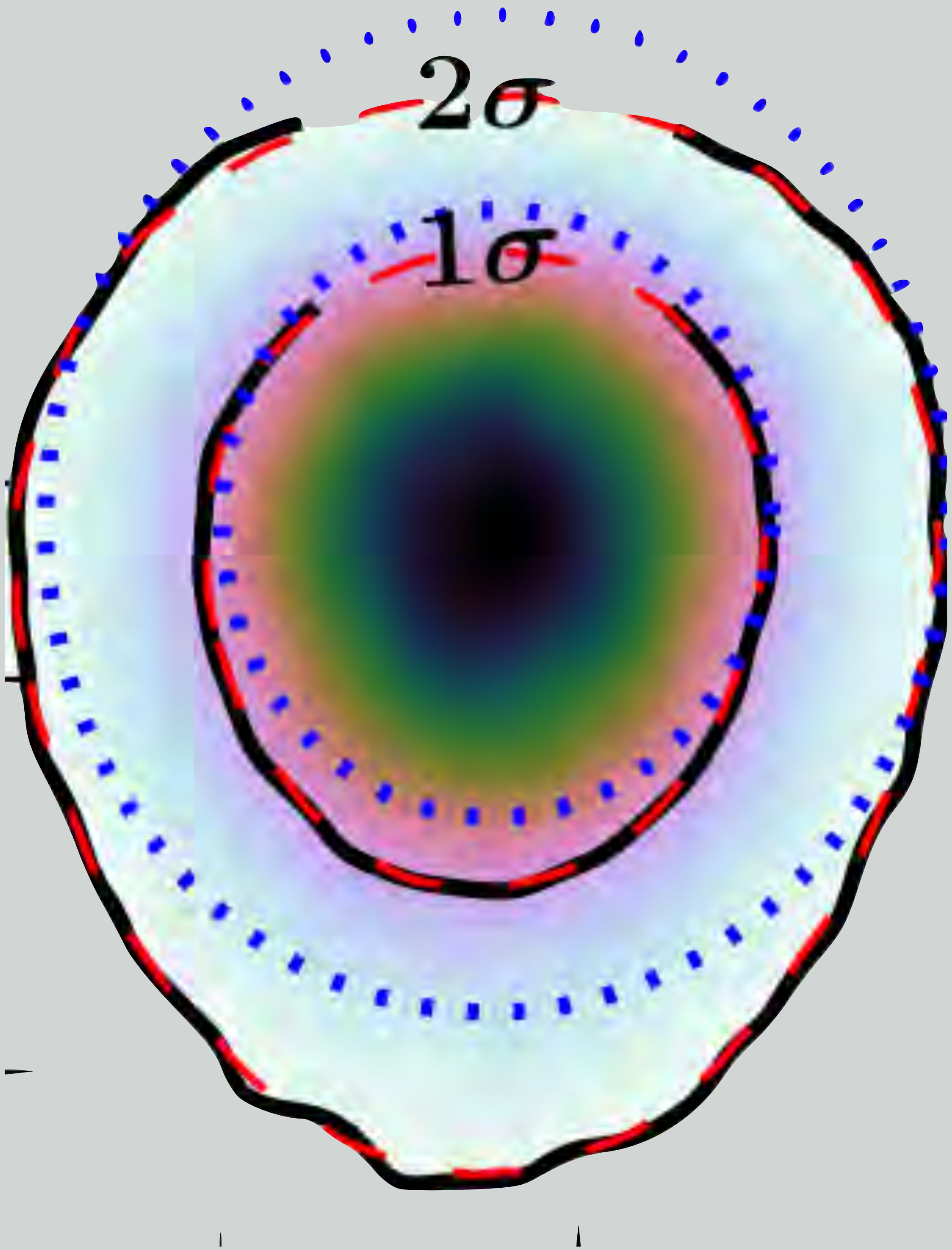


THEORETICAL UNCERTAINTY QUANTIFICATION AND PRECISION NUCLEAR PHYSICS

CHRISTIAN FORSSÉN

Department of Physics, Chalmers University of Technology, Sweden

FUSTIPEN workshop, GANIL, France, Mar. 14-18, 2016

INTRODUCTION

Uncertainty quantification in ab initio nuclear theory

Ab initio nuclear physics - Nucleonic degrees of freedom

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

σ_{model}

AIM: Connection with underlying theory

- 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 METHODS: NCSM, CC, IM-SRG, …

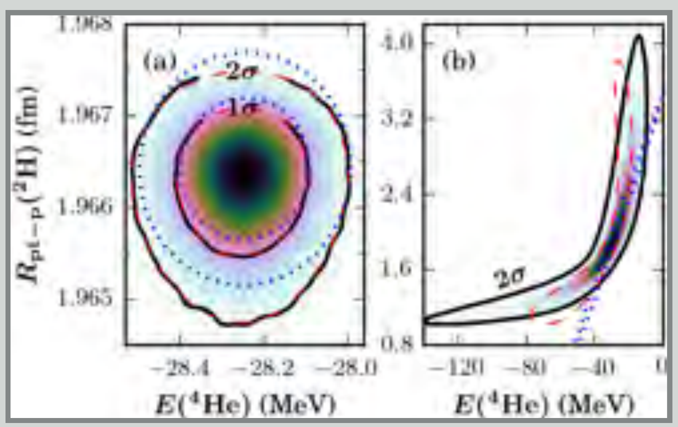
$\sigma_{\text{num+method}}$

EACH STEP INTRODUCES UNCERTAINTIES

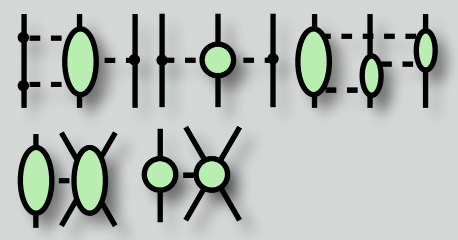
Overview of our research efforts

We aim to develop the technology and ability to:

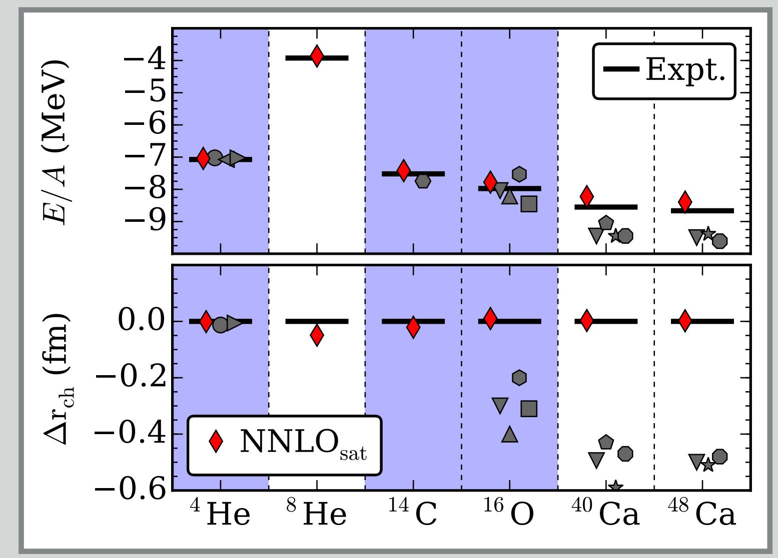
1. Diversify and extend the statistical analysis and perform a sensitivity analysis of input data.



2. Continue efforts towards higher orders of the chiral expansion, and possibly revisit the power counting.



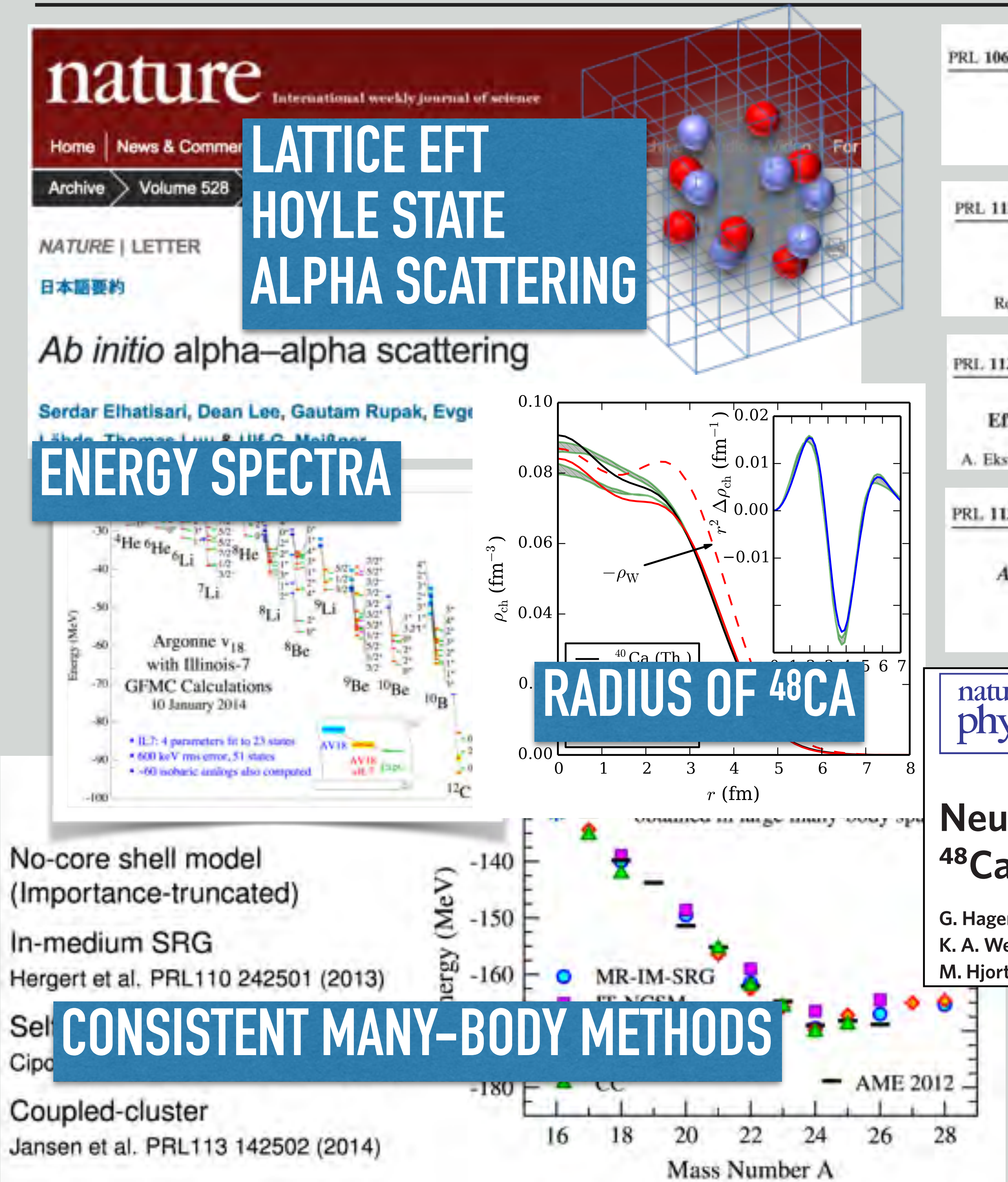
3. Explore alternative strategies of informing the model about low-energy many-body observables.

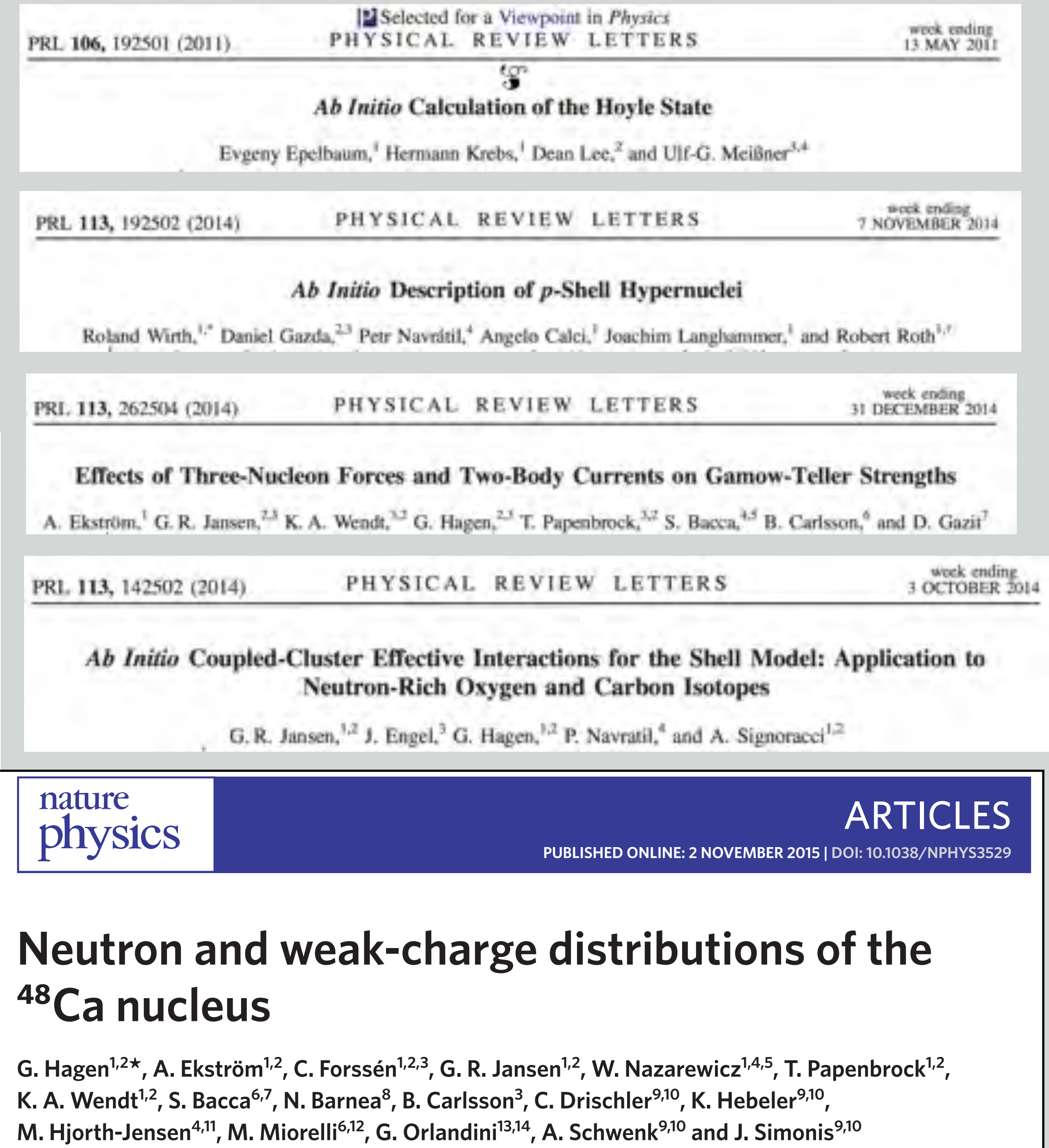


THE NUCLEAR FEW- AND MANY-BODY PROBLEMS

Ab initio methods

Ab initio capabilities (a selection)




PRL 106, 192501 (2011) — Selected for a Viewpoint in *Physics* — PHYSICAL REVIEW LETTERS — week ending 13 MAY 2011

***Ab Initio* Calculation of the Hoyle State**

Evgeny Epelbaum,[1] Hermann Krebs,[1] Dean Lee,[2] and Ulf-G. Meißner[3,4]

PRL 113, 192502 (2014) — PHYSICAL REVIEW LETTERS — week ending 7 NOVEMBER 2014

***Ab Initio* Description of *p*-Shell Hypernuclei**

Roland Wirth,[1,*] Daniel Gazda,[2,3] Petr Navrátil,[4] Angelo Calci,[1] Joachim Langhammer,[1] and Robert Roth[1,†]

PRL 113, 262504 (2014) — PHYSICAL REVIEW LETTERS — week ending 31 DECEMBER 2014

Effects of Three-Nucleon Forces and Two-Body Currents on Gamow-Teller Strengths

A. Ekström,[1] G. R. Jansen,[2,3] K. A. Wendt,[3,2] G. Hagen,[2,3] T. Papenbrock,[3,2] S. Bacca,[4,5] B. Carlsson,[6] and D. Gazit[7]

PRL 113, 142502 (2014) — PHYSICAL REVIEW LETTERS — week ending 3 OCTOBER 2014

***Ab Initio* Coupled-Cluster Effective Interactions for the Shell Model: Application to Neutron-Rich Oxygen and Carbon Isotopes**

G. R. Jansen,[1,2] J. Engel,[3] G. Hagen,[1,2] P. Navratil,[4] and A. Signoracci[1,2]

nature physics — ARTICLES — PUBLISHED ONLINE: 2 NOVEMBER 2015 | DOI: 10.1038/NPHYS3529

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

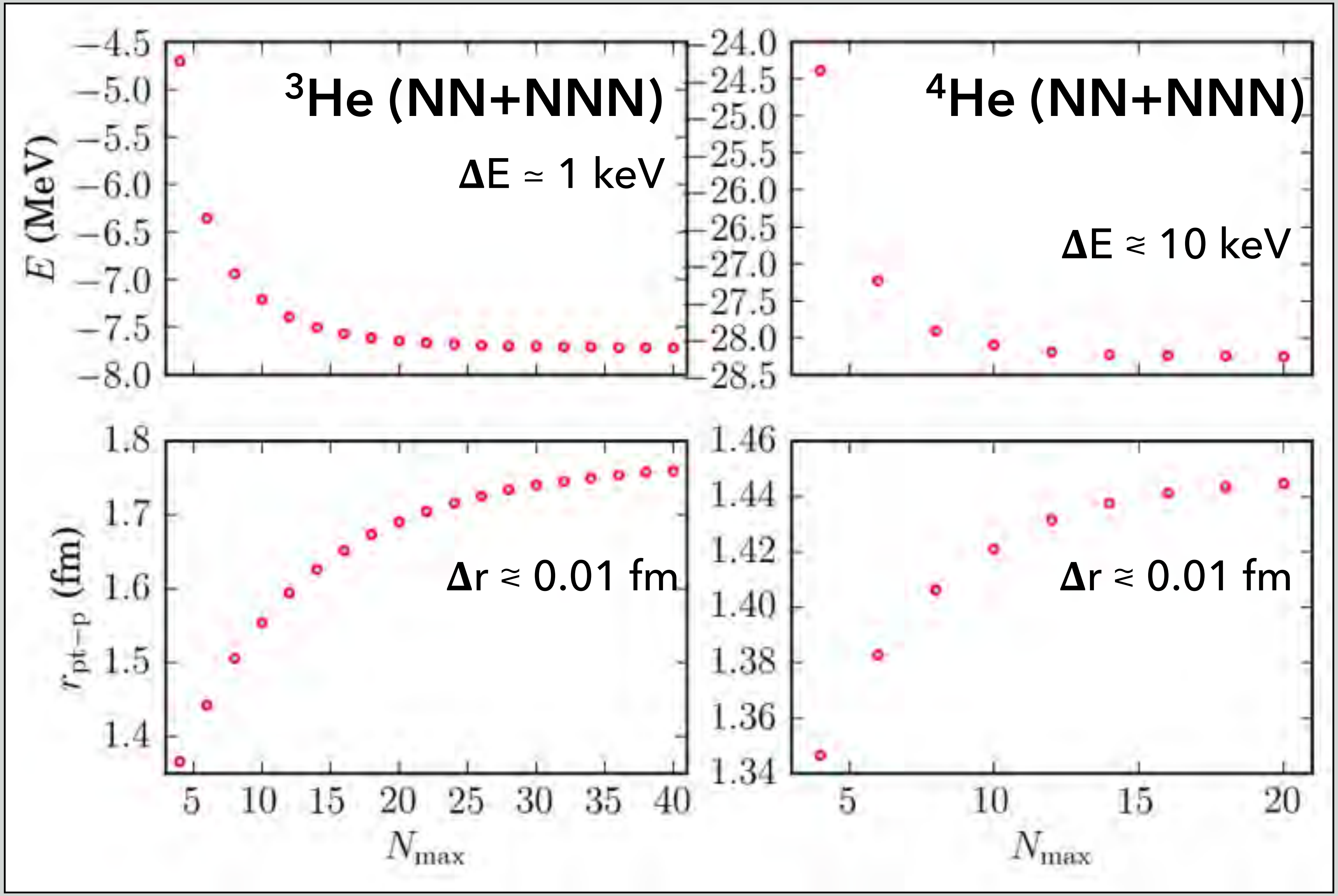
G. Hagen[1,2★], A. Ekström[1,2], C. Forssén[1,2,3], G. R. Jansen[1,2], W. Nazarewicz[1,4,5], T. Papenbrock[1,2], K. A. Wendt[1,2], S. Bacca[6,7], N. Barnea[8], B. Carlsson[3], C. Drischler[9,10], K. Hebeler[9,10], M. Hjorth-Jensen[4,11], M. Miorelli[6,12], G. Orlandini[13,14], A. Schwenk[9,10] and J. Simonis[9,10]

Several Many-Body Solvers:

GFMC, NCSM, Coupled Cluster, Many-Body Perturbation Theory, Hyperspherical harmonics, NCSM-RGM, Gamow Shell Model, Continuum Shell-Model, Self-Consistent Green's Functions, Faddeev, Bogoliubov CC, Gorkov SCGF, Monte Carlo Shell-Model, …

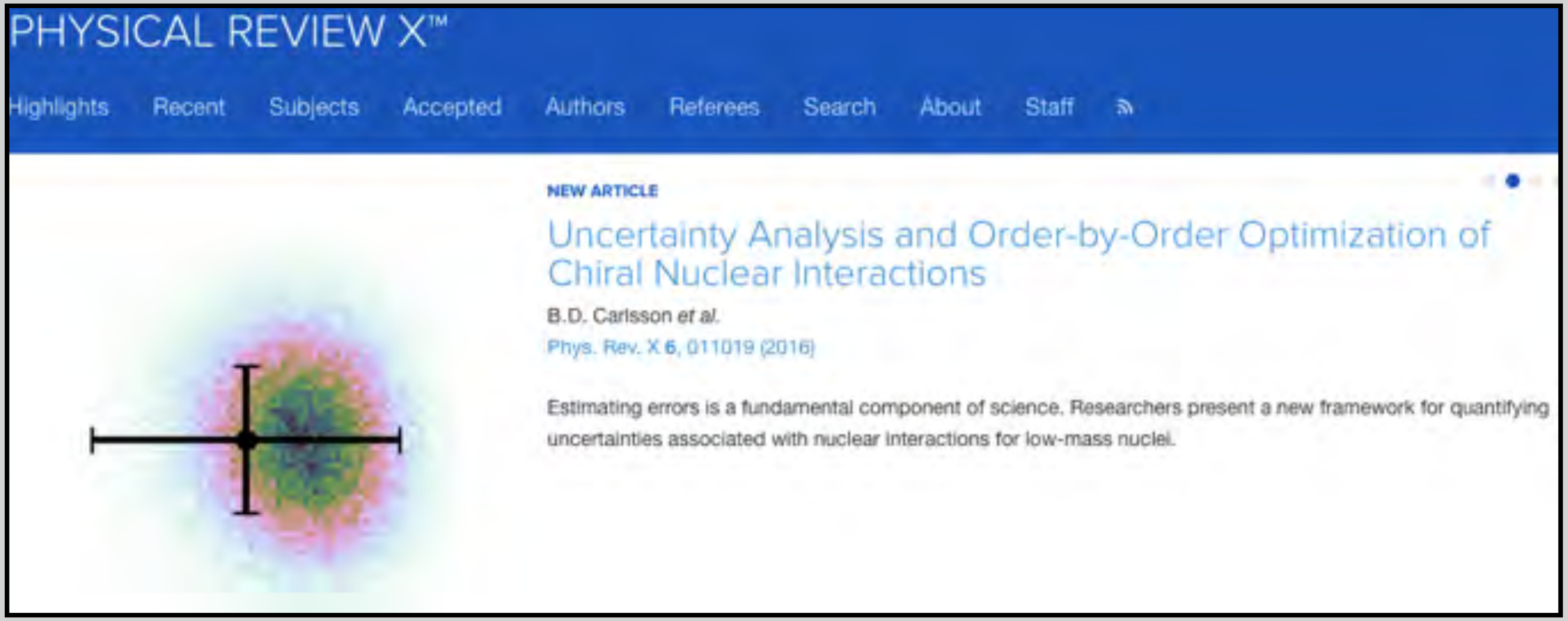
Few-body calculations

NCSM (rel. coord.)



~ 10 sec. ~ 45 sec.

Based on: B.D. Carlsson, A. Ekström, C. Forssén et al, Phys. Rev. X **6** (2016) 011019



THEORETICAL UNCERTAINTY QUANTIFICATION

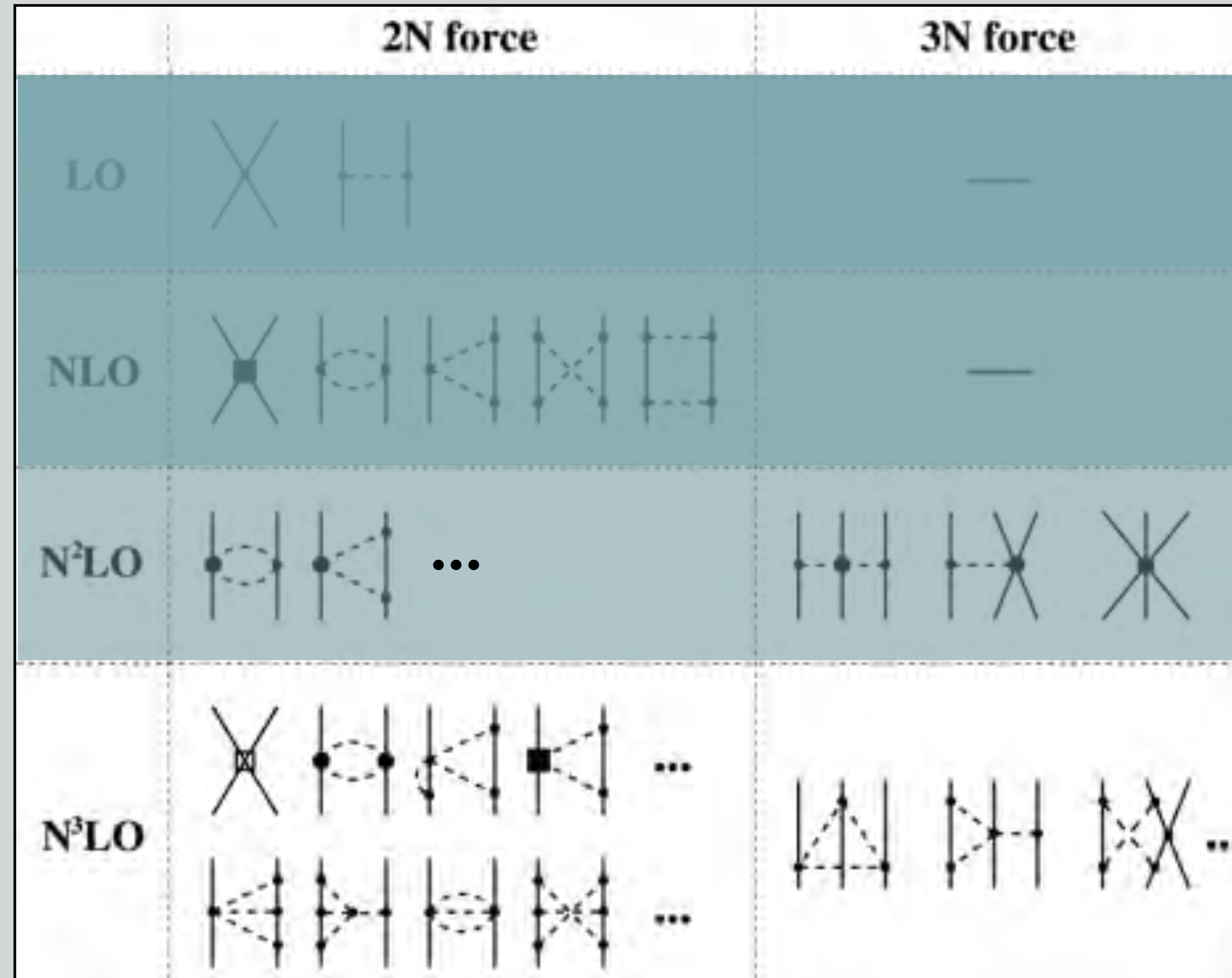
Ab initio (from few to many) with χ(p)EFT and error analysis

Chiral nuclear interactions

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.

$$\chi^2(\vec{p}) = \sum_i \left(\frac{O_i^{\mathrm{theo}}(\vec{p}) - O_i^{\mathrm{exp}}}{\sigma_{\mathrm{tot},i}} \right)^2$$



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

Optimization strategy

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

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

Standard approach:

1. **πN LECs determined first** from Pion-Nucleon scattering phase shifts or from NN phase shifts in peripheral waves
2. **(NN-only) objective function based on Nijmegen phase shift analysis**
   - Chi-by-eye optimization
   - N^3LO needed for high-accuracy fit up to T_{lab}=290 MeV
3. **NNN LECs determined at the end** given the NN part. Usually at NNLO. First results at N^3LO are coming.

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 technology significantly improved:

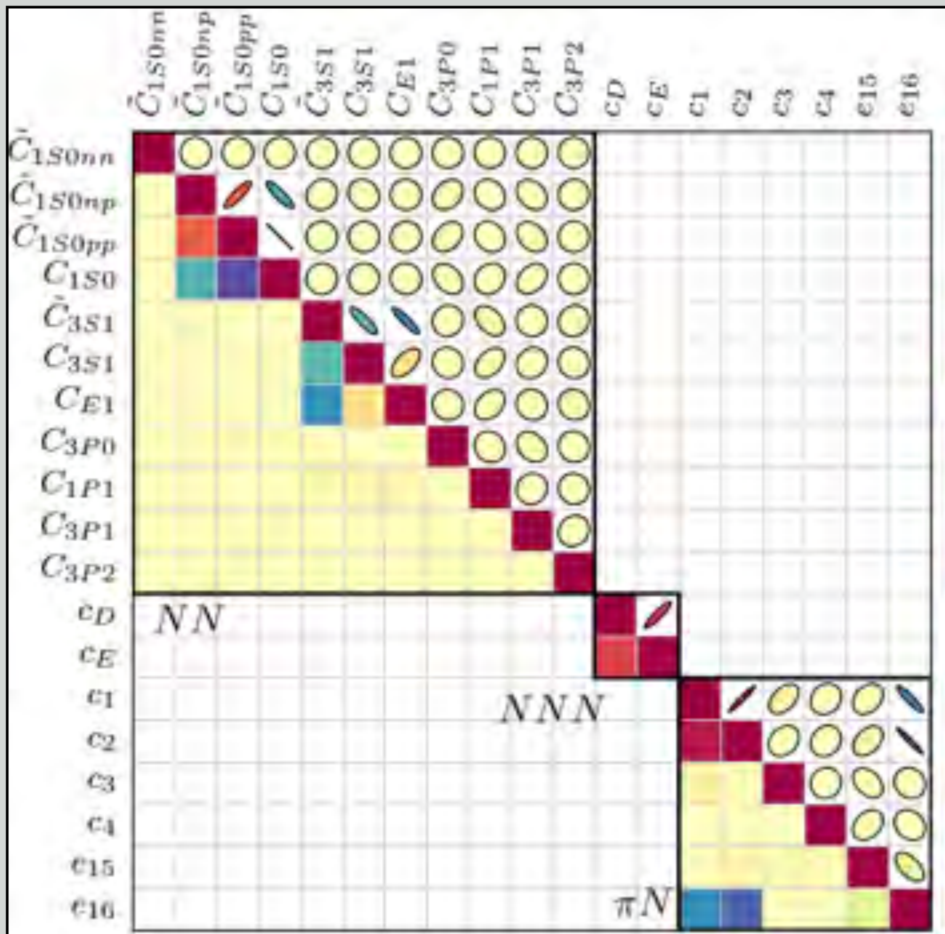
- Our first approach: Derivative-free optimization using POUNDerS*
- More efficient minimization algorithms (Levenberg-Marquardt, Newton), and statistical error analysis require **derivatives**

$$\frac{\partial r_i}{\partial p_j} \quad \text{and} \quad \frac{\partial^2 r_i}{\partial p_j \partial p_k}$$

- Numerical derivation using **finite differences** is plagued by **low numerical precision** and is **computationally costly.**
- Instead, we use **Algorithmic Differentiation** (AD).

Sequential optimization

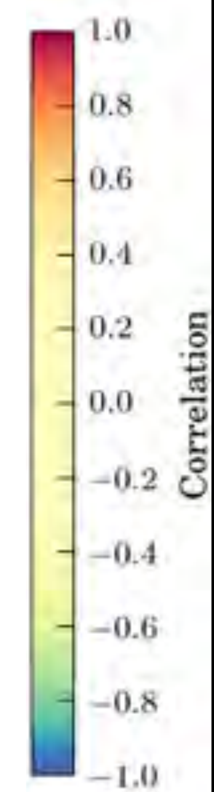
$$\chi^2(\vec{p}) \equiv \sum_i r_i^2(\vec{p}) = \underbrace{\sum_{j\in NN} r_j^2(\vec{p})}_{1} + \underbrace{\sum_{k\in \pi N} r_k^2(\vec{p})}_{2} + \underbrace{\sum_{l\in 3N} r_l^2(\vec{p})}_{3}$$



Sequential fit

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

This will imply huge statistical errors.



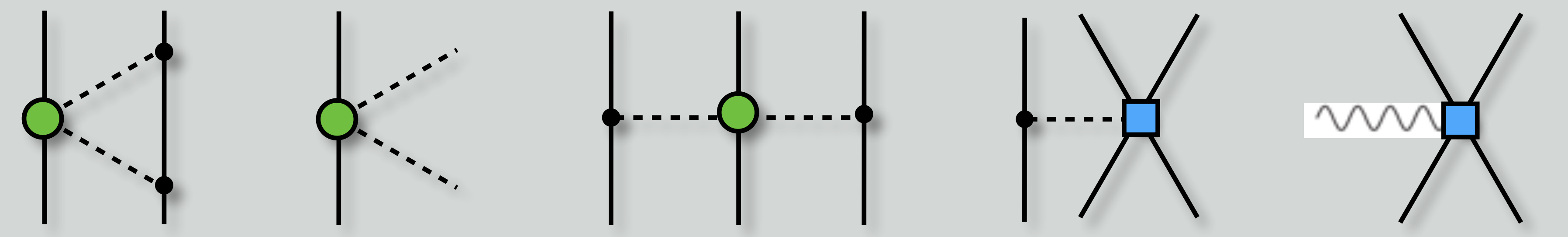
Simultaneous optimization

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

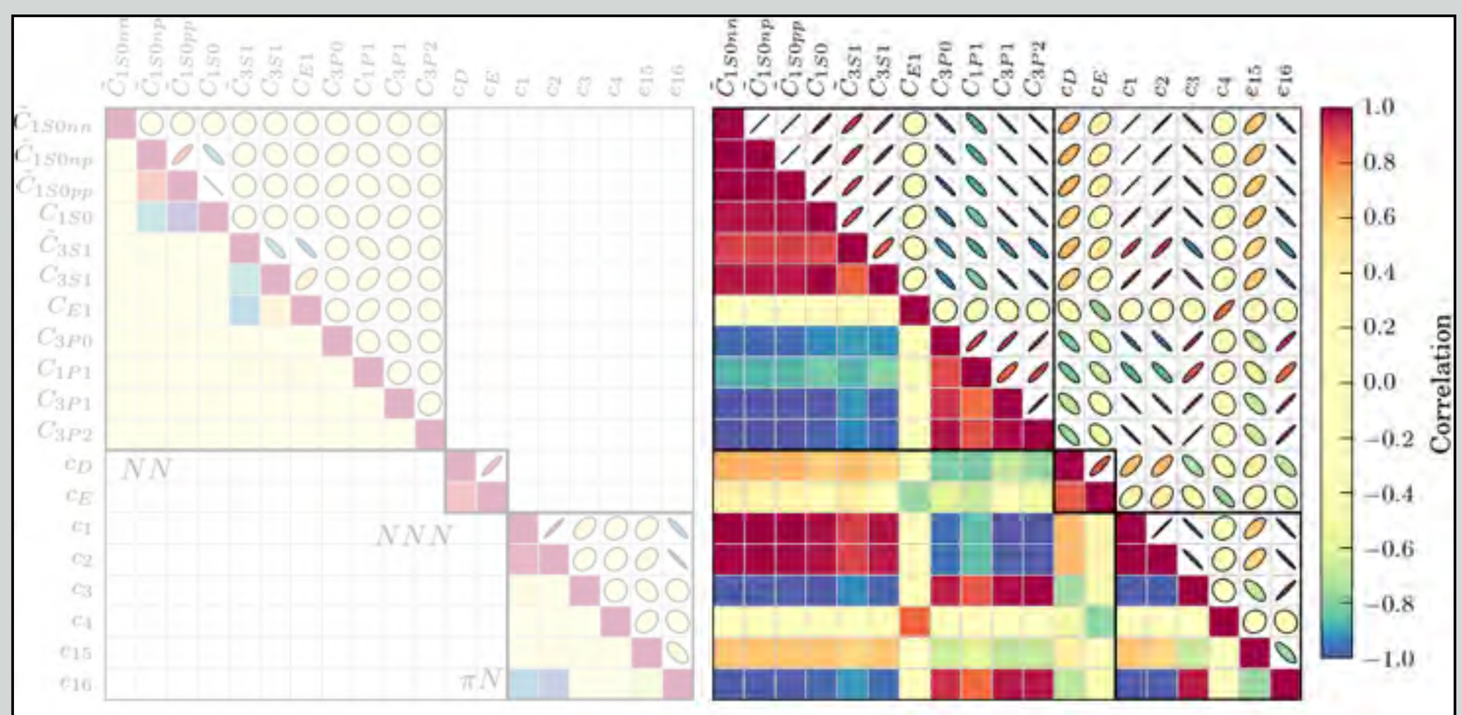
Simultaneous

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)



two-nucleon interaction | pion-nucleon scattering | three-nucleon interaction | three-nucleon interaction | external probe current



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)

Many-body predictions

A=4 bound state
- ^{4}He (binding energy, radius)
- $NCSM_{rel}$, N_{max}=20,ħΩ=36 MeV

A=16 bound state
- ^{16}O (binding energy, radius)
- Λ-CCSD(T), N_{max}=15,ħΩ=20 MeV

Total error budget

- The total error budget is

E.g. , NCSM — Neglected

$$\sigma^2_{\rm tot} = \sigma^2_{\rm exp} + \sigma^2_{\rm method} + \sigma^2_{\rm numerical} + \sigma^2_{\rm model}$$

- At a given chiral order v, the omitted diagrams should be of order

$$\mathcal{O}\left((Q/\Lambda_\chi)^{\nu+1}\right)$$

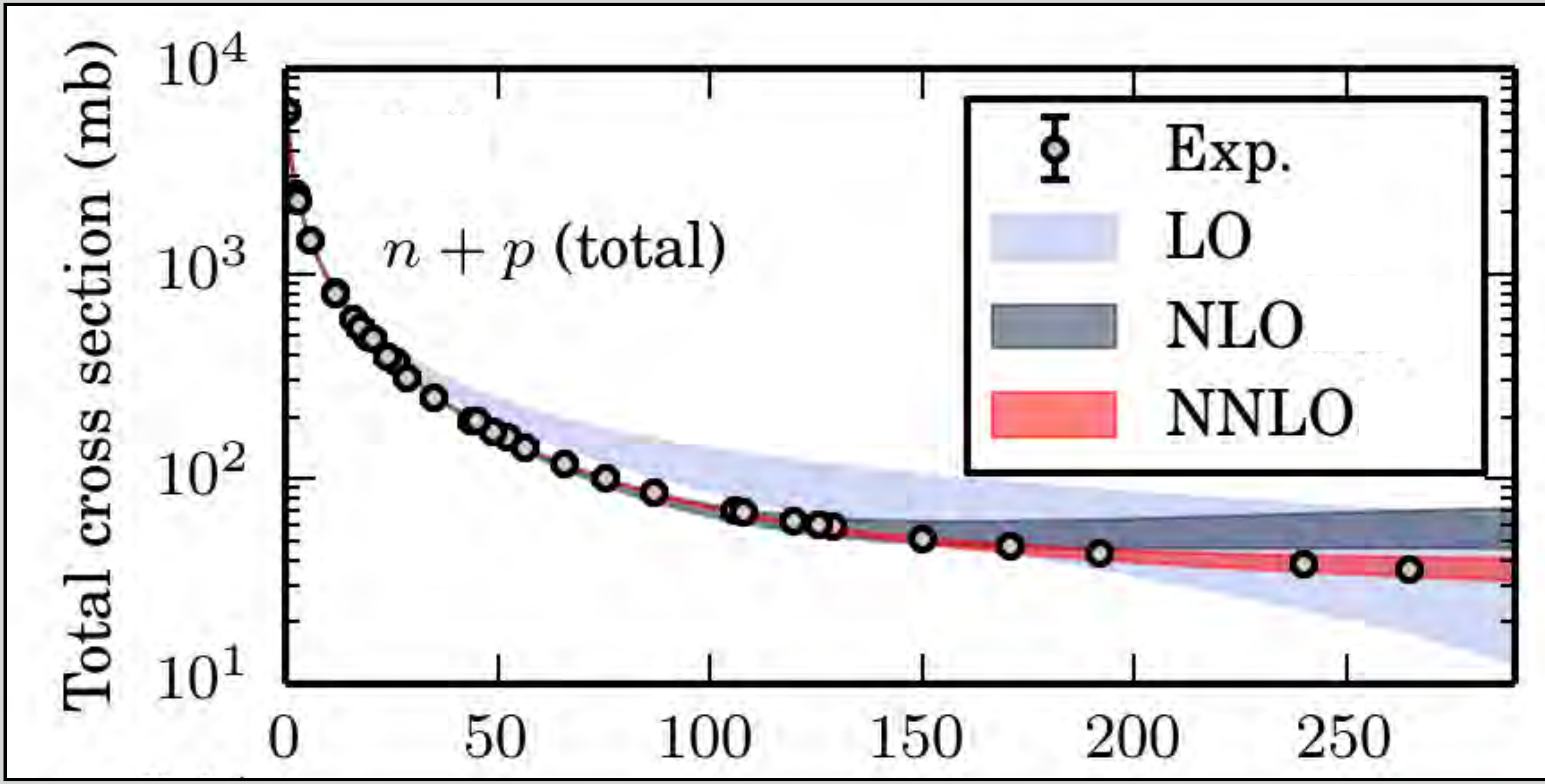
- Still needs to be converted to actual numbers $\sigma_{\rm model}$

- We translate this EFT knowledge into an error in the scattering amplitudes

$$\sigma^{\rm (amp)}_{\rm model,x} = C_x \left(\frac{Q}{\Lambda_\chi}\right)^{\nu+1}, \quad x \in \{NN, \pi N\}$$

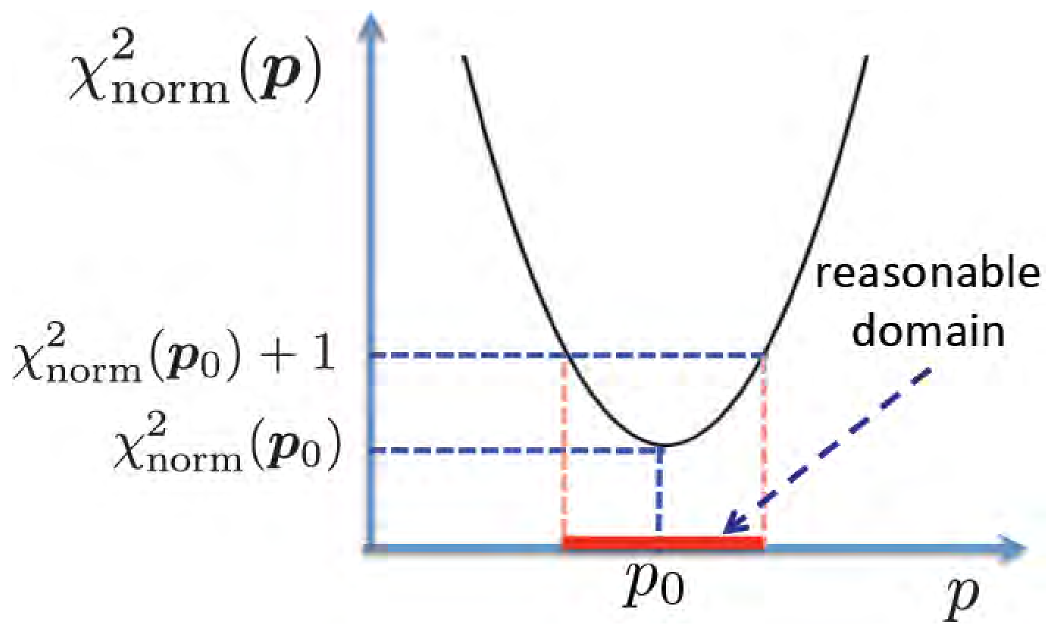
- which is then propagated to an error in the observable.

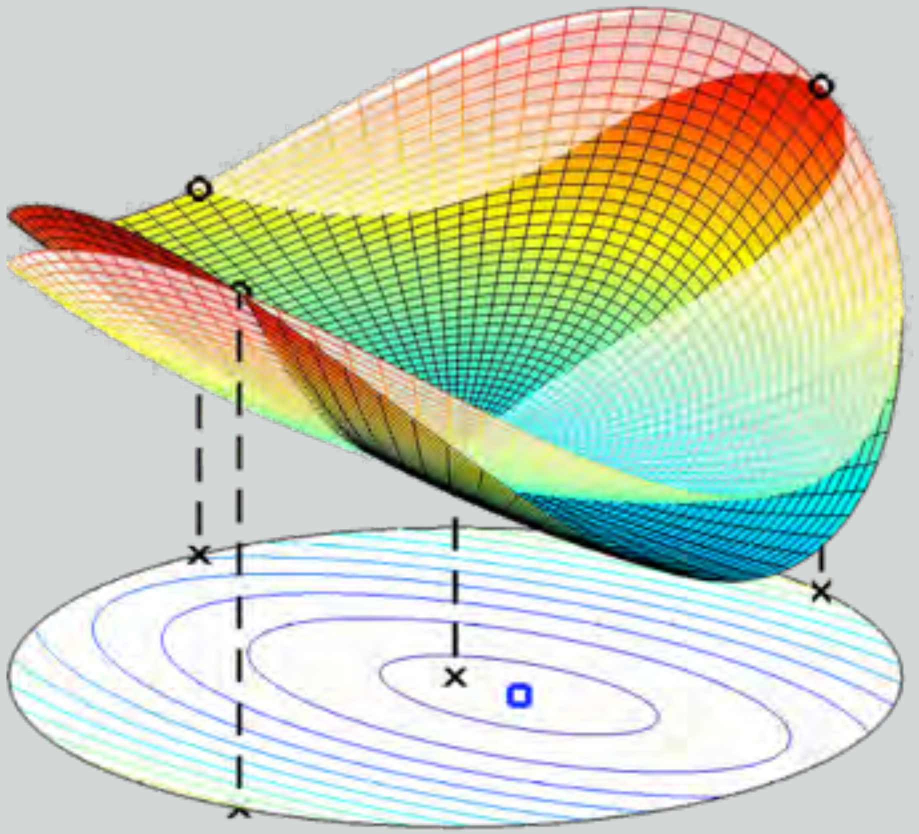
Total np cross section



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]





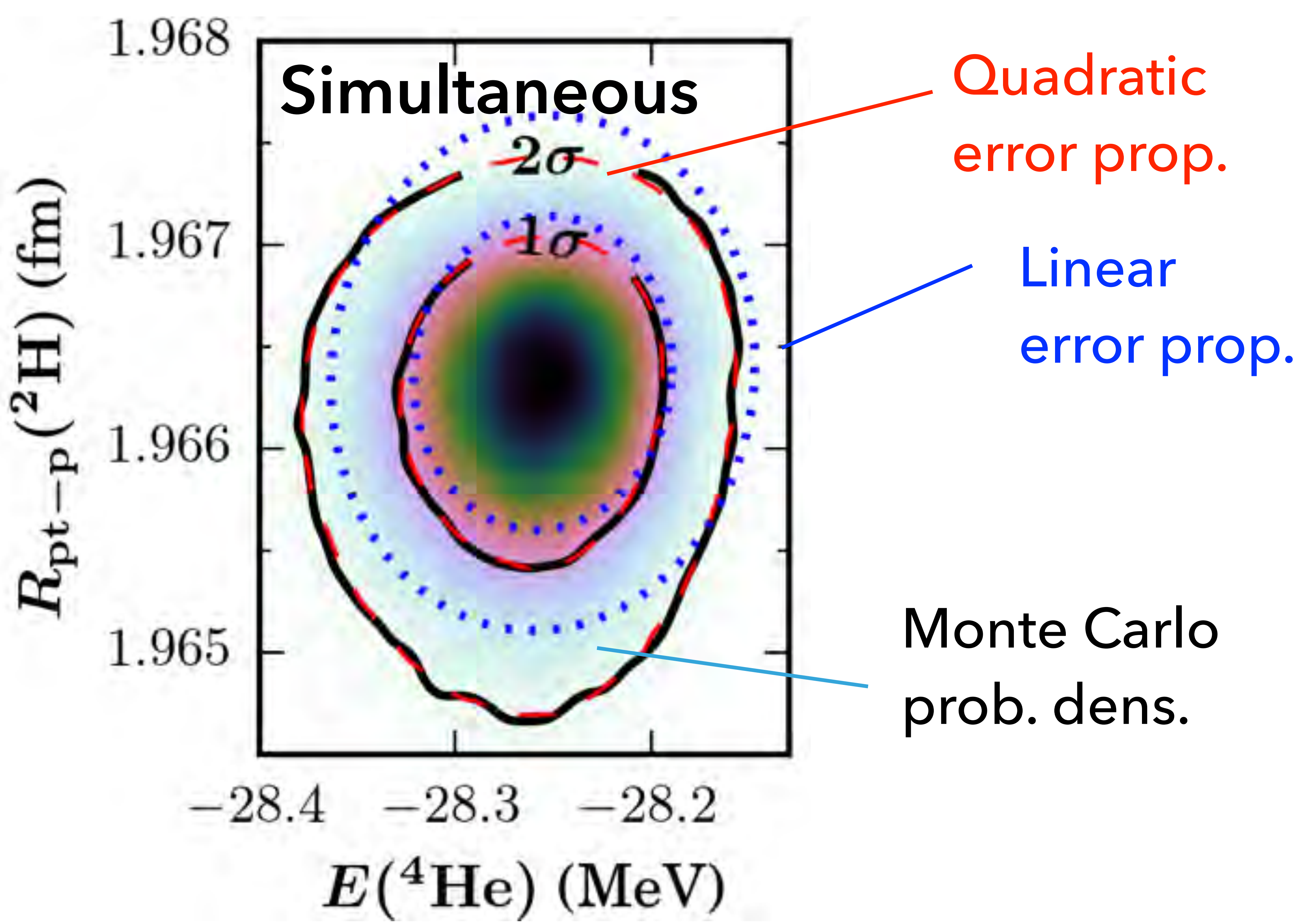
- From the hessian at $\mathbf{p}_0$ we can calculate a **covariance matrix** and from that a **correlation matrix**.

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

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

Quadratic error propagation vs Brute force sampling

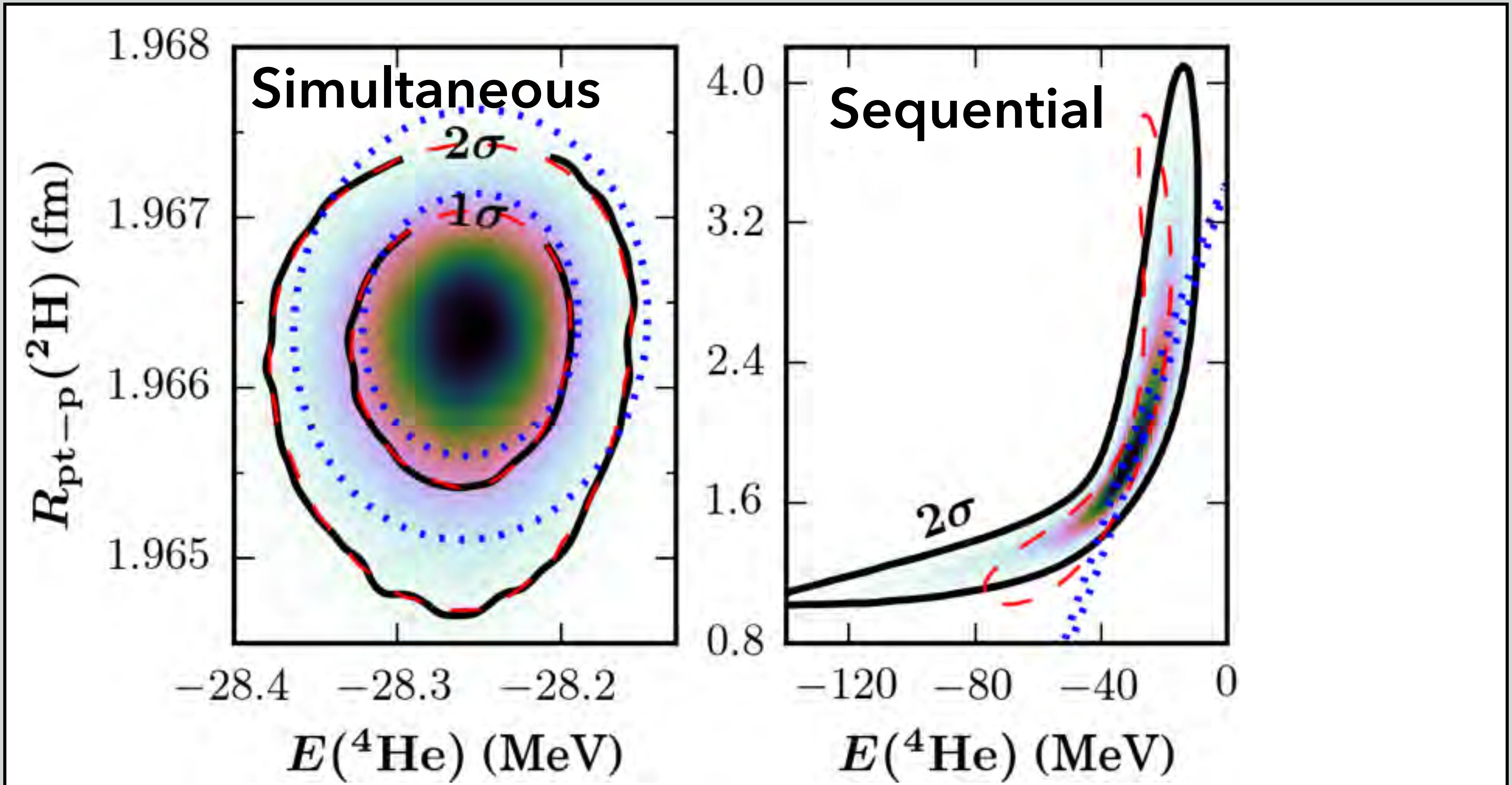
$$O(\mathbf{p}) \approx O(\mathbf{p}_0) + J_O \Delta\mathbf{p} + \frac{1}{2}\Delta\mathbf{p}^T H_O \Delta\mathbf{p}$$



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

Quadratic error propagation vs Brute force sampling

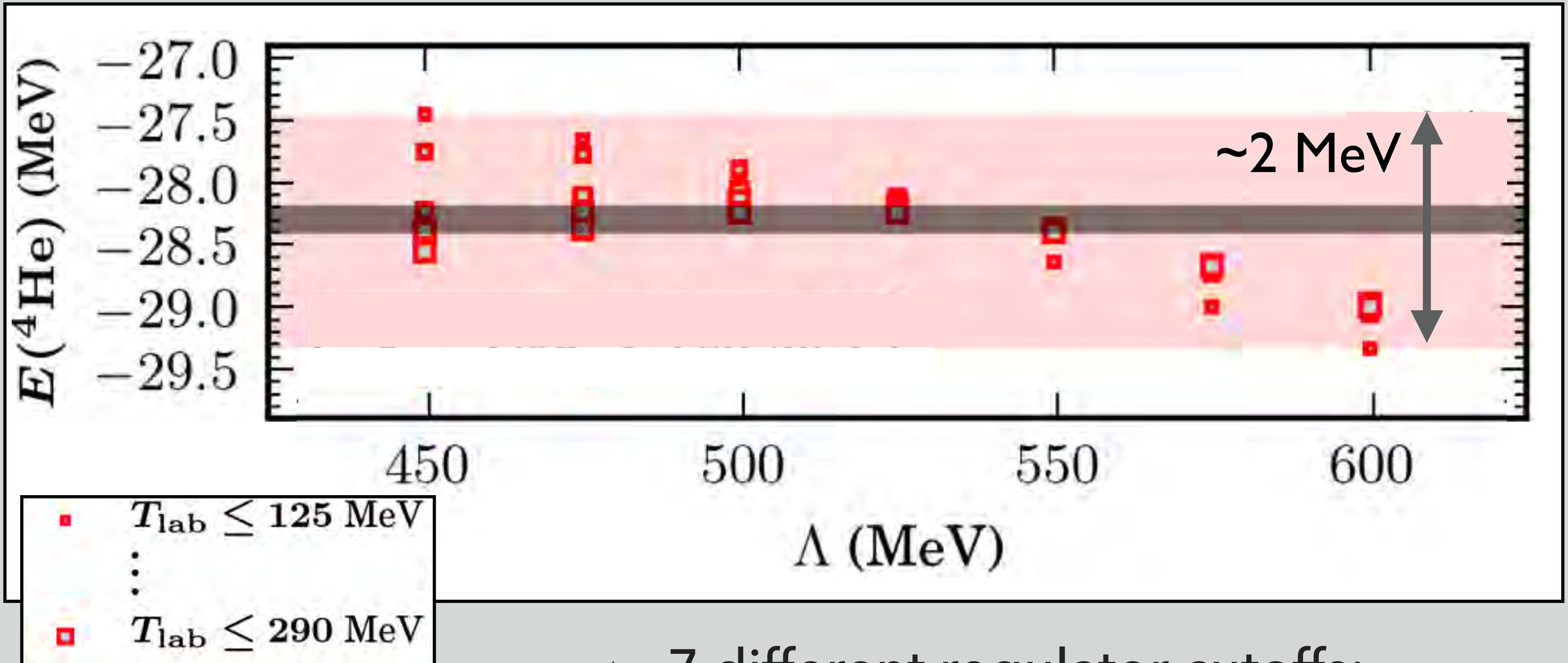
$$O(\mathbf{p}) \approx O(\mathbf{p_0}) + J_O \Delta\mathbf{p} + \frac{1}{2}\Delta\mathbf{p}^T H_O \Delta\mathbf{p}$$



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

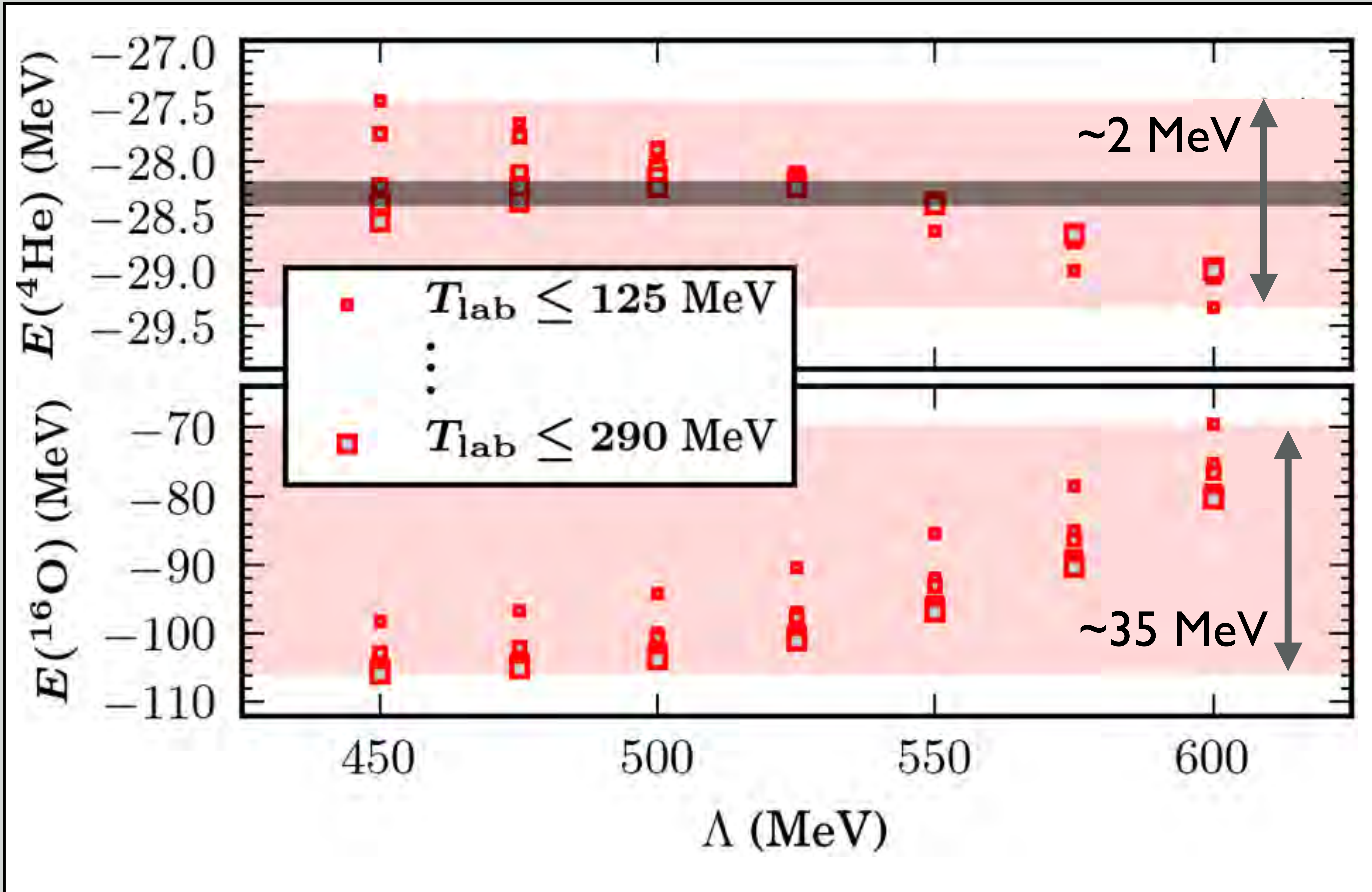
$E(^4\mathrm{He}) = -28^{+8}_{-18}$ (MeV)

Systematic uncertainties: input data, regulator cutoff



- 7 different regulator cutoffs: Λ=450, 475, …, 575, 600 MeV
- 6 different NN-scattering datasets $T_{lab} \in [0, T_{lab,max}]$, with $T_{lab,max}$=125, …, 290 MeV

Systematic uncertainties: input data, regulator cutoff



Do-it-yourself

All 42 different sim/sep potentials, as well as the respective covariance matrices are available as supplemental material.

$$\begin{aligned}\mathrm{Cov}(\mathrm{A},\mathrm{B}) &\equiv \mathbb{E}[(\mathcal{O}_\mathrm{A}(\mathbf{p})-\mathbb{E}[\mathcal{O}_\mathrm{A}(\mathbf{p})])(\mathcal{O}_\mathrm{B}(\mathbf{p})-\mathbb{E}[\mathcal{O}_\mathrm{B}(\mathbf{p})])] \\ &\approx \mathbb{E}[(\tilde{J}_{A,i}x_i + \frac{1}{2}\tilde{H}_{A,ij}x_ix_j - \frac{1}{2}\tilde{H}_{A,ii}\sigma_i^2) \\ &\times (\tilde{J}_{B,k}x_k + \frac{1}{2}\tilde{H}_{B,kl}x_kx_l - \frac{1}{2}\tilde{H}_{B,kk}\sigma_k^2)] \\ &= \tilde{\mathbf{J}}_A^T\mathbf{\Sigma}\tilde{\mathbf{J}}_B + \frac{1}{2}(\boldsymbol{\sigma}^2)^T(\tilde{\mathbf{H}}_A \circ \tilde{\mathbf{H}}_B)\boldsymbol{\sigma}^2,\end{aligned}$$

- LO-NLO-NNLO
- with 7 different cutoffs: 450,475,..,600 MeV
- from 6 different NN-scattering datasets

compute the derivatives of your own observables wrt LECs, then explore:

- cutoff variations
- order-by-order evolution
- LEC UQ/correlations

Based on: B. Acharya, B. D. Carlsson, A. Ekström, C. Forssén, and L. Platter, arXiv: 1603.01593

arXiv.org > nucl-th > arXiv:1603.01593

Nuclear Theory

Uncertainty quantification for proton–proton fusion in chiral effective field theory

B. Acharya, B. D. Carlsson, A. Ekström, C. Forssén, L. Platter

(Submitted on 4 Mar 2016)

Uncertainty Quantification for pp fusion in χEFT

Uncertainty quantification applied to pp fusion

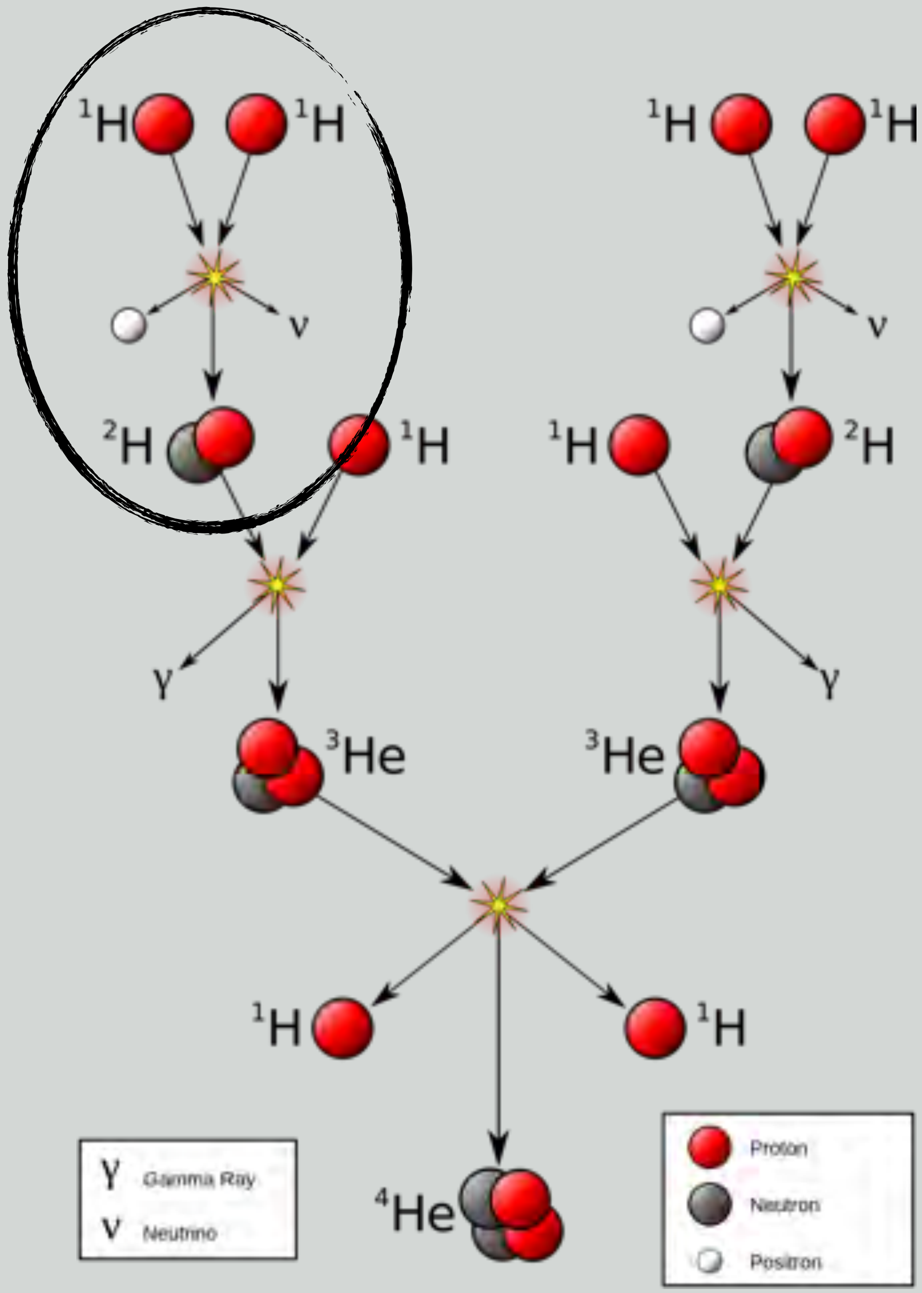
$$p + p \to d + e^{+} + \nu_e$$

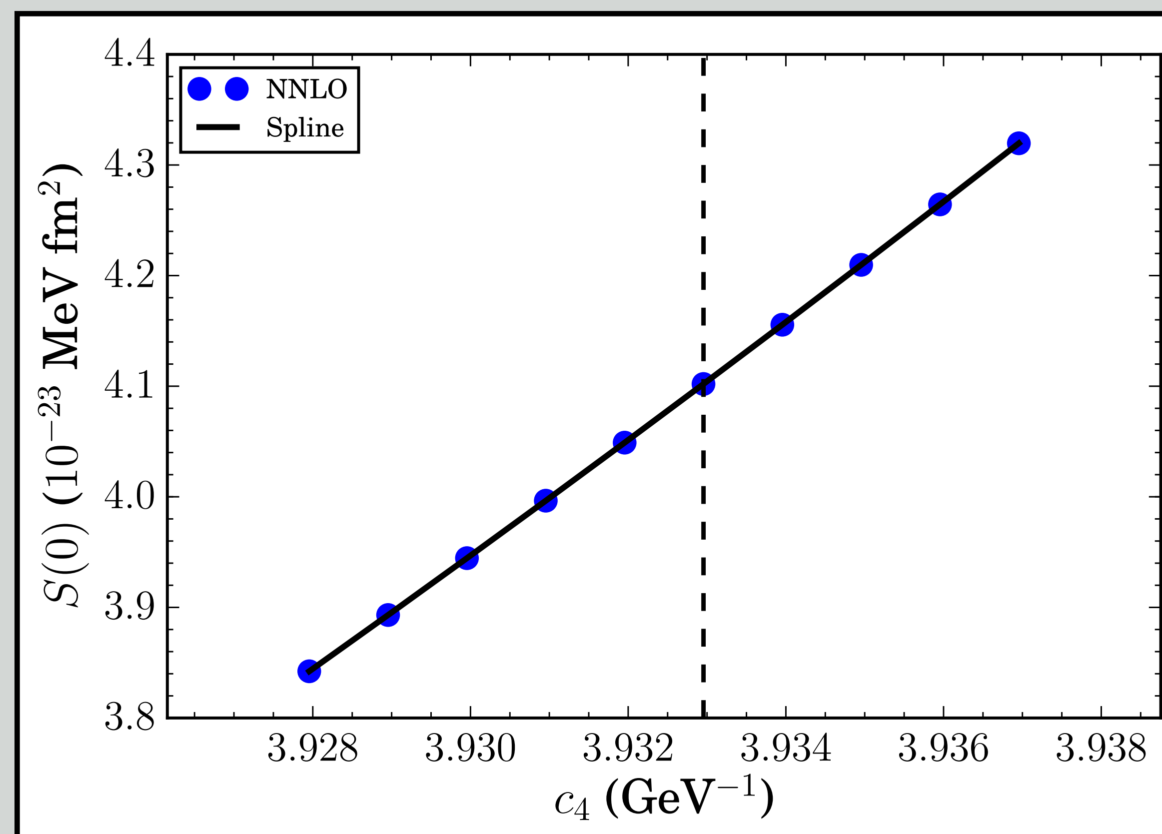
$$S(E) = \sigma(E) E e^{2\pi\eta}$$

$$\sigma(E) = \int \frac{\mathrm{d}^3 p_e}{(2\pi)^3} \frac{\mathrm{d}^3 p_\nu}{(2\pi)^3} \frac{1}{2E_e} \frac{1}{2E_\nu} \times$$

$$2\pi\delta\left(E + 2m_p - m_d - \frac{q^2}{2m_d} - E_e - E_\nu\right)$$

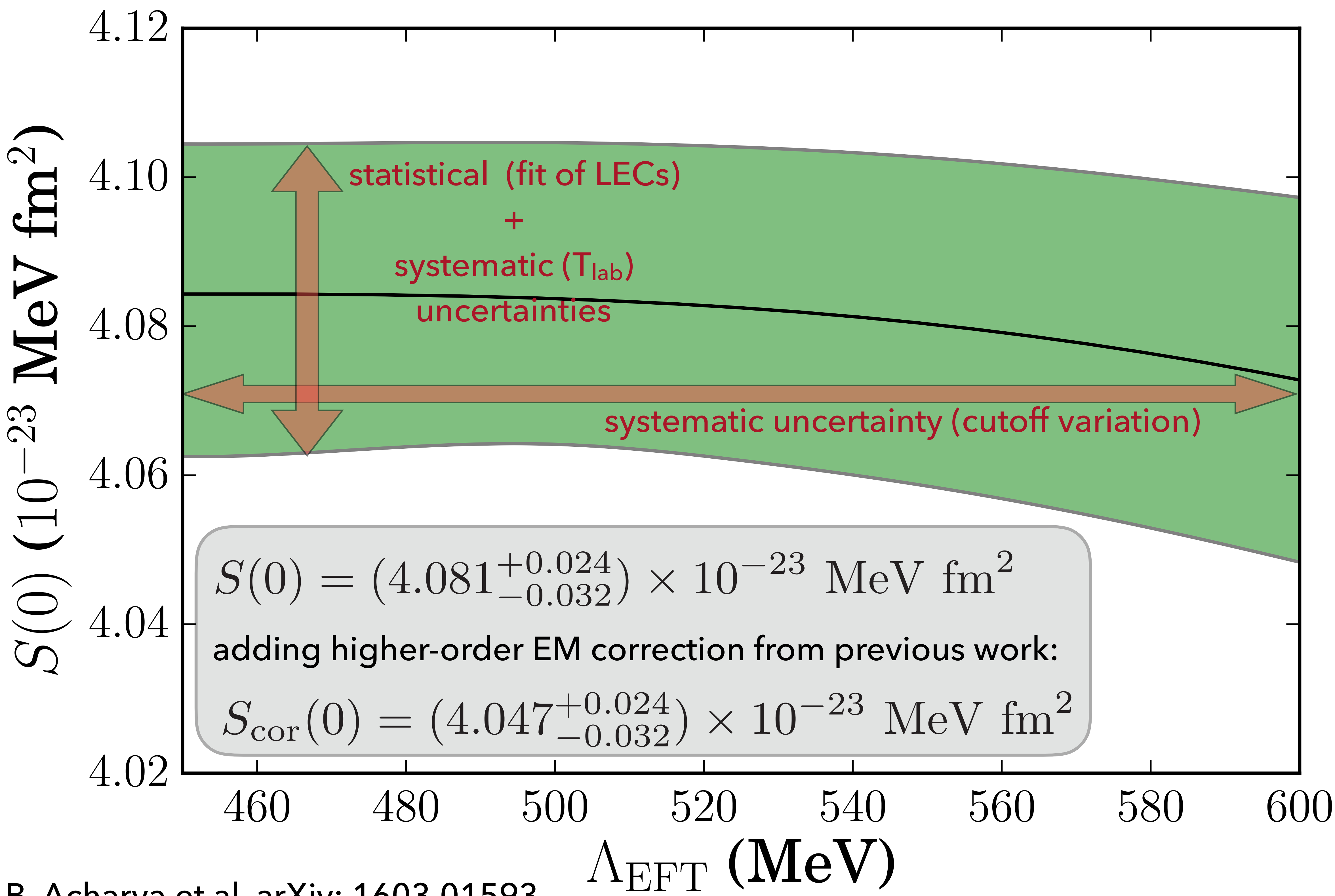
$$\frac{1}{v_{rel}} F(Z, E_e) \frac{1}{4} \sum |\langle f|\hat{H}_W|i\rangle|^2$$





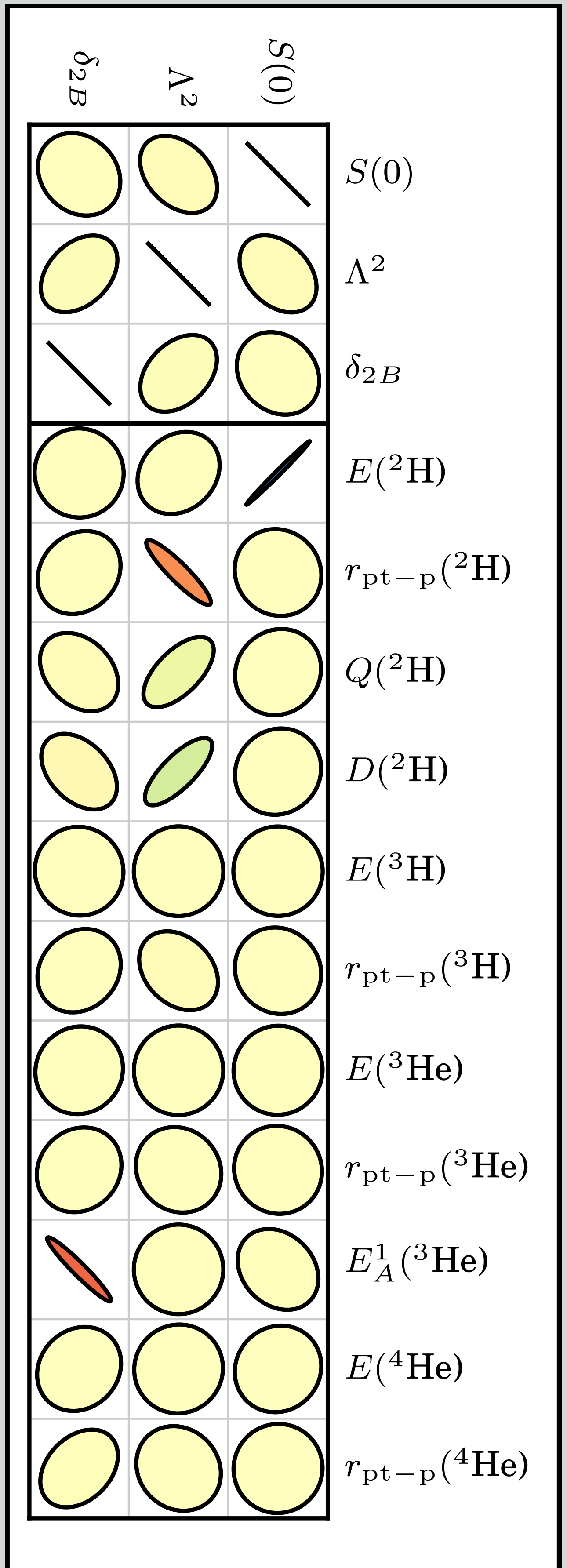
L. E. Marcucci et al PRL 110, 192503 (2013)
R. Schiavilla et al PRC 58, 1263 (1998)
J-W. Chen et al. PLB 720, 385 (2013)

Uncertainty quantification applied to pp fusion



B. Acharya et al, arXiv: 1603.01593

Uncertainty quantification applied to pp fusion



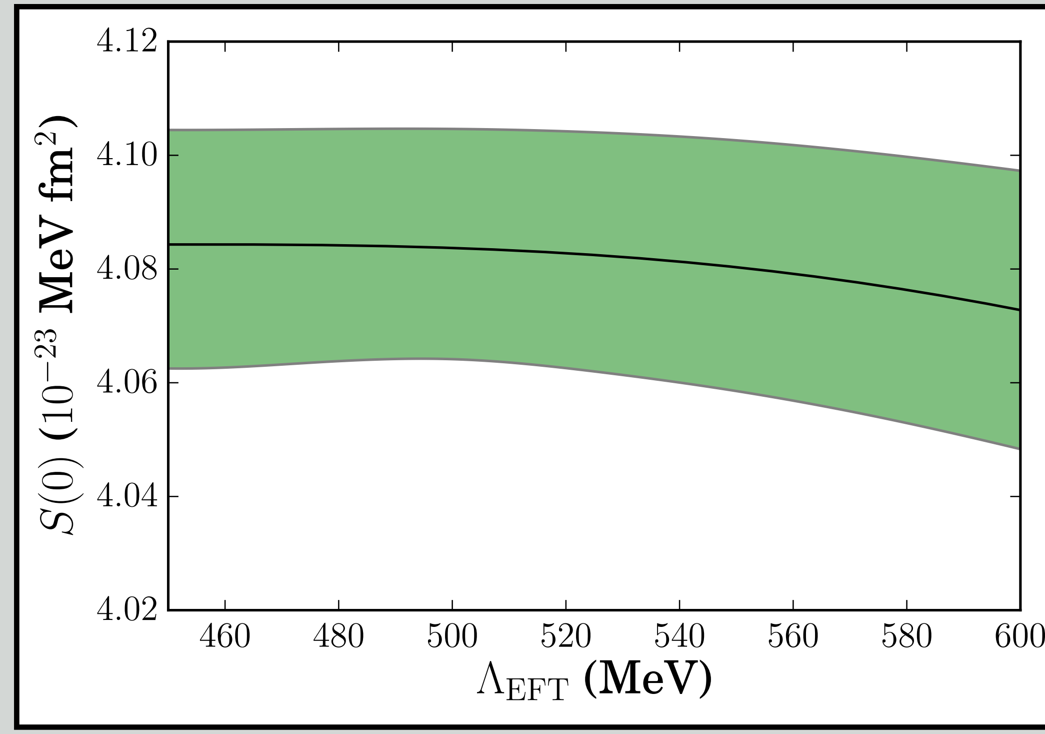
Correlation analysis:

S(0) - E(^{2}H): *phase space*

L^2-r(^{2}H): *radial overlap*

L^2-rQ(^{2}H): *radial overlap*

d$_{2B}$-E1A: *2B-current operator*



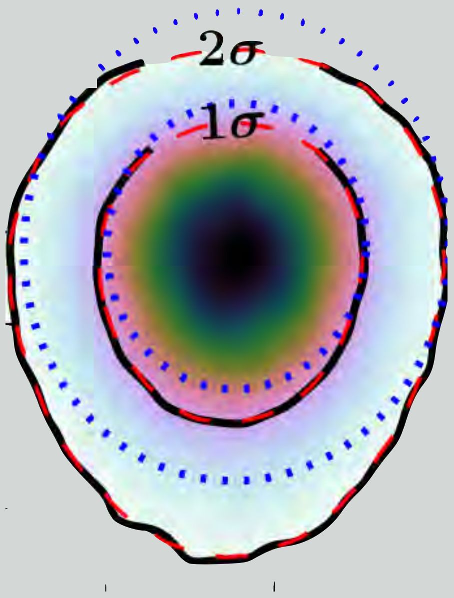
B. Acharya et al, arXiv: 1603.01593

- Insofar most consistent χEFT-study of this reaction
- Correlation study indicates sound statistical analysis
- Cutoff variation not large source of error
- Statistical error in S(0) is 3 times larger than what was previously thought
- Central value is most likely also larger due to previously neglected systematic uncertainties.

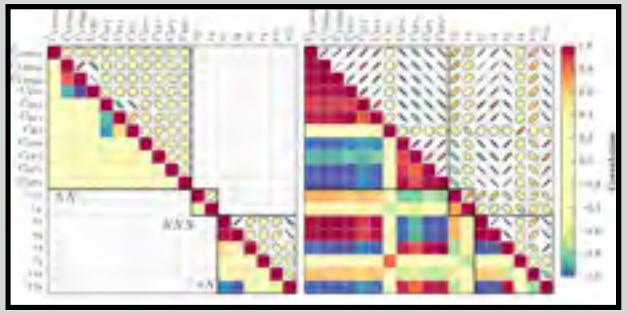
Conclusion

Summary

- **Uncertainty quantification** is a unique opportunity when employing **systematic approaches** (EFT + ab initio).

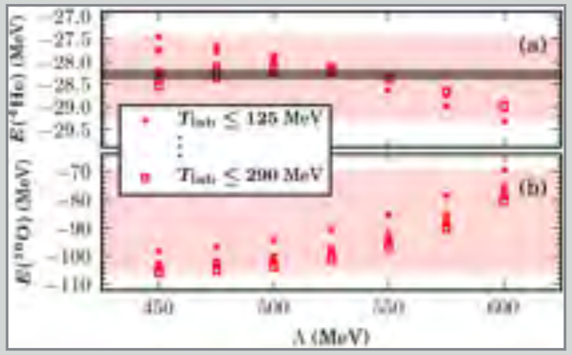


- First results for correlations, parameter uncertainties and **error propagation in the few and many-body sectors.**



- **Simultaneous optimization of all LECs** at LO, NLO, NNLO using NN, NNN and piN data is critical in order to:
  - capture all correlations between the parameters, and
  - reduce the statistical errors.

- **Covariance matrices** for optimized LO-NLO-NNLO potentials available for download



- **Small variations** in the nuclear interaction renders **large fluctuations** in predictions for heavier nuclei

Many thanks to my collaborators

- Boris Carlsson, Andreas Ekström, Dag Strömberg, Oskar Lilja, Mattias Lindby, Björn Mattsson (Chalmers)
- Gustav Jansen, Kyle Wendt (ORNL/UT)

and for the pp fusion calculations:

- Bijaya Acharya, Lucas Platter (UT)

and for the many-body calculations:

- Gaute Hagen, Thomas Papenbrock (ORNL/UT)

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