Eigenvector continuation in nuclear physics

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INT 19-2a: Nuclear Structure at the crossroads, Seattle, WA

July 4, 2019

SK, A. Ekström, K. Hebeler, A. Sarkar, D. Lee, A. Schwenk, in preparation

Outline

Genesis

Evolution

Exodus

Emulation

Motivation

Many physics problems are tremendously difficult...

- huge matrices, possibly too large to store
  - ever more so given the evolution of typical HPC clusters
- most exact methods suffer from exponential scaling
- **interest only in a few (lowest) eigenvalues**

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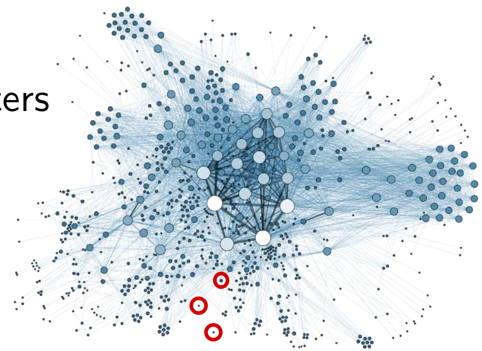

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Introducing eigenvector continuation

Frame et al., PRL **121** 032501 (2018)

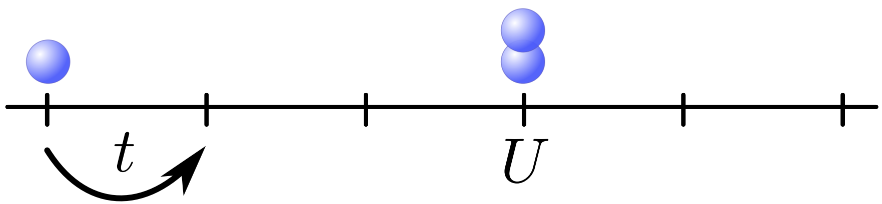
KDE Oxygen Theme

- novel numerical technique
- can solve otherwise untractable problems
- amazingly simple in practice
- broadly applicable
- **this talk: nuclear nails**

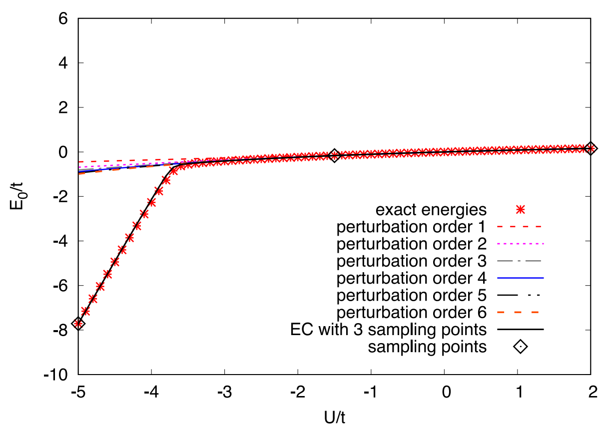
Hubbard model

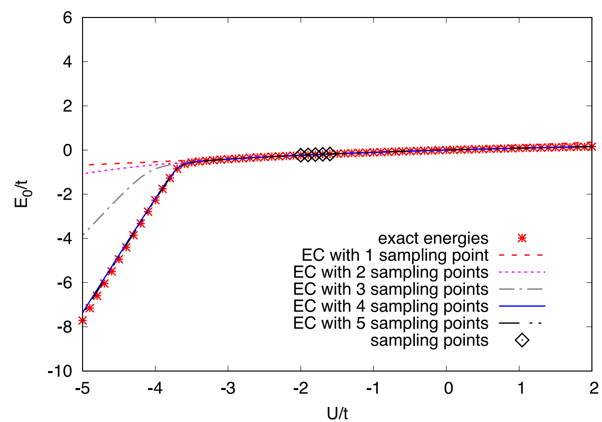
Frame et al., PRL **121** 032501 (2018)

- three-dimensional Bose-Hubbard model (4 bosons on $4 \times 4 \times 4$ lattice)
- hopping parameter t, on-site interaction $U \rightsquigarrow H = H(c = U/t)$



- Bose gas for $c > 0$, weak binding for $-3.8 < c < 0$, tight cluster for $c < -3.8$
- **eigenvector continuation can extrapolate across regimes**





General idea

Scenario

Frame et al., PRL **121** 032501 (2018)

- consider physical state (eigenvector) in a large space
- **parametric dependence of Hamiltonian $H(c)$ traces only small subspace**

Procedure

- calculate $|\psi(c_i)\rangle$, $i = 1, \ldots N_{\mathrm{EC}}$ in "easy" regime
- solve generalized eigenvalue problem $H|\psi\rangle = \lambda N|\psi\rangle$ with
  - $H_{ij} = \langle\psi_i|H(c_{\mathrm{target}})|\psi_j\rangle$
  - $N_{ij} = \langle\psi_i|\psi_j\rangle$

Prerequisite

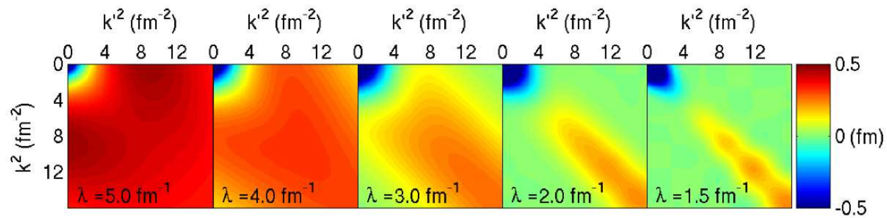
- smooth dependence of $H(c)$ on c
- enables analytic continuation of $|\psi(c)\rangle$ from c_{easy} to c_{target}

Part I

SRG evolution

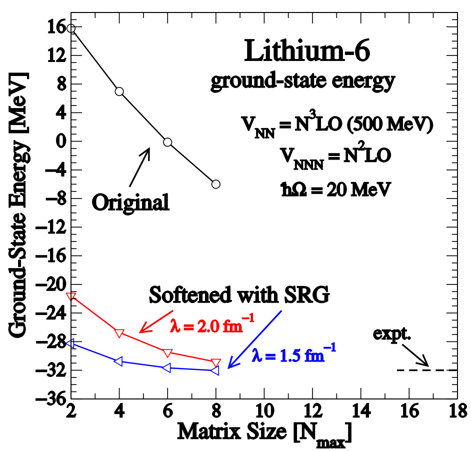
SRG evolution

- unitary transformation of Hamiltonian: $H \rightarrow H_\lambda = U_\lambda H U_\lambda^\dagger \rightsquigarrow V_\lambda$
- decouple low and high momenta at scale λ

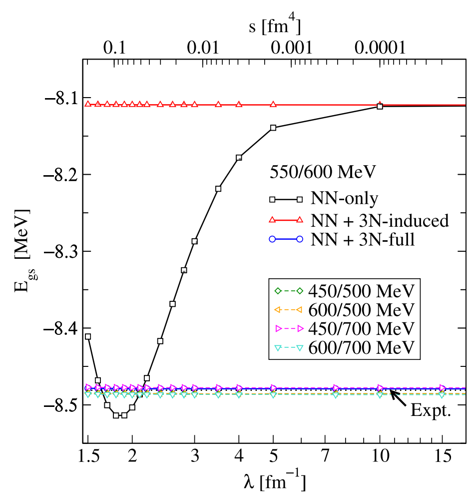


R. Furnstahl, HUGS 2014 lecture slides

- **interaction becomes more amenable to numerical methods...**
- **...at the cost of induced many-body forces!**



Bogner et al., PPNP 65 94 (2010)



Hebeler+Furnstahl, RPP **76** 126301 (2013)

SRG evolution = ODE solving

$$\frac{\mathrm{d}H_s}{\mathrm{d}s} = \frac{\mathrm{d}V_s}{\mathrm{d}s} = [[G, H_s], H_s]\,,\ \lambda = 1/s^{1/4}$$

ordinary differential equation ensures smooth parametric dependence

$\hookrightarrow$ **SRG evolution satisfies EC prerequisites!**

Reverse SRG

Consider A = 3,4 test cases

- EMN N3LO(500) interaction, Jacobi NCSM calculation

  Entem et al., PRC **96** 024004 (2017); A. Ekström implementation of Navratil et al., PRC **61** 044001 (2000)

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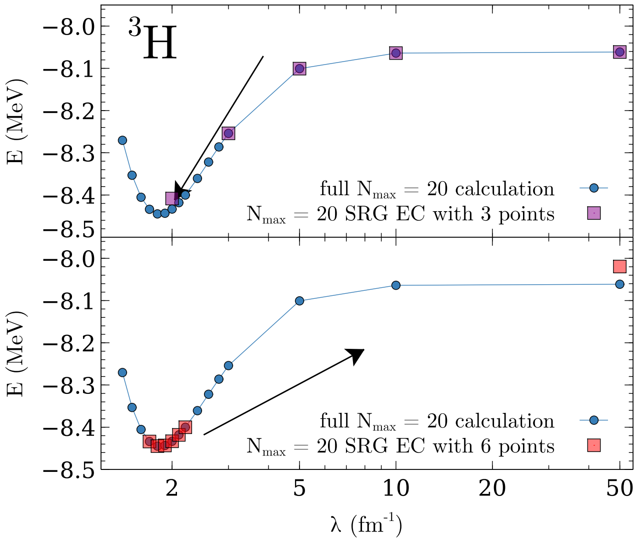
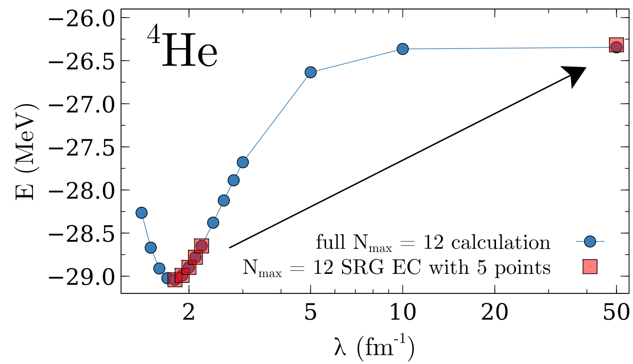


Not even induced 3N forces kept here!

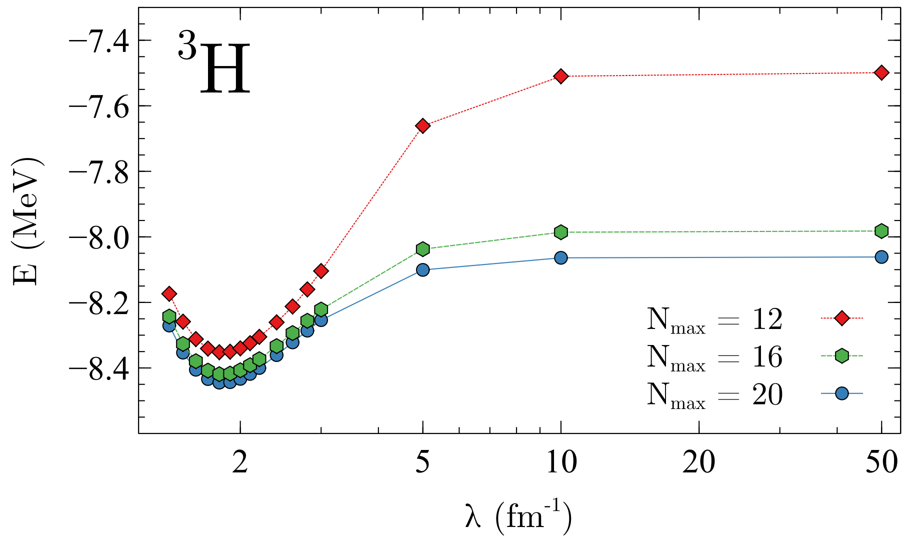


- possible to extrapolate back from small λ to bare interaction
- **information about missing many-body forces in wavefunctions**
  - not in any single wavefunction, but in how they change

Mind the gap

Still no free lunch, however...

- EC is a variational method
- **cannot go beyond what bare interaction gives in same model space!**



So now what?

Part II

Escaping the model space

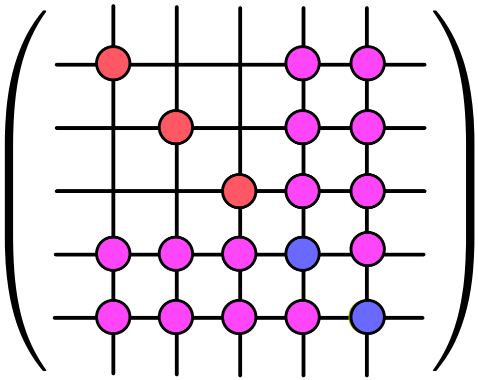
Model-space perturbation theory

- **consider a Hamiltonian diagonalized in a (small) subspace**

$$H = \begin{pmatrix} H_{\phi\phi} & H_{\phi\psi} \\ H_{\psi\phi} & H_{\psi\psi} \end{pmatrix}$$

$$N_0 = \dim H_{\phi\phi} \ll \dim H = N_1$$

$$H_{\phi\phi} = \mathrm{diag}(\{\lambda_i\}_{i=1,..N_0})$$



- factor out large number X from diagonal entries of $H_{\psi\psi}$
- perturbative expansion for lowest eigenvalue and vector

$$|\psi_1\rangle = \sum_{n=0}^{\infty} X^{-n} \left(\sum_{i=1}^{N_0} x_i^{(n)} |\phi_i\rangle + \sum_{j=N_0+1}^{N_1} x_j^{(n)} |\psi_j\rangle \right) \ , \ \lambda_1^{\mathrm{full}} = \sum_{n=0}^{\infty} X^{-n} \lambda_1^{(n)}$$

  - **matching powers gives coupled recursive expressions for $x_j^{(n)}$ and $\lambda_1^{(n)}$**

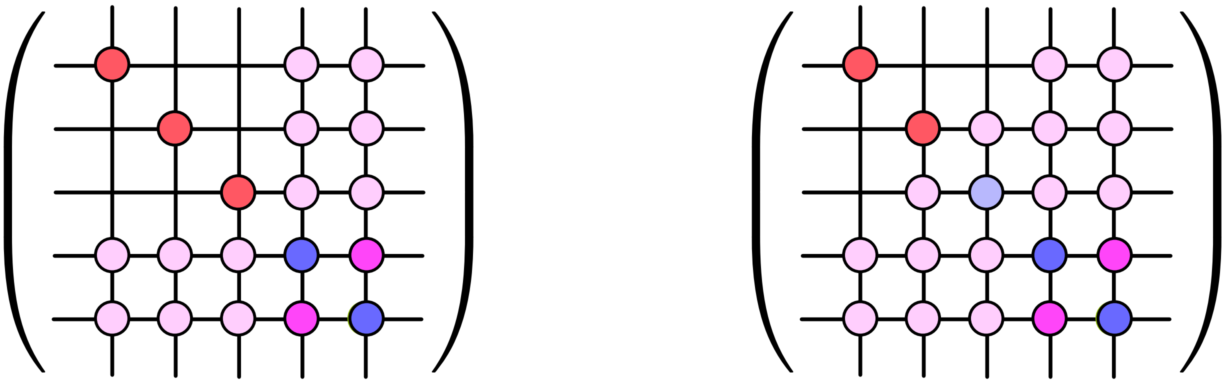
Model-space perturbation theory (cont'd)

Diagonalizing a small space can still be too expensive...

Model-space perturbation theory (cont'd)

Diagonalizing a small space can still be too expensive...

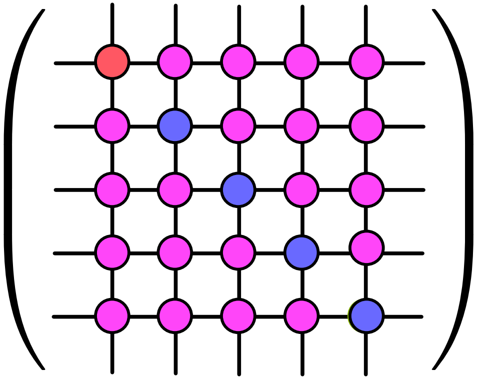
- actually, a partial diagonalization per se is ok ($\rightarrow$ Lanczos)
- but transforming the Hamiltonian is problematic...



- **cost for adjusting off-diagonal elements is significant**
  - scales with size of the full (large) space

Way out

Start from one-dimensional space ($N_{\max} = 0$)...



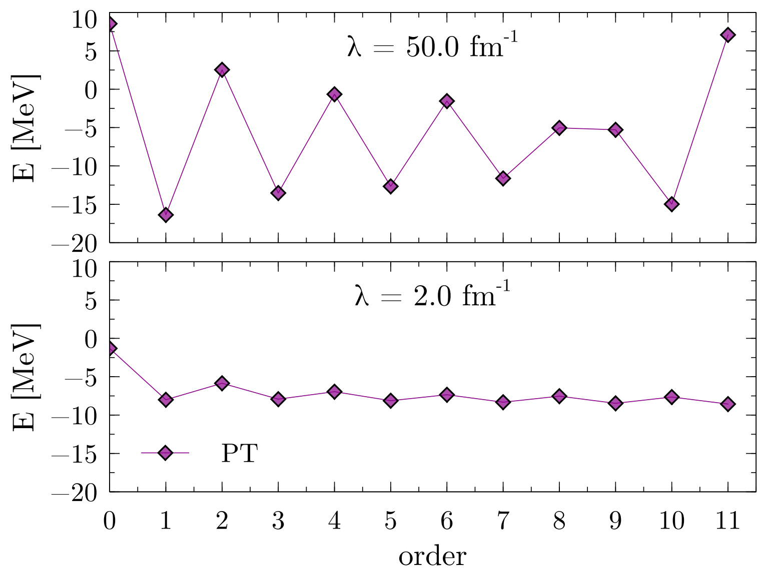
...i.e., directly use the given Hamiltonian

Failure

^{3}H NCSM calculation, $N_{\max} = 12$ model space

- EMN N3LO 500 interaction

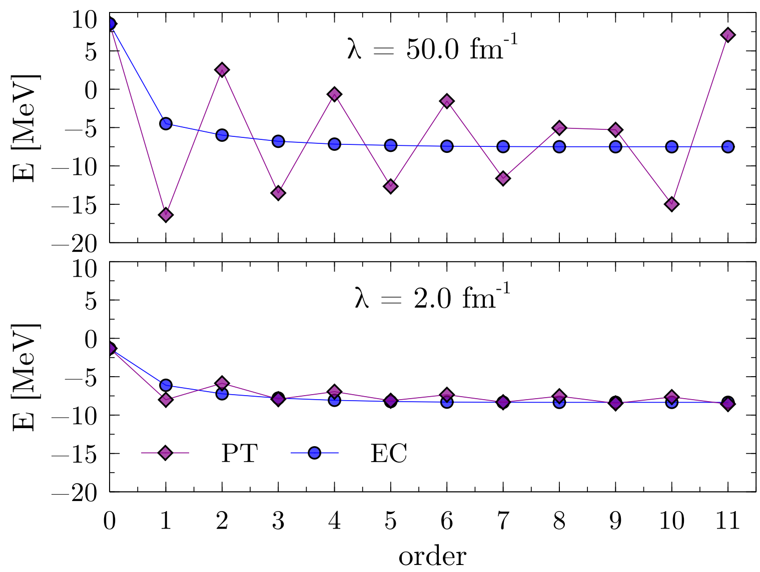
Entem et al., PRC **96** 024004 (2017)



- **perturbation theory does not converge!**
  - however, interaction clearly "more perturbative" for small SRG λ
  - convergence perhaps for very small λ

Saved by EC

- span space by the wavefunction corrections $|\psi_1^{(n)}\rangle \to x_j^{(n)}$, $n = 0, \cdots \text{order}$
- evaluate Hamiltonian between these states
- interpretation: $H = H_{\text{diag}} + c\, H_{\text{off-diag}}$, EC-extrapolate to $c = 1$



- **same input as PT, but now things converge (to the correct result!)**

Part III

EC as efficient emulator

Hamiltonian parameter spaces

- **consider now a Hamiltonian depending on several parameters:**

$$H = H_0 + V = H_0 + \sum_{k=1}^{d} c_k V_k \tag{1}$$

- in particular, V can be a chiral potential with LECs c_k
- Hamiltonian is element of d-dimensional parameter space
- typical for $\mathcal{O}(Q^3)$ calculation: 14 two-body LECs + 2 three-body LECs
- convenient notation: $\vec{c} = \{c_k\}_{k=1}^{d}$

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Generalized EC

- **EC construction is straightforward to generalize to this case:**
- simple replace $c_i \to \vec{c}_i$ in construction
  - $|\psi_i\rangle = |\psi(\vec{c}_i)\rangle$ for $i = 1, \cdot\cdot N_{\mathrm{EC}}$
  - $H_{ij} = \langle\psi_i|H(\vec{c}_{\mathrm{target}})|\psi_j\rangle$, $N_{ij} = \langle\psi_i|\psi_j\rangle$

Note: sum in Eq. (1) can be carried out in small (dimension = N_{EC}) space!

Need for emulators

1. Fitting of LECs to few- and many-body observables

- common practice now to use $A > 3$ to constrain nuclear forces, e.g.:
  - JISP16, NNLO_{sat}, α-α scattering

Shirokov et al., PLB **644** 33 (2007); Ekström et al., PRC **91** 051301 (2015); Elhatisari et al., PRL **117** 132501 (2016)

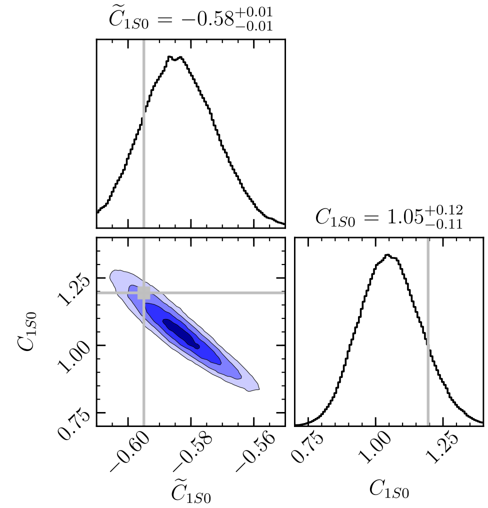
- **fitting needs many calculations with different parameters**

2. Propagation of uncertainties

- statistical fitting gives posteriors for LECs
- LEC posteriors propagate to observables

Wesolowski et al., JPG **46** 045102 (2019)

- **need to sample a large number of calculations**
- cf. talks yesterday by Sarah and Gautam



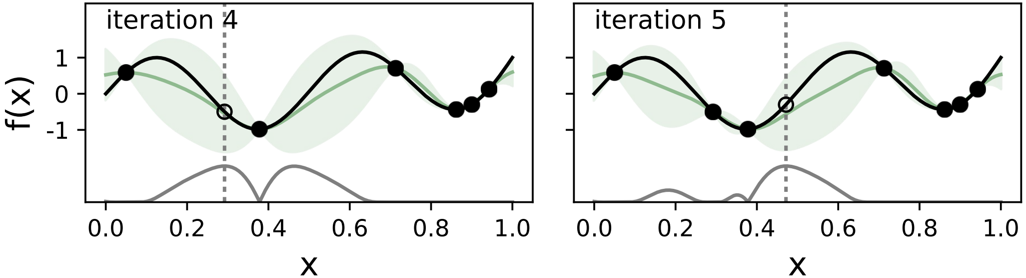
Emulators

Exact calculations can be prohibitively expensive!

Options

- **multi-dimensional polynomial interpolation**
  - simplest possible choice
  - typically too simple, no way to assess uncertainty

- **Gaussian process**



  - statistical modeling, iteratively improvable
  - interpolation with inherent uncertainty estimate

Ekström et al., arXiv:1902.00941

Recall

Eigenvector continuation can extrapolate!

Interpolation and extrapolation

Hypercubic sampling

- **want to cover parameter space $S = \{\vec{c}_i\}$ efficiently**
- Latin Hypercube Sampling can generate near random sample
- for examples that follow:
  - sample each component $c_k \in [-2, 2]$
  - vary d LECs, fix the rest at $\mathrm{NNLO}_{\mathrm{sat}}$ point

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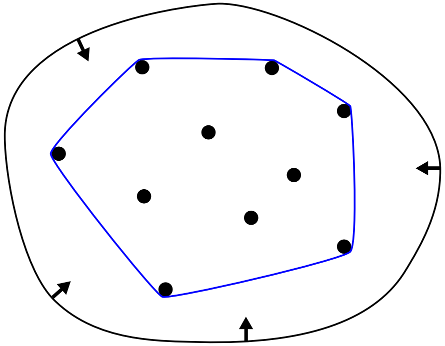
Ekström et al., PRC **91** 051301 (2015);

Convex combinations

- **distinguish interpolation and extrapolation target points**
- interpolation region is convex hull of the $\{\vec{c}_i\}$
  - $\text{conv}(S) = \sum_i \alpha_i \vec{c}_i$ with $\alpha_i \geq 0$ and $\sum_i \alpha_i = 1$
- extrapolation for $\vec{c}_{\text{target}} \notin \text{conv}(S)$
- **EC can handle both!**

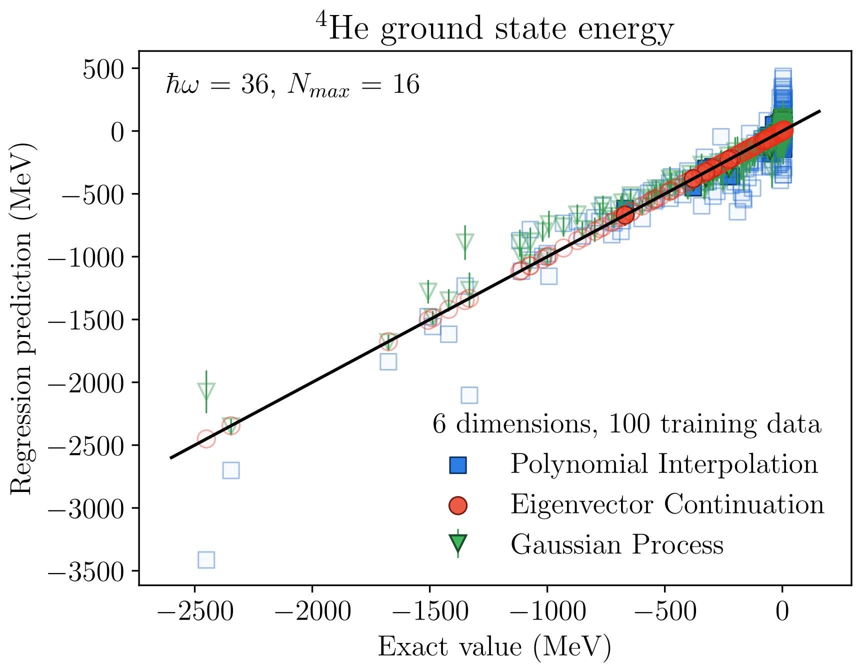


Pbroks13, Wikimedia Commons

Performance comparison: energy

Cross validation

- **compare emulation prediction agains exact result for set** $\{\vec{c}_{\mathrm{target},j}\}_{j=1}^{N}$
- underlying calculation: Jacobi NCSM (again)
- transparent symbols indicate extrapolation targets



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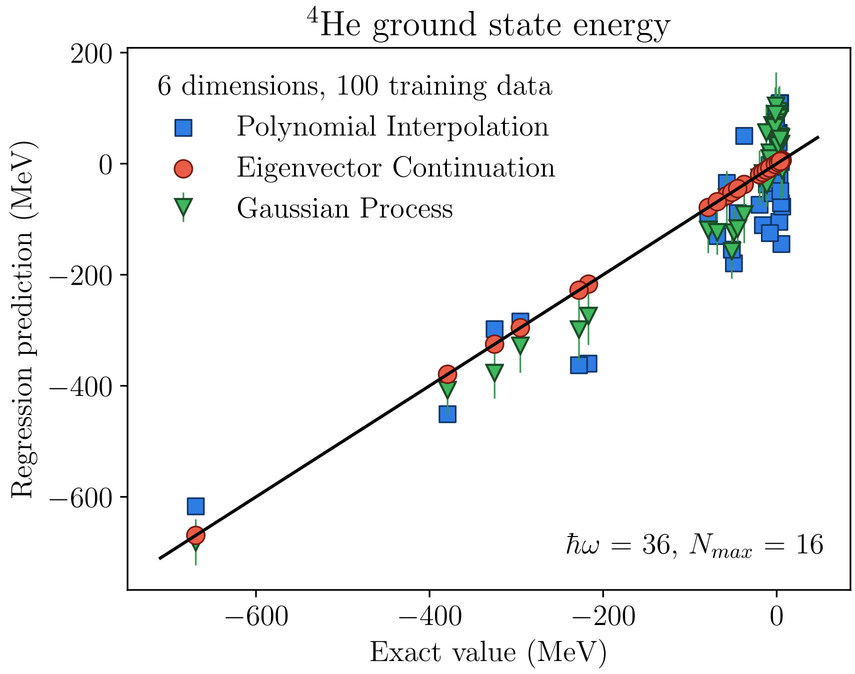

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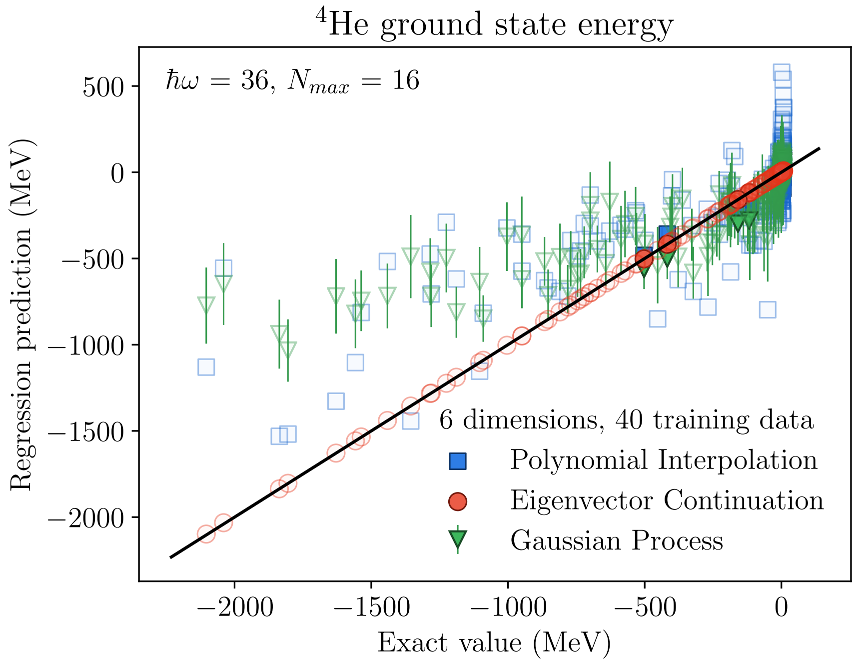
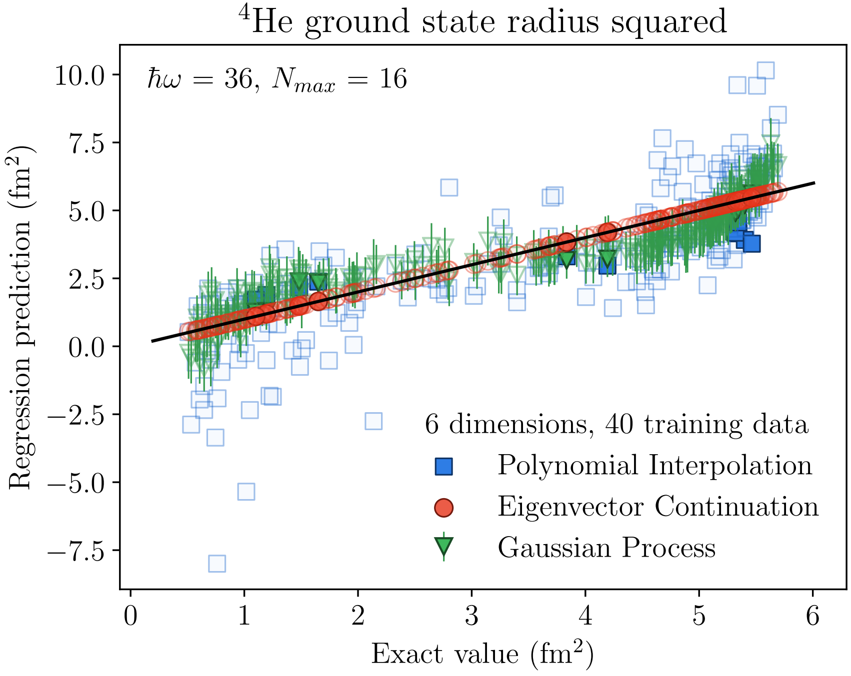


Performance comparison: radius

Operator evaluation

- generalized eigenvalue problem
- EC gives not only energy, but also a continued wavefunction
- **straightforward (and inexpensive) to evaluate arbitrary operators**



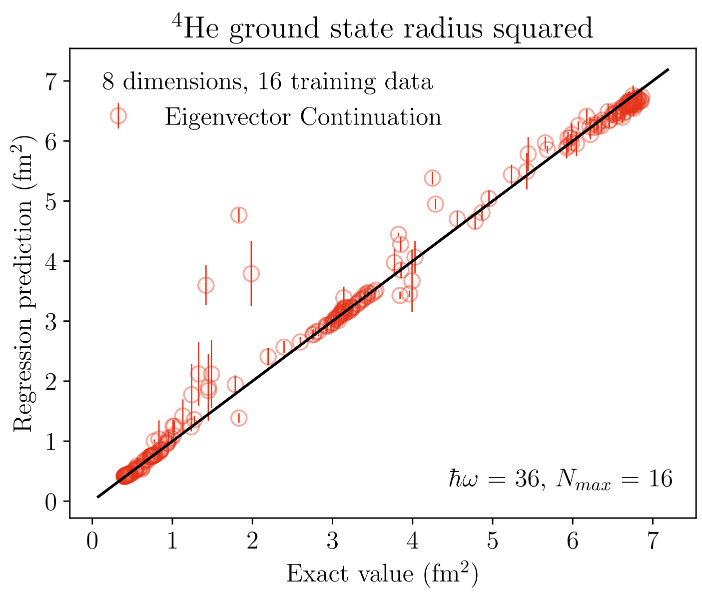
EC uncertainty estimate

- **EC is a variational method**
  - projection of Hamiltonian onto a subspace
  - dimension of this subspace determines the accuracy
  - rate of convergence currently being analyzed

D. Lee + A. Sarkar, work in progress

Bootstrap approach

- **leave out basis vectors one at a time, take mean and standard deviation**



Summary and outlook

This talk

- **eigenvector continuation can be used to reverse SRG**
  - conceptually interesting: implicit information about induced forces
- **convergent perturbative model-space extension**
  - effectively tame divergent expansion coefficients
  - interesting as computational method
- **eigenvector continuation efficient emulator**
  - highly competitive, accurate and efficient
  - can both interpolate and extrapolate from training set

Future directions

- larger systems, other methods (in particular: m-scheme NCSM)
- combined model-space and SRG EC
- application for large-scale uncertainty quantification

Thanks...

...to my collaborators:

- A. Schwenk, K. Hebeler (TU Darmstadt)
- A. Ekström (Chalmers U.)
- D. Lee, A. Sarkar (Michigan State U.)

...for funding:

SFB 1245

DFG Deutsche Forschungsgemeinschaft

German Research Foundation

...and to you, for your attention!