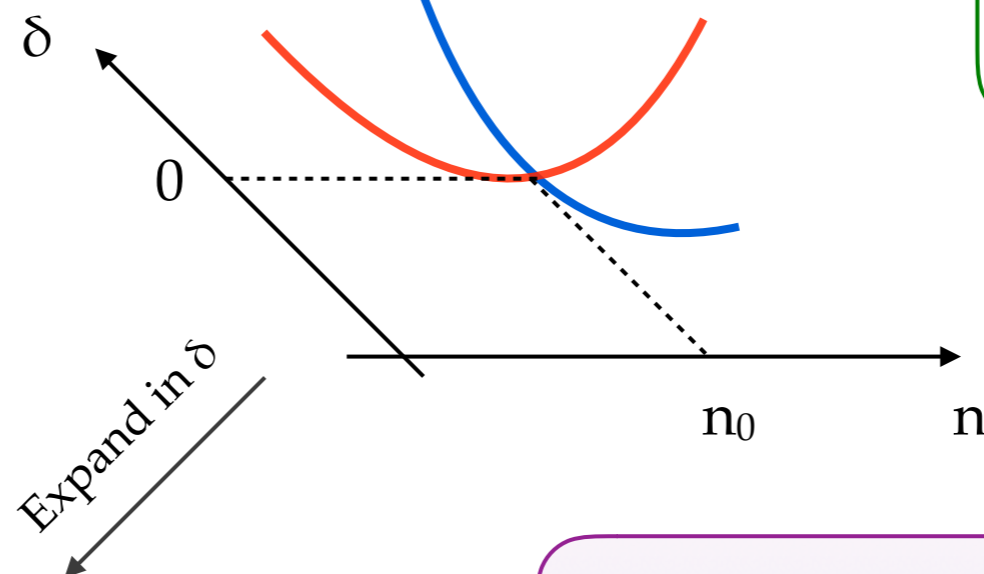
$$E(n, \delta = 0)/A \approx E_0 + (K/2) \eta^2$$

5. Symm. energy slope

4. Symmetry energy

$$E_{\text{sym}}(n) \approx S_v + L \eta$$

$$E(n, \delta)/A = E(n, 0)/A + E_{\text{sym}}(n) \delta^2$$



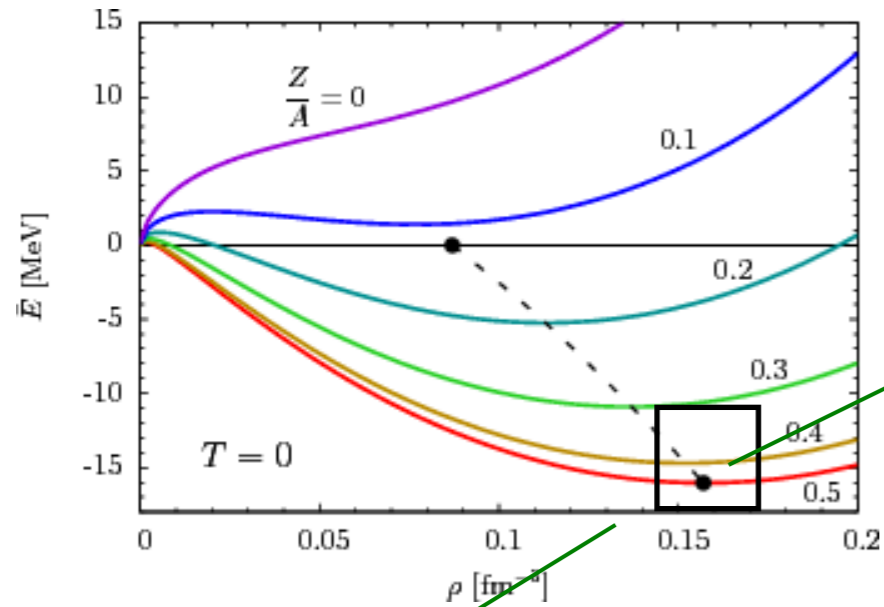
$$\eta = (n - n_0)/(3n_0)$$

$$\delta = (n_n - n_p)/n$$

Pure neutron matter

$$E(n, 1)/A \approx (E_0 + S_v) + L \eta$$

Equation of state of neutron-star matter



1. Saturation density

2. Saturation energy

$$E_0 = E(n_0, 0)/A$$

3. Incompressibility

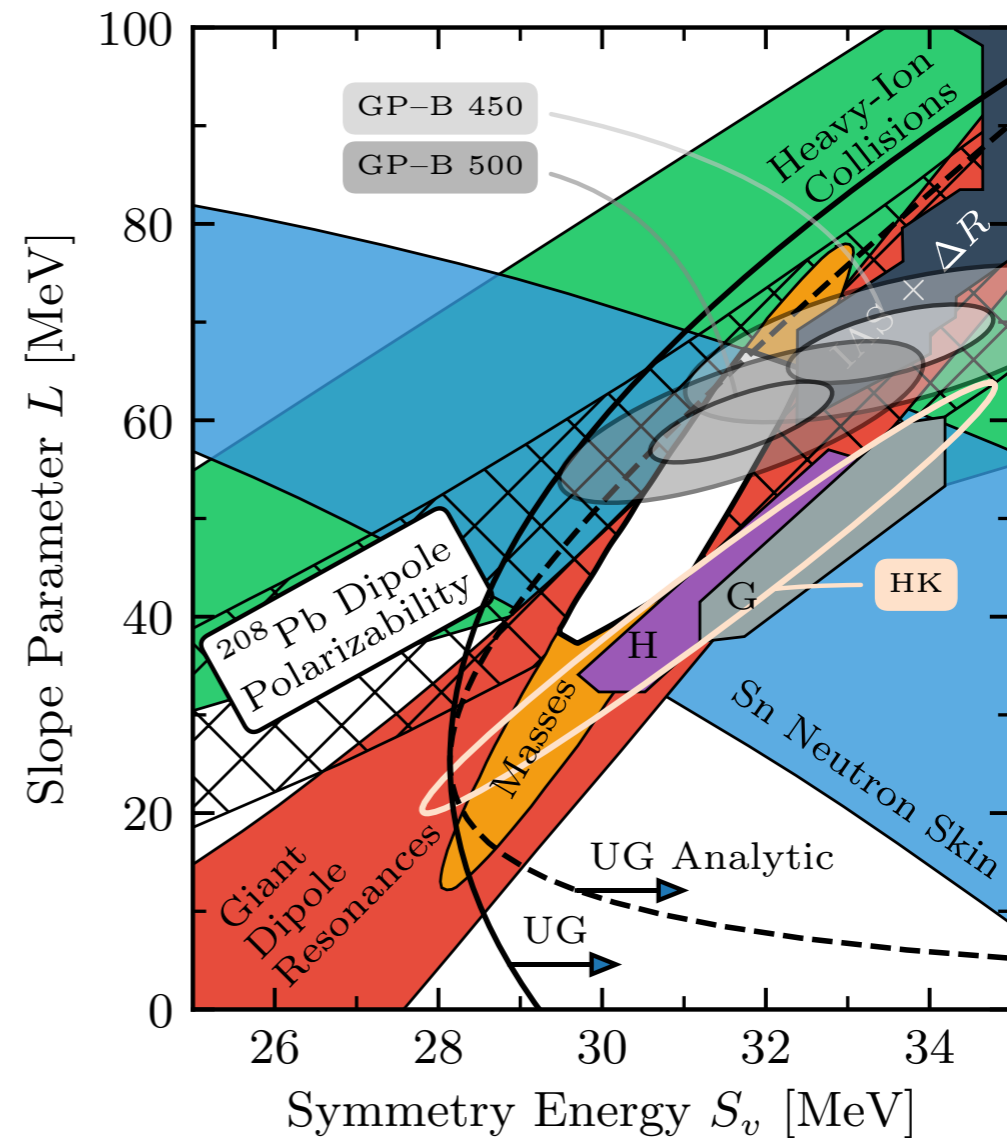
$$E(n, \delta = 0)/A \approx E_0 + (K/2) \eta^2$$

5. Symm. energy slope

4. Symmetry energy

$$E_{\text{sym}}(n) \approx S_v + L \eta$$

$$E(n, \delta)/A = E(n, 0)/A + E_{\text{sym}}(n) \delta^2$$



[Drischler et al. 2021]

Simulating nuclear matter

- ⊙ Modelling of nuclear matter

- **Homogeneous system** of nucleons interacting via strong interactions (Coulomb switched off)
- Thermodynamic limit ($A \rightarrow \infty$, $\mathcal{V} \rightarrow \infty$, $n=A/\mathcal{V}$ constant)
- Pure neutron matter is simpler (weaker 3N forces, tensor components, ...)
- Basis: plane waves well suited (translational invariance)
- Calculations easier than for finite nuclei (no surface, symmetry breaking often negligible, ...)



- ⊙ Nuclear matter as a **theoretical laboratory** to test interactions & many-body methods

- ⊙ Long history of ab initio nuclear matter calculations

- **Interactions:** schematic interactions, OBE potentials, forces from chiral EFT, SRG evolution, ...
- **Many-body approaches:** exact, correlation-expansion (both non-perturbative and perturbative)



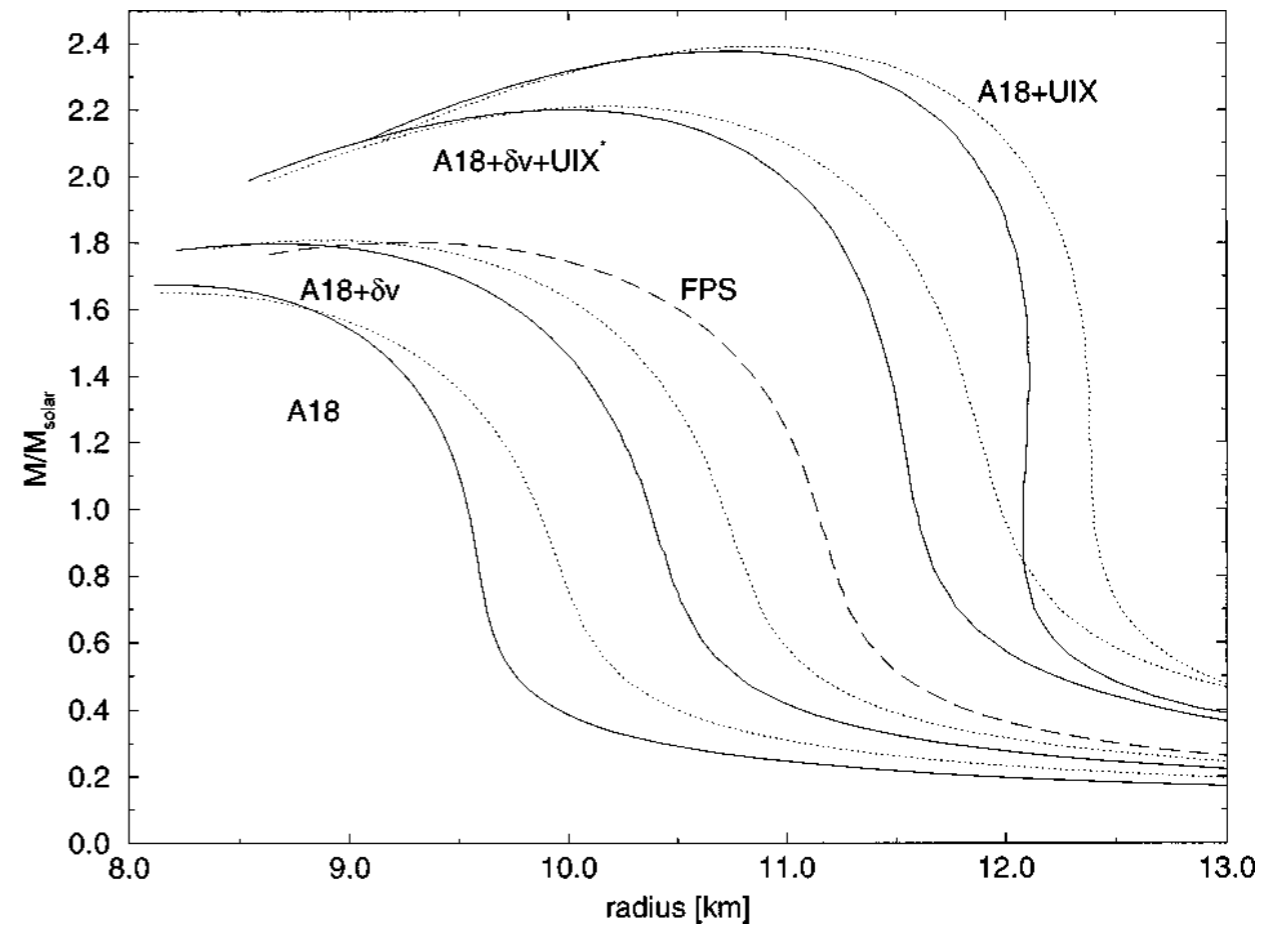
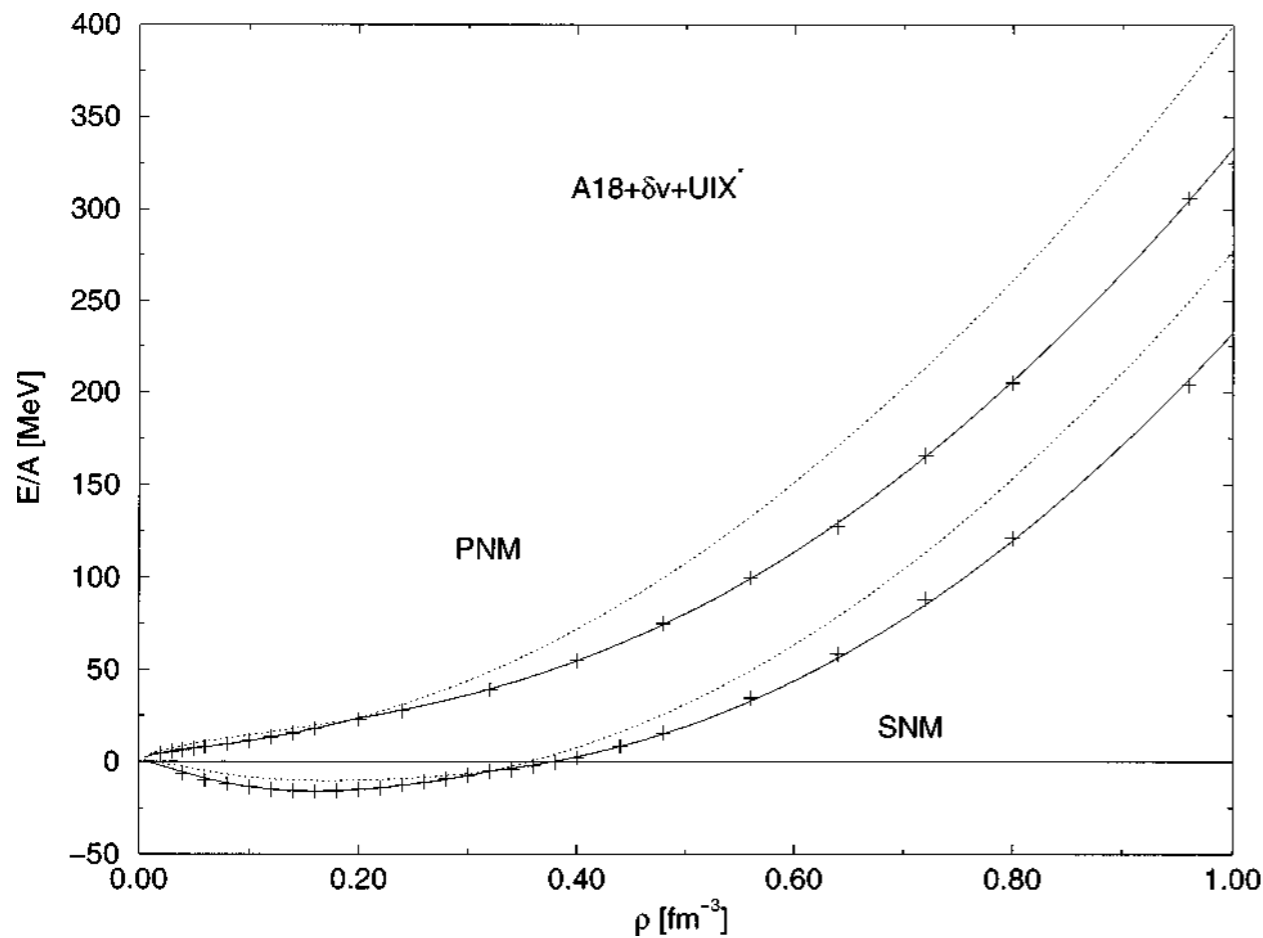
Frequent benchmarks between different calculations

First generation of ab initio results

© Akmal-Pandharipande-Ravenhall (APR) equation of state

[Akmal *et al.* 1998]

- “Milestone” calculation with AV18 + three-body forces (+ relativistic correction)

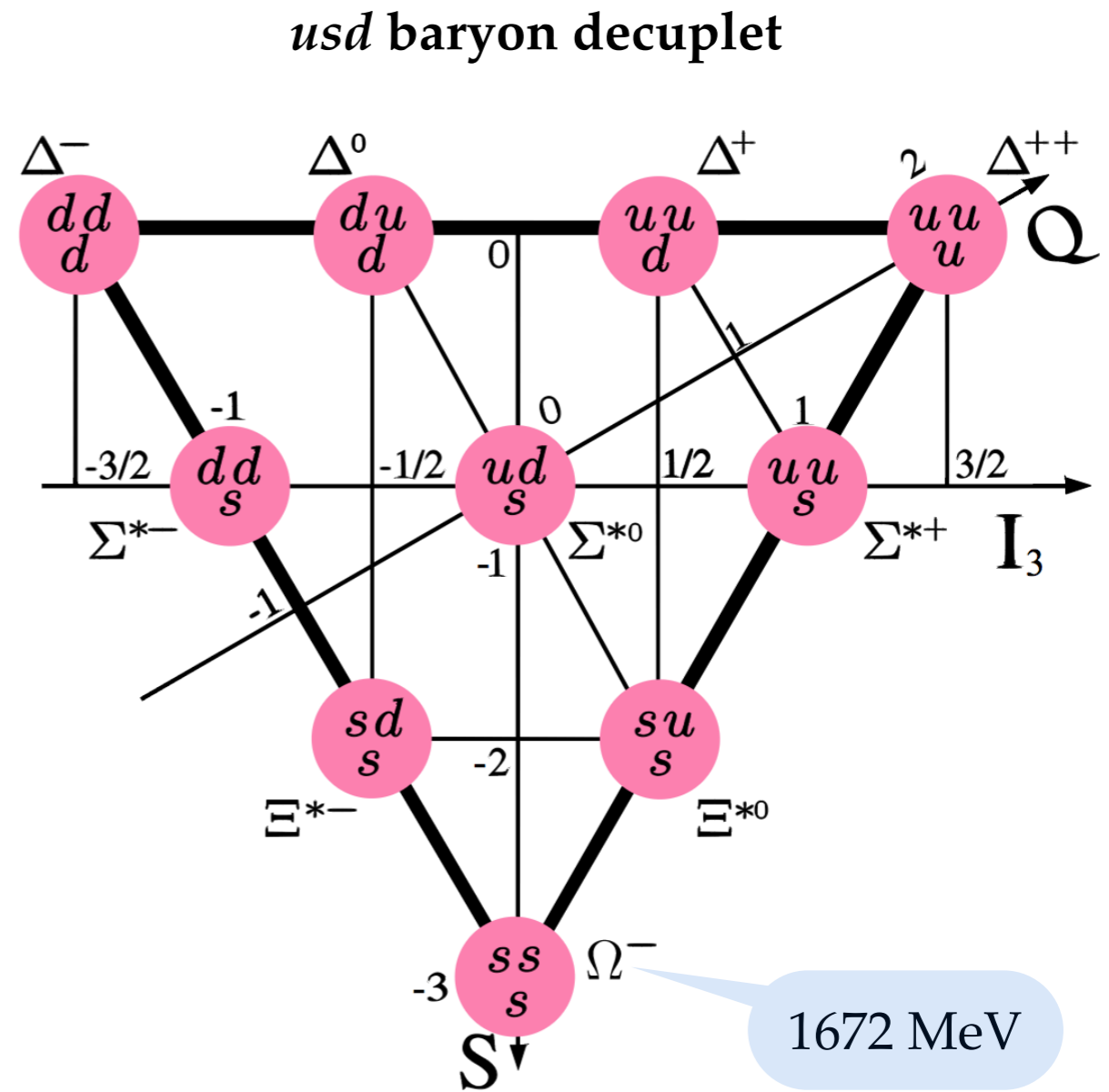
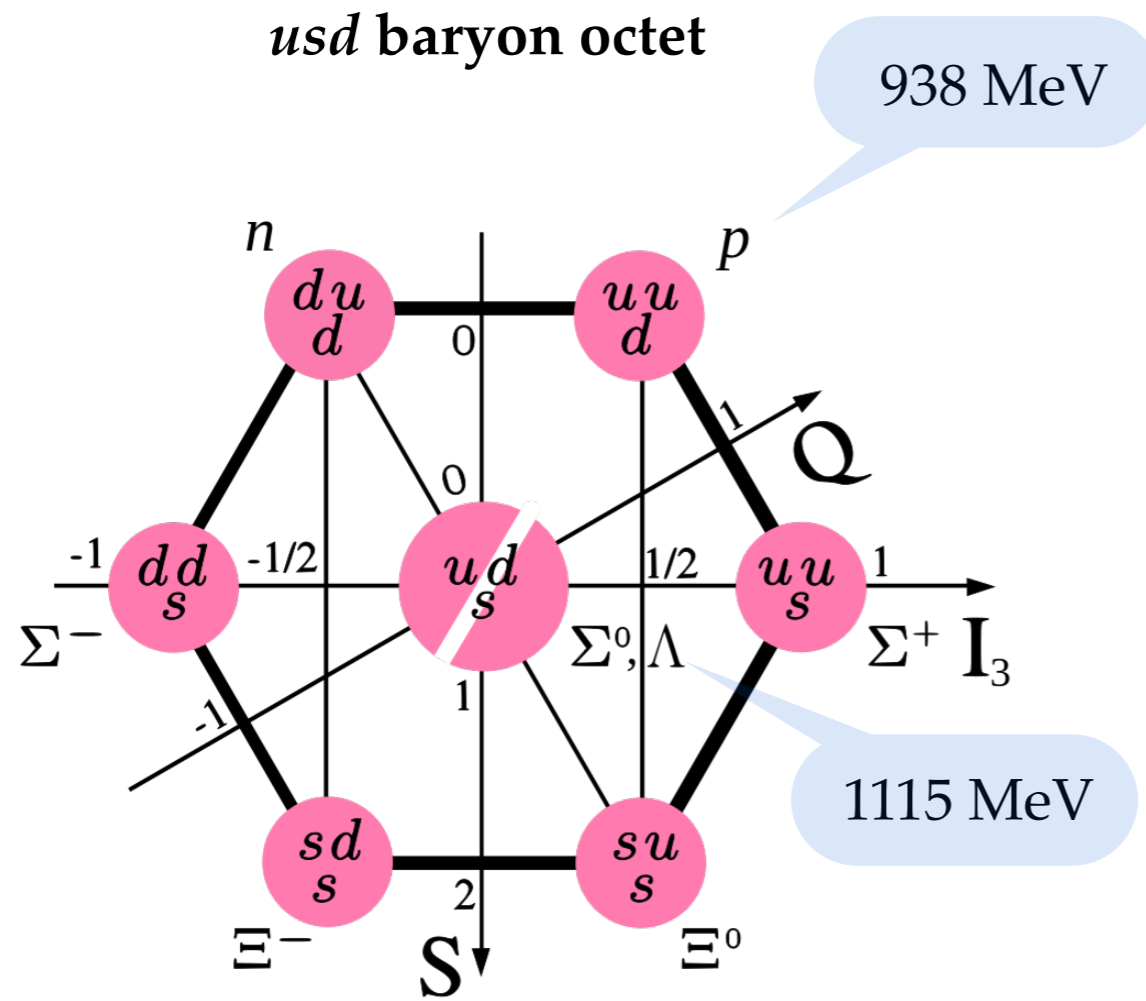


- Not many constraining data on the mass-radius relation at the time
- Is a **description in terms of only nucleons** realistic at such high densities?

Hyperons?

Quarks?

Hyperons

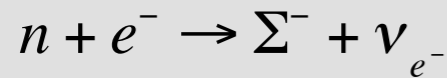
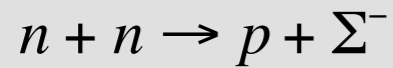
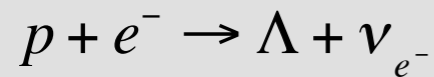
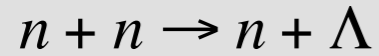


- ◎ **Hyperon:** a baryon containing one, two or three **s** quarks in addition to **u** and **d** quarks
 - Hyperons decay weakly (strangeness conserved by strong and EM interactions)
 - New quantum number: strangeness

Hyperon puzzle

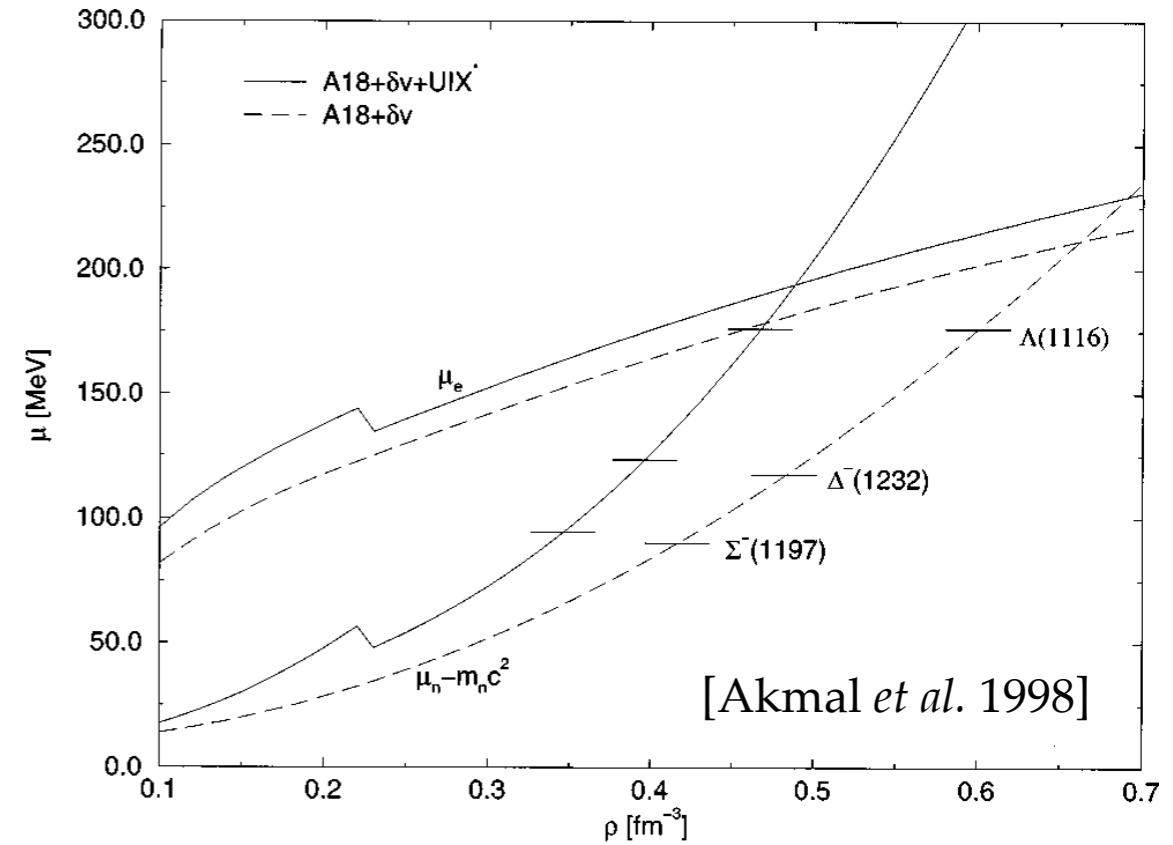
◎ Hyperon production

- Becomes energetically favourable at $n \sim 2-3 n_0$
- β -equilibrium equations get modified



$$\mu_{\Sigma^-} = \mu_n + \mu_{e^-} - \mu_{\nu_{e^-}}$$

$$\mu_{\Lambda} = \mu_n$$



- New degrees of freedom



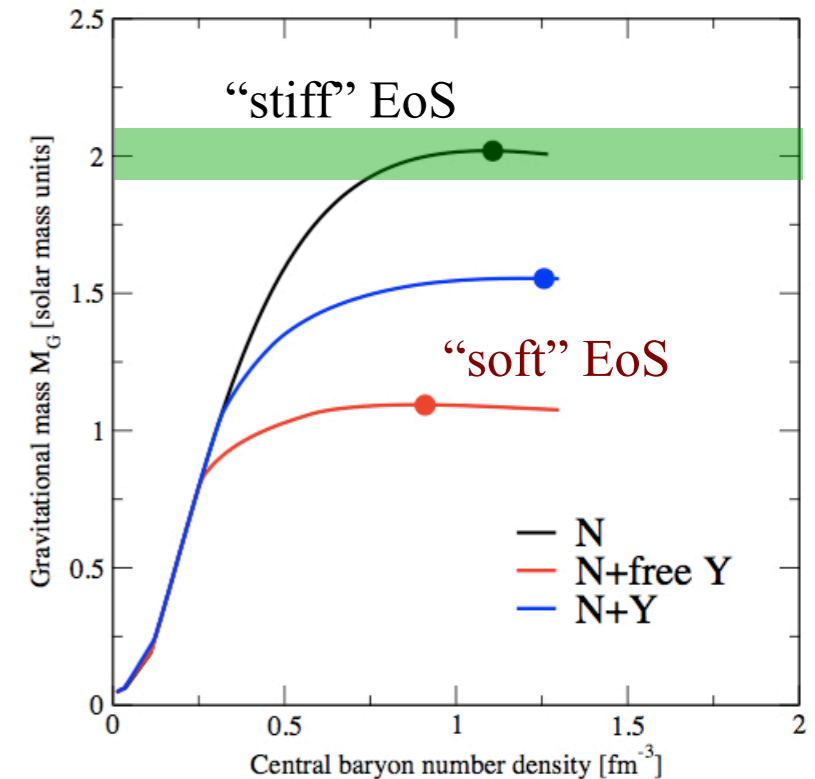
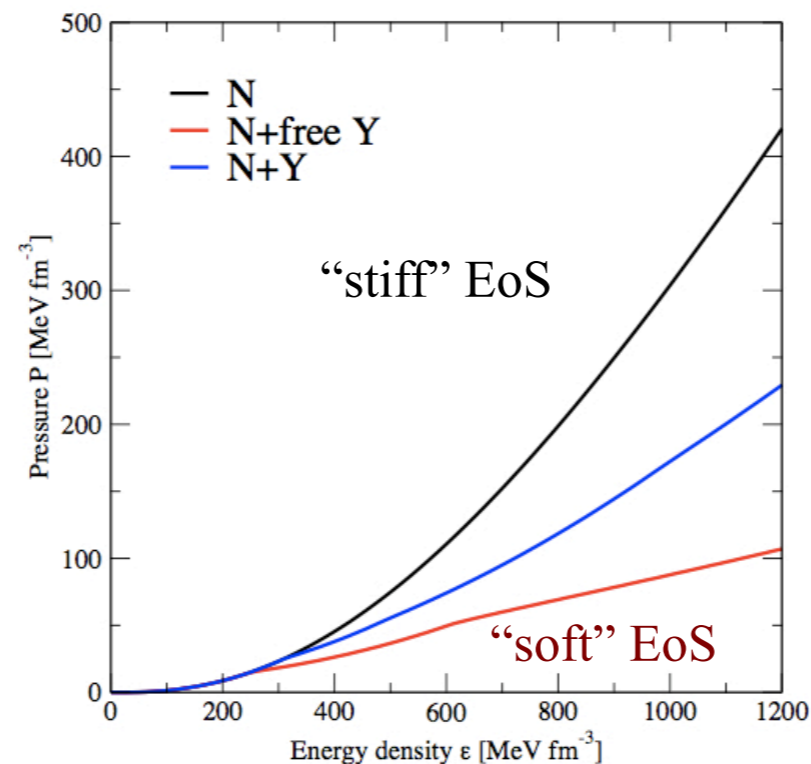
- Softening of the EoS



- Lower maximum mass



- In 2010, $2M_{\odot}$ star observed!

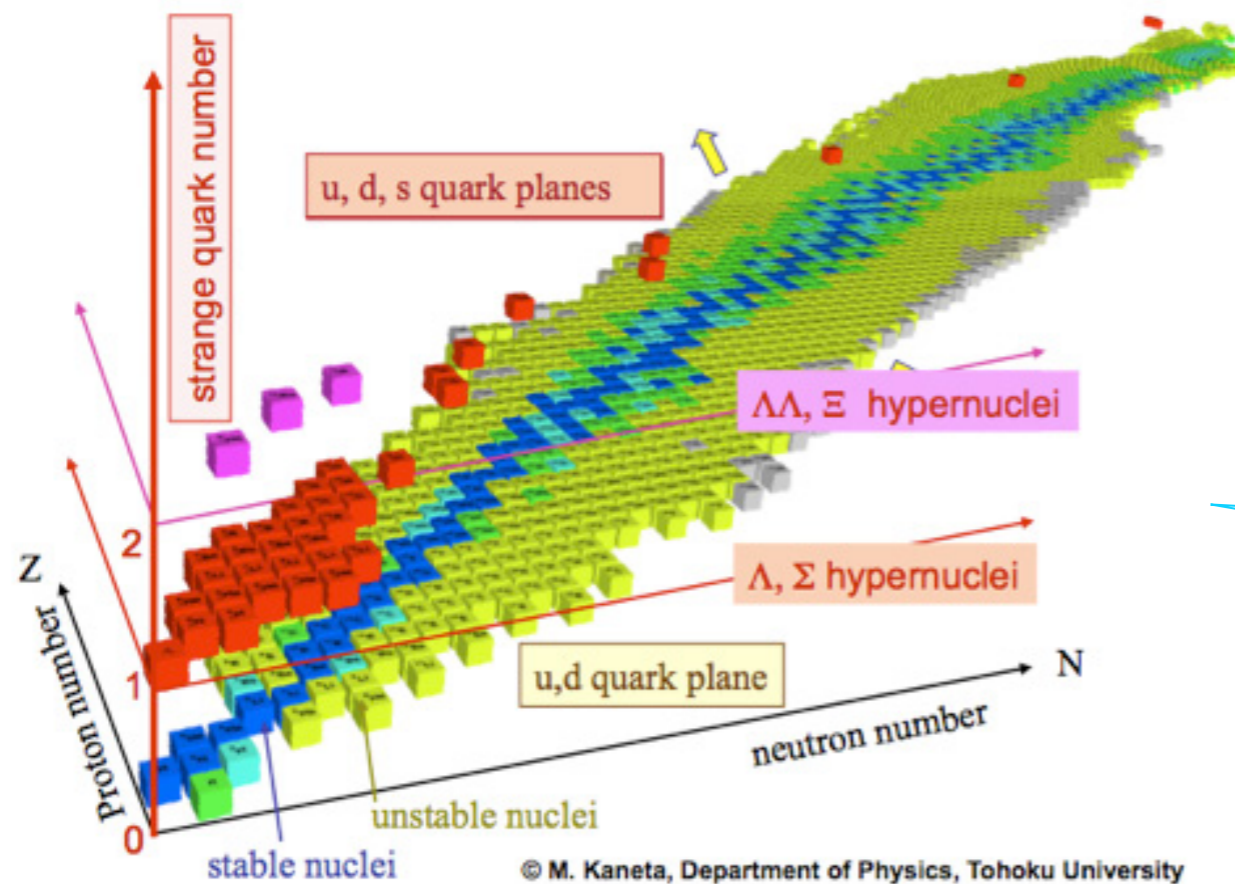


Hypernuclei & hyperon interactions

- ◎ **Hyperon-nucleon scattering**

- Difficult experiments, scarce data

- ◎ **Hypernuclei:** nuclei with at least one hyperon in addition to protons and neutrons



About 40 hypernuclei produced
+ various experiments planned

Idea: deduce YN interaction from
reverse-engineering NCSM results

- ◎ **Relativistic pp collisions**

- Study of correlations between strange baryonic products

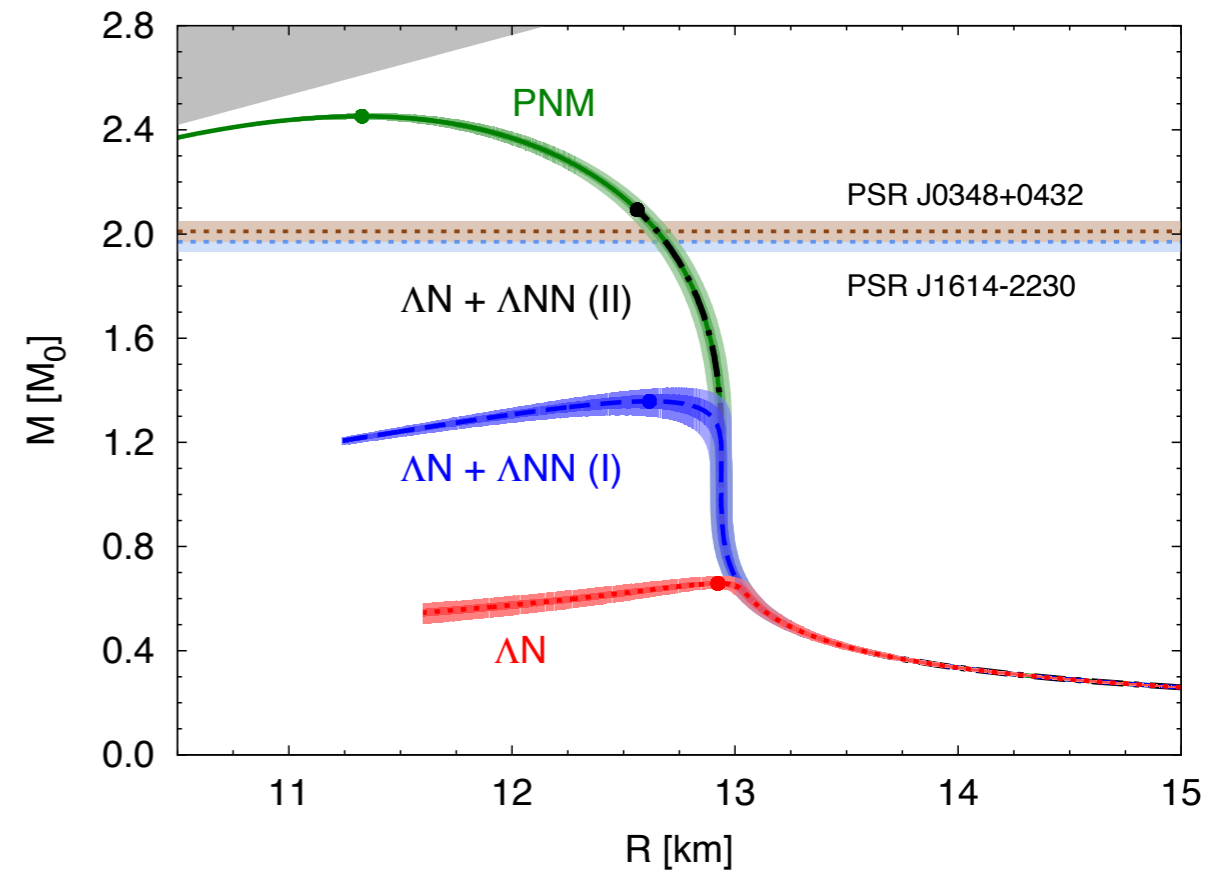
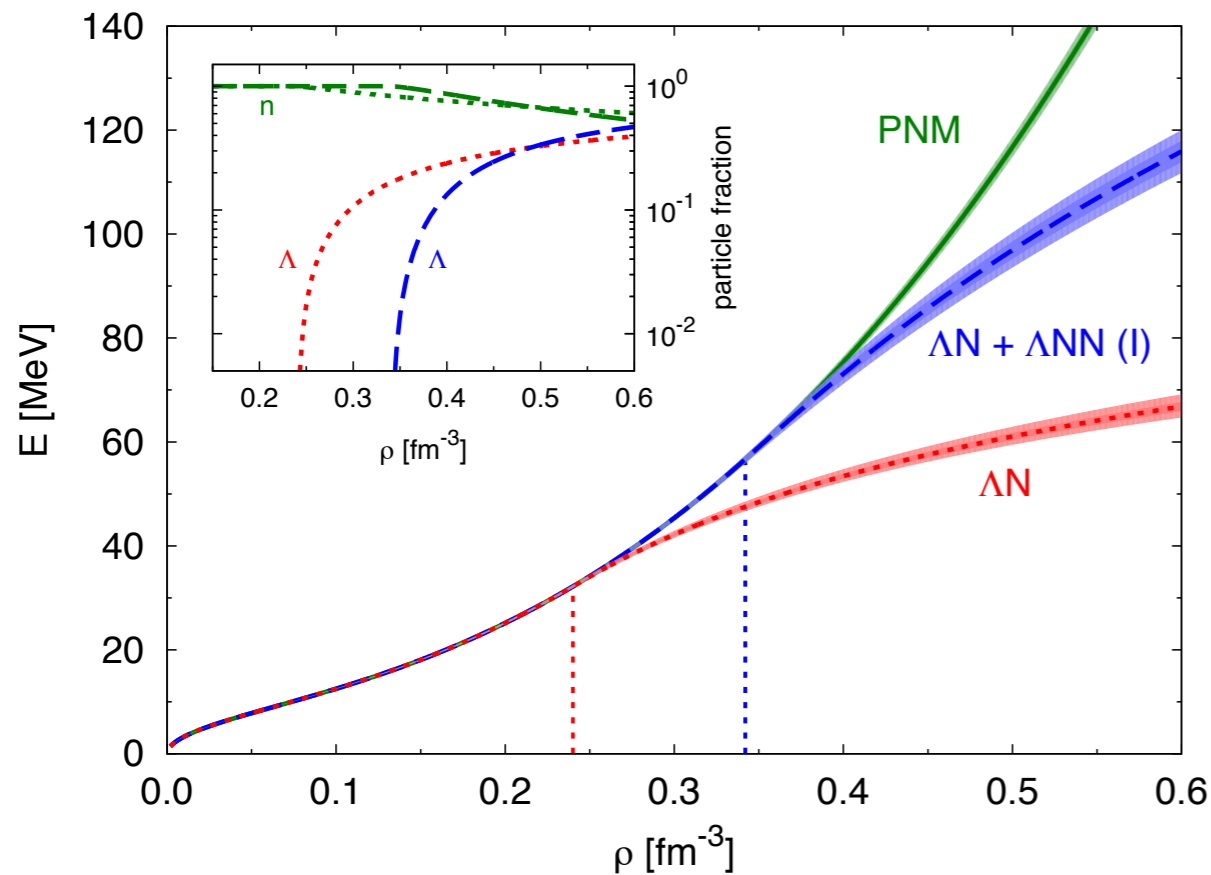
⇒ Possible game changer: **interactions from lattice QCD**

Hyperons in neutron stars

Modern calculations leave the problem open

- Strong sensitivity on (poorly known) YNN interactions

[Lonardoni *et al.* 2015]



Possible solutions:

- Poor knowledge of YN, YY, YN, YYN, YYY interactions
- Critical density not reached
- Transition to quark matter in the neutron star interior
- ?

Quark stars

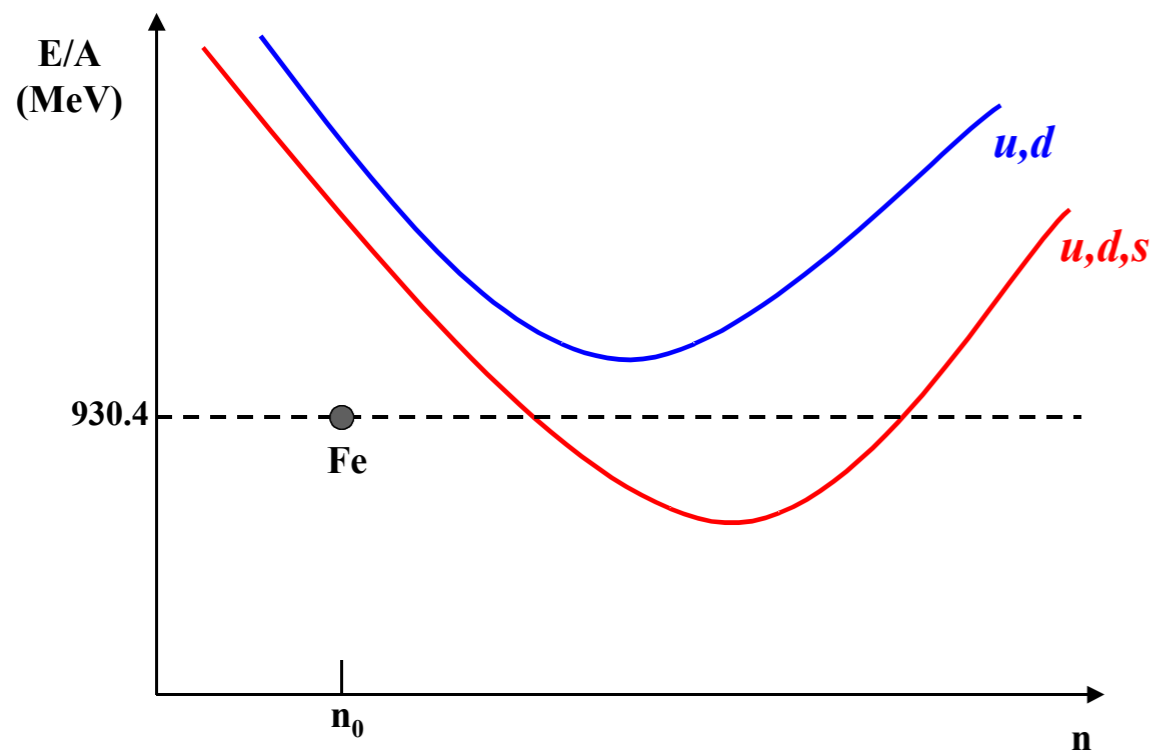
⊙ Hybrid stars → outer hadronic layers, deconfined quarks in the interior

○ Also leads to a softening of the equation of state

⊙ Stars made purely of quarks → “Strange stars”

Strange quark matter hypothesis

[Bodmer 1971, Terazawa 1979, Witten 1984]



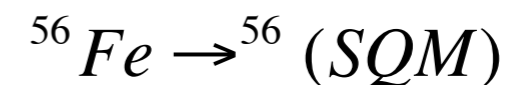
3-flavour u,s,d quark matter could be the **true ground state** of strongly interacting matter



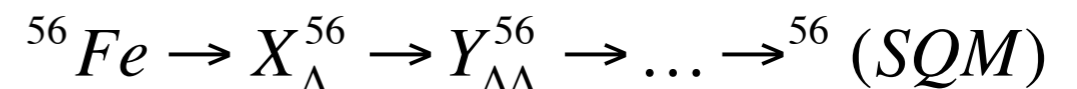
Why nuclei don't decay into droplets of strange quark matter?



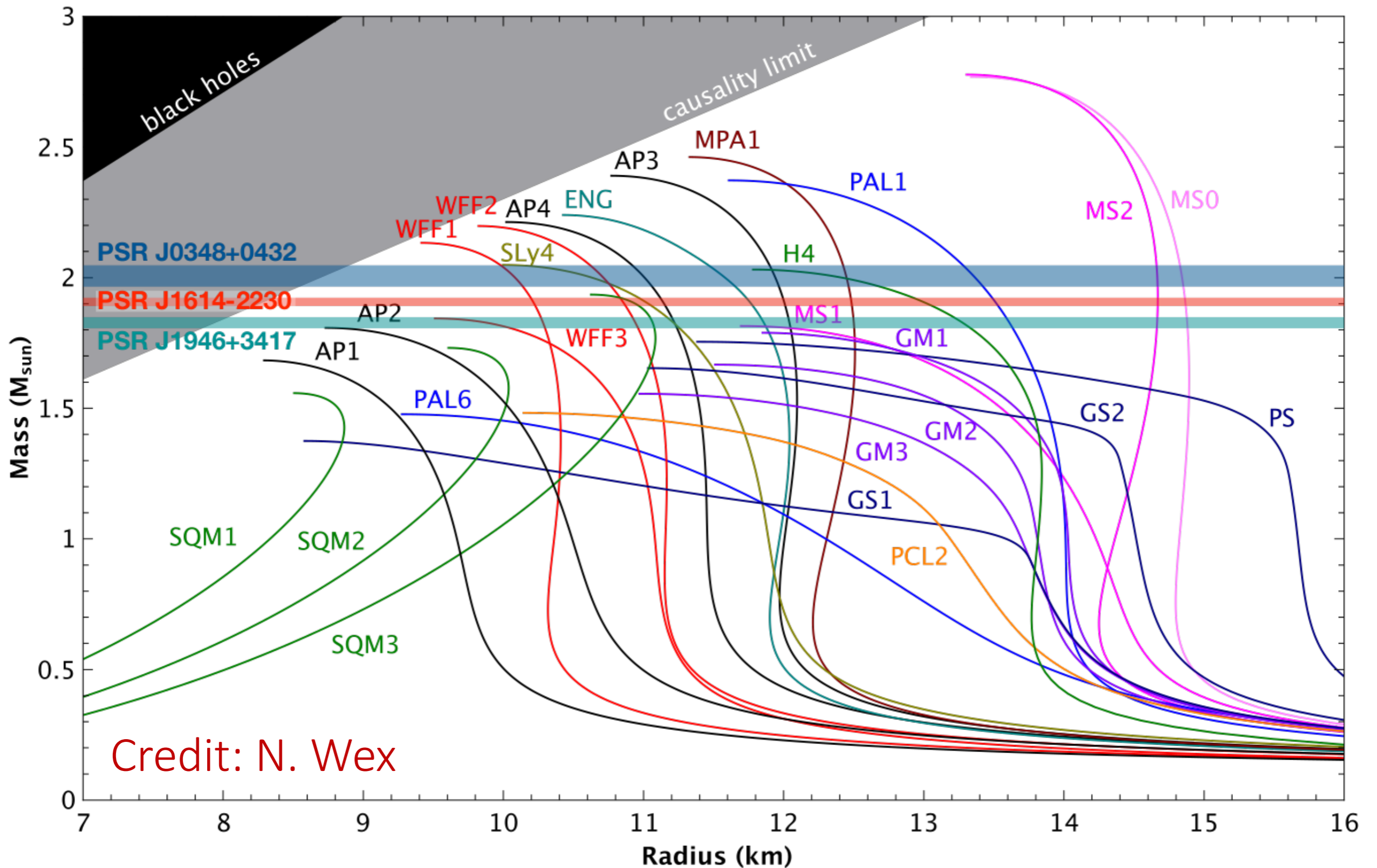
Probability for direct decay very small



Sequential decay energetically forbidden



Proliferation of EoS

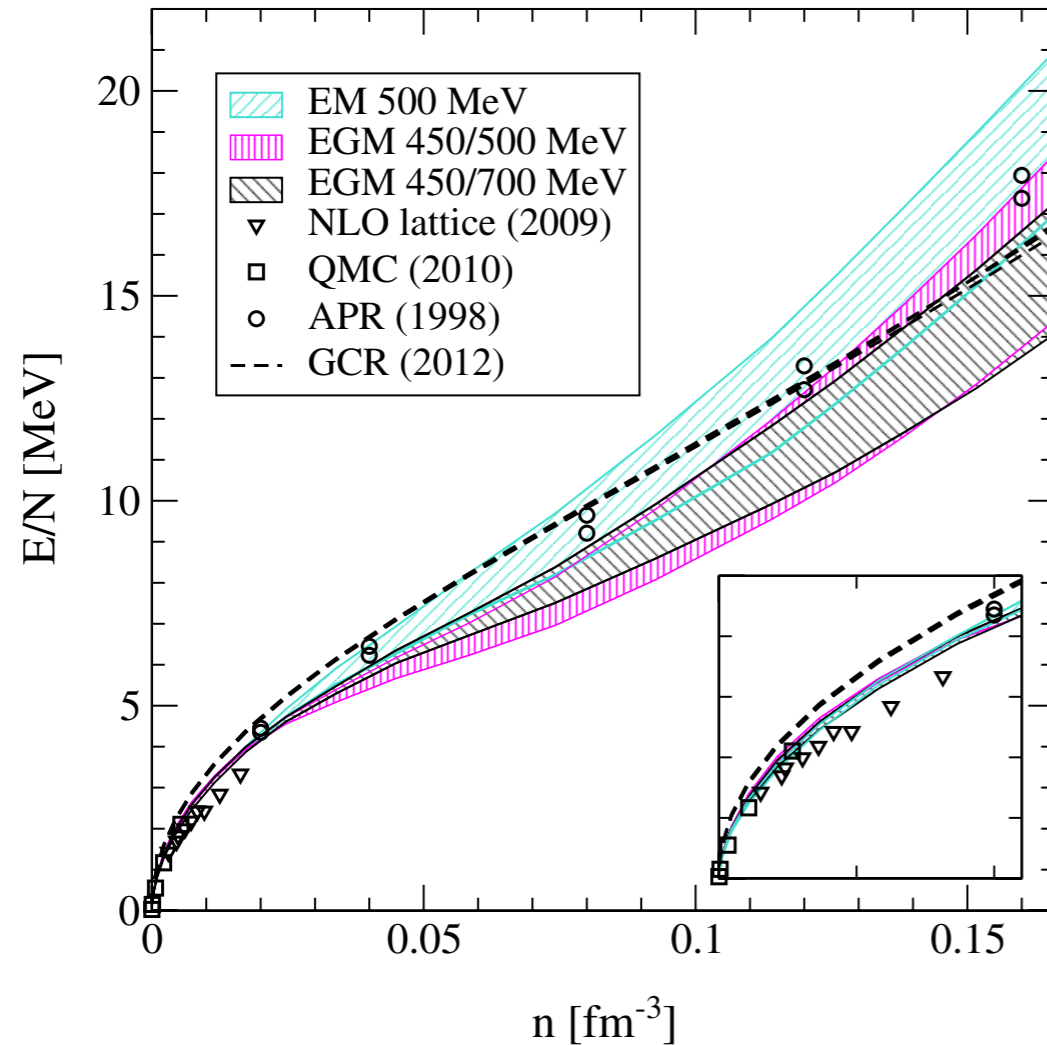


Chiral EFT

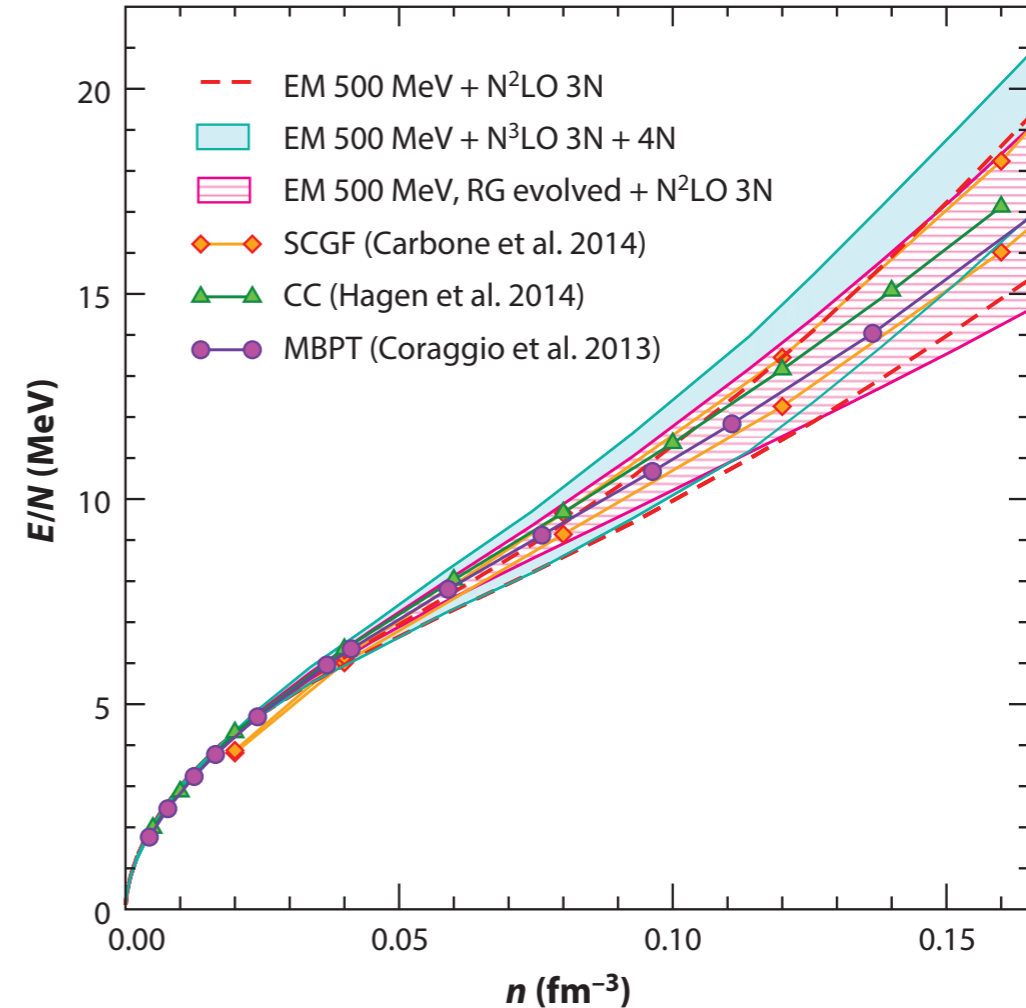
	NN forces	3N forces	4N forces
LO (Q^0)	2	—	—
NLO (Q^2)	7	—	—
N ² LO (Q^3)	0	2	—
N ³ LO (Q^4)	12	0	0
N ⁴ LO (Q^5)	0	?	?

⇒ No new 3N and 4N LECs in neutron matter until N⁴LO

Equation of state of neutron matter



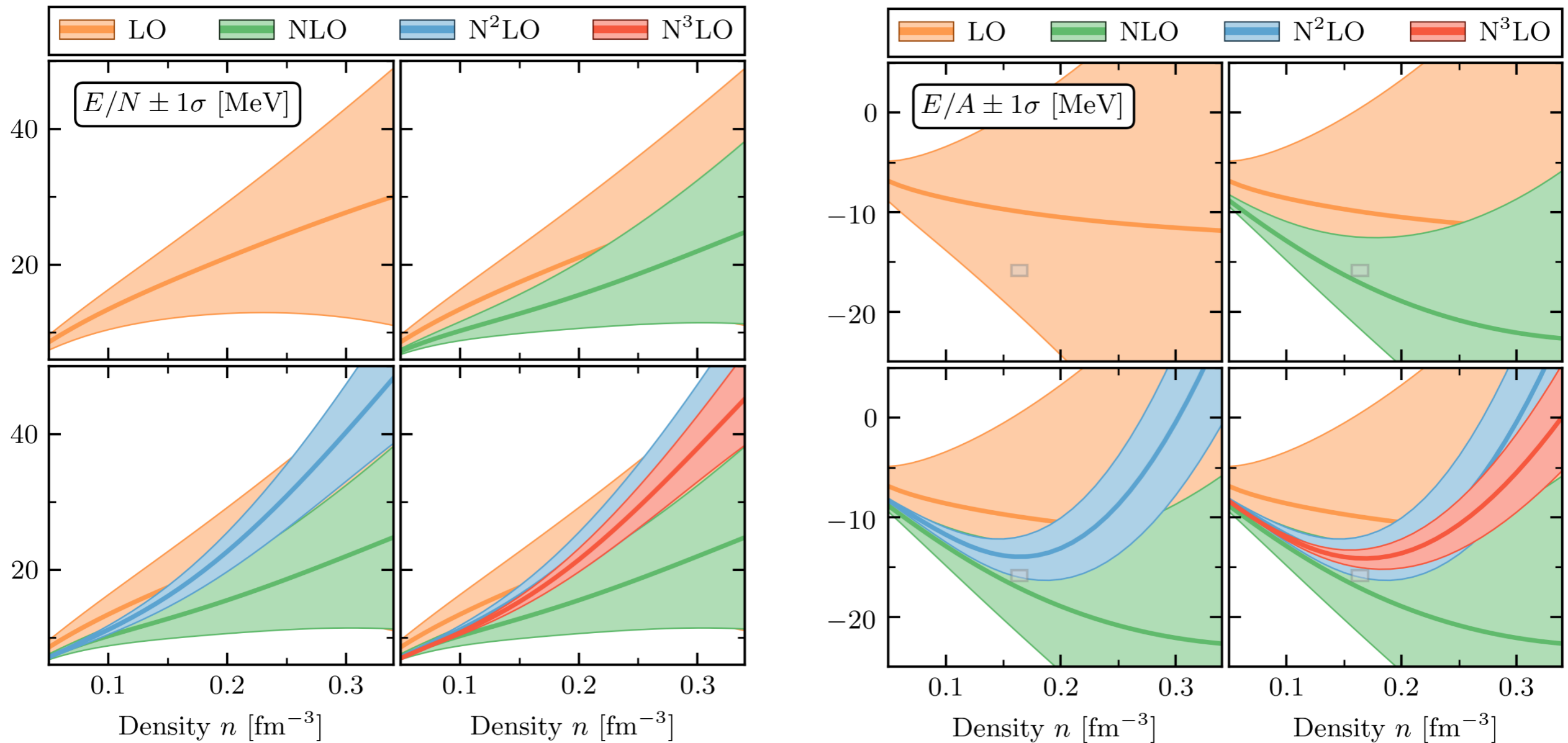
[Tews *et al.* 2013]



[Hebeler *et al.* 2015]

- ⊙ Benchmarks between several calculations (perturbative & non-perturbative)
- ⊙ Low-density part constrained by exact results
- ⊙ Uncertainties grow with density \rightarrow breakdown of chiral expansion

Equation of state of neutron & symmetric matter

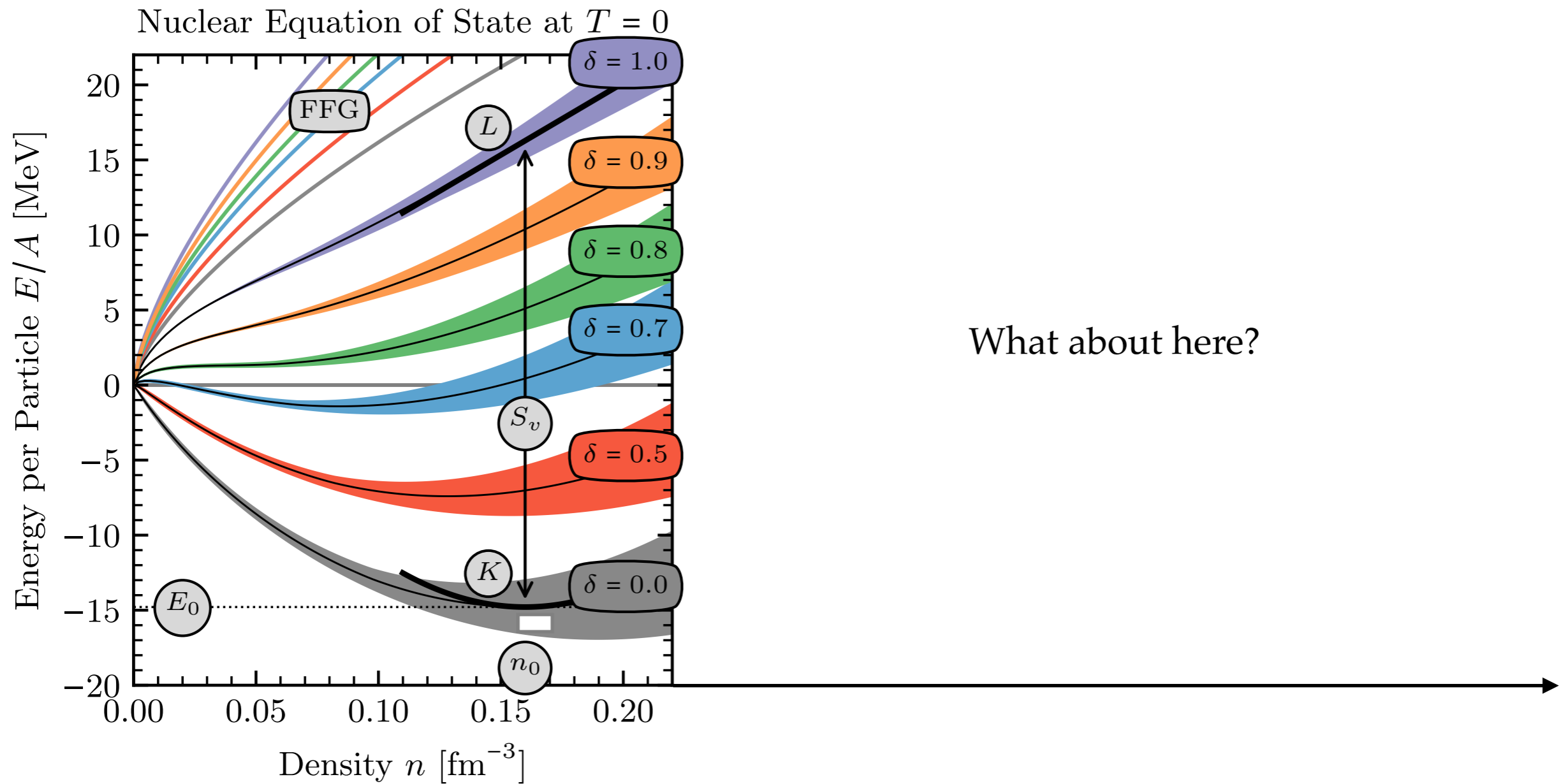


[Drischler *et al.* 2021]

- ⊙ Order-by-order convergence of chiral interactions
- ⊙ Going beyond N³LO currently problematic

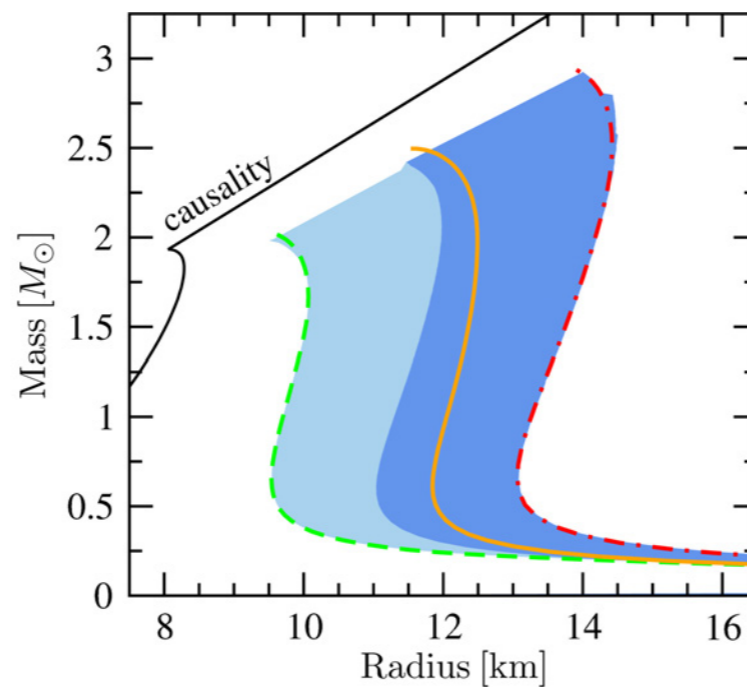
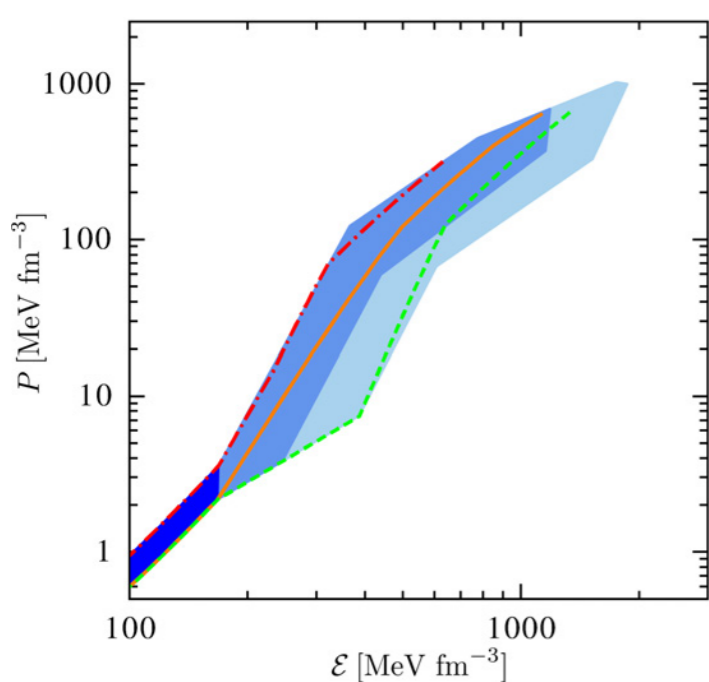
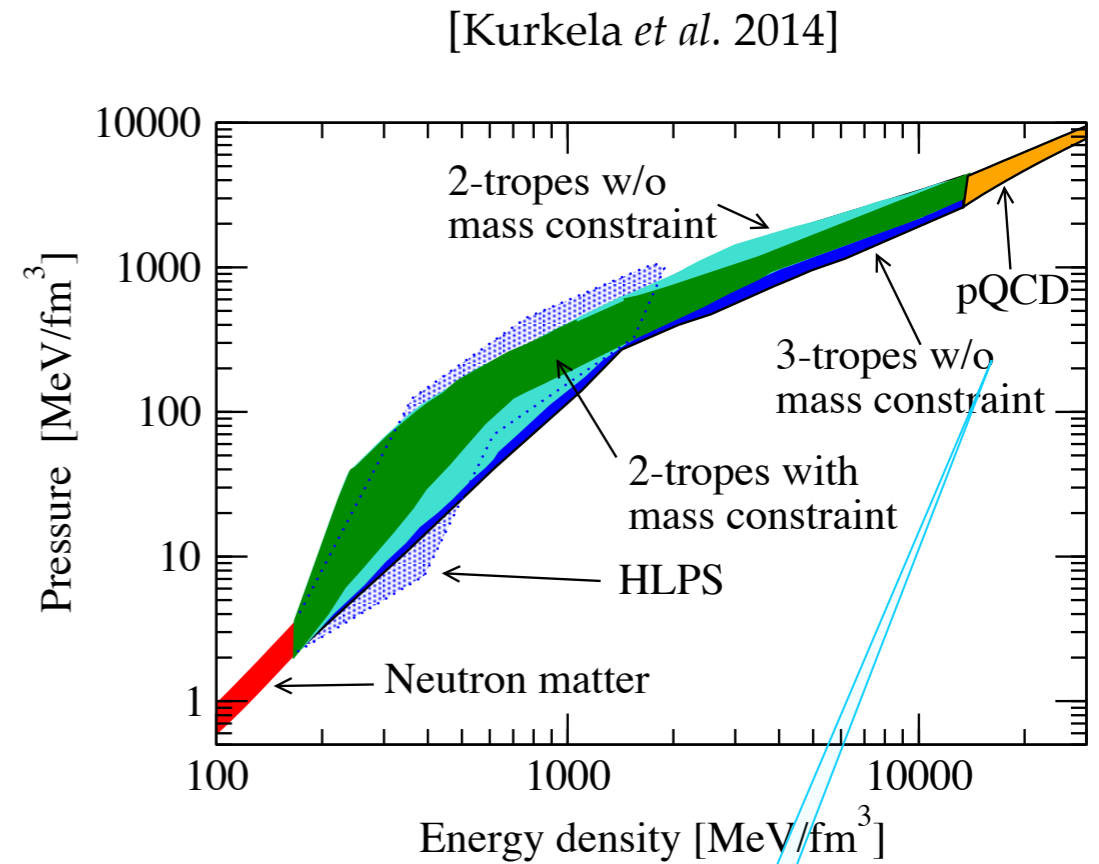
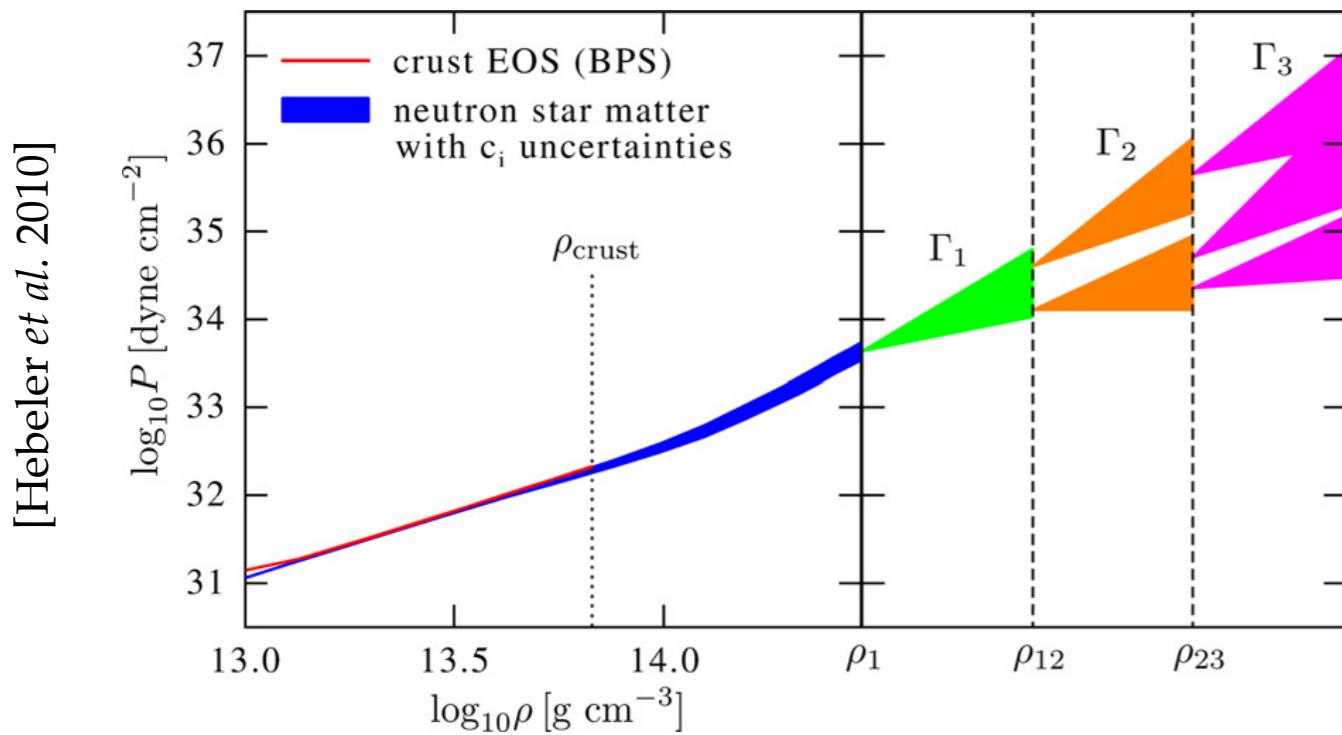
Limited applicability of chiral EoS

- Asymmetric matter can be computed as well...



High-density extrapolations

◎ Agnostic approach: series of piecewise polytropes

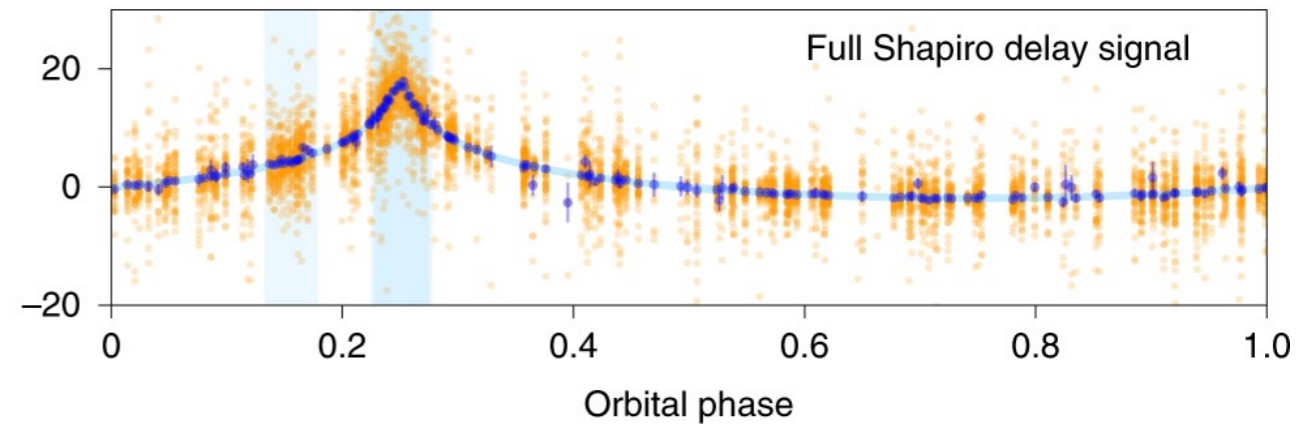


One can further constrain the very high density region
 → Perturbative QCD can be applied

Astrophysical constraints

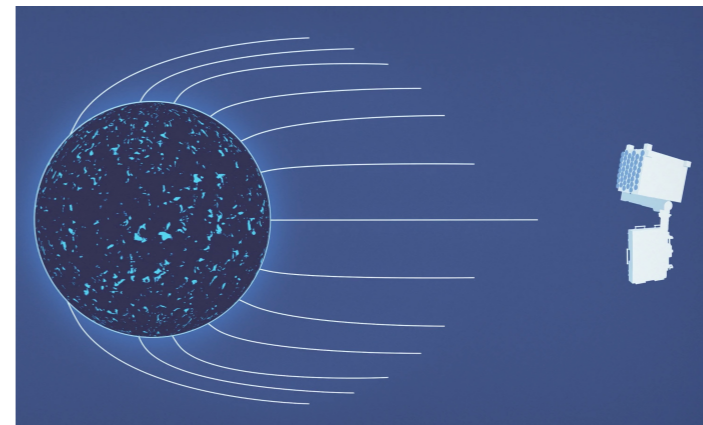
⊙ Measurements of NS masses

- Shapiro delay technique
- Measurements of $M > 2 M_{\odot}$



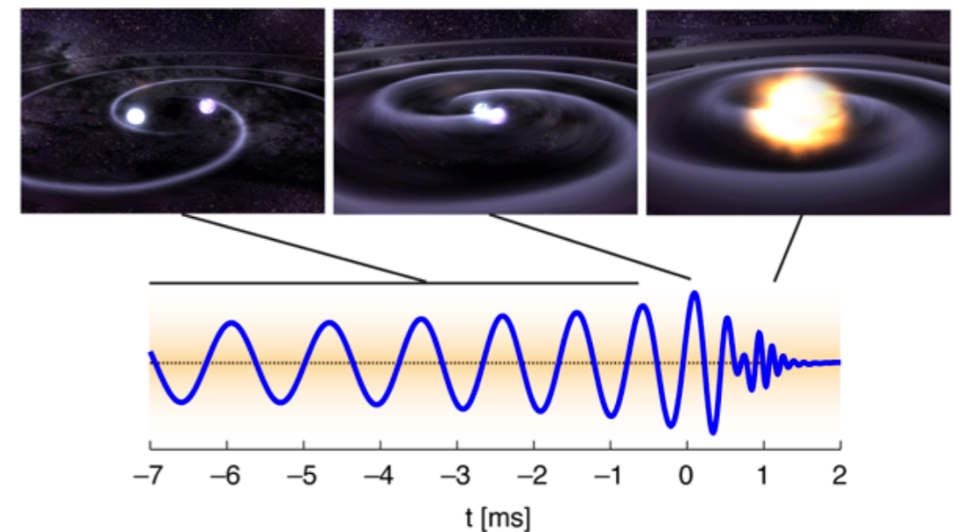
⊙ Measurements of NS radii

- NICER experiment → rotation of hot spots
- Measurements of $R \sim 12-13$ km



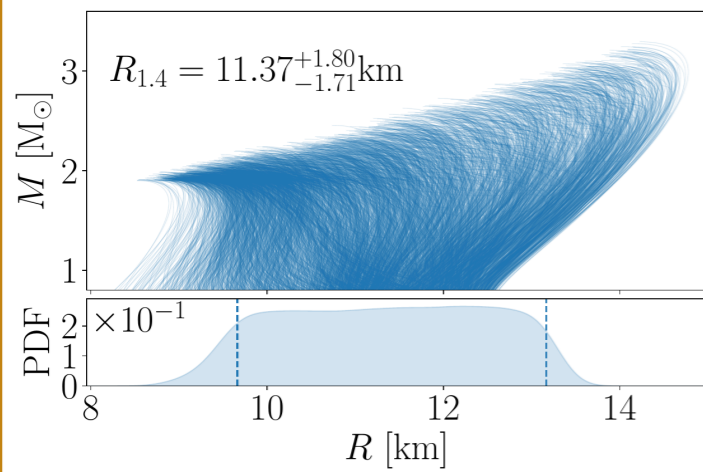
⊙ Gravitational waves / multi messenger observations

- GW signal → tidal deformability (→ radius)
- Oscillation frequency of merger remnant → radius
- Fate of merger remnant → maximum mass

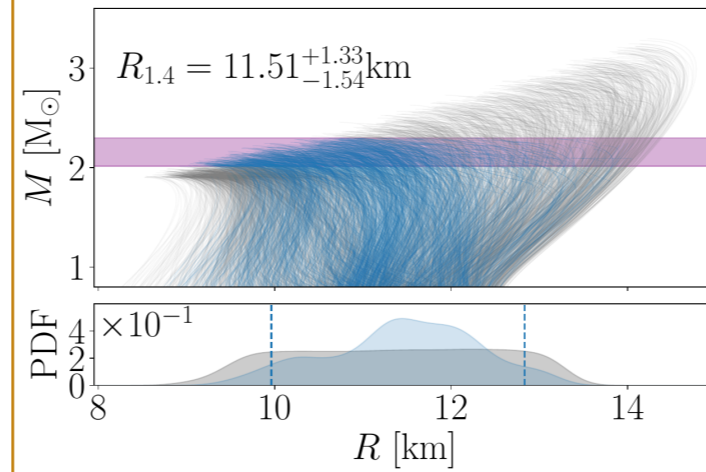


Multi-step analysis

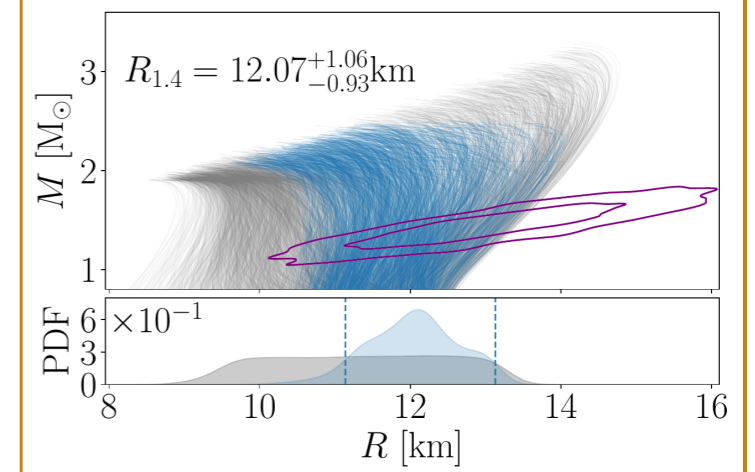
(A) Chiral effective field theory:
EOS derived with the chiral EFT
framework



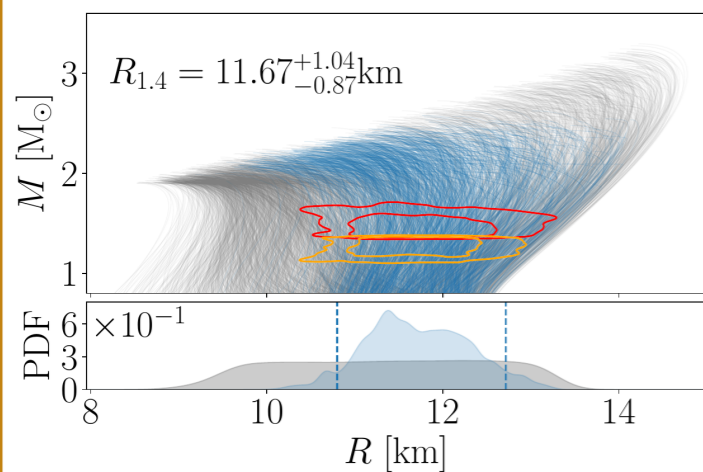
(B) Maximum Mass Constraints:
PSR J0740+6620/ PSR J0348+4032/ PSR
J1614-2230 and GW170817/AT2017gfo
remnant classification



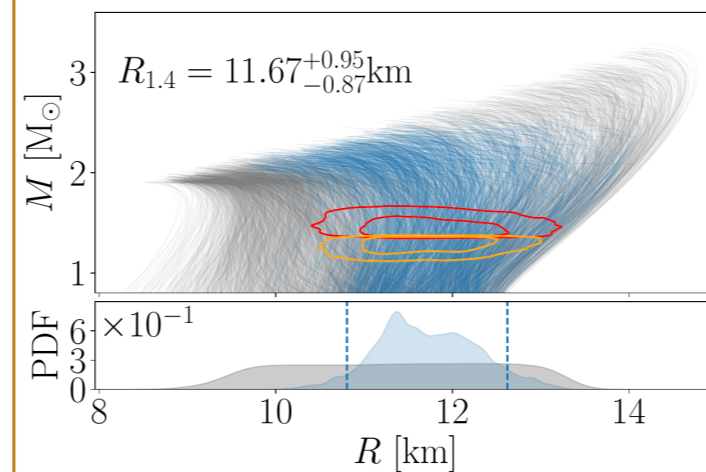
(C) NICER:
PSR J0030+0451



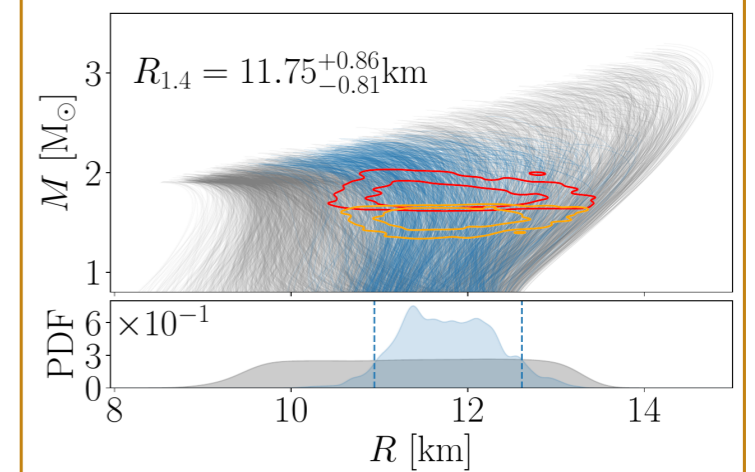
(D) GW170817:
reanalysis with
IMRPhenomPv2_NRTidalv2



(E) AT2017gfo:
analysis of the observed lightcurves



(F) GW190425:
reanalysis with
IMRPhenomPv2_NRTidalv2



References

- ⊙ **N. Chamel**, <http://www.astro.ulb.ac.be/~chamel/docs/lectures/chamel-russbach2010.pdf>
 - *Pedagogical introduction to neutron stars*
- ⊙ **A. Gal et al.**, Rev. Mod. Phys. **88** 035004 (2016)
 - *Review on hypernuclei and hypernuclear interactions*
- ⊙ **D. Lonardonì et al.**, Phys. Rev. Lett. **114** 092301 (2015)
 - *On the hyperon puzzle*
- ⊙ **A. Kurkela et al.**, Astrophys. J. **789** 127 (2014)
 - *Agnostic EoS with chiral EFT and pQCD constraints*
- ⊙ **R. De Petri et al.**, Astrophys. J. **881** 122 (2019)
 - *Two-family scenario (hadronic & quark stars) and mergers of compact objects*
- ⊙ **C. Drischler et al.**, Annu. Rev. Nucl. Part. Sci. **71** 1 (2021)
 - *Review on chiral EFT vs astrophysical constraints*
- ⊙ **T. Dietrich et al.**, Science **370** 1450 (2020)
 - *Multi-step analysis of astrophysical constraints*