Next Generation Ab Initio Nuclear Theory

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What is *ab initio* nuclear theory?

What is ab initio? R. Machleidt, Few Body Syst. **64** (2023)

"Microscopic nuclear theory is based on the tenet that atomic nuclei can be accurately described as collections of point-like nucleons interacting via two- and many-body forces obeying nonrelativistic quantum mechanics—and the concept of the *ab initio* approach is to calculate nuclei accordingly."

What is ab initio in nuclear theory? A. Ekström et al., Front. Phys. **11** (2023)

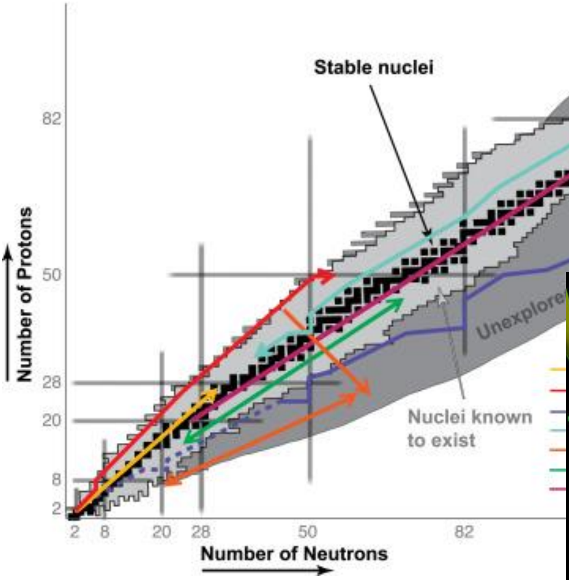
"We interpret the ab initio method as a systematically improvable approach employing Lagrangians, Hamiltonians, or energy density functionals derived from the Standard Model according to the principles of EFT. Subsequently solving for observables using numerically exact methods or, if necessary, controlled approximations that allow for systematic predictions with quantified uncertainties."

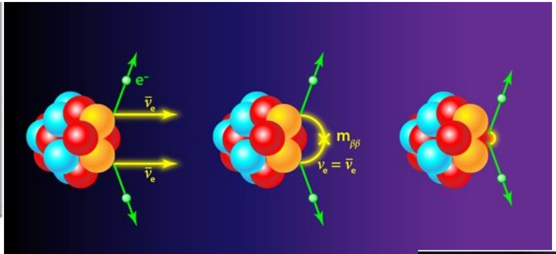
This week: microscopic with nucleon dofs; EFT principles; uncertainty quantification

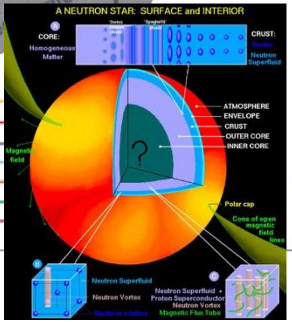
What problems does ab initio nuclear theory address?

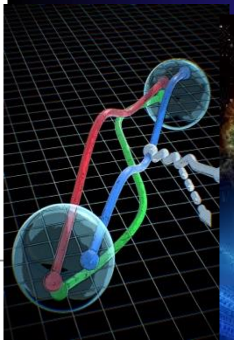
No longer just isolated nuclear structure; now reactions, electroweak probes, nuclear astrophysics, fundamental symmetries, …

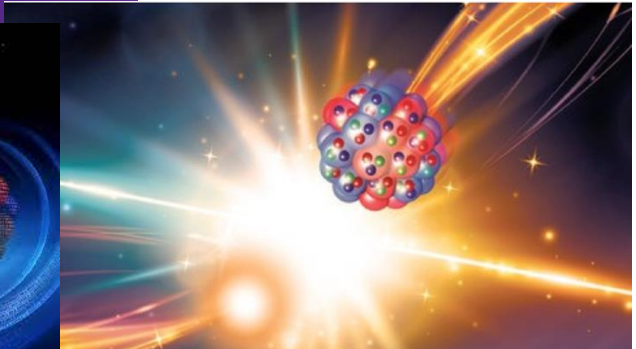
and many more!







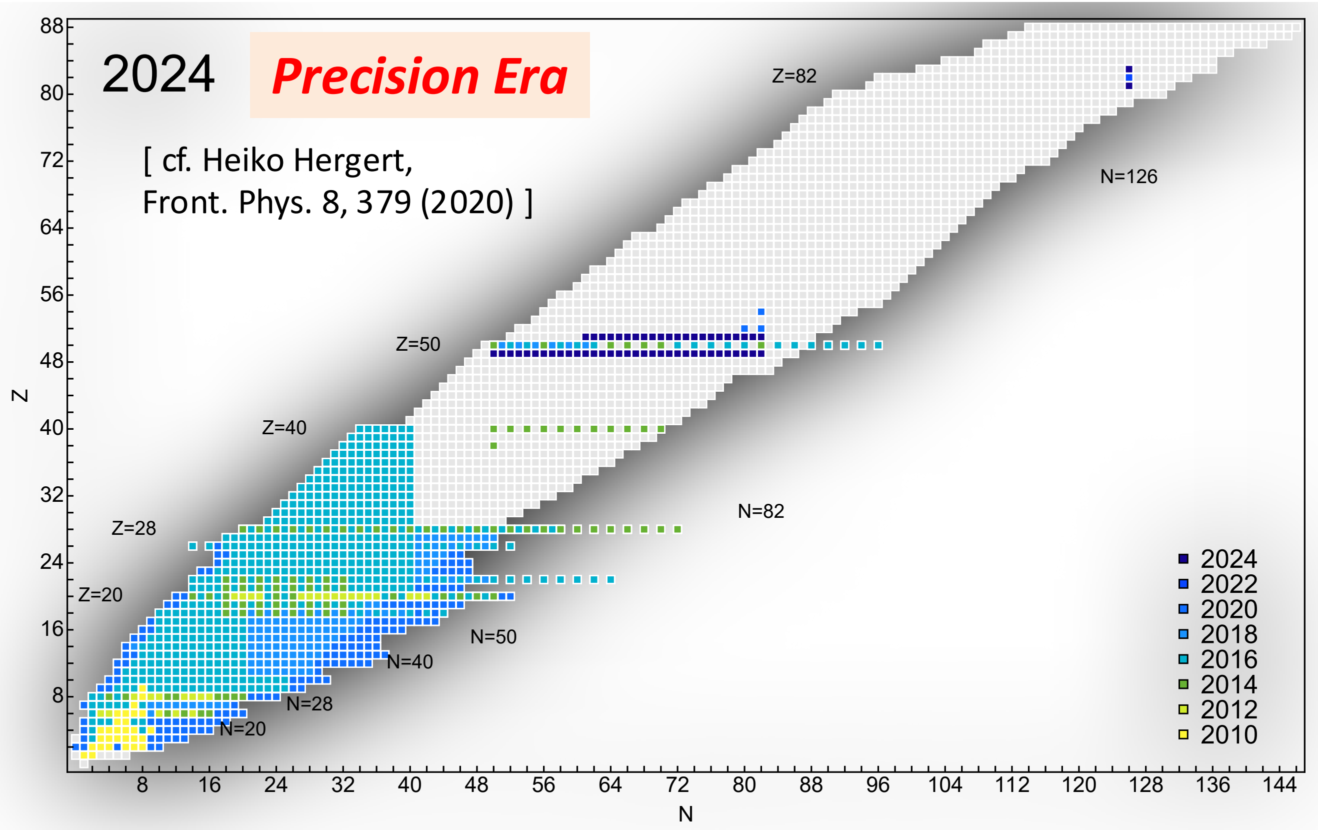




Amazing progress in ab initio calculations of nuclei

[from microscopic neutron+proton forces including 3N]

- Driven by EFT, RG, many-body algorithms, new technologies, …
- *Ab initio* calculations with multiple many-body methods, such as CI, IM-SRG, CC, lattice EFT, SCGF, QMC, …
- Enhanced interplay between ab initio theory and experiment



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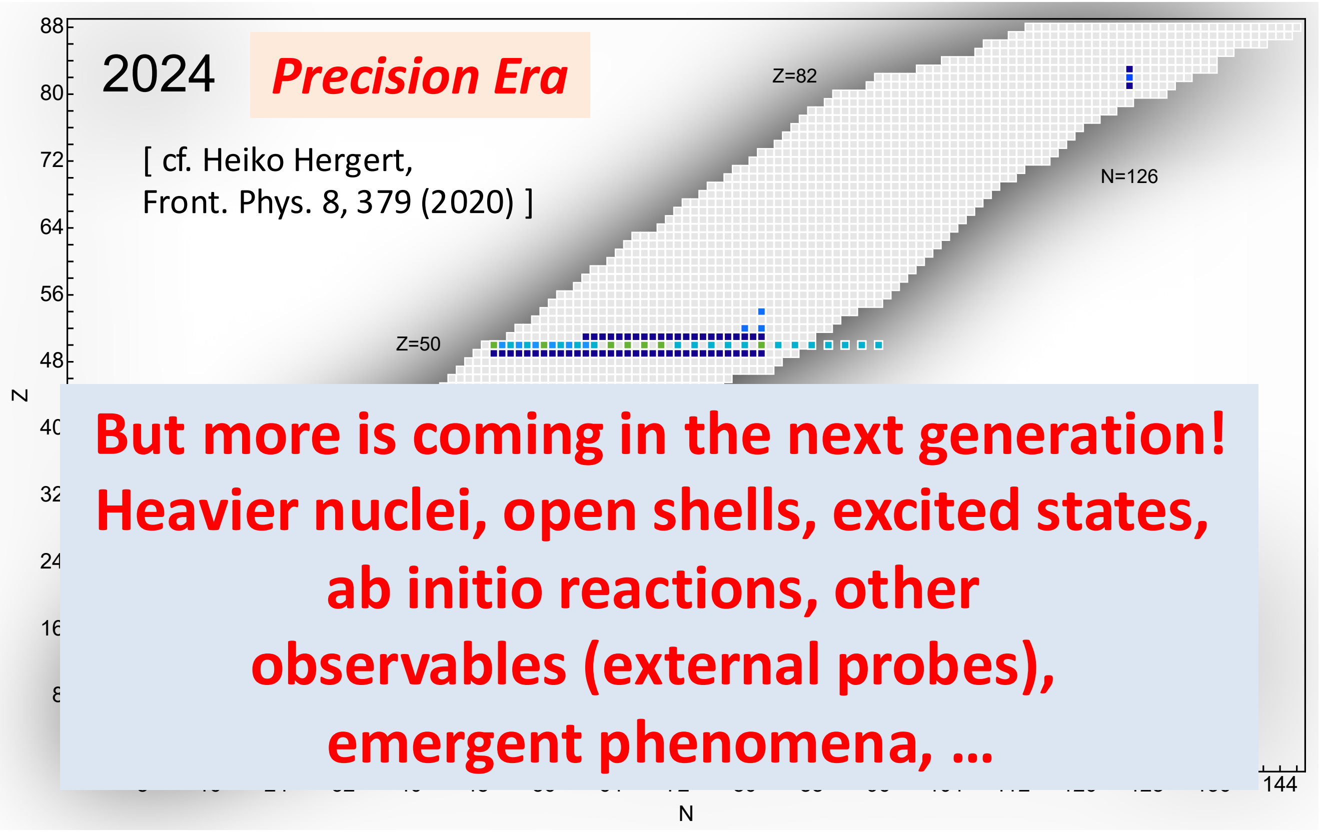


But more is coming in the next generation!
Heavier nuclei, open shells, excited states, ab initio reactions, other observables (external probes), emergent phenomena, …

Enabling factors for current generation ab initio

- Innovative experiment and its analysis
- Large-scale computational resources
- Shared (open source) software
- Large theory collaborations (funded and grass roots)
- Educational efforts (TALENT, ISNET, …) [Frontiers Overviews, …]
- New ideas from young people and from other fields
- Shared information through meetings like these (ECT*, INT, …)

How to ensure these are robust for the next generation?

Goals of the workshop

Foster future breakthroughs in ab initio theory with exchange of ideas

- Stepping up in predictive power and advancing the scope of applications
- Discuss the comparison of current ab initio theory with data and requirements for future applications.

Focus on three frontiers, which are intimately linked together:

1) Next generation many-nucleon interactions and electroweak currents.
2) Principled and robust propagation of uncertainties.
3) Novel many-body methods for nuclear theory.

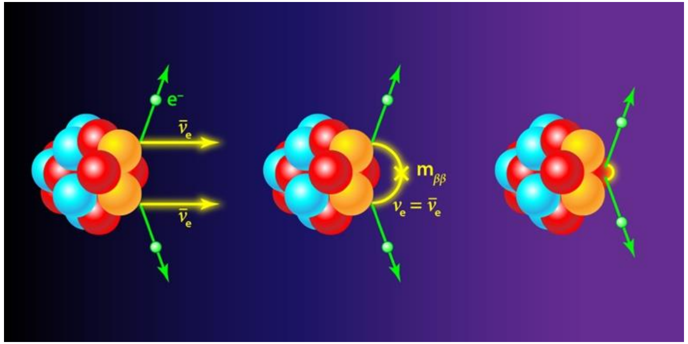
Effective Field Theory (EFT) methods

- Chiral EFT interactions and currents (H. Krebs)
  - Experiments for 3N forces (K. Sekiguchi)
  - Polarization phenomena in 2N and 3N (R. Skibiński)
- Pionless EFT (U. van Kolck)
- Unitarity expansion (H. Griesshammer, A. Kievsky)
- Uncertainty quantification for EFTs (D. Phillips, A. Gerzerlis)

- What is required by "consistent" EFT implementations?
- What interactions and currents (and EFTs) should many-body practitioners use? Are four-body forces needed? Deltas?
- How should we power count at finite density?
- How should we calibrate interactions and currents?

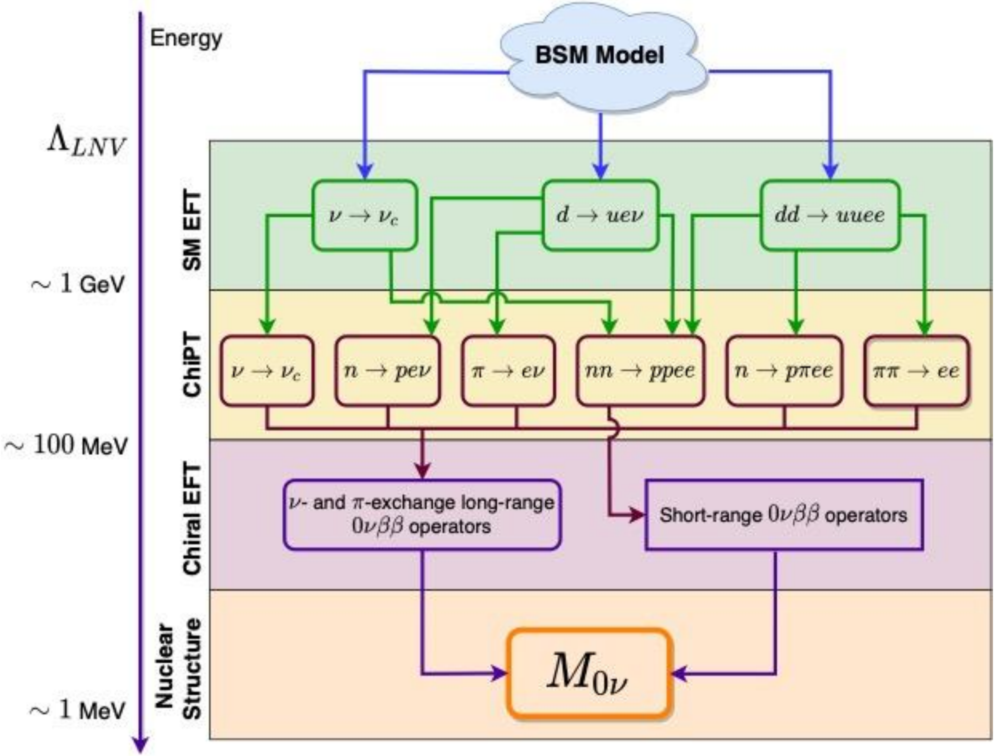
How should we connect to QCD and BSM physics?

Cascade of EFTs for neutrinoless double beta decay



[Cirigliano et al., J. Phys. G (2022)]

Lattice QCD for LECs



What about direct lattice QCD for nuclei? Next-to-next-to-?- generation

Uncertainty quantification: Bayesian inference checklist

Bayesian updating of knowledge

$$\mathrm{pr}(A|B,I) = \frac{\mathrm{pr}(B|A,I)\,\mathrm{pr}(A|I)}{\mathrm{pr}(B|I)} \Longrightarrow \underbrace{\mathrm{pr}(\boldsymbol{\theta}|\mathbf{y}_{\mathrm{exp}},I)}_{\text{posterior}} \propto \underbrace{\mathrm{pr}(\mathbf{y}_{\mathrm{exp}}|\boldsymbol{\theta},I)}_{\text{likelihood}} \times \underbrace{\mathrm{pr}(\boldsymbol{\theta}|I)}_{\text{prior}}$$

- ❑ Incorporate *all* sources of experimental and *theoretical* errors
- ❑ Formulate *statistical models* for uncertainties
- ❑ Use as informative priors as is reasonable; test sensitivity to priors
- ❑ Account for correlations in inputs (type x) and observables (type y)
- ❑ *Properly* propagate uncertainties through the calculation
- ❑ Use *model checking* to validate our models
- ❑ Interact with the experts (i.e., statisticians, applied mathematicians)

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Other frontier topics: multi-model inference, conformal prediction, experimental design, physics *discovery* through statistics, …

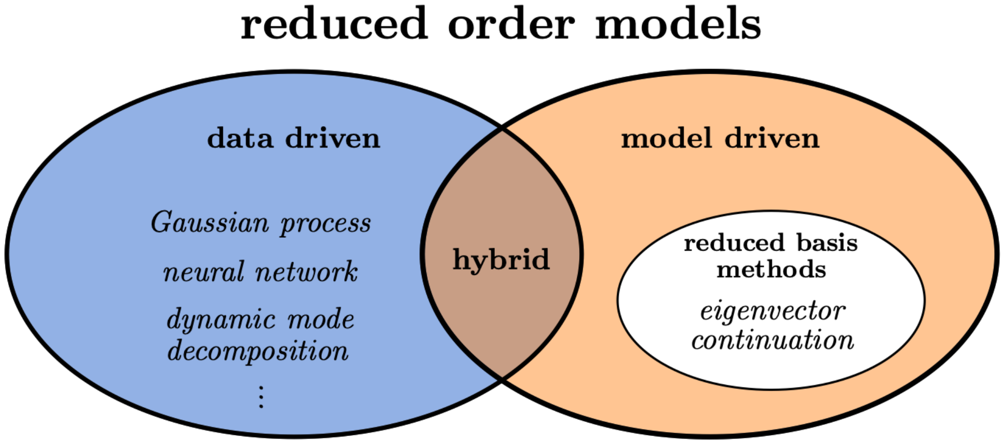
- ❑ *Properly* propagate uncertainties through the calculation
- ❑ Use *model checking* to validate our models
- ❑ Interact with the experts (i.e., statisticians, applied mathematicians)

Emulators

Need: to calculate with different parameters for calibration, UQ.

Exploit: much information in high-fidelity models is superfluous.

Solution: reduced-order model → emulator (fast & accurate™).



- **New technologies:** Parametric matrix models (D. Lee), …
- **Active learning:** Greedy algorithms to choose snapshots (C. Drischler)
- **New applications:** Few-body resonances (S. Koenig), …
- **Neural network emulators:** Light nuclei (A. Gezerlis) and …
- How can we extend the range of emulators for many-body applications?

Machine learning: Neural networks

- Neural network QMC for ab initio structure (Y. Yang)
- Neural quantum states (C. Barbieri)
- Physics-informed ANNs for many-body (L. Brevi)
- Other opportunities?

Emerging technologies for ab initio many-body

- Tensor factorization for ab initio (L. Zurek)
- Diagrammatic Monte Carlo (S. Broli)
- Many-body correlations at polynomial cost (A. Scalesi)
- Quantum formulas for ab initio (T. Otsuka)
- What else?

Ab initio approaches: Next generation

- Present and future of ab-initio (J. Vary, A. Schwenk)
- Low-resolution chiral interactions (P. Arthuis)
- What emergent phenomena can we study with ab initio? (D. Lee)
- In-medium SRG: deformed nuclei and more (H. Hergert)

- Resolving tension: Can we fit to only few-body data and accurately predict the energy and sizes and … of heavier nuclei?
- Is it ok to fine-tune to selected data?
- How far is the reach of the unitary limit in nuclei?
- Can relativistic heavy-ion experiments inform nuclear structure?
- What are the most important calculations for the next generation?

Electroweak physics and nuclear reactions

- Experiments to probe electroweak properties (R. Garcia Ruiz)
- Electrons-for-neutrinos experiments (L. Doria)
- Low-energy electron scattering for exotics (T. Suda)
- QMC for next-generation electroweak experiments (G. King)
- Electroweak radiative corrections (M. Gennari)
- Coupled-cluster theory and ν-nucleus scattering (S. Bacca)
- Electro-scattering on light nuclei and beyond (A. Gnech)
- Beta decays (S. Li Muli, Z. Li)
- Many-body theory for nuclear response (F. Marino)
- Nuclear response and correlations (A. Porro)
- QMC for dynamical pions and nucleons (L. Madeira)
- Ab initio reactions (J. Linares Fernandez)

To the speakers

- Look to the future in your talk: *next generation* tools and calculations!
- Emphasize innovative (potentially game changing) aspects.
- Make clear what you see as the opportunities and open challenges.
- Please keep your talk to 25 minutes to allow 10 minutes for discussion.

To the audience

- Critically discuss opportunities and challenges.
- Ask challenging (but respectful!) questions.
- Tell the organizers about topics for further (afternoon) discussion.

Thank you!