Skyrme EDFs with pions

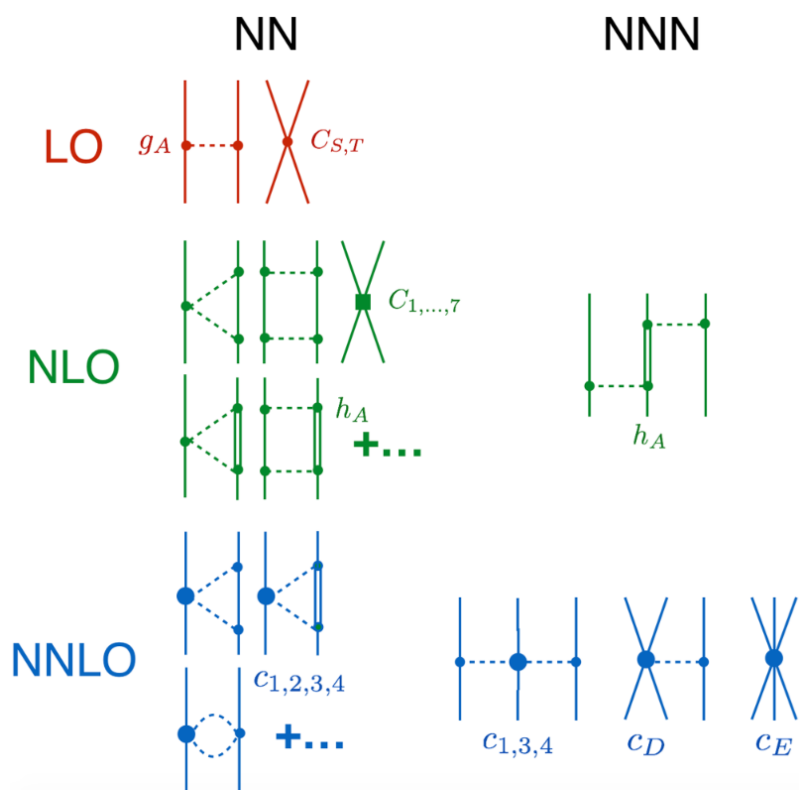
PRC **109**, 014319 (2024)

Lars Zurek

Mainz UQ workshop, June 28, 2024

Ab initio calculations with chiral EFT

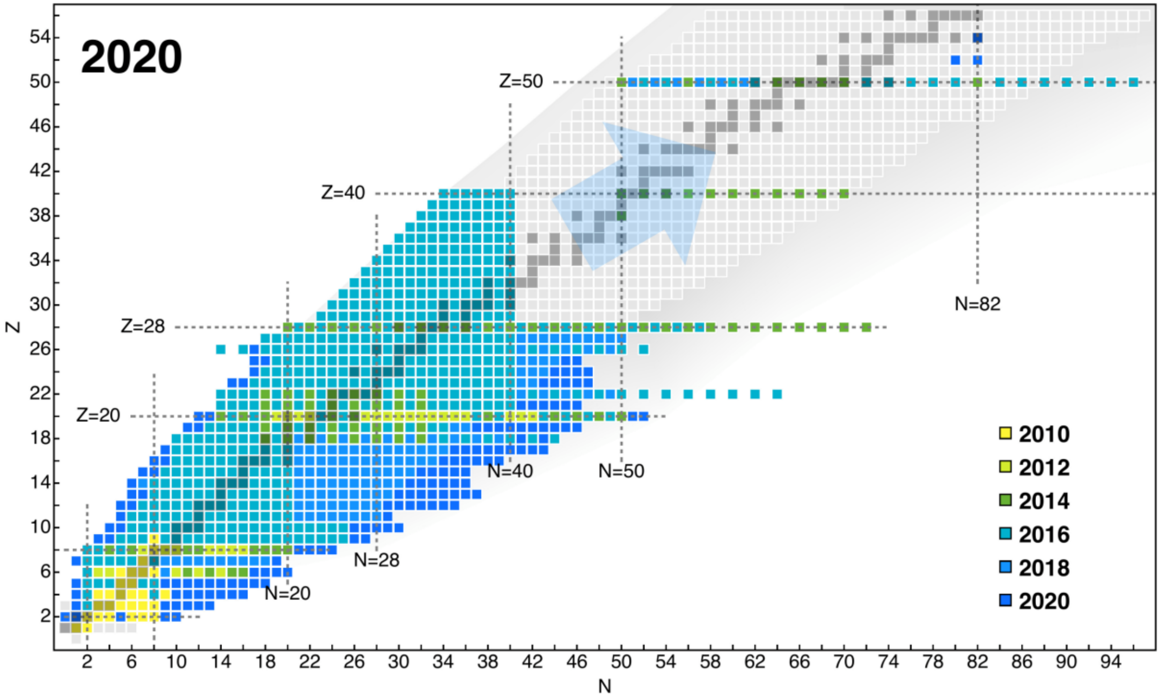
- Chiral effective field theory:
  expansion of nuclear interaction in typical momenta over breakdown scale
  - Systematically improvable
  - Uncertainty estimates “built-in”



Ekström et al., PRC **97** (2018)

Ab initio calculations with chiral EFT

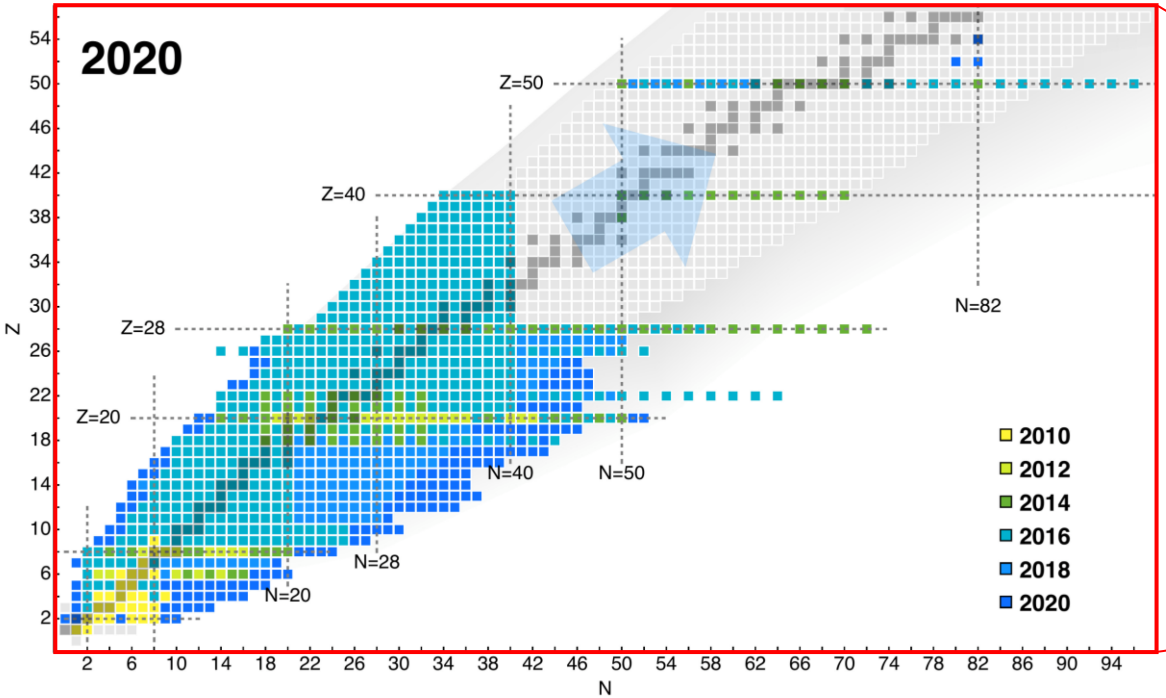
- Computationally expensive



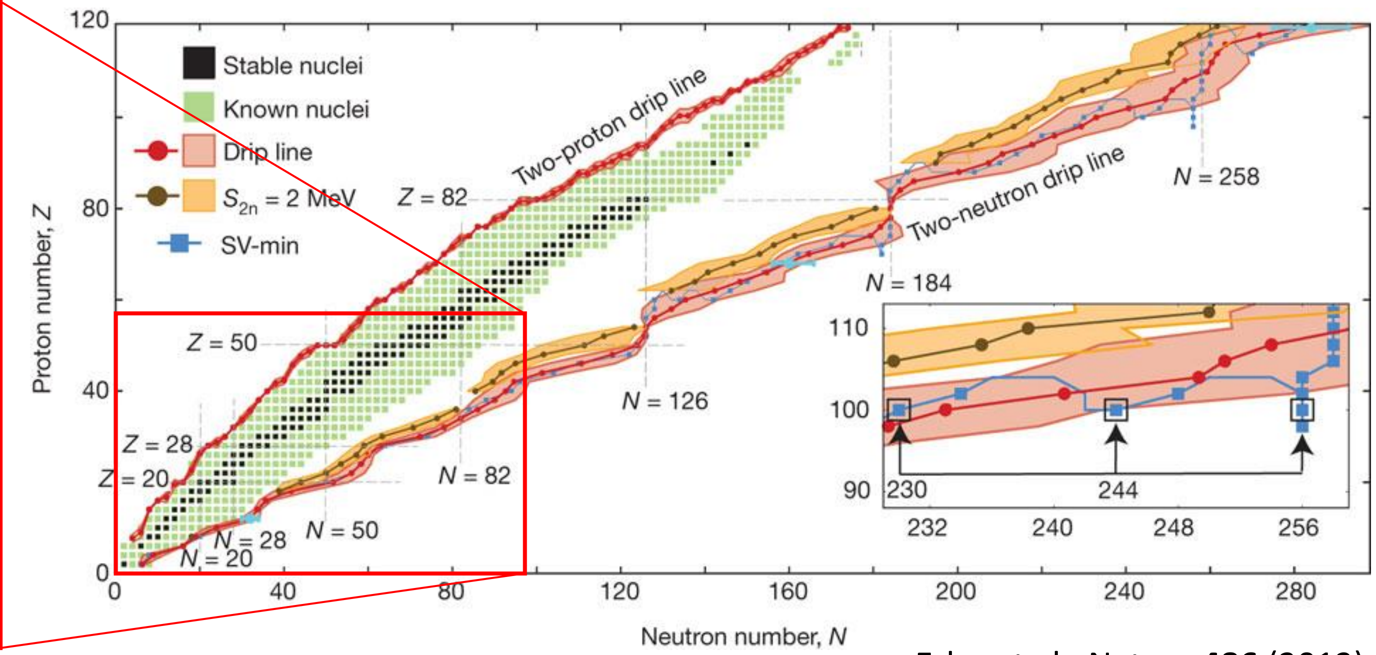
Hergert, FP **8** (2020)

Ab initio calculations with chiral EFT

- Computationally expensive
- Challenging to achieve similar accuracies as energy density functionals



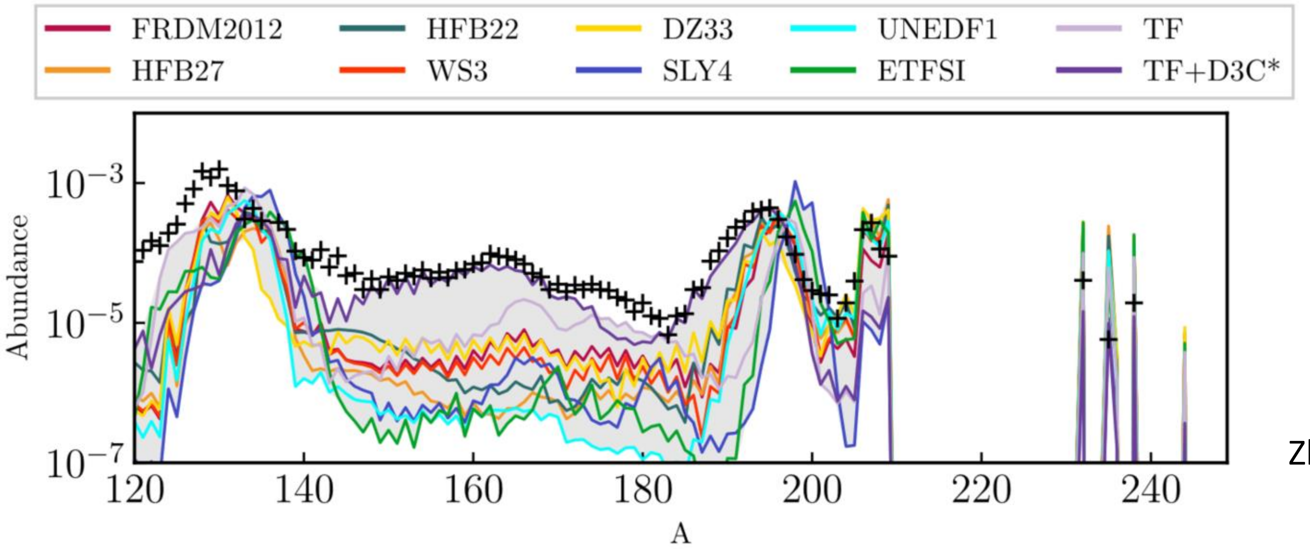
Hergert, FP **8** (2020)



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

Some EDF issues

- Extrapolation outside fitting region potentially uncontrolled



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

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

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

- Phenomenological construction of EDFs

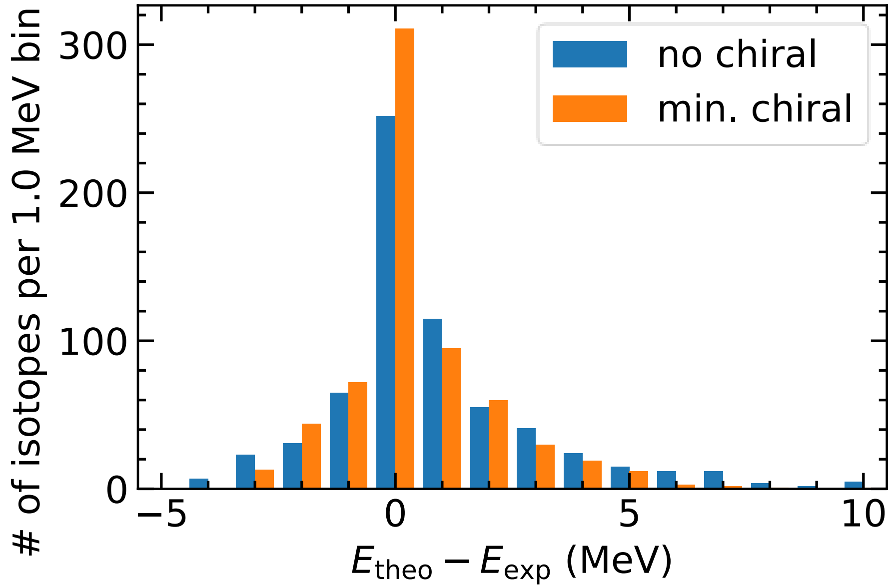
Quest for ab initio energy density functionals

- How to obtain EDFs from first principles
  or at least meaningfully connect EDFs and the ab initio approach?

Furnstahl, EPJA **56** (2020)
Marino et al., PRC **104** (2021)
Duguet et al., EPJA **59** (2023)
Fraboulet, Ebran, EPJA **60** (2024)

- Semi-phenomenological hybrid EDFs
  - Skyrme + pions from chiral EFT

Drut et al., PPNP **64** (2010)
Gebremariam et al., PRC **82** (2010)
Navarro Pérez et al., PRC **97** (2018)
LZ et al., PRC **109** (2024)



Idea

- 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

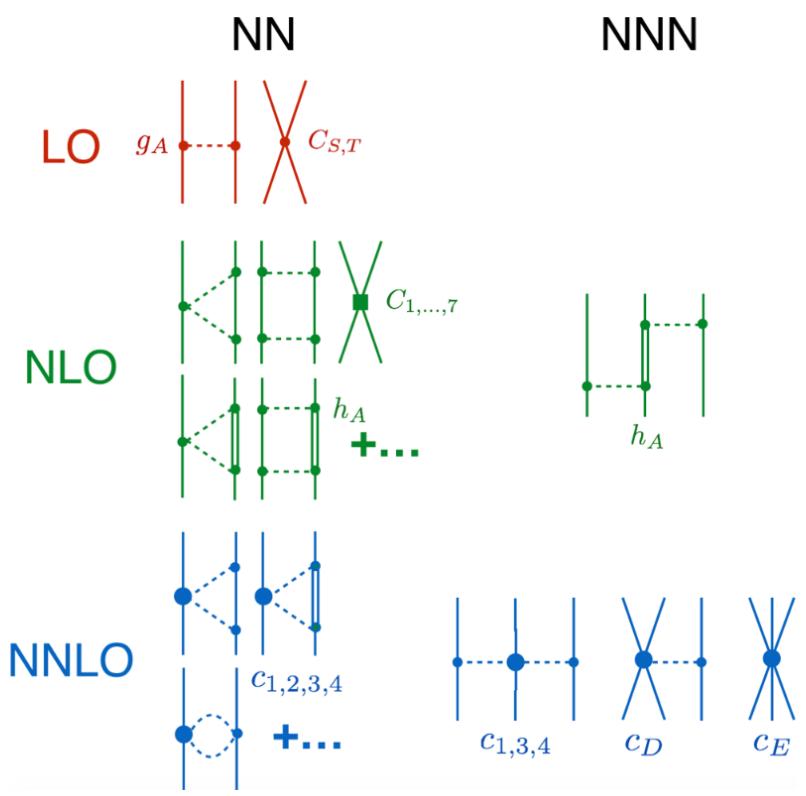
Sun et al., PRC **106** (2022)

Idea

- Skyrme EDF ~ effective HF contact interactions

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

  - Correlations and missing interactions implicitly included via fitting to data
- Increase resolution: add pions from chiral EFT



Ekström et al., PRC **97** (2018)

GUDE [guːdə]

Germany-USA Density-matrix expansion Energy density functionals

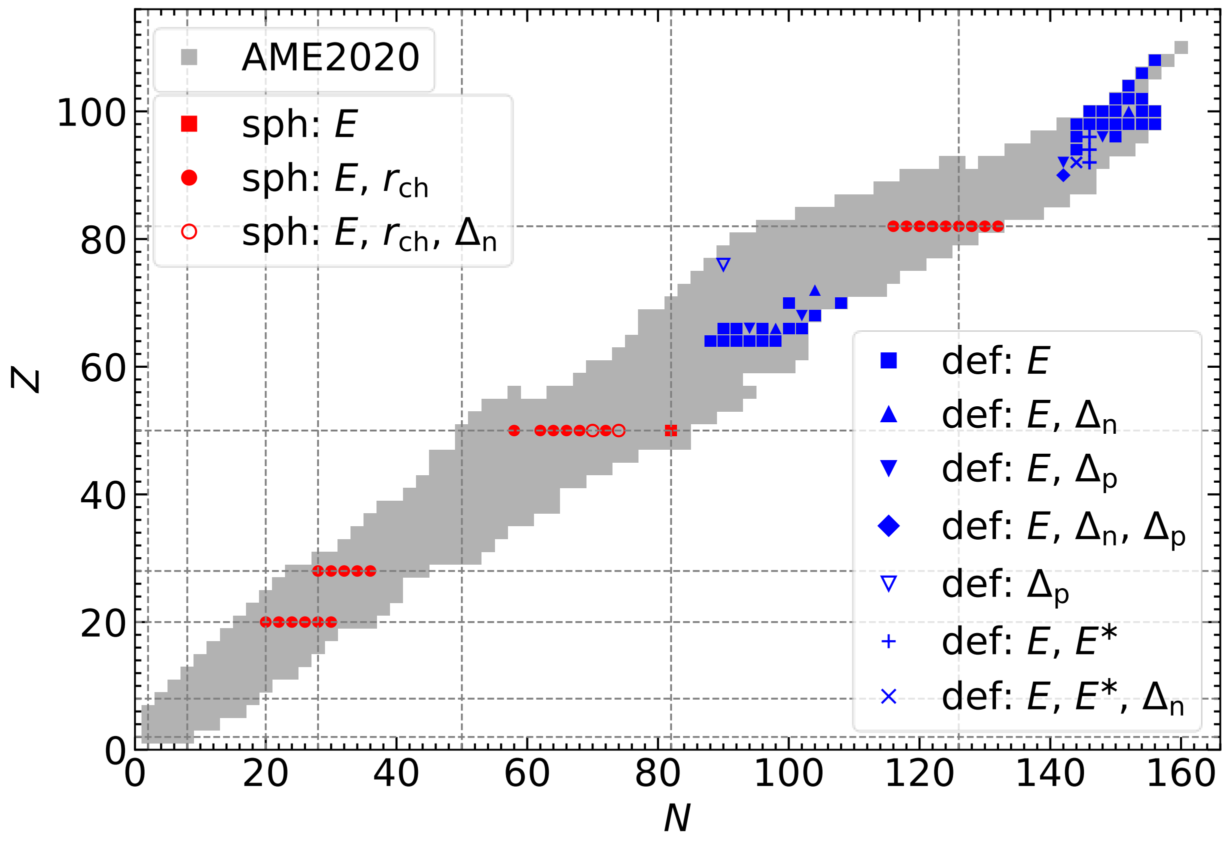
LZ et al., PRC **109** (2024)

- Semi-phenomenological hybrid EDFs
- Skyrme + HF long-range pions
  - At different chiral orders up to N^2LO, with and without Δs and 3N forces
  - No additional fit parameters
  - Refit 14 Skyrme parameters

Skyrme parameter optimization

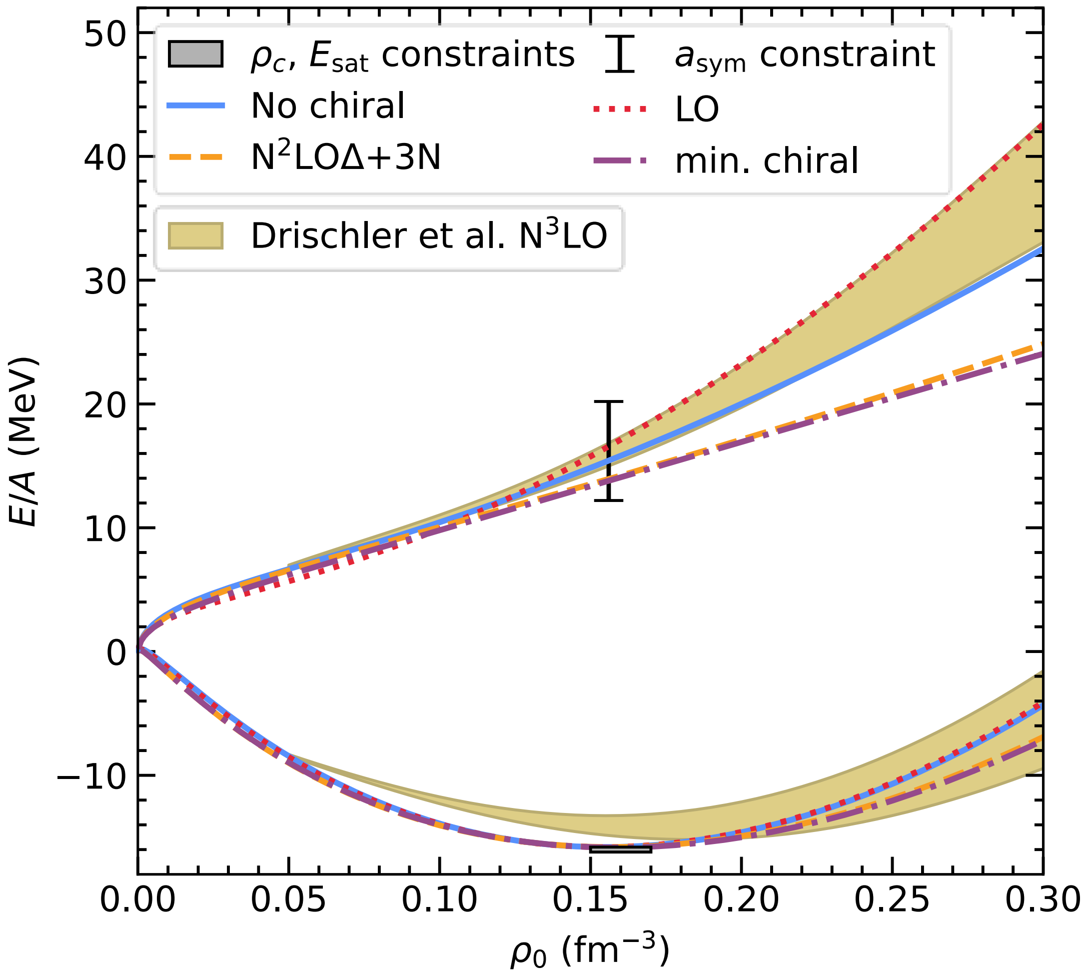
- Fit to 81 even-even nuclei
  - Binding energies, charge radii, odd-even mass staggerings, fission isomer energies
- Weights for observables from Bayesian posterior estimate for UNEDF1

Schunck et al., JPG **47** (2020)



Skyrme parameter optimization

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



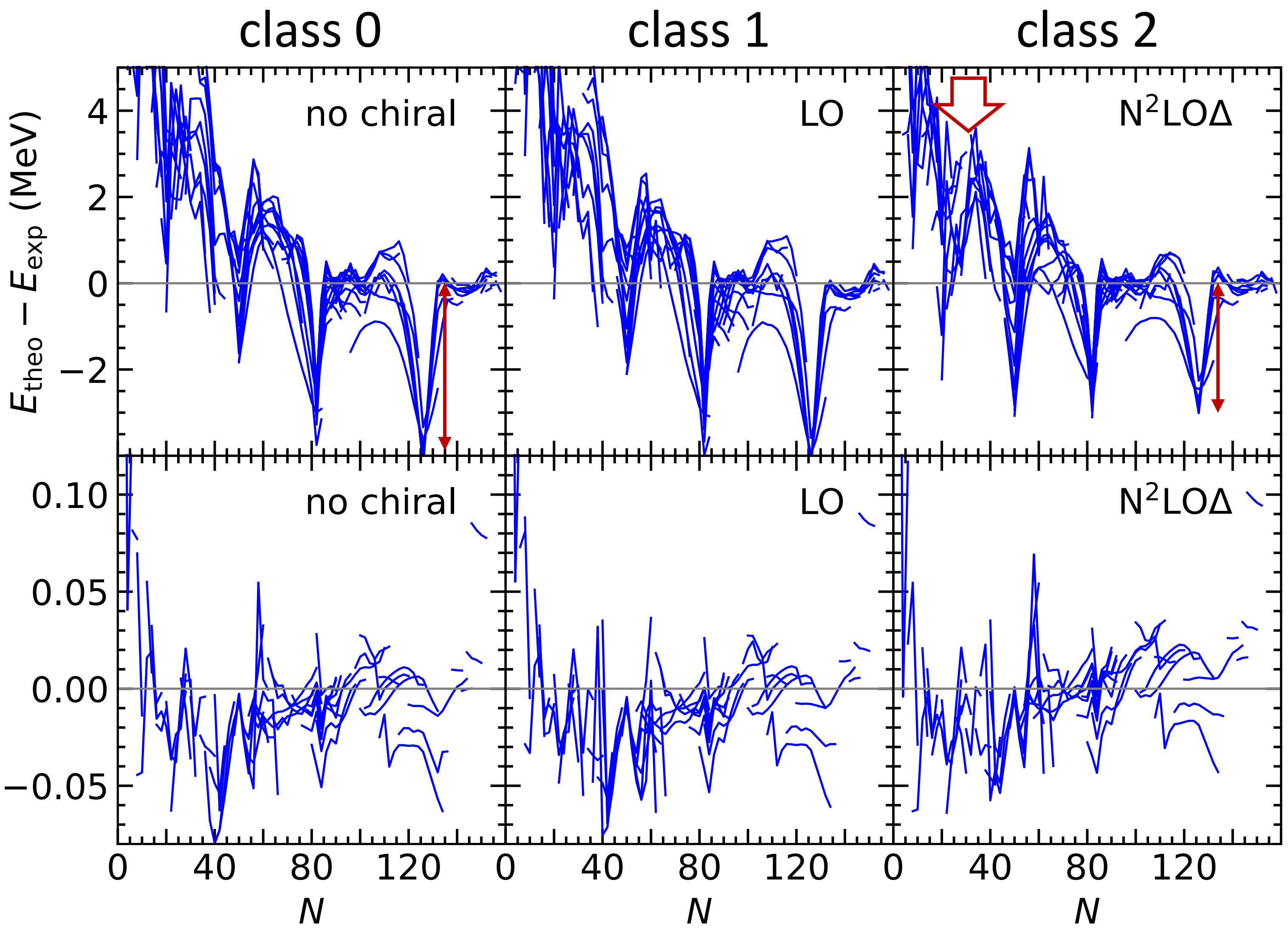
GUDE results

- We group EDFs in 3 classes

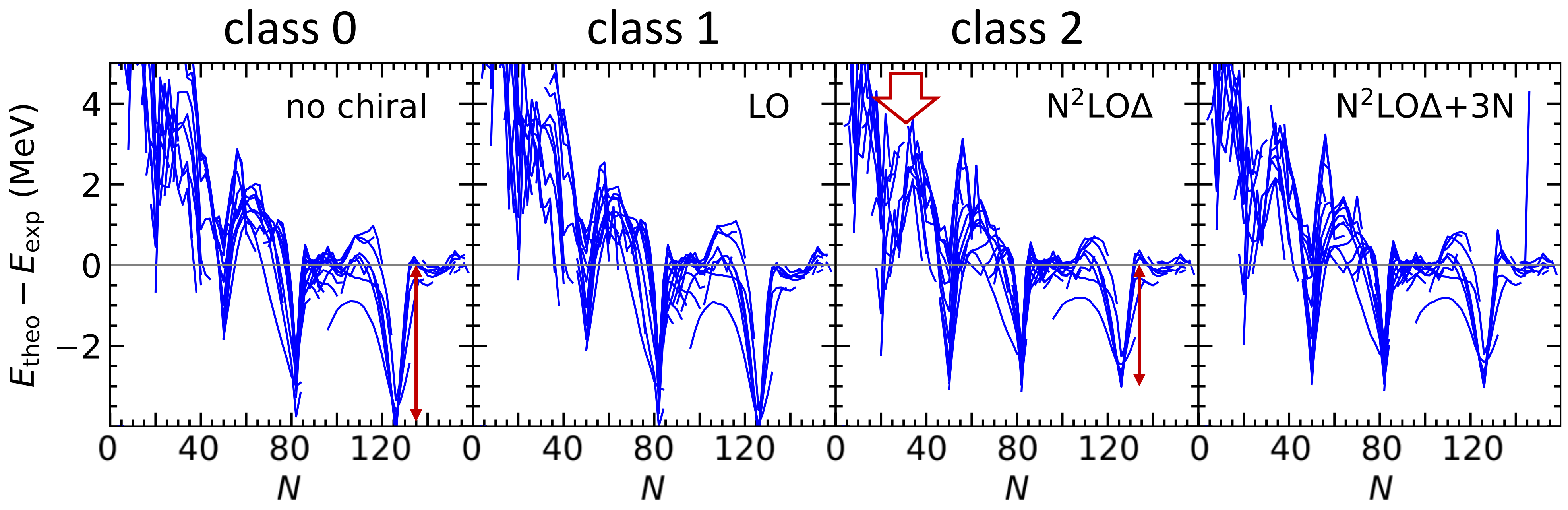
Class	0	1	2
Variants	no chiral	LO, NLO	NLOΔ(+3N), N^2LO(Δ,+3N)
χ^2	122	145	86 – 91
Binding energy rms deviation (MeV)	2.11	2.09 – 2.13	1.41 – 1.56

- Terms beyond NLO move global minima “closer” towards region allowed by nuclear matter parameter bounds
- Significant improvement beyond NLO: rms deviation reduced by 30%

GUDE results

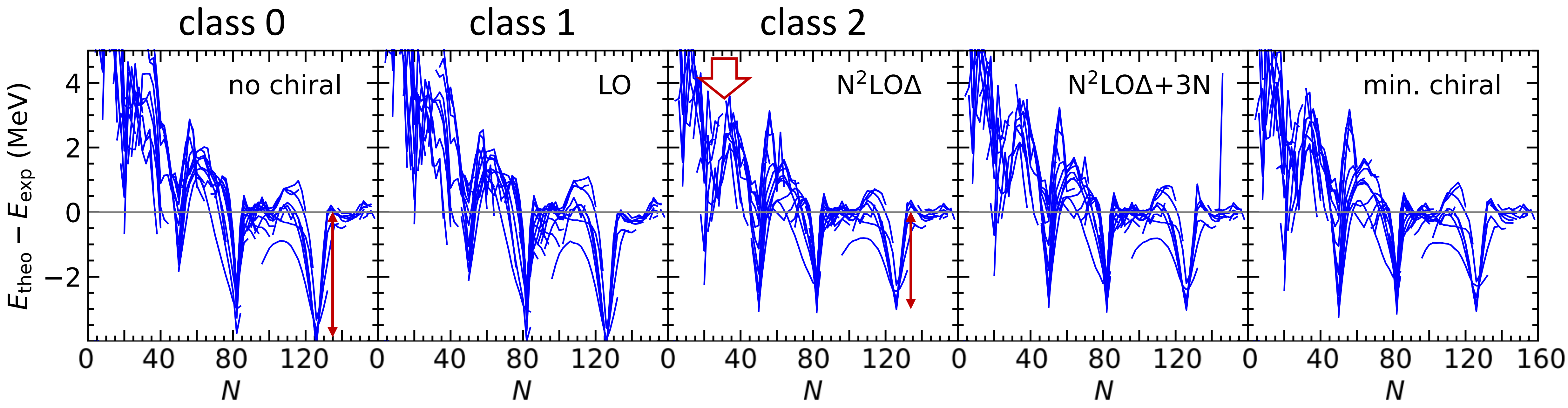


Analysis of pion contributions



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

Analysis of pion contributions



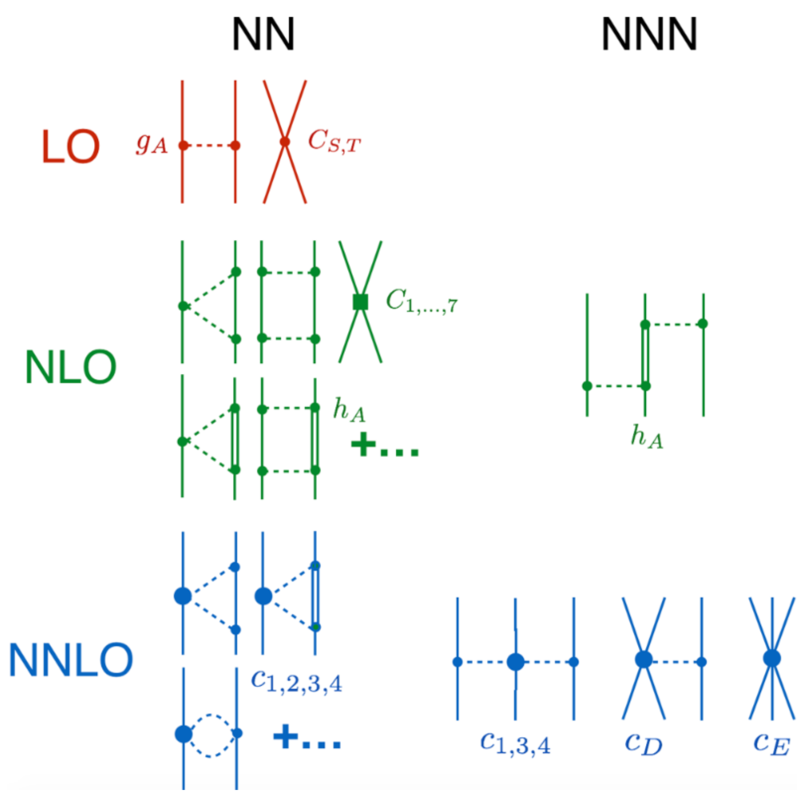
- Min. chiral EDF: minimal set of chiral terms that yield improvement
  - isoscalar N^2LO Hartree + LO Fock (in Slater approximation)

Analysis of pion contributions

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

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

  - Only mean-field contributions



Ekström et al., PRC **97** (2018)

(Not so) GUDE uncertainties

- First-order approximation of covariance matrix

$$\mathrm{Cov} \approx \frac{\chi^2(\mathbf{x})}{n_d - n_x}\left(J(\mathbf{x})^T J(\mathbf{x})\right)^{-1}$$

with $\chi^2(\mathbf{x}) = \|\mathbf{R}(\mathbf{x})\|^2$, $J(\mathbf{x})^T = \boldsymbol{\nabla} \otimes \mathbf{R}(\mathbf{x})$

Kortelainen et al., PRC **82** (2010)
Donaldson, Schnabel, Technometrics **29** (1987)

- Parameters at bound fixed
- Isovector parameters unconstrained
- a_{sym} uncertainty underestimated because L_{sym} at bound

min. chiral

parameter	$\mathbf{x}$	$\pm$ $\boldsymbol{\sigma}$
ρ_c (fm^{-3})	0.15832	0.00088
E (MeV)	−15.830	0.017
K (MeV)	223.6	6.8
M_{s}^{*-1}	0.9173	0.0033
a_{sym} (MeV)	28.58	0.33
L_{sym} (MeV)	30	
$C_0^{\rho\Delta\rho}$ (MeV fm^5)	22.5	1.0
$C_1^{\rho\Delta\rho}$ (MeV fm^5)	−38.8	19.2
$C_0^{\rho\nabla J}$ (MeV fm^5)	−61.4	5.3
$C_1^{\rho\nabla J}$ (MeV fm^5)	3.4	14.6
C_0^{JJ} (MeV fm^5)	−38.8	14.7
C_1^{JJ} (MeV fm^5)	−4.2	24.2
V_0^{n} (MeV fm^3)	−206.5	1.2
V_0^{p} (MeV fm^3)	−249.4	2.0

Parameter correlations

- Correlation coefficients

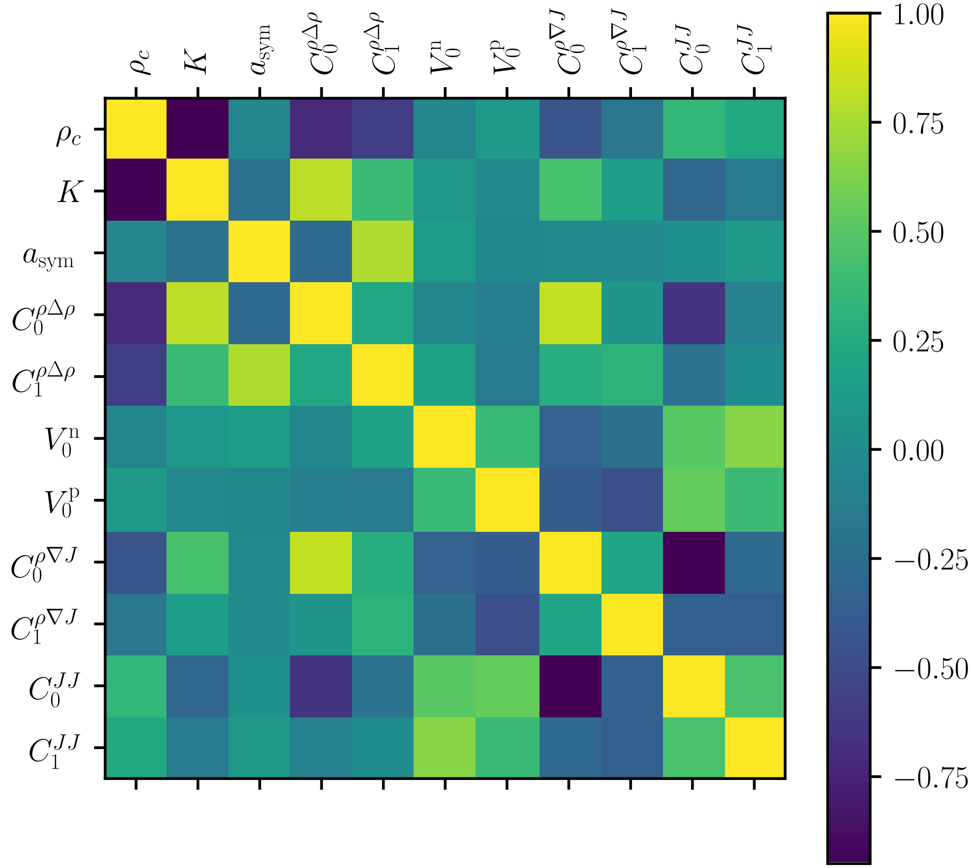
$$R_{k,l} = \frac{\mathrm{Cov}_{k,l}}{\sigma_k \sigma_l}$$

- Exclude E, M_s^{*-1}, L_sym from calculation to be able to compare different GUDE variants

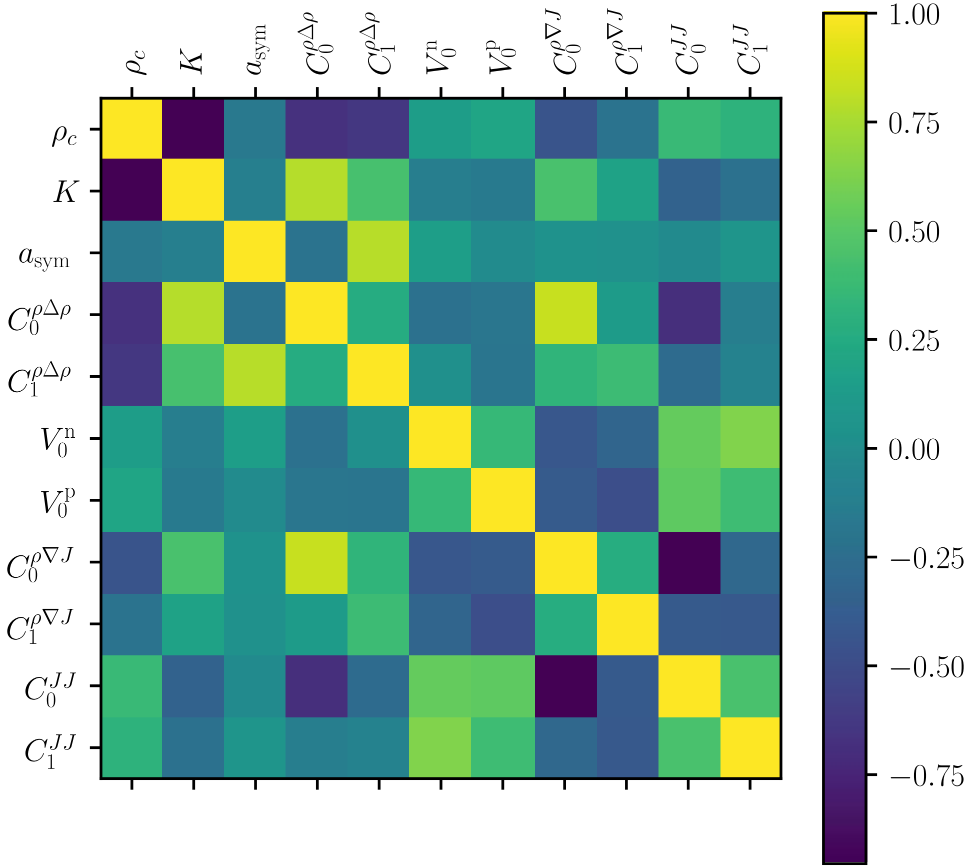
Parameter correlations

- Correlations depend little on the GUDE variant

N²LO+3N



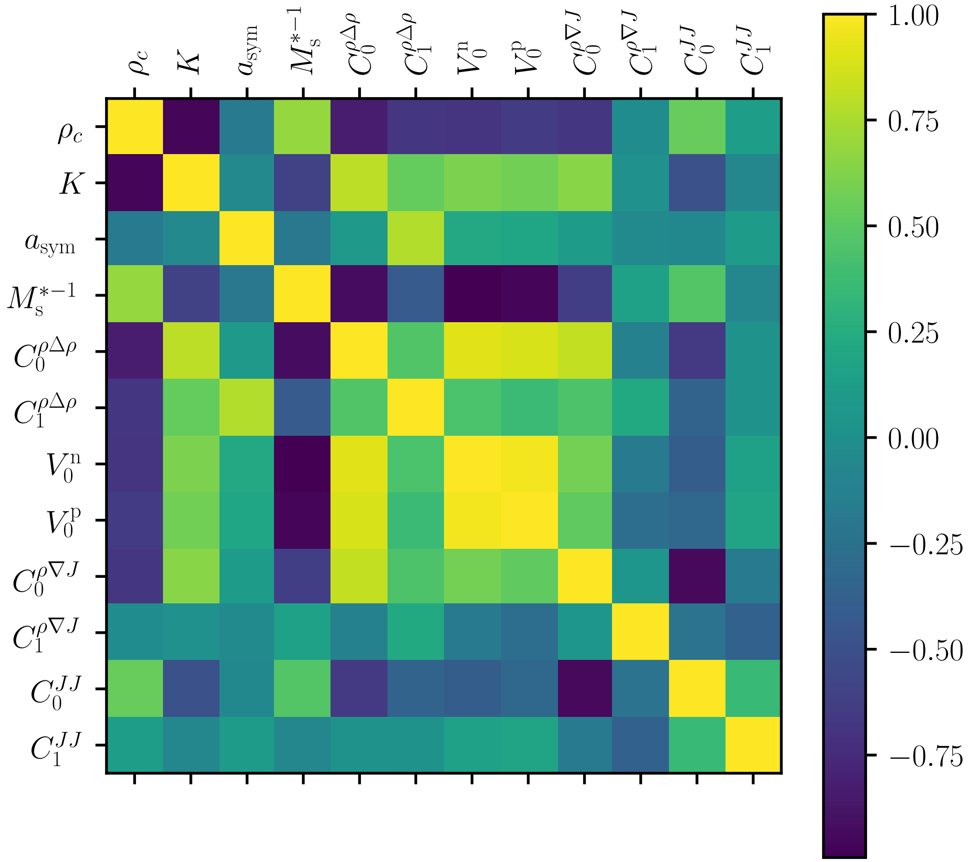
min. chiral



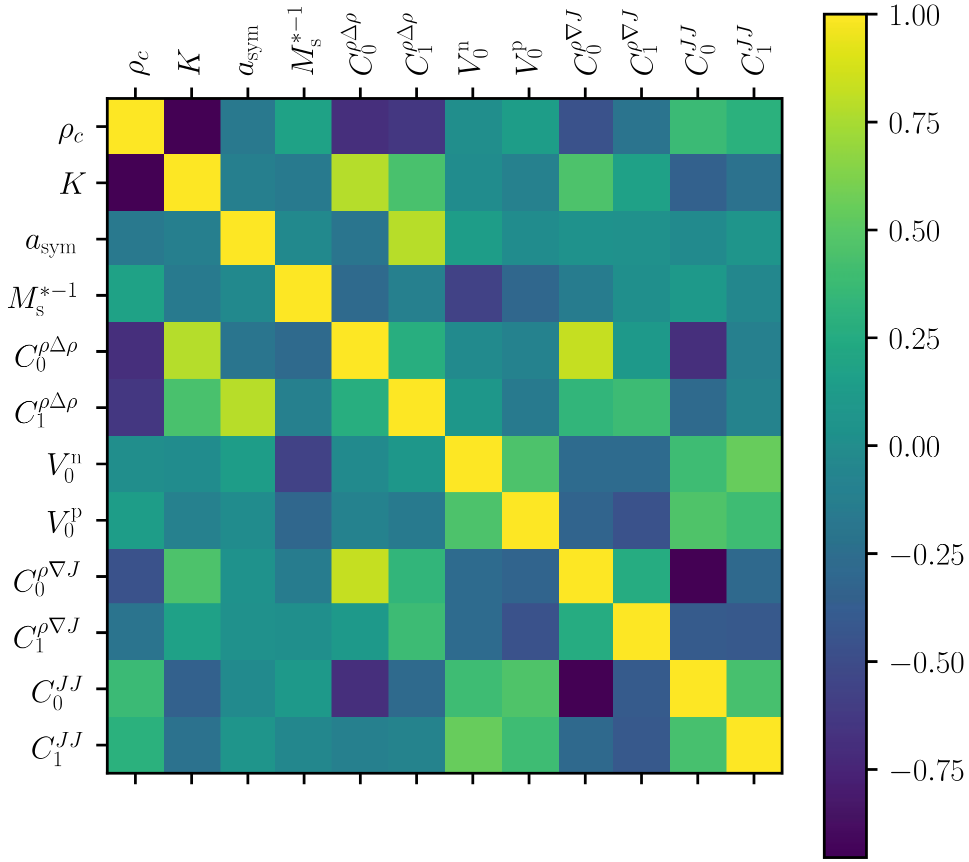
Parameter correlations

- Correlations depend ~~little~~ quite a lot (?) on the GUDE variant

N²LO+3N



min. chiral



Summary

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

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

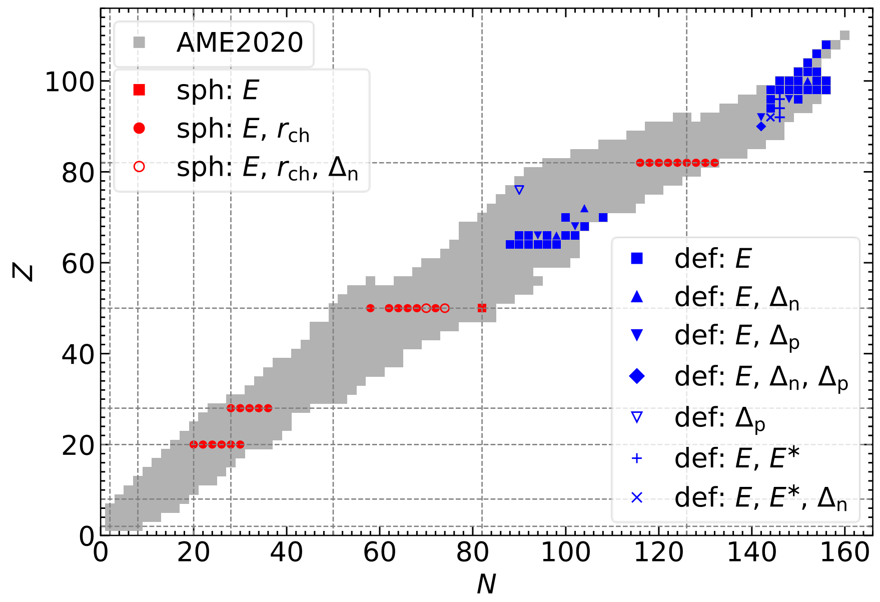
- Simple uncertainty analysis to be interpreted with caution because of parameters at bounds

Outlook

- Better uncertainty quantification
- Do pions help other EDF forms?

Outlook & Question

- Better uncertainty quantification
- Do pions help other EDF forms?

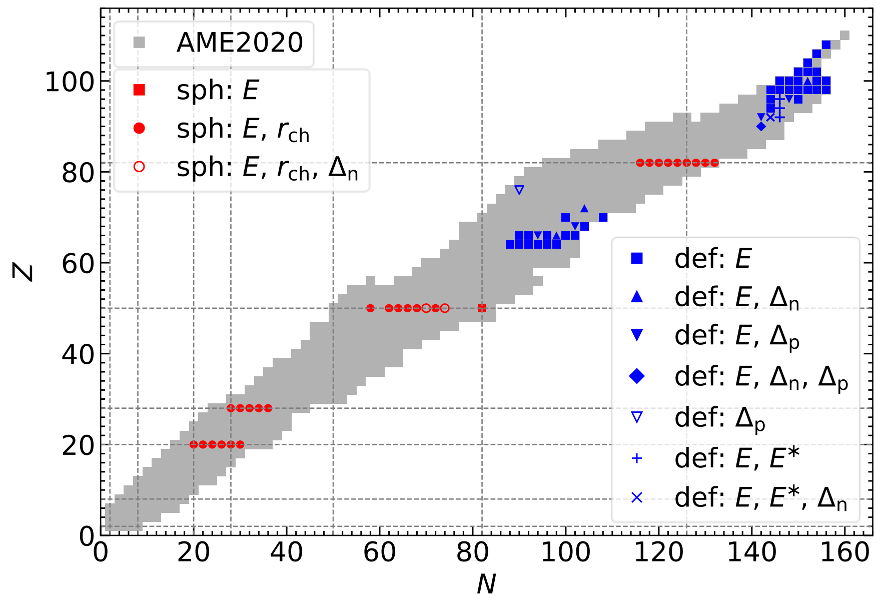


- GUDE functionals were fitted in a basis of 20 HO shells

# of HO shells	χ^2 for fixed parameters
18	759
20	87
22	?

Outlook & Question

- Better uncertainty quantification
- Do pions help other EDF forms?



- GUDE functionals were fitted in a basis of 20 HO shells

# of HO shells	χ^2 for fixed parameters
18	759
20	87
22	441

Questions

- Does it make sense to use nonconverged calculations? Should we extrapolate?
- How to power-count mean field contributions?
- How can we investigate reasons for improving description at shell closures?

Thanks

for your attention,
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Nicolas Schunck, and Achim Schwenk,
and to the organizers of the workshop!