Constraining the nuclear EoS by combining nuclear data and GW observations Michael McNeil Forbes Washington State University (Pullman) and University of Washington

## A Minimal Nuclear Energy Density Functional

• Bulgac, Forbes, Jin, Perez, Schunk arXiv:1708.08771 (accepted PRC 2018)

- 6-7 parameters
	- Better accuracy than other NEDF (without beyond mean-field corrections)
		- fewer parameters (others have 13-30)
		- Not fully optimized
	- Separation of dominant from subdominant parameters
	- Masses, Radii, Separation energies, Neutron matter
	- Suitable for dynamics (reasonably fission properties without tuning!)

#### Inspired by liquid drop E[*n*n, *n*p] = z }| {  $\overline{1}$ 1<br>
1<br><br><br><br>
1<br><br><br><br>  $\blacktriangledown$ <sup>+</sup> *<sup>W</sup>*<sup>0</sup> <sup>J</sup> · <sup>r</sup>*<sup>n</sup>* <sup>|</sup> {z }

- •Inspired by liquid drop formula
- 4-5 parameters:
- •Global mass fits (2375 nuclei) 2.6-2.8MeV compared to to 4-6 parameter Liquid Drop Formula (2.6-3.3MeV)
- •Also get 883 charge radii 0.041fm



Table II. Best fit parameters for the SeaLL1 functional (in bold) and the orbital-free approximation (next column in italic when different). The errors quoted for the fit parameters should be interpreted as estimating by how much this parameter can be independently changed while refitting the other and incurring a cost of at most  $\delta \chi_E < 0.1$  MeV.

*W*<sup>0</sup> and g are significant for fitting nuclear masses and radii.

$$
\mathcal{E}[n_{n}, n_{p}] = \underbrace{\overbrace{\frac{\hbar^{2}}{2m}(\tau_{n} + \tau_{p}) + \frac{\hbar^{2}}{\hbar^{2}(m_{\text{compgen}})}}^{\text{homogeneous}} + \sum_{\substack{\text{gradient} \\ \text{gradient}}}^{\text{2}} \left( a_{j} n^{5/3} + b_{j} n^{2} + c_{j} n^{7/3} \right) \beta^{2j} + \cdots + \sum_{q=n, p}^{\text{gradient}} \overbrace{\frac{\hbar^{2}}{2m} ||\vec{\nabla} n_{q}||^{2} + \underbrace{W_{0} \vec{J} \cdot \vec{\nabla} n}_{\text{spin-orbit}}}^{\text{gradient}} + \underbrace{\sum_{q=n, p}^{\text{max}} g_{\text{eff}}(\vec{r}) |v_{q}(\vec{r})|^{2}}_{\text{pairing}} - \frac{3e^{2}}{4} \left( \frac{n_{p}(\vec{r})}{3\pi} \right)^{4/3} + \underbrace{\frac{e^{2}}{2} \int d^{3} \vec{r}' \frac{n_{p}(\vec{r}) n_{p}(\vec{r}')}{\|\vec{r} - \vec{r}'\|} - \frac{3e^{2}}{4} \left( \frac{n_{p}(\vec{r})}{3\pi} \right)^{4/3}}_{\text{Coulomb}}
$$



$$
\mathcal{E}[n_n, n_p] = \frac{\frac{\hbar^2}{\hbar^2}(\tau_n + \tau_p) + \frac{\hbar^2}{\hbar^2}(\sigma_n + \tau_p) + \frac{2}{\hbar^2}(\sigma_n n^{5/3} + b_j n^2 + c_j n^{7/3}) \beta^{2j} + \frac{2}{\sigma^2}(\sigma_n n^{5/3} + b_j n^2 + c_j n^{7/3}) \beta^{2j} + \frac{\hbar^2}{\sigma^2} \frac{\hbar^2}{2m} \|\vec{\nabla} n_q\|^2 + \underbrace{W_0 \vec{J} \cdot \vec{\nabla} n}_{\text{spin-orbit}} + \underbrace{\sum_{q=n, p}^{n} g_{\text{eff}}(\vec{r}) |v_q(\vec{r})|^2}_{\text{pairing}} + \underbrace{\frac{e^2}{2} \int d^3 \vec{r}' \frac{n_p(\vec{r}) n_p(\vec{r}')}{\|\vec{r} - \vec{r}'\|} - \frac{3e^2}{4} \left(\frac{n_p(\vec{r})}{3\pi}\right)^{4/3}}_{\text{Coulomb}}
$$

# SeaLL1 NEDF

- •No effective mass good level densities
- •Orbital-free version from semi-classical expansion (2-fluid hydrodynamics)

◆4/3

$$
\mathcal{E}[n_n, n_p] = \frac{\hbar^2}{2m} (\tau_n + \tau_p) + \frac{\text{homogeneous}}{\text{homogeneous}}
$$
  
+ 
$$
\sum_{j=0}^{2} (a_j n^{5/3} + b_j n^2 + c_j n^{7/3}) \beta^{2j} + \frac{\beta^{2j}}{\text{Neutron skin}}
$$
  
NEDF  $\rho_0$   $- \epsilon_0$   $K_0$   $S$   $L$   $L_2$   ${}^{208}\text{Pb} \phantom{0}{}^{48}\text{Ca}$   
SeaLL1  $0.154$   $15.58$   $230.0$   $31.7$   $32.4$   $31.6$   $0.131$   $0.155$ 

 $\frac{1}{\sqrt{2\pi}}$ SeaLL1. All values in MeV unless otherwise specified. Table III. Saturation, symmetry, and neutron skin properties for

#### SeaLL1 NEDF |  $\blacksquare$ 0.49, 0.50 and 0.54 MeV for neutrons and protons, respectively. particle proton levels in 208Pb show that the *Z* = 82 gap is  $\blacksquare$

 $U$  unedfined for the empirical with the empirical with the empirical with the empirical  $U$ 

gauge the predictive power of NEDFs. To this purpose, we

 $\beta=(n_n-n_p)/(n_n+n_p)$ Inspired by UFG PCA reduces to 3 parameters ( $n_0$ ,  $\varepsilon_0$ ,  $S_2$ )  $K_0 \pm 25$ MeV and  $L_2$  not  $\rho_{\text{m}}(n-n)/(n+n)$  $\nu$  –  $(\nu n - \nu p) / (\nu n + \nu p)$ however, the SeaLL1 single-particle spectra, as  $\sim$  $E$ **Final pathway of**  $P$  $V_{\text{c}}$  of  $\Omega$  is the important  $V$  $\frac{1}{2}$  in the nuclear field  $\frac{1}{2}$  in this context.

tightly constrained and the excitation of the excitation of  $\sim$ is different of the more parameter) and in the  $\sim$ 

 $\beta^4$  terms fixed by neutron matter  $R<sup>4</sup>$  terms fived by  $\mathbb{P}$  performing constraints with constraints with constraints with constraints with constraints with constraints  $\mathbb{P}$ 

$$
\mathcal{E}[n_n, n_p] = \underbrace{\overbrace{\frac{\hbar^2}{2m}}^{kinetic}}_{\text{homogeneous}} + \underbrace{\overbrace{\sum_{\text{homogeneous} \text{gradient}}^{2}}_{\text{gradient}} \left( a_j n^{5/3} + b_j n^2 + c_j n^{7/3} \right) \beta^{2j} + \newline + \underbrace{\eta_s \sum_{q=n, p} \frac{\hbar^2}{2m} ||\vec{\nabla} n_q||^2}_{\text{spin-orbit}} + \underbrace{\sum_{q=n, p} g_{eff}(\vec{r}) |v_q(\vec{r})|^2}_{\text{pairing}} + \underbrace{e^2}{2} \int d^3 \vec{r}' \frac{n_p(\vec{r}) n_p(\vec{r}')}{\|\vec{r} - \vec{r}'\|} - \frac{3e^2}{4} \left( \frac{n_p(\vec{r})}{3\pi} \right)^{4/3} \newline
$$

Adjusts surface tension, diffuseness, pairing etc. Required and constrained by mass/radii fits

◆4/3

SeaLL1

NEDF



## Residuals

606 even-even nuclei:  $\chi_E$ =1.74MeV (1.46MeV w/o bias) Fit to 196 spherical nuclei

345 charge-radii  $\chi_r = 0.034$ fm

No beyond mean-field corrections Good for self-consistent dynamics CoM correction for spherical nuclei: 1.54MeV → 0.96MeV

2n (2p) separation energies  $\chi$ <sub>E</sub>=0.69MeV (0.59MeV) Lower than any other NEDF!

## Neutron Drip Line



## Density Profiles



Solid from De Vries et al. At. Data. Nucl. Data Tables 36, 495 – 536 (1987)

## Fission (for Free)



Similar <sup>240</sup>Pu fission behaviour as SkM\* but no tuning to match fission barriers

Other NEDFs have similar errors in barrier heights

# Subdominant and Free Parameters to Tune

### •Entrainment terms

GDR, Thomas-Kuhn-Reiche sum rule, Gamow-Teller resonance

- •Gradient terms/density-dependent kinetic terms Surface tension and diffuseness, Static dipole susceptibility Proton and neutron effective masses
- •Isospin-breaking pairing/spin-orbit coupling Spin-orbit splittings, Pairing gaps
- •Decoupled from primary mass fit parameters

$$
\mathcal{E}[n_n, n_p] = \underbrace{\overbrace{\frac{\hbar^2}{2m}}^{kinetic}}_{\text{homogeneous}} + \underbrace{\overbrace{\sum_{j=0}^{2}}^{homogeneous}}_{\text{gradient}}
$$
\n
$$
+ \eta_s \underbrace{\sum_{q=n, p} \overbrace{\frac{\hbar^2}{2m}}^{min}( \vec{v} n_q ||^2 + v_0 \vec{J} \cdot \vec{v} n + \overbrace{\sum_{q=n, p}^{2m} g_{eff}(\vec{r}) |v_q(\vec{r})|^2}^{gradient}
$$
\n
$$
+ \underbrace{\sum_{q=n, p}^{2m} g_{eff}(\vec{r}) |v_q(\vec{r})|^2}_{\text{pairing}}
$$
\n
$$
+ \underbrace{\frac{e^2}{2} \int d^3 \vec{r}' \frac{n_p(\vec{r}) n_p(\vec{r}')}{\|\vec{r} - \vec{r}'\|} - \frac{3e^2}{4} \left(\frac{n_p(\vec{r})}{3\pi}\right)^{4/3}}_{\text{Coulomb}}
$$

SeaLL1 NEDF

 $\beta=(n_n-n_p)/(n_n+n_p)$ 

Inspired by UFG

PCA reduces to 3 parameters (no, Eo, S2)

 $K_0 \pm 20$ MeV and  $L_2$  not tightly constrained (one more parameter)

 $\beta^4$  terms fixed by neutron matter

Nuclear Eos: L<sub>2</sub> 
$$
\neq
$$
 L

$$
\frac{\mathcal{E}(n_n,n_p)}{n} = \varepsilon_0(n) + \varepsilon_2(n) \left(\frac{n_n-n_p}{n}\right)^2 + \varepsilon_4(n) \left(\frac{n_n-n_p}{n}\right)^4 + \cdots
$$

- •Isospin expansion about symmetric nuclear matter
- $\varepsilon_0(n) = \varepsilon_0$  +  $\frac{1}{2}K_0\delta^2$  +  $O(\delta^3)$  $\varepsilon_2(n) = S_2 + L_2 + \frac{1}{2}K_0\delta^2 + O(\delta^3)$  $\varepsilon_4(n) = S_4 + L_4 + \frac{1}{2}K_0\delta^2 + O(\delta^3)$  $\delta=$  $n - n_0$  $3\mathfrak{n}_0$  $n = n_n + n_p$

Symmetry Properties

$$
\frac{\mathcal{E}(n,0) - \mathcal{E}(n/2,n/2)}{n} = \underbrace{(S_2 + S_4 + \cdots) + (\underbrace{L_2 + L_4 + \cdots})}_{S} \delta + \cdots
$$

- •Isospin expansion about symmetric nuclear matter
- L=L<sub>2</sub> Only if  $(n_n n_p)^4$  terms are insignificant

#### See also Lattimer NPA 928 (2014) 276

## Nuclear EoS: L2≠L



 $\cdot (n_n-n_p)^2$ Fit nuclei (masses, radii, skins etc.)

 $\cdot$   $(n_n-n_p)^4$ Seems needed for neutron matter Setting these to match neutron matter does not affect quality of fits

Bulgac, Forbes, Jin, Perez, Schunk: 1708.08771 (PRC 2018)

## Nuclear EoS: L2≠L



•Older functionals fit QMC without 3N

- •Hard to fit new QMC with  $(n_n-n_p)^2$
- $\cdot (n_n-n_p)^4$  fits neutron matter without affecting nuclear fits

QMC from Wlazłowski, Holt, Moroz, Bulgac, Roche, PRL 113 (2014) 182503 [1403.3753]









Skyrme and Relativistic Mean Field Theory

Still misses neutron matter

Possible that neutron matter is essentially independent of nuclei?

P.-G. Reinhard at ECT\*, Trento, Italy, 26-30 January, 2015, [https://sites.google.](https://sites.google) com/site/ectworkshopns2015/talks

Wednesday, March 14, 18





Skyrme and Relativistic Mean Field Theory

Still misses neutron matter

Possible that neutron matter is essentially independent of nuclei?

P.-G. Reinhard at ECT\*, Trento, Italy, 26-30 January, 2015, [https://sites.google.](https://sites.google) com/site/ectworkshopns2015/talks

Wednesday, March 14, 18

# Connect Nuclear EoS with Neutron Stars

•Expand from neutron matter

•Constrain with symmetric matter

### •Unified EoS

Compressible Liquid Drop Model (CLDM) matching Similar to Fortin et al. PRC 94 (2016) 035804

### •Parametrized Core

Characterize the speed of sound

# Connect Nuclear EoS with Neutron Stars

•Outer Crust

Tabulated Data

•Compressible Liquid Drop Model (CLDM)

Match outer crust to homogeneous matter

•Homogeneous Matter

EoS extrapolated from neutron matter

•Core

Parameterize speed of sound

with Sanjay Reddy (UW), Dake Zhou (UW), Sukanta Bose (WSU)

Outer Crust None

Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

Homogeneous Matter EoS extrapolated from neutron matter

#### •Outer Crust

i.e. Negele-Vautherin Augment if needed to ensure convexity

•No parameters

Outer Crust None

Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

Homogeneous Matter EoS extrapolated from neutron matter

- •Unified EoS Solve for Wigner-Seitz cell given homogeneous EoS
- •Two parameters
	- •C\_C Coulomb suppression
	- •sigma\_delta Isospin dependence Other surface parameter fixed to smoothly match to tabulated outer crust

sound Lattimer et al. NPA 432 (1985) <sup>646</sup> Steiner PRC 85 (012) 055804

Outer Crust None

Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

Homogeneous Matter EoS extrapolated from neutron matter

Core Parameterize speed of

- •Pure neutron matter: 4 a, α, b, β
- •Proton polaron: 3  $|\overline{\mu}_{\textup{p}}(\tilde{\mathsf{n}}_0),\overline{\mu}_{\textup{p}},\overline{\mathsf{m}}^*|$
- •Symmetric nuclear matter: 6  $n_0$ ,  $\epsilon_0$ ,  $K_0$ S2, L2, K2

Outer Crust None

Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

Homogeneous Matter EoS extrapolated from neutron matter

#### Start from pure Neutron matter

$$
E_n(n_n) = \frac{\mathcal{E}_n(n_n)}{n_n} = m_n c^2 + a \left(\frac{n_n}{\bar{n}_0}\right)^{\alpha} + b \left(\frac{n_n}{\bar{n}_0}\right)^{\beta}
$$

### Generally fits QMC data and trends



MAXIMUM MASS AND RADIUS OF NEUTRON STARS, AND *...* PHYSICAL REVIEW C **85**, 032801(R) (2012)

#### **Estate in Fig. 1. The intersections with the intersections with the intersections with the intersections with th** indicate central densities realized in these stars. each value of *E*sym the corresponding band shows the effect of different spatial and spin structure three-neutron interactions of the three-neutron interaction. In The inset shows the linear correlation between *E*sym and its density two-body interactions in the AFDMC, and the incorporation of  $R_{\Gamma}$  (2012)  $\Omega$ 201(D) Gandolfi et al. PRC 85 (2012) 032801(R)

three-neutron interactions corresponding to the bands for different

sound speed *cs* <sup>=</sup> <sup>√</sup>∂*p/*∂ϵ ! *<sup>c</sup>* for <sup>ρ</sup> <sup>≃</sup> (4–5)ρ0. To overcome

tions. These studies have been useful but not very constraining

#### Outer Crust None

 $\overline{C}$ 

once its strength is tuned to give a particular value of *E*sym.

respectively.

### Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

**Matter S. GANDOLFI, S. GANDOLFI, GANDOLFI, GANDOLFI, AND SANJAY REDDITION, AND SANJAY REDDITION, AND SANJAY RE** EoS extrapolated from neutron matter

> Core Parameterize speed of **for different equations of sound** 0 1234 Feb 1234 Feb 1234 The left panel shows the mass  $\sim$

for different values of the nuclear symmetry energy (*E*sym). For

Expand in powers of proton fraction

$$
x_p=\frac{n_p}{n_n+n_p}
$$

$$
E_{np}(n_n, n_p) = (1 - x_p)E_n(n_n) +
$$
  
+  $x_p (m_p c^2 + \Sigma^p(n_B)) +$   
+  $\frac{(2\pi^2)^{2/3}}{2m^*} x_p^{5/3} n_B^{2/3}$   
+  $x_p^2 f_2(n_B) + x_p^3 f_3(n_B) + \cdots$ 

Outer Crust None

Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

Homogeneous Matter EoS extrapolated from neutron matter

#### Bulk neutron matter

$$
E_{np}(n_n, n_p) = (1 - x_p)E_n(n_n) + x_p (m_p c^2 + \Sigma^p(n_B)) +
$$
  
+ 
$$
\frac{(2\pi^2)^{2/3}}{2m^*} x_p^{5/3} n_B^{2/3} + x_p^2 f_2(n_B) + x_p^3 f_3(n_B) + \cdots
$$

Outer Crust None

Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

Homogeneous Matter EoS extrapolated from neutron matter

Proton polaron Dilute proton gas in neutron background

QMC for chemical potential Roggero et al. PRL 112 (2014) 221103

$$
E_{np}(n_n, n_p) = (1 - x_p)E_n(n_n) +
$$
  
+ 
$$
\frac{x_p(m_pc^2 + \Sigma^p(n_B))}{2m^*}x_p^{5/3}n_B^{2/3} +
$$
  
+ 
$$
x_p^2f_2(n_B) + x_p^3f_3(n_B) + \cdots
$$

Outer Crust None

Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

Homogeneous Matter EoS extrapolated from neutron matter



#### Polaron Parameters

 $\cdot \mu_p(\tilde{n}_0)$ Chemical potential at saturation

 $\bullet$   $\mathfrak{u}_p$ Location of minimum

#### Proton gas Fermi energy Proton effective mass

$$
E_{np}(n_n, n_p) = (1 - x_p)E_n(n_n) ++ x_p (m_p c^2 + \Sigma^p(n_B)) ++ \frac{(2\pi^2)^{2/3}}{2m^*} x_p^{5/3} n_B^{2/3} + x_p^2 f_2(n_B) + x_p^3 f_3(n_B) + \cdots
$$

Outer Crust None

Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

Homogeneous Matter EoS extrapolated from neutron matter

Expand and match symmetric nuclear matter

$$
\frac{\mathcal{E}(n_n, n_p)}{n} = \varepsilon_0(n) + \varepsilon_2(n) \left(\frac{n_n - n_p}{n}\right)^2
$$

Fix up to  $x_p^5 f_5(n_B)$ 

$$
E_{np}(n_n, n_p) = (1 - x_p)E_n(n_n) + x_p (m_p c^2 + \Sigma^p(n_B)) +
$$
  
+ 
$$
\frac{(2\pi^2)^{2/3}}{2m^*} x_p^{5/3} n_B^{2/3} + x_p^2 f_2(n_B) + x_p^3 f_3(n_B) + \cdots
$$

Outer Crust None

Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

Homogeneous Matter EoS extrapolated from neutron matter

Expand and match symmetric nuclear matter

$$
\frac{\mathcal{E}(n_n, n_p)}{n} = \varepsilon_0(n) + \varepsilon_2(n) \left(\frac{n_n - n_p}{n}\right)^2
$$

Fix up to  $x_p^5 f_5(n_B)$ 

$$
\epsilon_0(n) = \frac{\epsilon_0}{\epsilon_2(n)} + \frac{1}{2}K_0\delta^2 + O(\delta^3)
$$
  
\n
$$
\epsilon_2(n) = \frac{S_2 + L_2 + \frac{1}{2}K_2\delta^2 + O(\delta^3)}{n - n_0}, \qquad n = n_n + n_p
$$

Outer Crust None

Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

Homogeneous Matter EoS extrapolated from neutron matter

#### Parametrize speed of sound  $C= c_s^2/c^2$



for *n*tr*,*<sup>2</sup> and the chiral TPE+*VE,*<sup>1</sup> interaction. Black dots indicate t[he maximal central densitie](https://arxiv.org/abs/1801.01923)s reached Tews, Carlson, Gandolfi, Reddy [arXiv:1801.01923]

Outer Crust None

Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

Homogeneous Matter EoS extrapolated from neutron matter

Parametrize speed of sound  $C(\mathcal{E})=c_s^2/c^2$ Quadratic polynomial as function of energy-density (Easy to invert to get EoS)

 $\bullet \mathcal{E}_{c}$ 

Transition from homogeneous matter

#### $\bullet$   $C_{\text{max}}$ Maximum of polynomial

 $\bullet$   $\epsilon$ <sub>max</sub>

Location of maximum

Outer Crust None

Compressible Liquid Drop Model (CLDM) Match outer crust to homogeneous matter

Homogeneous Matter EoS extrapolated from neutron matter

# Live Demos on Binder (or CoCalc, etc.)

- •Reproducible science
- LIGO analysis
- •[https://github.com/losc-tutorial/LOSC\\_Event\\_tutorial](https://github.com/losc-tutorial/LOSC_Event_tutorial)
- •Parameter Exploration
- •[https://github.com/mforbes/binder\\_tov\\_explorer](https://github.com/mforbes/binder_tov_explorer)

## Explore Parameters

Initialization Cell [

#### 2 Mass/Radius Relationships  $\overline{\mathbf{v}}$

#### In  $[21]$ :

\*pylab inline --no-import-all import tools  $data = tools.DataFrame(KEY)$ data.explore parameters();

Populating the interactive namespace from numpy and matplotlib



[https://github.com/mforbes/binder\\_tov\\_explorer](https://github.com/mforbes/binder_tov_explorer)

Wednesday, March 14, 18

## Principal Components

1 principal component(s) better than 50%. (Next component constrained at 117%)



[https://github.com/mforbes/binder\\_tov\\_explorer](https://github.com/mforbes/binder_tov_explorer)

## Principal Components



9 principal component(s) better than 10%. (Next component constrained at 10%)



[https://github.com/mforbes/binder\\_tov\\_explorer](https://github.com/mforbes/binder_tov_explorer)

# Missing? Lots!

- Phase transitions
- •Clustering
- •Pasta
- Finite T
- •Out of equilibrium
- •Core?!?

## Conclusions

•New Minimal Nuclear Functional SeaLL1

- •Good static and dynamic properties
- Suggests L2≠L
- •Parametrize Neutron Star EoS from Neutron Matter
- •Explore parameter sensitivity
- Share results and code