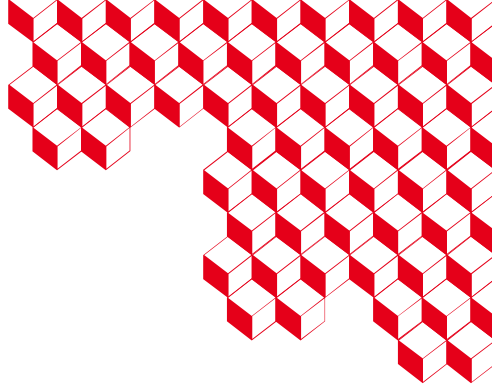


ESNT WORKSHOP

Emulation of PGCM calculations using the eigenvector continuation method

A. Roux

T. Duguet, J-P. Ebran, V. Somà, M. Frosini

24/05/2024

Outline

Part 1 : general considerations

- Introduction
- GCM formalism
- GCM workflow
- Emulator workflow
- Emulator quality
- Grassmannian distance

Part 2 : results

- The model
- Subspace distance
- Brute-force self-learning
- Fixed common space
- Under and over training
- Emulator quality vs subspace distance
- Computational cost

Part 1 : general considerations Introduction

PGCM ⟶ Projected Generator Coordinate Method

- Beyond mean-field approximation of A-body nuclear problem (HFB)
- Static correlations & collective spectroscopy

EC ⟶ Eigenvector Continuation*

- Emulate eigensolutions of parametrized hamiltonian

PGCM-EC

- Same underlying formalism
- Taking advantage of

$$H^{\mu} = \sum_{k=1}^{n_p} \mu^k h_k$$

- Emulate PGCM for arbitrary μ with negligible cost
- Uncertainty propagation

* D.Frame et al, PRL 121, 032508 (2018)

A.Ekstrom, G.Hagen, arXiv:1910.02922v1 (2019)

T.Duguet et al, arXiv:2310.19419v1 (2023)

Part 1 : general considerations GCM formalism

PGCM state → $|\Psi\rangle = \sum_q f_q P |\Phi_q\rangle$ → Constrained HFB states

$\delta \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = 0$

Symmetry restoring projection (N, Z, J)

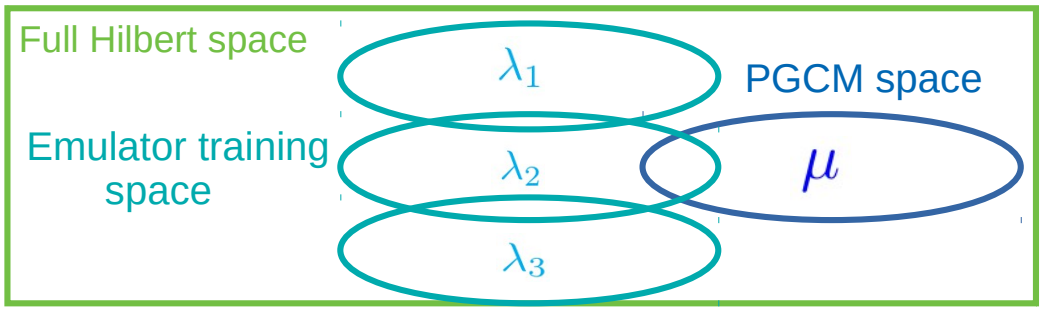
PGCM → f_q obtained by extremizing energy in physically-inspired small-dimensional subspace

Strong point of PGCM

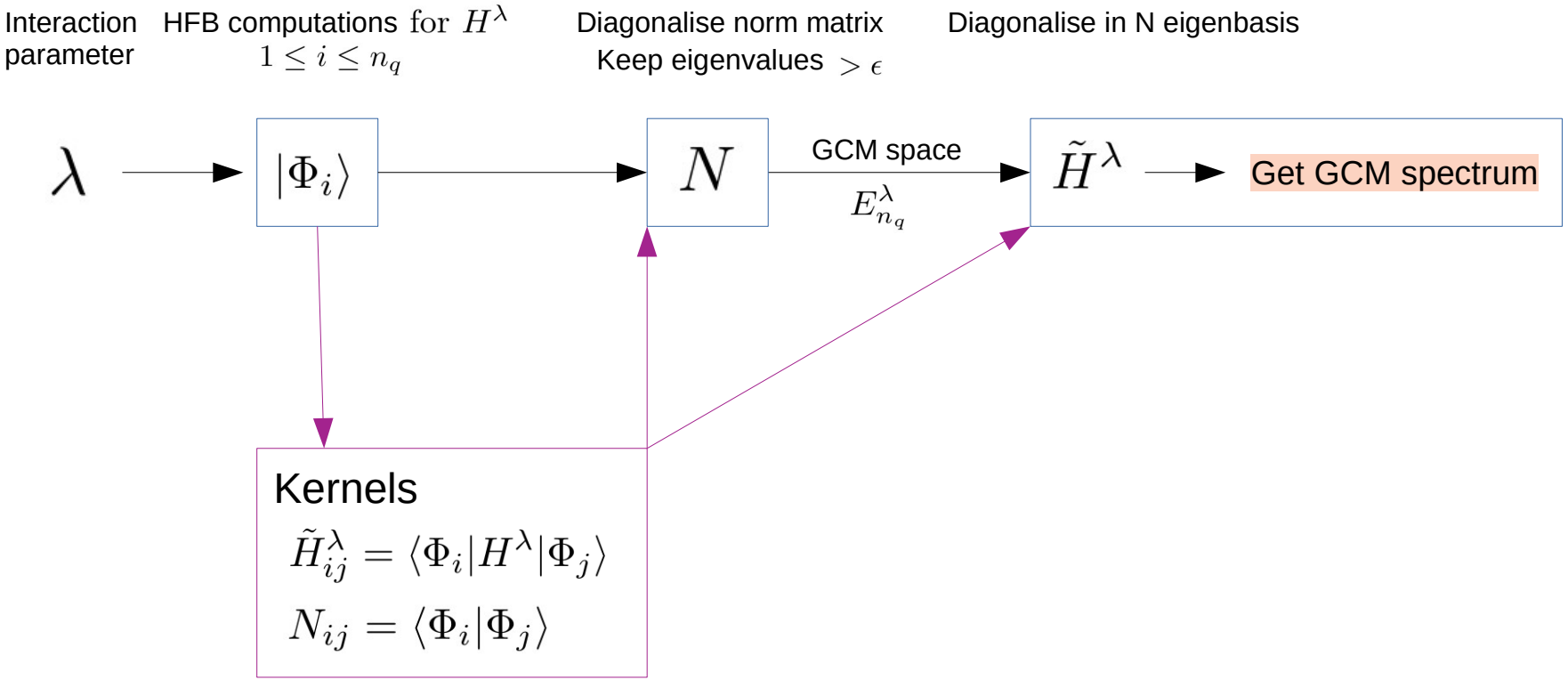
→ Ab initio collective spectroscopy

Emulator → needs to emulate both coefficients and subspace

Challenging point for emulator



Part 1 : general considerations GCM workflow



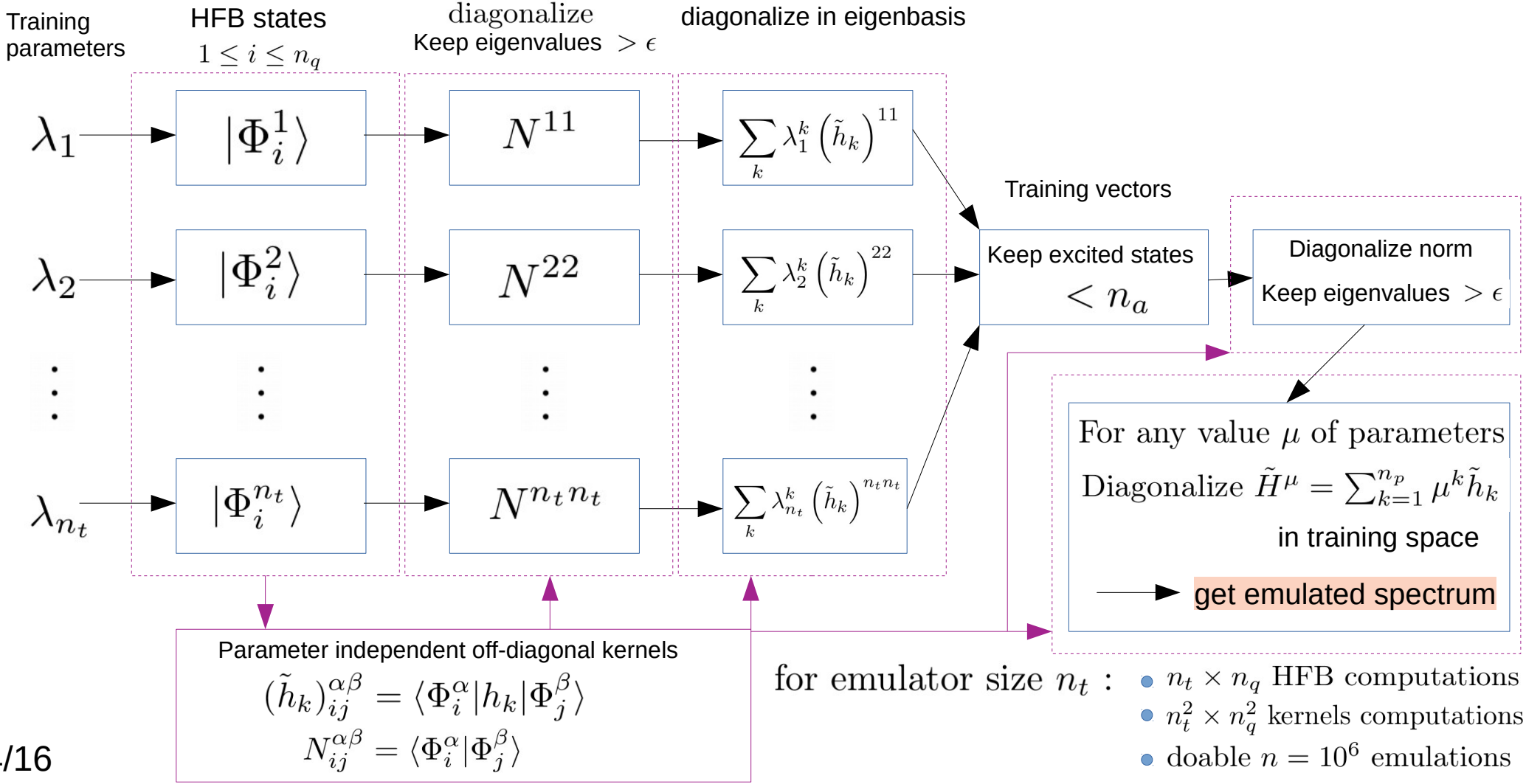
For n GCM computations :

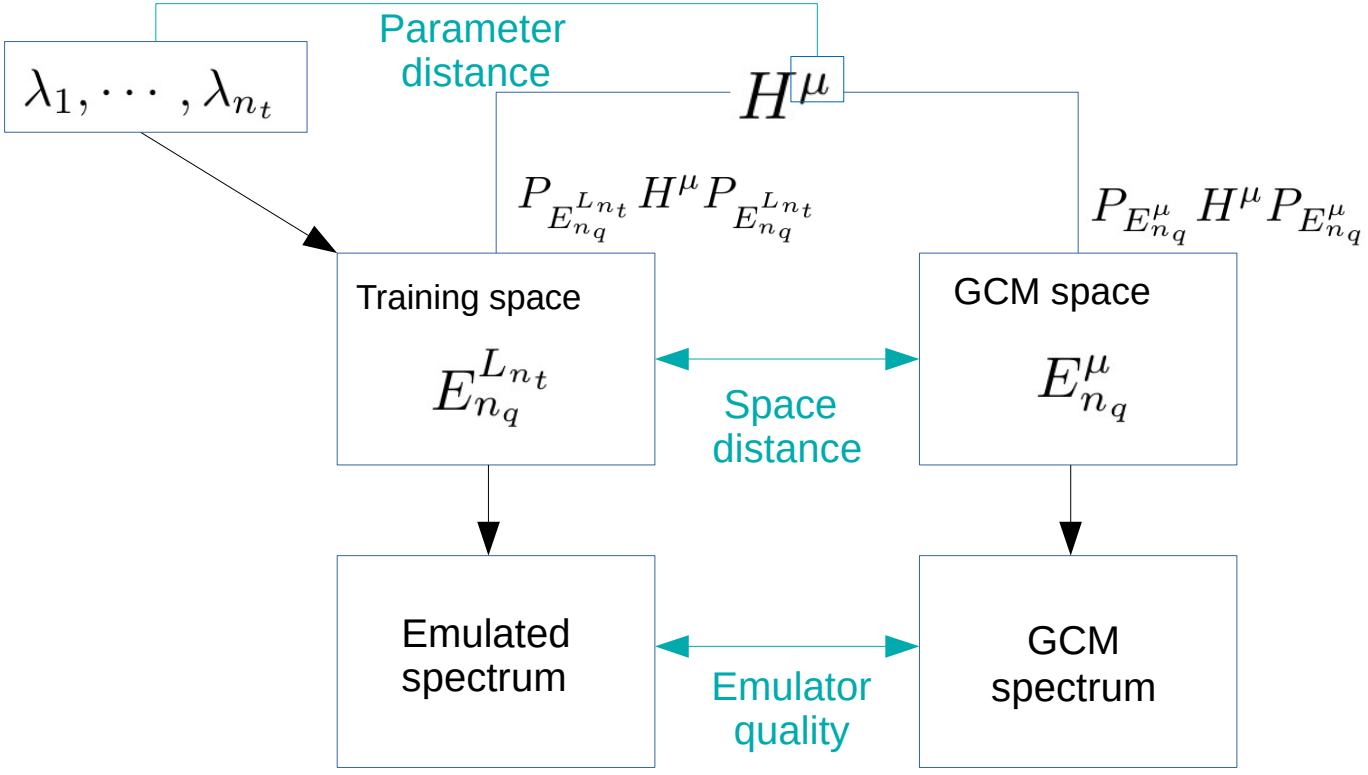
- $n \times n_q$ HFB computations
- $n \times n_q^2$ kernels computations

Numerically undoable

$n \simeq 10^6$

Part 1 : general considerations Emulator workflow





- Parameter distance : Euclidean distance
- Space distance : Grassmannian distance
- Emulator quality : relative error

Are they correlated ?

- $\mathcal{H}$, n-dimensional Hilbert space
- $\mathrm{Gr}\,(k, \mathcal{H})$ set of k-dimensional linear subspace of $\mathcal{H}$
  - ⟶ $= O(n)/\left(O(k) \times O(n-k)\right)$
  - ⟶ homogeneous space
  - ⟶ riemannian manifold
    - ◆ geodesic distance
- For $V_1 \in \mathrm{Gr}\,(k, \mathcal{H})$, $V_2 \in \mathrm{Gr}\,(l, \mathcal{H})$, $k < l$ *

  define $\Omega^-(V_2) = \{W \in \mathrm{Gr}\,(k, \mathcal{H}) \mid W \subset V_2\} \subset \mathrm{Gr}\,(k, \mathcal{H})$
- $\delta(V_1, V_2) =$ minimal geodesic distance from V_1 to $\Omega^-(V_2)$
- $\delta(V_1, V_2) = 0 \iff V_1 \subset V_2$ or $V_2 \subset V_1$

  ⟶ δ is a premetric

*Ye and Lim, SIAM (2016)

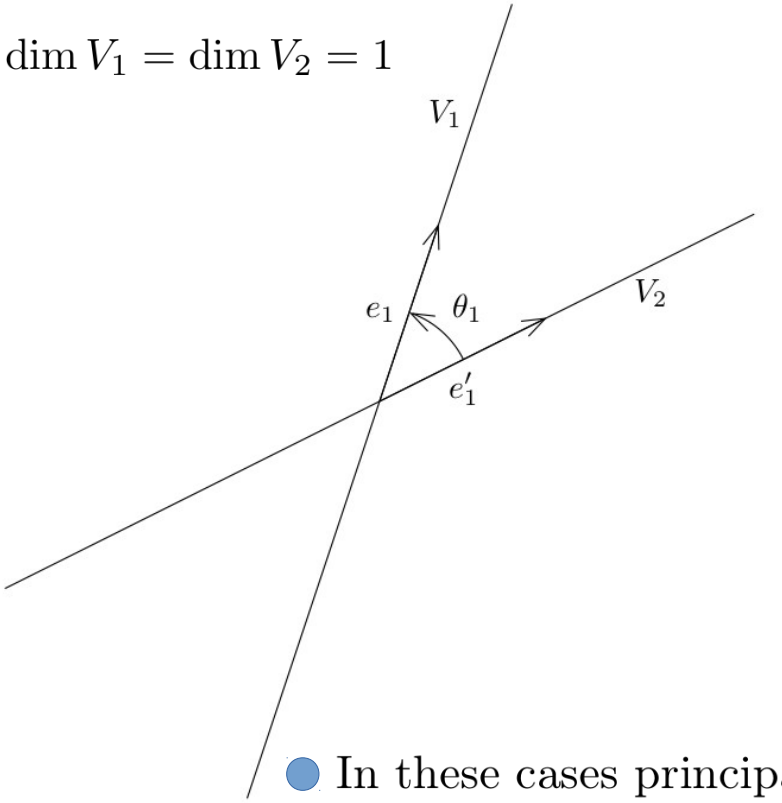
- Readily computable

  $(u_i)_{1 \le i \le k}$ orthonormal basis of V_1

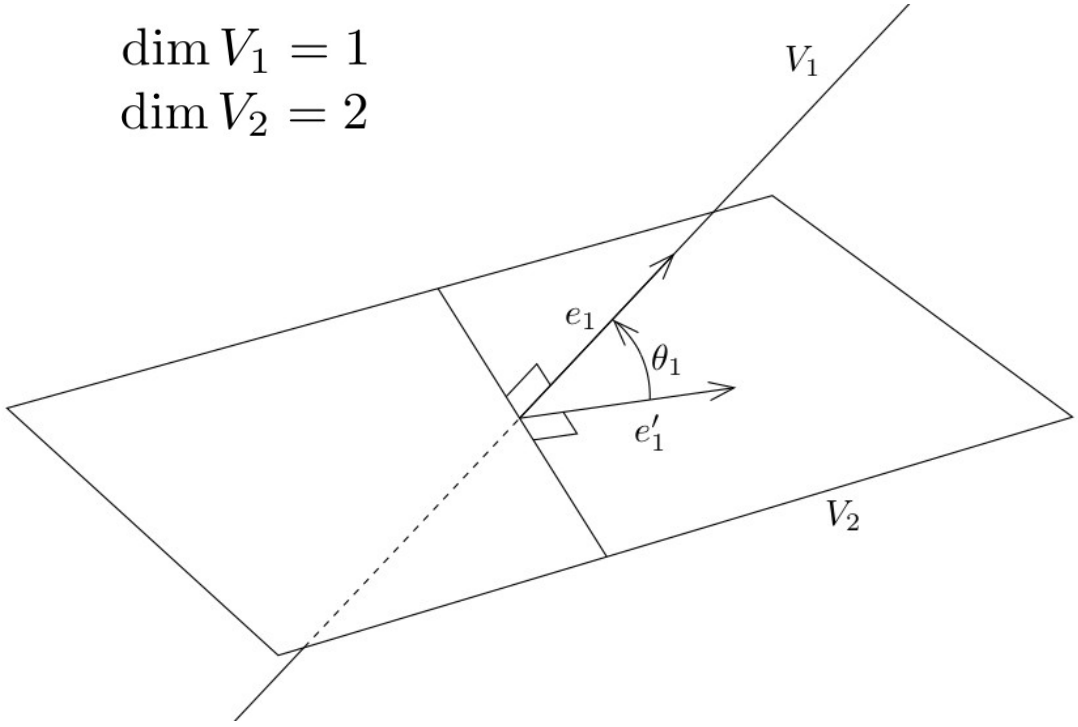
  $(v_i)_{1 \le i \le l}$ orthonormal basis of V_2
- $X_{ij} = \langle u_i, v_j \rangle$ ⟶ SVD
- $S = (s_1, \cdots, s_m) = (\cos\theta_1, \cdots, \cos\theta_m)$

  $0 \le \theta_i \le \frac{\pi}{2}$ principal angles $\quad m = \min(k, l)$
- $\delta(V_1, V_2) = \left(\sum_{i=1}^{m} \theta_i^2\right)^{\frac{1}{2}} \le \frac{\pi}{2}\sqrt{m}$
- upper bound attained iff V_1 and V_2 are orthogonal

$\dim V_1 = \dim V_2 = 1$



$\dim V_1 = 1$
$\dim V_2 = 2$



- In these cases principal angle θ_1 is the angle between subspace V_1 and V_2

  $\longrightarrow \delta(V_1, V_2) = |\theta_1|$

- When $\dim V_1 = 1$ and $\dim V_2 = 2$

  $\delta(V_1, V_2)$ is smallest distance between V_1 and all 1-dimensional subspaces of V_2

- ^{20}Ne Nucleus
- No particule number & J^2 projections
- Brink & Boecker interaction $(4+2$ parameters)

$$V^{\mathrm{BB}} = \sum_{i=0}^{1} (w_i - m_i P_\sigma P_\tau)\, e^{-(\boldsymbol{r}_1-\boldsymbol{r}_2)^2/\mu_i^2} + \text{kinetic \& COM correction}$$

$\longrightarrow \quad n_p = 4$

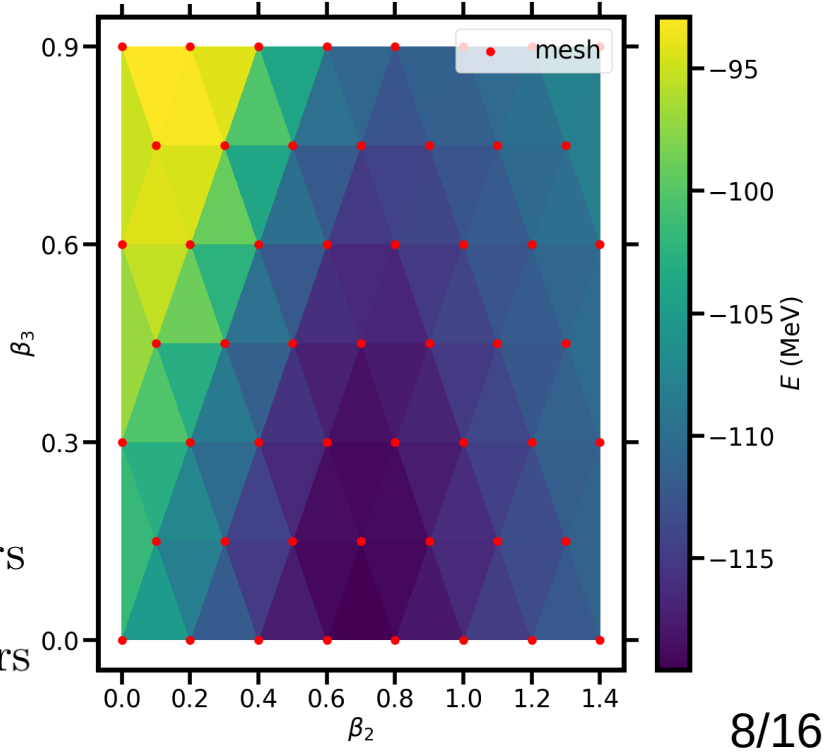
- mesh on β_2, β_3 with $n_q = 53$ points
- basis truncation : 8 oscillator shells
- Latin Hypercube Sampling in $[\lambda_0 - 10, \lambda_0 + 10]^4$ with $n_{\mathrm{pes}} = 50$ points
- 50×53 HF states $\longrightarrow$ computation time : 736 hours
- $\frac{(50\times53)^2}{2} \times 6$ kernels $\longrightarrow$ computation time : 2703 hours

Nominal parametrization

$w_0 = -72.21$ MeV
$m_0 = -68.39$ MeV
$w_1 = -595.55$ MeV
$m_1 = -206.05$ MeV

$\mu_0 = 1.4$ fm
$\mu_1 = 0.7$ fm

Fixed at nominal values



- ^{20}Ne Nucleus
- No particule number & J^2 projections
- Brink & Boecker interaction $(4+2$ parameters)

$$V^{\mathrm{BB}} = \sum_{i=0}^{1} (w_i - m_i P_\sigma P_\tau)\, e^{-(\boldsymbol{r}_1-\boldsymbol{r}_2)^2/\mu_i^2} + \text{kinetic \& COM correction}$$

$\longrightarrow \quad n_p = 4$

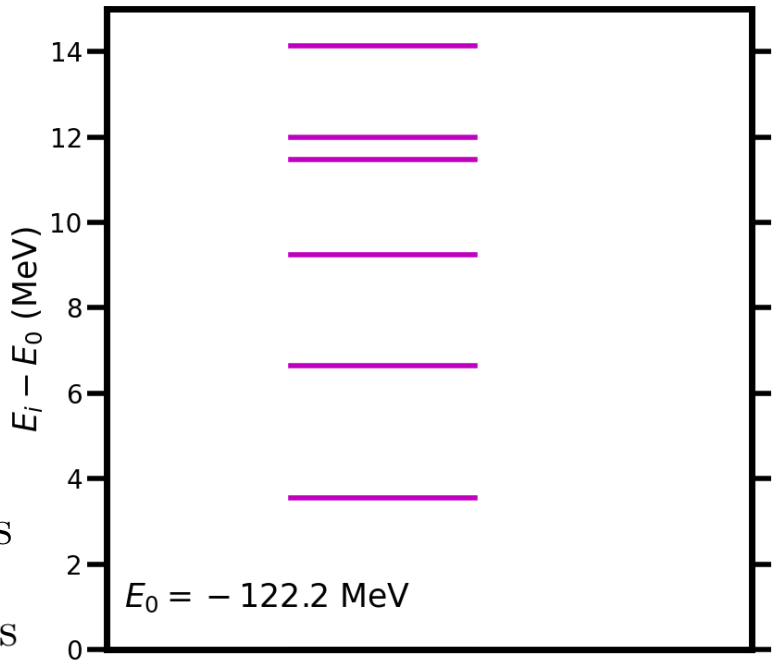
- mesh on β_2, β_3 with $n_q = 53$ points
- basis truncation : 8 oscillator shells
- Latin Hypercube Sampling in $[\lambda_0 - 10, \lambda_0 + 10]^4$ with $n_{\mathrm{pes}} = 50$ points
- 50×53 HF states $\longrightarrow$ computation time : 736 hours
- $\frac{(50\times53)^2}{2} \times 6$ kernels $\longrightarrow$ computation time : 2703 hours

Nominal parametrization

$w_0 = -72.21$ MeV
$m_0 = -68.39$ MeV
$w_1 = -595.55$ MeV
$m_1 = -206.05$ MeV

$\mu_0 = 1.4$ fm
$\mu_1 = 0.7$ fm

Fixed at nominal values



Part 2 : Results Subspace distance

- for each $1 \leq i \leq 50$ compute $E_{53}^{\lambda_i}$ with $\epsilon = 10^{-6}$

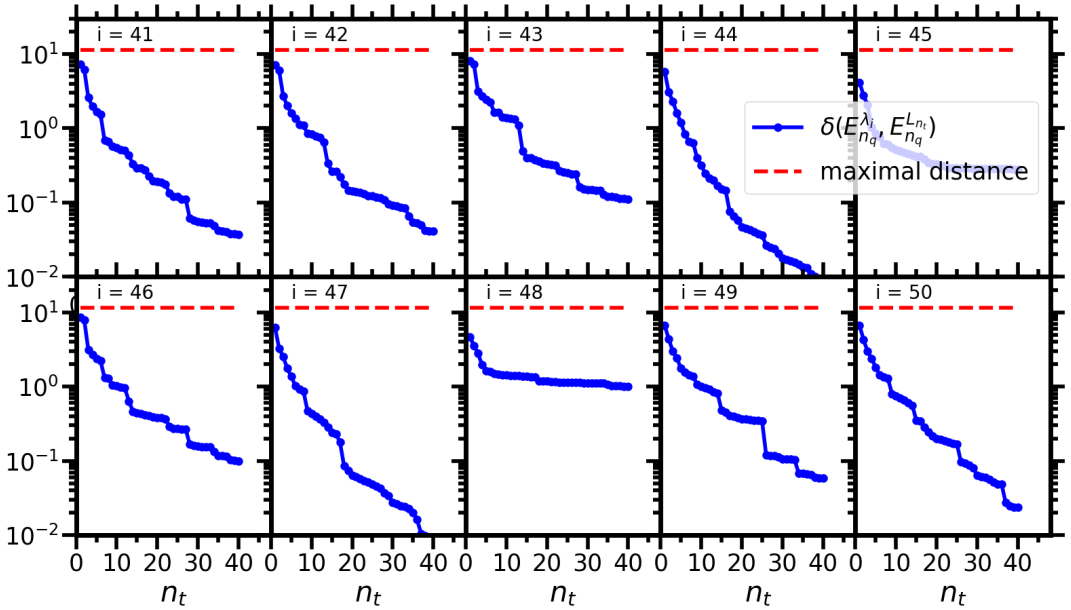
  for $1 \leq i \leq n_t$ concatenate basis of $E_{53}^{\lambda_i}$

  diagonalize norm matrix with $\epsilon^{L_{n_t}} = 10^{-8}$

  get space $E_{53}^{L_{n_t}}$

  compute $\delta\left(E_{53}^{\lambda_i}, E_{53}^{L_{n_t}}\right)$ for $41 \leq i \leq 50$

n_t	1	10	40
mean d_{space}	6.546	0.825	0.168
dispersion d_{space}	1.322	0.367	0.290



- Distance decrease quasi-exponentially for (essentially) all $41 \leq i \leq 50$
- $\delta\left(E_{53}^{\lambda_{43}}, E_{53}^{L_{40}}\right) \simeq \delta\left(E_{53}^{\lambda_{45}}, E_{53}^{L_{40}}\right) \simeq 0.1$ and $\delta\left(E_{53}^{\lambda_{48}}, E_{53}^{L_{40}}\right) \simeq 1$

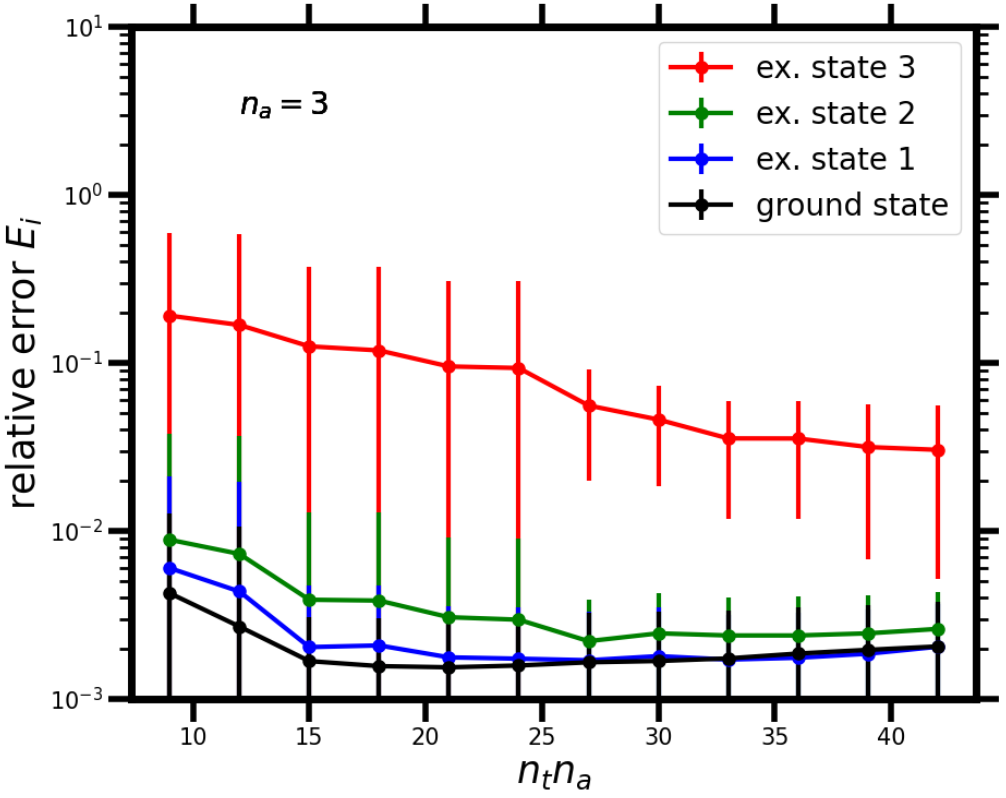
  $\longrightarrow$ $E_{53}^{\lambda_{43}}$, $E_{53}^{\lambda_{45}}$ and $E_{53}^{\lambda_{48}}$ not fully emulated by training space

Part 2 : Results Brute-force self-learning

- For $1 \leq n_t < n_{t\ \max}$ take as $n_t + 1$ training point the one minimizing ground state relative error

- For $n_a = 3$ very good reprodution of E_0 E_1 E_2
  - ⟶ Best relative error : 0.3 % (~ 0.4 MeV)

  good reprodution of E_3
  - ⟶ Best relative error : 3 % (~ 4 MeV)



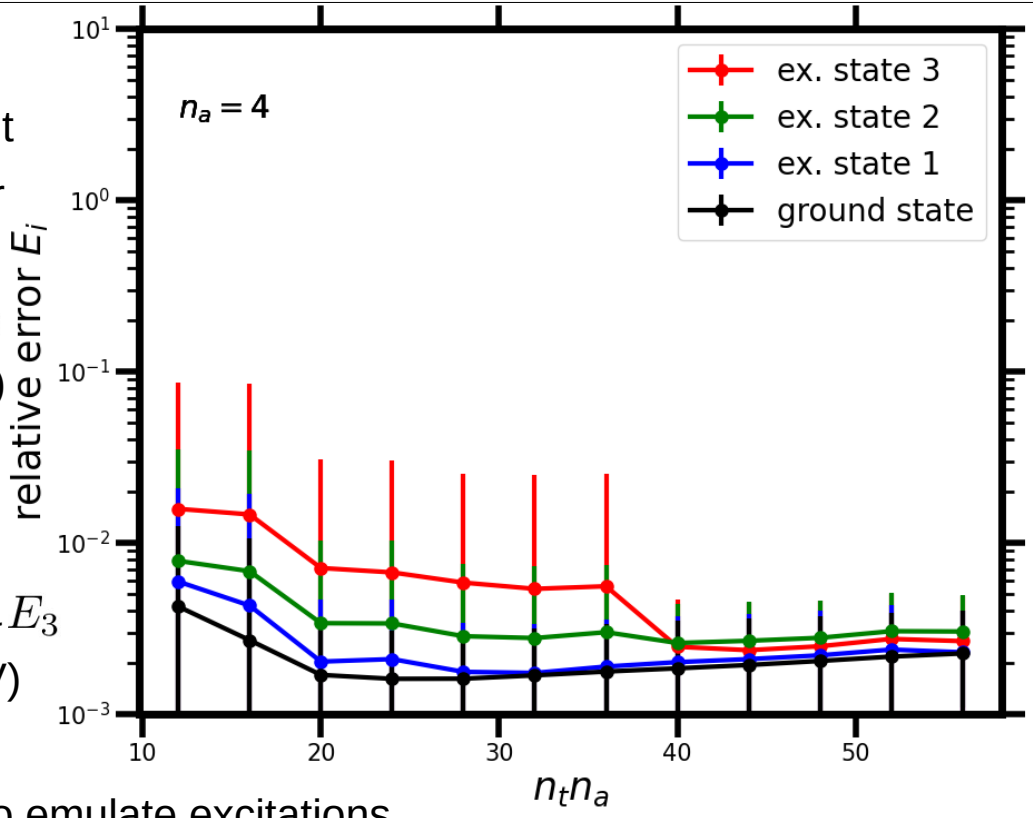
Part 2 : Results Brute-force self-learning

- For $1 \leq n_t < n_{t\ \max}$ take as $n_t + 1$ training point the one minimizing ground state relative error

- For $n_a = 3$ very good reprodution of E_0 E_1 E_2
  - ⟶ Best relative error : 0.3 % (~ 0.4 MeV)

  good reprodution of E_3
  - ⟶ Best relative error : 3 % (~ 4 MeV)

- For $n_a = 4$ very good reprodution of $E_0 E_1$ E_2 & E_3
  - ⟶ Best relative error : 0.3 % (~ 0.4 MeV)



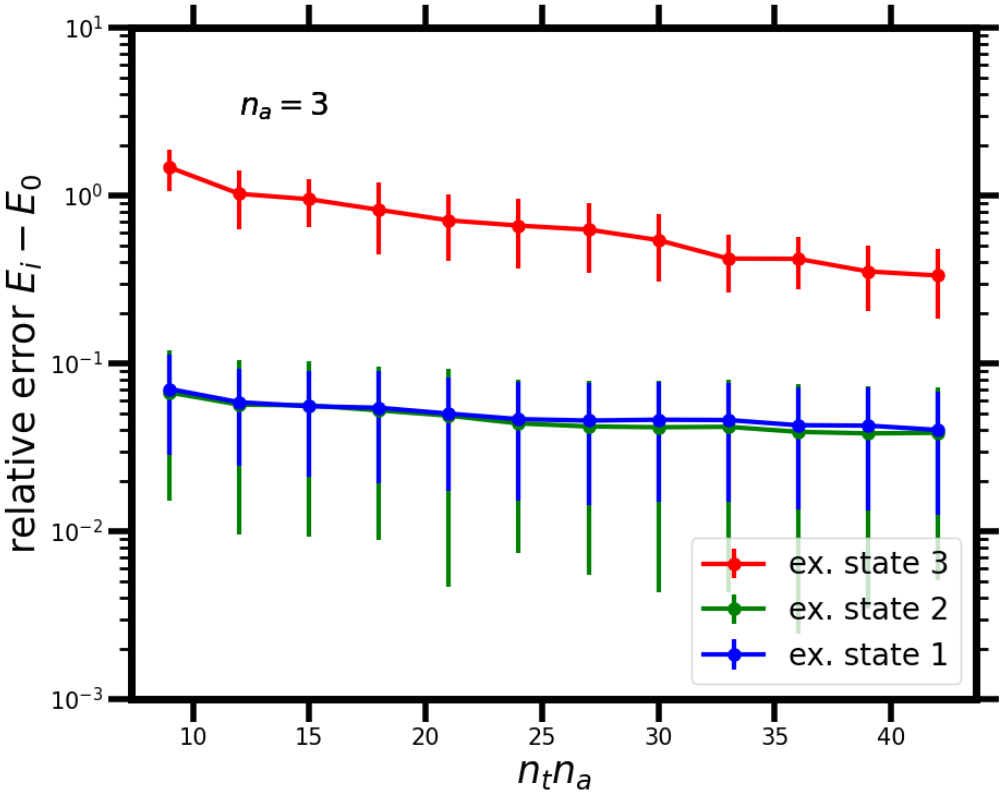
- Training on excited states is necessary to emulate excitations
- Very good accuracy
- For $n_t \geq 6$ accuracy slowly degrades

Part 2 : Results Brute-force self-learning

- For $1 \leq n_t < n_{t\ \max}$ take as $n_t + 1$ training point the one minimizing ground state relative error

- For $n_a = 3$ good reprodution of excitations 1 & 2
  - → Best relative error : 4 % (~ 160 keV)

    bad reprodution of excitation 3
  - → Best relative error : 20 % (~ 800 keV)

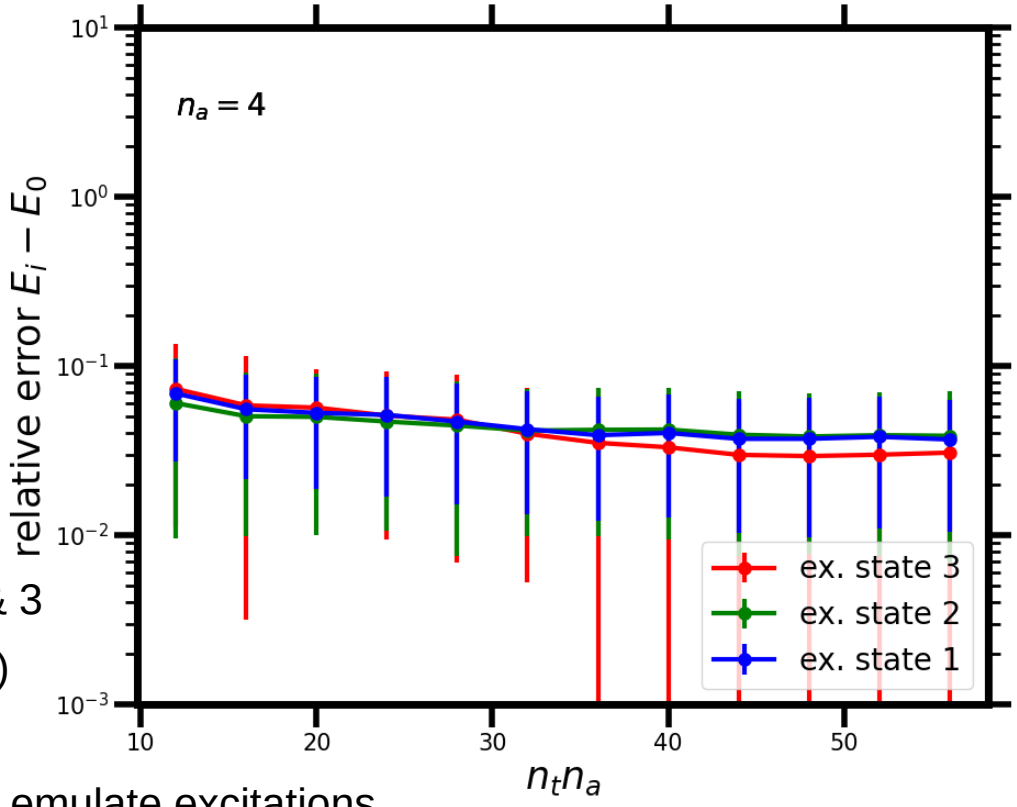


Part 2 : Results Brute-force self-learning

- For $1 \leq n_t < n_{t\ \max}$ take as $n_t + 1$ training point the one minimizing ground state relative error

- For $n_a = 3$ good reprodution of excitations 1 & 2
  - → Best relative error : 4 % (~ 0.16 MeV)
  - bad reprodution of excitation 3
  - → Best relative error : 20 % (~ 0.8 MeV)

- For $n_a = 4$ good reprodution of excitations 1, 2 & 3
  - → Best relative error : 4 % (~ 0.16 MeV)

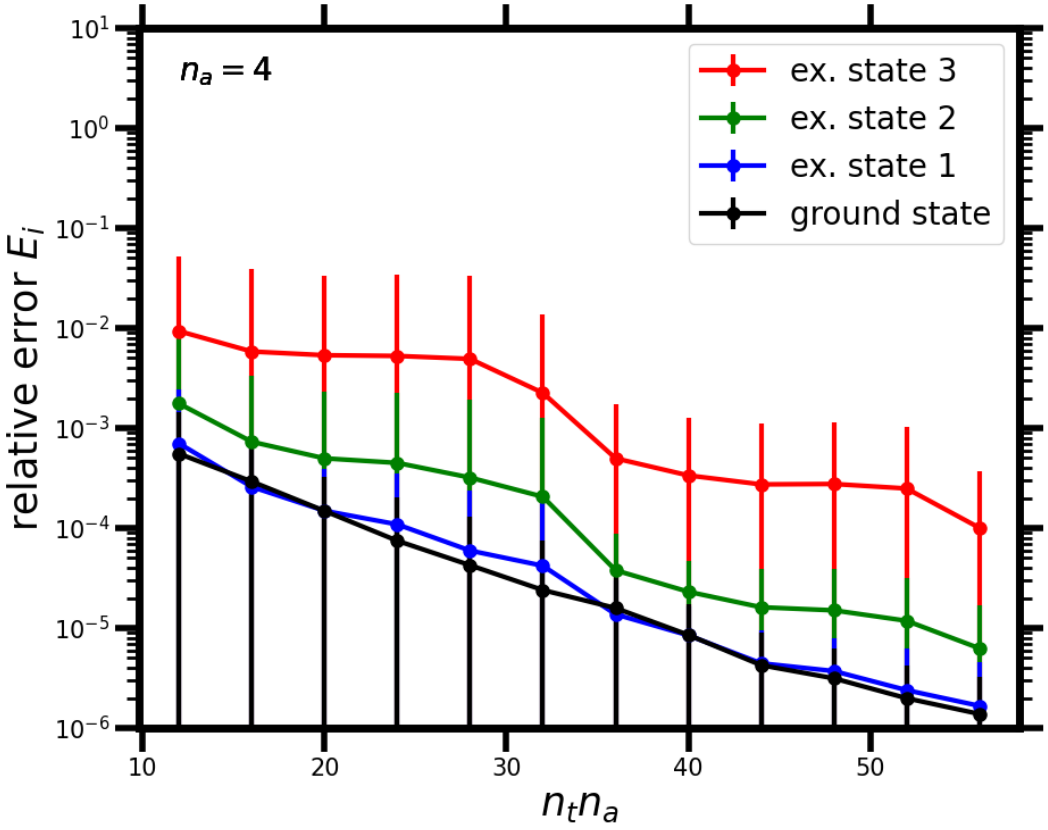


- Training on excited states is necessary to emulate excitations
- Good accuracy but not fantastic
- For large n_t accuracy keeps improving slowly

Part 2 : Results Emulator vs simulator in fixed common space

- Do emulation & GCM in a fixed common space
  - Emulation of GCM coefficients
  - No need to emulate GCM space
- Best relative errors

E_0 & E_1	0.0002 %
E_2	0.001 %
E_3	0.01 %

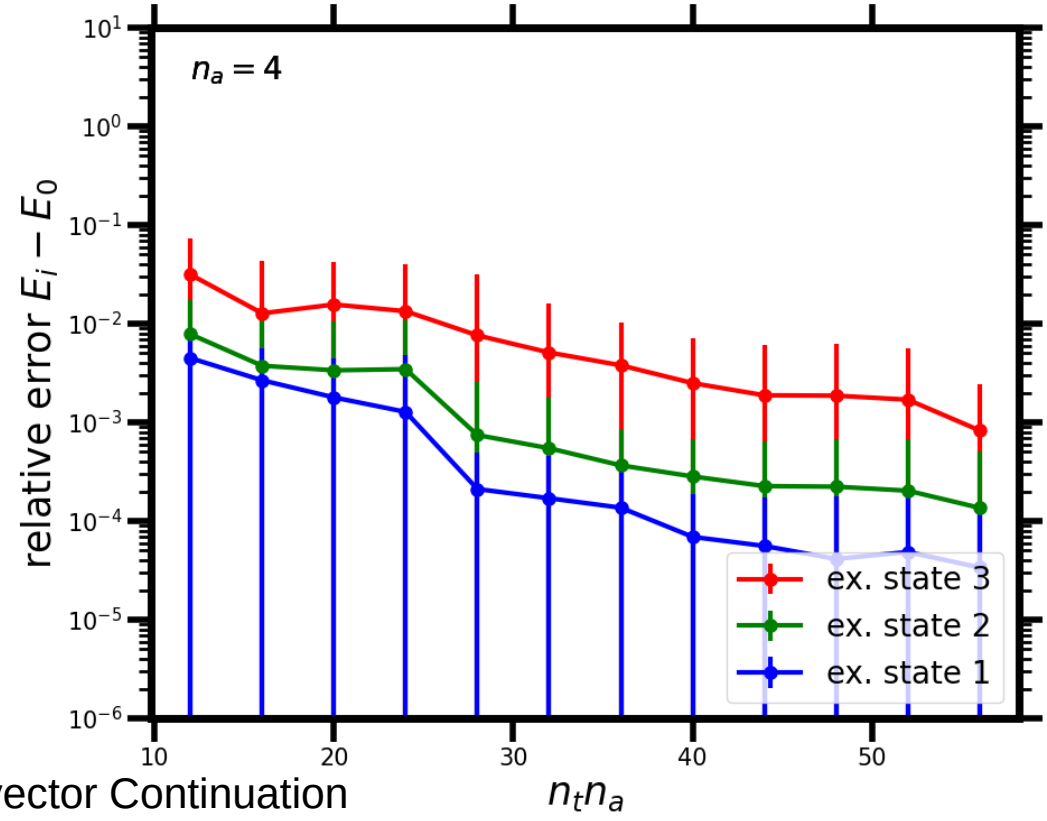


Part 2 : Results Emulator vs simulator in fixed common space

- Do emulation & GCM in a fixed common space
  - Emulation of GCM coefficients
  - No need to emulate GCM space

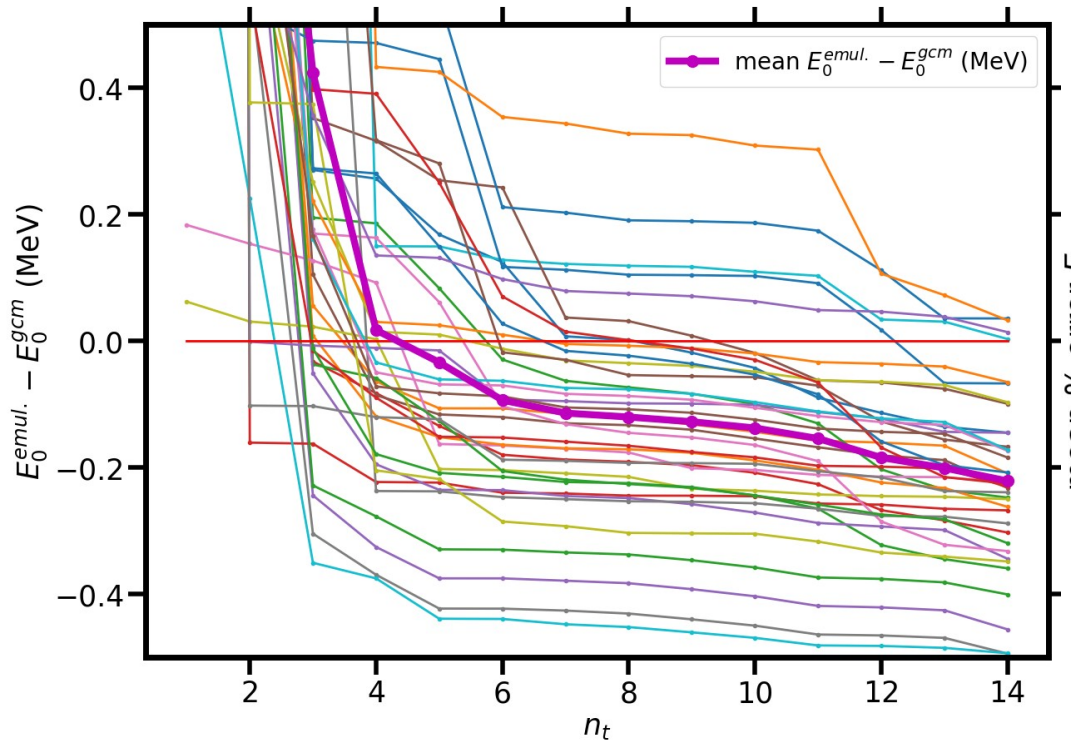
- Best relative errors

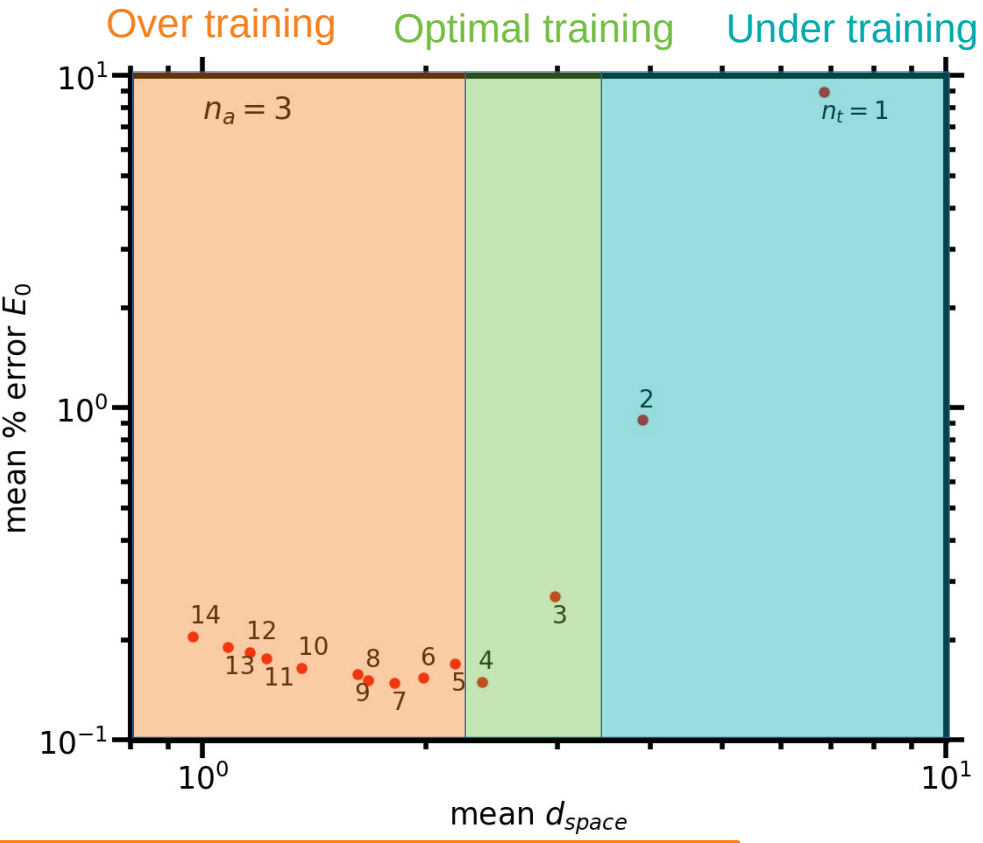
E_0 & E_1	0.0002 %
E_2	0.001 %
E_3	0.01 %
$E_1 - E_0$	0.003 %
$E_2 - E_0$	0.01 %
$E_3 - E_0$	0.1 %



- Agrees with previous work on Eigenvector Continuation
  - → Lee, Frame & Sarkar → Hergert
- GCM subspace emulation is the limiting factor
  - → Need to investigate subspace distance

Part 2 : Results Under-training and over-training





- Variational principle

→ for $n_t \geq 5$ emulator is better than GCM

→ Emulator becomes a super GCM with additional coordinate μ

Part 2 : Results Correlation of emulator quality with subspace distance

- Mean ground-state energy error strongly correlated with mean distance

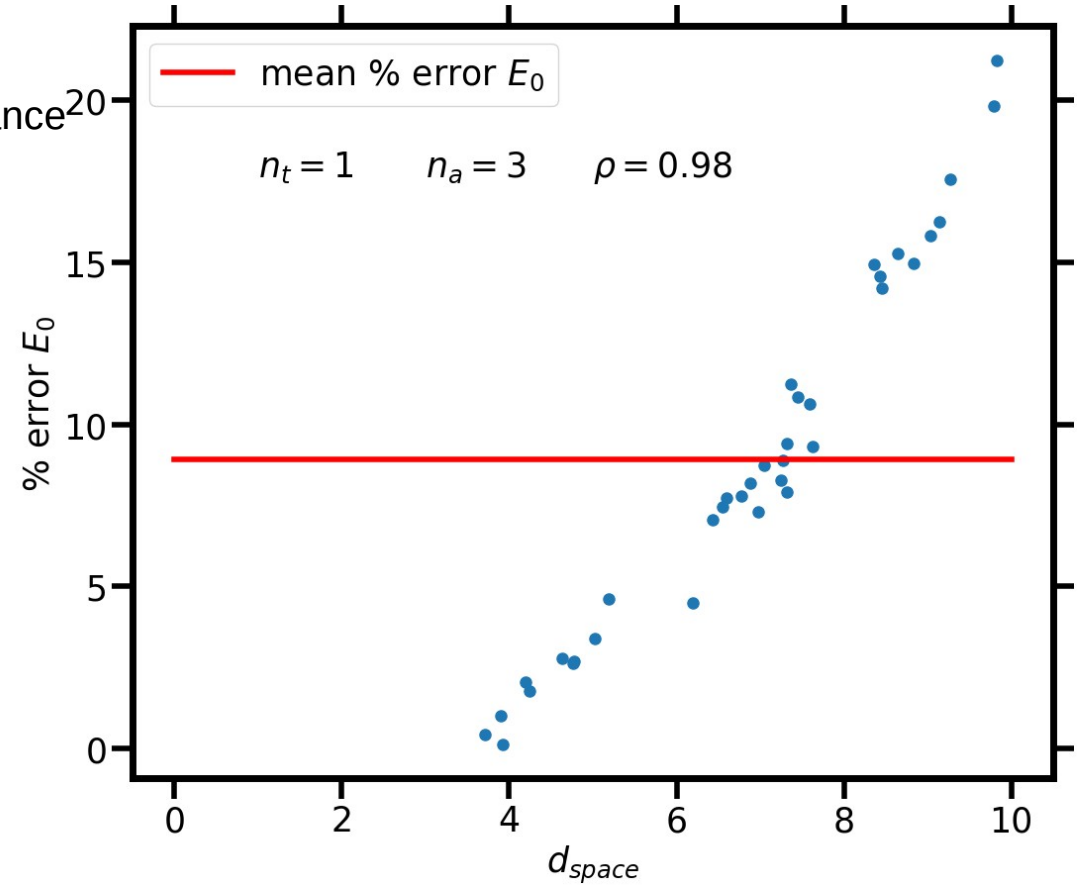
For $n_a = 3$ and $n_t = 1$

Distance from 4 to 10

Mean error around 10%

Strong correlation between error and distance to training

→ (Large) error dominated by GCM space too distant from training space



Part 2 : Results Correlation of emulator quality with subspace distance

- Mean ground-state energy error strongly correlated with mean distance

For $n_a = 3$ and $n_t = 1$

Distance from 4 to 10

Mean error around 10%

Strong correlation between error and distance to training

→ (Large) error dominated by GCM space too distant from training space

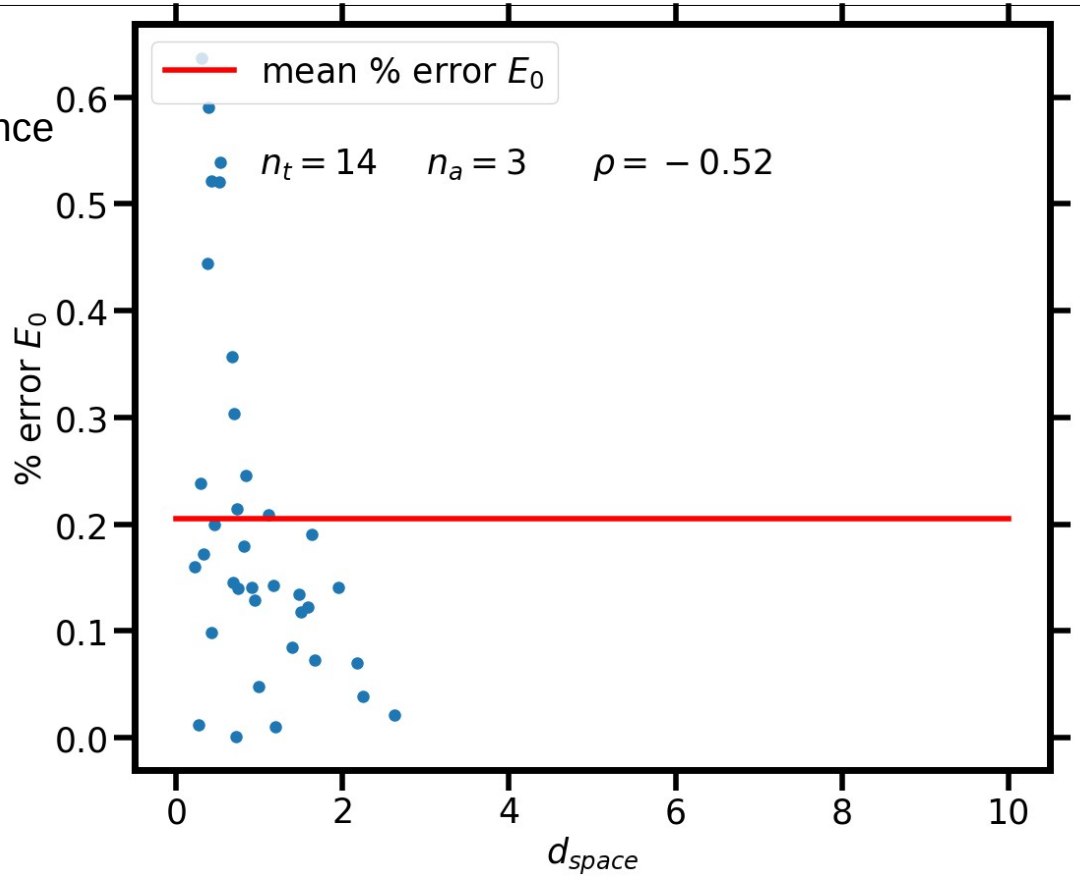
- For $n_a = 3$ and $n_t = 14$

All distances to training space reduced to ~1

Mean error down to 0.2 %

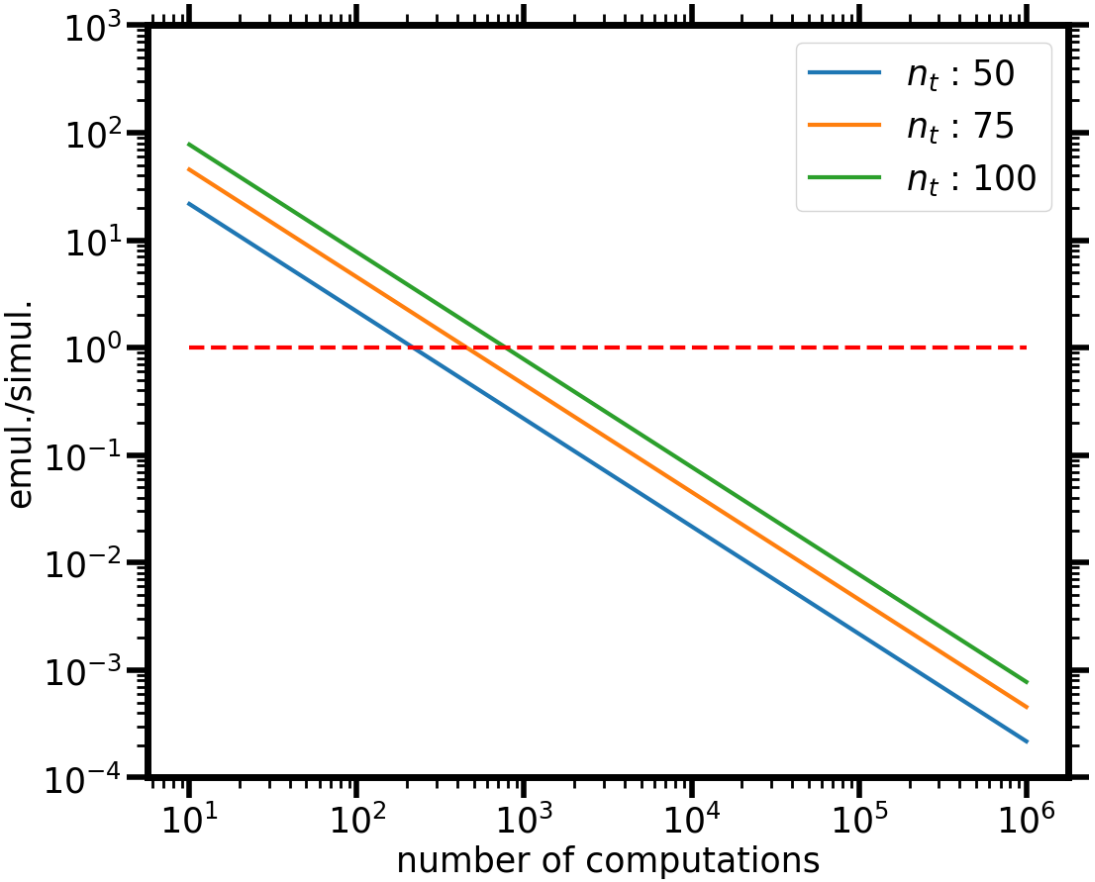
Residual error dispersion not correlated with residual distance

→ Due to over-training



Part 2 : Results Computational cost

- For large emulators :
  - → Gain for large computation number
    - For 10^6 computations : gain of 10^4
    - To be compared with 10^5 from Erkstrom et al. (2019)



Conclusion & perspectives

Conclusion

-Good reproduction of absolute and excitation enrgies

-Large computational speedup

-Emulation limited by lack of common space

Perspectives

-Emulation of charge radii (already done but not shown)

-Including projection on J and emulation of electromagnetic transitions

-Moving to Chiral EFT Hamiltonians

-Large scale applications and sensitivity analysis