

# **Precision nuclear theory**

#### Christian Forssén Chalmers University of Technology

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# Many thanks to my collaborators















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$$y_{\exp} + \delta y_{\exp} = y_{th}(\boldsymbol{\alpha})$$

Credit W. Nazarewicz, INTRANS 2024









$$y_{\exp} + \delta y_{\exp} = y_{th}(\boldsymbol{\alpha}) + \delta y_{th}$$

With complete uncertainty quantification this relation turns into a statistical model

# Scientific goals in ab initio nuclear theory

- Model the strong interaction at low-energy
  - At the most fundamental level, the strong interaction is described by Quantum Chromodynamics (QCD);



- Atomic nuclei can presumably be described with relevant low-energy degrees of freedom—nucleons and pions—and residual interactions;
- Effective field theories (EFTs) offer a systematic approach to this problem.
- Infer the parameters (low-energy constants = LECs) of chiral EFT from lowenergy observables such as NN scattering phase shifts, few-nucleon observables.
- Universal framework for few- and many-nucleon modeling
  - Universal framework for modeling of strongly-interacting many-nucleon systems.
  - Solve the many-nucleon problem with controlled approximations.
- Predictive power
  - Linking nuclear structure and observables to fundamental forces.
  - Reliably predict scientifically relevant nuclear observables.

### Why ab initio is more like Gruyère than Champagne 9



(\*)A. Ekström, cf, G.Hagen, G. R. Jansen, W.G. Jiang, and T. Papenbrock, Frontiers in Phys. (2023)

# Reach of ab initio nuclear theory



Image credit: Heiko Hergert

# Reach of ab initio nuclear theory



#### Image credit: Heiko Hergert

# Accuracy: N3LO<sub>TX</sub> (work in progress)

- Optimization includes NN observables, <sup>4</sup>He and <sup>16</sup>O energy and radius.
- Enabled by the use of fast & accurate emulators (reduced-order models)

Baishan Hu, Weiguang Jiang, A. Ekström, cf, G. Hagen. T. Papenbrock (2025) in prep.



## From accuracy to precision in ab initio theory

- Model the strong interaction at low-energy
  - Effective field theories (EFTs) offer a systematic description of this physics.
  - Truncating your EFT implies an understanding of the importance of terms beyond the truncation order.
- Bayesian parameter estimation and model checking
  - The inference of EFT parameters using low-energy observables.
  - Also other parameters might be of interest. E.g.,
    - Can we infer the breakdown scale of the EFT?
    - Can we rigorously test the EFT model assumptions?
- Predictive power strongly linked to precision
  - Predict scientifically relevant nuclear observables with quantified uncertainties.

# Learning from data via Bayesian statistics

#### Model calibration via Bayes' theorem

Likelihood Prior Posterior  $pr(\boldsymbol{\alpha} \mid \mathcal{D}, I) = \frac{pr(\mathcal{D} \mid \boldsymbol{\alpha}, I)pr(\boldsymbol{\alpha} \mid I)}{pr(\mathcal{D} \mid I)}$ 

**Marginal likelihood** 

- The prior encodes our knowledge about parameter values before analyzing the data
- The likelihood is the probability of observing the data given a set of parameters
- The marginal likelihood (or model evidence) provides normalization of the posterior.
- The posterior is the inferred probability density for the parameters.

Statistical models (for ab initio predictions)

$$y_{exp} = \tilde{y}(\boldsymbol{\alpha}) + \delta y_{EFT} + \delta y_{method} + \delta \tilde{y}_{em} + \delta y_{exp}$$



# The present: *ab initio* predictions with quantified uncertainties

**Selected examples** 

#### Ab initio predictions link the skin of <sup>208</sup>Pb to nuclear forces



#### **History Matching**

We explore 10<sup>9</sup> different interaction parameterizations

Confronted with A=2-16 data + NN scattering information

Find 34 non-implausible interactions

#### **Model calibration**

Importance resampling

#### Model checking

Inspect ab initio model and error estimates

B. Hu et al (Nature Phys. 2022)

# <u>Prediction</u>: small skin thickness 0.14-0.20 fm in mild (1.5 sigma) tension with PREX results.

#### Physics predictions with (complex) precision models

#### Searches for BSM physics via high-precision beta decay

$$\frac{d\omega^{1^{+}\beta^{-}}}{dE\frac{d\Omega_{k}}{4\pi}\frac{d\Omega_{\nu}}{4\pi}} = \frac{4}{\pi^{2}} \left(E_{0} - E\right)^{2} kEF^{-}(Z_{f}, E) C_{\text{corr}} \left|\langle \|\hat{L}_{1}^{A}\|\rangle\right|^{2} \times 3\left(1 + \delta_{1}^{1^{+}\beta^{-}}\right) \left[1 + a_{\beta\nu}^{1^{+}\beta^{-}}\vec{\beta} \cdot \hat{\nu} + b_{\text{F}}^{1^{+}\beta^{-}}\frac{m_{e}}{E}\right],$$

A. Glick-Magid et al., Phys. Lett. B 832 (2022) 137259





Predictive modelling of rare isotopes such as heavy oxygen isotopes

> Y. Kondo et al., Nature 620, (2023), 965



## Ab initio predictions of deformed nuclei



#### **FEATURED IN PHYSICS**

#### <u>Multiscale Physics of Atomic Nuclei from First</u> <u>Principles</u>

Z. H. Sun, A. Ekström, C. Forssén, G. Hagen, G. R. Jansen, and T. Papenbrock

Phys. Rev. X 15, 011028 (2025)





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Global Sensitivity Analysis of R<sub>42</sub>

### Nuclear radii in Ca isotopes: pairing / superfluidity

Ab initio computations based on chiral EFT interactions fail to reproduce the parabolic radius trend in the Ca isotopes where is the pairing? - missing correlations

- interaction

A. Scalesi et al., Eur. Phys. J. A 60 (2024) 209

A. Scalesi et al., unpublished (2025)

See Alberto's talk this afternoon



#### **Nuclear radii in Ca isotopes: pairing**



### Ab initio predictions of deformed nuclei



#### **Nuclear radii in Ca isotopes: pairing**



# **Summary and future**

- The concept of tension in science relies on statements of uncertainties
- It is natural to strive for accuracy in theoretical modeling; but actual predictive power is more associated with quantified precision.
- Ab initio methods +  $\chi$ EFT + Bayesian statistical methods in combination with fast & accurate emulators is enabling **precision nuclear theory**.
- Future frontiers of ab initio nuclear structure theory:
  - Symmetry-breaking and restoration schemes for open-shell / deformed nuclei (see Alberto Scalesi's talk this afternoon)
  - Efficient handling of many-body forces for converging heavy (A>200) nuclear systems.
  - Predict scientifically relevant nuclear structure observables across the nuclear chart with quantified uncertainties (e.g. nuclear beta decay observables for BSM searches; <sup>225</sup>Ra PT-violating electric dipole moment)