Bundesministerium für Bildung und Forschung

TECHNISCHE UNIVERSITÄT DARMSTADT

EDFs with local chiral interactions: Pionifying Skyrme

arXiv: 2307.13568

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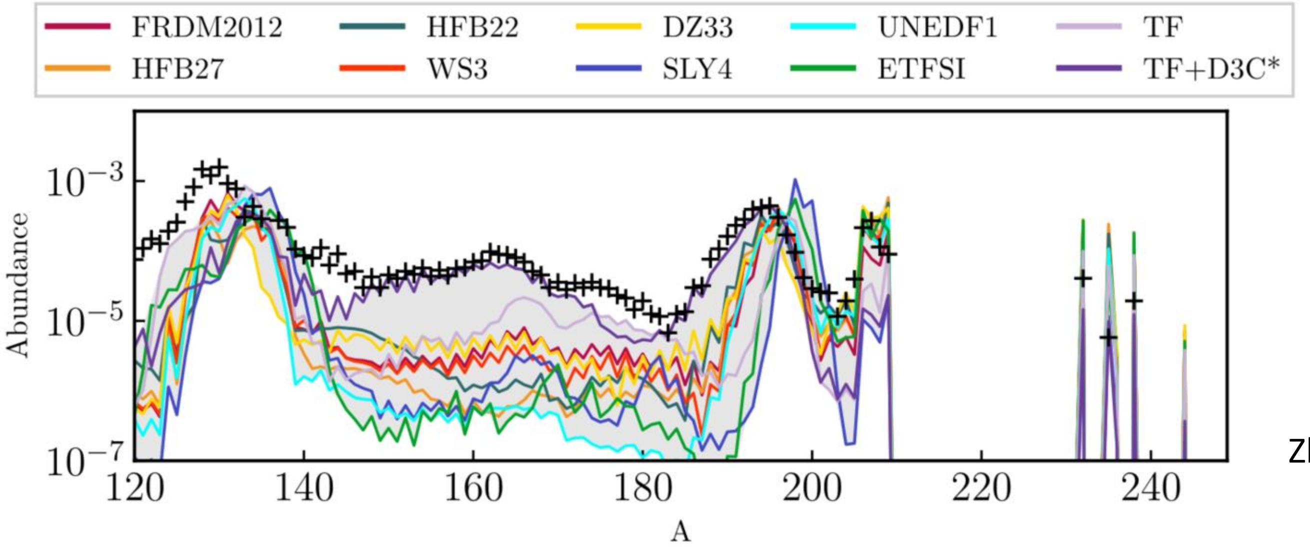
ESNT EDF workshop, November 22, 2023

Some EDF issues

- Extrapolation outside fitting region potentially uncontrolled



Zhu et al., ApJ **906** (2021)

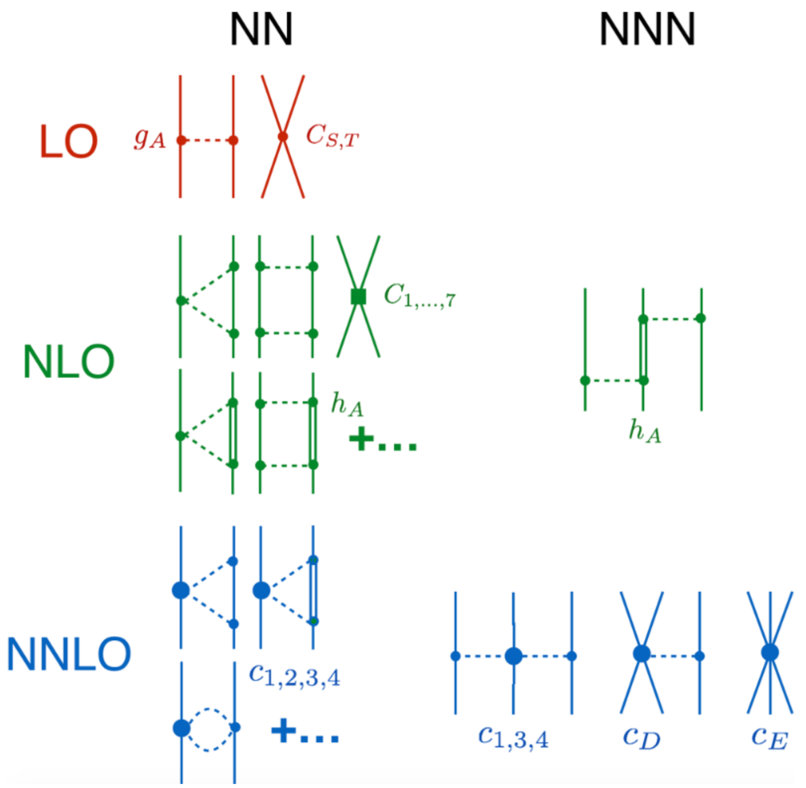
- How to assess uncertainties?
- Have standard EDFs reached their accuracy limit?

McDonnell et al., PRL **114** (2015)

- Phenomenological construction of EDFs

Ab initio calculations with chiral EFT

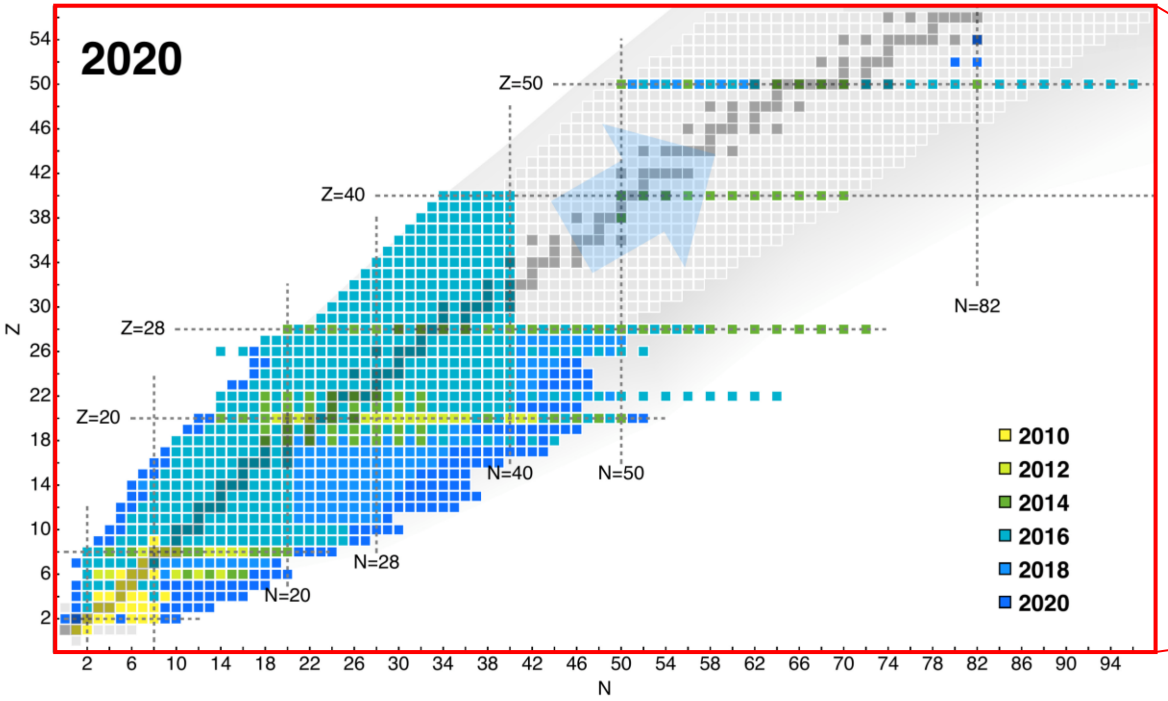
- Chiral effective field theory:
  expansion of nuclear interaction in typical momenta over breakdown scale
  - Systematically improvable
  - Uncertainty estimates “built-in”



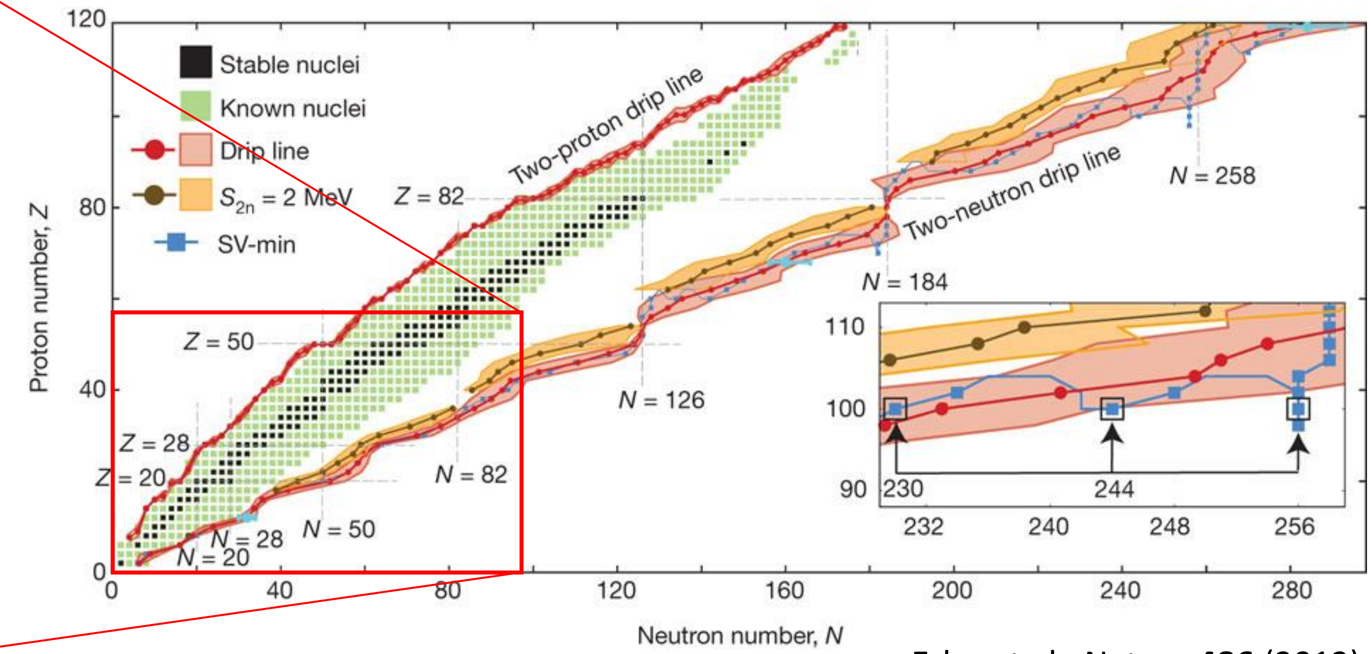
Ekström et al., PRC **97** (2018)

Ab initio calculations with chiral EFT

- Challenging to achieve similar accuracies as EDFs
- Computationally more expensive



Hergert, FP **8** (2020)



Erler et al., Nature **486** (2012)

Quest for ab initio energy density functionals

- How to connect energy density functionals and the ab initio approach?

  Salvioni et al., JPG **47** (2020)
  Furnstahl, EPJA **56** (2020)
  Marino et al., PRC **104** (2021)
  Duguet et al., EPJA **59** (2023)

- Schematic of ab initio calculations:
  - Potential from chiral EFT
  - Solve on mean-field level
  - Build correlations on top via correlation expansion method

→ Adjust short-range part of potential instead of using correlation expansion

  - cf. encapsulate triples from CCSD(T) in CCSD by adjusting 3N contact

Sun et al., PRC **106** (2022)

Quest for ab initio energy density functionals

- Semi-phenomenological hybrid EDFs
  - Increase resolution: add pions from chiral EFT to Skyrme
  - No additional fit parameters
  - Refit Skyrme parameters
  - Encouraging results, but puzzling systematics

→ Revisit EDF construction

Drut et al., PPNP **64** (2010)
Gebremariam et al., PRC **82** (2010)

Navarro Pérez et al., PRC **97** (2018)

Zurek et al., arXiv:2307.13568 (2023)

Semi-phenomenological hybrid EDFs

- Employed at HFB level
- Consider only even-even nuclei

$$E = E_{\mathrm{H}}^{\chi} + E_{\mathrm{F}}^{\chi} + E_{\mathrm{Skyrme}} + E_{\mathrm{Coulomb}} + E_{\mathrm{pair}} + E_{\mathrm{kin}}$$

$$E_{\mathrm{Skyrme}} = \sum_{t=0,1} \int \mathrm{d}\mathbf{R} \Big[\big(C_t^{\rho\rho} + C_{tD}^{\rho\rho} \rho_0^{\gamma} \big) \rho_t^2 + C_t^{\rho\tau} \rho_t \tau_t + C_t^{\rho\Delta\rho} \rho_t \Delta\rho_t + C_t^{\rho\nabla J} \rho_t \boldsymbol{\nabla} \cdot \mathbf{J}_t + C_t^{JJ} J_{t,ab} J_{t,ab} \Big]$$

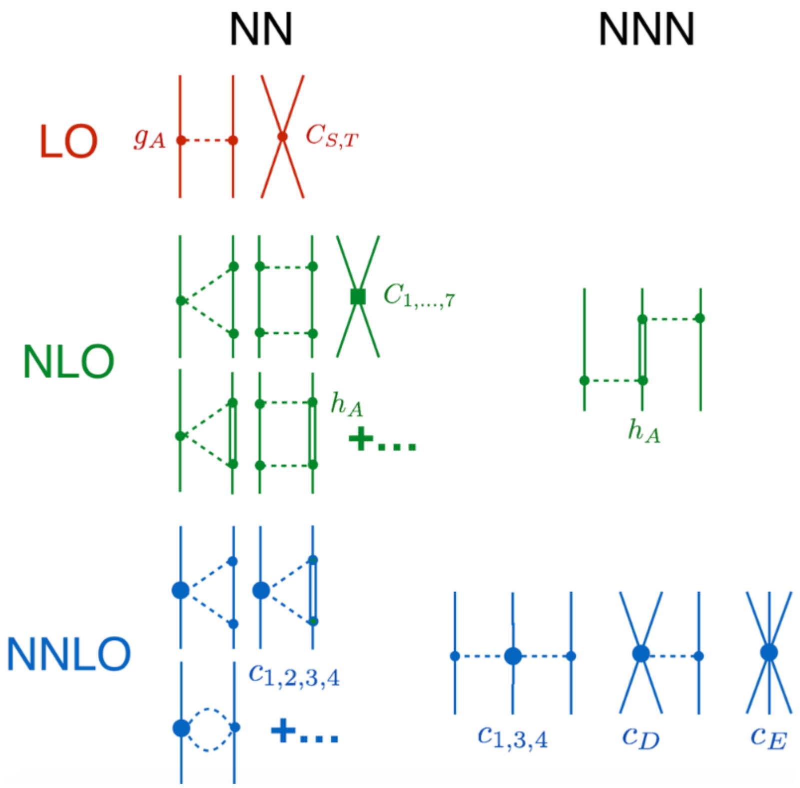
$$E_{\mathrm{pair}} = \frac{1}{4} \sum_{q=\mathrm{n,p}} \int \mathrm{d}\mathbf{R}\, V_0^q \left(1 - \frac{1}{2} \frac{\rho_0}{0.16\ \mathrm{fm}^{-3}} \right) \tilde{\rho}_q^2$$

- 14 parameters

Chiral pion exchanges

- At different chiral orders up to N²LO
- With / without Δ isobars and 3N forces
- Local coordinate-space regulator

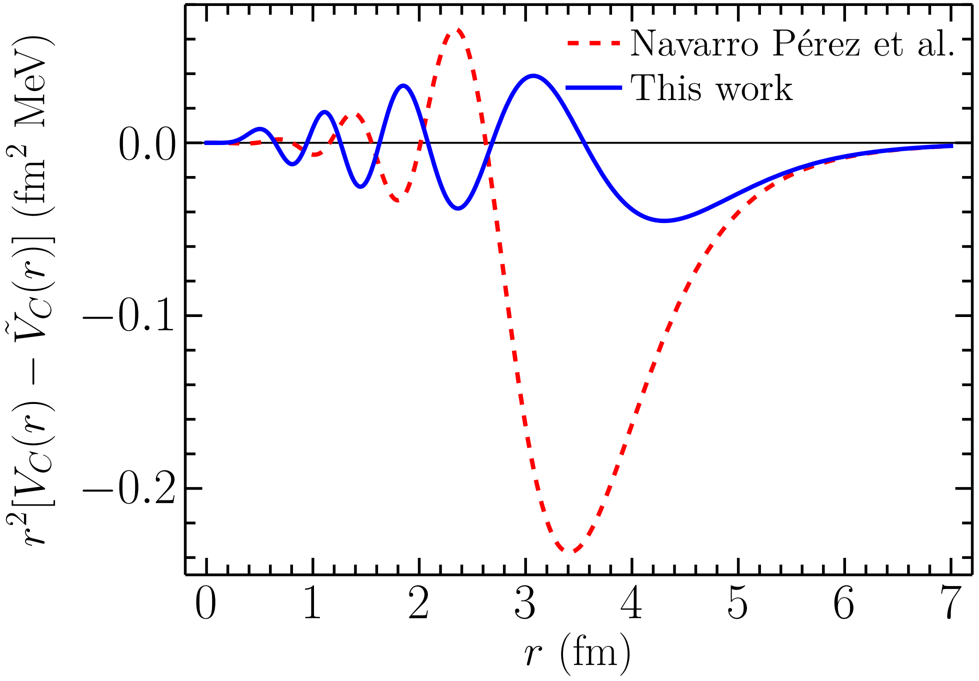
Krebs et al., EPJA **32** (2007)
Epelbaum et al., EPJA **51** (2015)



Ekström et al., PRC **97** (2018)

Chiral pion exchanges

- Hartree term: approximate potentials by sums of 5 Gaussians



- 5 MeV deviation from exact Hartree energy in ^{208}Pb at N^{2}LO (4 GeV)

Chiral pion exchanges

- Fock term in local form
  - Approximate one-body density matrices via density-matrix expansion

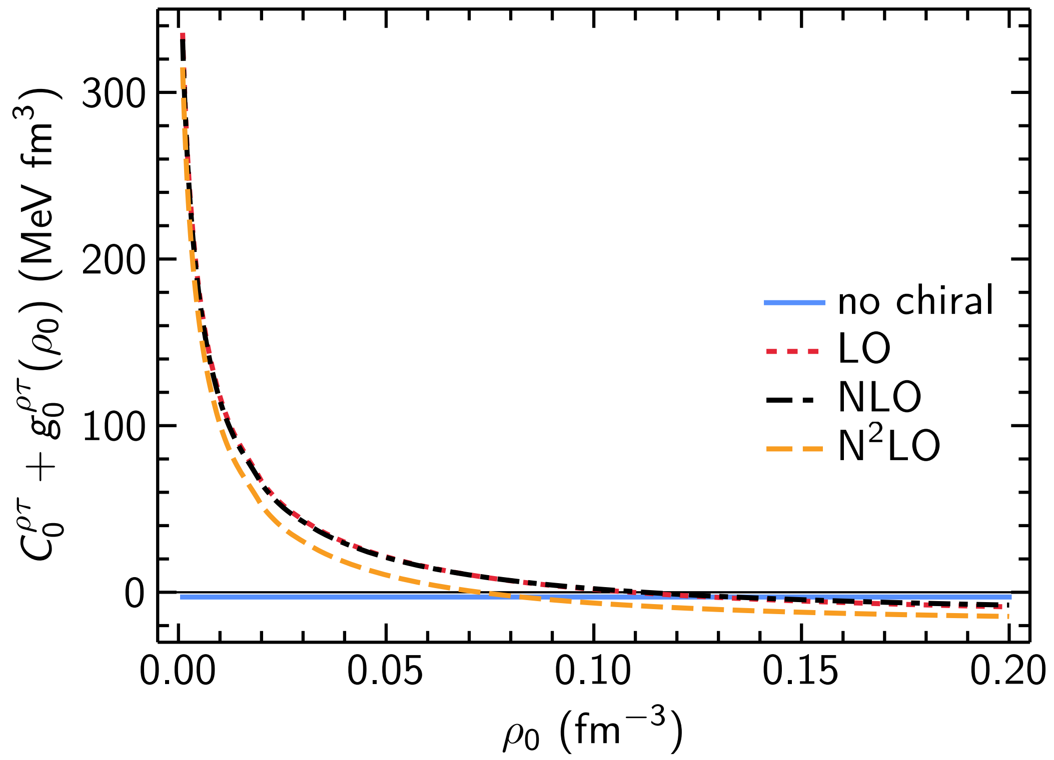
Gebremariam et al., PRC **82** (2010), NPA **851** (2011)

  - Extension of Slater approximation

Slater, PR **81** (1951)

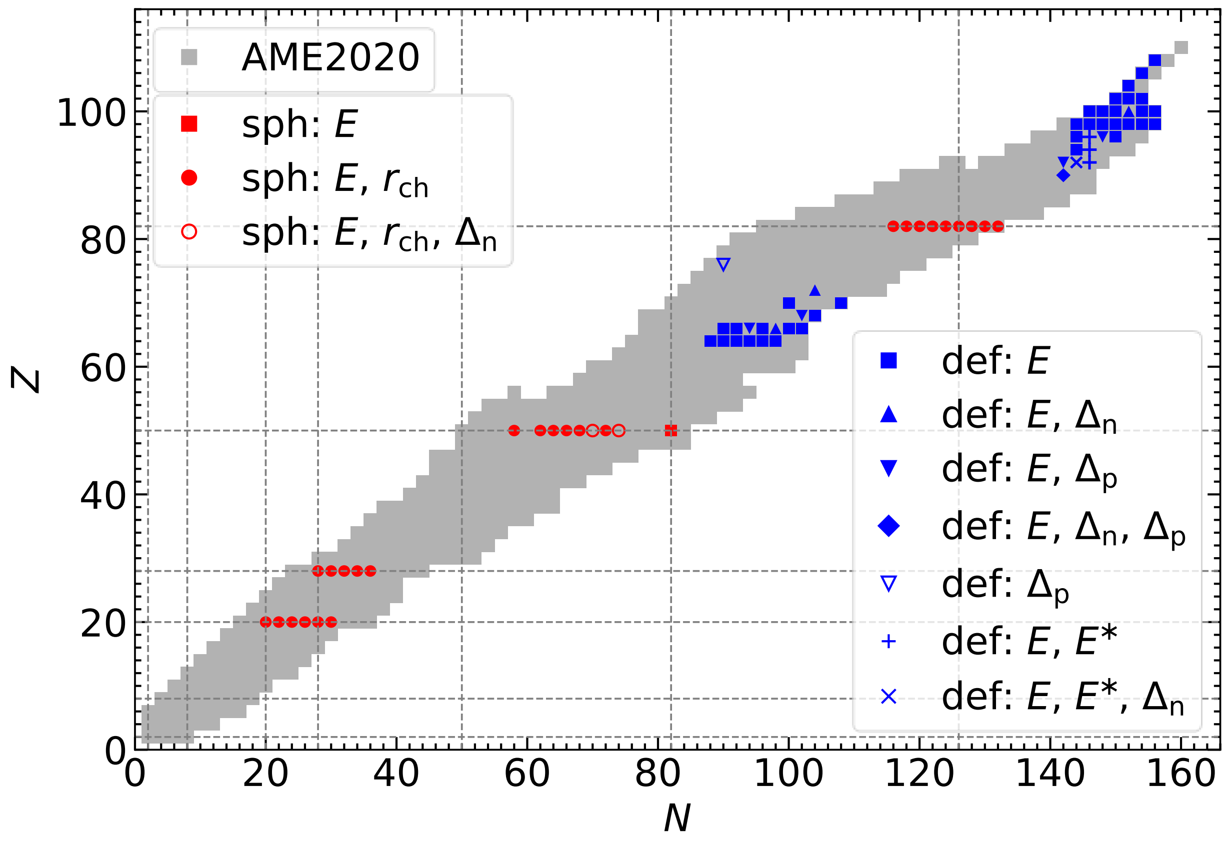
$$\rho(\mathbf{x}_1, \mathbf{x}_2) = \frac{3 j_1(k_\mathrm{F}(\mathbf{R}) r)}{k_\mathrm{F}(\mathbf{R}) r} \rho(\mathbf{R})$$

  - Finite-range potential → EDF with density-dependent contacts



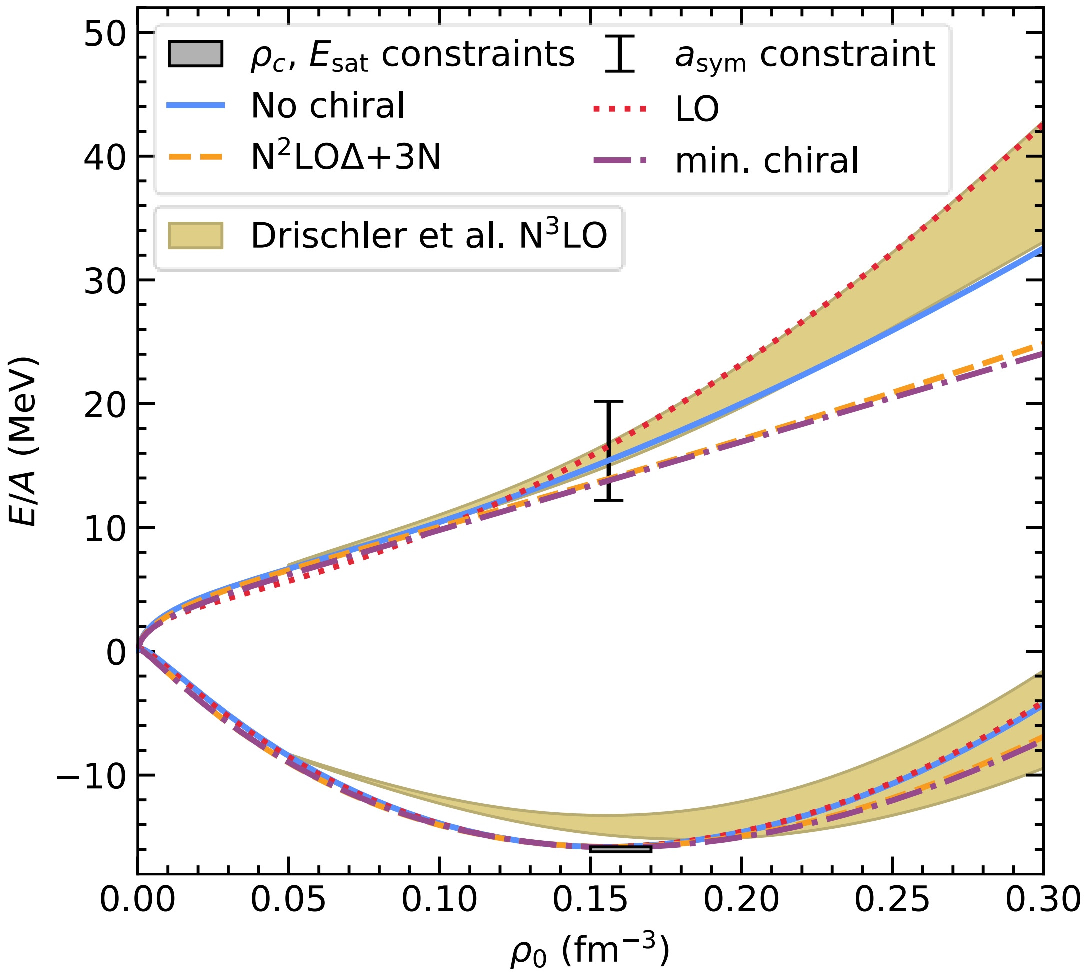
Skyrme parameter optimization

- Fit to 81 nuclei
  - Binding energies, charge radii, odd-even mass staggerings, fission isomer energies
- Weights for observables from Bayesian posterior estimate for UNEDF1
  Schunck et al., JPG **47** (2020)
- Find constrained minimum using POUNDERS
  Wild et al., JPG **42** (2015)



Skyrme parameter optimization

- Infinite nuclear matter parameters are constrained to physically plausible region in fit



GUDE [guːdə]

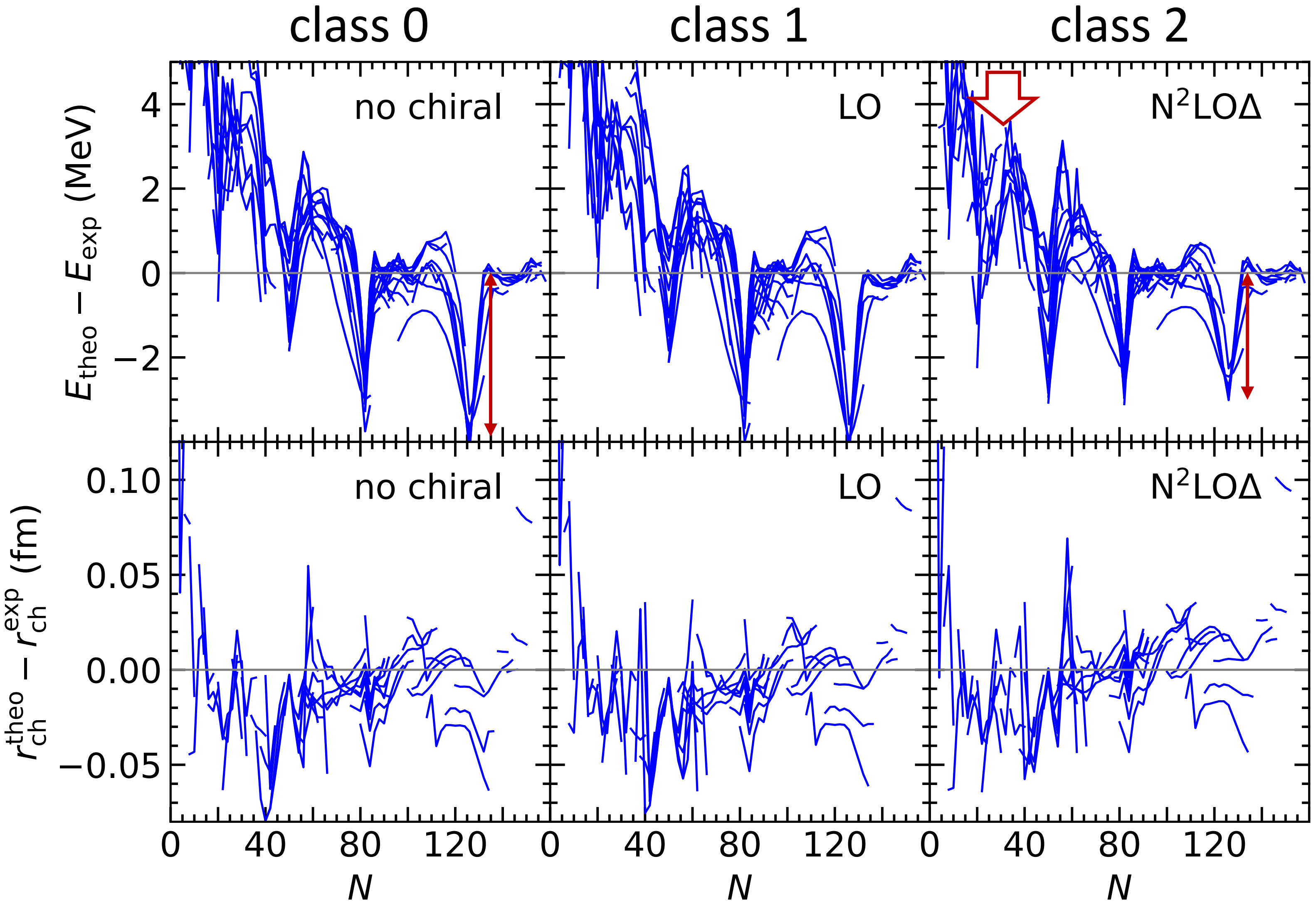
Germany-USA Density-matrix expansion Energy density functionals

- We group EDFs in 3 classes

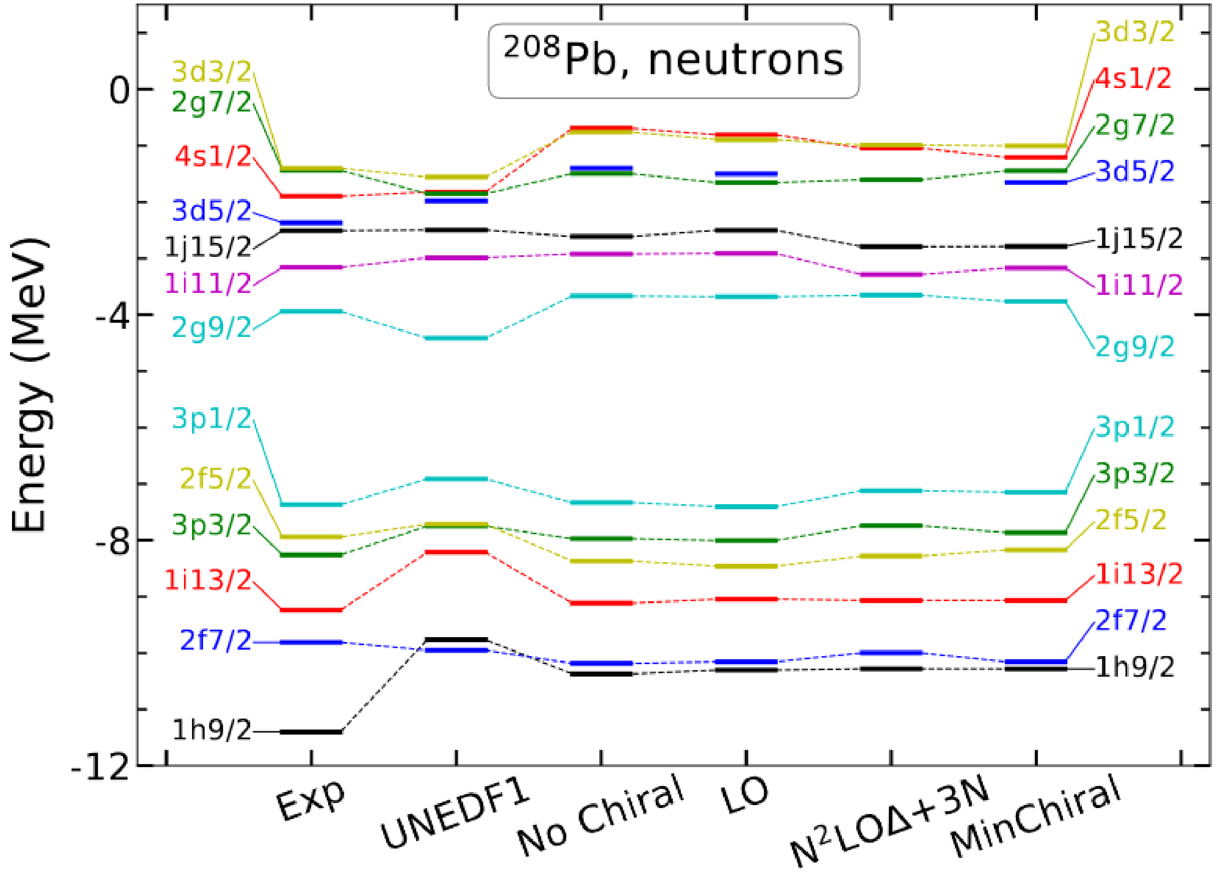
Class	0	1	2
Variants	no chiral	LO, NLO	NLOΔ(+3N), N^2LO(Δ,+3N)
χ^2	122	145	86 – 91
Binding energy rms deviation (MeV)	2.11	2.09 – 2.13	1.41 – 1.56

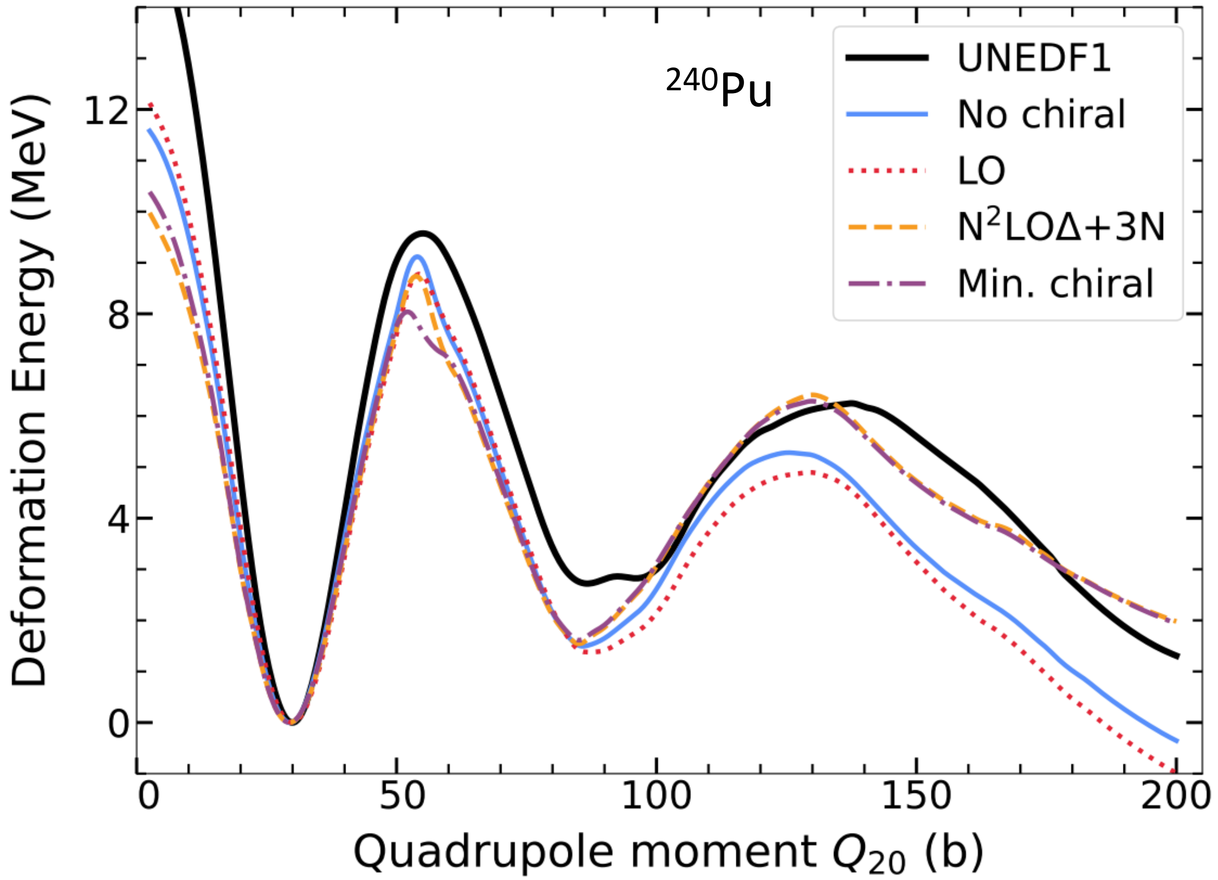
- Terms beyond NLO move global minima “closer” towards region allowed by nuclear matter parameter bounds
- Significant improvement beyond NLO

GUDE results

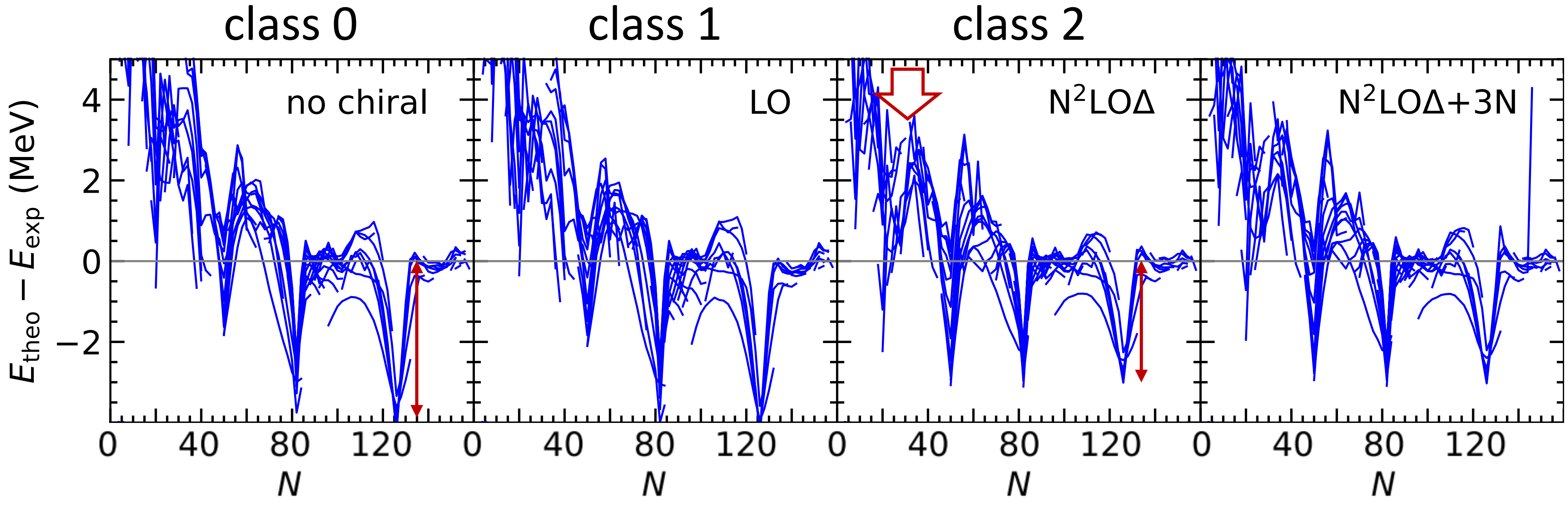


GUDE results



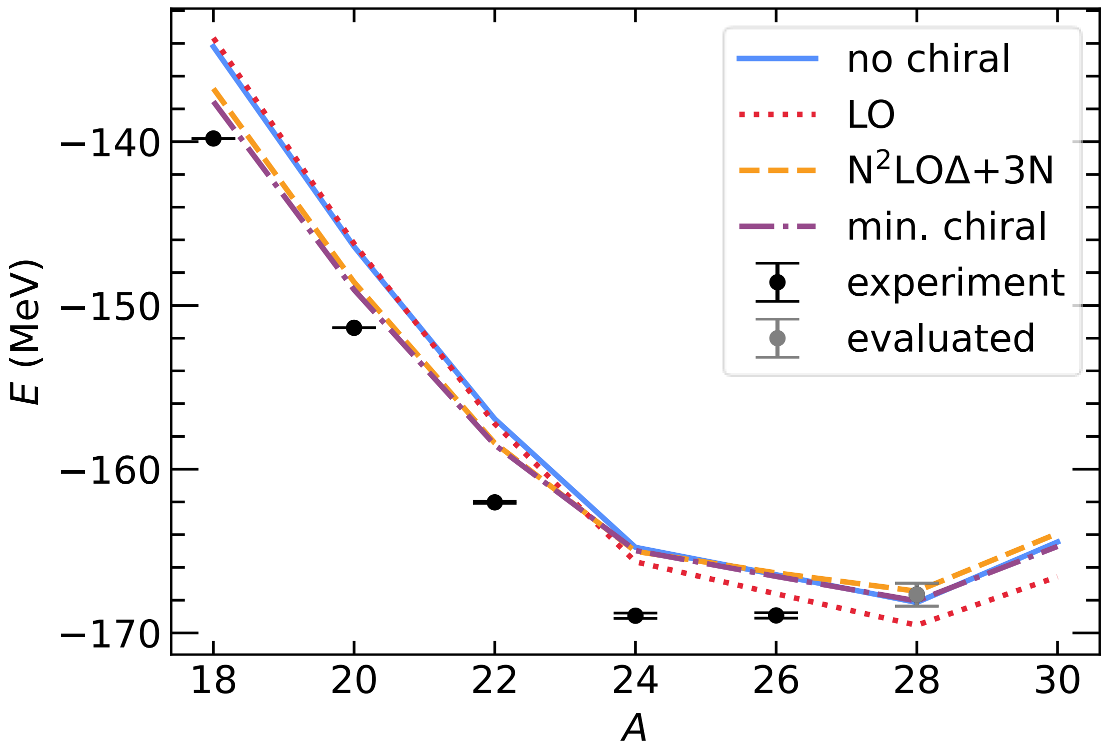


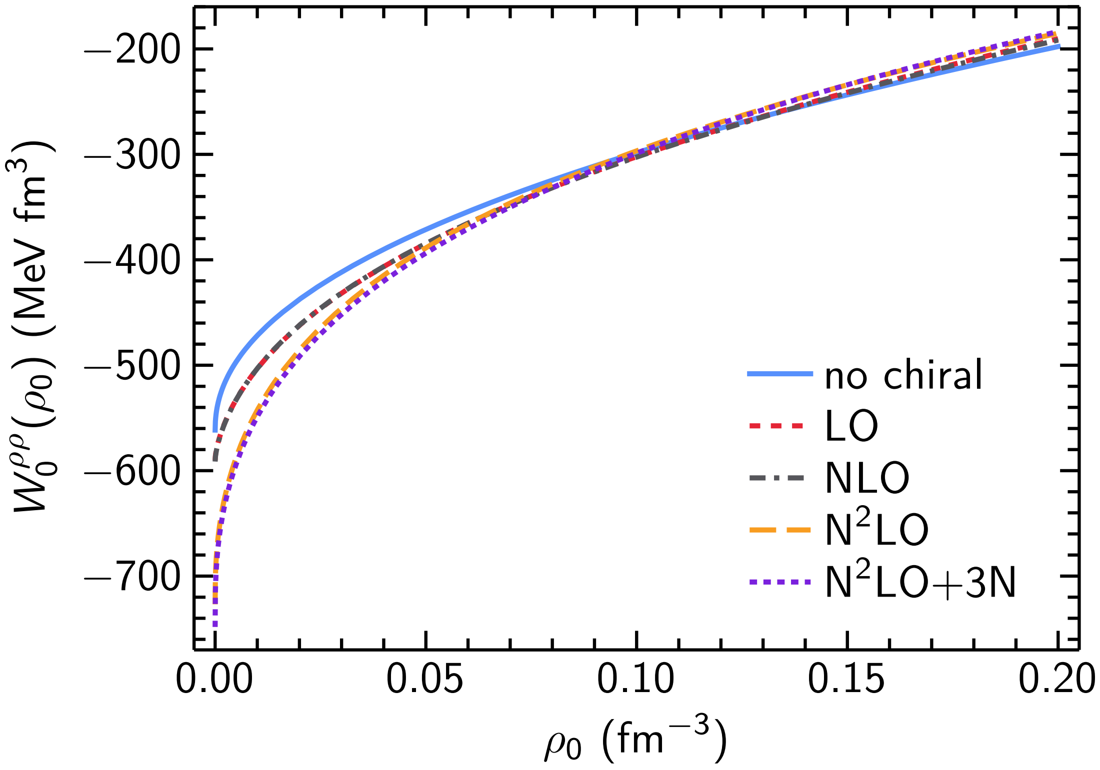
Analysis of pion contributions



- 3N pion exchanges have no effect

Analysis of pion contributions





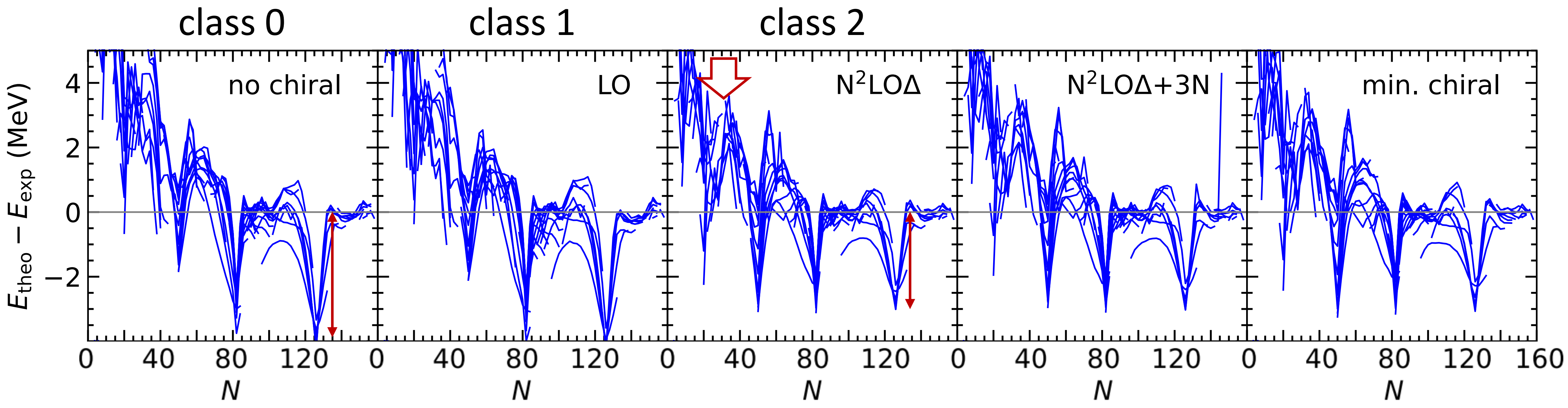
- 3N pion exchanges have no effect
  - Already effectively incorporated via density-dependent Skyrme contact

Analysis of pion contributions

- 3N pion exchange effect might appear from
  - fitting to neutron-rich nuclei
  - Changing regularization scheme

- Leave out density dependent contact?

Analysis of pion contributions

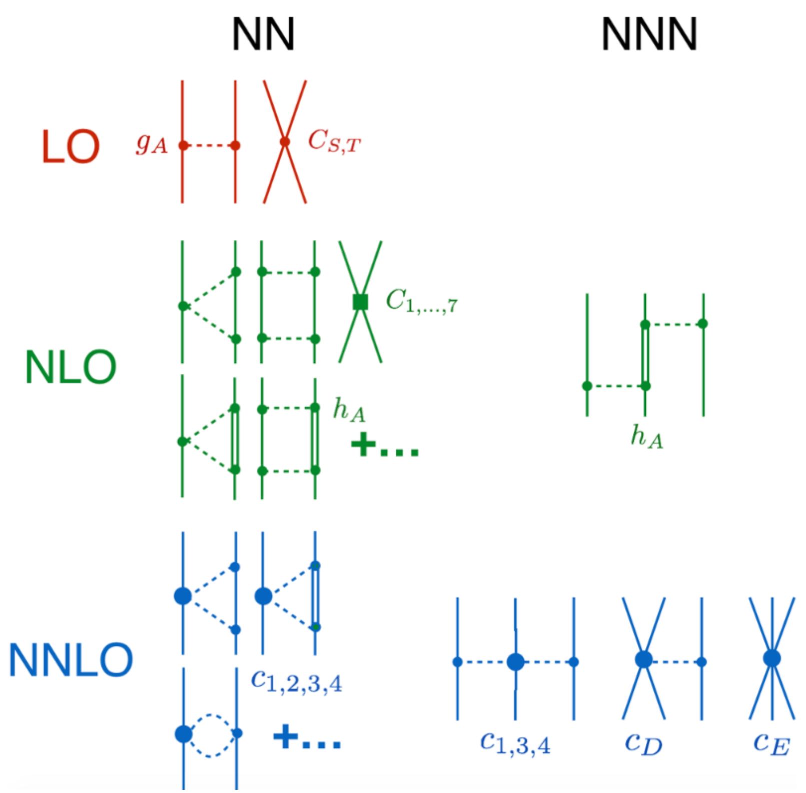


- Min. chiral EDF: minimal set of chiral terms that yield improvement
  - isoscalar N^2LO Hartree + LO Fock (in Slater approximation)

Analysis of pion contributions

- Chiral power counting does not carry over
  - Here: structure of contacts does not change with chiral order

$$E_{\mathrm{Skyrme}} = \sum_{t=0,1}\int \mathrm{d}\mathbf{R}\left[\left(C^{\rho\rho}_{t0} + C^{\rho\rho}_{tD}\rho_0^{\gamma}\right)\rho_t^2 + C^{\rho\tau}_t \rho_t \tau_t + C^{\rho\Delta\rho}_t \rho_t \Delta\rho_t + C^{\rho\nabla J}_t \rho_t \boldsymbol{\nabla}\cdot\mathbf{J}_t + C^{JJ}_t J_{t,ab} J_{t,ab}\right],$$



Ekström et al., PRC **97** (2018)

Summary

- Towards ab initio EDFs: add parameter-free pion exchanges to Skyrme EDF
  - Significant improvement beyond NLO:
    binding energy rms deviation decreased by 30%

→ Pions help with simultaneous description of finite nuclei and infinite matter

Outlook

- Different regularization scheme
- Changes of fit data set
  - Fit to ab initio pseudodata
- Do pions help other EDF forms?

Thanks for your attention

and to my collaborators
Scott Bogner, Toño Coello Pérez, Dick Furnstahl,
Rodrigo Navarro Pérez, Nicolas Schunck, and Achim Schwenk