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MANY-BODY EMULATORS FOR NUCLEAR STRUCTURE

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European Research Council
Established by the European Commission

Hirschegg Workshop

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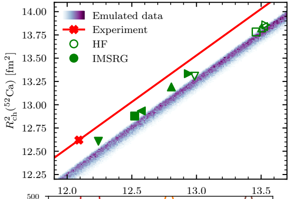
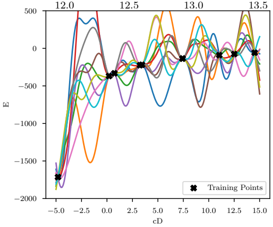
OUTLINE

- ☐ Eigenvector-continuation (EC)-based Hartree-Fock (HF) emulator
  Companys Franzke et al. arXiv:2510.08362 (2025)
  - ▷ Motivation
  - ▷ Emulator construction
  - ▷ Results for calcium radius puzzle
- ☐ Gaussian process (GP) emulators
  - ▷ Idea and construction
  - ▷ Preliminary results





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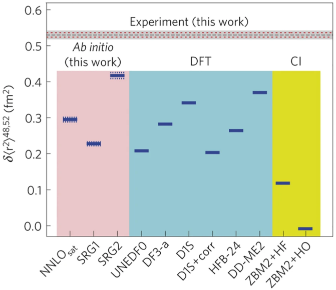
MOTIVATION

- Modern nuclear Hamiltonians from chiral effective field theory
  - Interactions depend on LECs c_i
    $\hat{V} = \hat{V}_0 + \sum_i c_i \hat{V}_i$
  - Need to be fit to experimental data
- **Radius puzzle** for ^{52}Ca - ^{48}Ca
  - Steep increase of charge radii cannot be explained



Garcia Ruiz et al., Nat. Phys. (2016).

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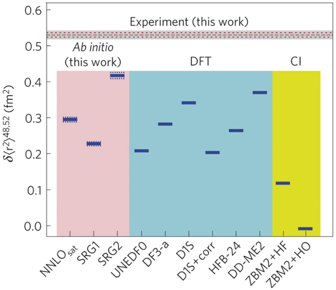
- **Radius puzzle** for ^{52}Ca - ^{48}Ca
  - Steep increase of charge radii cannot be explained
- Sensitivity study of LEC variations
  - Finding exact solution or approximations has a high computational cost

$\Longrightarrow$ Emulator for extracting solutions for different LEC values
König et al., PLB (2020)
Ekström, Hagen, PRL (2019)



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EIGENVECTOR CONTINUATION (EC)

- For Hamiltonians $\hat{H}(c)$ with smooth parametric dependence
  - For example $\hat{H} = \hat{H}_0 + c \cdot \hat{H}_1$
- Diagonalize Hamiltonian in reduced subspace of training vectors

$$HX = \epsilon NX$$

- With matrix elements

$$H_{pq} = \langle \Psi^{(p)} | \hat{H}(c) | \Psi^{(q)} \rangle$$

$$N_{pq} = \langle \Psi^{(p)} | \Psi^{(q)} \rangle$$

- Two different applications
  - This talk: as an **emulator** tool
  - Solution known for some c_i
  - Exact solutions used as EC basis
    e.g. König et al., PLB (2020)
    Furnstahl et al., PLB (2020)
    Companys et al., PRC (2023)
  - Other applications: as a perturbation theory resummation tool
    e.g. Demol et al., PRC (2020)
    Companys et al., PLB (2022)

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NON-SYMMETRIC FORMULATION

FROM SUN ET AL., PRX (2025)

- ☐ **Problem:** Since the Slater-Determinants are not a subspace, the emulated energies can lie below the HF energy even at the training points.

- ☐ **Goal:** Get emulator to reproduce training states at the training points

- ☐ Normal EC: Operator kernel $\mathbf{H}_{ij} = \langle \Phi^{\mathrm{HF}}(c_i) | \hat{H}(c) | \Phi^{\mathrm{HF}}(c_j) \rangle$

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- Normal EC: Operator kernel $\mathbf{H}_{ij} = \langle \Phi^{\mathrm{HF}}(c_i) | \hat{H}(c) | \Phi^{\mathrm{HF}}(c_j) \rangle$
- Non-symmetric EC: Operator kernel $\mathbf{H}_{ij} = \langle \Phi^{\mathrm{HF}}(c_i) | \hat{H}_{c_j}(c) | \Phi^{\mathrm{HF}}(c_j) \rangle$
- $\hat{H}_{c_j}(c)$ is the one-body part of $\hat{H}(c)$ normal ordered with respect to $|\Phi^{\mathrm{HF}}(c_j)\rangle$

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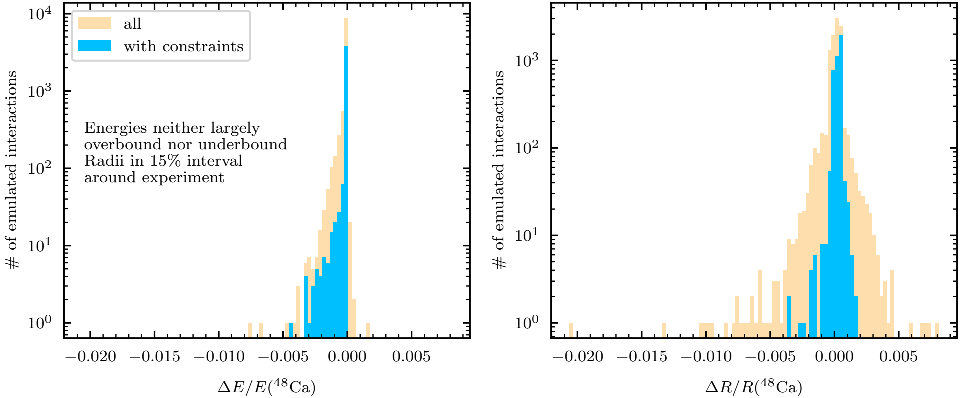
HARTREE-FOCK-BASED EMULATOR

- Eigenvector continuation (EC) based emulator
  - Diagonalization in submanifold spanned by training vectors
- Hartree Fock (HF) used for training
  - HF approximates charge radii well for softer chiral interactions
- Ground state from EC can be used to extract other observables
- Training state is not necessarily recovered at the training point for normal EC
  $\Longrightarrow$ **Training state recovered** using method from Sun et al., Phys. Rev. X (2025)
- For **validation** exact HF energies for 10000 random points were calculated

INTERACTION DISTRIBUTION

CROSS VALIDATION/EMULATOR ERROR



- ☐ Energy and radius error both below 0.5%

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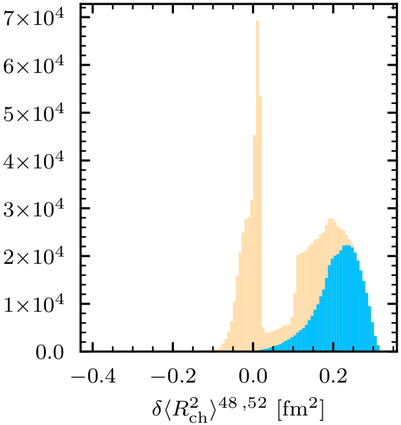
RESULTS FOR CALCIUM RADIUS PUZZLE

CAN 3N VARIATIONS EXPLAIN RADIUS INCREASE FROM $R^2_{^{52}\mathrm{Ca}}$ TO $R^2_{^{48}\mathrm{Ca}}$?



- HF emulator for calcium for very large LEC ranges
  - Variation of 3N LECs, NN interaction fixed N^{3}LO (here EM500 $\lambda = 1.8\,\mathrm{fm}^{-1}$):

c_1	$-0.81\,\mathrm{GeV}^{-1}$
c_3	$\in [-6.2\,\mathrm{GeV}^{-1}, -0.2\,\mathrm{GeV}^{-1}]$
c_4	$\in [0.4\,\mathrm{GeV}^{-1}, 10.4\,\mathrm{GeV}^{-1}]$
c_D	$\in [-5, 10]$
c_E	$\in [-2, 2]$

- For 3N variation at HF level no interaction with $\delta R^2 > 0.31\,\mathrm{fm}^2$

$\Longrightarrow$ **Main message:** At HF level 3N variations do not support experimental value

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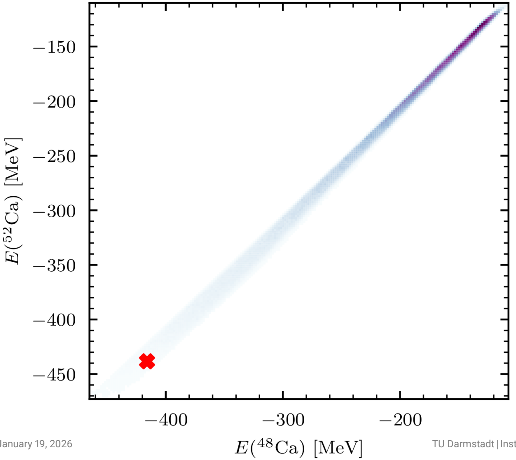
RESULTS FOR CALCIUM RADIUS PUZZLE

HIGHLY CORRELATED RADII



- Energies highly correlated
  - Experimental value on correlation line

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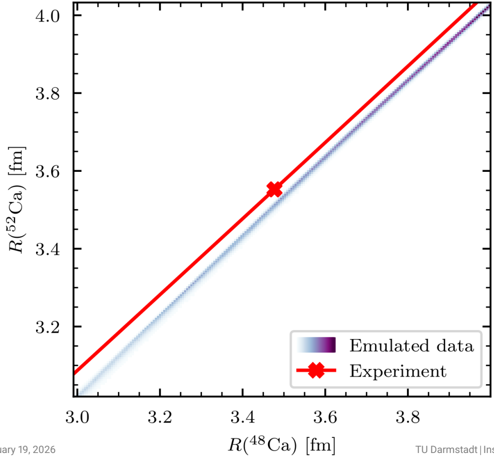

- ☐ Energies highly correlated
  - ▷ Experimental value on correlation line
- ☐ Radii highly correlated
  - ▷ Experimental value not on correlation line
- ☐ For 3N variation at HF level no interaction with $\delta R^2 > 0.31\,\mathrm{fm}^2$

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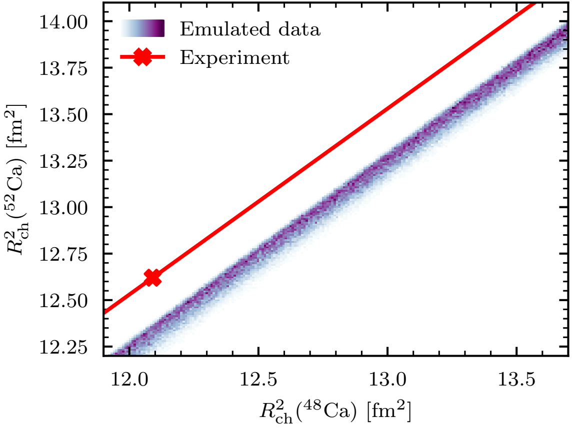
RESULTS FOR CALCIUM RADIUS PUZZLE

WHAT ABOUT A DIFFERENT NN INTERACTION?



- Before: 1.8/2.0 (EM) NN interaction
- Here: N^{3}LO EMN 450 SRG-evolved $\lambda = 1.8$ fm^{-1}
- For 3N variation at HF level no interaction with $\delta R^2 > 0.31\,\text{fm}^2$
- **Additional challenge:** Emulator less accurate, probably due to unbound training states

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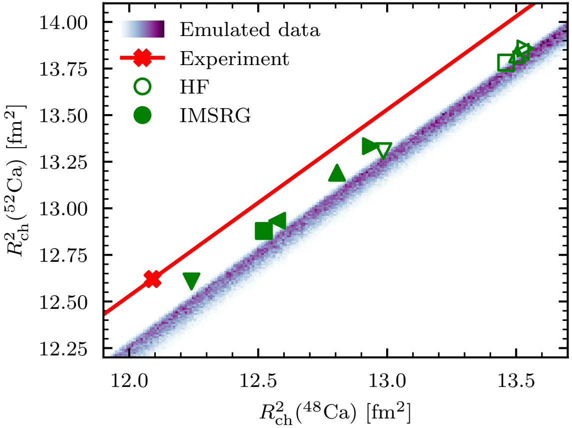
RESULTS FOR CALCIUM RADIUS PUZZLE

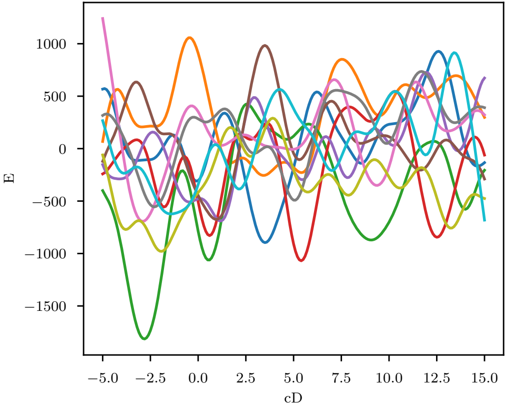
BEYOND HARTREE-FOCK



- Selected IMSRG calculations do not simultaneously reach experimental δR^2 and radii or energies
- Even in preliminary test set: Corrections for δR^2 from HF to IMSRG of up to 40%
- **Challenge:** IMSRG corrections for δR^2 can be large and are difficult to predict

GAUSSIAN PROCESSES

C. E. V. RASMUSSEN AND C. K. I. V. WILLIAMS, *GAUSSIAN PROCESSES FOR MACHINE LEARNING* (2005)



- ☐ **Goal**: Emulate IMSRG
- ☐ Data driven approach
  - ▷ No need for the full ground state
- ☐ Emulated observable function out of multivariate normal distribution

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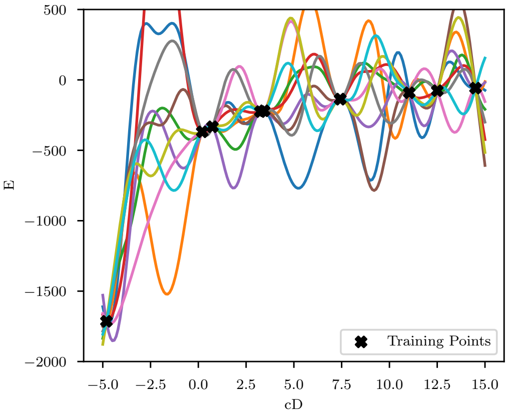

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- Multivariate normal restricted through training points

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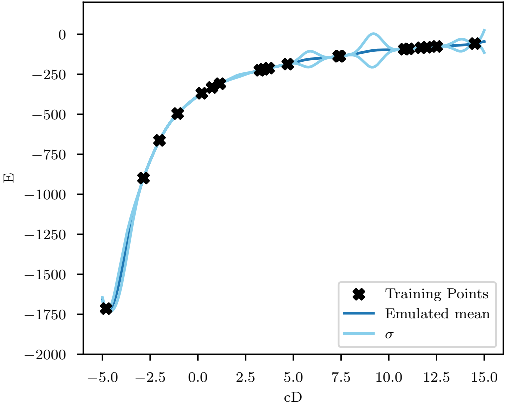

- **Goal**: Emulate IMSRG
- Data driven approach
  - ▷ No need for the full ground state
- Emulated observable function out of multivariate normal distribution
- Multivariate normal restricted through training points
- Mean of multivariate normal as emulated observable
- Standard deviation can give estimate for emulation error

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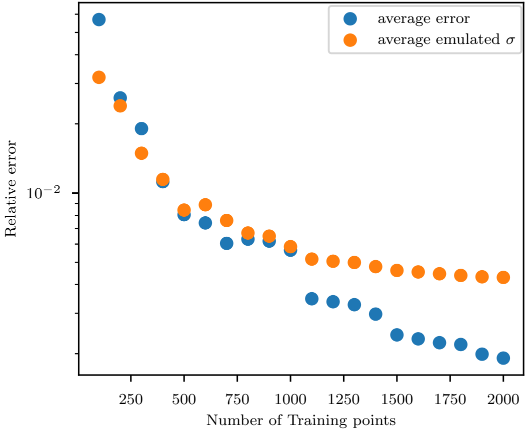
GAUSSIAN PROCESSES

HYPERPARAMETERS AND COVARIANCE FUCTION

- Hyperparameters enter through covariance function
  - Possible choice RBF kernel: $k(x_a, x_b) = \sigma \exp\left(\frac{-1}{2\ell^2}\|x_a - x_b\|^2\right)$
  - σ and l hyperparameters
  - $\frac{-1}{2\ell^2}$ can be matrix for multidimensional x
- Hyperparameters need to be optimized
  - With cross validation and minimized emulator error
  - Or maximize posterior likelihood/ minimize negative logarithmic likelihood

PRELIMINARY RESULTS FOR THE RADIUS



- Emulator trained from data generated with EC emulator from previous project
- Negative logarithmic likelihood minimized for hyperparameter optimization
- Different training point numbers
- Emulated error and error on a test set for radius emulators
- Good emulator accuracy for radius emulator

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NEXT STEPS

- ☐ Reduce training point number
  - ▷ Active subspace learning
  - ▷ Can emulators optimized on HF then be trained on IMSRG?
- ☐ Improve hyperparameter optimization
  - ▷ So far highly dependent on the minimizer
  - ▷ Possibly with gradient-based minimizers or sampling
- ☐ Go to IMSRG for training

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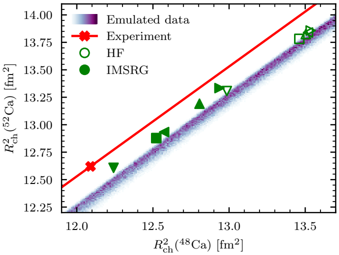
SUMMARY

THANK YOU FOR YOUR ATTENTION!!

- ☐ Emulator at HF level with ‰ accuracy for energies and radii
  - ▷ Other ground-state observables accessible as well
- ☐ At HF level:
  - ▷ 3N variations cannot explain the increase in charge radii
- ☐ Discrepancy to IMSRG for δR^2 too large for our large 3N LEC variation
- ☐ GPs promising for IMSRG emulator
  - ▷ So far implemented at HF level



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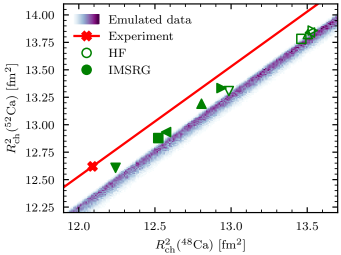

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