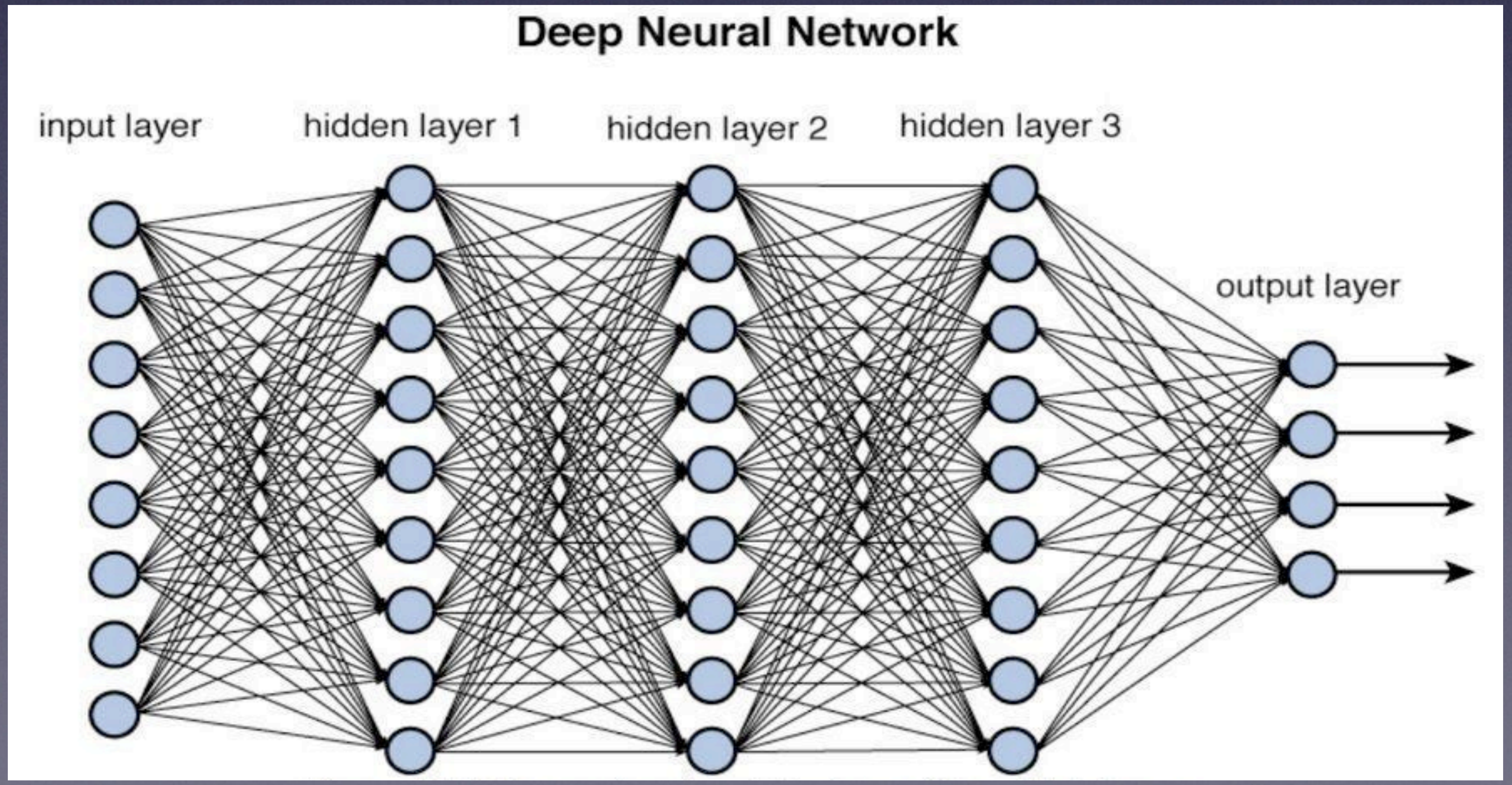
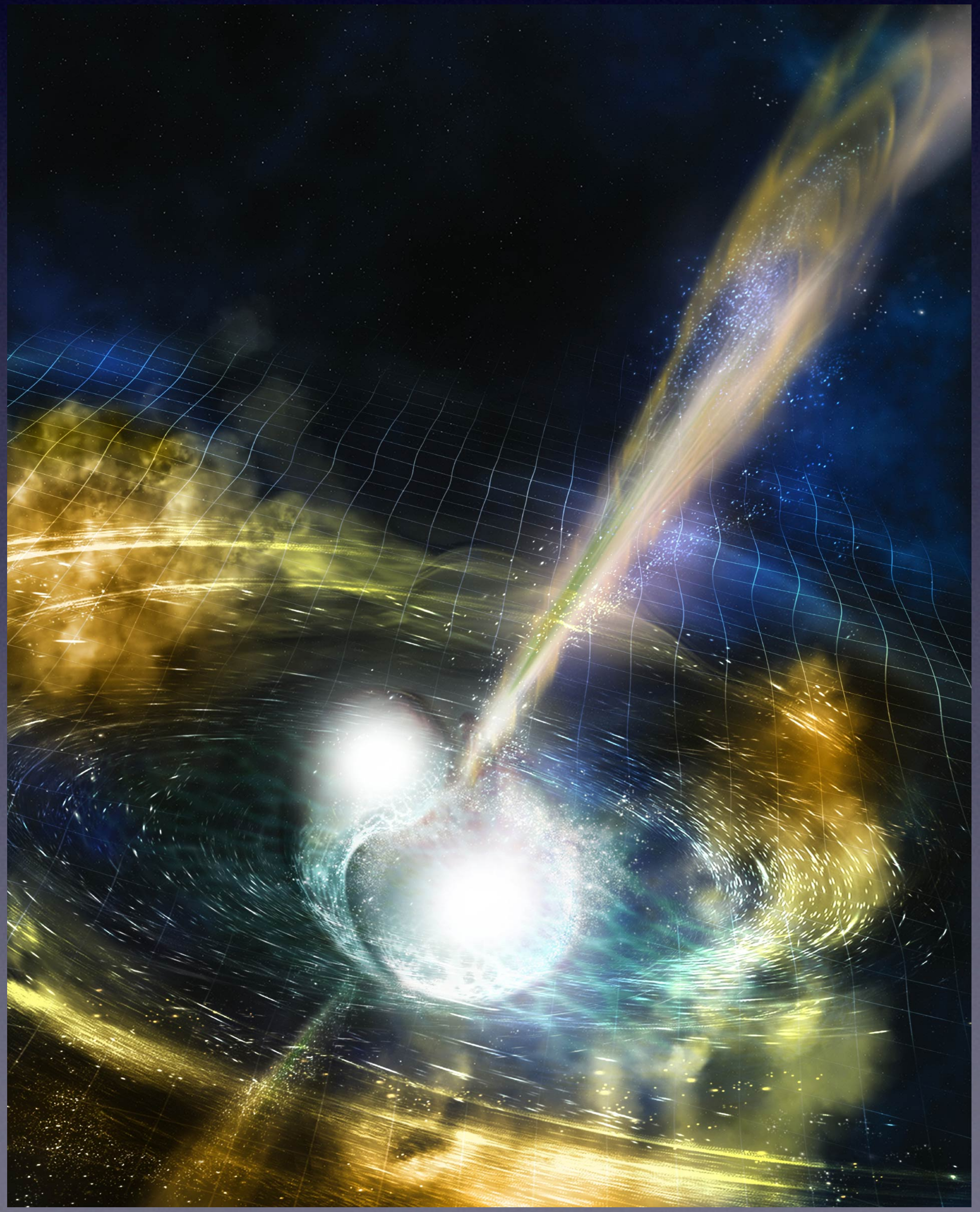
Applications of Machine Learning to Nuclear Theory

J. Piekarewicz





Old, Recent, and NEW friends!

Guacamole with chapulines (crickets!)

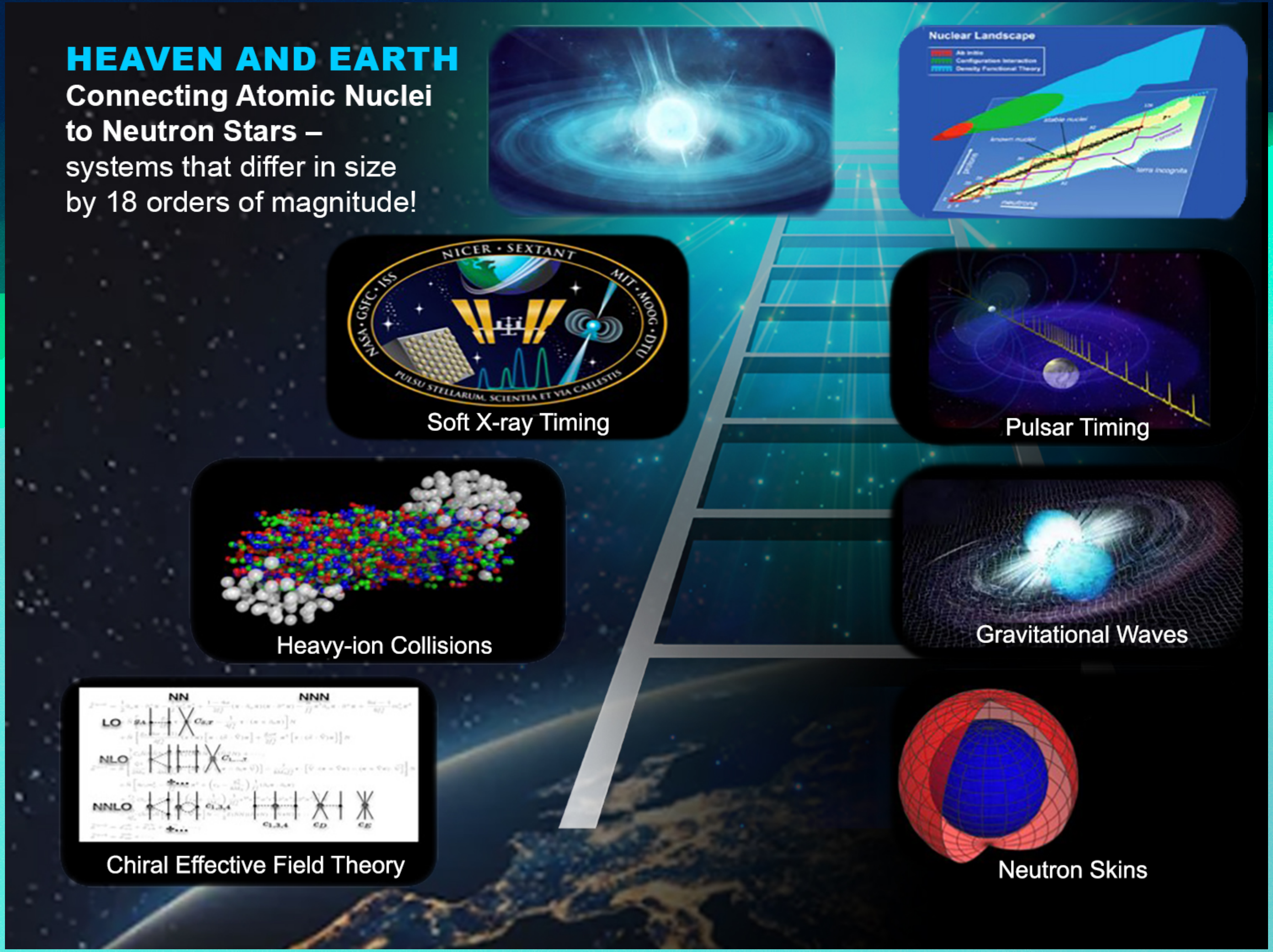
... and of course,

please do not eat tuna

in this unit ...

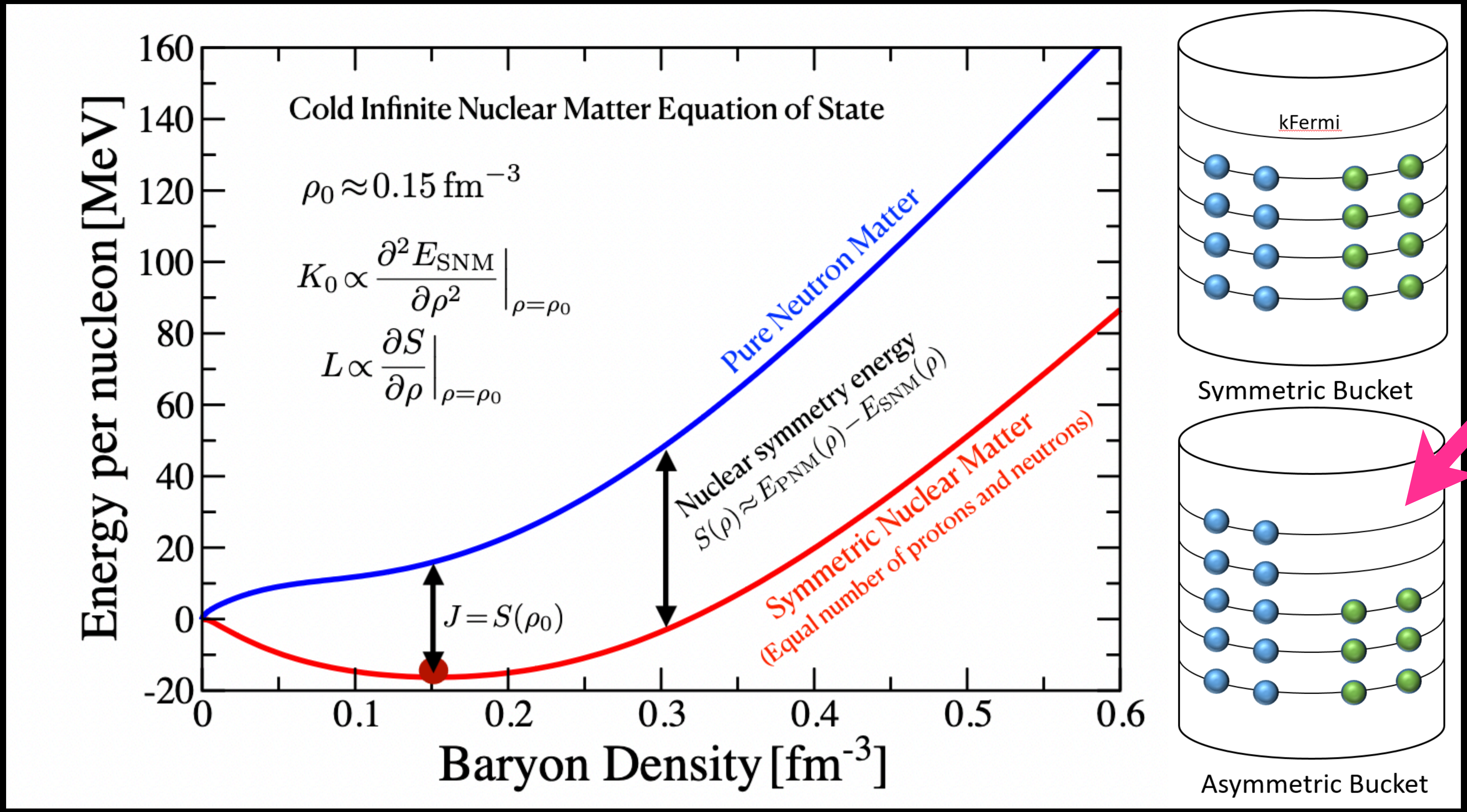
Heaven and Earth: Nuclear EOS Density Ladder

No single method can constrain the EOS over the entire density domain. Instead, each rung on the ladder provides information that can be used to determine the **EOS** at neighboring rungs

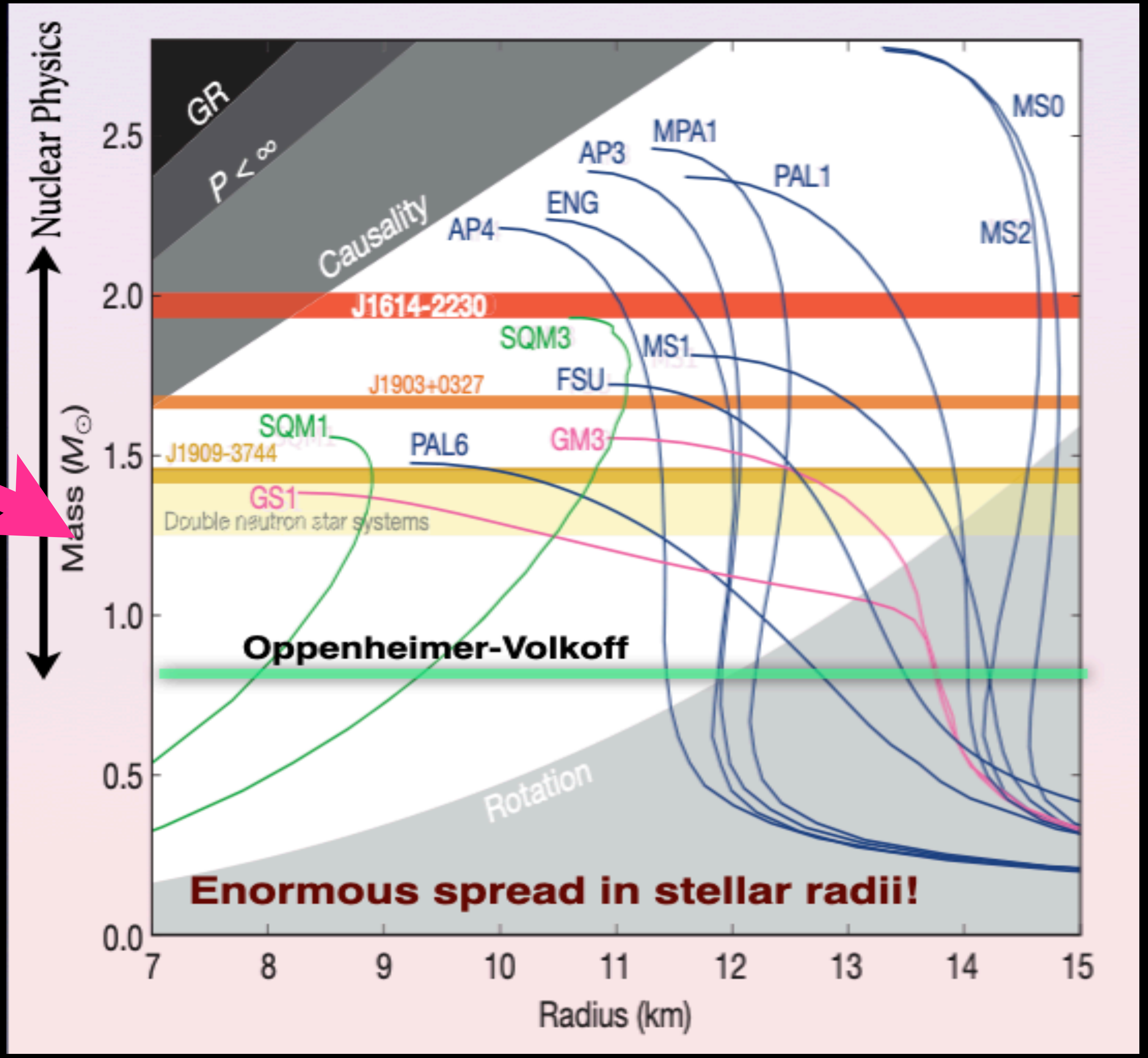


Multimessenger Astronomy!

Neutron Stars and The Equation of State of Neutron-Rich Matter



Micro-Macro Connection



Only Physics that the TOV equation is sensitive to is the Equation of State

$$S(\rho_0) \approx \Big(E_{\rm PNM} - E_{\rm SNM}\Big)(\rho_0) = J$$

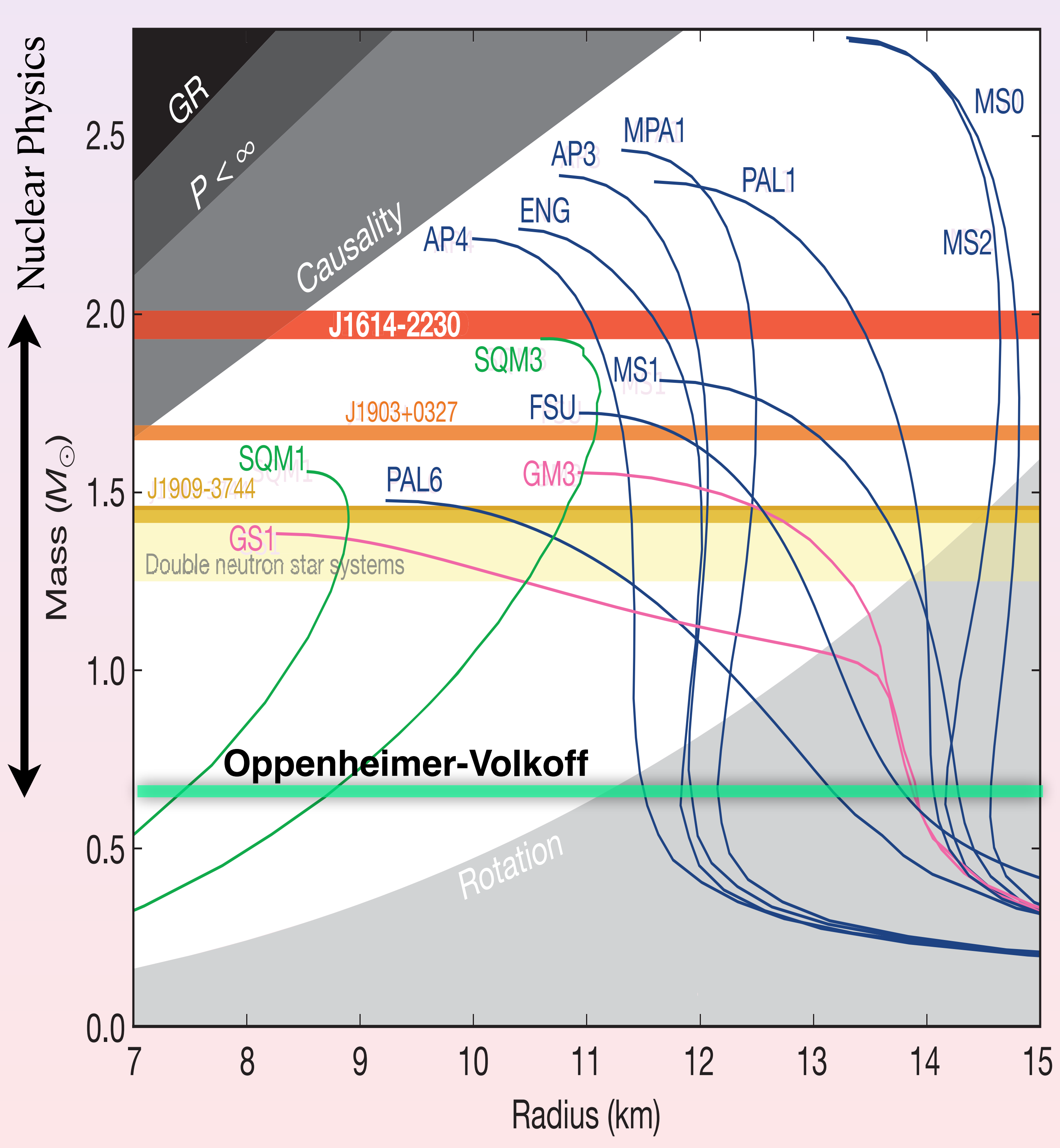
$$P_{\rm PNM} \approx \frac{1}{3} L \rho_0 \ (\text{Pressure of PNM})$$

"Stiff" ⟶ L large
"Soft" ⟶ L small

PREX constrains L!

Nuclear science plays a fundamental role in understanding the structure, dynamics, and composition of neutron stars!

Increase from 0.7 to 2 Msun is entirely due to repulsive nuclear interactions at short distances and transfers ownership to us!

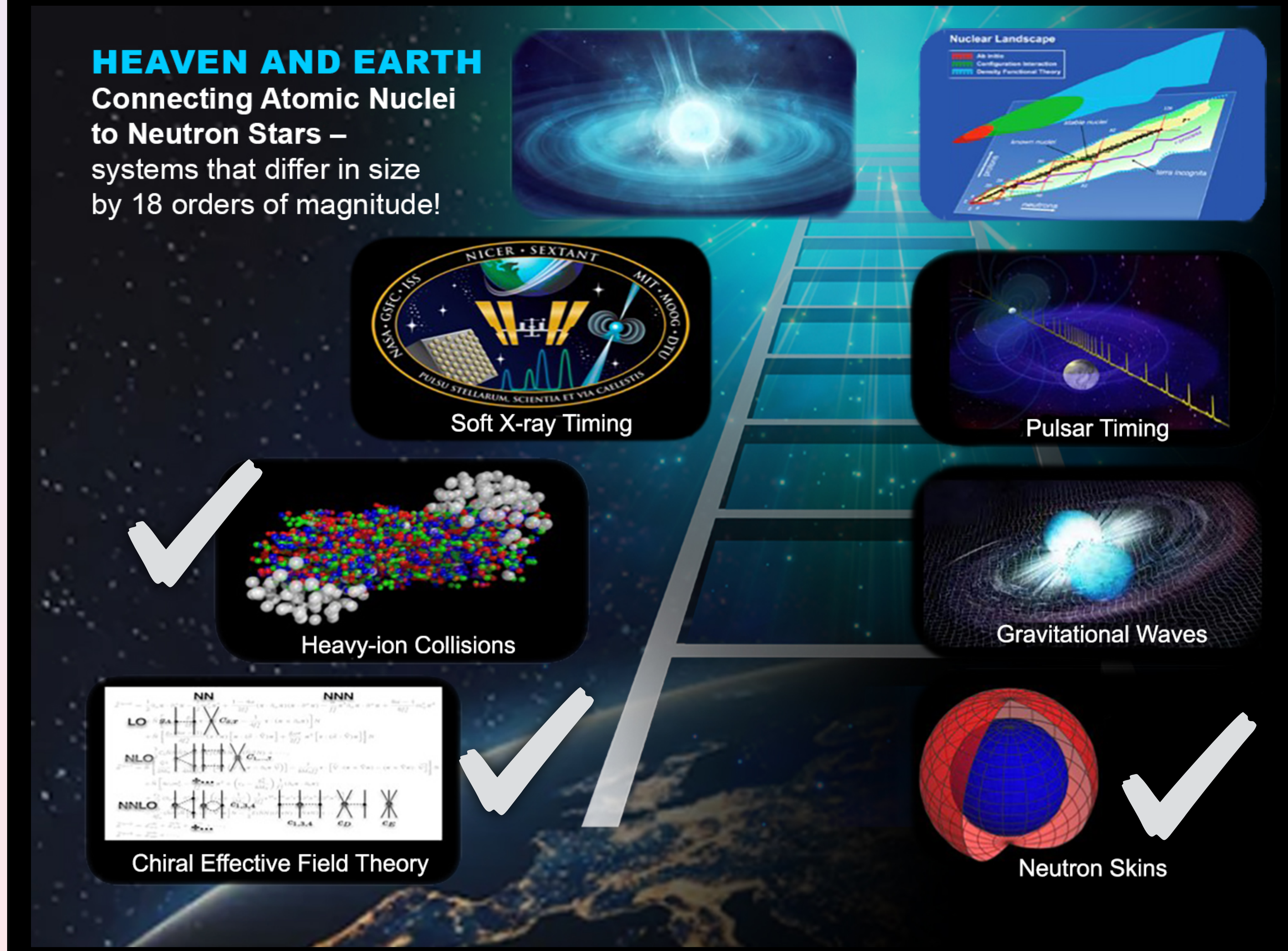


$$\frac{dM}{dr} = 4\pi r^2 \mathcal{E}(r)$$

$$\frac{dP}{dr} = -G\frac{\mathcal{E}(r)M(r)}{r^2}\left[1+\frac{P(r)}{\mathcal{E}(r)}\right]\left[1+\frac{4\pi r^3 P(r)}{M(r)}\right]\left[1-\frac{2GM(r)}{r}\right]^{-1}$$

Need an EOS: $P = P(\mathcal{E})$ relation

Nuclear Physics Critical

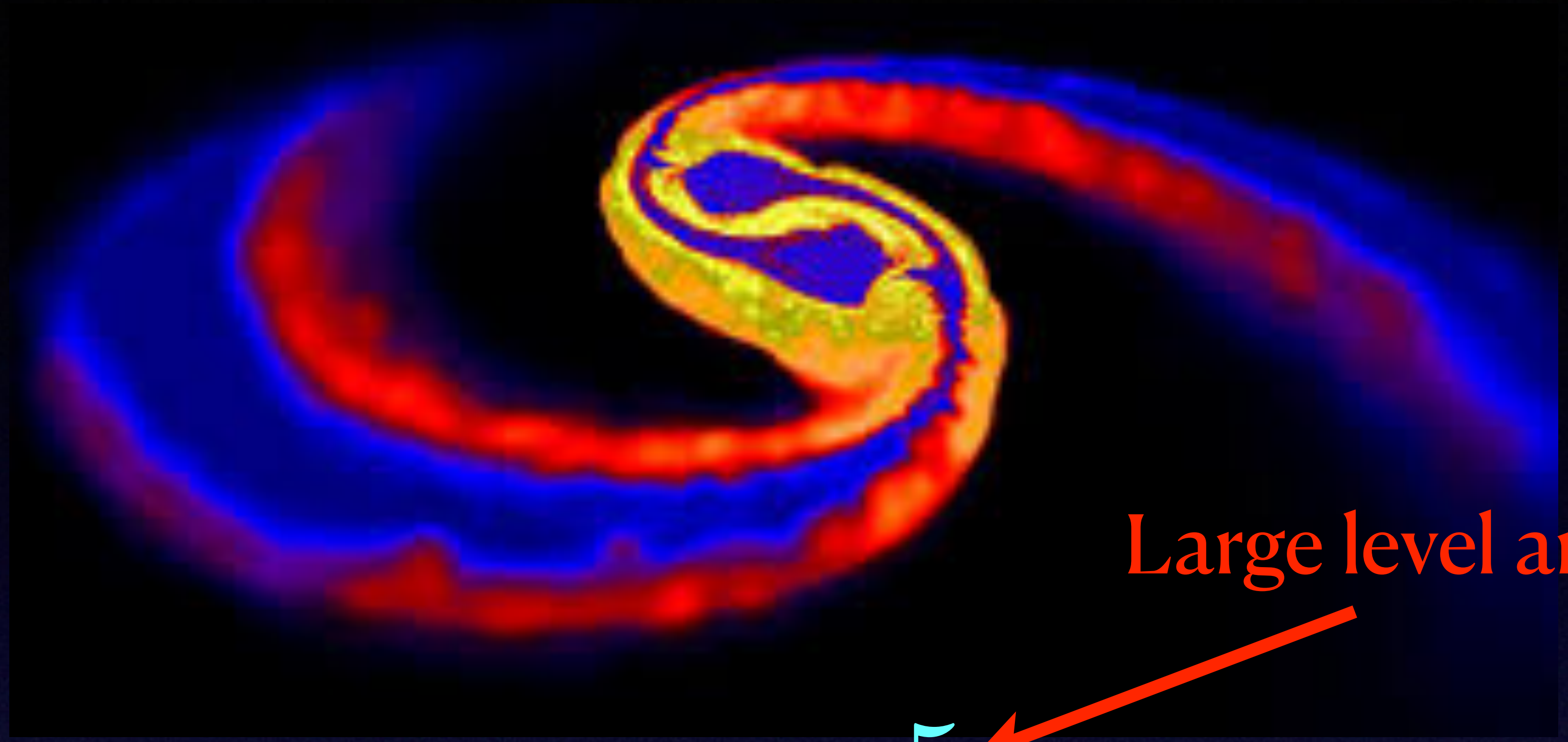


Nuclear Physics and Neutron Stars

Tidal Polarizability and Neutron-Star Radii (2017)

Tidal Polarizability(Deformability):

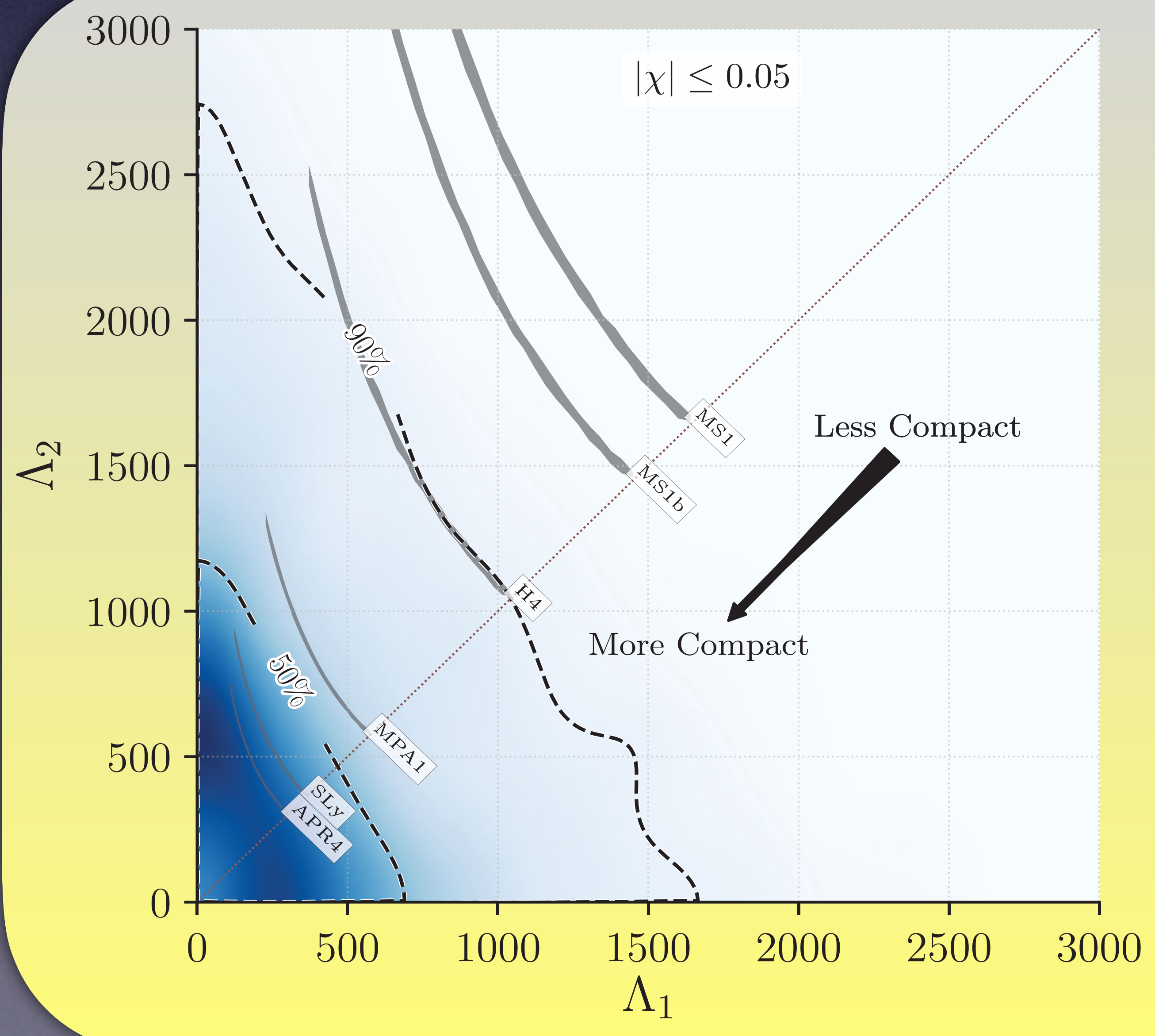
- Tidal field induces a mass polarization
- A time dependent mass quadrupole emits gravitational waves



Large level arm!

Micro-Macro

$$Q_{ij} = \Lambda \mathcal{E}_{ij} \qquad \Lambda = k_2 \left(\frac{c^2 R}{2GM}\right)^5 = k_2 \left(\frac{R}{R_s}\right)^5$$



GW170817 rules out very large neutron star radii!

Neutron Stars must be compact

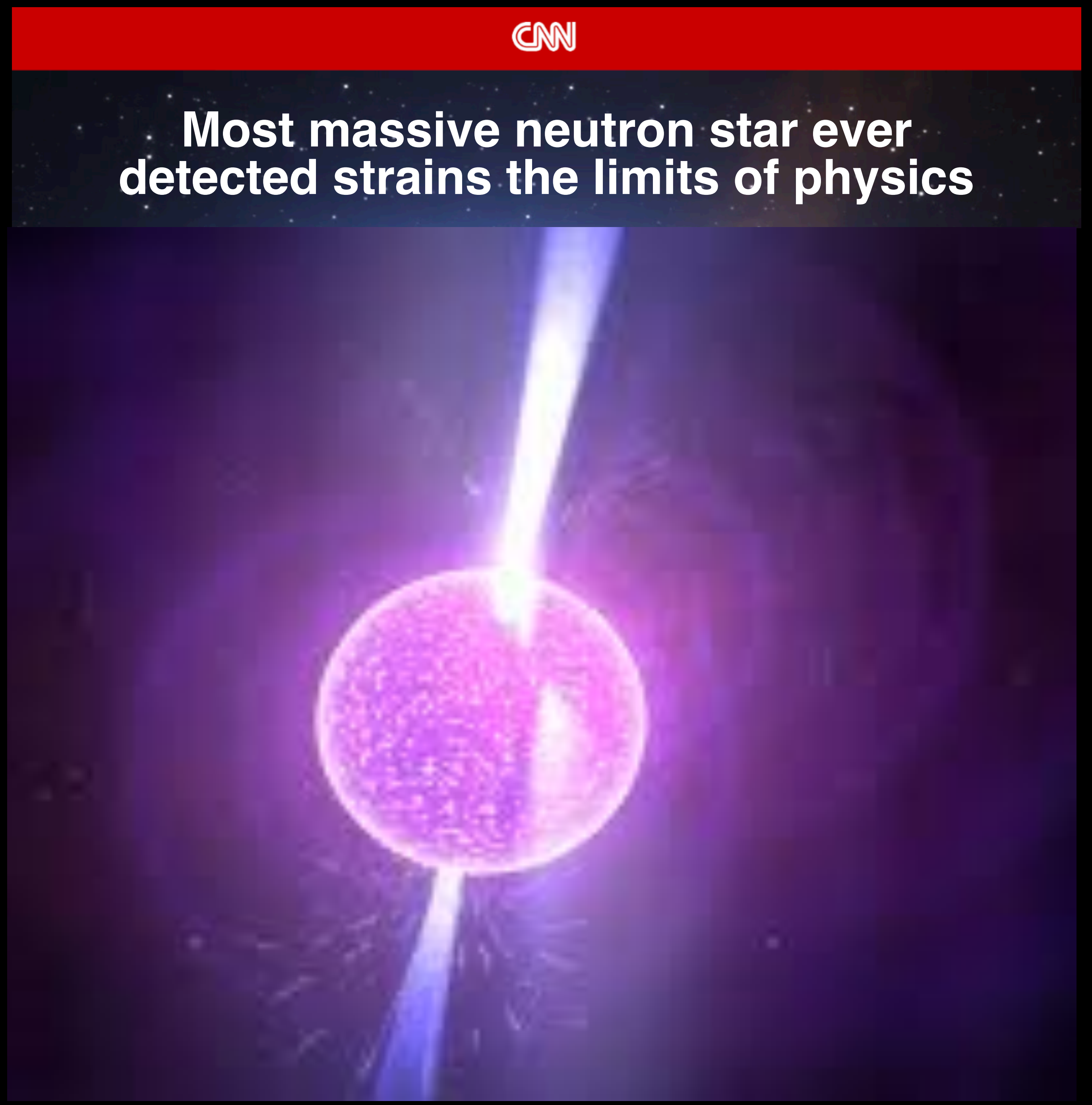
$$\Lambda_{1.4} = 390^{+190}_{-120}\ (90\%)$$

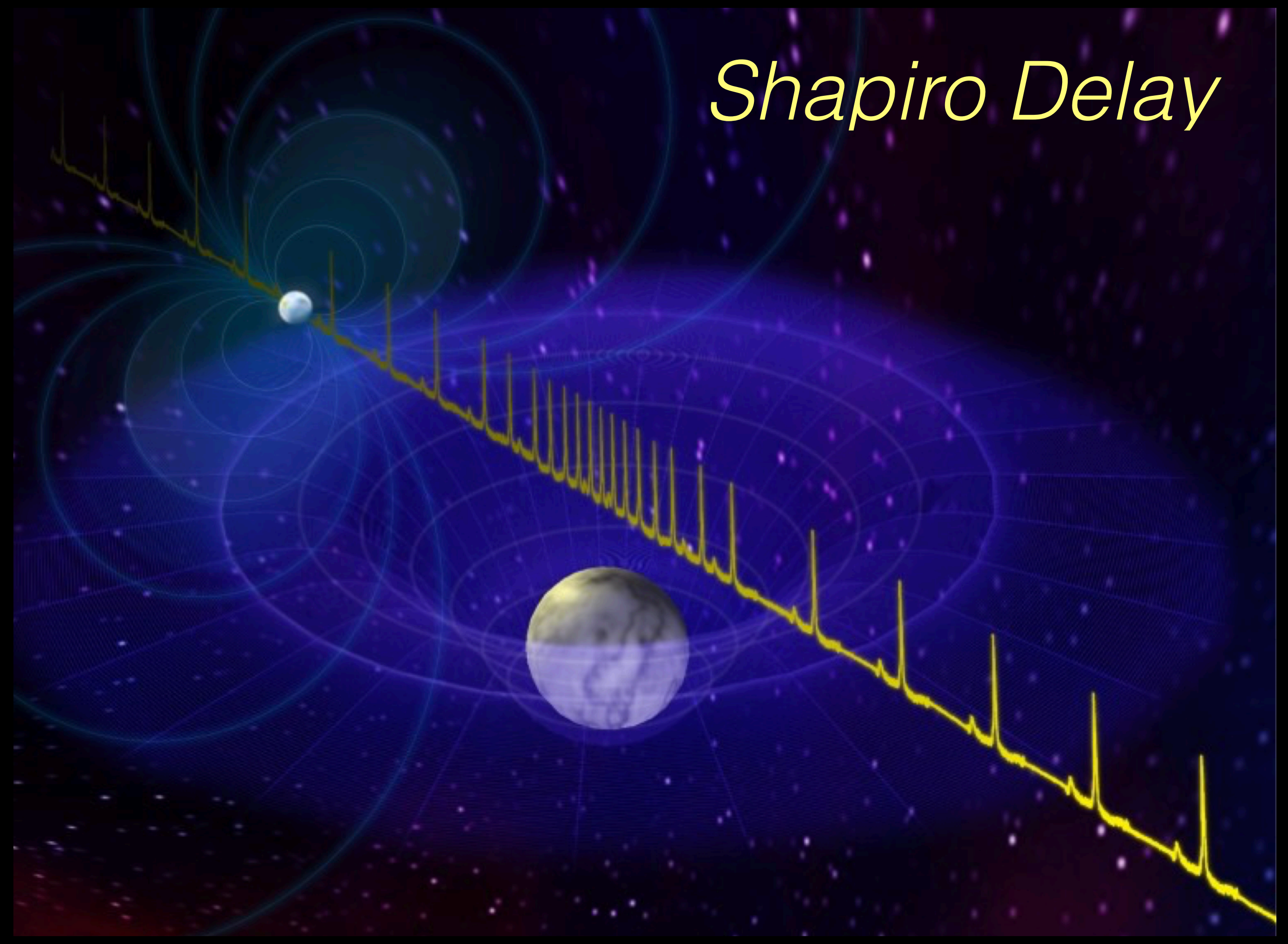
(Latest LIGO/Virgo analysis)

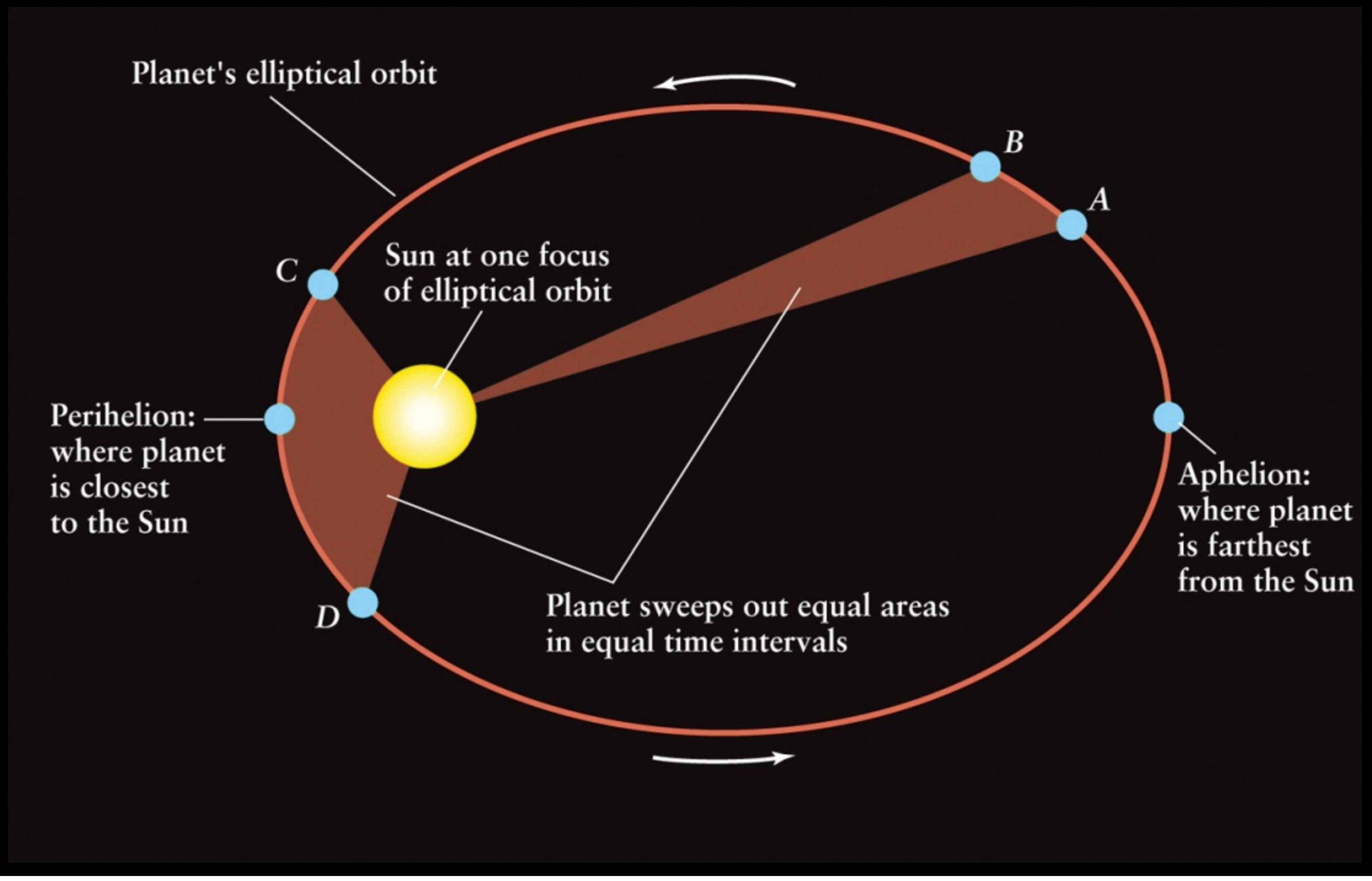
Soft EOS! Small L!

The tidal polarizability measures the "fluffiness" (or stiffness) of a neutron star against deformation. Very sensitive to stellar radius!

Measuring Heavy Neutron Stars (2019)
Shapiro Delay: General Relativity to the Rescue

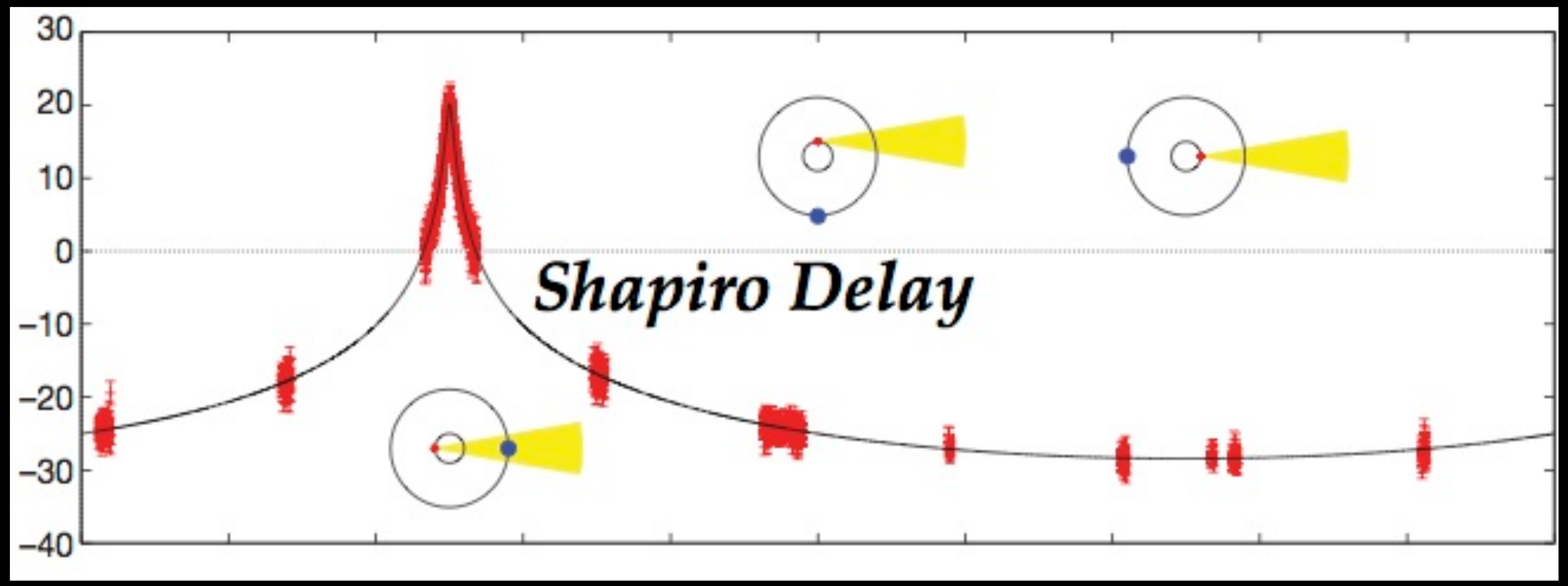






Newtonian Gravity sensitive to the total mass of the binary
Kepler's Third Law

$$G(M_{\rm ns}+M_{\rm wd}) = 4\pi^2\frac{a^3}{P^2}$$



Shapiro delay — a purely General Relativistic effect can break the degeneracy

$$\delta t = \frac{2GM_{\rm WD}}{c^3}\ln\left(\frac{4R_\star R_\oplus}{d^2}\right) \approx 10\mu s$$

Stiff EOS!
Large L!

$$M = 2.08 \pm 0.07 M_\odot$$

Cromartie/Fonseca et al. (2020)

Neutron-star Interior Composition Explorer (NICER)
Simultaneous Mass and Radius Measurements (2019-2021)

NICER was launched from Kennedy's Space Center on June 3, 2017 aboard SpaceX Falcon 9 Rocket and docked at the International Space Station two days later.

NICER measures the compactness of the Neutron Star by looking at back of the star!

Pulse Profile: The stellar compactness controls the light profile from the hot spot

$$\xi = \frac{2GM}{c^2 R} = \frac{R_S}{R}$$

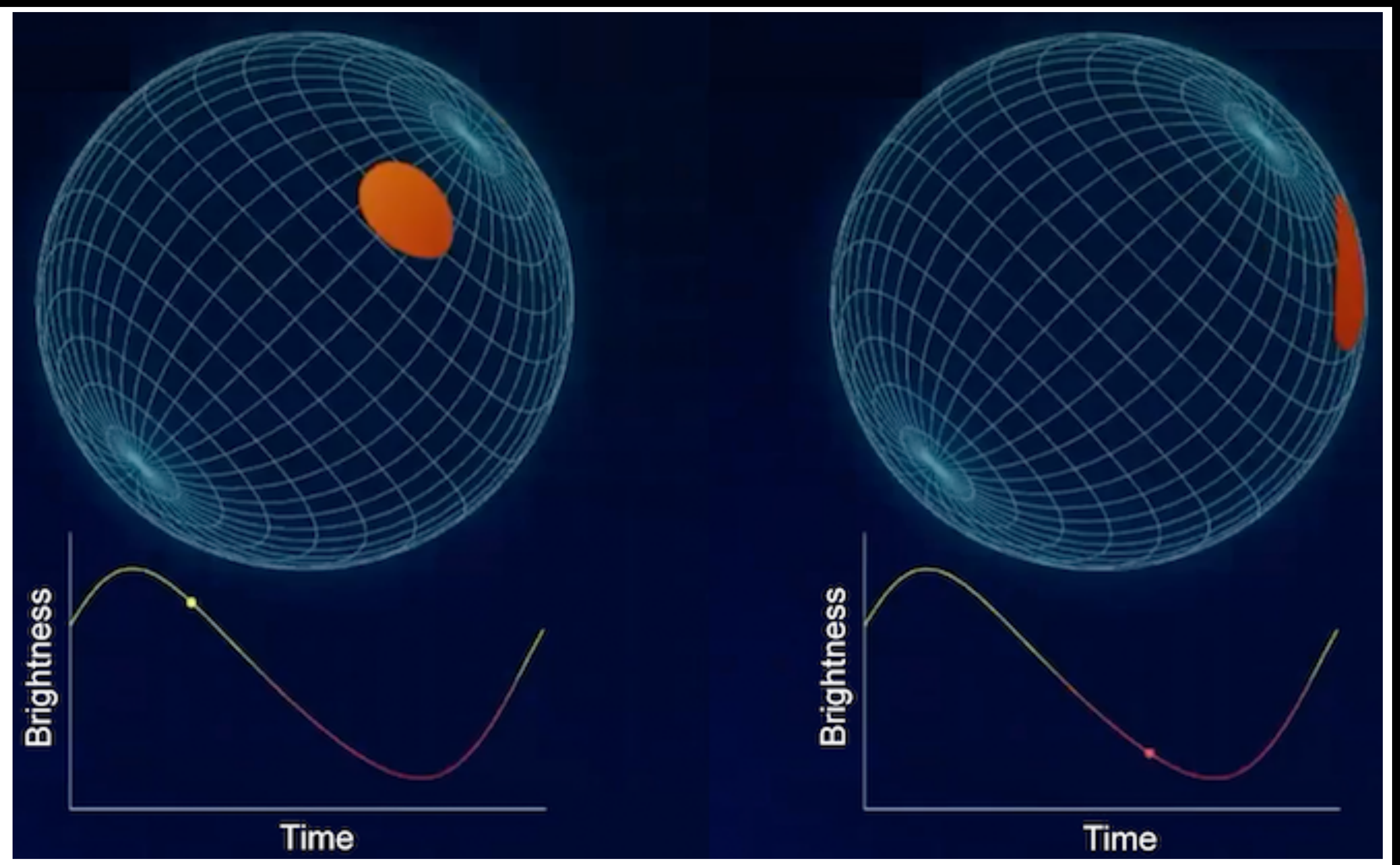
$M = 2.08 \pm 0.07\, M_\odot$
Shapiro delay: Cromartie *et al.* (2020)

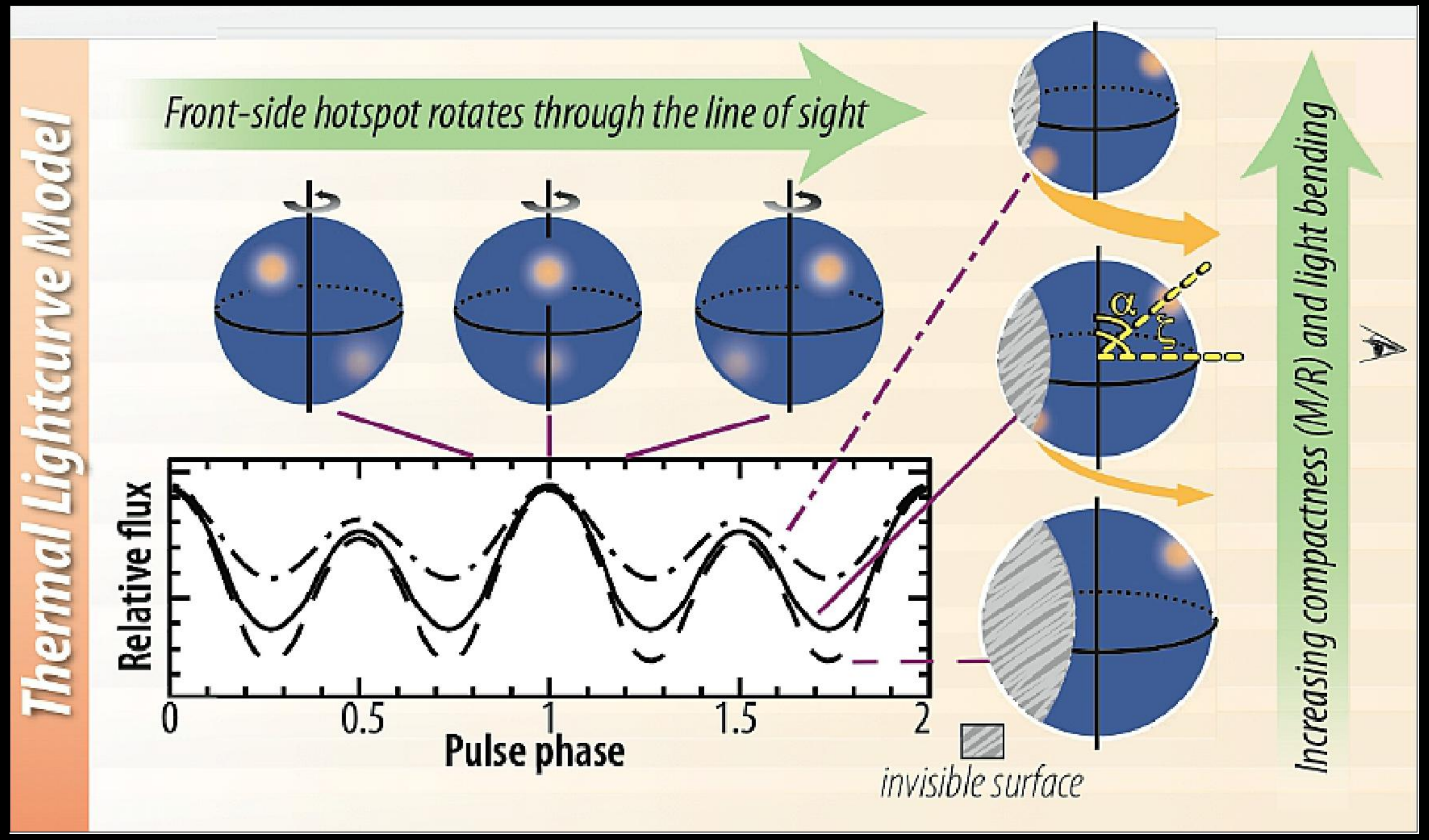
$R_{2.0} = 12.39^{+1.30}_{-0.98}$ km
Riley *et al.* (2021)

$R_{2.0} = 13.7^{+2.6}_{-1.5}$ km
Miller *et al.* (2021)

Micro-Macro

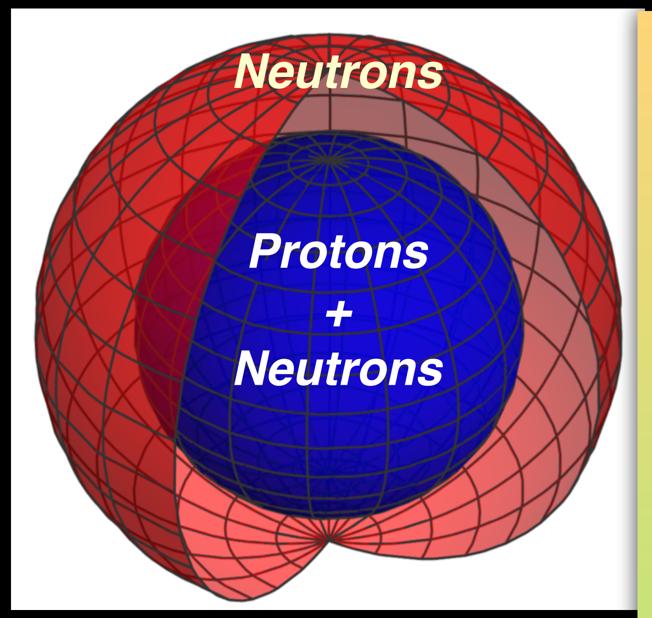
Stiff EOS! Large L!

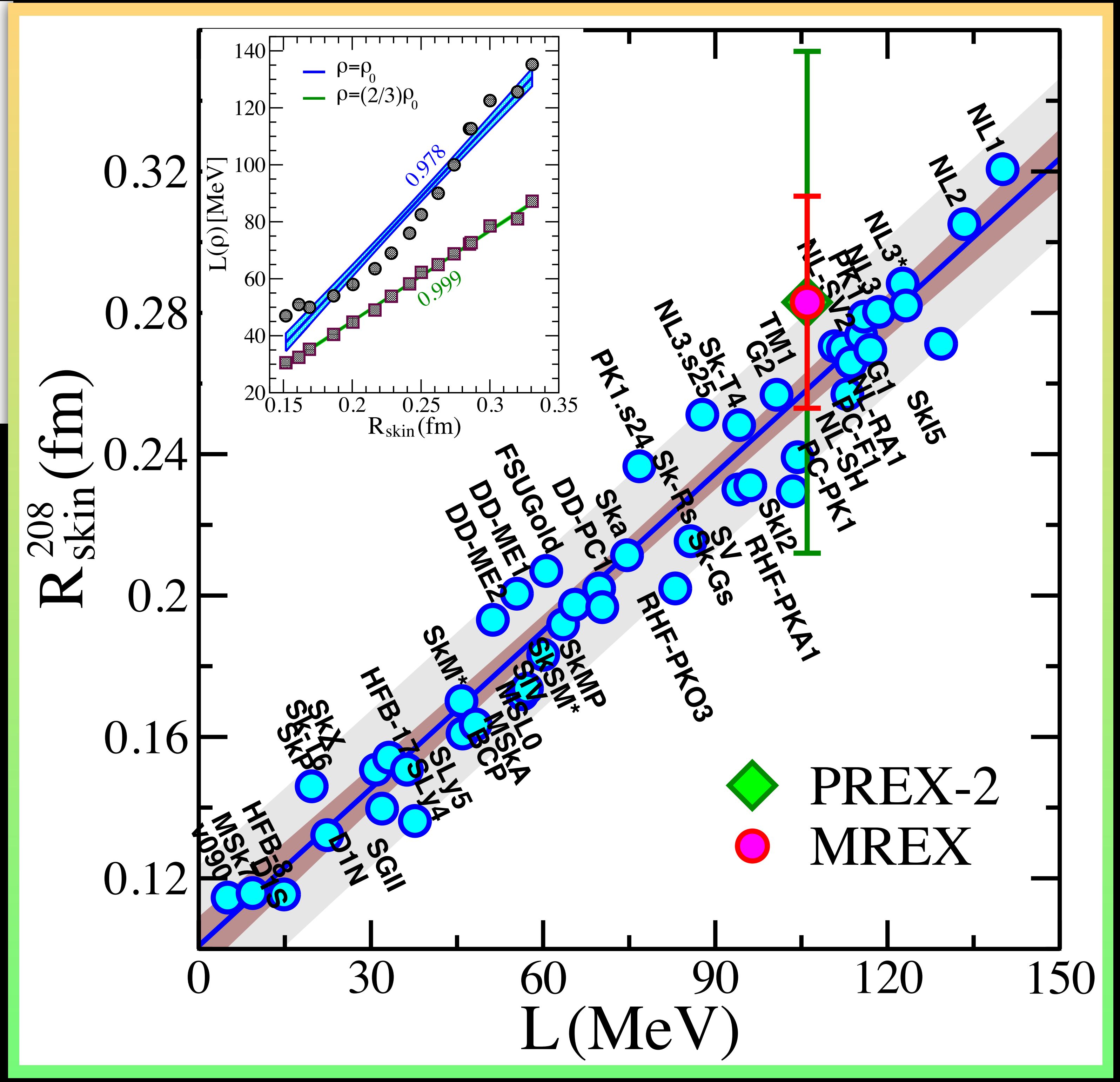




Heaven and Earth

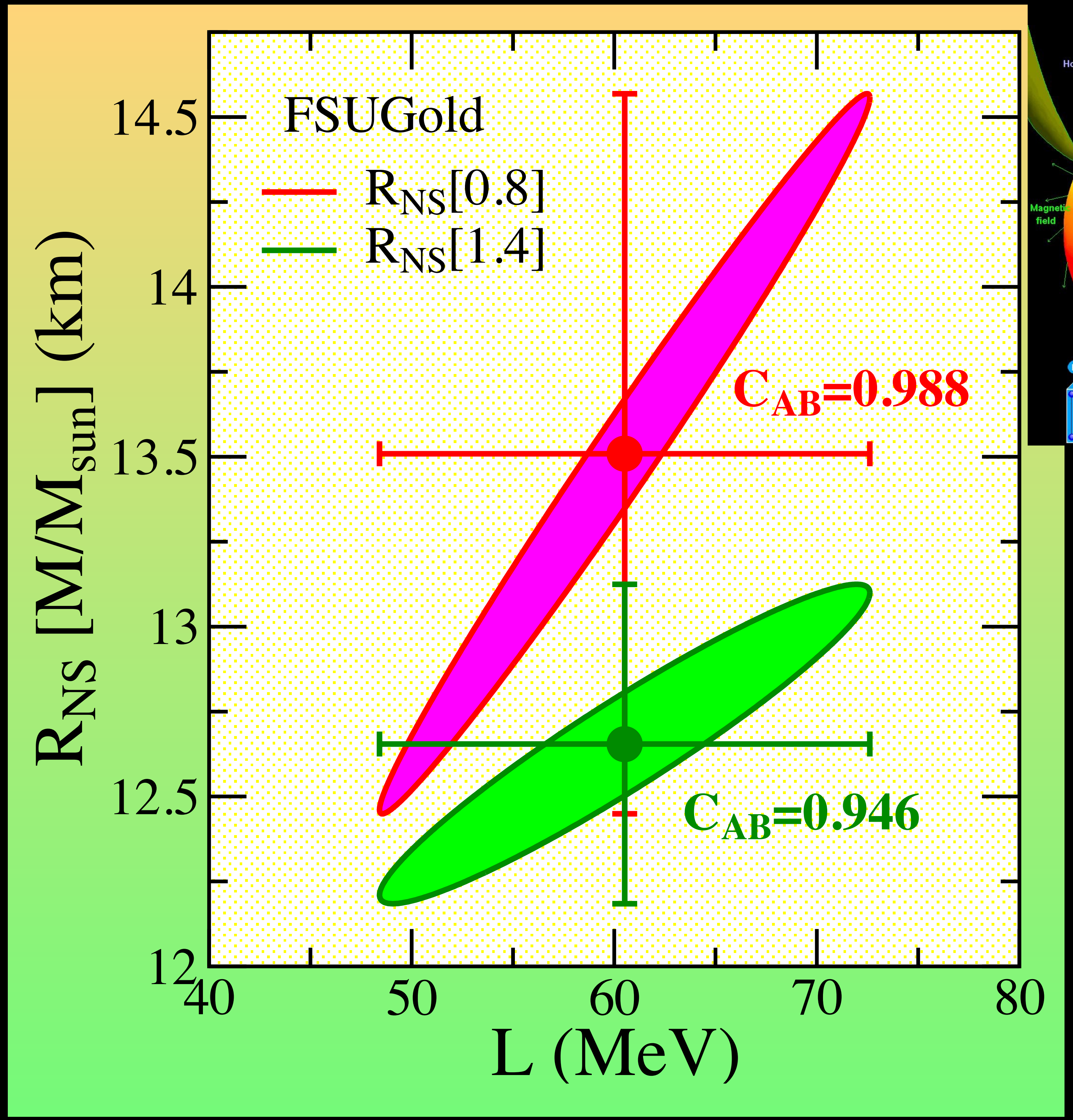
Laboratory Constraints on the EOS

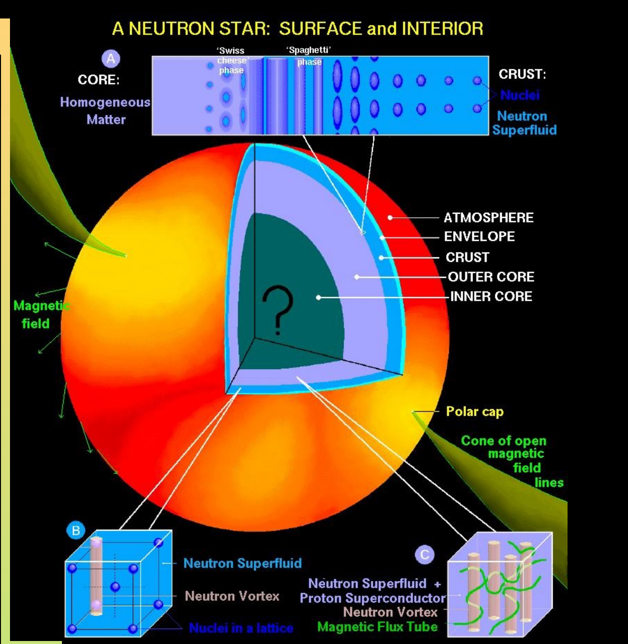




18 orders

magnitude



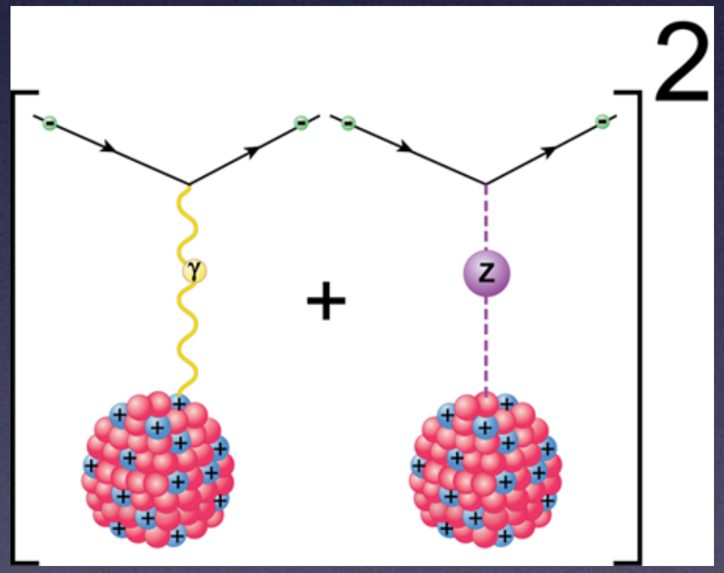


The slope of the symmetry energy L controls both the neutron skin of heavy nuclei as well as the radius of (low mass) neutron stars — objects that differ in size by 18 orders of magnitude!

Parity Violating e-Nucleus Scattering

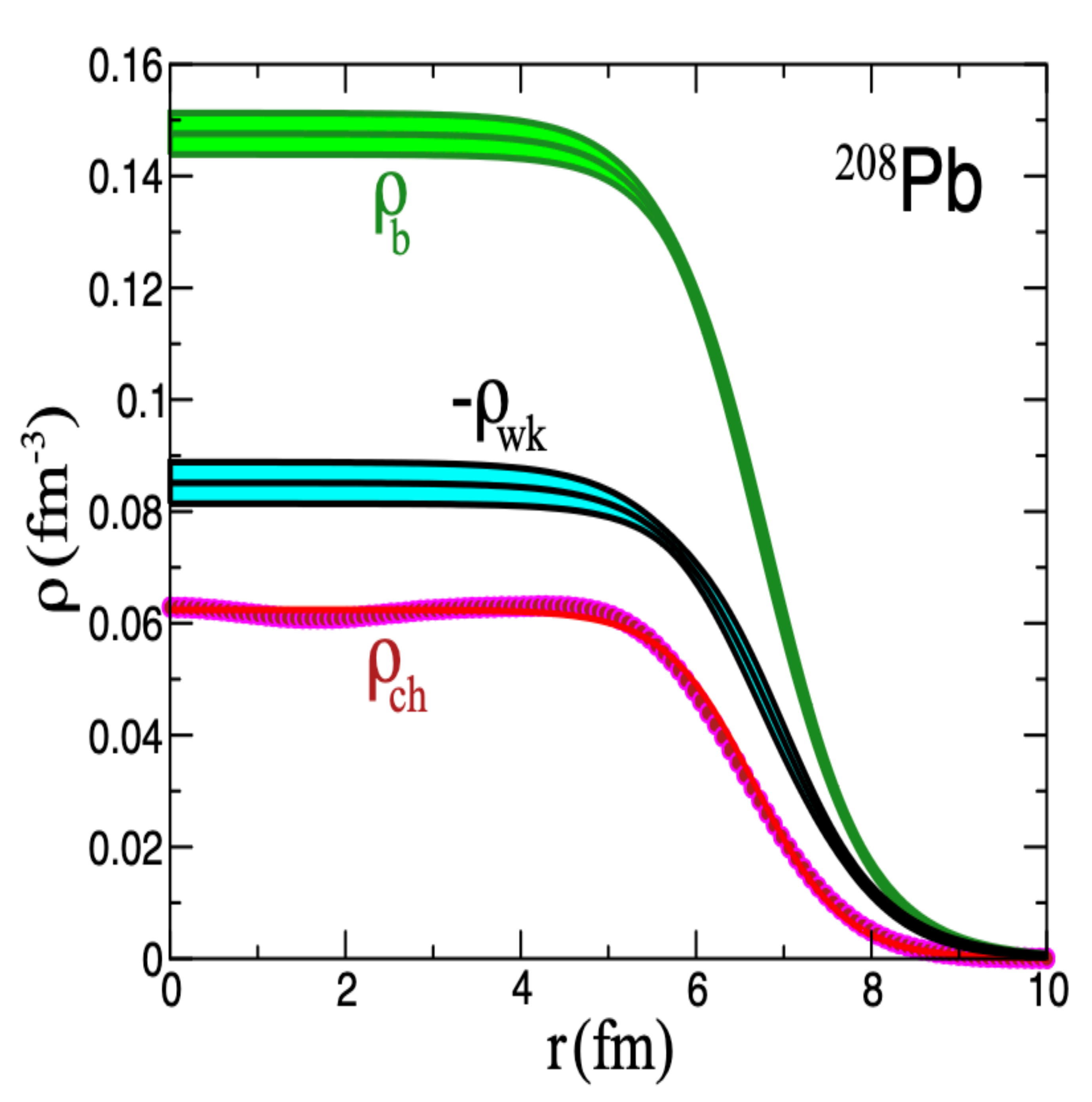
Searching for an accurate picture of the neutron distribution

- Charge (proton) density known with enormous precision
  - Probed via parity-conserving elastic e-scattering
- Weak-charge (neutron) density known very poorly known
  - Probed via parity-violating elastic e-scattering



$$A_{\rm PV} \equiv \left[\frac{\left(\frac{d\sigma}{d\Omega}\right)_R - \left(\frac{d\sigma}{d\Omega}\right)_L}{\left(\frac{d\sigma}{d\Omega}\right)_R + \left(\frac{d\sigma}{d\Omega}\right)_L}\right] = \left(\frac{G_{\rm F}Q^2}{4\pi\alpha\sqrt{2}}\right)\frac{F_{wk}(Q^2)}{F_{ch}(Q^2)} \simeq 10^{-6}$$

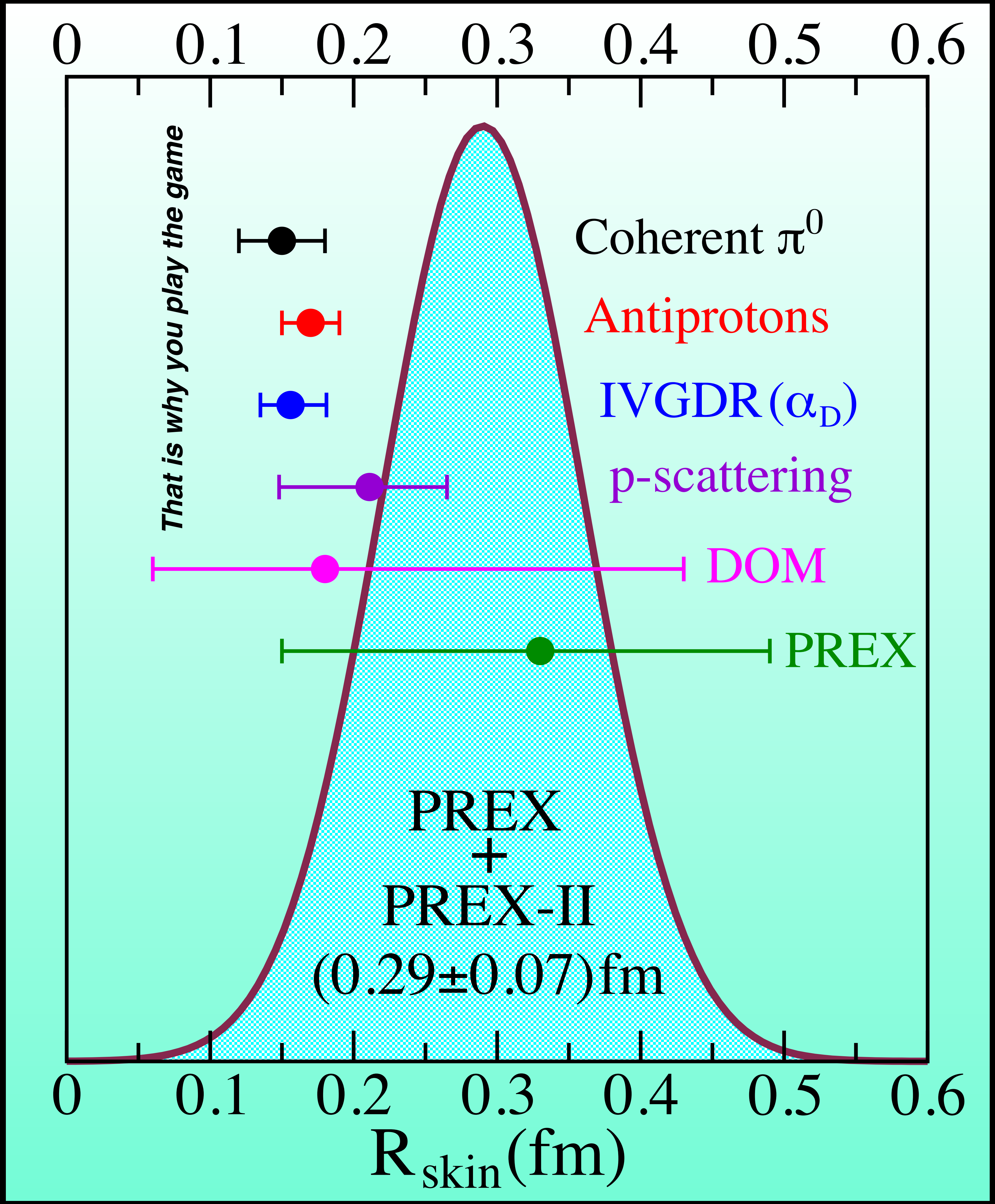
- *Electric-charge density dominated by protons*
- *Weak-charge density dominated by neutrons*



	up-quark	down-quark	proton	neutron
γ-coupling	$+2/3$	$-1/3$	$+1$	0
Z_0-coupling	$\approx +1/3$	$\approx -2/3$	≈ 0	-1

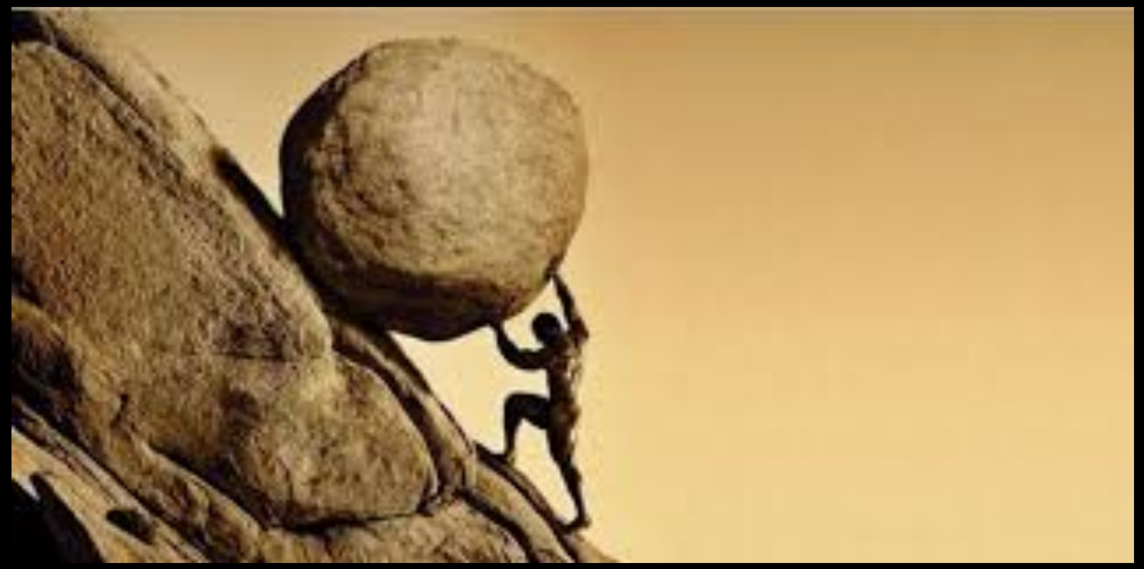
$$g_{\rm v} = 2t_z - 4Q\sin^2\theta_{\rm W} \approx 2t_z - Q$$

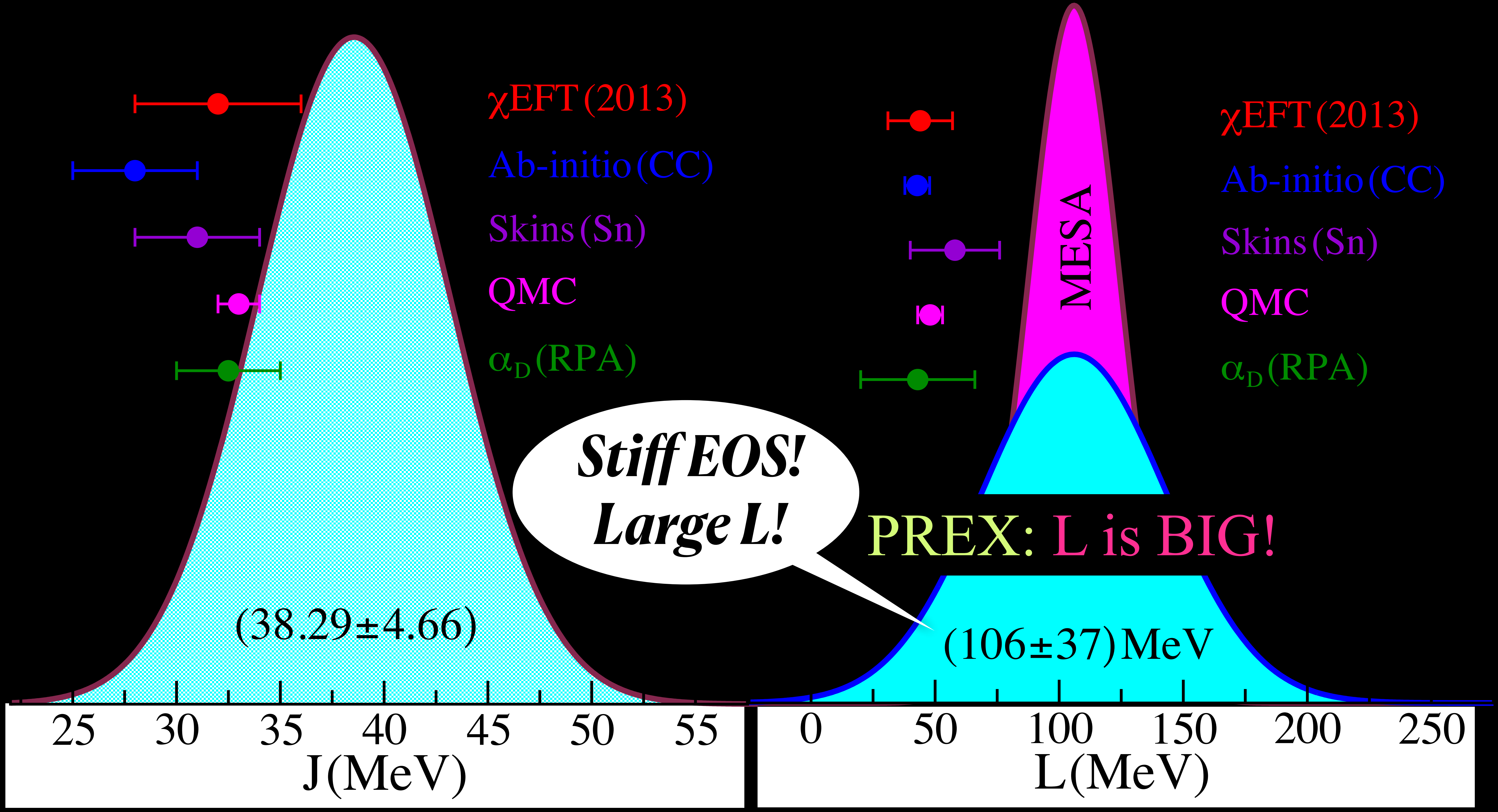
PREX-2 (Oct 29, 2020)
Ciprian Gal - DNP Meeting
Adhikari et al., PRL 126, 172502 (2021)



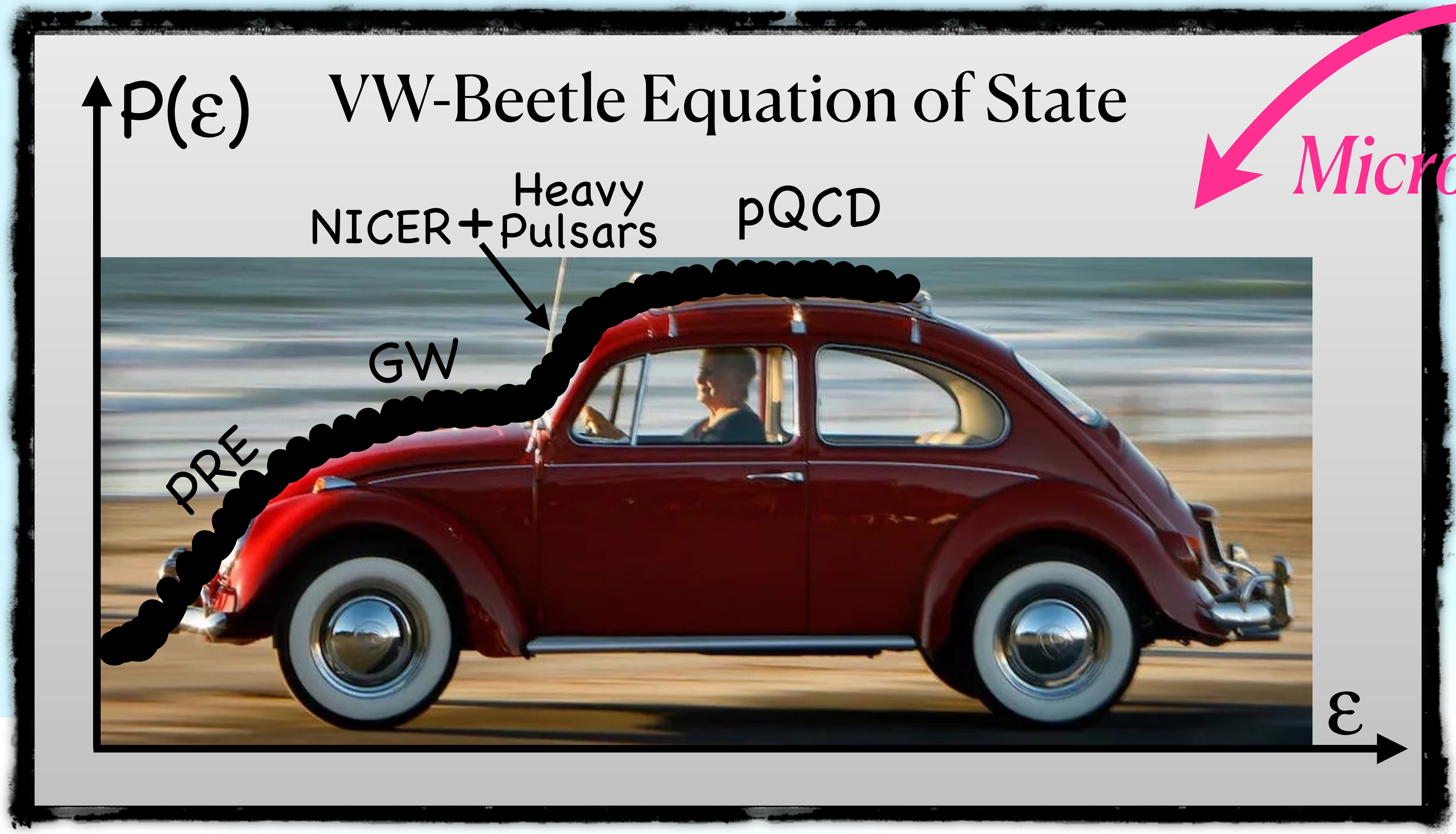
Conservation of difficulty: PVES provides the cleanest constraint on the EOS of neutron-rich matter in the vicinity of saturation density

Heroic effort from our experimental colleagues

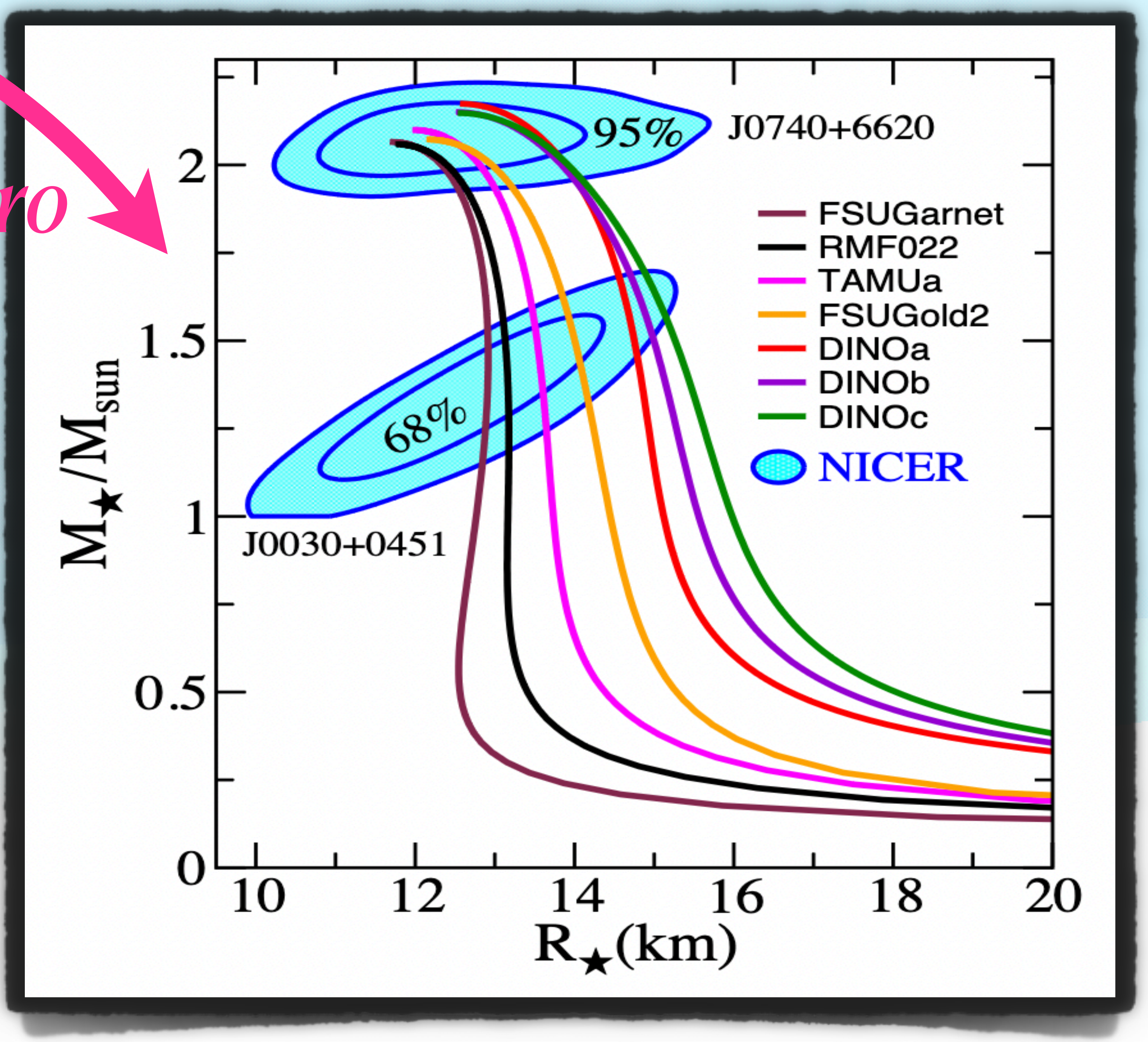


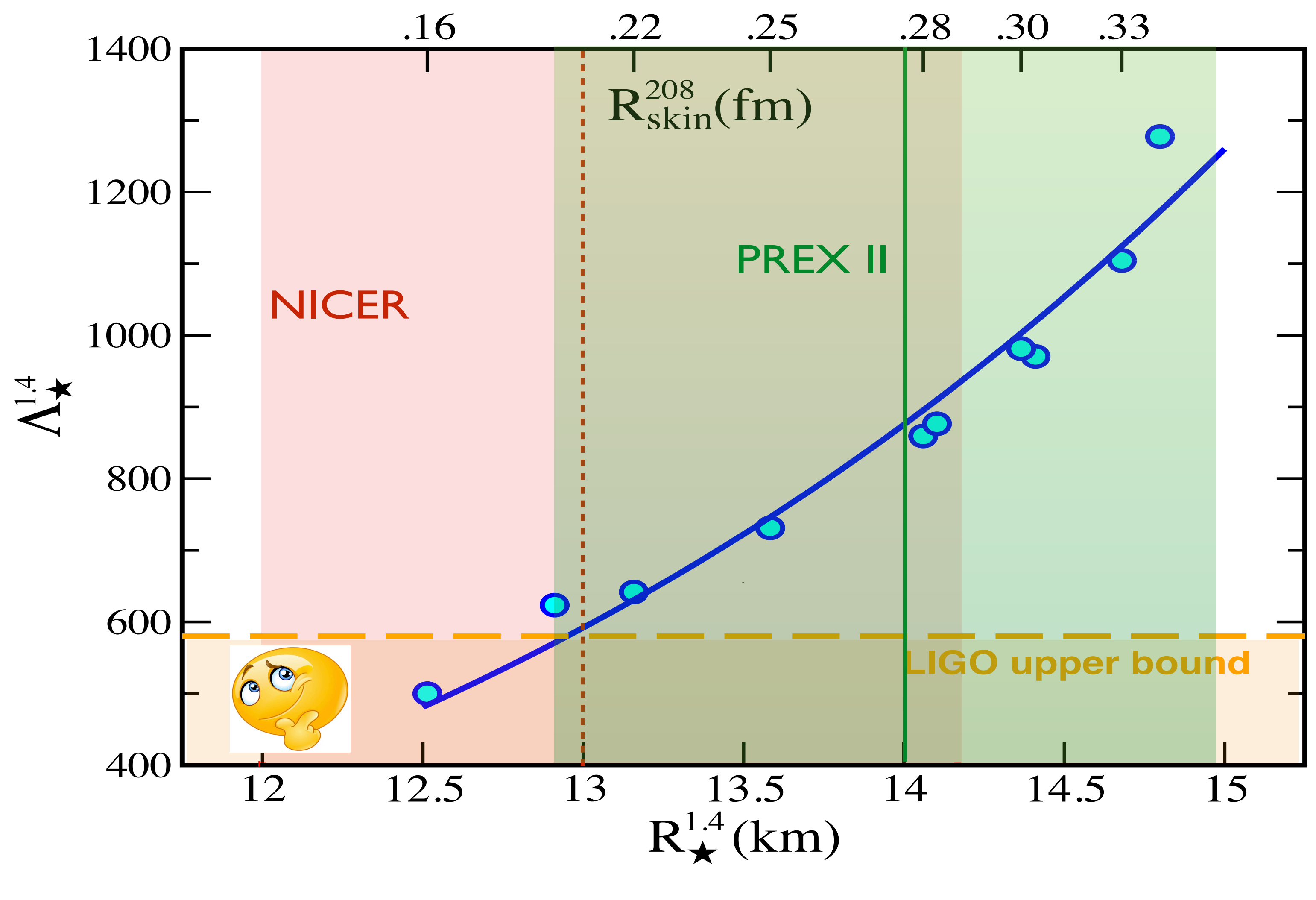


The Dawn of a Golden Era in Neutron-Star Physics



Micro-Macro





Tantalizing Possibility

- *Laboratory Experiments suggest large neutron radii for Pb* $\lesssim 1\rho_0$
- *Gravitational Waves suggest small stellar radii* $\gtrsim 2\rho_0$
- *Electromagnetic Observations suggest large stellar masses* $\gtrsim 4\rho_0$

Exciting possibility: If all are confirmed, this tension may be evidence of a softening/stiffening of the EOS (phase transition?)

The composition of the outer crust and the r-process

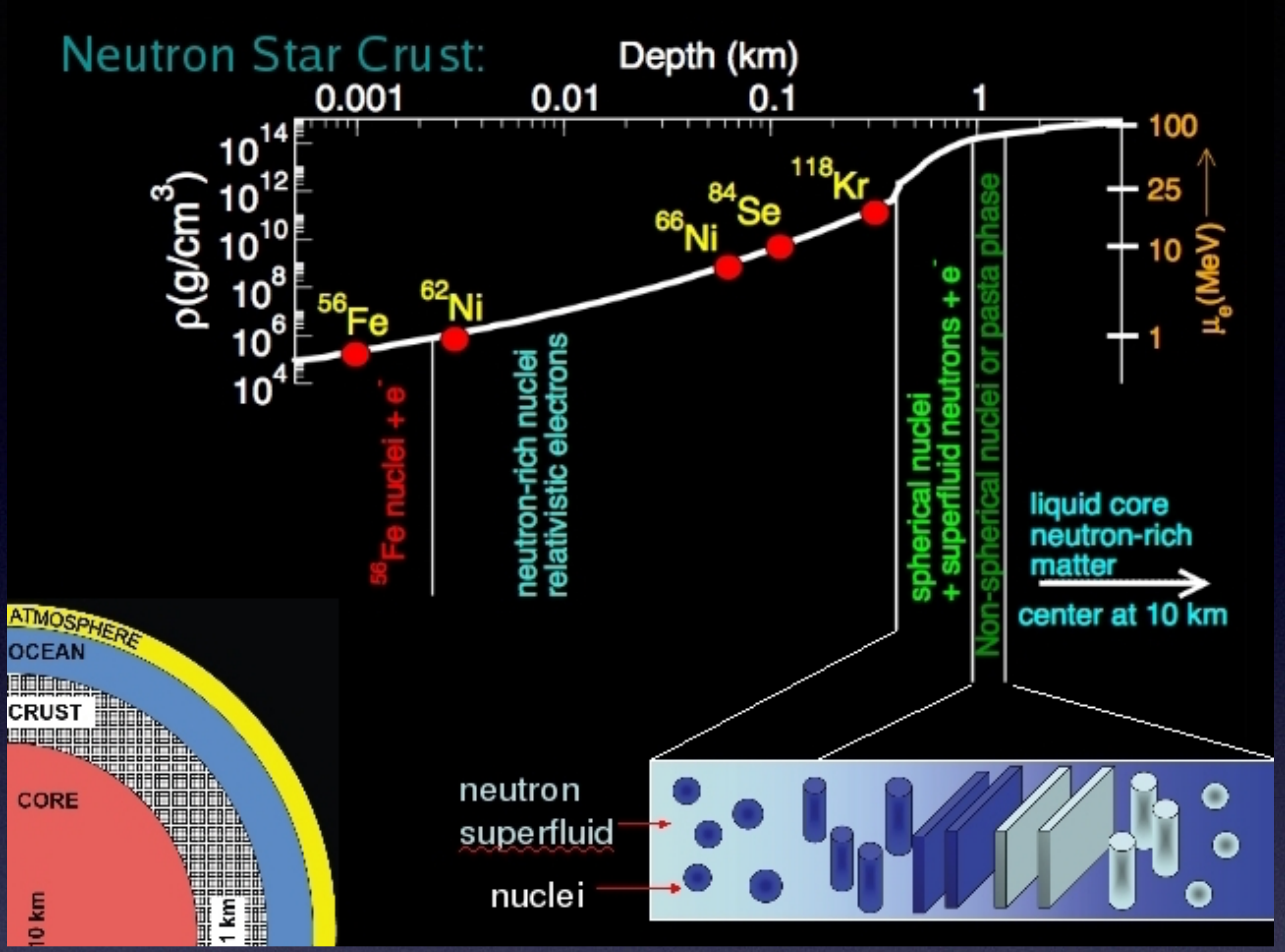
Enormous sensitivity to nuclear masses!

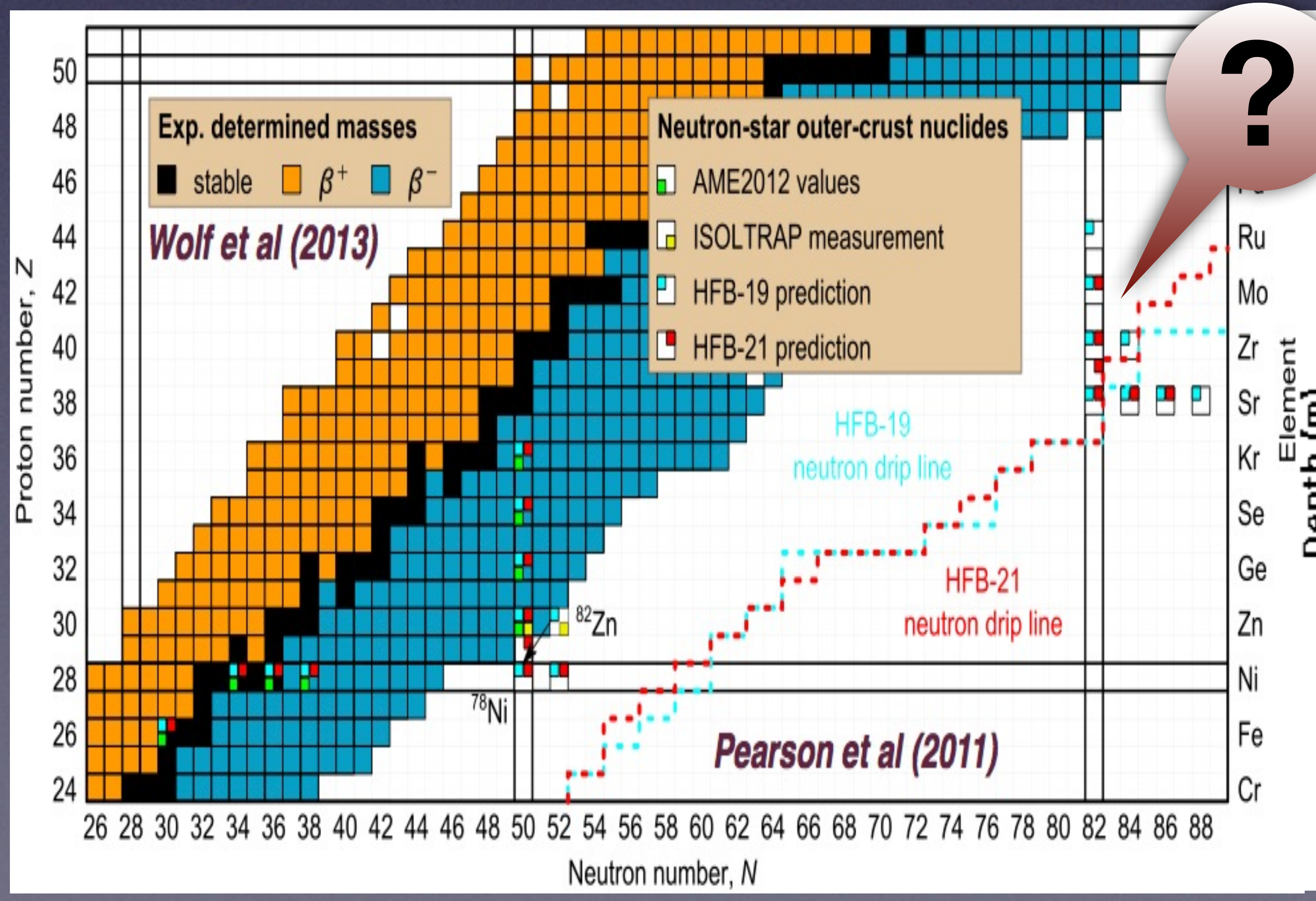
Outer Crust: Lattice of neutron-rich nuclei imbedded in e-gas (N=50,82)

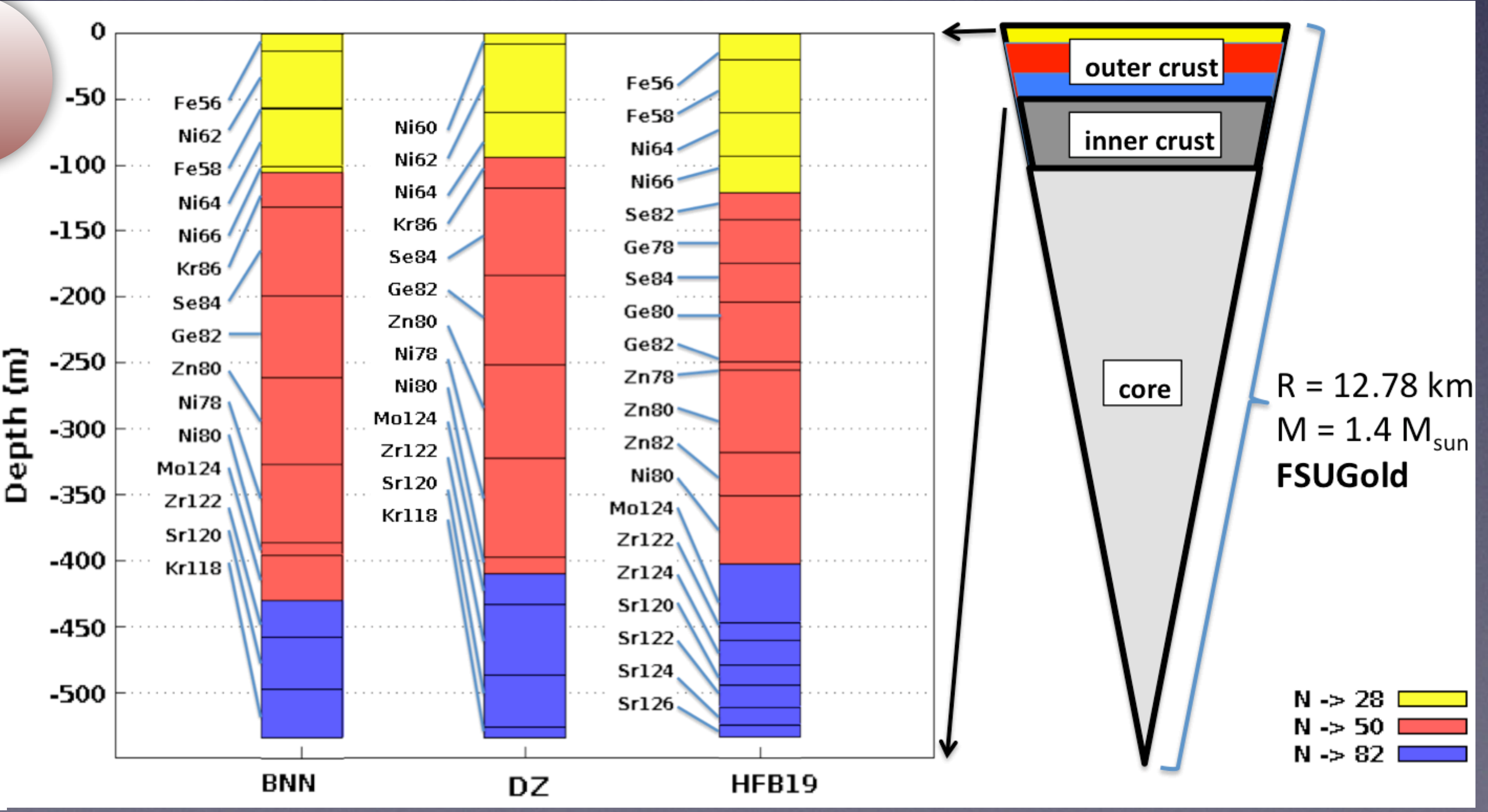
r-Process: Seed nuclei imbedded in a high neutron-flux environment reach neutron drip line

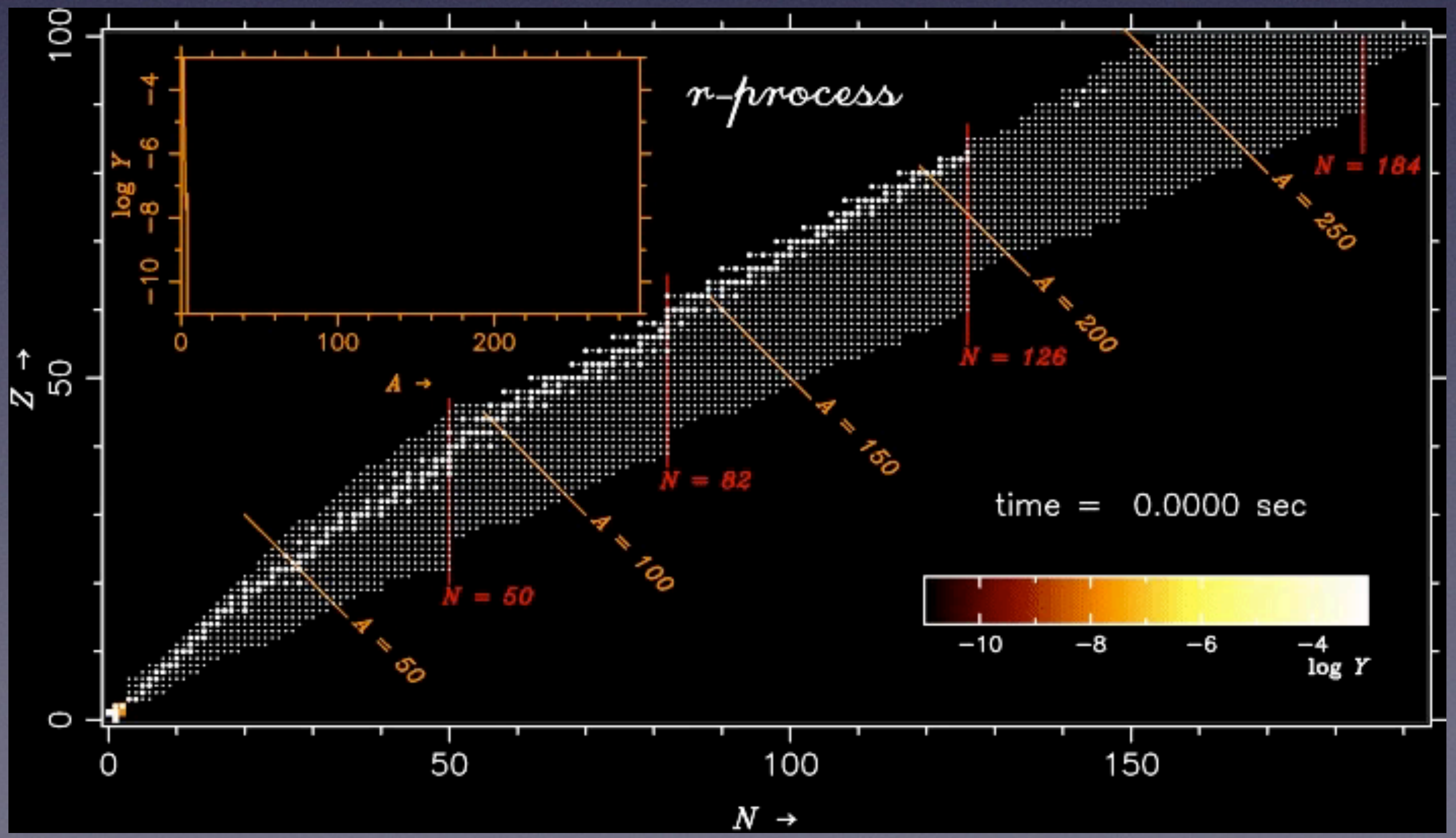
RIB Facilities: Unlikely to reach drip lines

Theory/Experiment partnership!









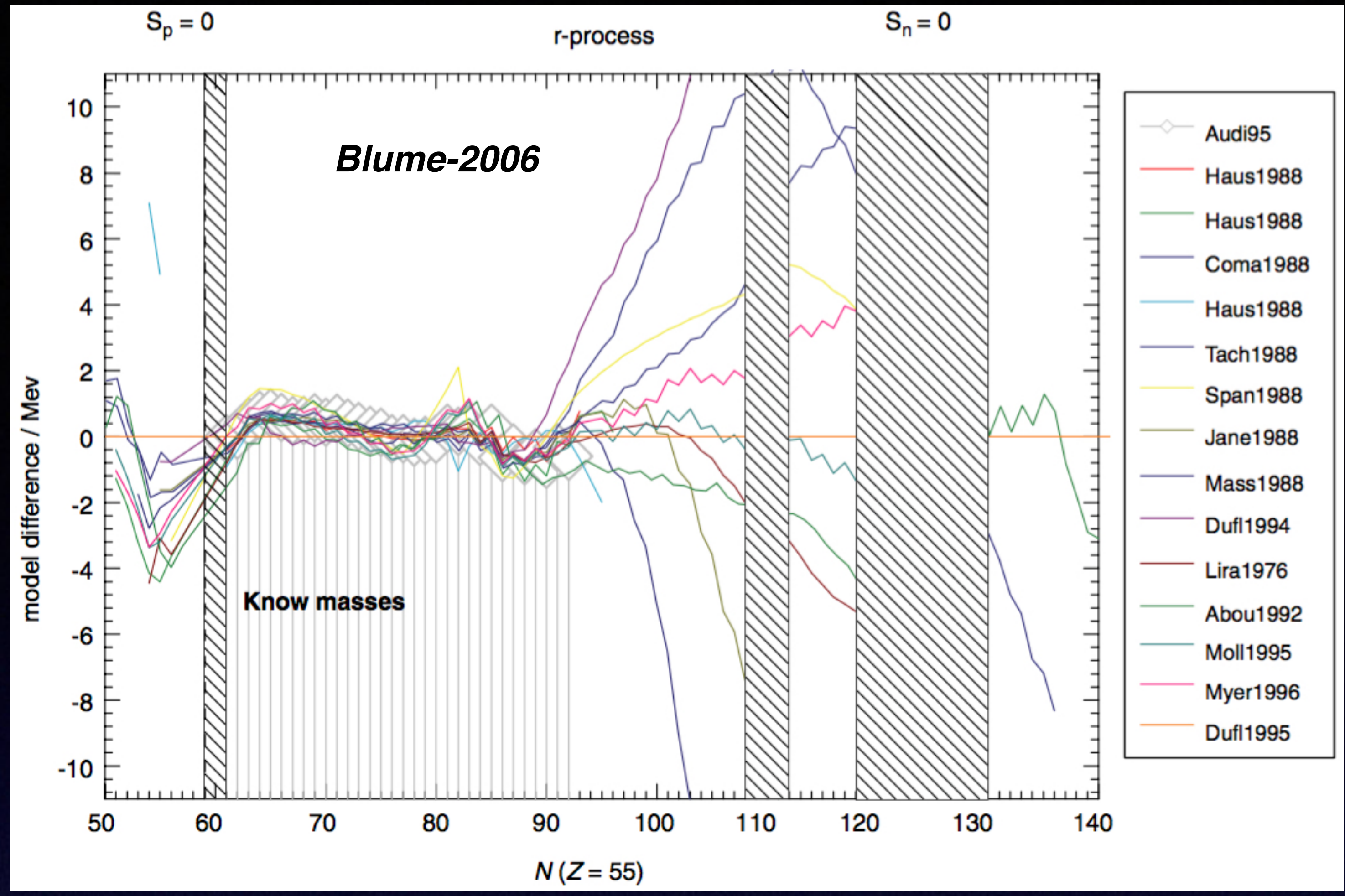
Nuclear Theory meets Machine Learning

- Use DFT to predict nuclear masses
- Train BNN by focusing on residuals

} *The paradigm*

$$M(N,Z) = M_{DFT}(N,Z) + \delta M_{BNN}(N,Z)$$

- Systematic scattering greatly reduced
- Predictions supplemented by theoretical errors

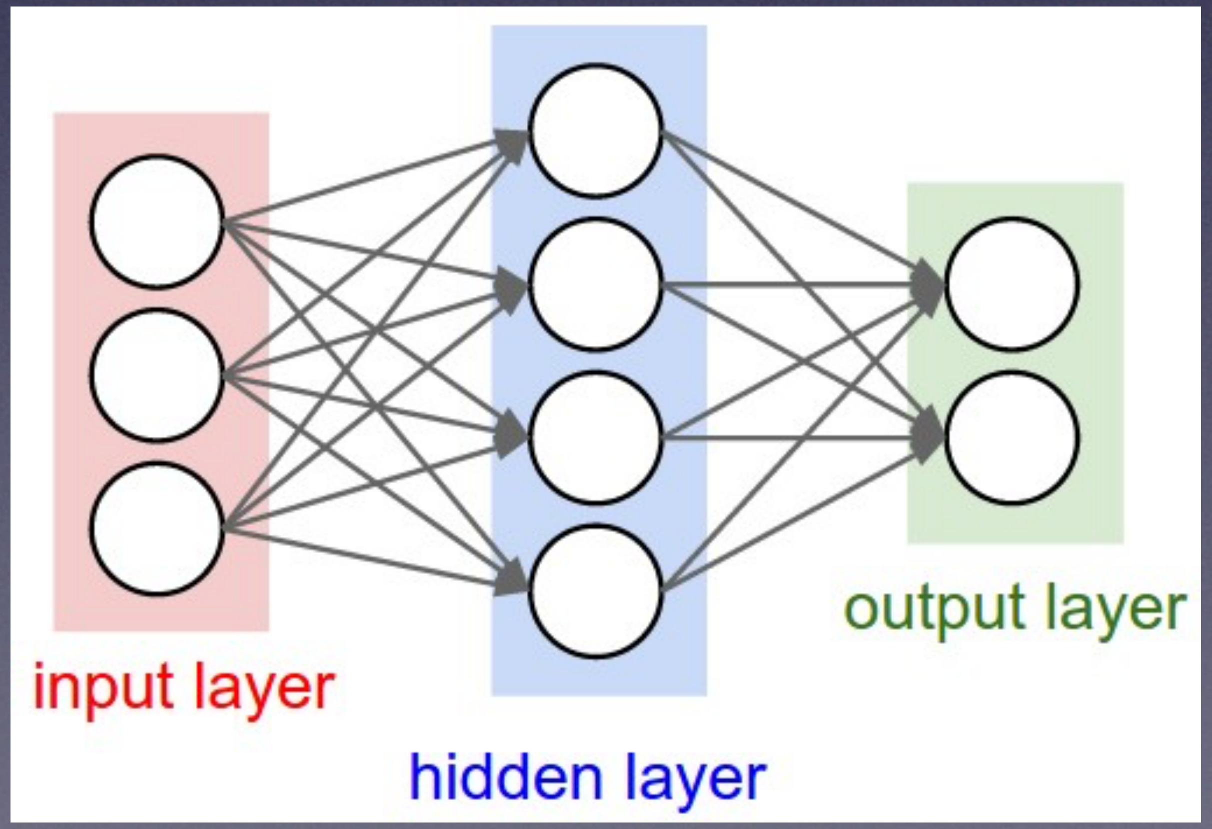


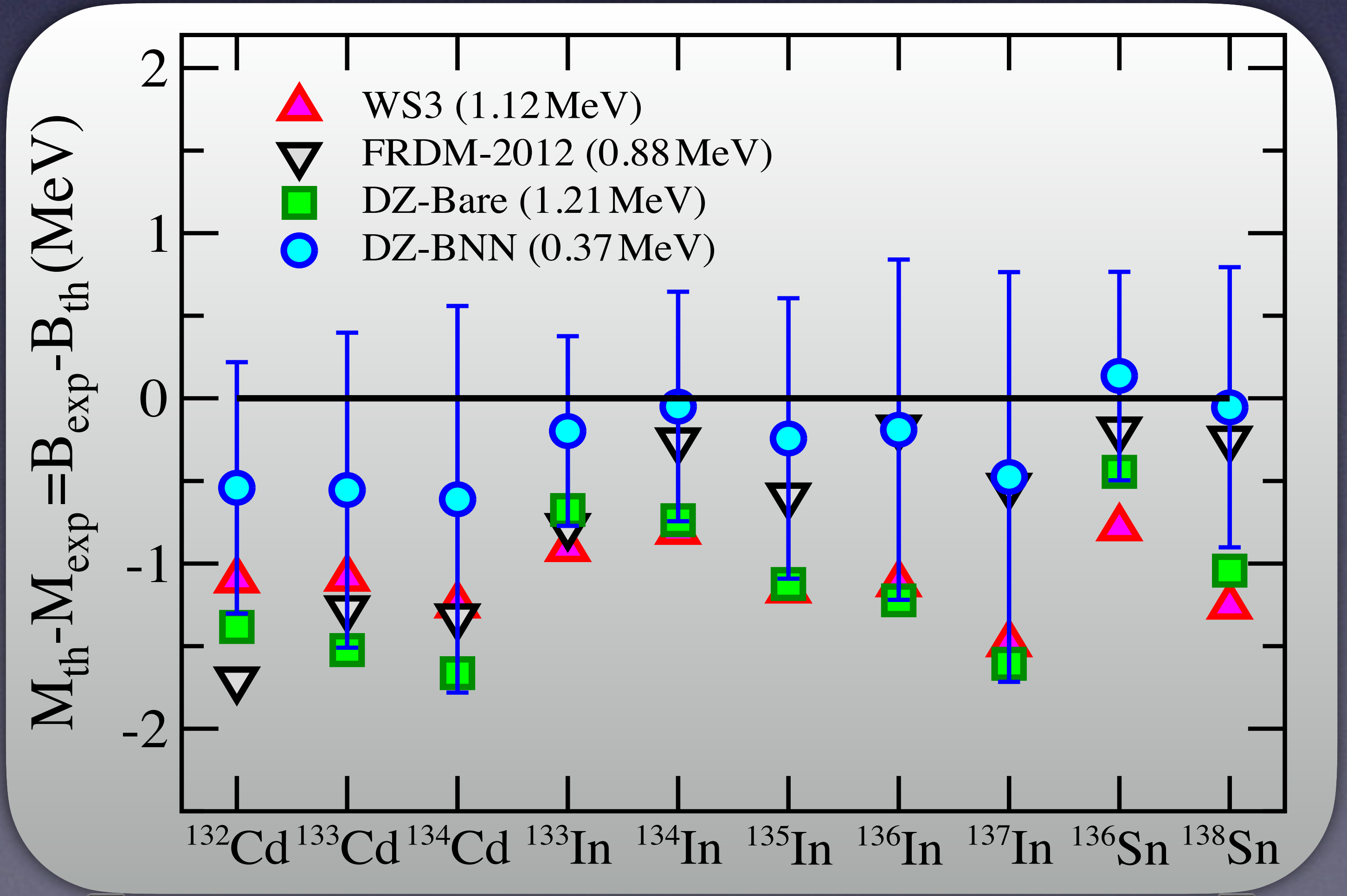
A very sad state of affairs

Train with AME2012 then predict AME2016

Re-generating Richard Feynman

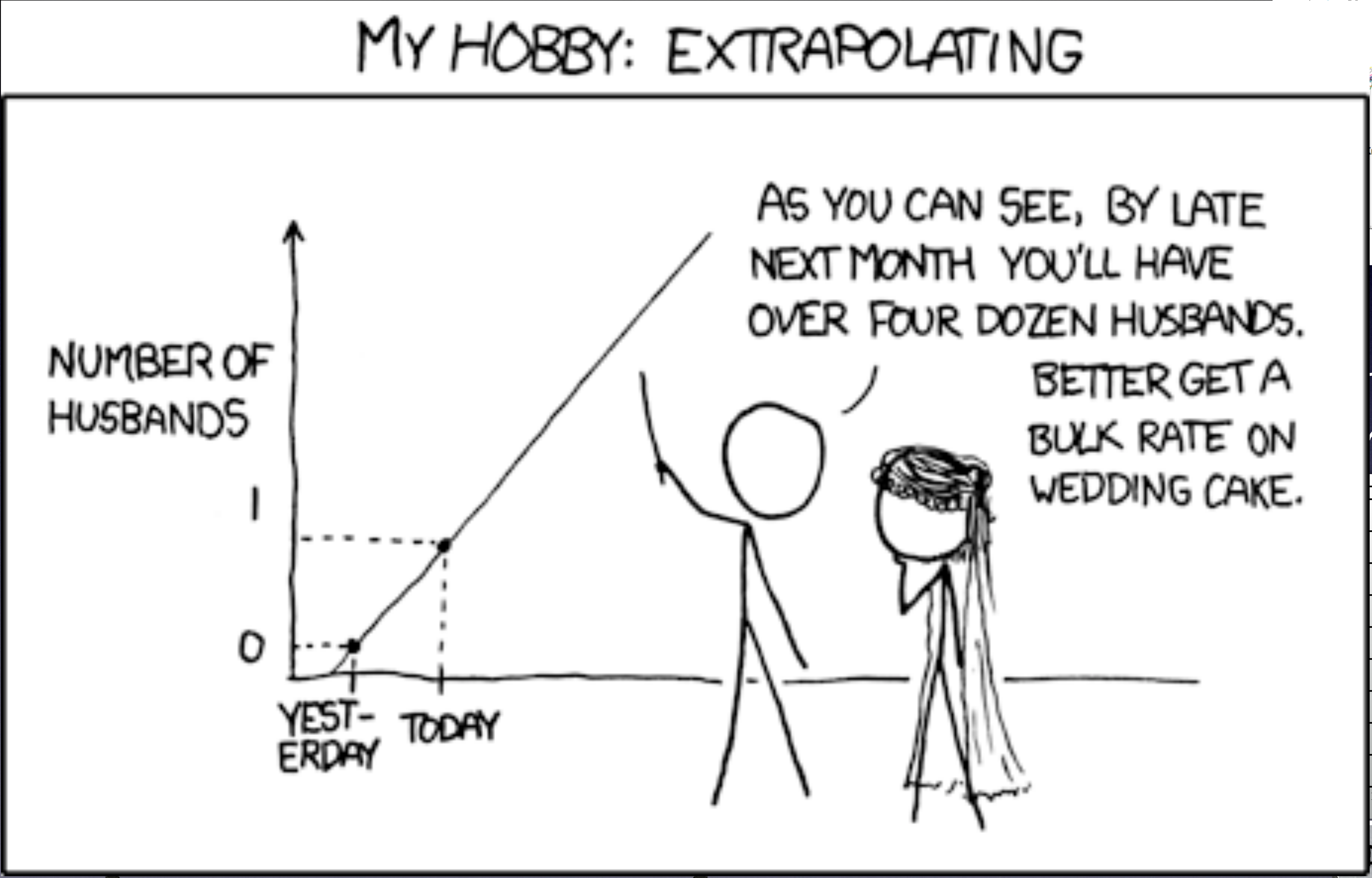
Refine Theory

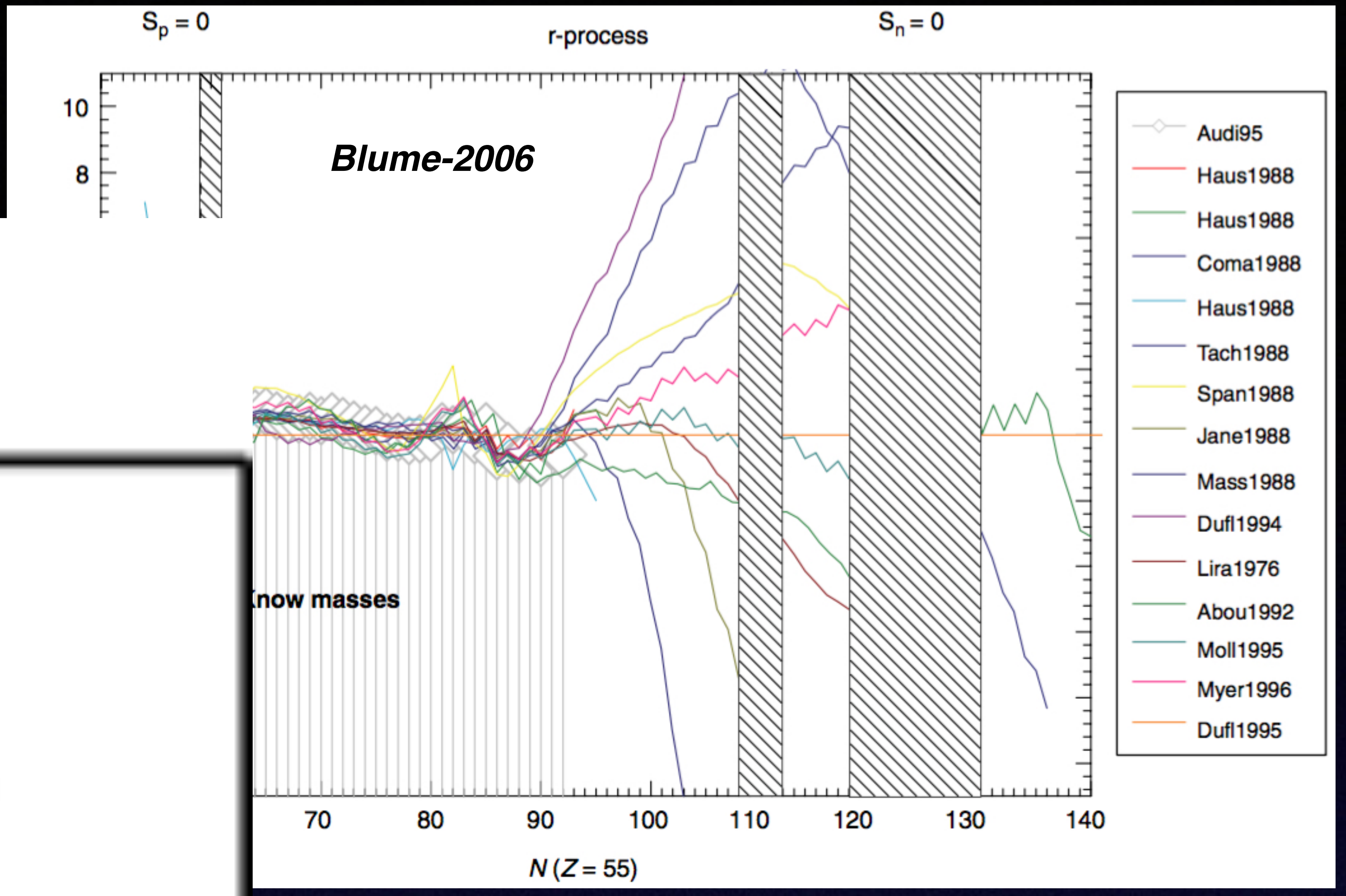




Duflo-Zuker + BNN

The Dangers of Extrapolation!

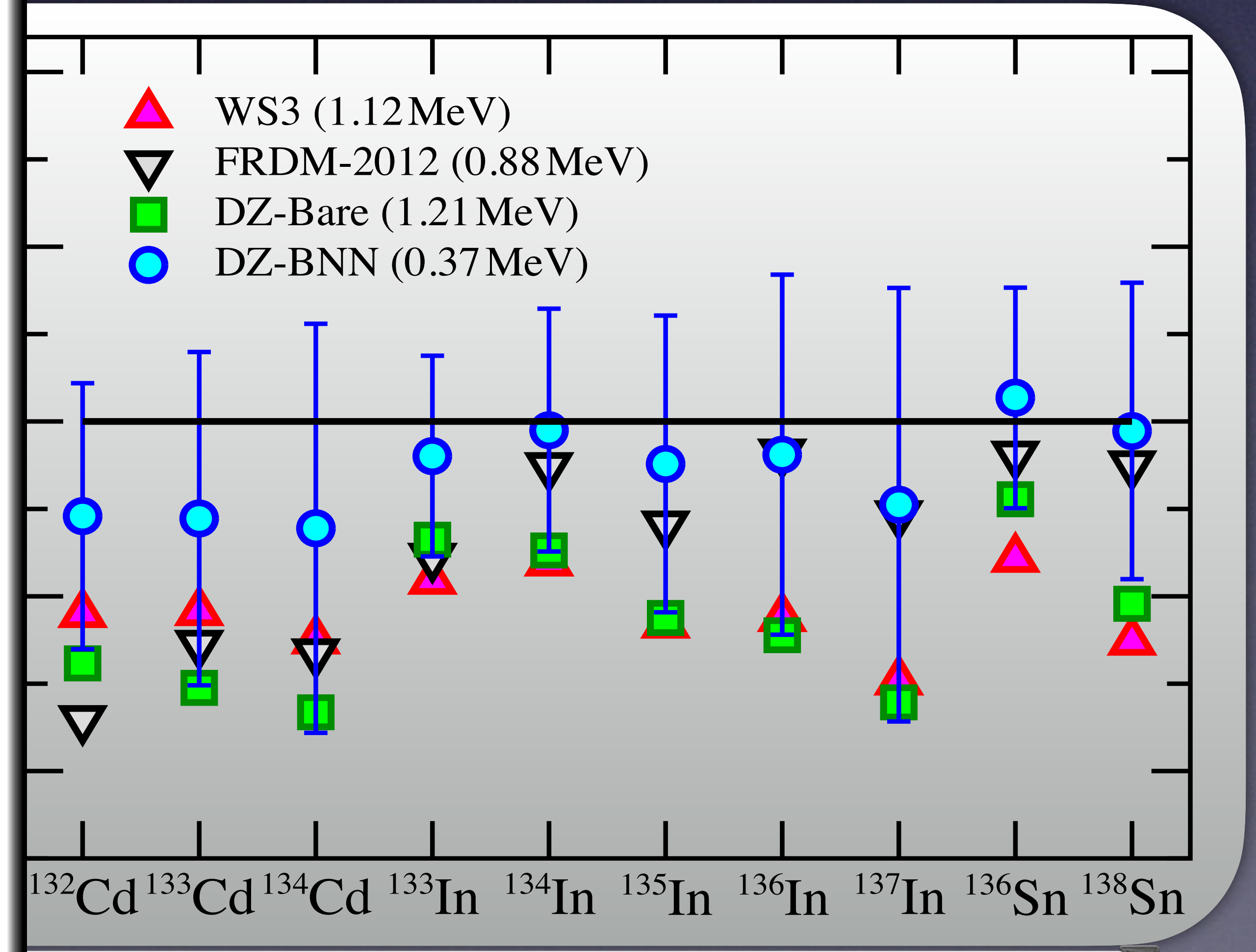




ry sad state of affairs

rain with AME2012

hen predict AME2016



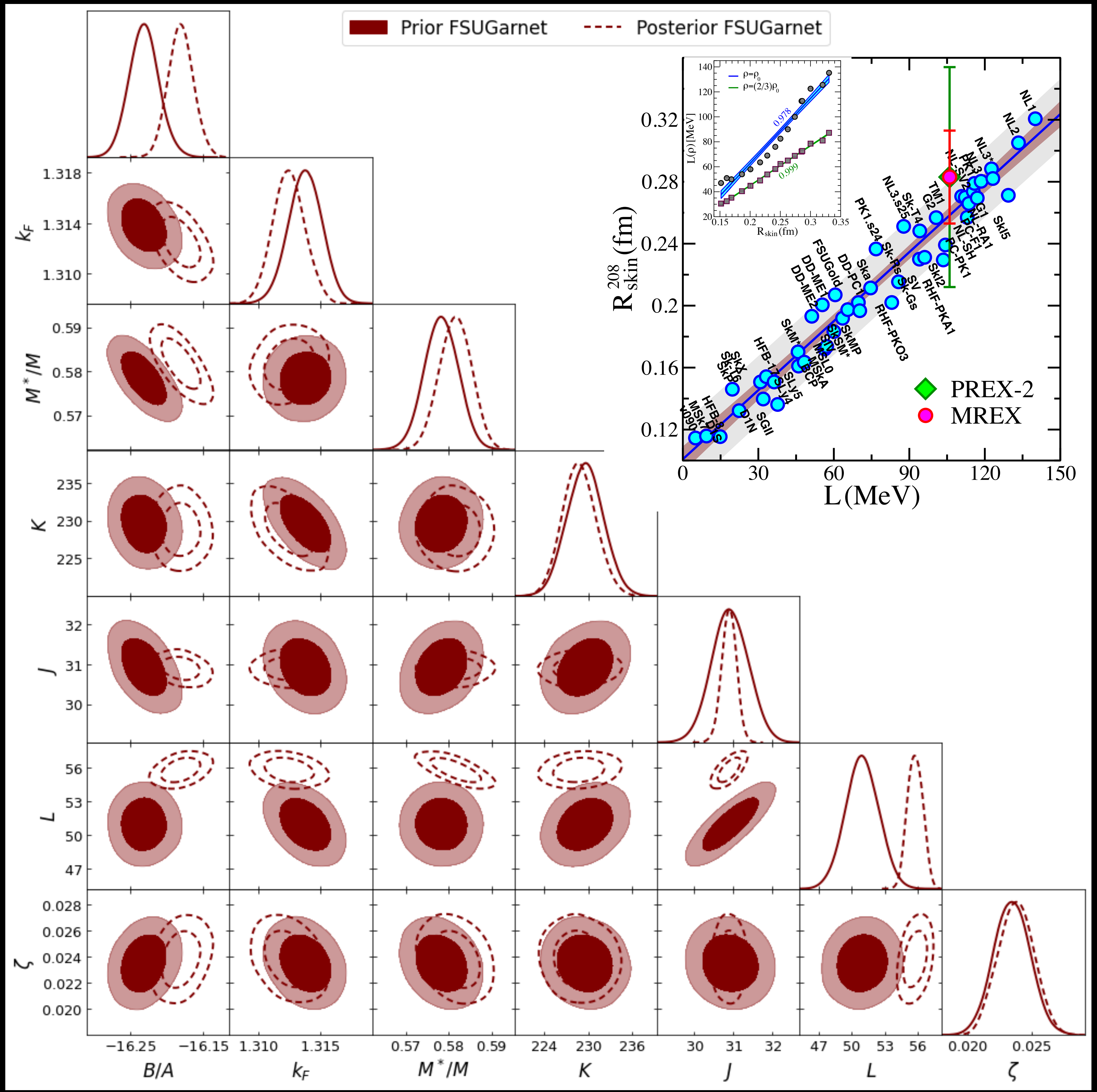
uflo-Zuker + BNN

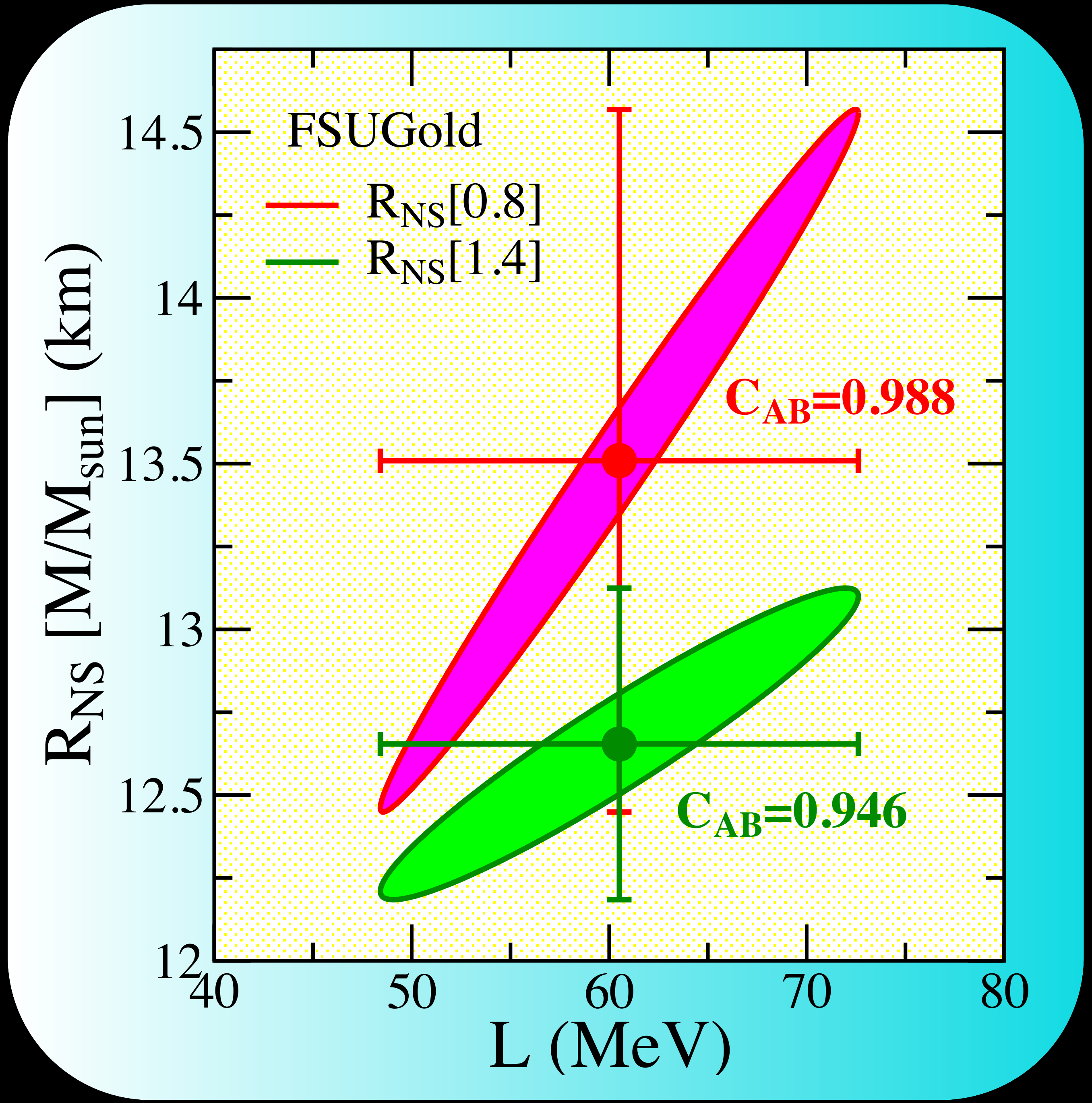
Bayesian Inference for Uncertainty Quantification: Model building for the understanding of atomic nuclei, neutron stars, and unveiling correlations

$$\mathcal{L}_{\rm Yukawa} = \bar{\psi}\left[g_{\rm s}\phi - \left(g_{\rm v}V_\mu + \frac{g_\rho}{2}\tau\cdot\mathbf{b}_\mu + \frac{e}{2}(1+\tau_3)A_\mu\right)\gamma^\mu\right]\psi$$

$$\mathcal{L}_{\rm self} = \frac{\kappa}{3!}(g_{\rm s}\phi)^3 - \frac{\lambda}{4!}(g_{\rm s}\phi)^4 + \frac{\zeta}{4!}g_{\rm v}^4(V_\mu V^\mu)^2 + \Lambda_{\rm v}\left(g_\rho^2\,\mathbf{b}_\mu\cdot\mathbf{b}^\mu\right)\left(g_{\rm v}^2 V_\nu V^\nu\right)$$

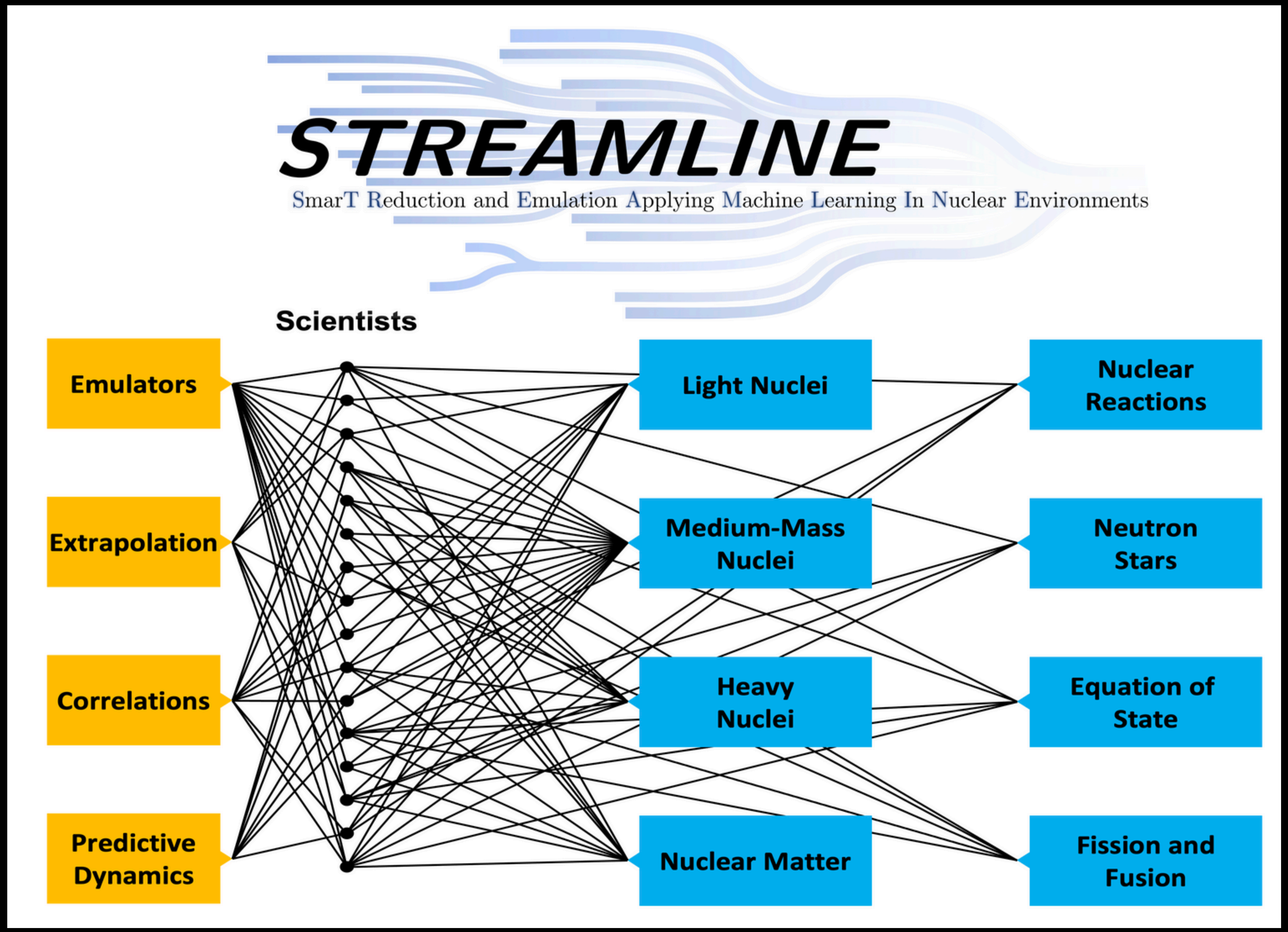
$$(g_{\rm s}, g_{\rm v}, g_\rho, \kappa, \lambda, \Lambda_{\rm v}) \Longleftrightarrow (\rho_0, \epsilon_0, M^*, K, J, L)$$





Neutron skins and stellar radii (quantities that differ by 18 orders of magnitude) are both sensitive to L!

Emulators and Reduced Order Models

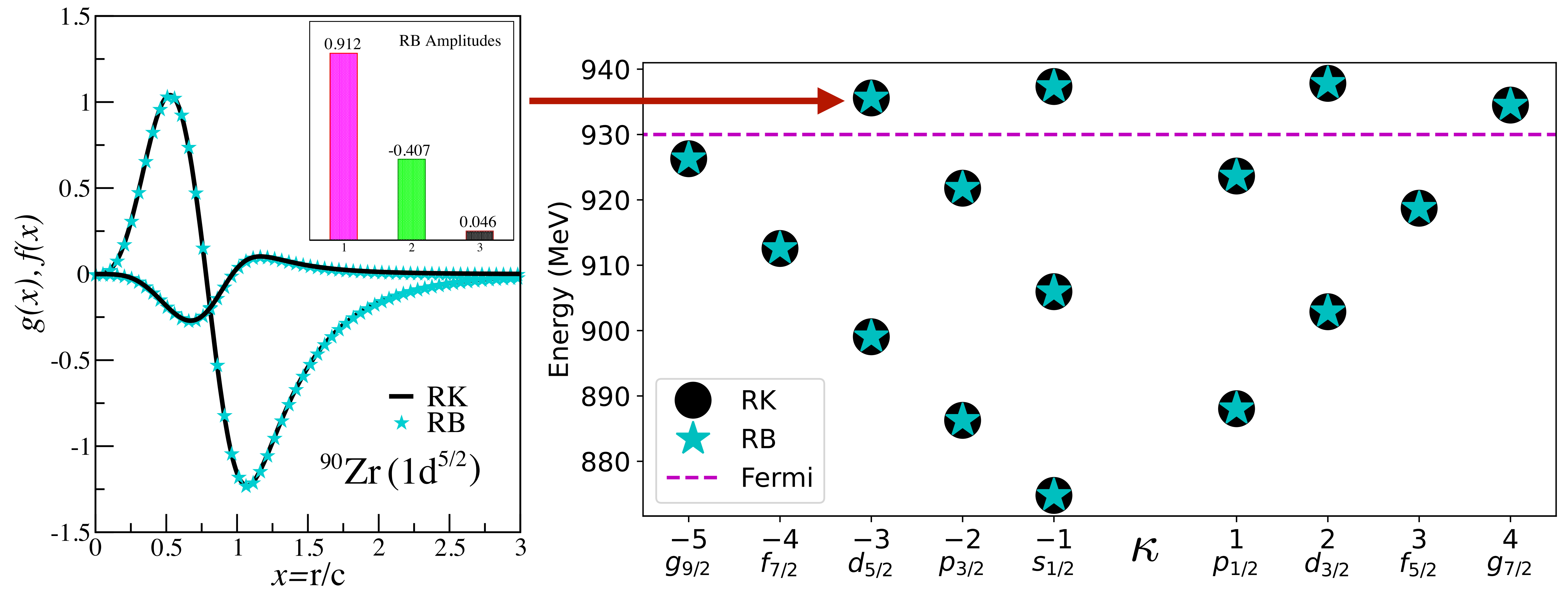


A universal reduced basis for the calibration of covariant energy density functionals

Amy L. Anderson* and J. Piekarewicz†
Department of Physics, Florida State University, Tallahassee, FL 32306, USA

(Dated: June 5, 2024)

The reduced basis method is used to construct a "universal" basis of Dirac orbitals that may be applicable throughout the nuclear chart to calibrate covariant energy density functionals. Relative to our earlier work using the non-relativistic Schrödinger equation, the Dirac equation adds an extra layer of complexity due to the existence of negative energy states. However, once this problem is mitigated, the resulting reduced basis is able to accurately and efficiently reproduce the high-fidelity model at a fraction of the computational cost. We are confident that the resulting reduced basis will serve as a foundational element in developing rapid and accurate emulators. In turn, these emulators will play a critical role in the Bayesian optimization of covariant energy density functionals.



Emulators are statistical ML models that faithfully reproduce the behavior of a complex physical system at a "tiny" fraction of the computational cost!

Conclusions: We have entered the golden era of neutron-star physics

- Astrophysics: What is the minimum mass of a black hole?
- C.Matter Physics: Existence of Coulomb-Frustrated Nuclear Pasta?
- General Relativity: Can BNS mergers constrain stellar radii?
- Nuclear Physics: What is the EOS of neutron-rich matter?
- Particle Physics: What exotic phases inhabit the dense core?
- Machine Learning: Extrapolation to where no man has gone before?

Neutron Stars are the natural meeting place for interdisciplinary, fundamental, and exciting science!

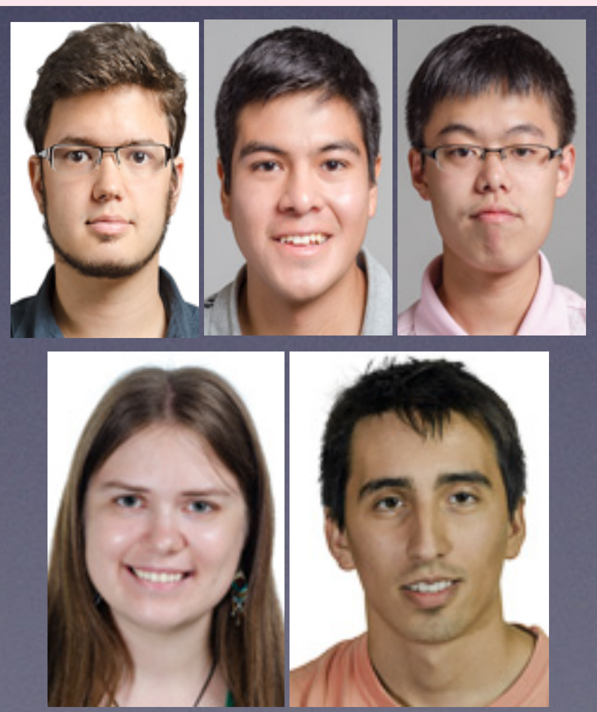
My FSU Collaborators

- Genaro Toledo-Sanchez
- Karim Hasnaoui
- Bonnie Todd-Rutel
- Brad Futch
- Jutri Taruna
- **Farrukh Fattoyev**
- **Wei-Chia Chen**
- **Raditya Utama**

Brendan Reed

My Outside Collaborators

- B. Agrawal (Saha Inst.)
- M. Centelles (U. Barcelona)
- G. Colò (U. Milano)
- C.J. Horowitz (Indiana U.)
- W. Nazarewicz (MSU)
- N. Paar (U. Zagreb)
- M.A. Pérez-Garcia (U. Salamanca)
- P.G.- Reinhard (U. Erlangen-Nürnberg)
- X. Roca-Maza (U. Milano)
- D. Vretenar (U. Zagreb)

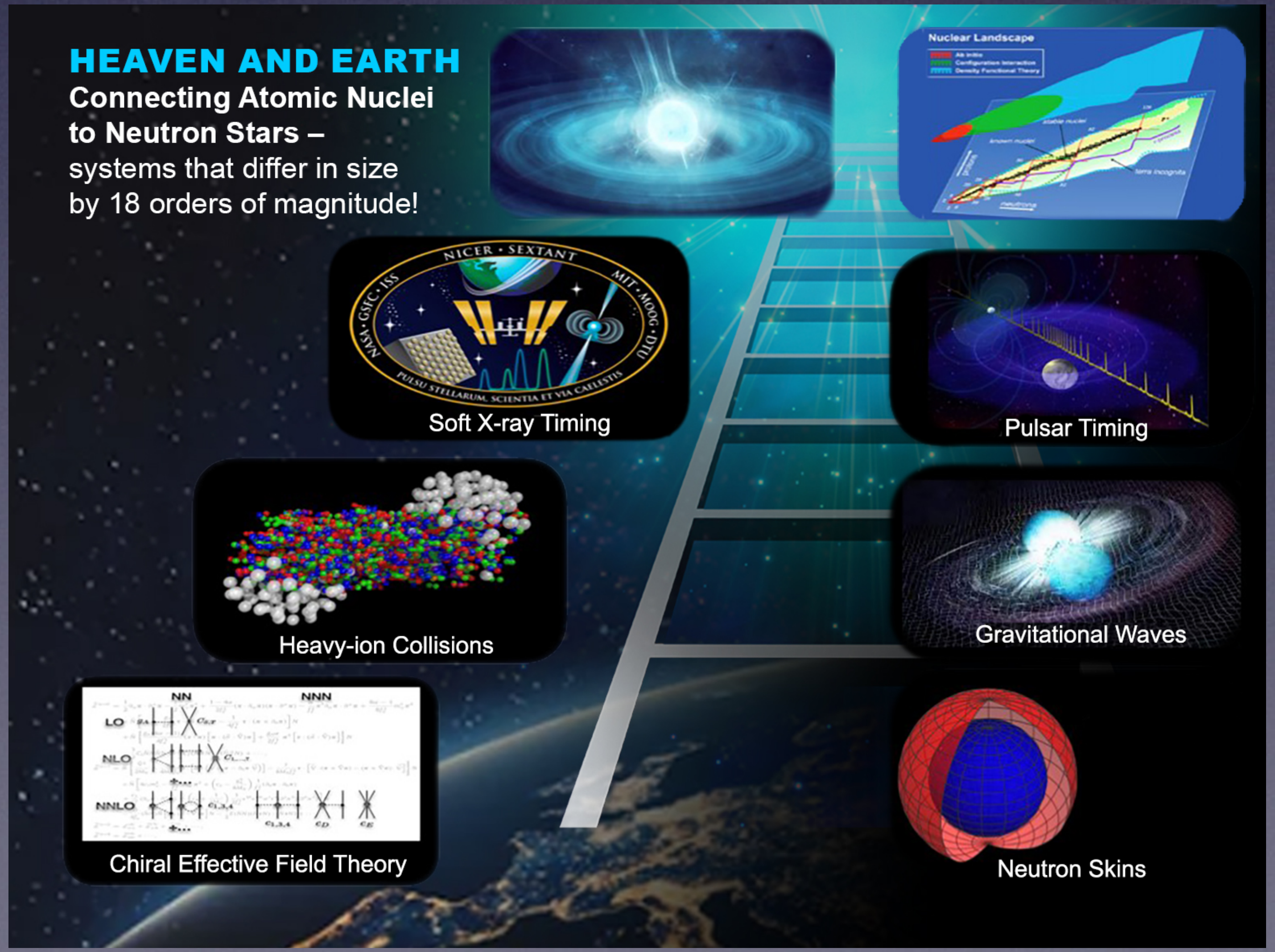


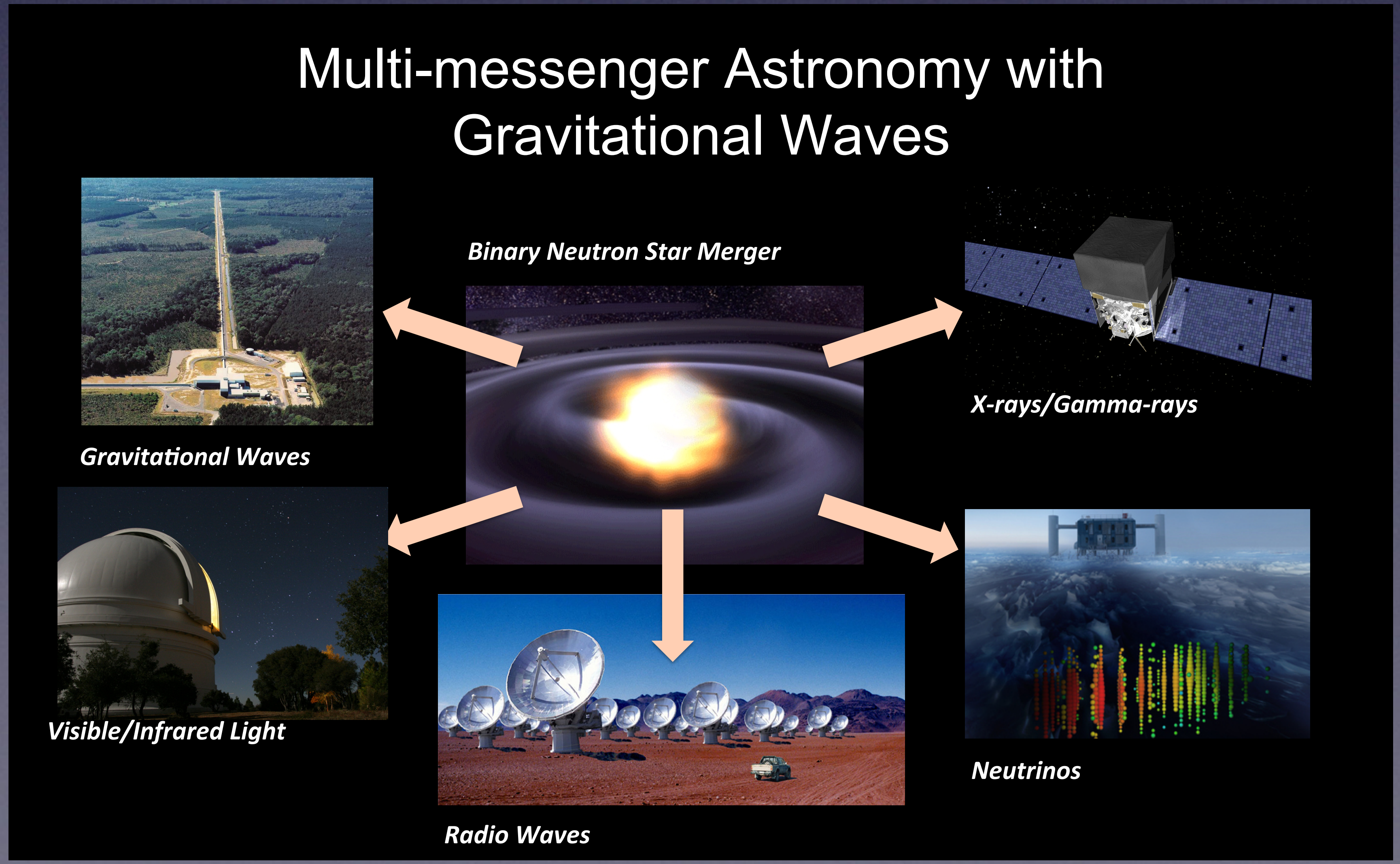
The “Old” Generation

- **Pablo Giuliani**
- **Daniel Silva**
- **Junjie Yang**

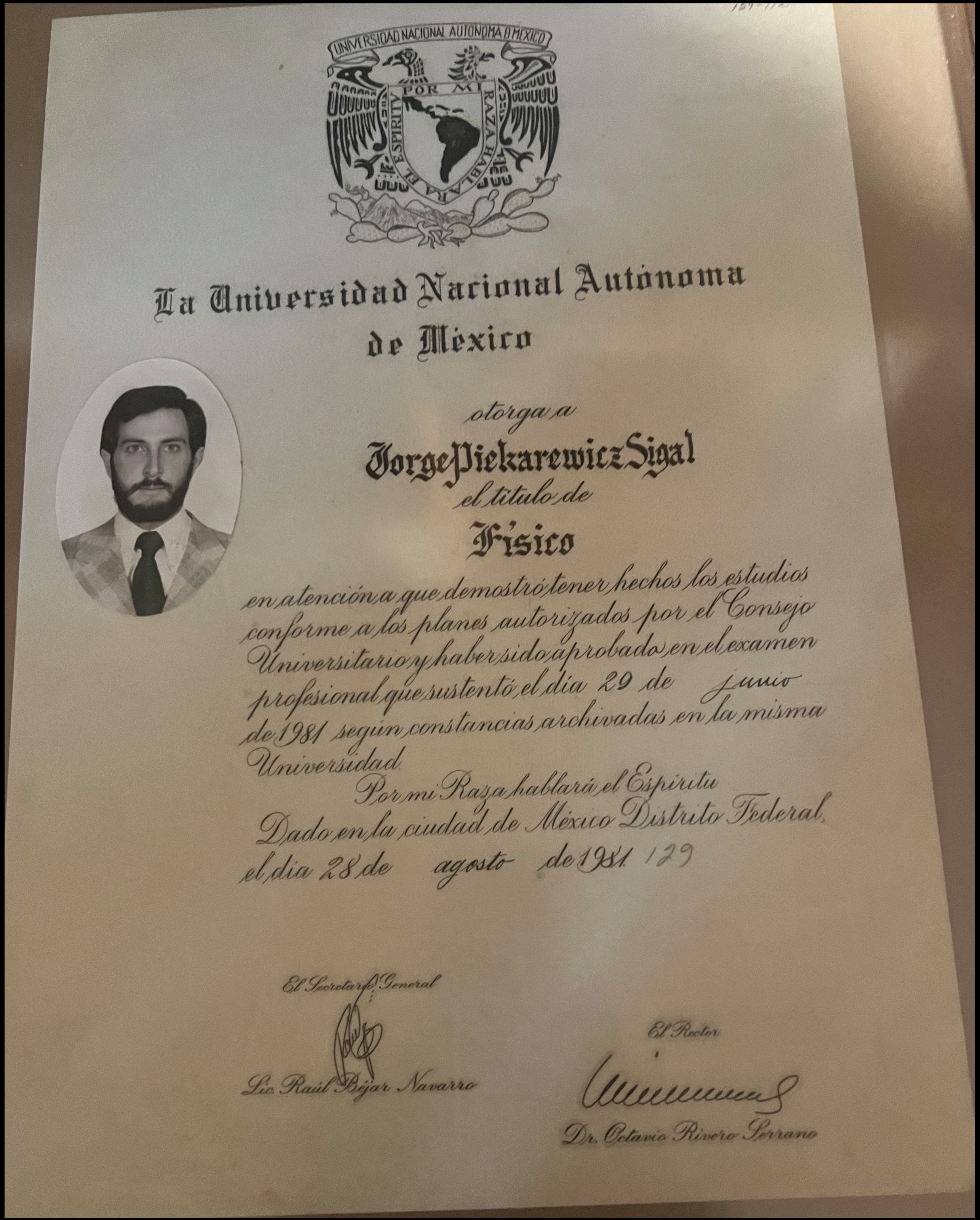
The New Generation

- **Amy Anderson**
- **Marc Salinas**





Muchas Gracias!!


UNIVERSIDAD NACIONAL AUTONOMA D MEXICO
POR MI RAZA HABLARA EL ESPIRITU

La Universidad Nacional Autónoma de México

otorga a

Jorge Piekarewicz Sigal

el título de

Físico

en atención a que demostró tener hechos los estudios conforme a los planes autorizados por el Consejo Universitario y haber sido aprobado en el examen profesional que sustentó el día 29 de junio de 1981 según constancias archivadas en la misma Universidad

Por mi Raza hablará el Espíritu

Dado en la ciudad de México Distrito Federal, el día 28 de agosto de 1981 129

El Secretario General

Lic. Raúl Béjar Navarro

El Rector

Dr. Octavio Rivero Serrano

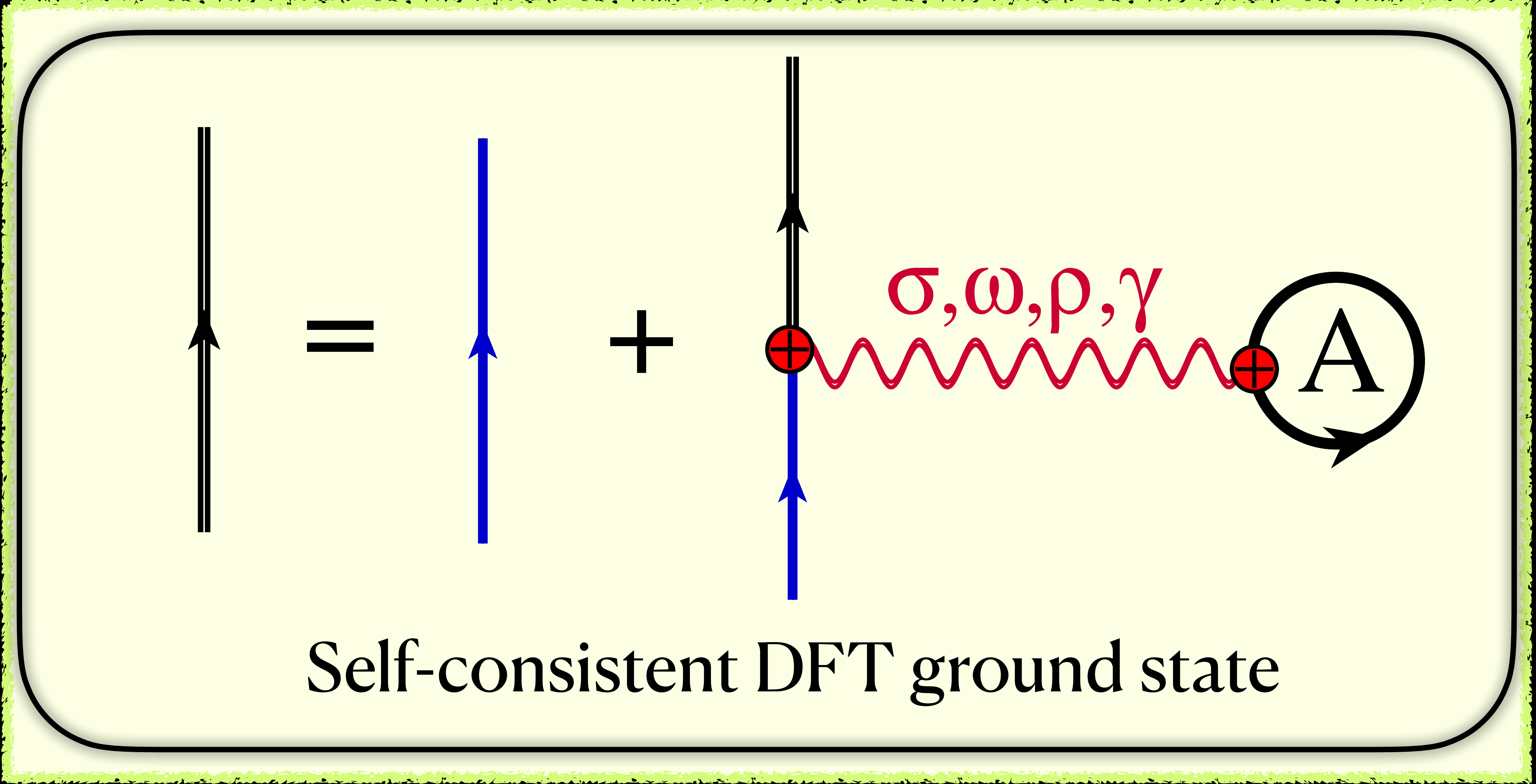
Backup Slides

Covariant Density Functional Theory

$$\mathcal{L}_{\rm Yukawa} = \bar{\psi}\left[g_{\rm s}\phi - \left(g_{\rm v}V_\mu + \frac{g_\rho}{2}\tau\cdot\mathbf{b}_\mu + \frac{e}{2}(1+\tau_3)A_\mu\right)\gamma^\mu\right]\psi$$

$$\mathcal{L}_{\rm self} = \frac{\kappa}{3!}(g_{\rm s}\phi)^3 - \frac{\lambda}{4!}(g_{\rm s}\phi)^4 + \frac{\zeta}{4!}g_{\rm v}^4(V_\mu V^\mu)^2 + \Lambda_{\rm v}\left(g_\rho^2\,\mathbf{b}_\mu\cdot\mathbf{b}^\mu\right)\left(g_{\rm v}^2 V_\nu V^\nu\right)$$

- σ: intermediate range scalar attraction (2π exchange)
- ω: short-range vector repulsion (contact term in χEFT)
- ρ: isospin (flavor) dependent short-range interaction
- γ: long-range Coulomb repulsion between protons



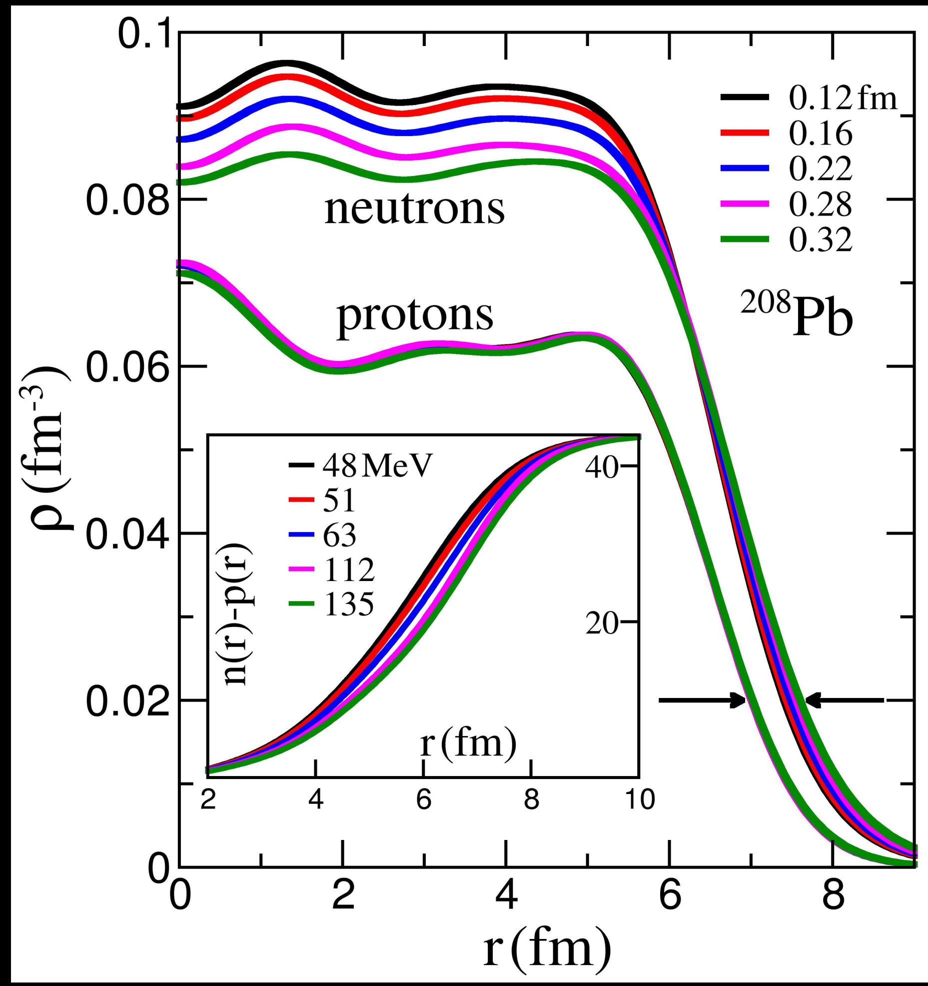
Walter Kohn
Nobel Laureate
Chemistry 1998

Anatomy of a self-consistent Covariant DFT calculation

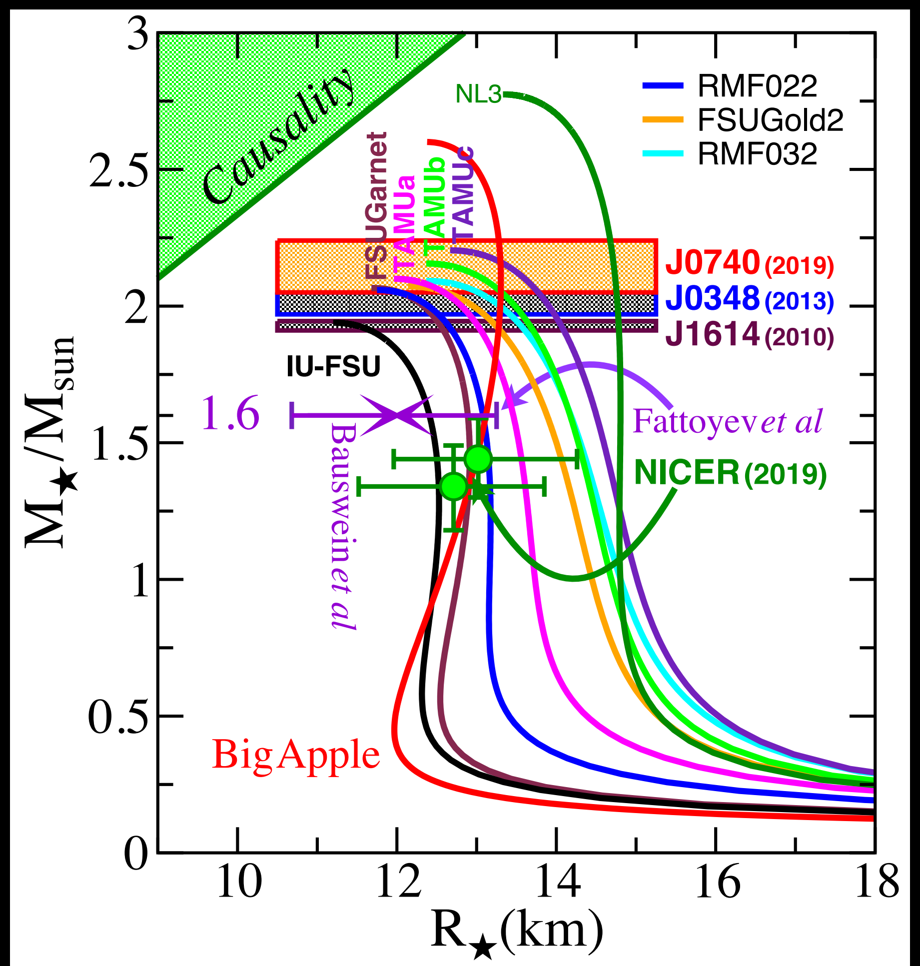
The Hohenberg-Kohn Theorem: The ground state energy can be obtained variationally: the density that minimizes the total energy is the exact ground state density

- Empirical parameters calibrated to physical observables
- Ground state properties emerge from functional minimization

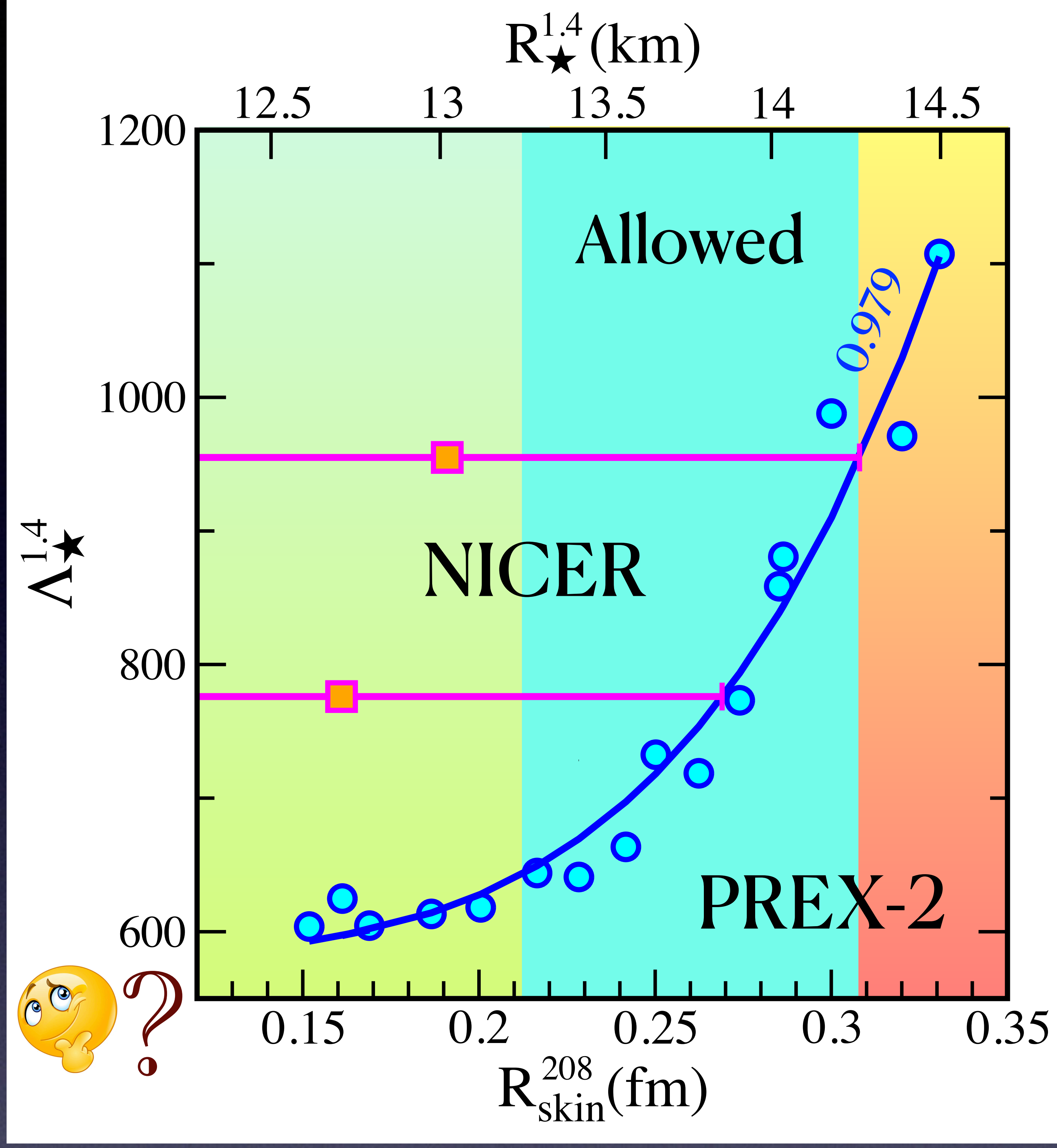
From finite nuclei to neutron stars!

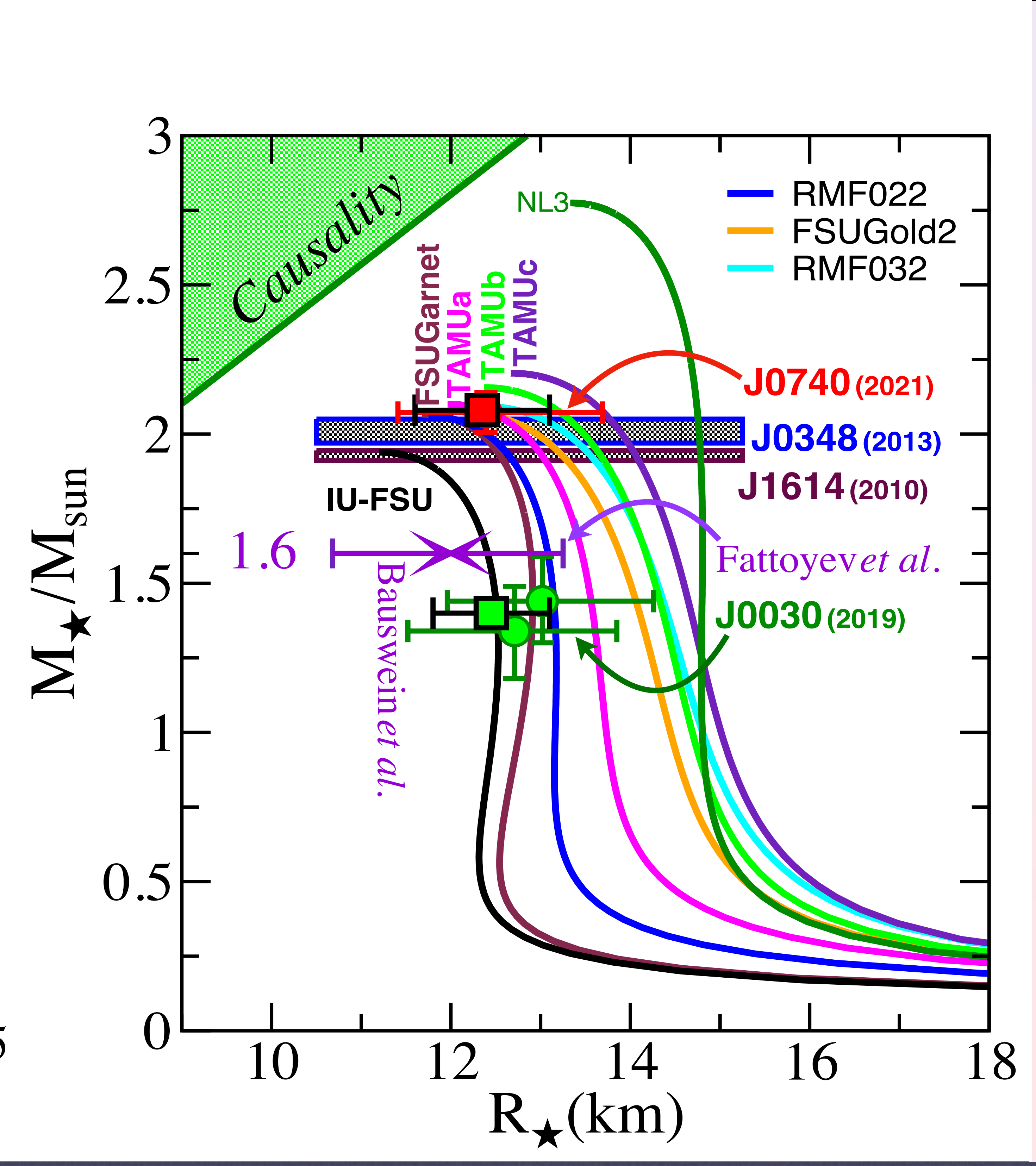


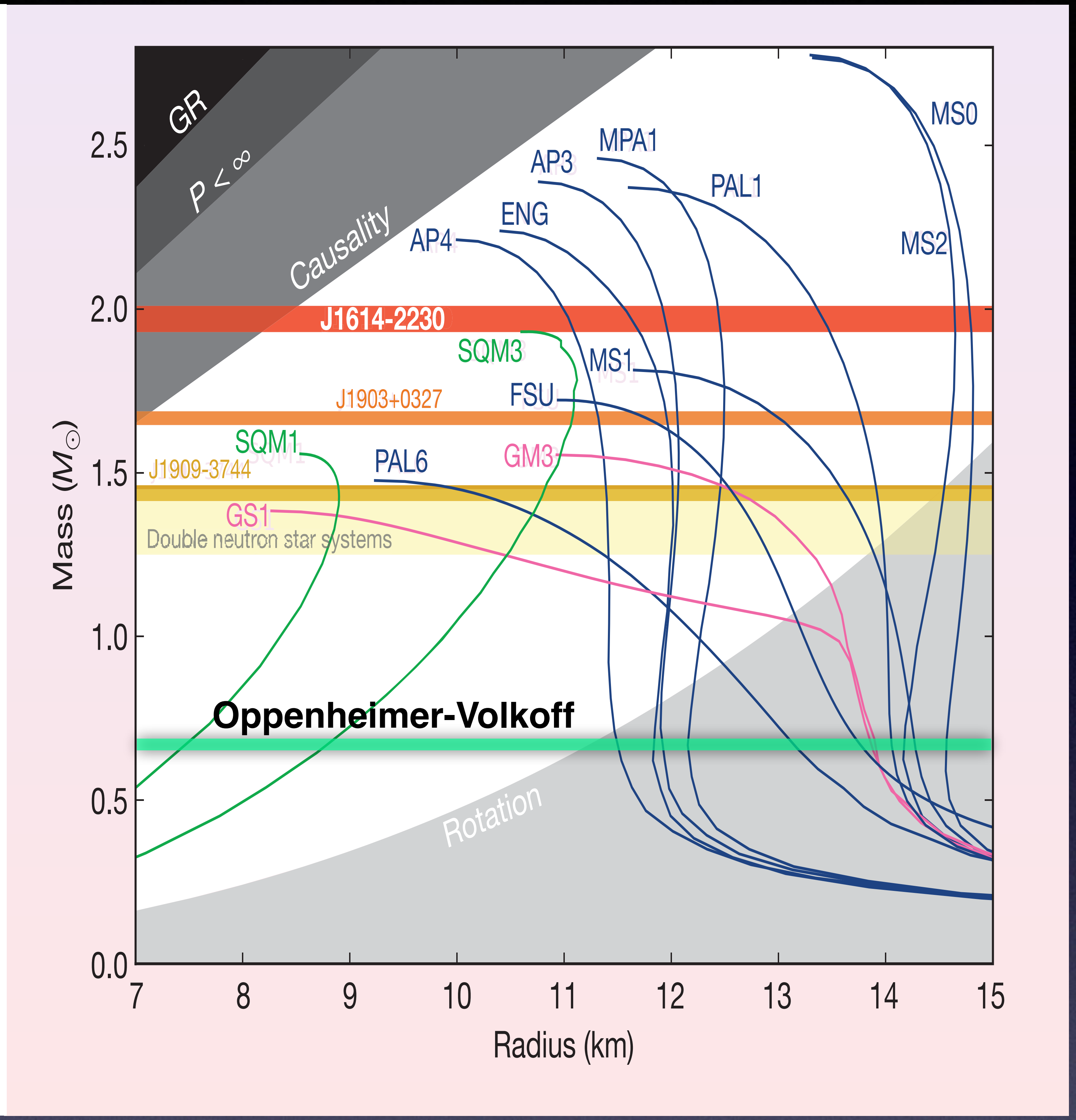
18 orders ⟷ magnitude

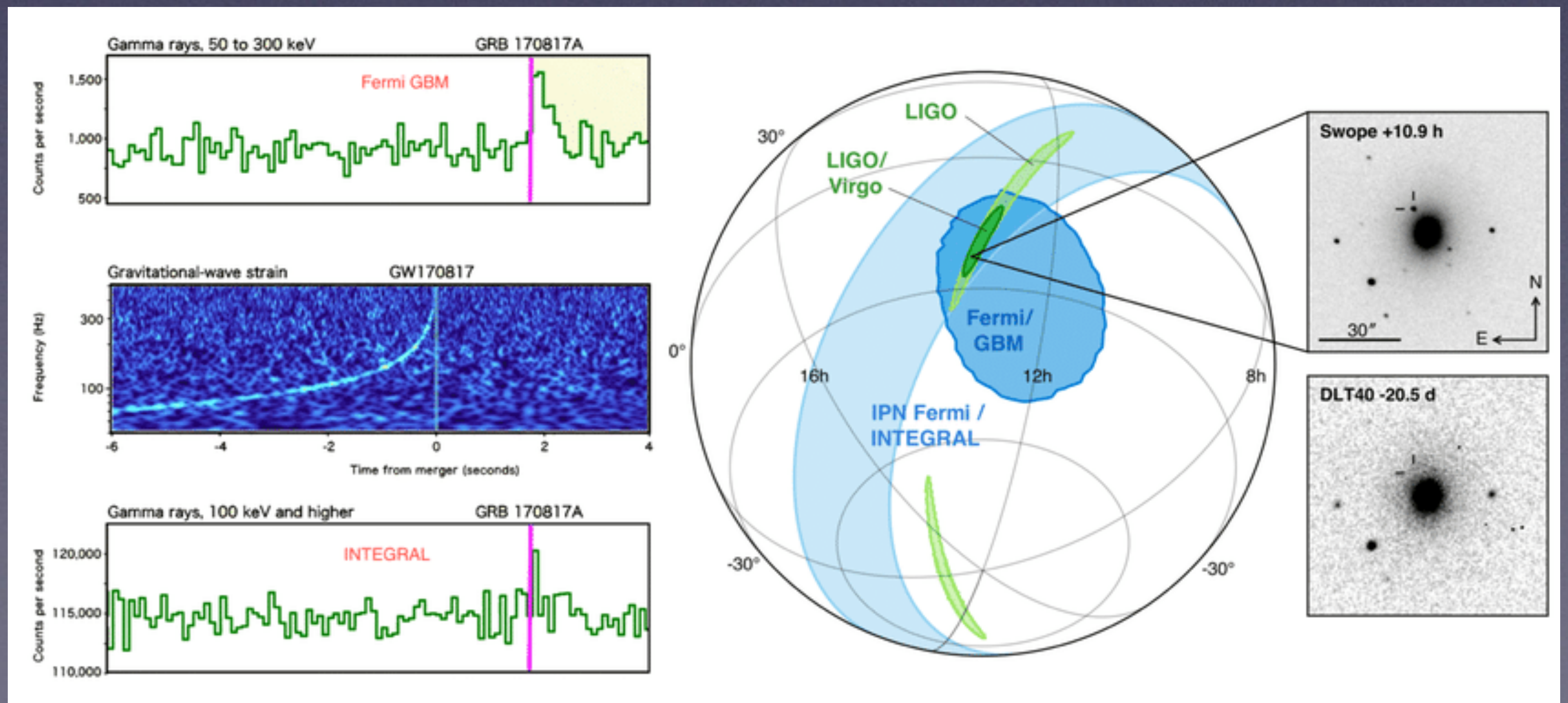


The Dawn of a Golden Era in Neutron-Star Physics





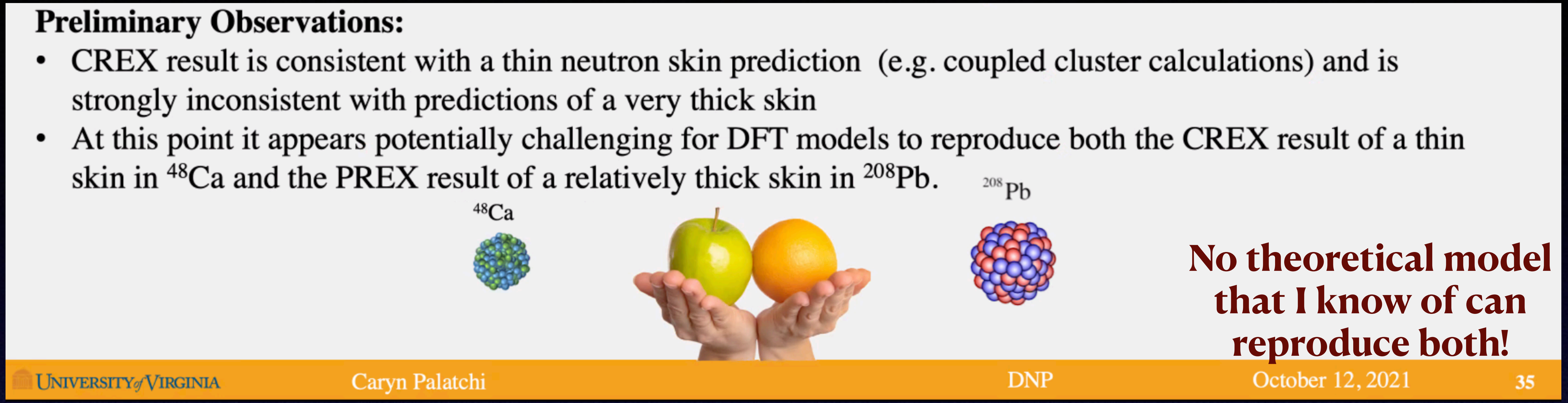




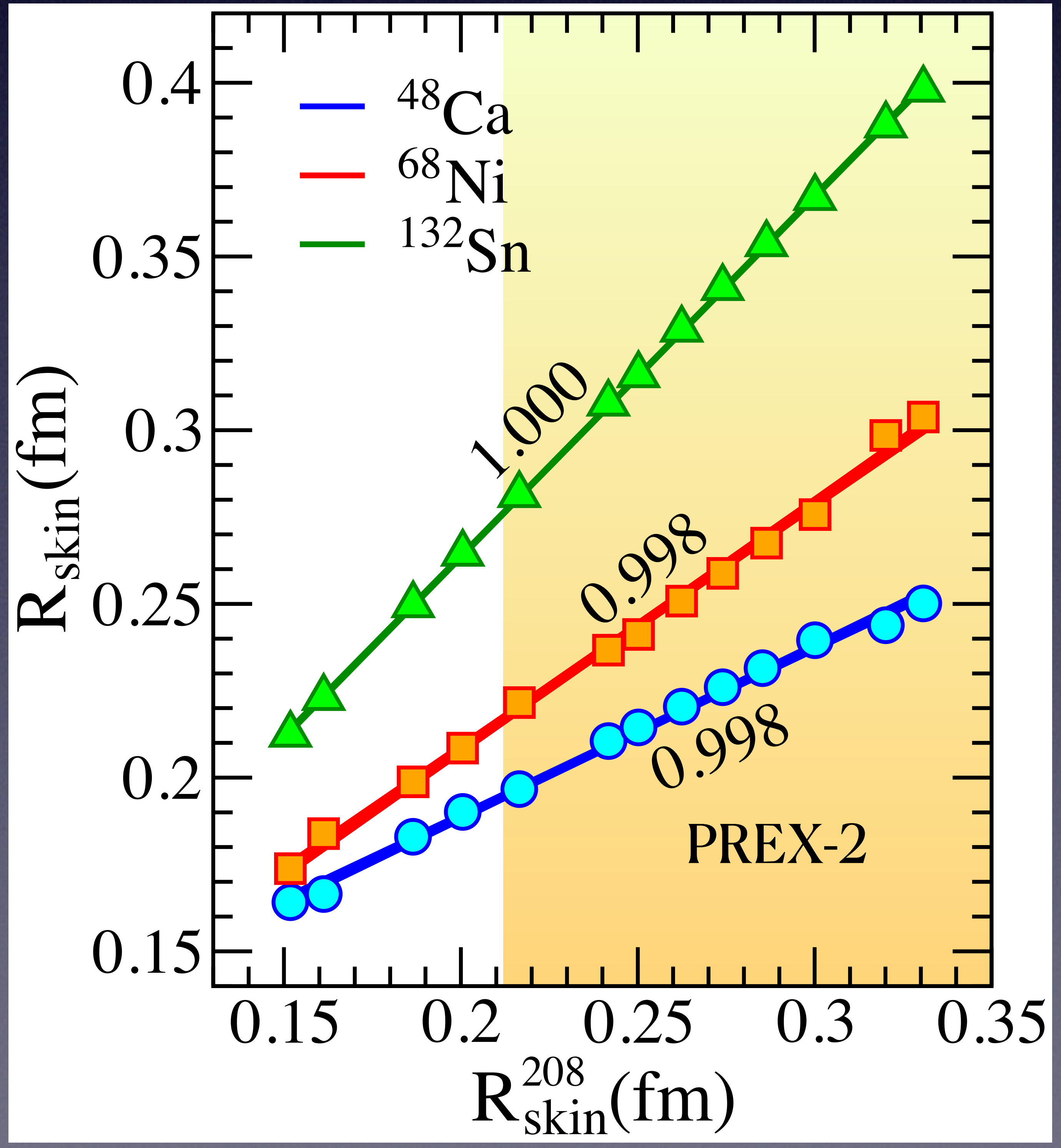
What have we learned since GW170817

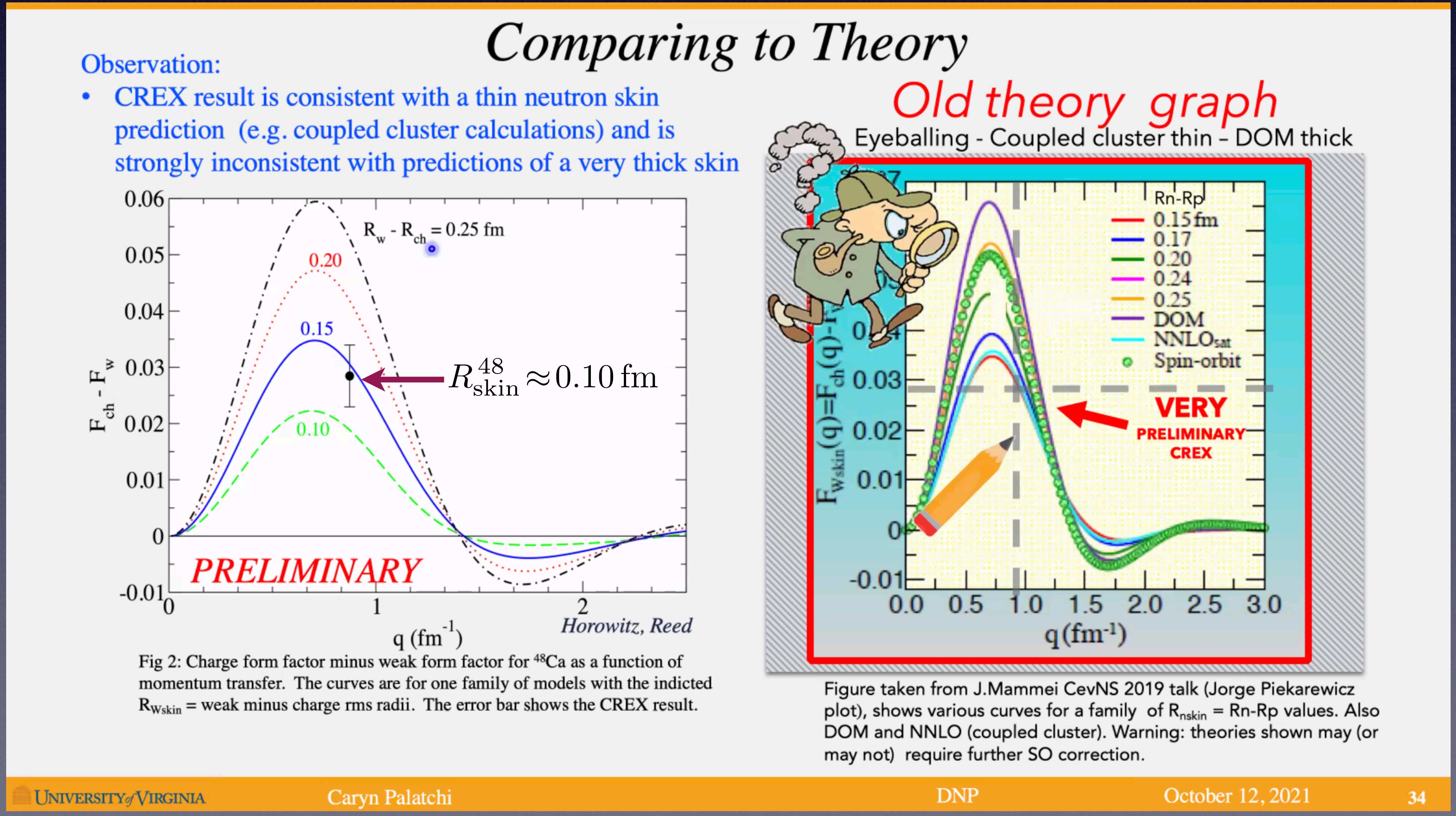
- PREX suggest a **stiff** EOS around saturation density
- LIGO-Virgo favor a **soft** EOS at around $2n_0$
  although see Gamba et al., PRD 103, 124015 (2021)
- NICER/Pulsar Timing suggest a **stiff** EOS at $\sim 4n_0$

Who Ordered That?

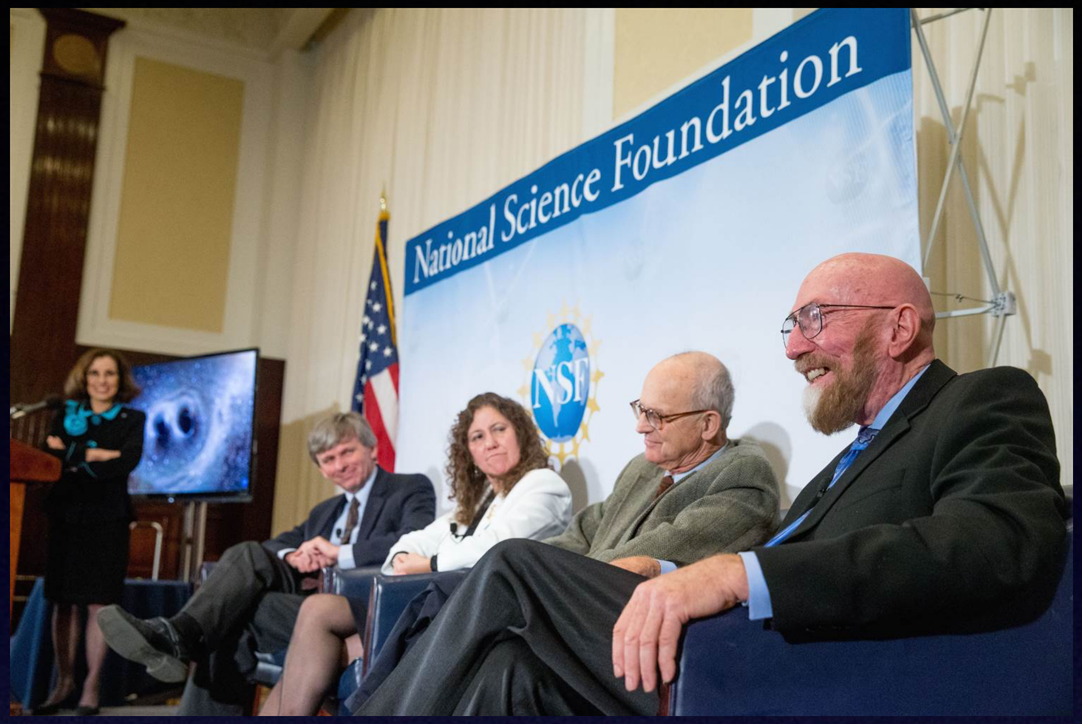


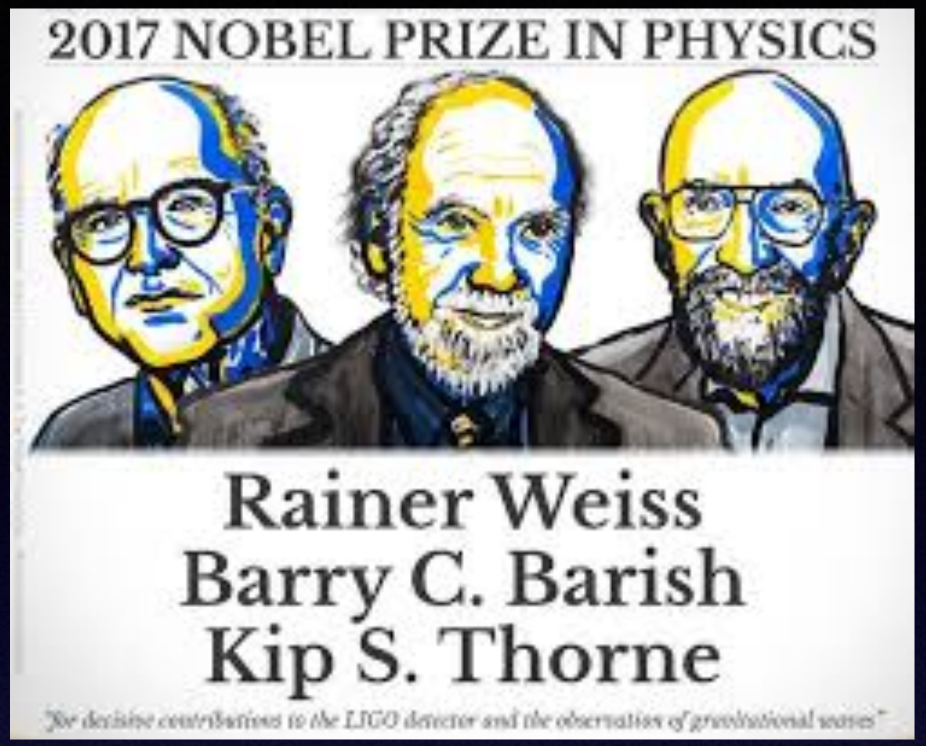
Isidor Isaac Rabi





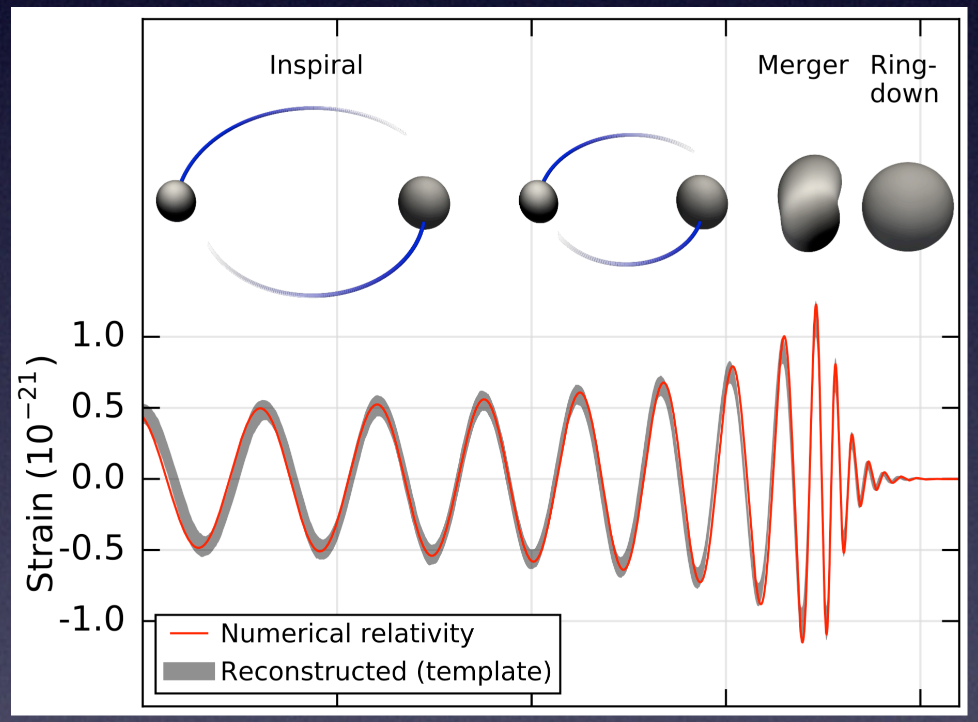
"We have detected gravitational waves; we did it"
David Reitze, February 11, 2016

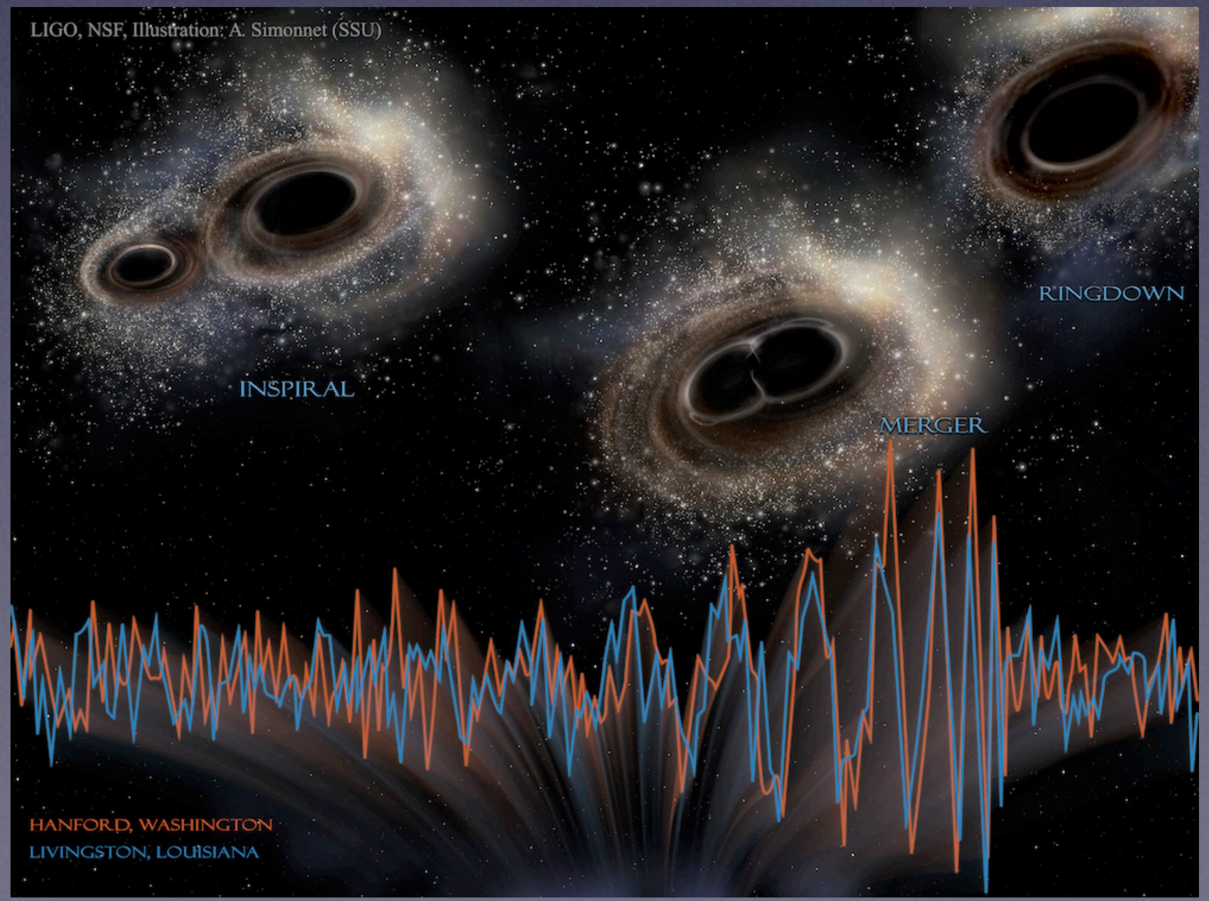


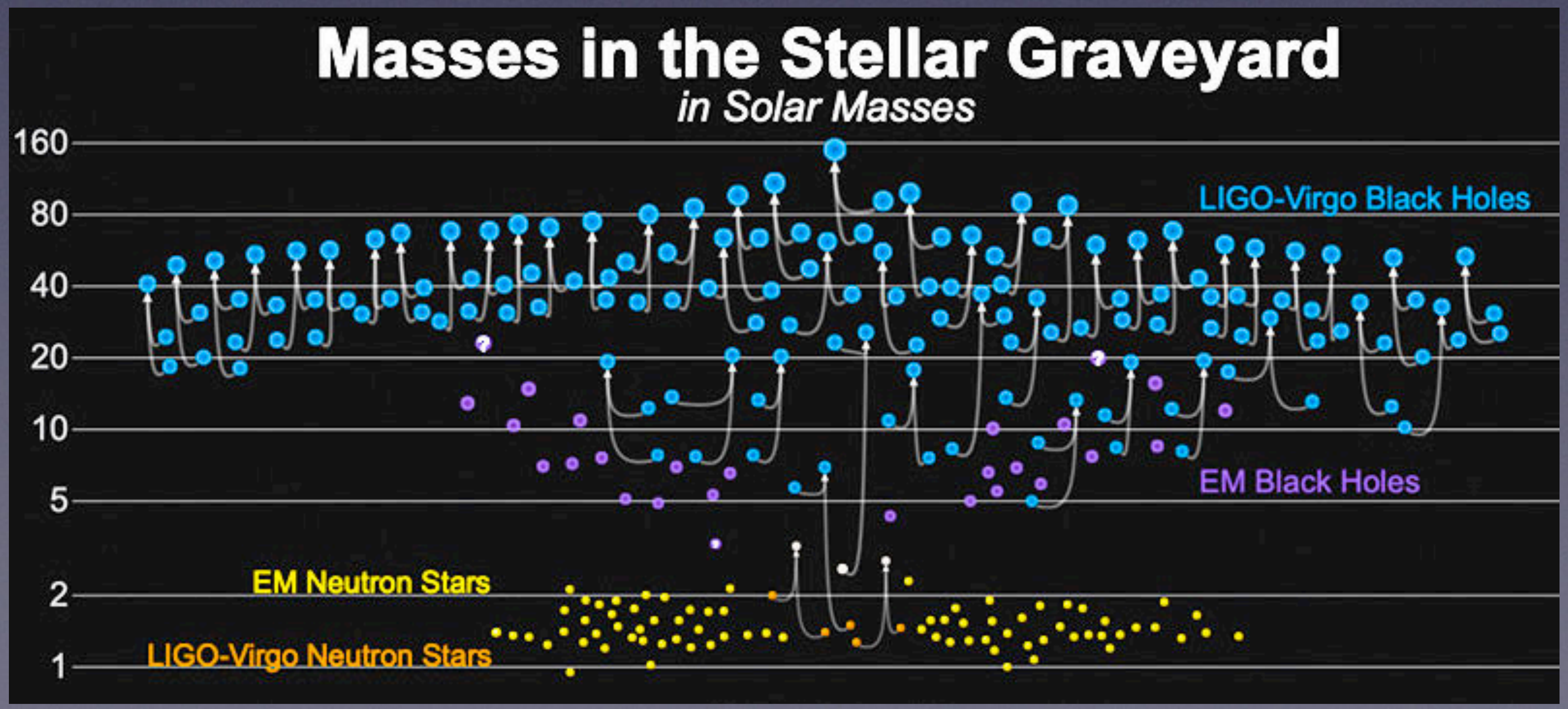


- The dawn of a new era: GW Astronomy
  - Initial black hole masses are 36 and 29 solar masses
  - Final black hole mass is 62 solar masses;

    3 solar masses radiated in Gravitational Waves!

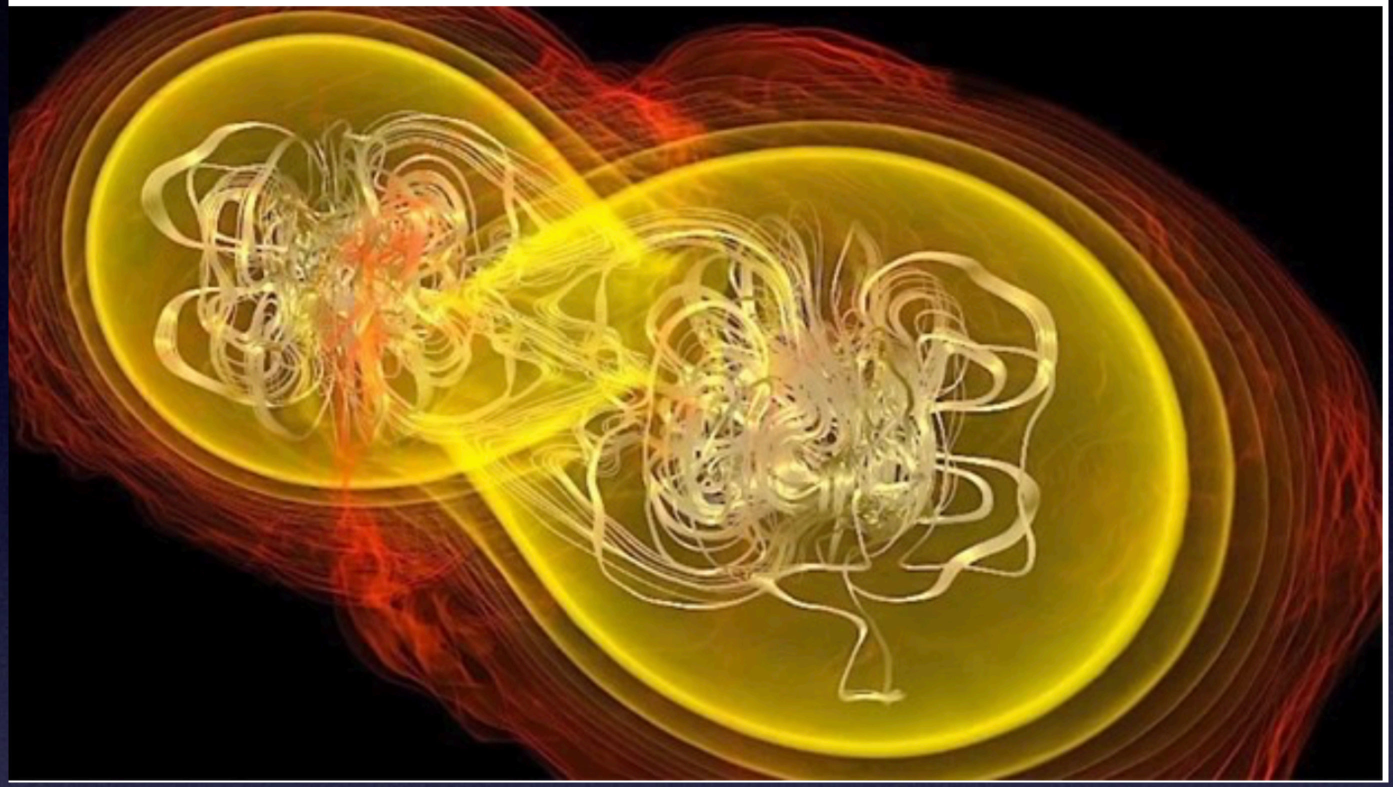






The New Periodic Table of the Elements

Colliding neutron stars revealed as source of all the gold in the universe



The optical counterpart SSS17a produced at least 5% solar masses (10^{29} kg!) of heavy elements - demonstrating that NS-mergers play a role in the r-process