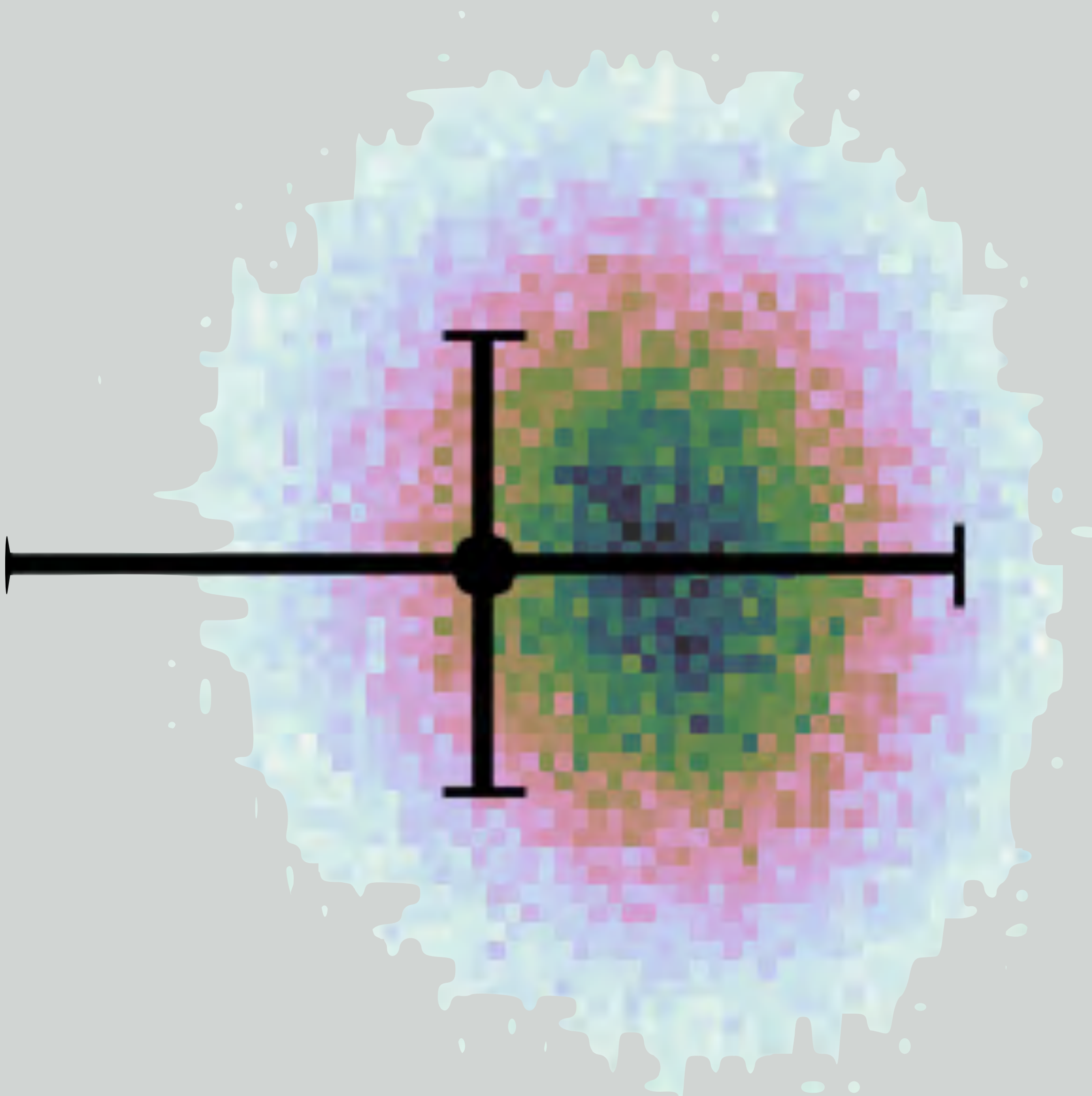


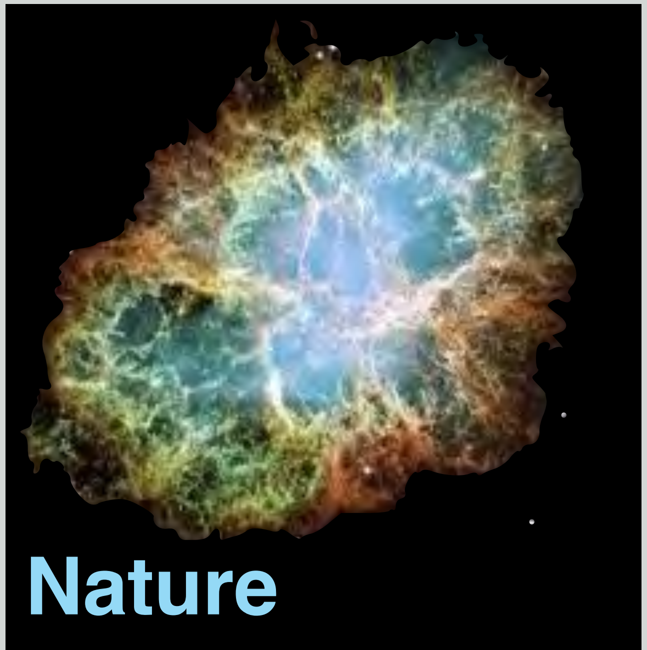
NUCLEAR FORCES AND THEORETICAL UNCERTAINTIES

CHRISTIAN FORSSÉN

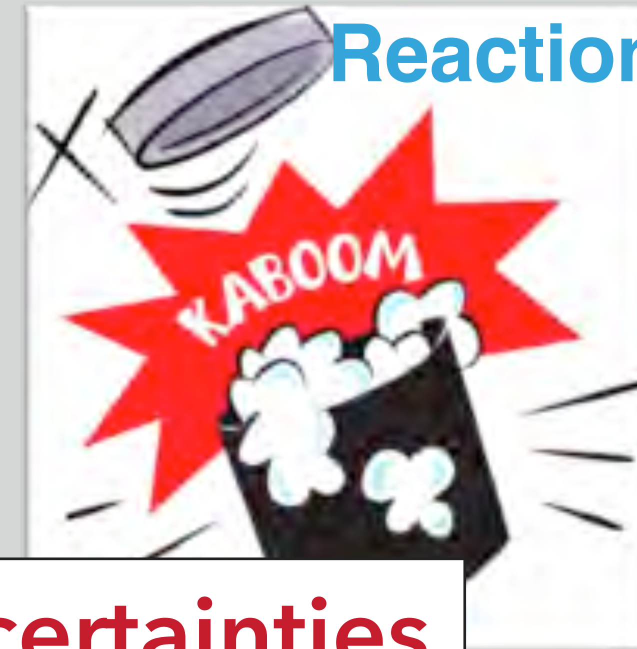
Department of Physics, Chalmers University of Technology, Sweden

NUSTAR annual meeting, GSI, Darmstadt, March 2, 2017

The scientific method



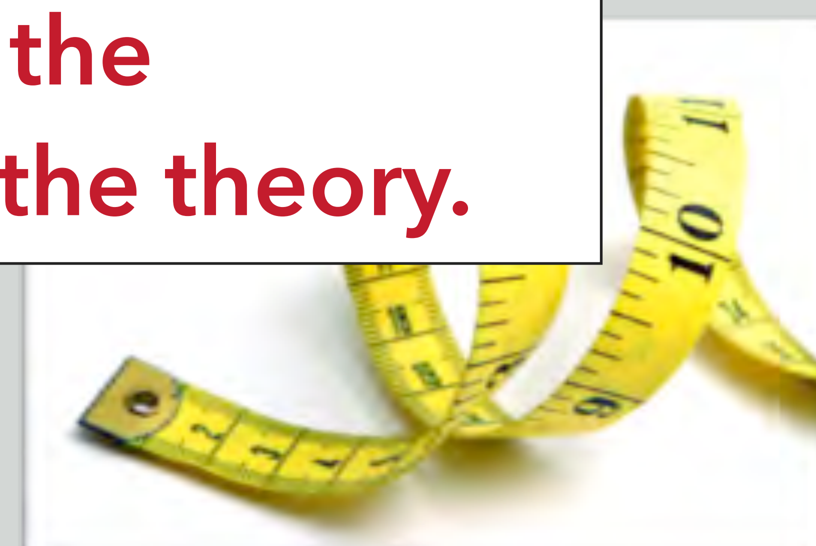
Manifests itself in

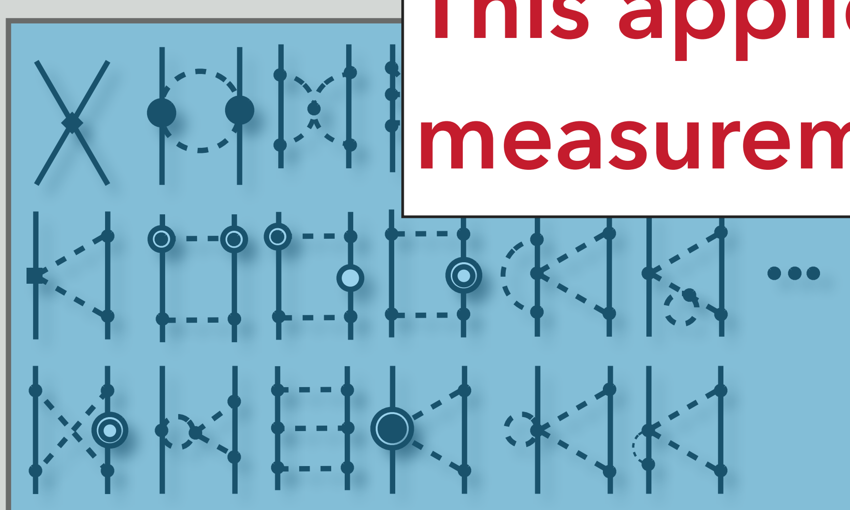


Reactions

accessible to

The quantification of uncertainties is absolutely critical for progress. This applies BOTH to the measurement and to the theory.





inspire

Theories

AB INITIO NUCLEAR PHYSICS – NUCLEONIC DEGREES OF FREEDOM

OUR AIM: A credible program for uncertainty quantification in nuclear theory

- Start from nucleonic degrees of freedom and construct an effective inter-nucleon force.

  Connection with QCD

  σ_{model}

- This force will have to be constrained by data.

  σ_{data}

  REALISTIC INTERACTIONS: NN scattering data reproduced

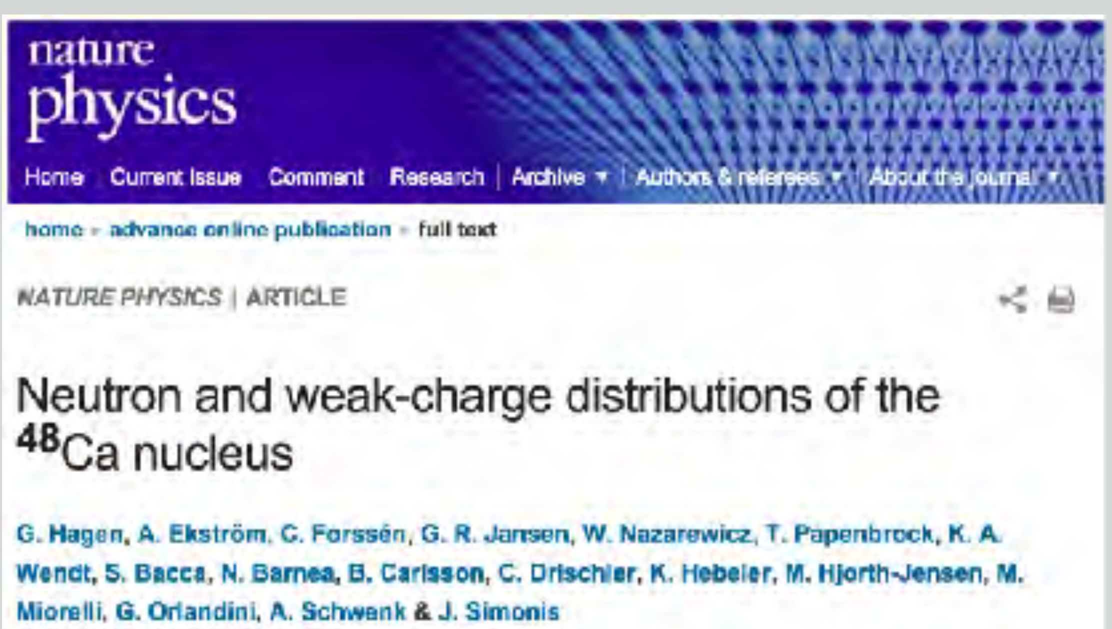
- Solve the few- or many-nucleon problem and compute observables.

  AB INITIO many -body methods

  $\sigma_{\mathrm{num+method}}$

AB INITIO APPROACHES

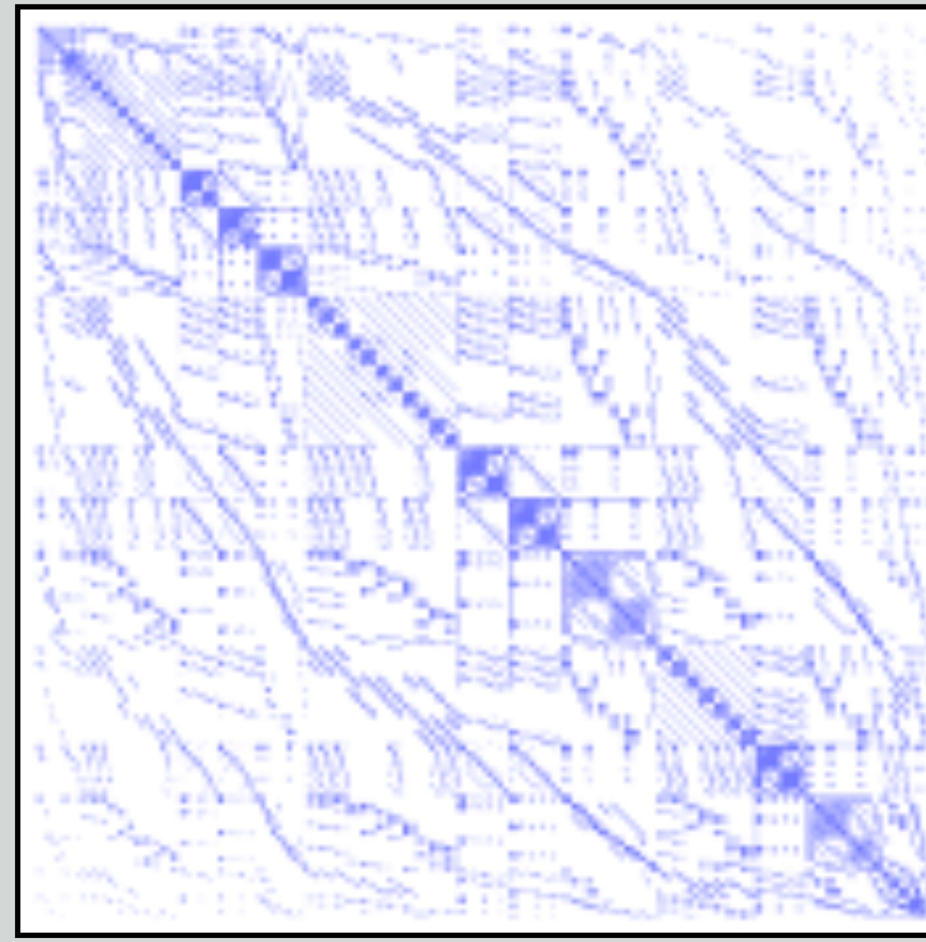
- Consider an A-nucleon system described by a well defined microscopic Hamiltonian
- *Ab initio* methods solve the relevant QM many-body equations without uncontrolled approximations
- Controlled approximations, e.g. number of channels, are allowed since they can be systematically improved.
- Converged results are considered precise *ab initio* results.
- *Ab initio* methods: No-Core Shell Model, Coupled clusters, Green's function Monte Carlo, In- Medium SRG, Lattice EFT

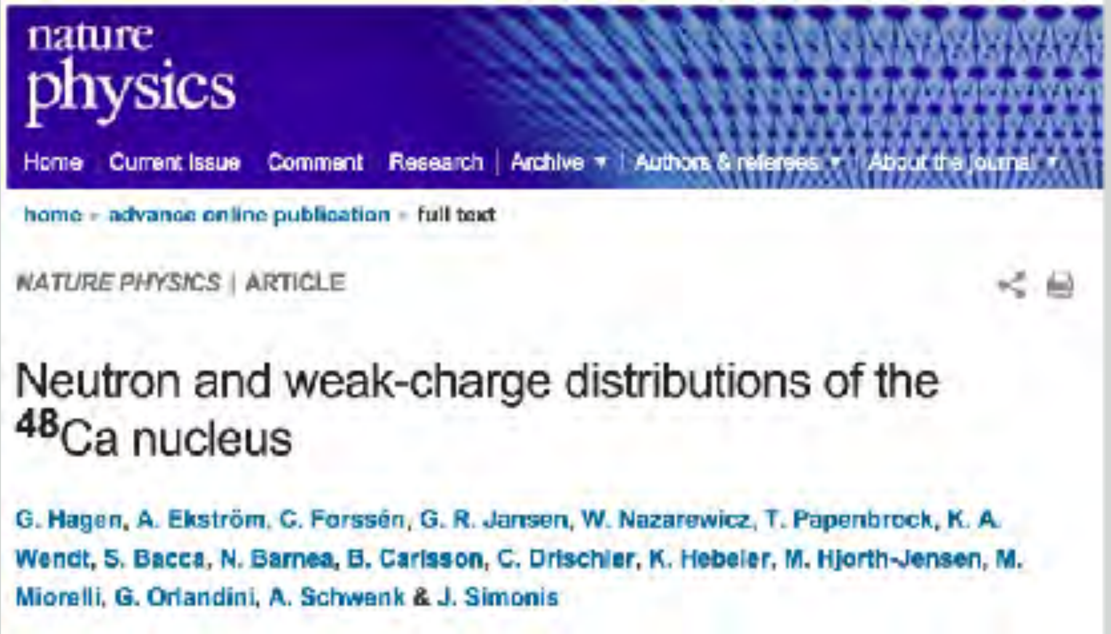


AB INITIO APPROACHES

TECHNOLOGY EXAMPLE: LARGE-SCALE MATRIX DIAGONALIZATION

- Current limit: $N_{dim} = 10^{10}$
- Sparse, BUT: $N_{non\text{-}zero}=5\times10^{14}$, equivalent to 6 PB data
- In effect, we perform 2.5×10^{9} multiplications / sec / machine





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NATURE PHYSICS | ARTICLE

Neutron and weak-charge distributions of the ^{48}Ca nucleus

G. Hagen, A. Ekström, C. Forssén, G. R. Jansen, W. Nazarewicz, T. Papenbrock, K. A. Wendt, S. Bacca, N. Barnea, B. Carlsson, C. Drischler, K. Hebeler, M. Hjorth-Jensen, M. Miorelli, G. Orlandini, A. Schwenk & J. Simonis

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Archive › Volume 528 › Issue 7580 › Letters › Article

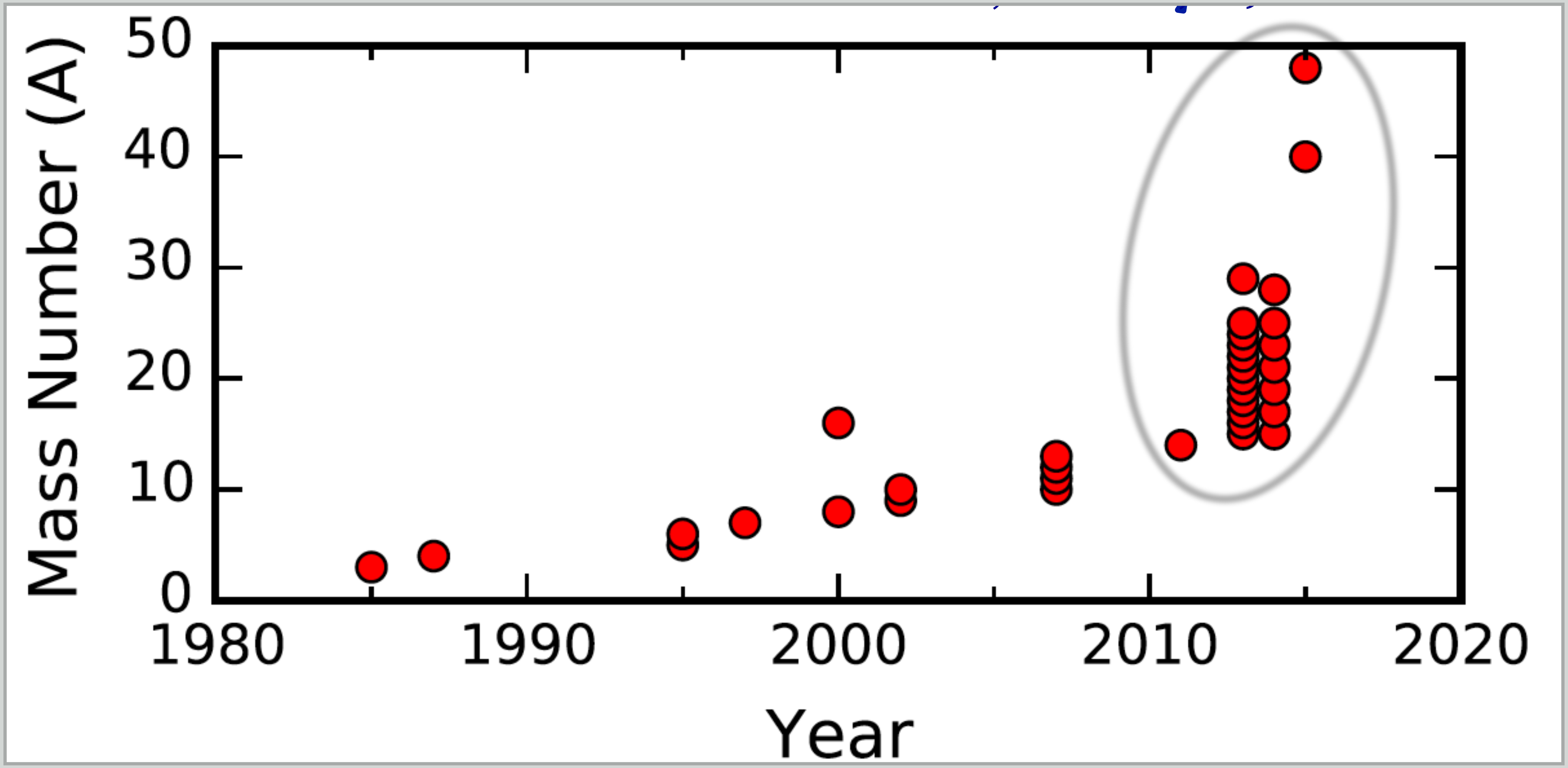
NATURE | LETTER

日本語要約

Ab initio alpha–alpha scattering

Serdar Elhatisari, Dean Lee, Gautam Rupak, Evgeny Epelbaum, Hermann Krebs, Timo A. Lähde, Thomas Luu & Ulf-G. Meißner

TREND IN REALISTIC AB INITIO CALCULATIONS



"Computational capabilities exceed accuracy of available interactions "

[Binder et al, Phys. Lett. B 736 (2014) 119]

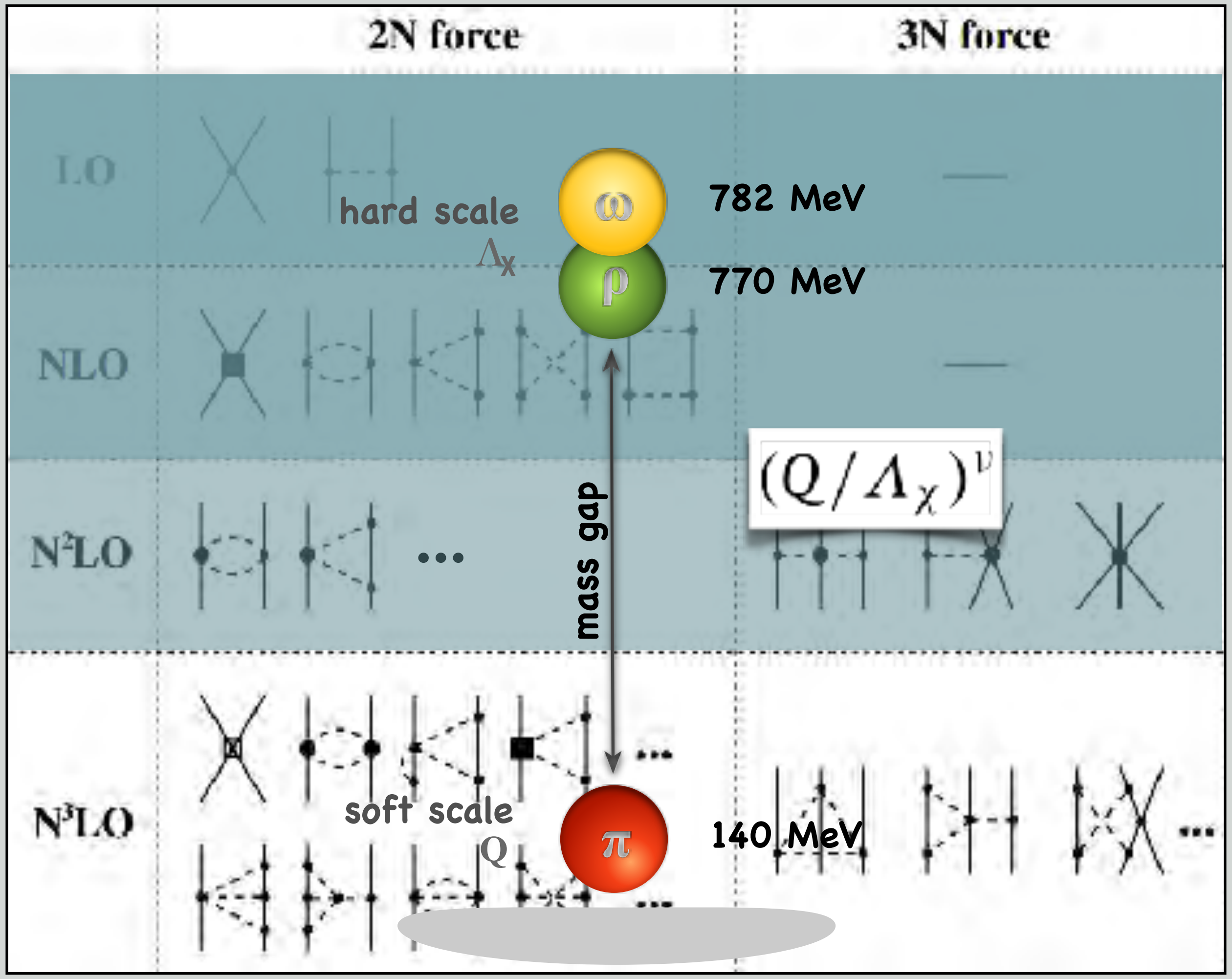
EFFECTIVE THEORIES

- Utilize a separation of scales.
- Long distance solved explicitly (e.g. known symmetries); short-distance unresolved – capture in LECs.
- Power counting; expansion parameter(s) – e.g., ratio of scales.

CHIRAL EFFECTIVE FIELD THEORY

Chiral EFT

- Systematic low-energy expansion: $(Q/\Lambda_\chi)^\nu$
- Connects several sectors: πN, NN, NNN, j_N
- Short-range physics included as contact interactions.
- LECs need to be fitted to data.



Chiral EFT

- E. Epelbaum, H. Hammer, U. Meissner Rev. Mod. Phys. **81** (2009) 1773
- R. Machleidt, D. Entem, Phys. Rep. **503** (2011) 1

FRONTIERS IN LOW-ENERGY NUCLEAR PHYSICS (AB INITIO THEORY)

New territory frontier

- Heavier systems
- Away from closed shells
- Hypernuclei

Continuum frontier

- Approaching the drip lines
- Unified theory of structure and reactions

Precision and accuracy frontiers

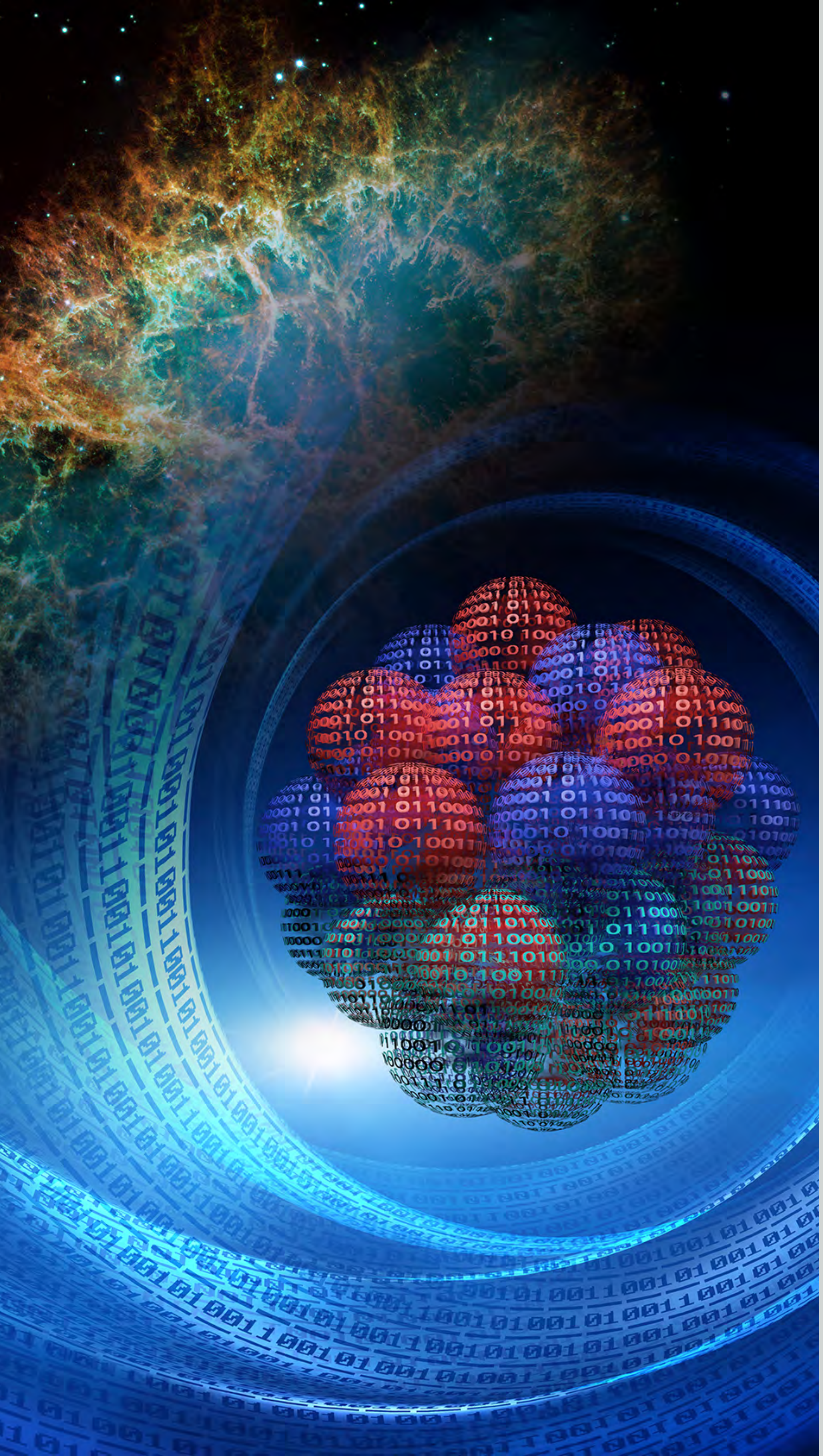
- Accurate results
- Precise results:
  - Uncertainty quantification, Error propagation

Service frontier

- Deliver reliable input to other communities
- Cross sections, masses, etc ($0\nu\beta\beta$, dark matter, astrophysics processes, ...)

Technology frontier

- New computational hardware
- Algorithms, applied mathematics



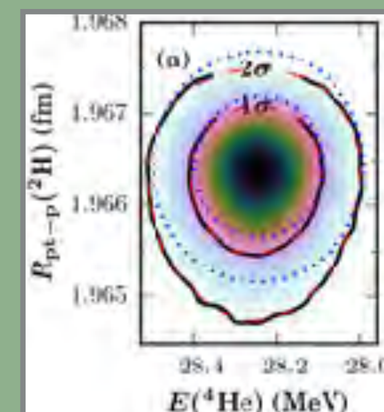
THE ACCURACY AND PRECISION FRONTIER

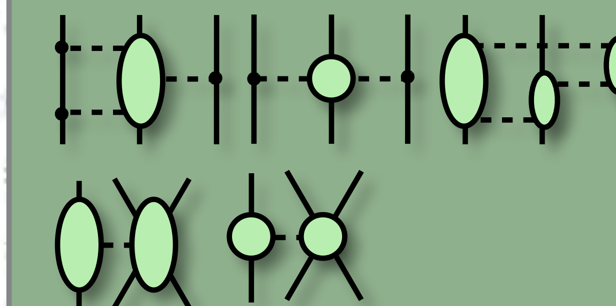
Overview of our research efforts

We aim to develop the technology and ability to:

- **Does nuclear-physics phenomena emerge in a "from few to many" ab initio approach?**
- **Is available few-body data sufficient to constrain this model? Does the model become fine-tuned?**

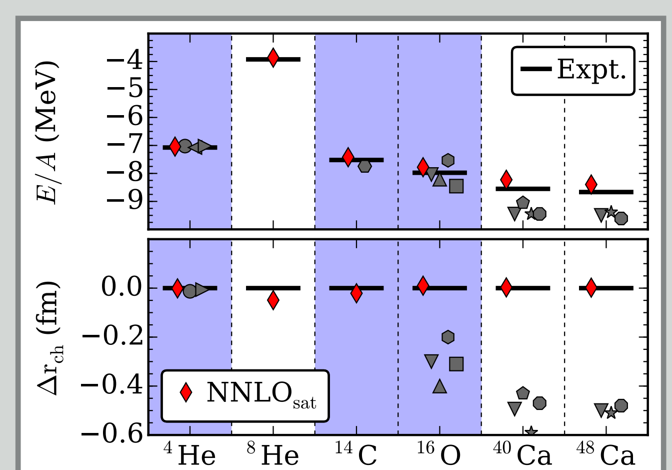
Diversify and extend the **statistical analysis** of chiral-EFT based nuclear interactions in a **data-driven** approach.

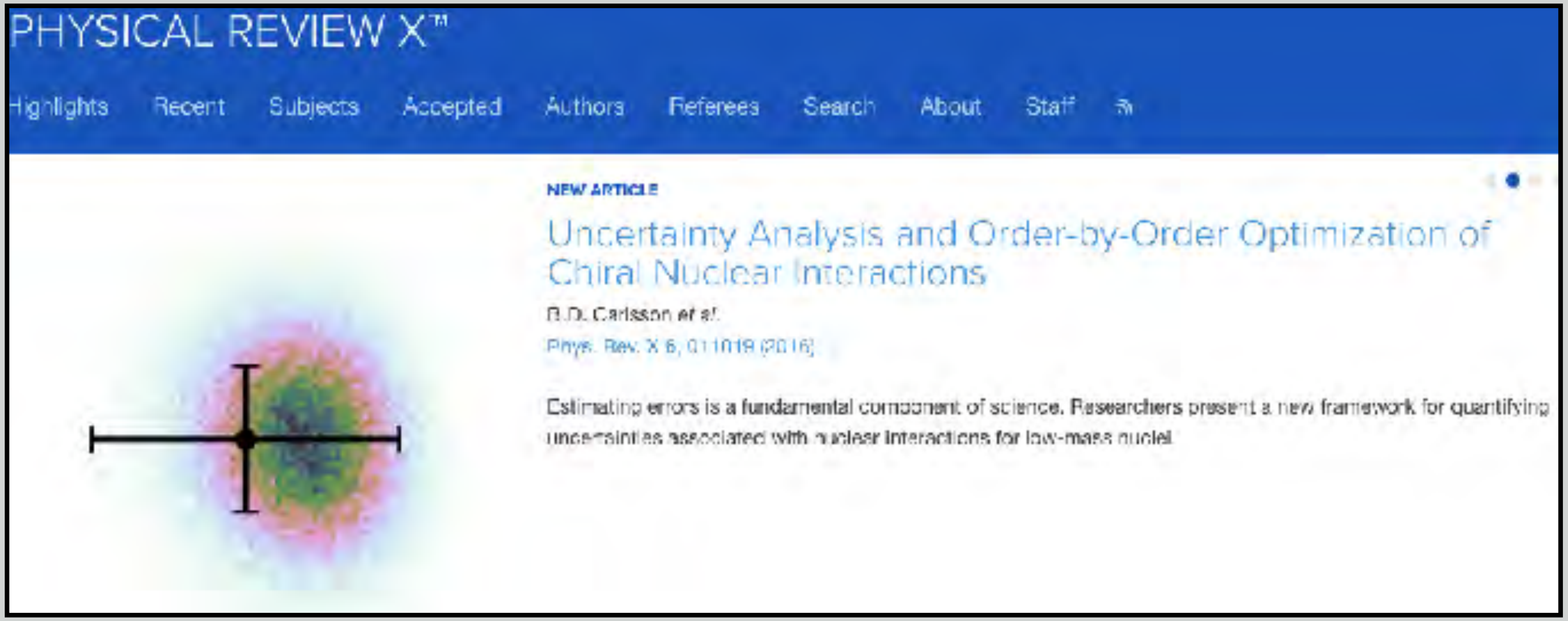




- **Can/should emergent phenomena be used to constrain the model?**
- **How to quantify systematic uncertainties in such an approach?**

Explore **alternative strategies of informing** the model about low-energy many-body observables.





THEORETICAL UNCERTAINTY QUANTIFICATION

Ab initio nuclear physics with χEFT and error analysis

Optimization strategy

Low-energy constants (LECs) enter through contact interactions and need to be fitted to experimental data.

$$\chi^2(\vec{p}) \equiv \sum_i \left(\frac{O_i^{\text{theo}}(\vec{p}) - O_i^{\text{expr}}}{\sigma_{\text{tot},i}} \right)^2 \equiv \sum_i r_i^2(\vec{p})$$

Optimization

- **Standard approach:** sequential, chi-by-eye optimization; fits to phase shifts; N^3LO needed for high-accuracy fit up to T_{lab}=290 MeV.
- From 2013: **Optimization technology** significantly improved.
- From 2015: Fits to **experimental data including uncertainties**.
- From 2016: **Algorithmic Differentiation (AD)** to get precise derivatives.

Input and technology

πN scattering
- WI08 database
- T_{lab} between 10-70 MeV
- N_{data} = 1347
- χEFT(Q^4) to avoid underfitting

NN scattering
- SM99 database
- T_{lab} between 0-290 MeV
- N_{data} = 2400(np) + 2045(pp)
- χEFT(Q^0,Q^2,Q^3)

All 6000 residuals computed on 1 node in ~90 sec.

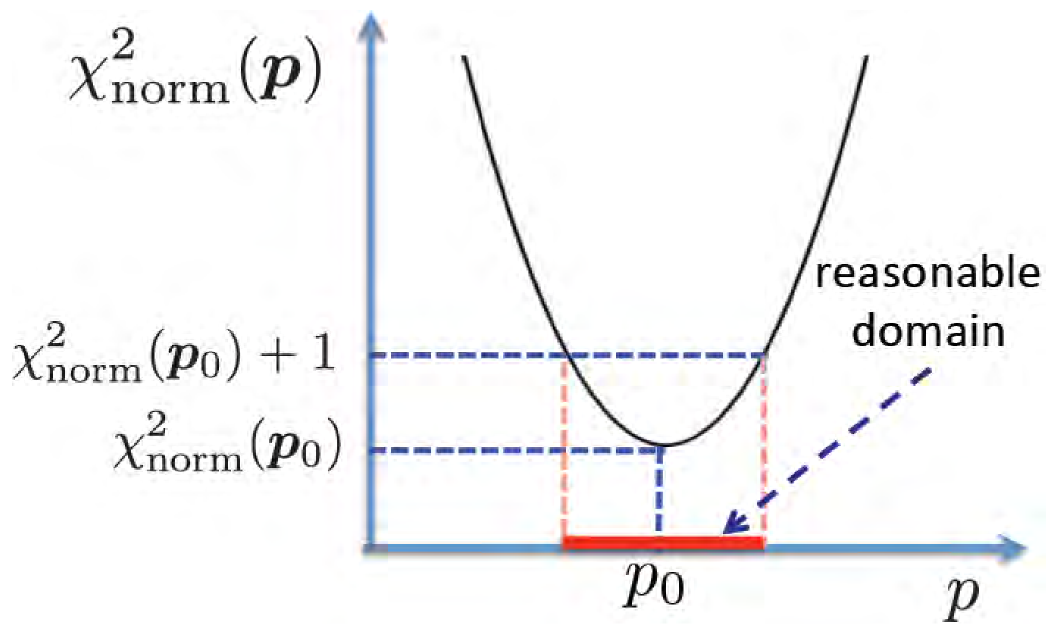
A=3 bound states
- ^{3}H,^{3}He (binding energy, radius, ^{3}H half life)

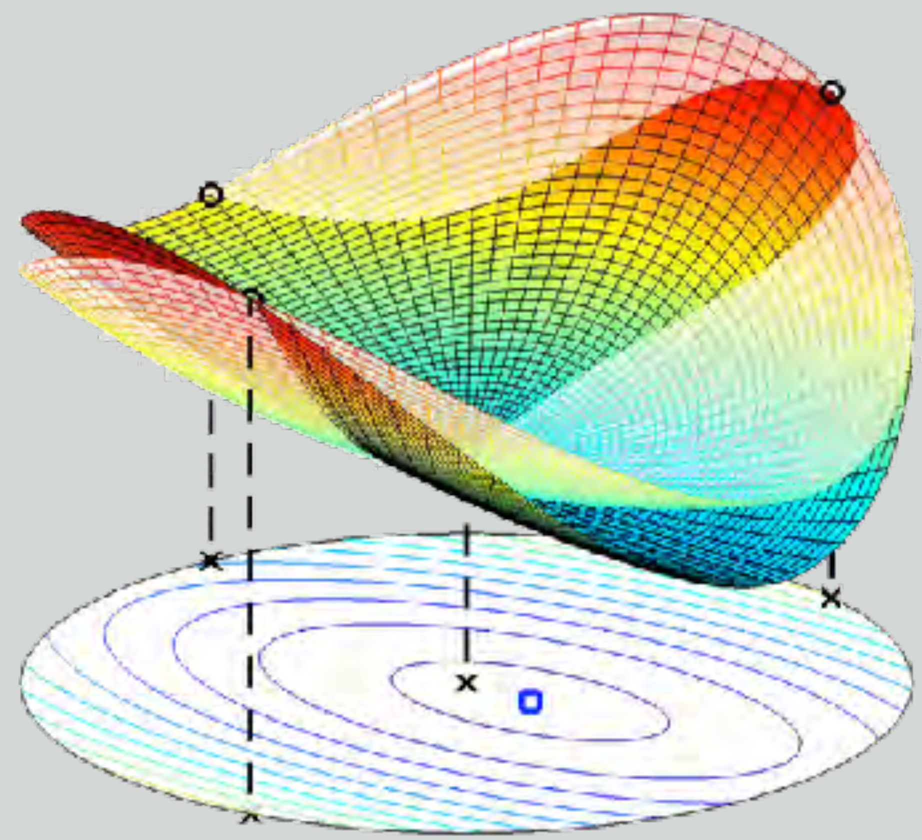
On 1 node in ~10 sec

+ derivatives! (×2-20 cost)

Statistical error analysis

- In a minimum there will be an **uncertainty in the optimal parameter values $\mathbf{p}_0$** given by the χ^2 surface.[1]





- From the hessian at $\mathbf{p}_0$ we can calculate a **covariance matrix** and from that a **correlation matrix**.

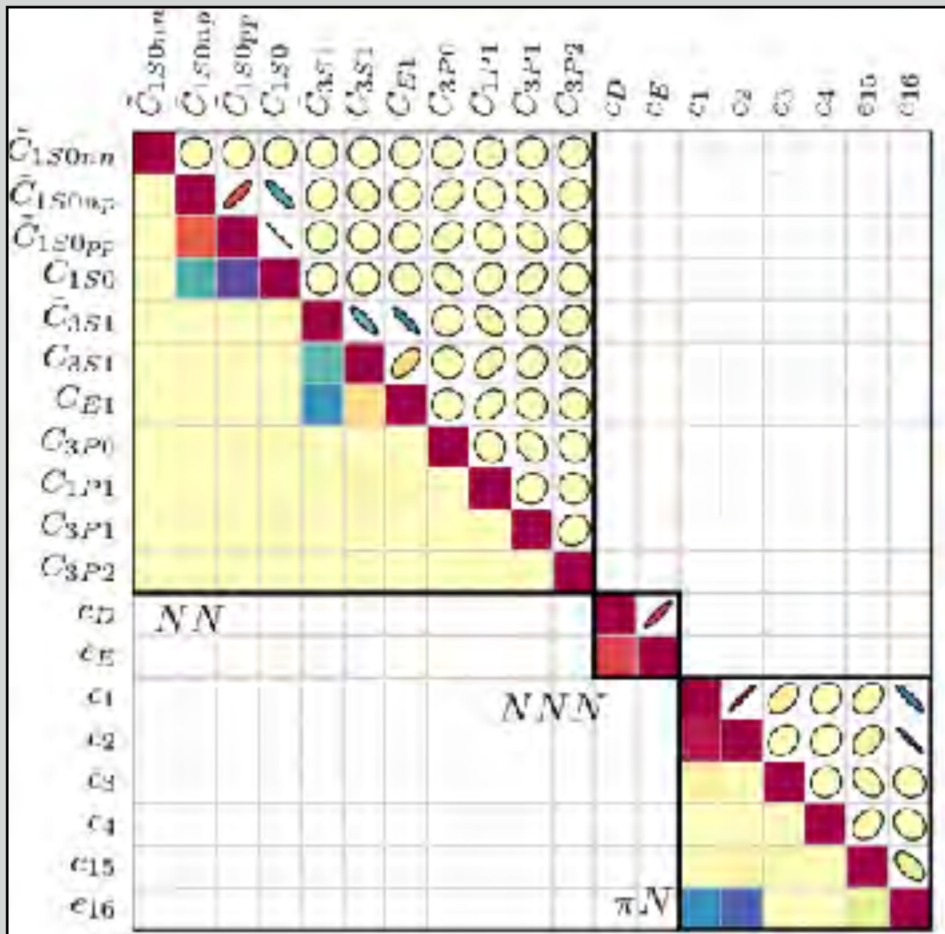
[1] J Dobaczewski et al 2014 J. Phys. G: Nucl. Part. Phys. 41 074001

HESSIAN	COVARIANCE MATRIX	CORRELATION MATRIX
$H_{ij} = \frac{1}{2}\left.\frac{\partial^2\chi^2}{\partial x_i \partial x_j}\right\|_{\mathbf{x}=\mathbf{x}_\mu}$	$\mathbf{\Sigma} = \frac{\chi^2}{N_{df}}\mathbf{H}^{-1}$	$R_{ij} = \frac{\Sigma_{ij}}{\sqrt{\Sigma_{ii}\Sigma_{jj}}}$

Sequential optimization

$$\chi^2(\vec{p}) \equiv \sum_i r_i^2(\vec{p}) = \sum_{j\in NN} r_j^2(\vec{p}) + \sum_{k\in \pi N} r_k^2(\vec{p}) + \sum_{l\in 3N} r_l^2(\vec{p})$$

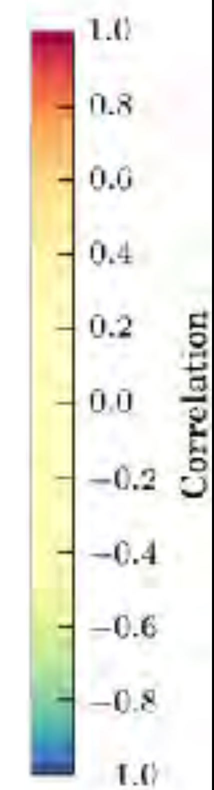
2 **1** **3**



Sequential fit

By construction no correlations between πN, NN, NNN groups of parameters.

This will imply huge statistical errors.



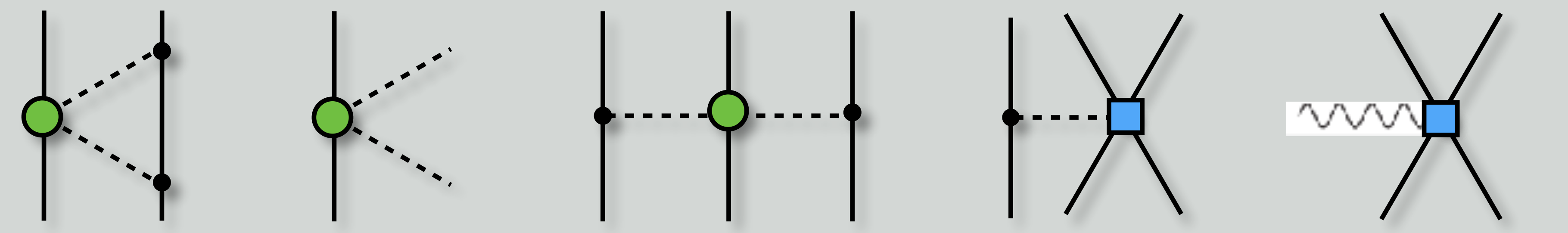
Simultaneous optimization

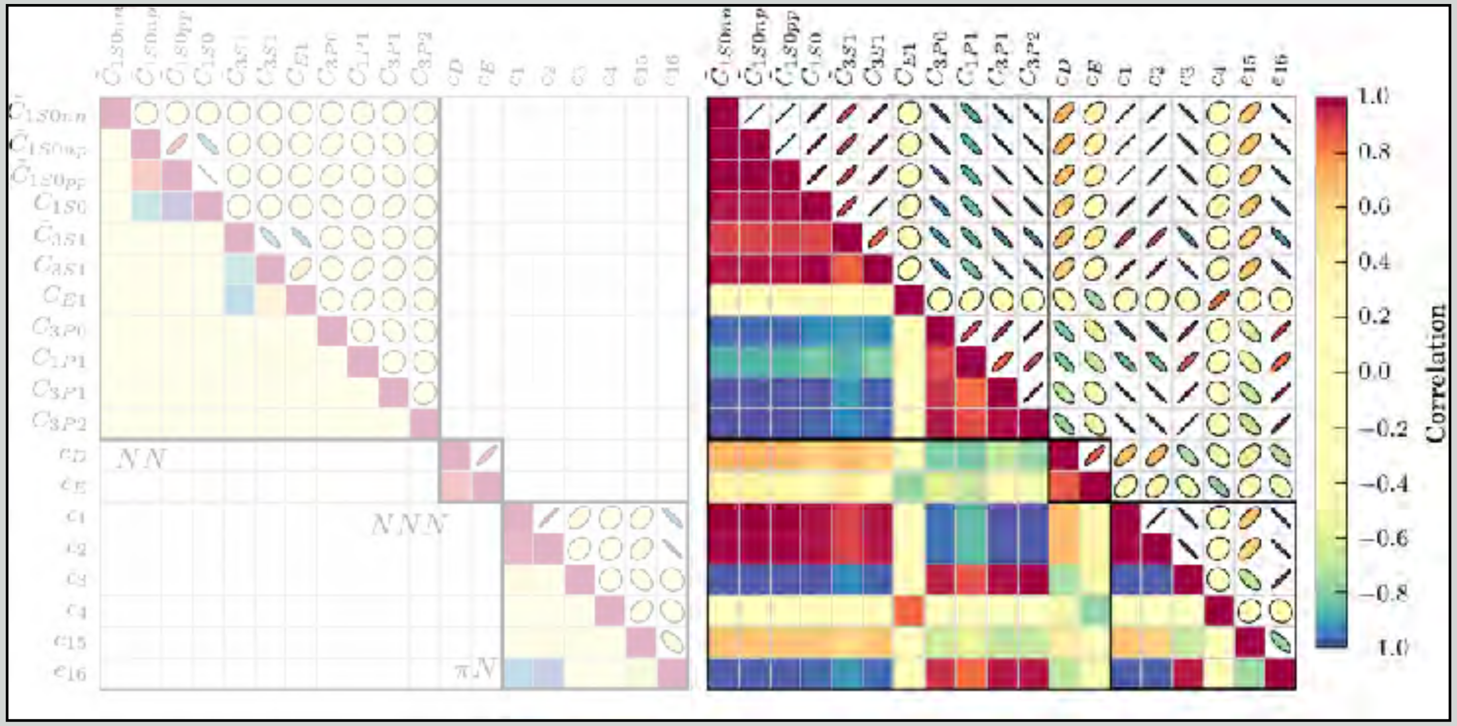
$$\chi^2(\vec{p}) \equiv \sum_i r_i^2(\vec{p}) = \sum_{j\in NN} r_j^2(\vec{p}) + \sum_{k\in \pi N} r_k^2(\vec{p}) + \sum_{l\in 3N} r_l^2(\vec{p})$$

Simultaneous

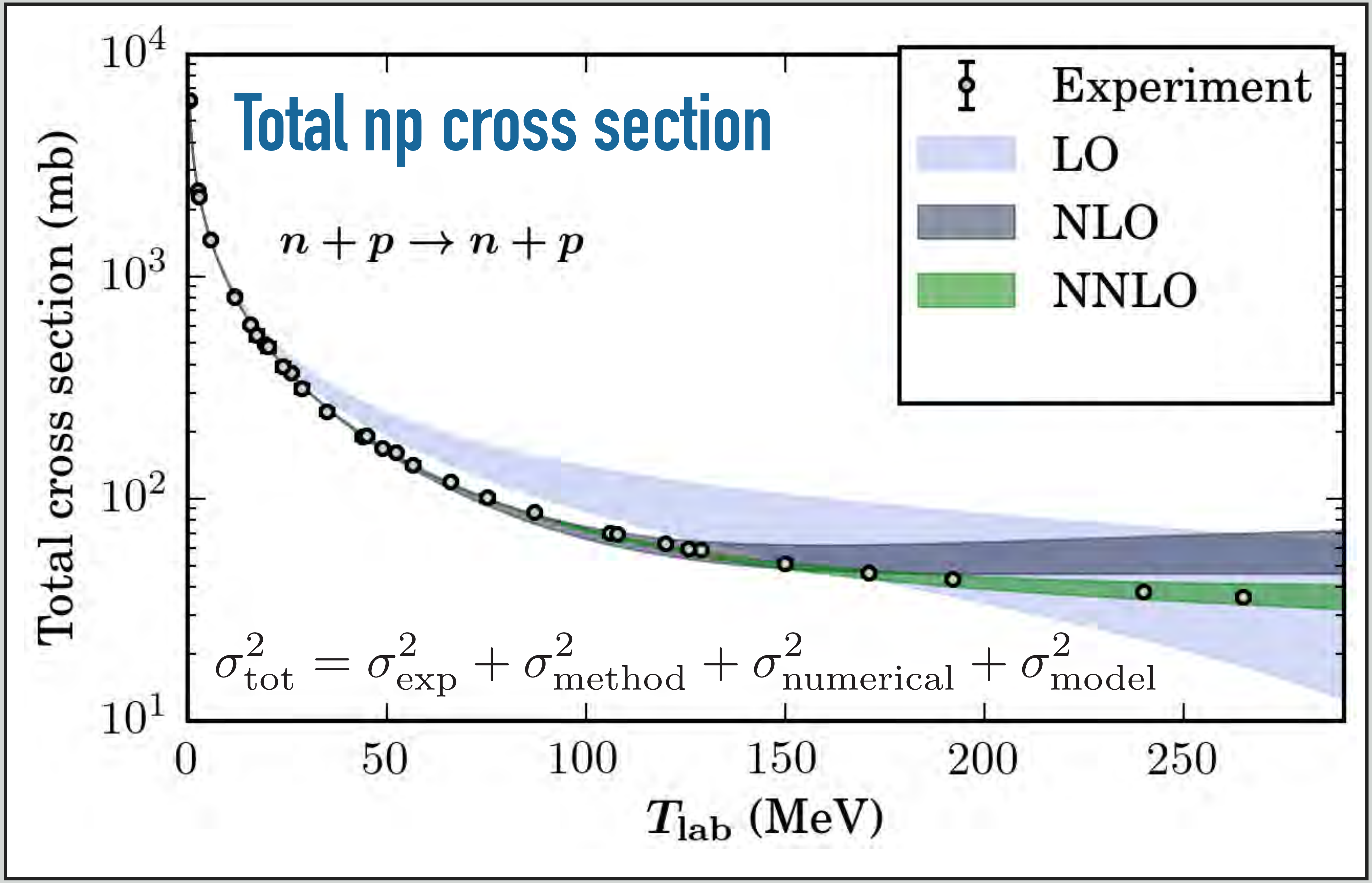
BUT, the same LECs appear in the expressions for various low-energy processes

- e.g. the c_i (green dot)
- and c_D (blue square)



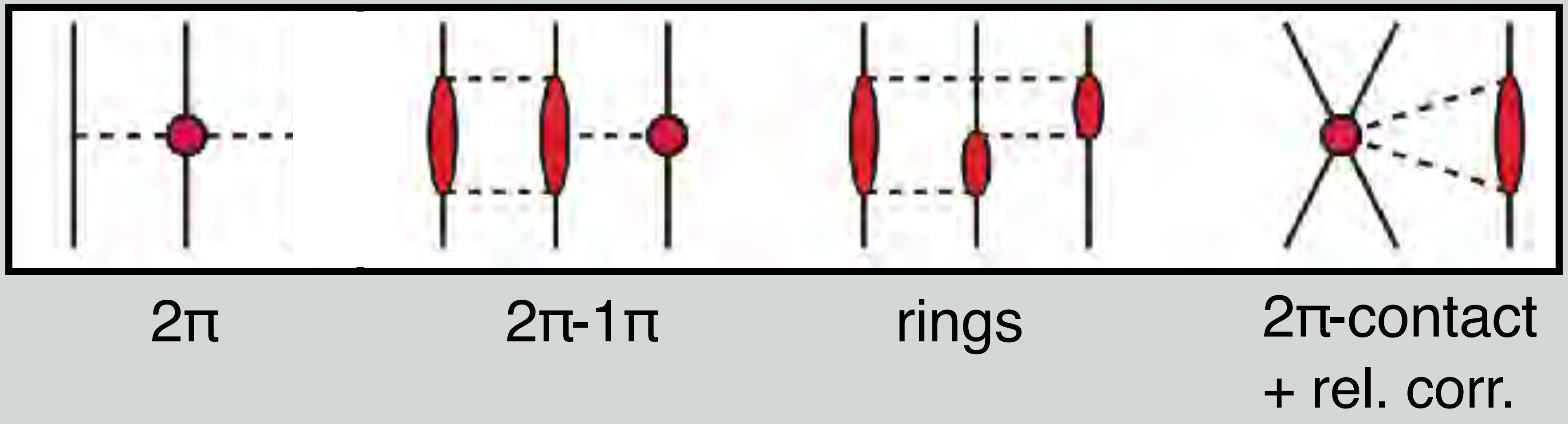


Order-by-order convergence

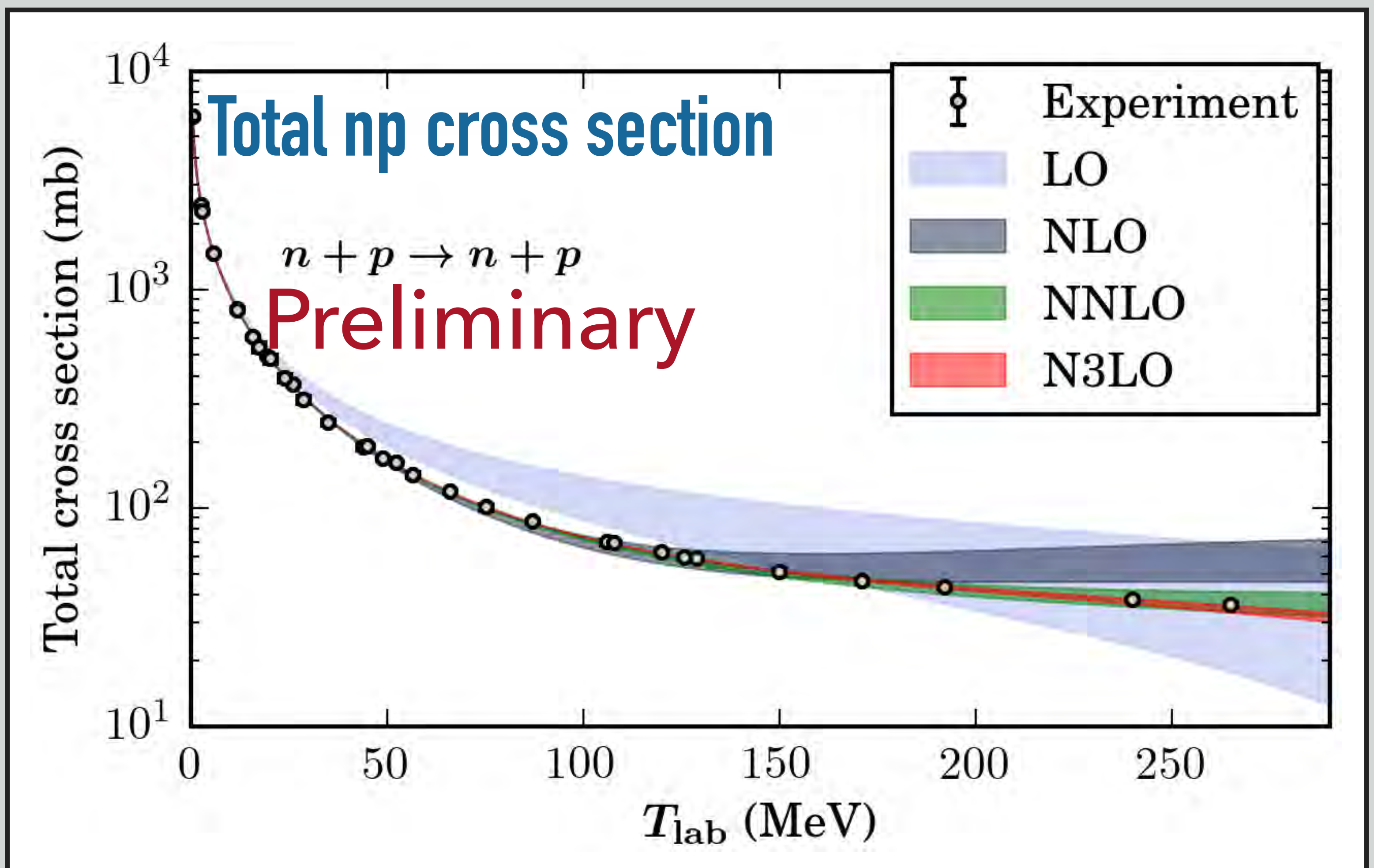


Order-by-order convergence

N3LO optimizations are challenging



41 parameters to optimize,
No new parameters in the three-nucleon force.
3NF matrix elements recently made available (K. Hebeler)



@N3LO:

- at least 100 minima
- all with a good description of πN, NN, NNN data

Possible solutions:

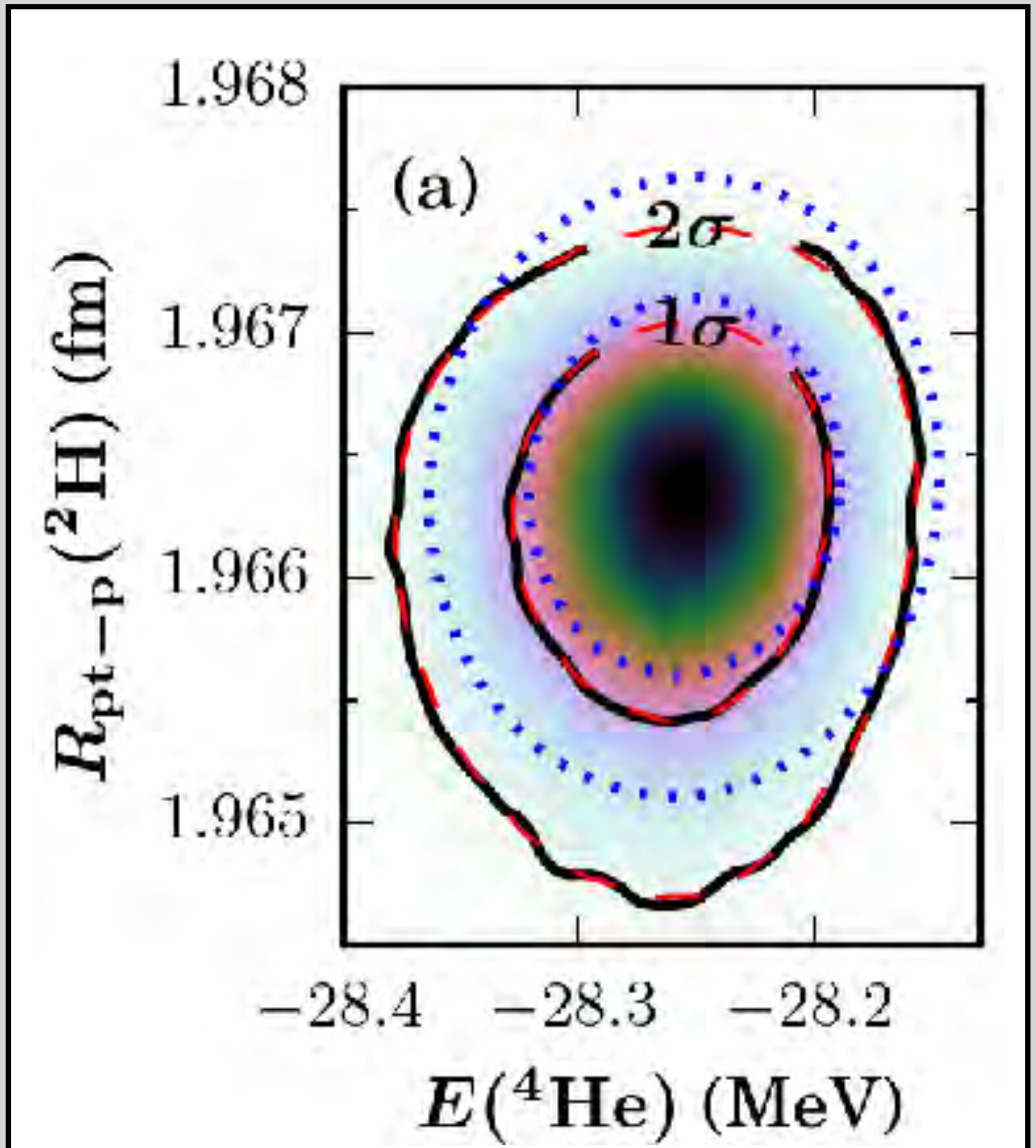
- Additional data… NNN scattering,
- Additional data… Heavier systems
- Bayesian statistics…

are all **computationally very costly**

Uncertainty quantification in the few-body sector

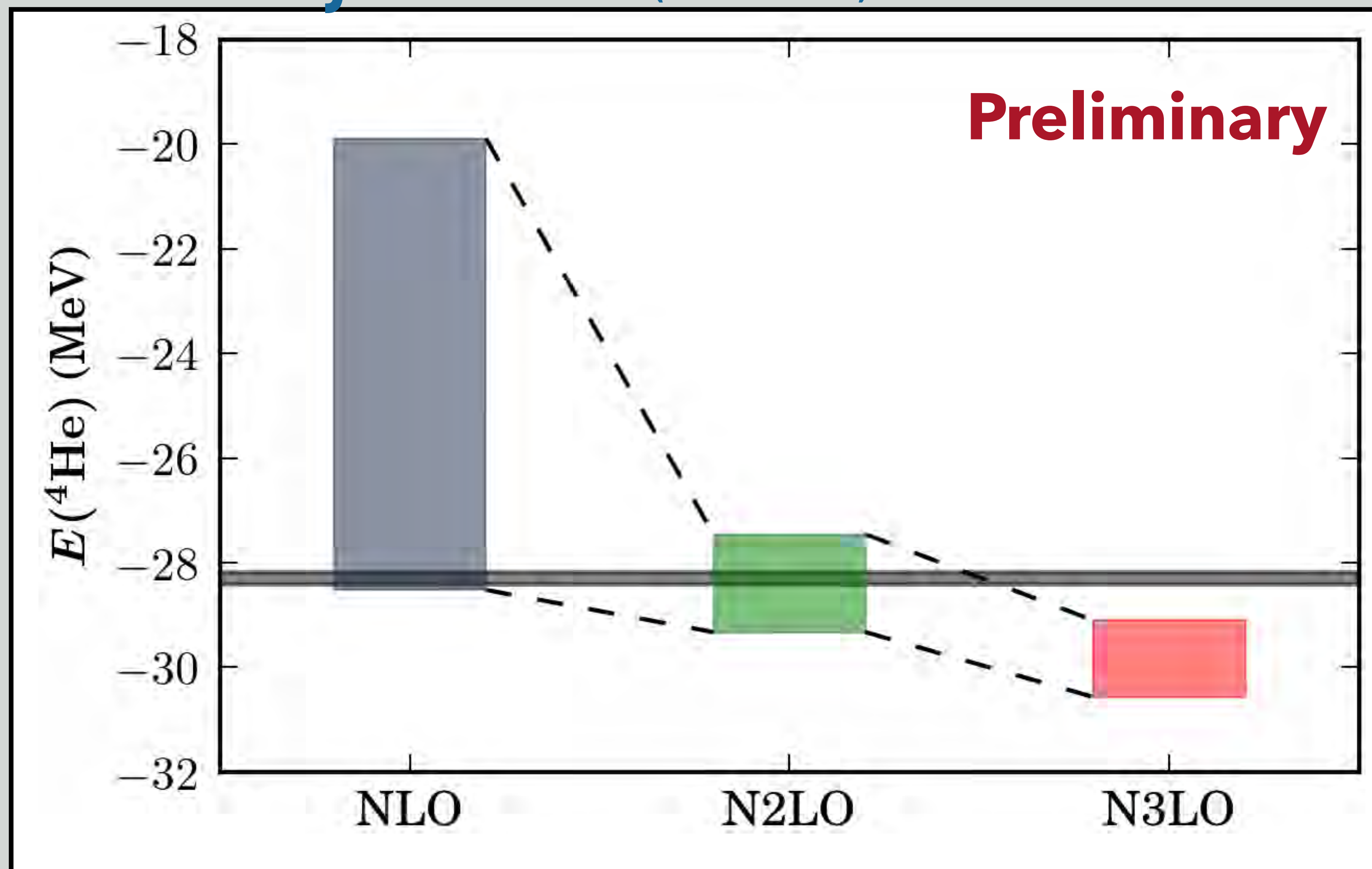
Statistical error propagation

$$O(\mathbf{p}) \approx O(\mathbf{p}_0) + J_O \Delta\mathbf{p} + \frac{1}{2}\Delta\mathbf{p}^T H_O \Delta\mathbf{p}$$



$E(^4He) = -28.24^{+9}_{-11}$ (MeV)

Systematic (model) error estimate



Bands indicate effects of cutoff variation and different truncations in the NN database.

Conclusion

OUTLOOK

We’re in a golden age for low-energy nuclear physics theory

- EFT and RG have become important tools for precision when combined with ab initio many-body methods.
  Finally – rapid progress on theoretical uncertainty quantification!
- Synergies of analytic theory, computation, and experiment.
- How accurate can we make our Hamiltonians?
- The use of advanced computational methods and new technologies are key for progress.
- Stay tuned!

We’re entering the era of *precision nuclear physics*!

Many thanks to my collaborators

- **Boris Carlsson**, **Andreas Ekström**, Daniel Gazda, Håkan Johansson, Emil Ryberg, Daniel Sääf (Chalmers)
- Gustav Jansen, Gaute Hagen, Thomas Papenbrock (ORNL/UT)
- Morten Hjorth-Jensen (MSU/UiO), Witek Nazarewicz (MSU)
- Kai Hebeler, Achim Schwenk, Kyle Wendt (TU Darmstadt)

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"UNCERTAINTY IS AN UNCOMFORTABLE POSITION. . . ." BUT CERTAINTY IS AN ABSURD ONE."

Voltaire