TECHNISCHE UNIVERSITÄT DARMSTADT

# MANY-BODY EMULATORS FOR NUCLEAR STRUCTURE

Margarida Companys Franzke

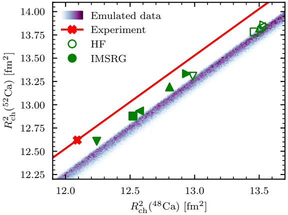
PAINT26 workshop at TRIUMF

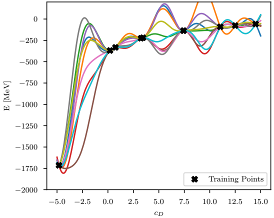
European Research Council
Established by the European Commission

# OUTLINE

- ☐ Eigenvector-continuation (EC)-based Hartree-Fock (HF) emulator
  Companys Franzke et al., arXiv:2510.08362 (2025)
  - ▷ Motivation: the calcium radius puzzle
    Garcia Ruiz et al., Nat. Phys. (2016).
  - ▷ Emulator construction
  - ▷ Results for calcium radius puzzle

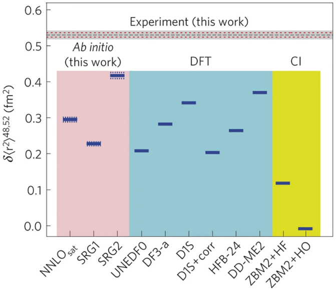
- ☐ Gaussian process (GP) emulators
  - ▷ Idea and construction
  - ▷ Preliminary results



# MOTIVATION

- Modern nuclear Hamiltonians from $\chi$EFT
  - 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
    $\delta\langle r^2\rangle^{48,52} = R^2_{\mathrm{ch}}(^{52}\mathrm{Ca}) - R^2_{\mathrm{ch}}(^{48}\mathrm{Ca})$




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

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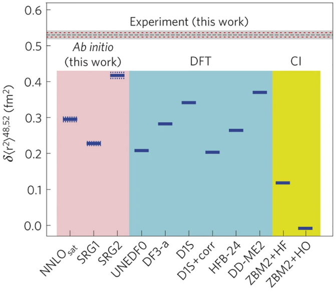
    $\delta\langle r^2\rangle^{48,52} = R^2_{\mathrm{ch}}(^{52}\mathrm{Ca}) - R^2_{\mathrm{ch}}(^{48}\mathrm{Ca})$
- Sensitivity study of LEC variations
  - Explain uncertainties

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




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

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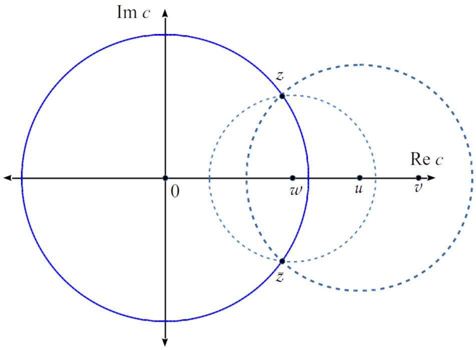
# EIGENVECTOR CONTINUATION (EC)

## GENERAL IDEA

- For Hamiltonians $\hat{H}(c)$ with smooth parametric dependence
  - For example $\hat{H} = \hat{H}_0 + c \cdot \hat{H}_1$

- Based on **analytical continuation** of eigenvalue spectrum outside original domain
  Frame *et al.*, PRL (2018)
  - Eigenvector less sensitive to variation in $c$




Frame, arXiv:1905.02782 (2019)

# 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
  - First part: as an **emulator** tool
  - Solution known for some $c$ values
  - 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 (PT) resummation tool
    e.g. Demol et al., PRC (2020)
    Companys et al., PLB (2022)

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# SPECIALTY OF HF EMULATORS

## FROM SUN ET AL., PRX (2025)

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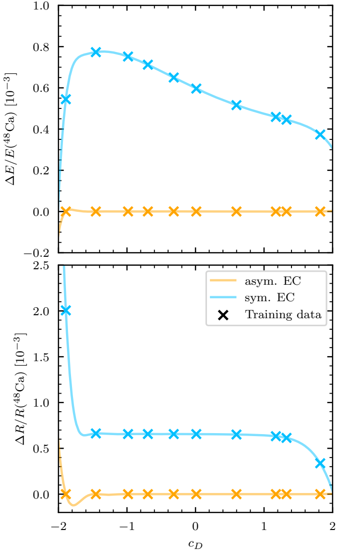
- Normal EC: Operator kernel $\mathbf{H}_{ij} = \langle \Phi^{\mathrm{HF}}(c_i) | \hat{H}(c) | \Phi^{\mathrm{HF}}(c_j) \rangle$
- Non-symmetric EC: Operator kernel $\mathbf{H}_{ij} = \langle \Phi^{\mathrm{HF}}(c_i) | \hat{H}_{c_j}(c) | \Phi^{\mathrm{HF}}(c_j) \rangle$
- $\hat{H}_{c_j}(c)$ is the one-body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




Companys Franzke et al., arXiv:2510.08362 (2025)

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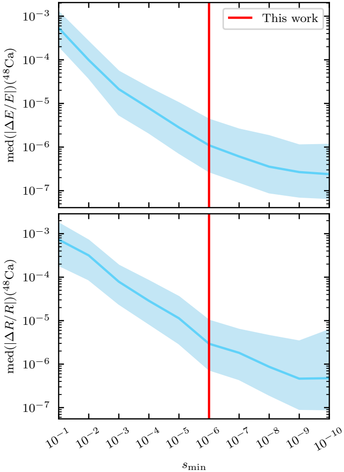
# REGULARIZATION FOR NUMERICAL STABILITY

- ☐ Norm matrix can get singular
  - ▷ Singular value decomposition (SVD) $N = L\Sigma R^T$
  - ▷ $\Sigma$ has diagonal entries close to zero
- ☐ Cut out small singular values ($< s_{min}$) for more numerical stability:
  $L \rightarrow \tilde{L}$, $\Sigma \rightarrow \tilde{\Sigma}$ and $R \rightarrow \tilde{R}$
- ☐ Project norm and operator kernel onto regularized subspace:
  $\tilde{H} = \tilde{\Sigma}^{-1/2}\tilde{L}^T H \tilde{R}\tilde{\Sigma}^{-1/2}$
- ☐ 100 training points and $s_{min} = 10^{-6}$ dimension reduces to $\approx 70$




Companys Franzke et al., arXiv:2510.08362 (2025)

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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., PRX (2025)
- For **validation** exact HF energies for $10,000$ random points were calculated

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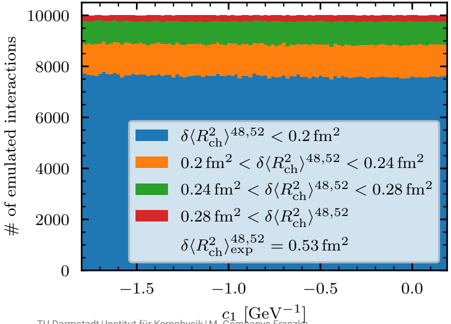
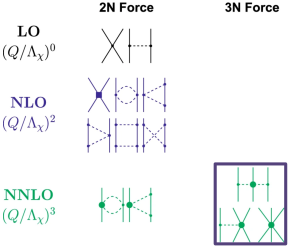
# INTERACTION AND TRAINING MANIFOLD

- ☐ HF emulator for calcium for very large 3N LEC ranges with fixed NN interaction fixed $N^3LO$ (here EM500 $\lambda = 1.8\,\mathrm{fm}^{-1}$)
- ☐ Variation of $c_1$ has little influence on $\delta R^2$

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



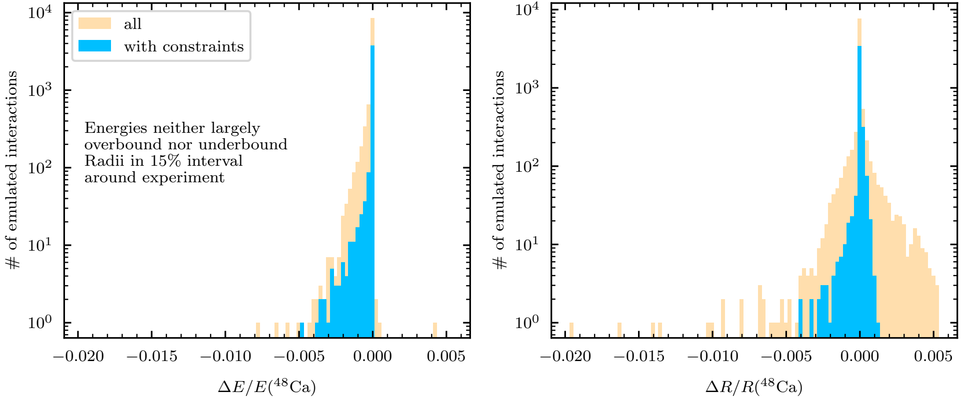




Machleidt and Sammarruca, Eur. Phys. J. A (2020)

Companys Franzke et al., arXiv:2510.08362 (2025)

# INTERACTION DISTRIBUTION

## CROSS VALIDATION/EMULATOR ERROR




- ☐ Energy and radius error both below 0.5%

Companys Franzke et al., arXiv:2510.08362 (2025)

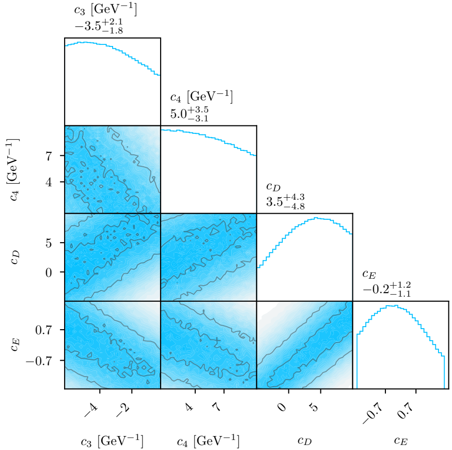
# RESULTS FOR CALCIUM RADIUS PUZZLE

## RESTRICT THE TRAINING MANIFOLD

- ☐ What if we restrict the training points to the same constraints as the emulated points?

$$-466\,\text{MeV} < E(^{48}\text{Ca}) < -100\,\text{MeV}$$

$$2.95\,\text{fm} < R(^{48}\text{Ca}) < 4.00\,\text{fm}$$



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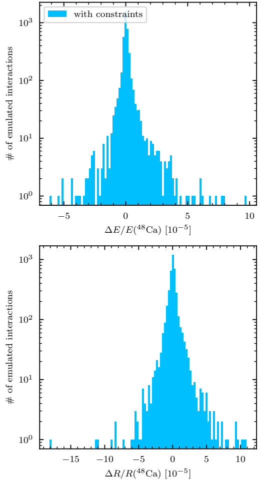
- Accuracy on constraint emulation data improves to $\approx 10^{-4}$
- Accuracy for unconstrained emulation data worsens ($|\frac{\Delta E}{E}| > 1$, $|\frac{\Delta R}{R}| \approx 0.5$)
- From here we use the restricted training set



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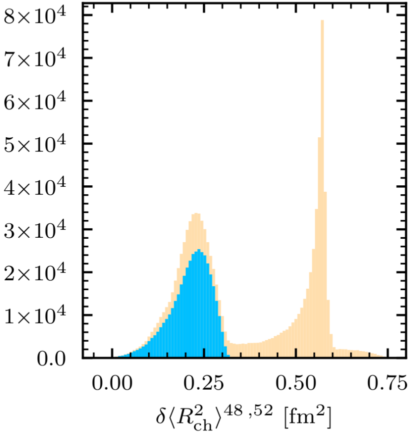
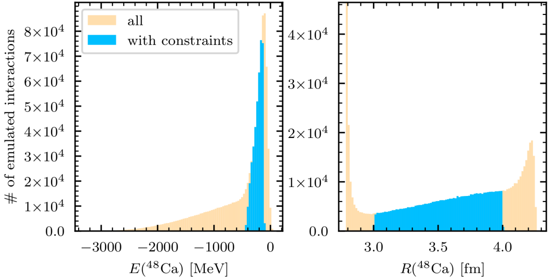
# RESULTS FOR CALCIUM RADIUS PUZZLE

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




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

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



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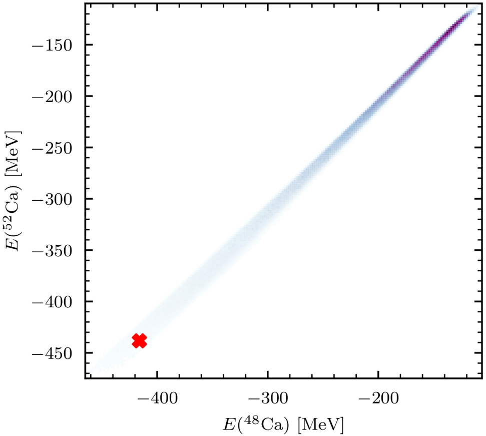
# RESULTS FOR CALCIUM RADIUS PUZZLE

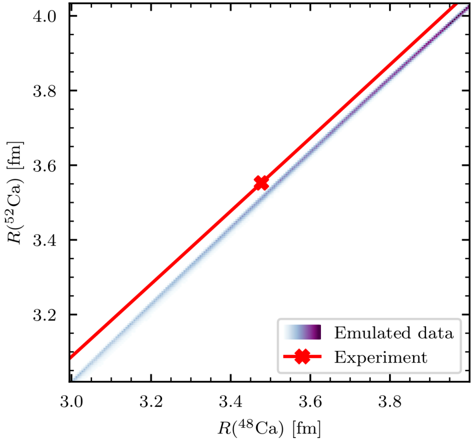
## HIGHLY CORRELATED ENERGIES




- Energies highly correlated
  - Experimental value on correlation line

# RESULTS FOR CALCIUM RADIUS PUZZLE

## HIGHLY CORRELATED RADII




- ☐ 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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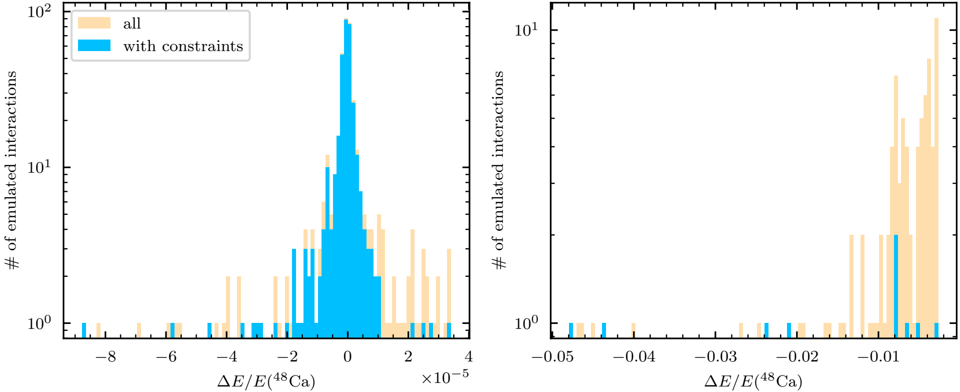
# RESULTS FOR CALCIUM RADIUS PUZZLE

## WHAT ABOUT A DIFFERENT NN INTERACTION?




- ☐ Constrained training set for $N^3LO$ EMN 450 unevolved would require to many training points

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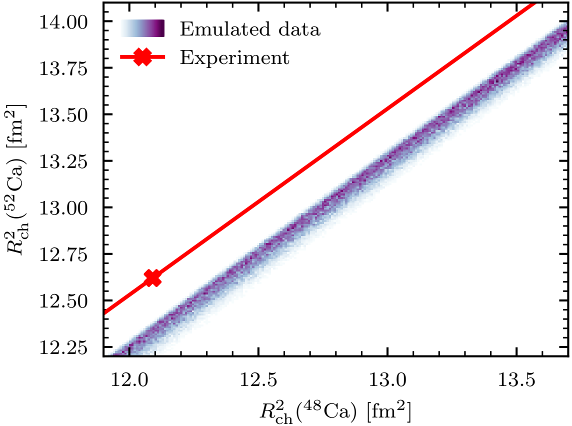
# RESULTS FOR CALCIUM RADIUS PUZZLE

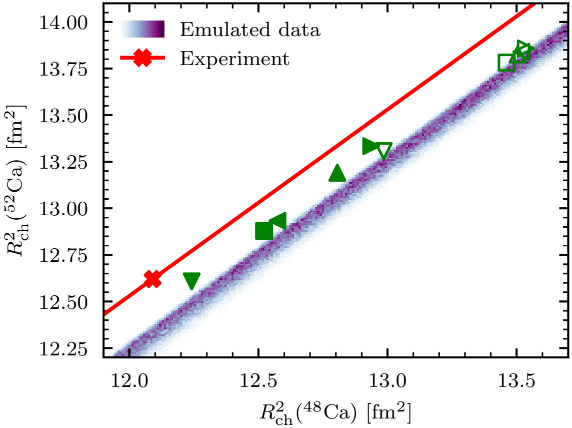
## WHAT ABOUT A DIFFERENT NN INTERACTION?




- ☐ 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 $\delta R^2 > 0.31\,\mathrm{fm}^2$
- ☐ **Additional challenge:** Emulator less accurate, probably due to unbound training states

# RESULTS FOR CALCIUM RADIUS PUZZLE

## BEYOND HARTREE-FOCK




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

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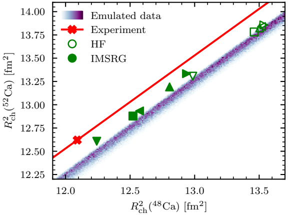
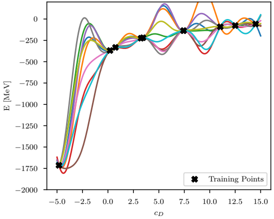
# OUTLINE

- ☐ Eigenvector-continuation (EC)-based Hartree-Fock (HF) emulator
  Companys Franzke et al., arXiv:2510.08362 (2025)
  - ▷ Motivation: the calcium radius puzzle
    Garcia Ruiz et al., Nat. Phys. (2016).
  - ▷ Emulator construction
  - ▷ Results for calcium radius puzzle
- ☐ Gaussian process (GP) emulators
  - ▷ Idea and construction
  - ▷ Preliminary results



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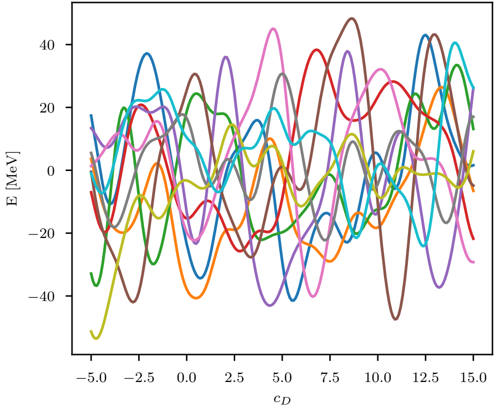
# GAUSSIAN PROCESSES

## MOTIVATION

- **Goal**: Emulate IMSRG
- EC excellent method for emulator construction, BUT wave function needed
- IMSRG does not give access to the full wave function
- Data driven approach
  - No need for the full ground state

# GAUSSIAN PROCESSES

## METHOD




Companys Franzke et al., in prep.

- Emulated observable function out of multivariate normal distribution
- Left: Exploratory $c_D$ variations at HF level

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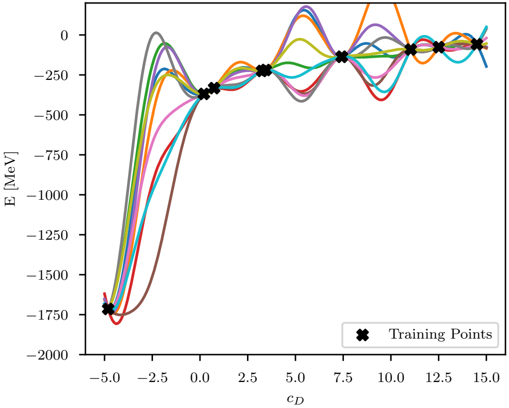


Companys Franzke et al., in prep.

- ☐ Emulated observable function out of multivariate normal distribution
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- ☐ Multivariate normal restricted through training points

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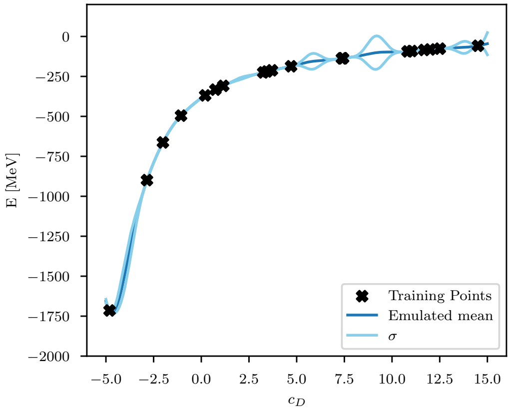


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- ☐ Emulated observable function out of multivariate normal distribution
- ☐ Left: Exploratory $c_D$ variations at HF level
- ☐ Multivariate normal restricted through training points
- ☐ Mean of multivariate normal as emulated observable
- ☐ Standard deviation can give estimate for emulation error
- ☐ Mean and standard deviation are influenced by hyperparameters in training process

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# GAUSSIAN PROCESSES

## HYPERPARAMETERS AND COVARIANCE FUNCTION

- Hyperparameters enter through covariance function
  - Possible choice radial basis function (RBF) kernel:
    $k(x_a, x_b) = \sigma \exp\left((x_a - x_b)\frac{-1}{2\ell^2}(x_a - x_b)\right)$
  - $\sigma$ and $\ell$ hyperparameters
    - $\rightarrow$ $\frac{-1}{2\ell^2}$ correlation-length (matrix)
- Hyperparameters need to be optimized
  - With cross validation and minimized emulator error or
  - Maximize posterior likelihood/minimize negative logarithmic likelihood

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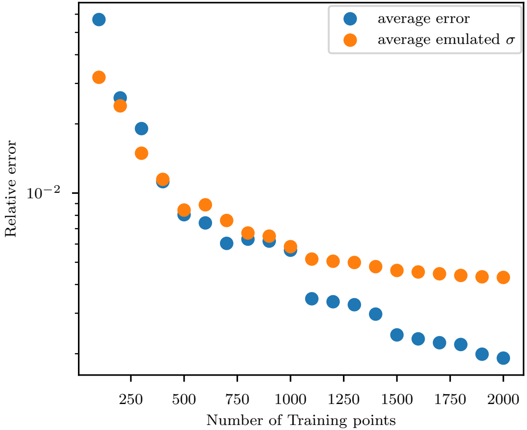
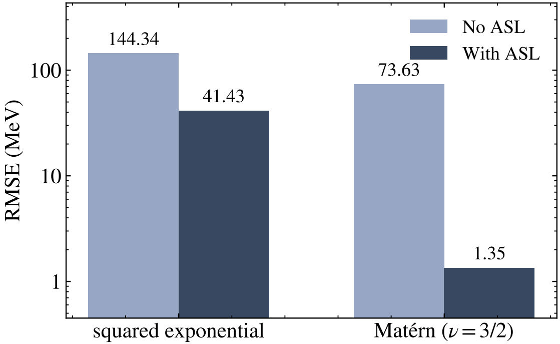
# PRELIMINARY RESULTS FOR THE RADIUS




- 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

# ACTIVE SUBSPACE LEARNING (ASL)




work with Tom Plies

- ☐ Number of correlation-length hyperparameters grows quadratically with number of varied parameters (LECs)
- ☐ Idea active subspace learning: Diagonalize correlation-length matrix for linear relation between number of hyperparameters and LECs
- ☐ Important spatial directions in the parameter space need to be identified
- ☐ Technically, cost can be further reduced by removing less important spatial directions

# NEXT STEPS

- ☐ Reduce training point number
  - ▹ Further test active subspace learning
  - ▹ Can emulators optimized on HF then be trained on IMSRG?
- ☐ Improve hyperparameter optimization
  - ▹ Can we optimize them to get a good emulated error?
- ☐ Look for alternatives to find the emulation error
- ☐ Go to IMSRG for training

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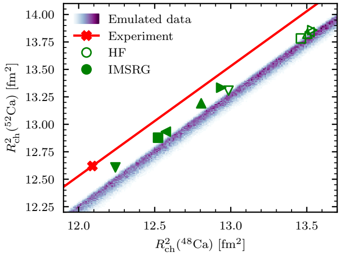
# SUMMARY

- 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 $\delta R^2$ too large for our large 3N LEC variation
- GPs promising for IMSRG emulator
  - So far implemented at HF level




**Collaborators**: T. Plies, A. Tichai, K. Hebeler and A. Schwenk

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**THANK YOU FOR YOUR ATTENTION!!**

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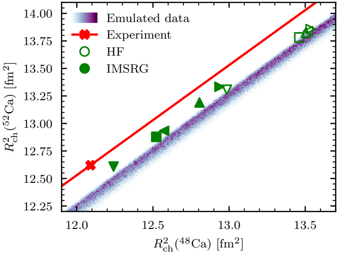


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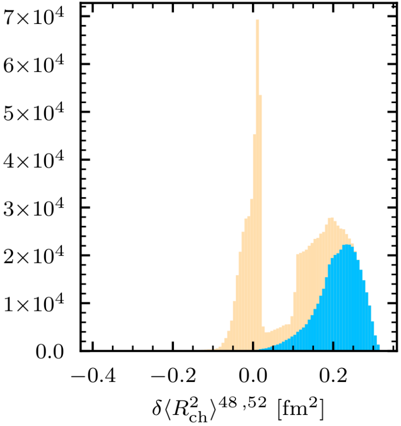
# BACK UP

## RESULTS FOR UNCONSTRAINED TRAINING POINTS




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

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