ESNT WORKSHOP

Fast emulation of large-scale ab-initio description of collective excitations

Rationale of the approach and (very) preliminary results

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Outline

Introduction

- Projected Generator Coordinate Method
- Examples of recent PGCM computations

PGCM-EC emulator project and goals

PGCM-EC Algorithm

- Brief review of PGCM
- General idea of a PGCM-EC emulator
- Presentation of simplified preliminary algorithm

Model specifications

Results

PGCM A whole new world of possibilities for ab initio studies

PGCM = zero-order of PGCM-PT

State-specific/multi-reference/symmetry-conserving perturbation theory

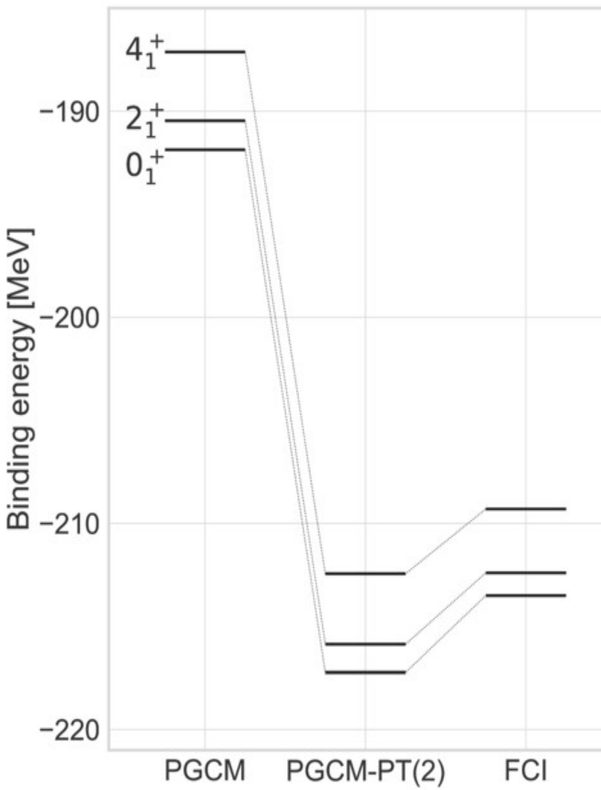
M. Frosini et al, EPJA (2022)

$$|\Psi_{\text{PGCM-PT}}\rangle = \Omega^{\text{PT}} |\Psi_{\text{PGCM}}\rangle$$

Dynamical collective correlations (Ω^{PT}) — Static collective correlations ($|\Psi_{\text{PGCM}}\rangle$)

- PGCM not converged for absolute energies

→ Large correction from dynamical correlations



^{20}Ne

$e_{\max} = 4$

N^3LO NN interaction (Hüther et al 2020)

$l_{\text{srg}} = 1.88 \text{fm}^{-1}$

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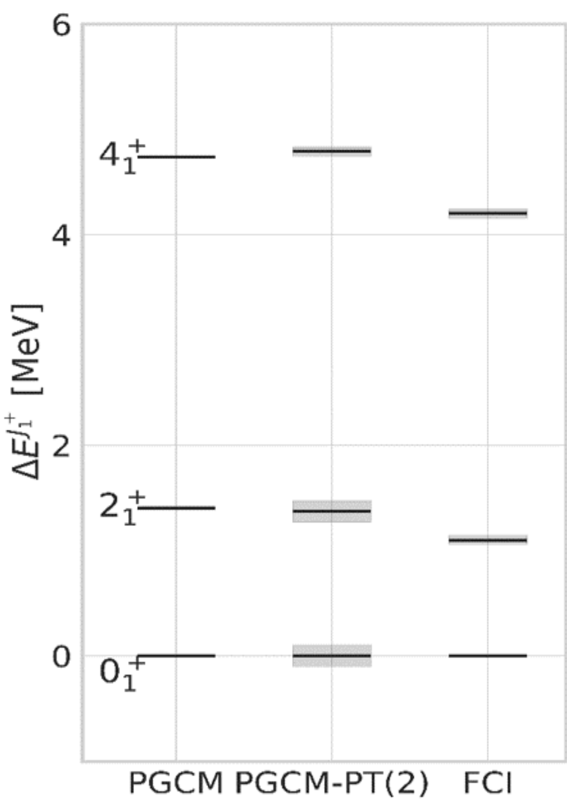

- PGCM not converged for absolute energies

  → Large correction from dynamical correlations

- PGCM is converged for excitation energies

  → Cancellation of dynamical correlations

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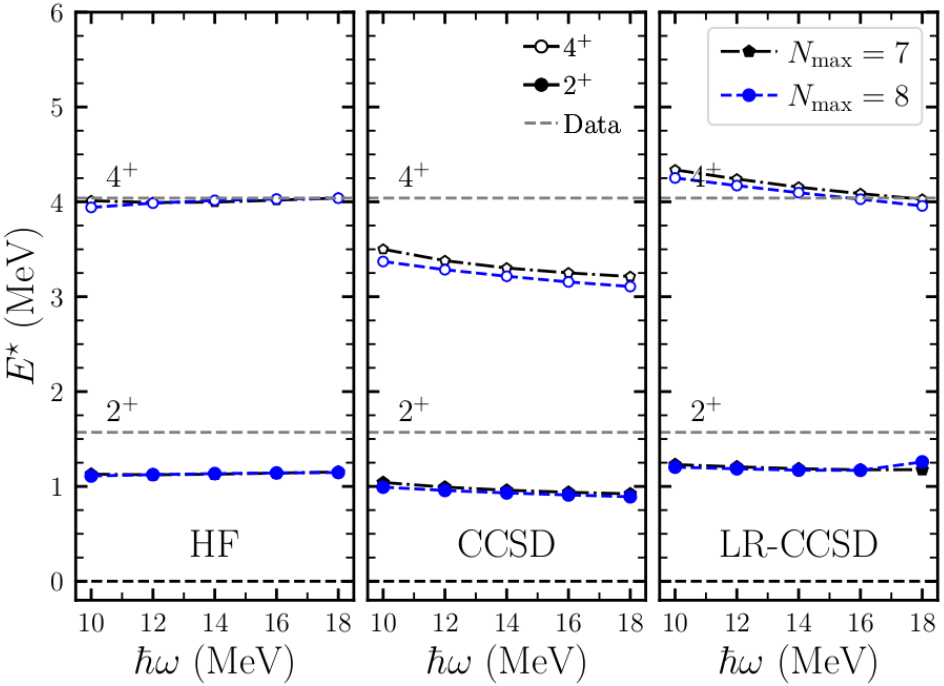
State-specific/multi-reference/symmetry-conserving perturbation theory

M. Frosini et al, EPJA (2022)

A. Ekström et al (2023)



- PGCM not converged for absolute energies
  - → Large correction from dynamical correlations
- PGCM is converged for excitation energies
  - → Cancellation of dynamical correlations

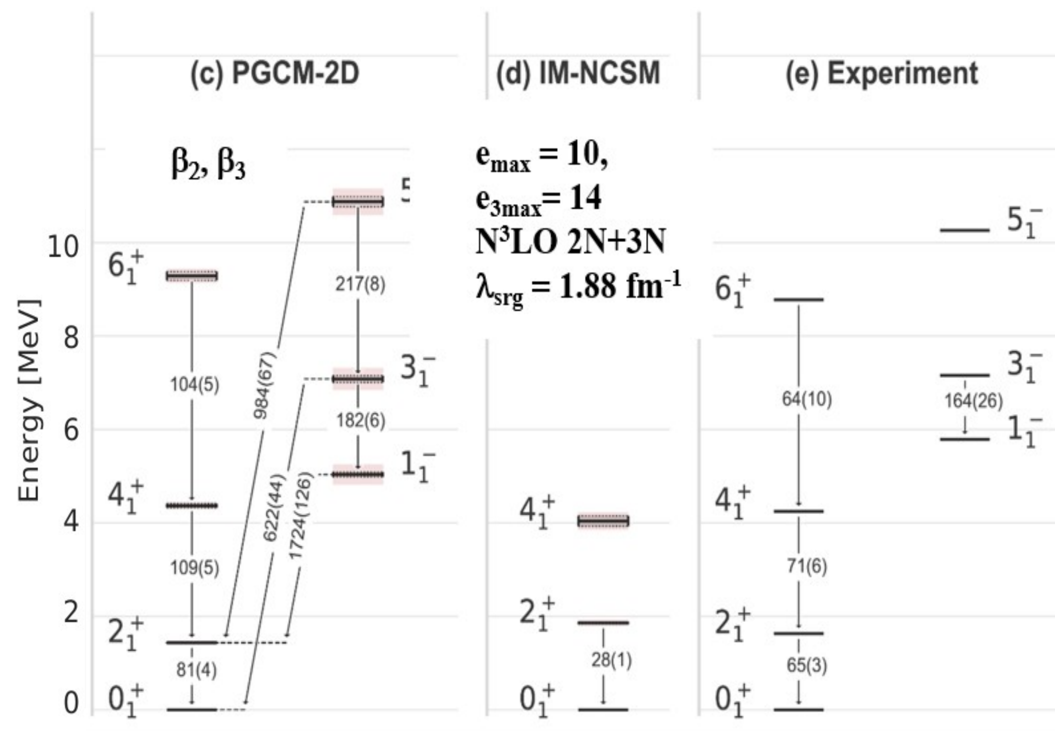
★ Confirmed by Projected Coupled Cluster approach

PGCM appropriate for ab-initio spectroscopy

PGCM A whole new world of possibilities for ab initio studies

- Low-lying collective spectroscopy

- PGCM $^{20}\mathrm{Ne}$
- Excellent account of exp. data
  - → Chiral order uncertainty $\simeq 100\ \mathrm{KeV}$
- Good agreement of ground-state band with IM-NCSM
  - → Many-body uncertainty $\simeq 100\ \mathrm{KeV}$

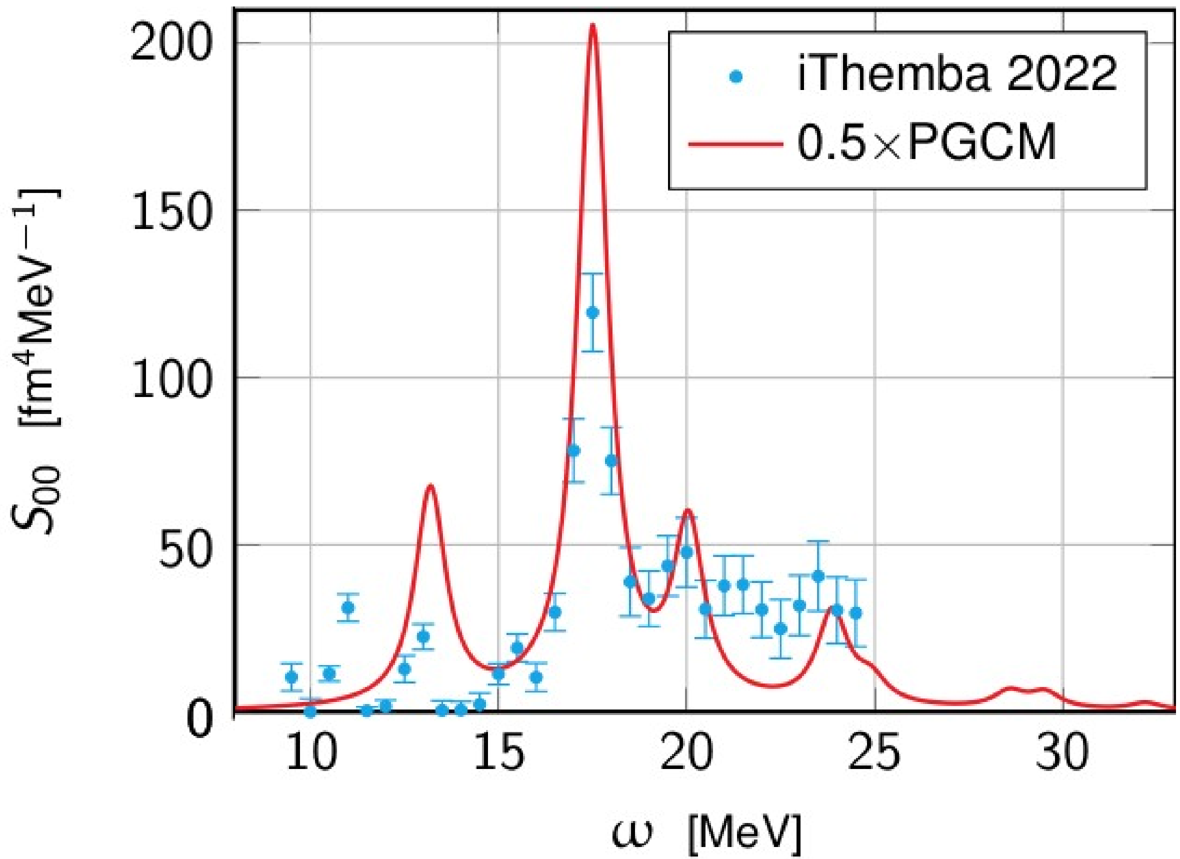


[Frosini et al., EPJA58 (2022) 63]

PGCM A whole new world of possibilities for ab initio studies

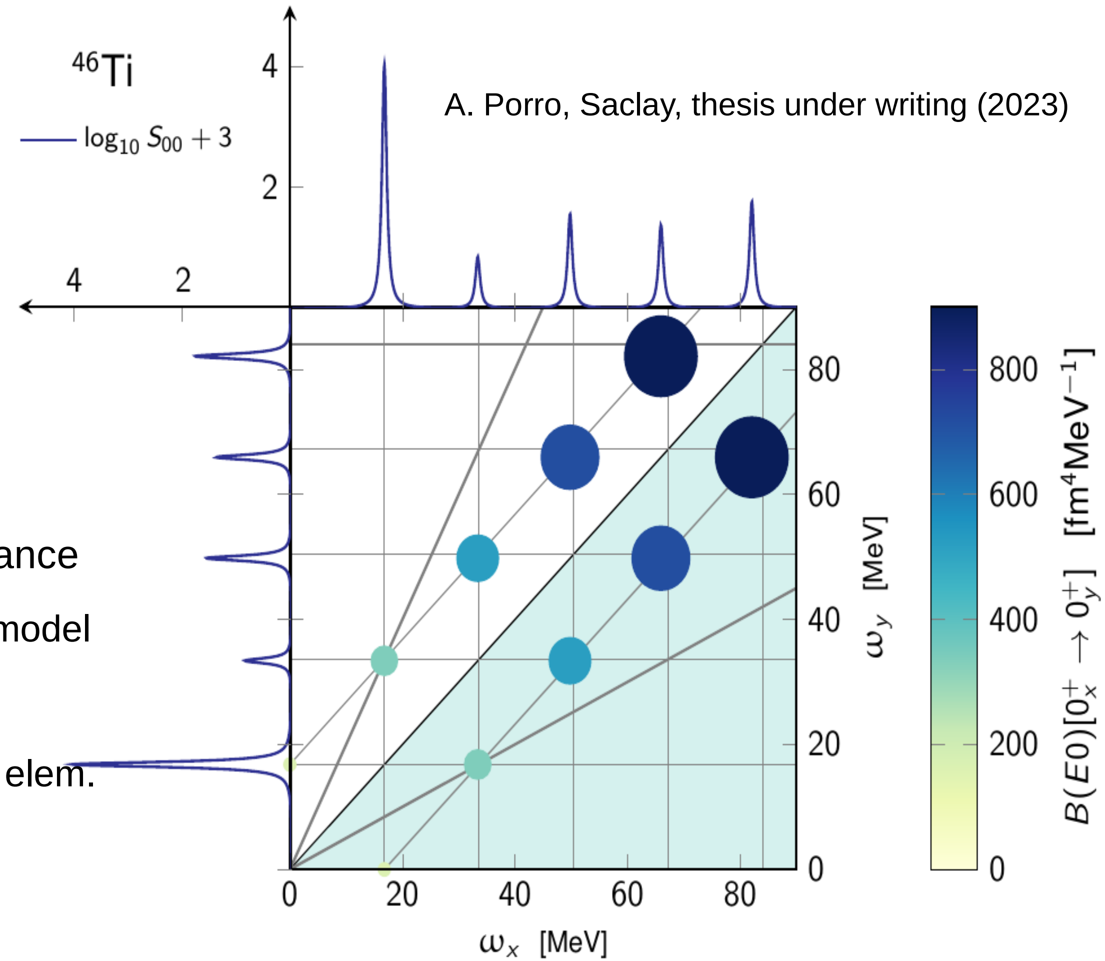
- Low-lying collective spectroscopy
- Giant resonances
  - $^{28}\mathrm{Si}$ monopole strength distribution vs exp. data

A. Porro, Saclay, thesis under writing (2023)



PGCM A whole new world of possibilities for ab initio studies

- Low-lying collective spectroscopy
- Giant resonances & multi-phonon



◆ Multi-phonon states on top of monopole resonance

→ Correspondance with harmonic oscillator model

★ HO spectrum

★ Linear growth of (n, n+1) $B\left(E_0\right)$ matrix elem.

→ Practically inaccessible in QRPA

→ First ab initio prediction of this type

PGCM A whole new world of possibilities for ab initio studies

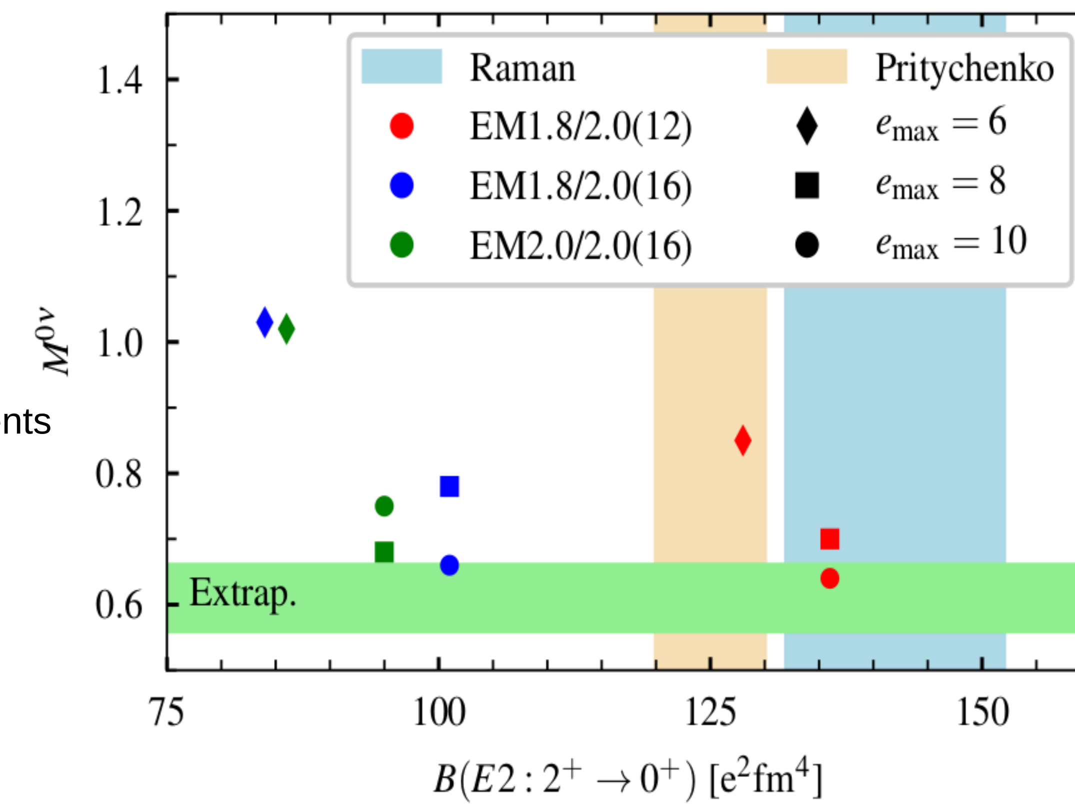
- Low-lying collective spectroscopy

- Giant resonances & multi-phonon

- Neutrinoless double-beta decay

    - State of the art computation of matrix elements

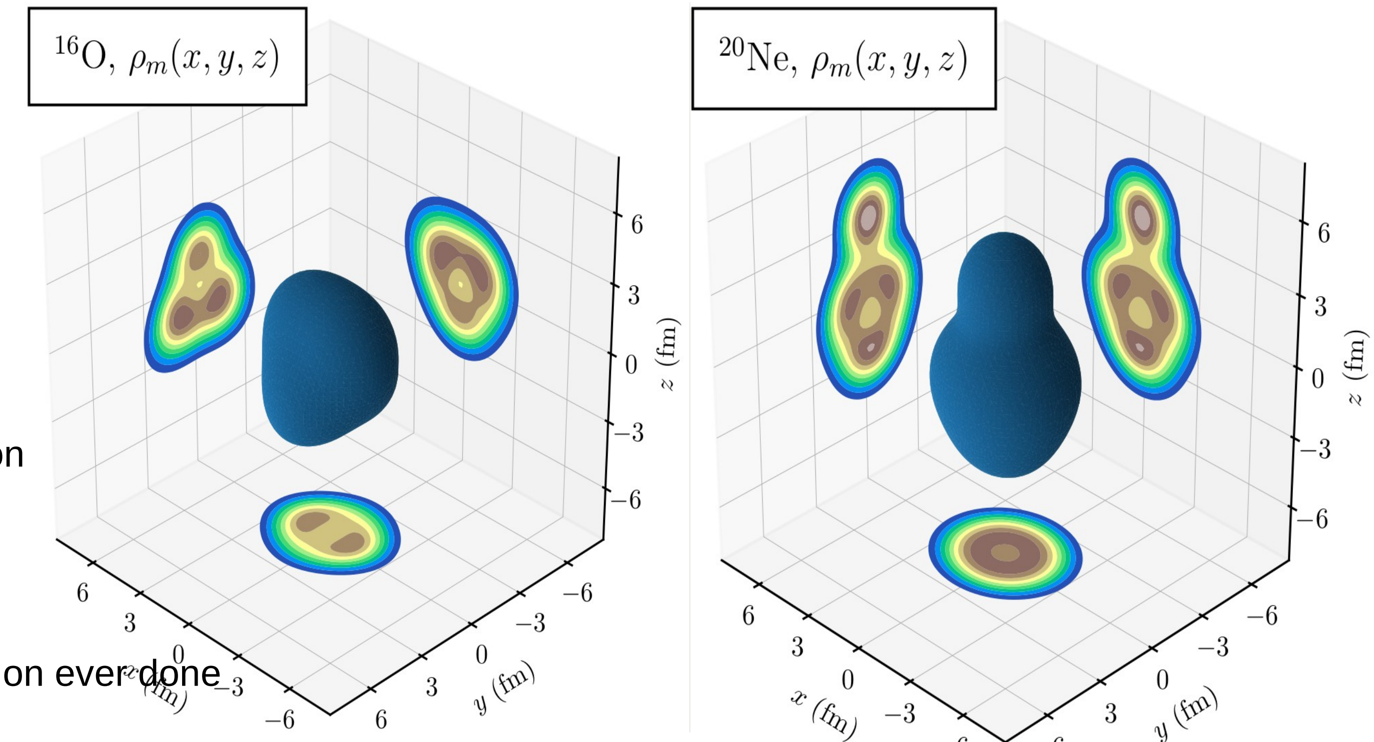
J. M. Yao et al, PRL (2020)



PGCM A whole new world of possibilities for ab initio studies

- Low-lying collective spectroscopy
- Giant resonances & multi-phonon
- Neutrinoless double-beta decay
- Clustering
  - Ground-state intrinsic density distribution
    - → $^{16}\mathrm{O}$: tetrahedral clustering
    - → $^{20}\mathrm{Ne}$: $^{16}\mathrm{O}$ clustering + alpha
    - → Most advanced PGCM computation ever done

B. Bally et al., in preparation (2023)



PGCM A whole new world of possibilities for ab initio studies

- Low-lying collective spectroscopy
- Giant resonances & multi-phonon
- Neutrinoless double-beta decay
- Clustering

}

PGCM-EC project

Combine all these aspects with EC

Numerical implementations of the collaboration

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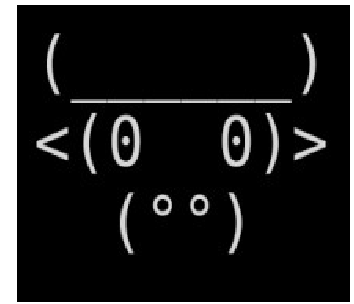
TAURUS

B. Bally, A. Sanchez-Fernandez & T. Rodriguez



Advanced multidimensional PGCM

- HFB states → Break N, Z, J^2, Π & time reversal
  → Constraints on Y_1^m, Y_2^m, Y_3^m, r^2 & Δ
- Symmetry restoration N, Z, J^2, Π

- Hamiltonian → Chiral Hamiltonian
  → Gogny effective interaction
  → Shell-model valence interaction

PGCM-EC emulator project

Goals

- Sensitivity analysis & error propagation for ab initio calculations of collective excitations
- Easy inclusion of collective excitations within fit of future chiral EFT interactions
- Large scale database of ab initio prediction of collective excitations with statistical analysis

Preliminary tests

- One-dimensional GCM on $\beta_{20} \leftrightarrow Y_2^0$
- No $U(1)$ symmetry breaking = HF
- No J^2 projection
- Brink & Boecker soft interaction $(4 + 2$ parameters$)$

Necessary for full-fledged project

- Access to (SRG-evolved) splitted chiral Hamiltonian
- Access to state-of-the-art post-processing statistical tools

PGCM-EC Algorithm review of PGCM

(1) $H(\lambda) = H^\lambda$

Set of HFB states $\left\{|\Phi^\lambda(q)\rangle\right\}_{q\in\{q_1,\cdots,q_{n_q}\}}$

Constrained to $\langle\Phi^\lambda(q)|Q|\Phi^\lambda(q)\rangle = q$

q Deformation parameter

no λ dependence → P^σ_M

projection

$$P^\sigma_M|\Phi^\lambda(q)\rangle \equiv \frac{d_\sigma}{v_G}\sum_{\Theta=1}^{n_\Theta} D^{\sigma *}_{MM}(\Theta)U(\Theta)|\Phi^\lambda(q)\rangle$$

$P^\sigma_M|\Phi^\lambda(q)\rangle$ — PGCM ansatz →

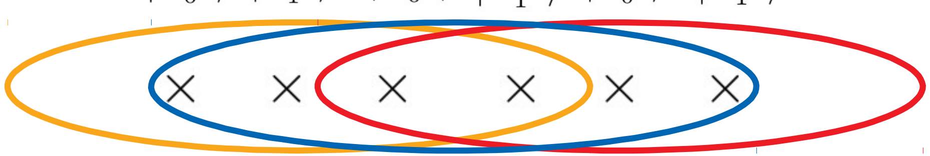
$$|\Psi^\lambda_a\rangle = \sum_{q=1}^{n_q} f^\lambda_a(q)\; P^\sigma_M|\Phi^\lambda(q)\rangle \text{ with } \delta\frac{\langle\Psi^\lambda_a|H^\lambda|\Psi^\lambda_a\rangle}{\langle\Psi^\lambda_a|\Psi^\lambda_a\rangle} = 0$$

Full Hilbert space

H^{λ_0}

λ_0 nominal param.

$|\Psi^{\lambda_1}_0\rangle$ $|\Psi^{\lambda_1}_1\rangle$ $|\Psi^{\lambda_0}_0\rangle$ $|\Psi^{\lambda_0}_1\rangle$ $|\Psi^{\lambda_2}_0\rangle$ $|\Psi^{\lambda_2}_1\rangle$



$\text{Vect}\left\{|\Phi^{\lambda_1}(q)\rangle\right\}_q \equiv V^{\lambda_1}$ $\text{Vect}\left\{|\Phi^{\lambda_0}(q)\rangle\right\}_q \equiv V^{\lambda_0}$ $\text{Vect}\left\{|\Phi^{\lambda_2}(q)\rangle\right\}_q \equiv V^{\lambda_2}$

(2) ↕ Hill-Wheeler-Griffin eq.

Solve Generalized Eigenvalue Problem

→ $\left\{f^\lambda_a(q)\right\}_{q\in\{q_1,\cdots,q_{n_q}\}}$

- Objective EC

→ Emulate (1) and (2)

PGCM-EC Algorithm review of PGCM

1

$H(\lambda) = H^\lambda$

Set of HFB states $\{|\Phi^\lambda(q)\rangle\}_{q\in\{q_1,\cdots,q_{n_q}\}}$

Constrained to $\langle\Phi^\lambda(q)|Q|\Phi^\lambda(q)\rangle = q$

q Deformation parameter

no λ dependence: P^σ_M

projection →

$$P^\sigma_M|\Phi^\lambda(q)\rangle \equiv \frac{d_\sigma}{v_G}\sum_{\Theta=1}^{n_\Theta} D^{\sigma *}_{MM}(\Theta)U(\Theta)|\Phi^\lambda(q)\rangle$$

2

$P^\sigma_M|\Phi^\lambda(q)\rangle$

PGCM ansatz →

$$|\Psi^\lambda_a\rangle = \sum_{q=1}^{n_q} f^\lambda_a(q)\; P^\sigma_M|\Phi^\lambda(q)\rangle \text{ with } \delta\frac{\langle\Psi^\lambda_a|H^\lambda|\Psi^\lambda_a\rangle}{\langle\Psi^\lambda_a|\Psi^\lambda_a\rangle} = 0$$

$$\sum_{q'=1}^{n_q}\left(\langle\Phi^\lambda(q)|H^\lambda P^\sigma_M|\Phi^\lambda(q')\rangle - E^\lambda_a\langle\Phi^\lambda(q)|P^\sigma_M|\Phi^\lambda(q')\rangle\right) f^\lambda_a(q') = 0$$

→ Off-diagonal projected Hamiltonian and Norm kernels

→ $n_q \times n_q$ diagonalisation : negligible numerical cost

$$\langle\Phi^\lambda(q)|H^\lambda P^\sigma_M|\Phi^\lambda(q')\rangle = \frac{d_\sigma}{v_G}\sum_{\Theta=1}^{n_\Theta} D^{\sigma *}_{MM}(\Theta)\langle\Phi^\lambda(q)|H^\lambda\; U(\Theta)\;|\Phi^\lambda(q')\rangle$$

$$\langle\Phi^\lambda(q)|P^\sigma_M|\Phi^\lambda(q')\rangle = \frac{d_\sigma}{v_G}\sum_{\Theta=1}^{n_\Theta} D^{\sigma *}_{MM}(\Theta)\langle\Phi^\lambda(q)|U(\Theta)\;|\Phi^\lambda(q')\rangle$$

→ Off-diagonal Hamiltonian and Norm kernels

→ $n_q^2 n_\Theta$ kernels → PGCM cost $n_q^2 n_\Theta \times N^4$

→ Computed via off-diagonal Wick Th./Pfaffian

Balian & Brezin (1969) Robledo (2009)

Porro & Duguet (2022) Bally & Duguet (2018)

PGCM-EC Algorithm EC extrapolation

Goal

- $N_{\text{sim.}} \gg 1$ PGCM computations on H^μ for $\mu \in \{\mu_1, \cdots, \mu_{N_{\text{sim.}}}\} \subset \mathbb{R}^{n_p}$

Emulator

- Apply EC on H^μ for training set $\{|\Psi_a^{\lambda_i}\rangle\}_{\substack{0\leq i<n_t \\ 0\leq a<n_a}} \longrightarrow n_t \ll N_{\text{sim.}}$

$$\longrightarrow |\Psi_c^\mu\rangle_{\text{EC}} = \sum_{ia} g_{ac}^{\lambda_i\mu} |\Psi_a^{\lambda_i}\rangle$$

with $g_{ac}^{\lambda_i\mu}$ solution of $\sum_{ia} \left[\langle\Psi_b^{\lambda_j}|H^\nu|\Psi_a^{\lambda_i}\rangle - E_c^\mu \langle\Psi_b^{\lambda_j}|\Psi_a^{\lambda_i}\rangle\right] g_{ac}^{\lambda_i\mu} = 0$ HWG-type equation

Additional hypothesis

- Linear dependence of H^μ on μ $\longrightarrow H^\mu = \sum_{k=1}^{n_p} \mu^k H_k$

$$\langle\Psi_b^{\lambda_j}|H^\mu|\Psi_a^{\lambda_i}\rangle = \sum_{k=1}^{n_p} \mu^k \langle\Psi_b^{\lambda_j}|H_k|\Psi_a^{\lambda_i}\rangle \longrightarrow$$

$$\langle\Psi_a^{\lambda_i}|H_k|\Psi_b^{\lambda_j}\rangle \quad \langle\Psi_a^{\lambda_i}|\Psi_b^{\lambda_j}\rangle$$

Precompute & store

Removes μ dependence complexity

Low dimensionality diagonalisation $n_t n_a \simeq n_q$ $\simeq$ PGCM cost

PGCM-EC Algorithm elementary kernels computation

Express μ-independent kernels in terms of off-diagonal elementary kernels

$\lambda_{i,j}, a, b$ dependent

$\lambda_{i,j}$ dependent
a, b **independent**

$$\frac{\langle \Psi_a^{\lambda_i} | H_k | \Psi_b^{\lambda_j} \rangle}{\langle \Psi_a^{\lambda_i} | \Psi_b^{\lambda_j} \rangle} = \sum_{qq'\Theta} f_a^{\lambda_i *}(q) f_b^{\lambda_j}(q') D_{MM}^{\sigma *}(\Theta) \langle \Phi^{\lambda_i}(q) | H_k \; U(\Theta) \, | \Phi^{\lambda_j}(q') \rangle$$

→ Costly part of the computation

→ $n_q^2 n_\Theta \times n_t^2 n_p \times n_{\text{nuclei}} \; n_{\text{interactions}}$

	λ_0	λ_1	λ_2
λ_0	$\langle \Phi_q^{\lambda_0} \| H_k U_\Theta \| \Phi_{q'}^{\lambda_0} \rangle$	$\langle \Phi_q^{\lambda_0} \| H_k U_\Theta \| \Phi_{q'}^{\lambda_1} \rangle$	$\langle \Phi_q^{\lambda_0} \| H_k U_\Theta \| \Phi_{q'}^{\lambda_2} \rangle$
λ_1	$\langle \Phi_q^{\lambda_1} \| H_k U_\Theta \| \Phi_{q'}^{\lambda_0} \rangle$	$\langle \Phi_q^{\lambda_1} \| H_k U_\Theta \| \Phi_{q'}^{\lambda_1} \rangle$	$\langle \Phi_q^{\lambda_1} \| H_k U_\Theta \| \Phi_{q'}^{\lambda_2} \rangle$
λ_2	$\langle \Phi_q^{\lambda_2} \| H_k U_\Theta \| \Phi_{q'}^{\lambda_0} \rangle$	$\langle \Phi_q^{\lambda_2} \| H_k U_\Theta \| \Phi_{q'}^{\lambda_1} \rangle$	$\langle \Phi_q^{\lambda_2} \| H_k U_\Theta \| \Phi_{q'}^{\lambda_2} \rangle$

→ massive computation of kernels
→ do this for all nuclei
→ Ab initio, Gogny, Skyrme

→ HPC challenge

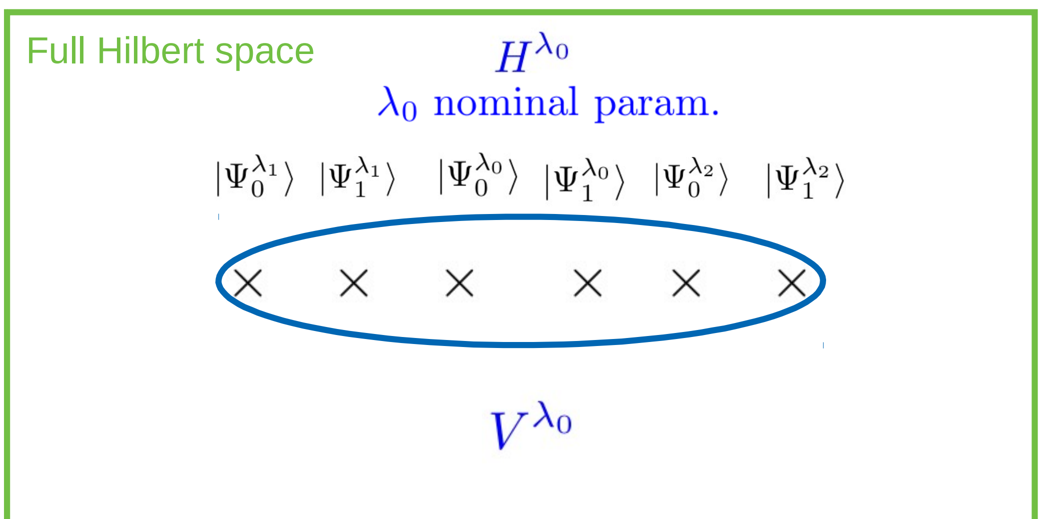
→ n_t training PGCM calculations
→ Computable with available technology
→ **Training on excited states without additional cost**

PGCM-EC Algorithm preliminary simplification

Costly part of the computation $\longrightarrow \langle \Phi^{\lambda_i}(q) | H_k \, U(\Theta) \, | \Phi^{\lambda_j}(q') \rangle$

- First step $|\Phi^{\lambda}(q)\rangle \xrightarrow[\lambda_0 \text{ nominal param.}]{\text{for all } \lambda} |\Phi^{\lambda_0}(q)\rangle$
  - (Too ?) drastic complexity reduction

    $\langle \Phi^{\lambda_i}(q) | H_k \, U(\Theta) \, | \Phi^{\lambda_j}(q') \rangle \longmapsto \langle \Phi^{\lambda_0}(q) | H_k \, U(\Theta) \, | \Phi^{\lambda_0}(q') \rangle$
  - Only $f_a^{\lambda}(q)$ carry training parameters dependence



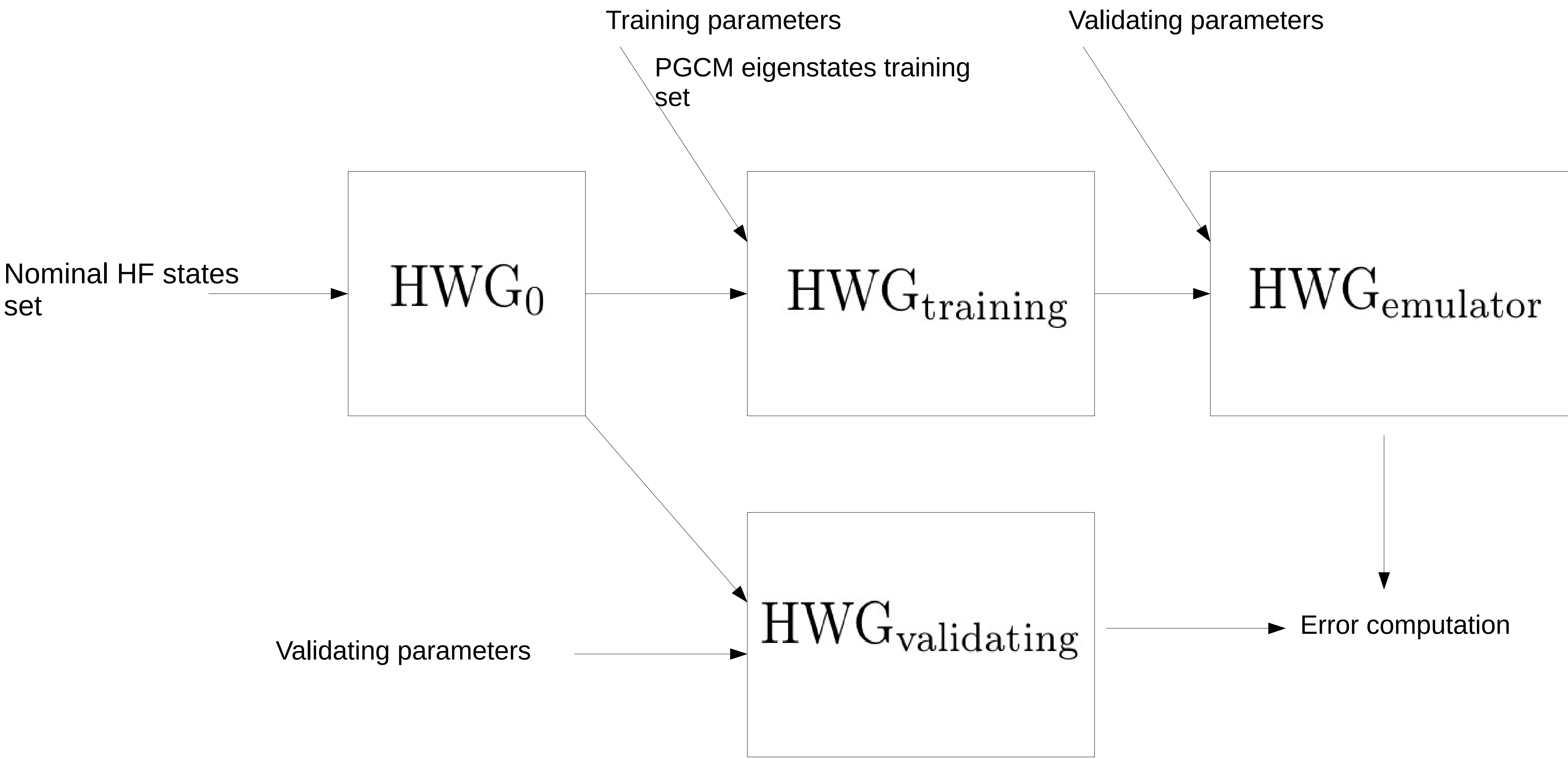
A First step (today)

$$V^{\lambda_1} \simeq V^{\lambda_2} \simeq \cdots \simeq V^{\lambda_{n_t}} \simeq V^{\lambda_0}$$

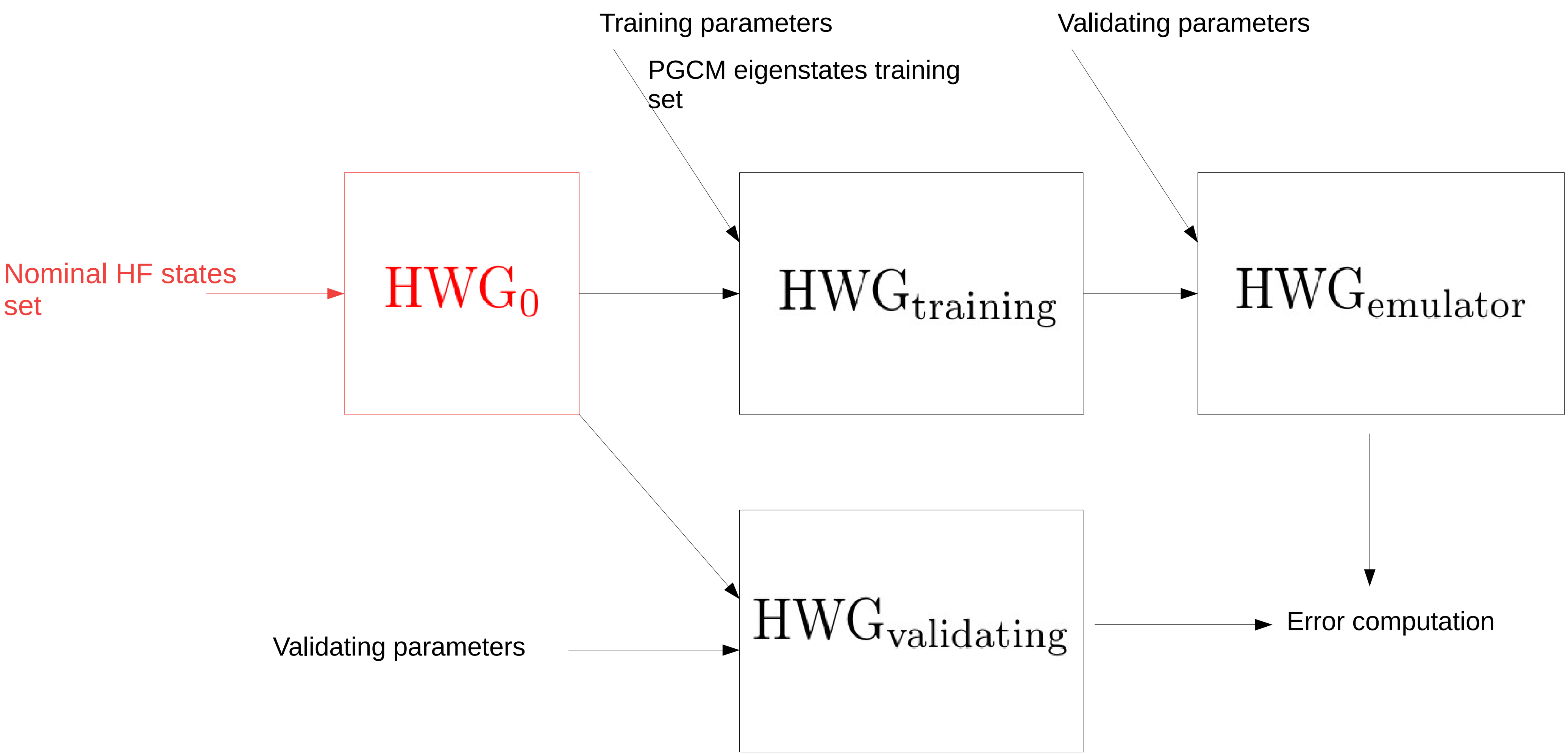
B Next step : emulate V^{λ}

$\longrightarrow$ To be investigated next

PGCM-EC Algorithm Preliminary implementation



PGCM-EC Algorithm Preliminary implementation



PGCM-EC Algorithm Preliminary implementation

Set of HF states $\left\{|\Phi^{\lambda_0}(q_i)\rangle\right\}_{1\leq i\leq n_q}$

Generating V^{λ_0}

→

HWG_0

$\langle\Phi^{\lambda_0}(q_i)|H_k|\Phi^{\lambda_0}(q_j)\rangle$ $\quad 1\leq i,j\leq n_q$

$\langle\Phi^{\lambda_0}(q_i)|\Phi^{\lambda_0}(q_j)\rangle$

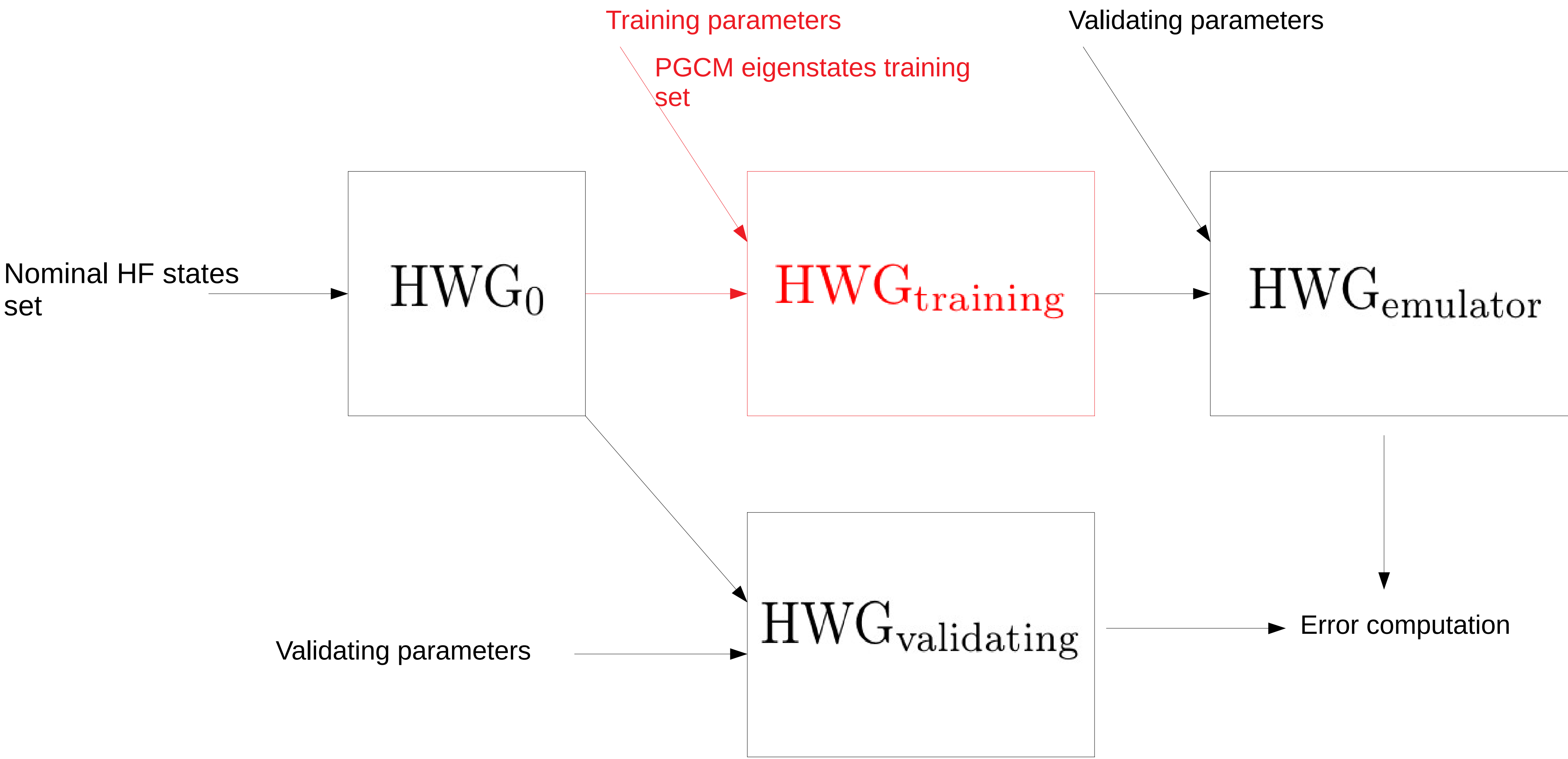
↓ Diagonalize norm matrix

$\left\{|\Theta_i^0\rangle\right\}_{1\leq i\leq \dim\, V^{\lambda_0}} \subset V^{\lambda_0}$

$\langle\Theta_i^0|H_k|\Theta_j^0\rangle$ $\quad 0\leq i,j\leq \dim\, V^{\lambda_0}$

$\langle\Theta_i^0|\Theta_j^0\rangle = \delta_{ij}$

PGCM-EC Algorithm Preliminary implementation



PGCM-EC Algorithm Preliminary implementation

$$\mathrm{HWG}_0$$

$$\{\mu_n\}_{1\leq n\leq n_t} \subset \mathbb{R}^{n_p}$$

$$\{a_m\}_{1\leq m\leq n_a} \subset \mathbb{N}$$

$$\mathrm{HWG}_{\mathrm{training}} \qquad 0 \leq i,j \leq \dim V^{\lambda_0}$$

$$H_{ij}^{\mu_n} = \langle \Theta_i^0 | H^{\mu_n} | \Theta_j^0 \rangle = \sum_k \langle \Theta_i^0 | H_k | \Theta_j^0 \rangle \mu_n^k$$

$$H^{\mu_n} | \Psi_{a_m}^{\mu_n} \rangle = E_{a_m}^{\mu_n} | \Psi_{a_m}^{\mu_n} \rangle$$

$$\langle \Psi_{a_m}^{\mu_n} | H_k | \Psi_{a_{m'}}^{\mu_{n'}} \rangle$$

$$\langle \Psi_{a_m}^{\mu_n} | \Psi_{a_{m'}}^{\mu_{n'}} \rangle$$

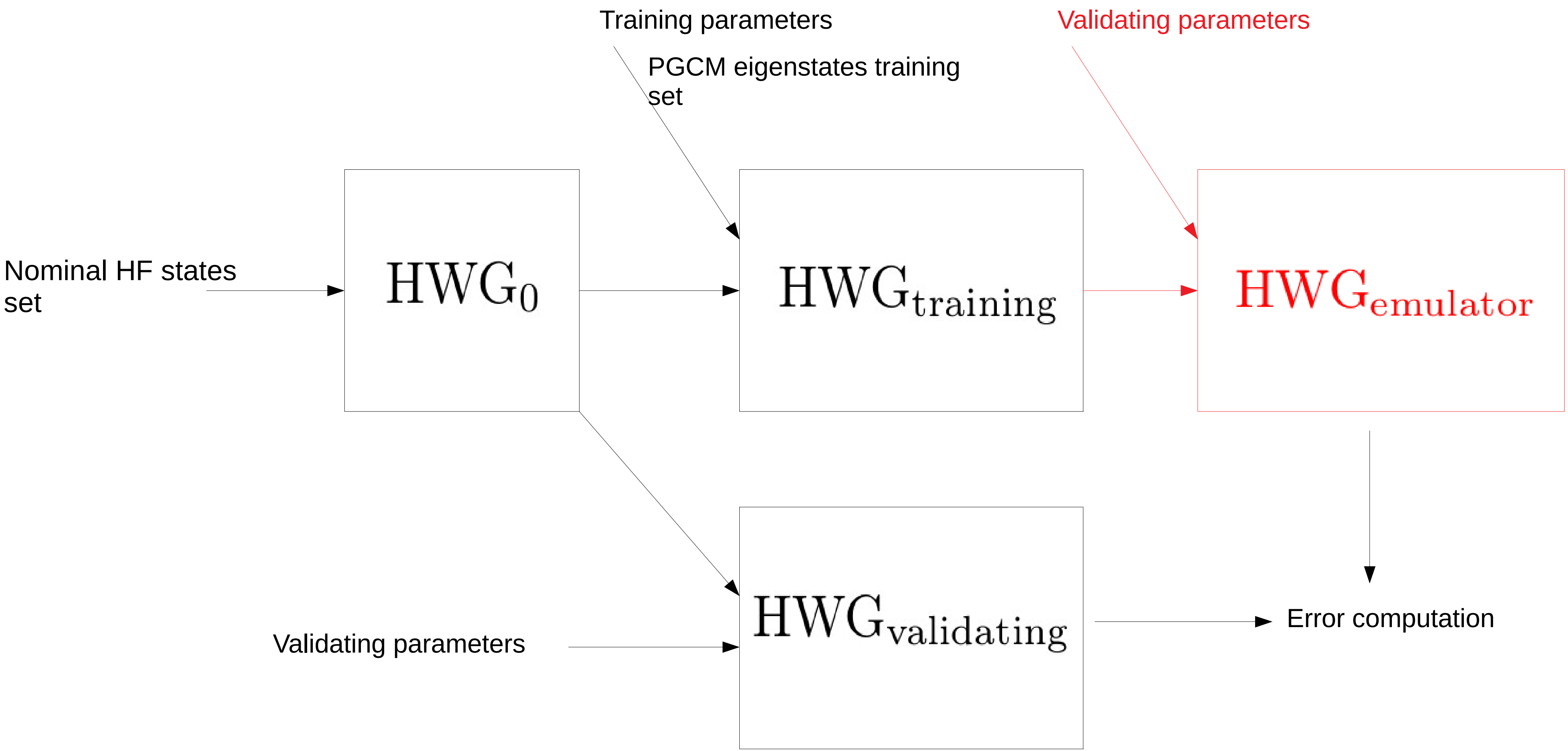
Diagonalize norm matrix

$$0 \leq i,j \leq \dim V^{\mathrm{train.}}$$

$$\langle \Theta_i^{\mathrm{train.}} | H_k | \Theta_j^{\mathrm{train.}} \rangle$$

$$\langle \Theta_i^{\mathrm{train.}} | \Theta_j^{\mathrm{train.}} \rangle = \delta_{ij}$$

PGCM-EC Algorithm Preliminary implementation



PGCM-EC Algorithm Preliminary implementation

$\mathrm{HWG}_{\mathrm{training}}$

$\{\lambda_n\}_{1\leq n\leq n_{\mathrm{val}}} \subset \mathbb{R}^{n_p}$

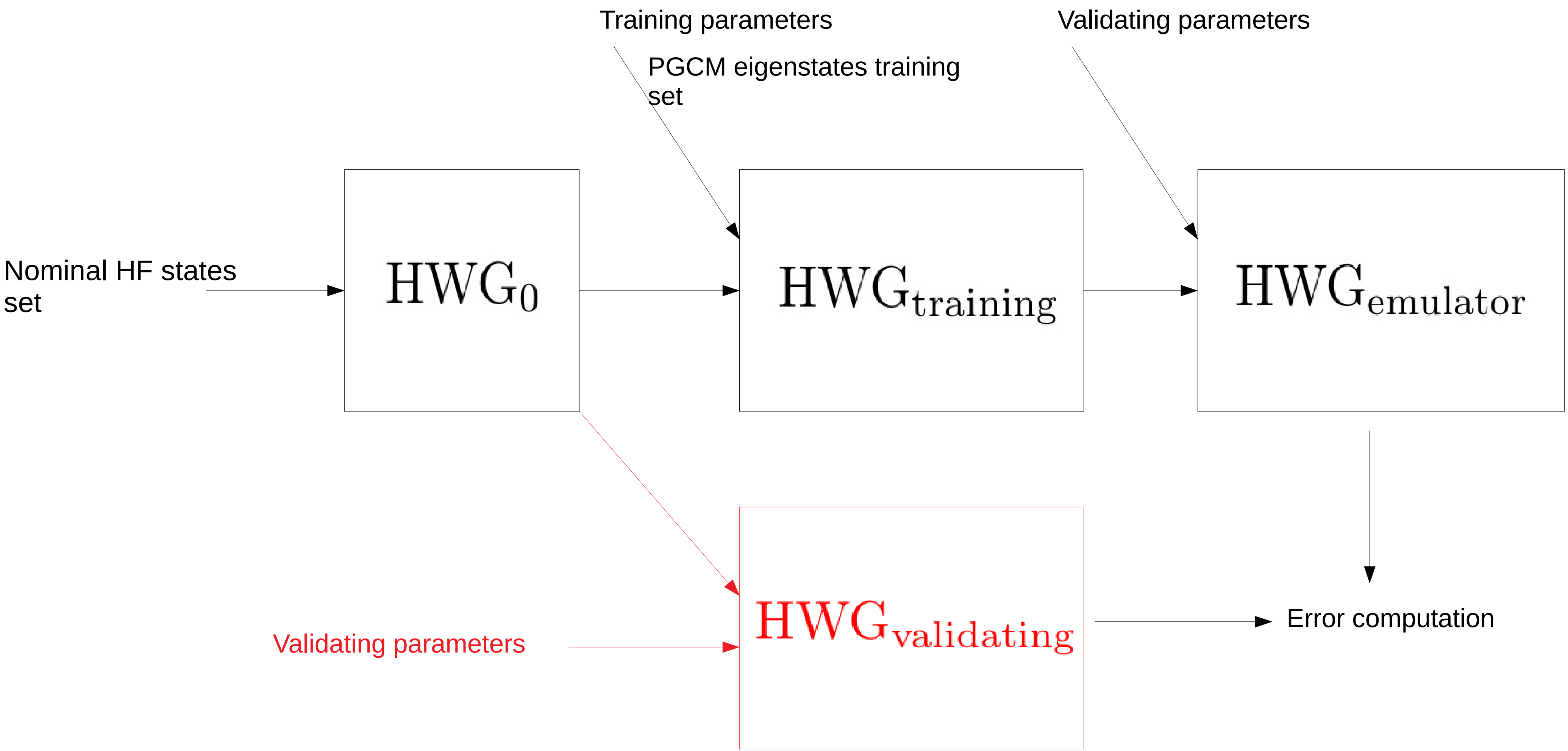
$\mathrm{HWG}_{\mathrm{emulator}}$

$0 \leq i,j \leq \dim V^{\mathrm{train.}}$

$$H_{ij}^{\lambda_n} = \langle \Theta_i^{\mathrm{train.}} | H^{\lambda_n} | \Theta_j^{\mathrm{train.}} \rangle = \sum_k \langle \Theta_i^{\mathrm{train.}} | H_k | \Theta_j^{\mathrm{train.}} \rangle \lambda_n^k$$

$$H^{\lambda_n} | \Psi_a^{\lambda_n} \rangle_{\mathrm{emul.}} = E_a^{\lambda_n} | \Psi_a^{\lambda_n} \rangle_{\mathrm{emul.}}$$

PGCM-EC Algorithm Preliminary implementation



PGCM-EC Algorithm Preliminary implementation

HWG_0

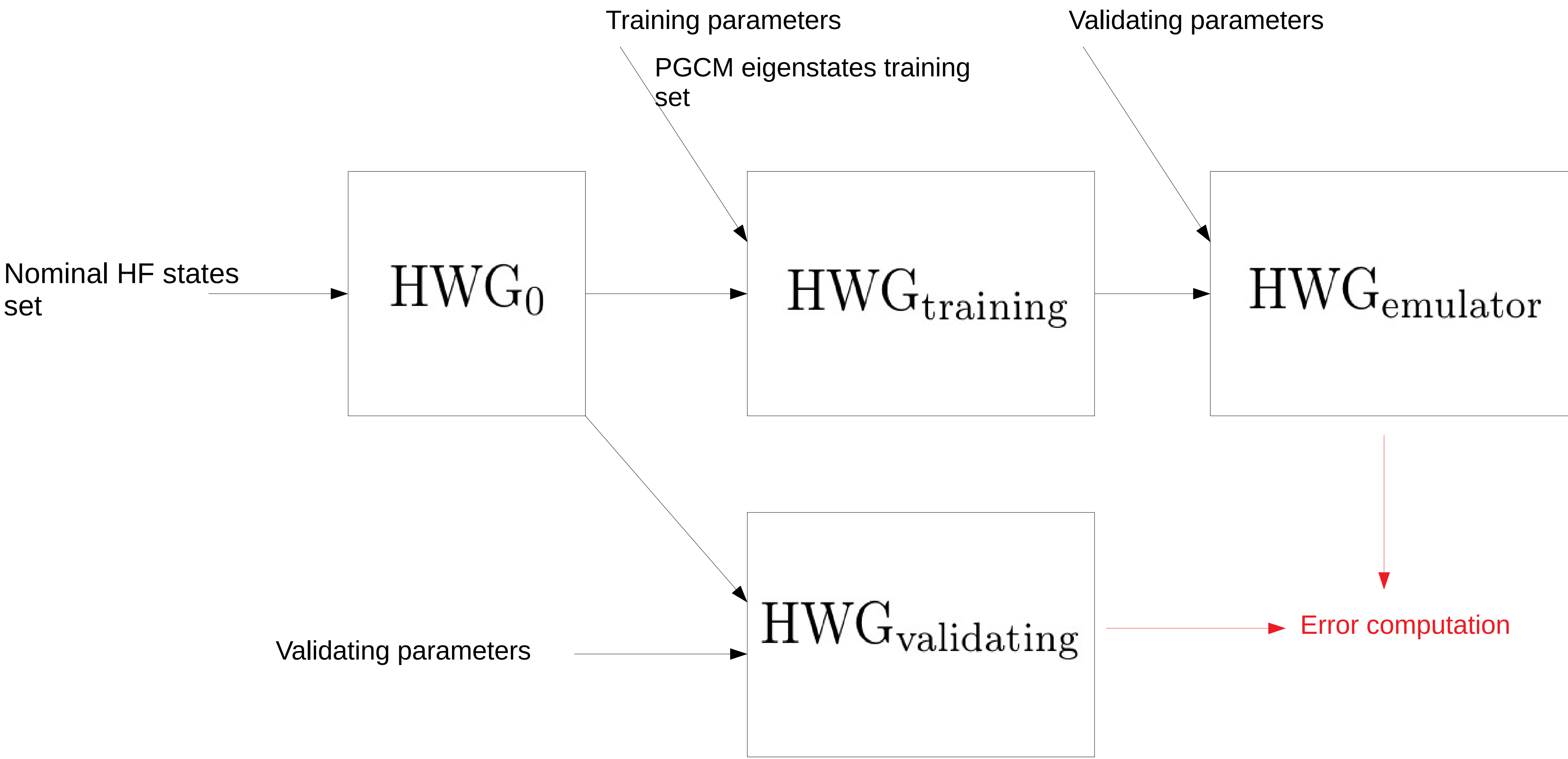
$\{\lambda_n\}_{1\leq n\leq n_{\mathrm{val}}} \subset \mathbb{R}^{n_p}$

$\mathrm{HWG}_{\mathrm{validating}}$ $\quad 0 \leq i, j \leq \dim V^{\lambda_0}$

$$H_{ij}^{\lambda_n} = \langle \Theta_i^0 | H^{\lambda_n} | \Theta_j^0 \rangle = \sum_k \langle \Theta_i^0 | H_k | \Theta_j^0 \rangle \lambda_n^k$$

$$H^{\lambda_n} | \Psi_a^{\lambda_n} \rangle = E_a^{\lambda_n} | \Psi_a^{\lambda_n} \rangle$$

PGCM-EC Algorithm Preliminary implementation



PGCM-EC Algorithm Preliminary implementation

Error computations

- Absolute energies
- Excitation energies
- Radii
- States distance → To be implemented soon

Preliminary computation model definition

- ^{20}Ne Nucleus
- Brink & Boecker interaction $(4+2$ parameters$)$

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

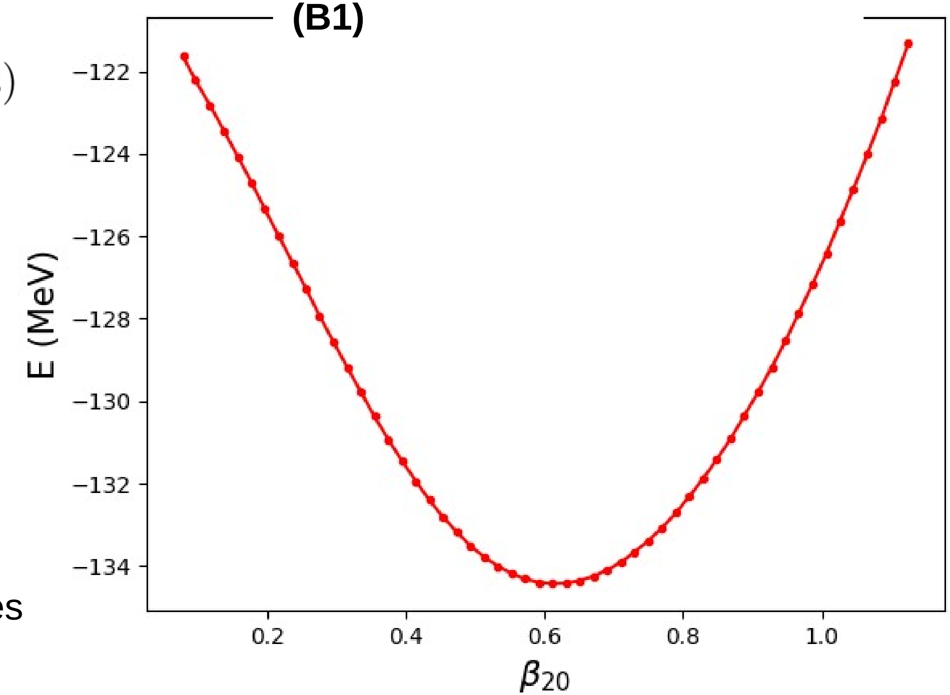
$$+ \text{ kinetic \& COM correction}$$

$w_0 = -72.21$ 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

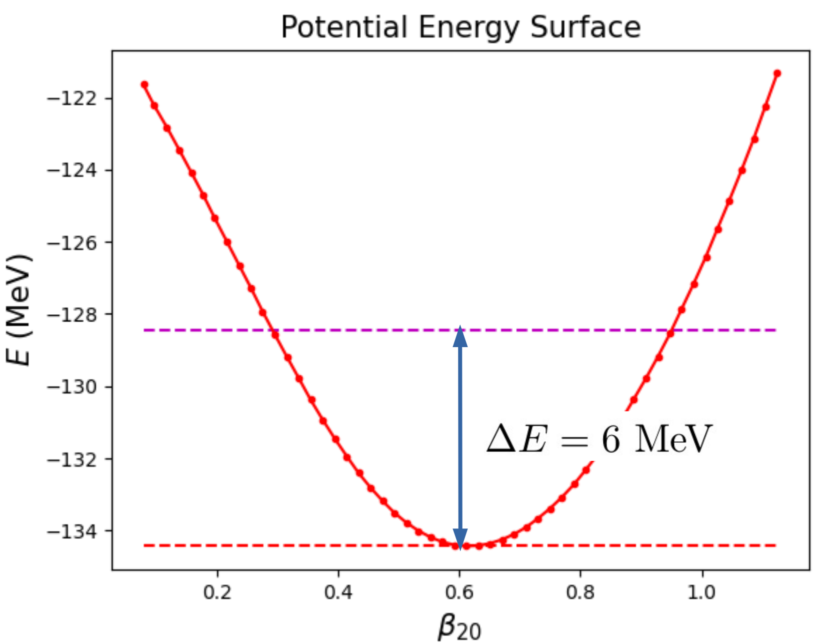
Fix at nominal values

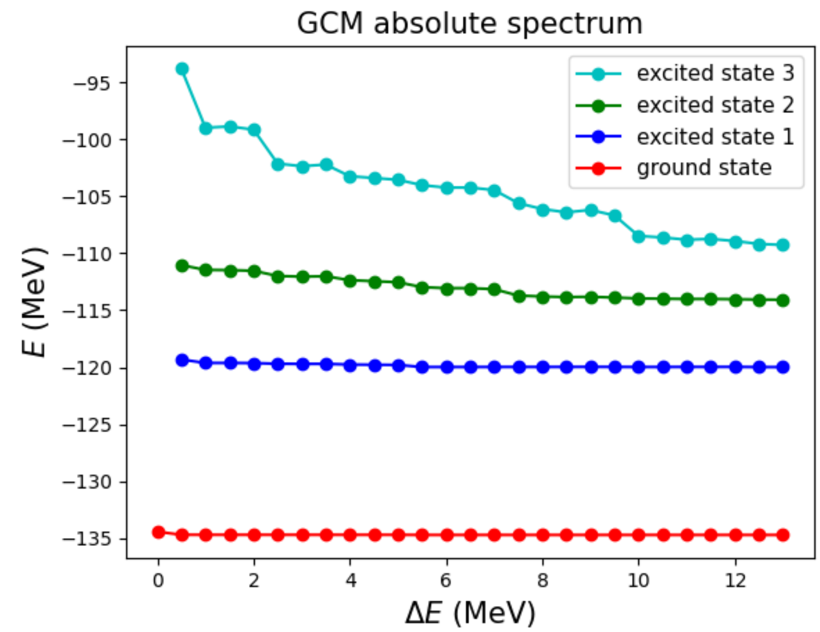
PES for nominal parameters (B1)

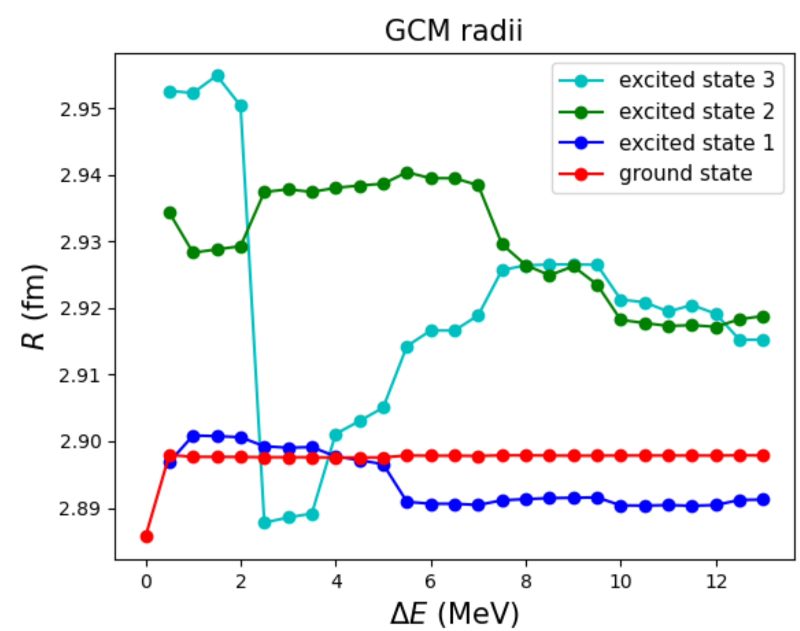


Nominal GCM computation Convergence

- Convergence of GCM energies & radii vs GCM truncation
  - → Nominal parametrization (B1)
  - → Energy cut on HF set
  - → Energies converged for E_0 + vibrational excitations E_1 & E_2
  - → Radii converged for R0 & R1
  - → Evaluation of GCM truncation error
    - $E_{n+1} - E_n$
    - $R_{n+1} - R_n$







Nominal GCM computation Effective dimension

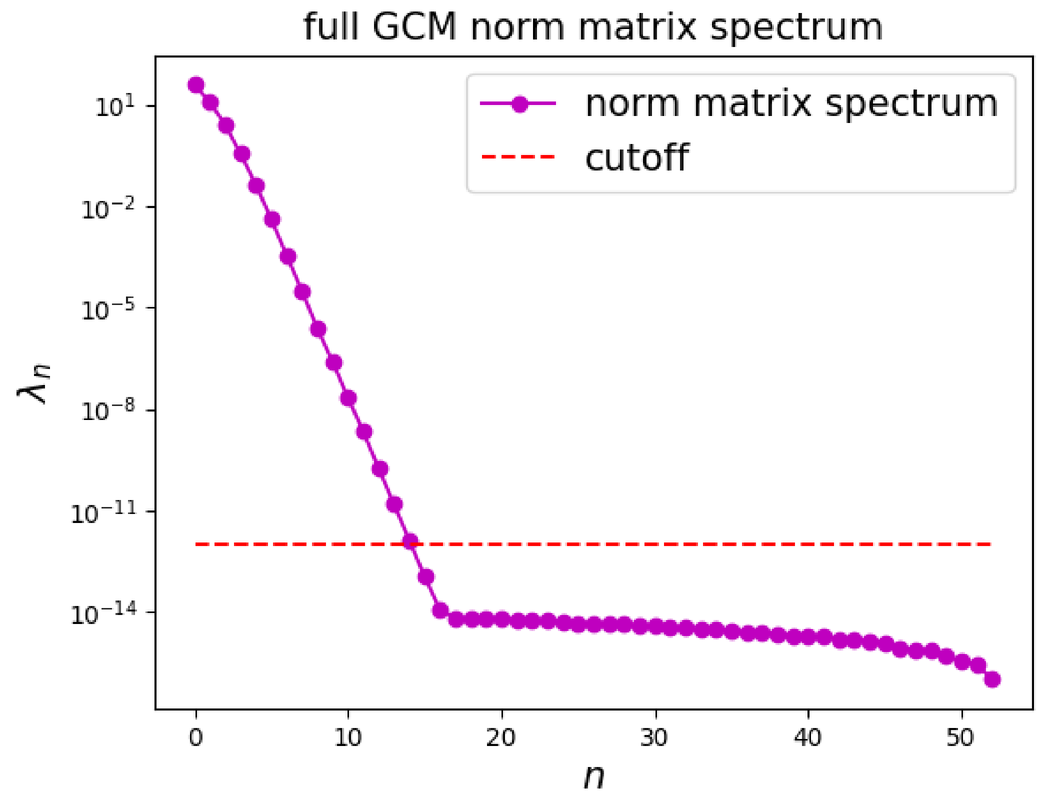
- Norm matrix spectrum

→ $\text{cutoff} = 10^{-12}$

→ Number of eigenvalues above cutoff

◆ Effective dimension of V^{λ_0}

	Size	**Dimension**
GCM set	53	15



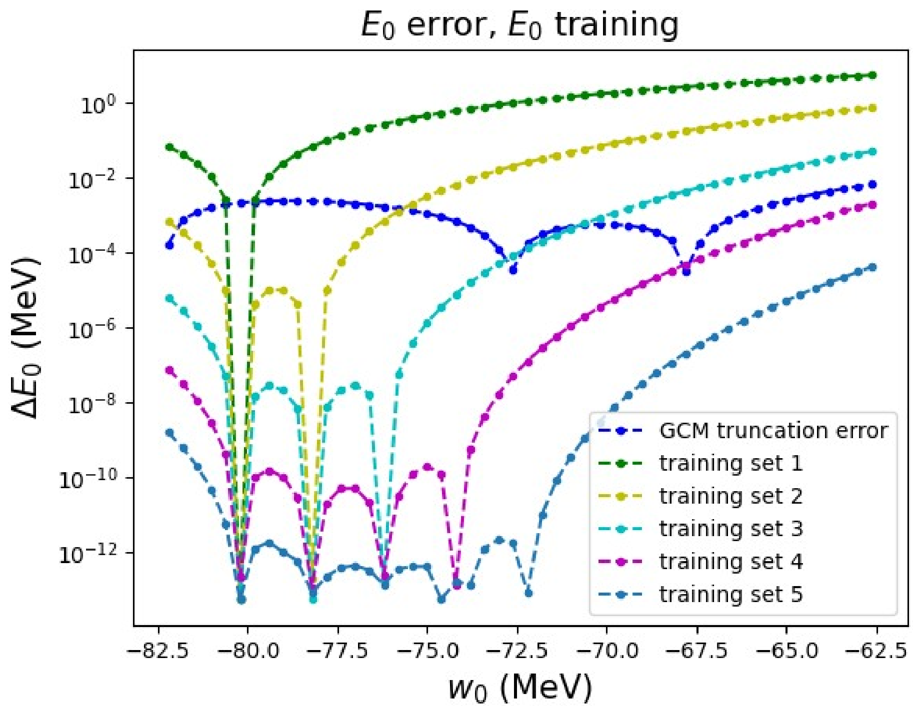
1 parameter GCM-EC Ground-state training

- One-dimensional emulator (w_0)

→ Ground-state training $\mathrm{TS}_0^{\mathrm{ex.}} = \{0\}$

→ Training set of parameters

$$\mathrm{TS}_1^{\mathrm{par.}} = \{-80.21\}$$
$$\mathrm{TS}_2^{\mathrm{par.}} = \{-80.21, -78.21\}$$
$$\mathrm{TS}_3^{\mathrm{par.}} = \{-80.21, -78.21, -76.21\}$$
$$\mathrm{TS}_4^{\mathrm{par.}} = \{-80.21, -78.21, -76.21, -74.21\}$$
$$\mathrm{TS}_5^{\mathrm{par.}} = \{-80.21, -78.21, -76.21, -74.21, -72.21\}$$



→ Excellent (good) interpolation (extrapolation) of ground-state energy

→ Excellent (good) interpolation (extrapolation) of ground-state radii

	Size	**Dimension**
GCM set	53	15
$\mathrm{TS}_1^{\mathrm{par.}}$	1	1
$\mathrm{TS}_2^{\mathrm{par.}}$	2	2
$\mathrm{TS}_3^{\mathrm{par.}}$	3	3
$\mathrm{TS}_4^{\mathrm{par.}}$	4	4
$\mathrm{TS}_5^{\mathrm{par.}}$	5	5

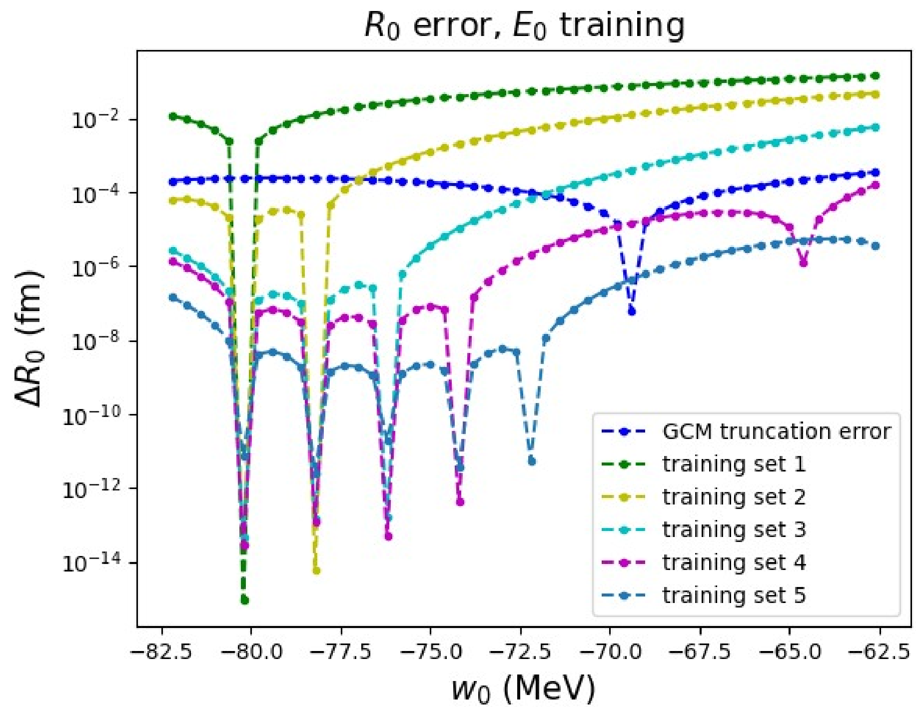
1 parameter GCM-EC Ground-state training

- One-dimensional emulator (w_0)

→ Ground-state training $\mathrm{TS}_0^{\mathrm{ex.}} = \{0\}$

→ Training set of parameters

$$\mathrm{TS}_1^{\mathrm{par.}} = \{-80.21\}$$
$$\mathrm{TS}_2^{\mathrm{par.}} = \{-80.21, -78.21\}$$
$$\mathrm{TS}_3^{\mathrm{par.}} = \{-80.21, -78.21, -76.21\}$$
$$\mathrm{TS}_4^{\mathrm{par.}} = \{-80.21, -78.21, -76.21, -74.21\}$$
$$\mathrm{TS}_5^{\mathrm{par.}} = \{-80.21, -78.21, -76.21, -74.21, -72.21\}$$



	Size	Dimension
GCM set	53	15
$\mathrm{TS}_1^{\mathrm{par.}}$	1	1
$\mathrm{TS}_2^{\mathrm{par.}}$	2	2
$\mathrm{TS}_3^{\mathrm{par.}}$	3	3
$\mathrm{TS}_4^{\mathrm{par.}}$	4	4
$\mathrm{TS}_5^{\mathrm{par.}}$	5	5

→ Excellent (good) interpolation (extrapolation) of ground-state energy

→ Excellent (good) interpolation (extrapolation) of ground-state radii

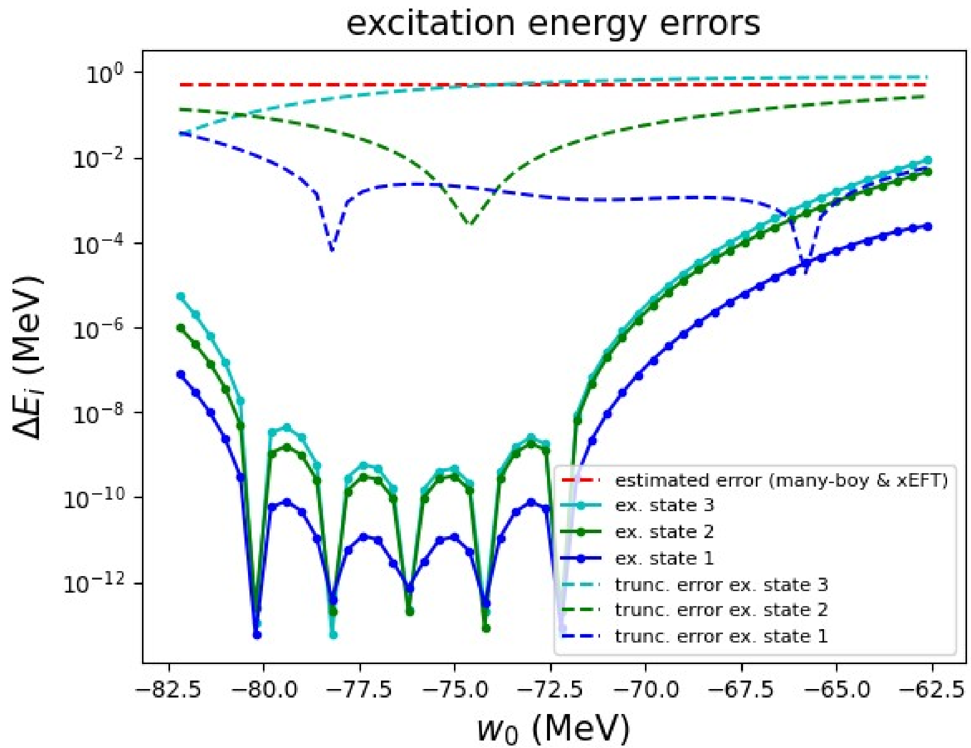
1 parameter GCM-EC Separate training for excited states

- Separate training for excited states

$$\mathrm{TS}_1^{\mathrm{ex.}} = \{1\}$$
$$\mathrm{TS}_2^{\mathrm{ex.}} = \{2\}$$
$$\mathrm{TS}_3^{\mathrm{ex.}} = \{3\}$$

- Common training for parameters

$$\mathrm{TS}_5^{\mathrm{par.}} = \{-80.21, -78.21, -76.21, -74.21, -72.21\}$$



→ Excellent (good) interpolation (extrapolation) of excitation energies

	Size	**Dimension**
GCM set	53	15
$\mathrm{TS}_1^{\mathrm{ex.}}$	5	5
$\mathrm{TS}_2^{\mathrm{ex.}}$	5	5
$\mathrm{TS}_3^{\mathrm{ex.}}$	5	5

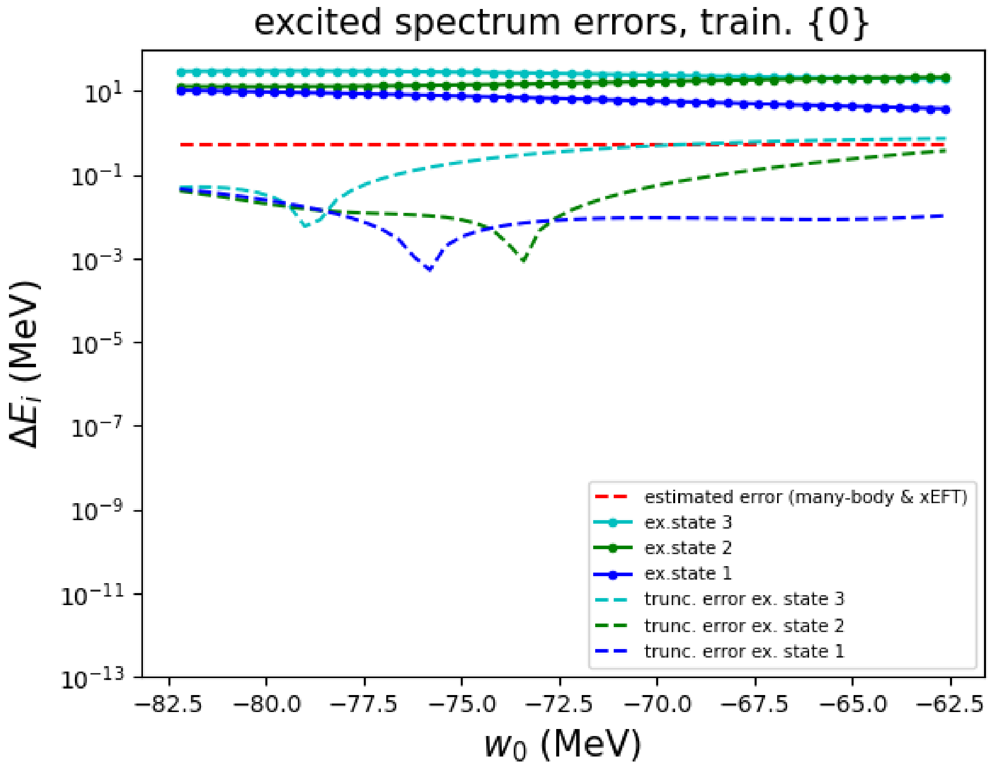
1 parameter GCM-EC Ground-state training for excited states

- Training on ground state

$$\mathrm{TS}_0^{\mathrm{ex.}} = \{0\}$$

$$\mathrm{TS}_5^{\mathrm{par.}}$$

→ Cannot reproduce excited states



	Size	**Dimension**
GCM set	53	15
$\mathrm{TS}_0^{\mathrm{ex.}}$	5	5

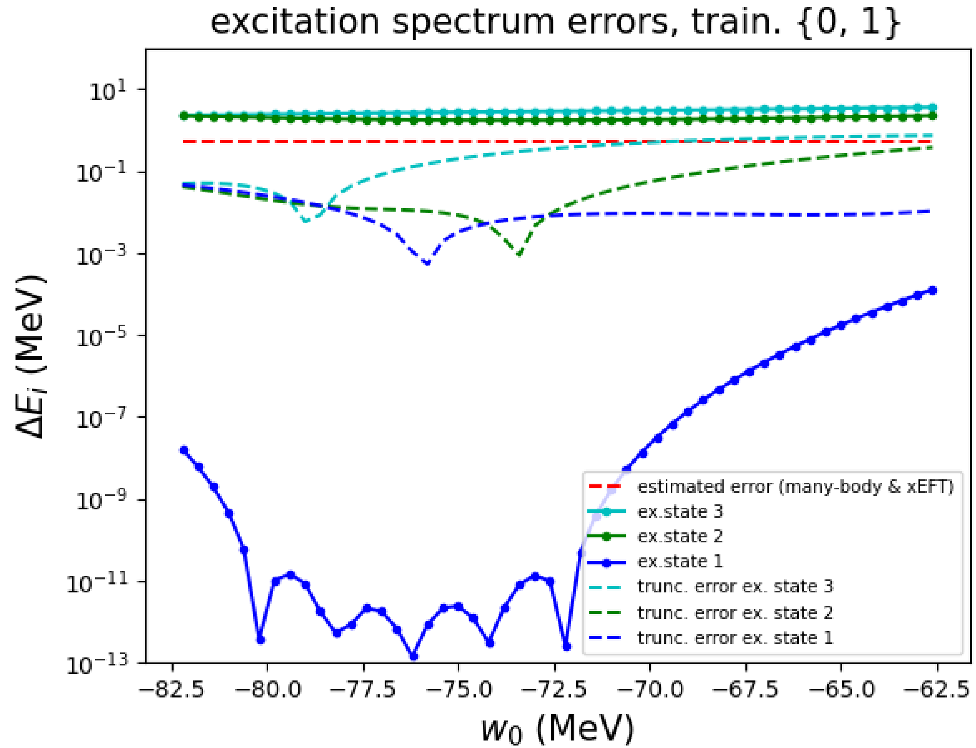
1 parameter GCM-EC Excited-state training for excited states

- Adding first excited state to training

$$\mathrm{TS}_{01}^{\mathrm{ex.}} = \{0, 1\}$$

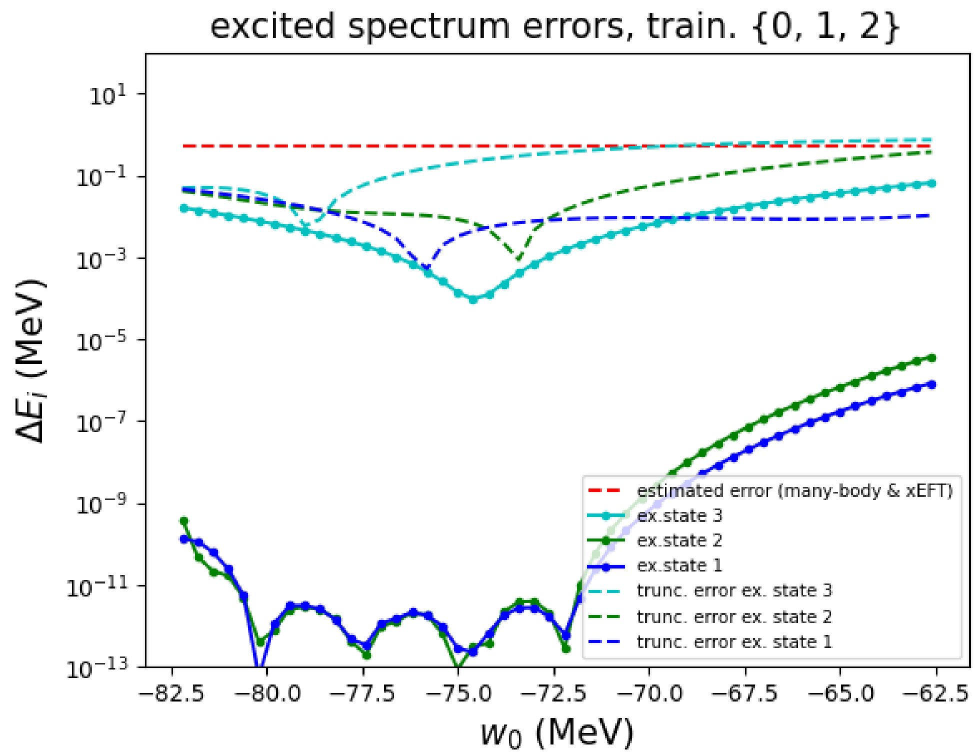
$$\mathrm{TS}_{5}^{\mathrm{par.}}$$

→ First excitation energy immediately ok



	Size	Dimension
GCM set	53	15
$\mathrm{TS}_{01}^{\mathrm{ex.}}$	10	10

1 parameter GCM-EC Excited-state training for excited states



- Adding second excited state to training

$$\mathrm{TS}^{\mathrm{ex.}}_{012} = \{0, 1, 2\}$$

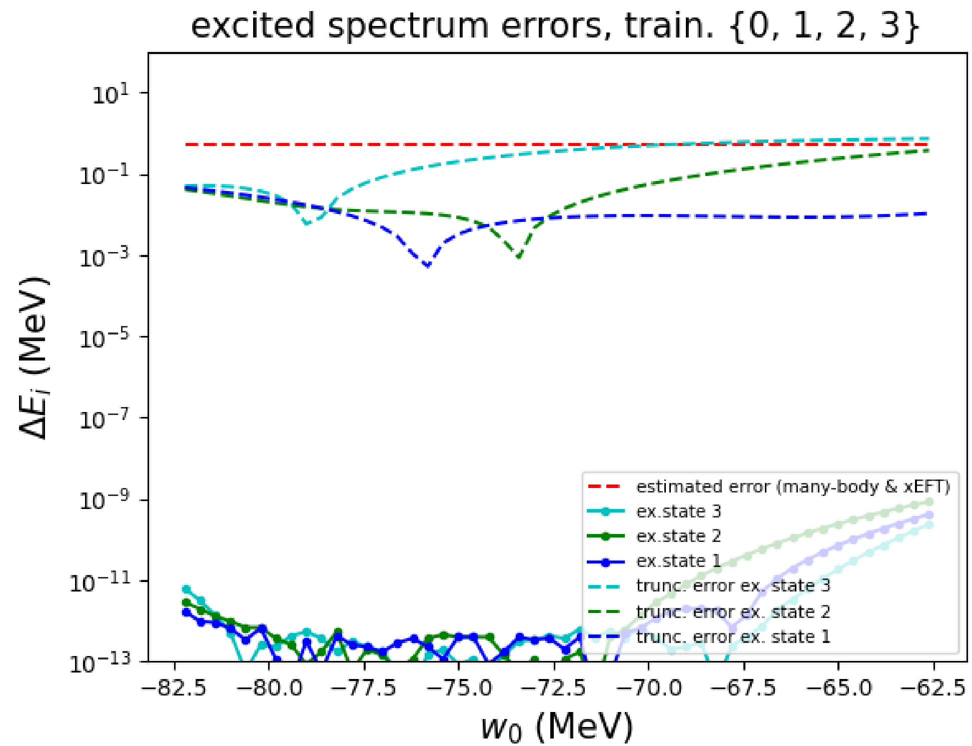
$$\mathrm{TS}^{\mathrm{par.}}_{5}$$

⟶ First excitation energy ok

⟶ Second excitation energy now also ok

	Size	**Dimension**
GCM set	53	15
$\mathrm{TS}^{\mathrm{ex.}}_{012}$	15	14

1 parameter GCM-EC Excited-state training for excited states



- Adding third excited state to training

$$\mathrm{TS}^{\mathrm{ex.}}_{0123} = \{0, 1, 2, 3\}$$

$$\mathrm{TS}^{\mathrm{par.}}_{5}$$

→ First three excitation energies ok

- Training set span full GCM space

	Size	**Dimension**
GCM set	53	15
$\mathrm{TS}^{\mathrm{ex.}}_{0123}$	20	15

4 parameter GCM-EC random parameter training

- Regular rectangular mesh of $[\lambda_0 - 10, \lambda_0 + 10]^4$ with $4^4 = 256$ points

  $\rightarrow$ sketchy, should use **latin hypercube sampling**

- Random mesh partition into $\mathrm{TS}^{\mathrm{param.}}_{\mathrm{train.}}$ and $\mathrm{TS}^{\mathrm{param.}}_{\mathrm{val.}}$

  $\longrightarrow \quad |\mathrm{TS}^{\mathrm{param.}}_{\mathrm{train.}}| = n_t$

- Emulator cost function

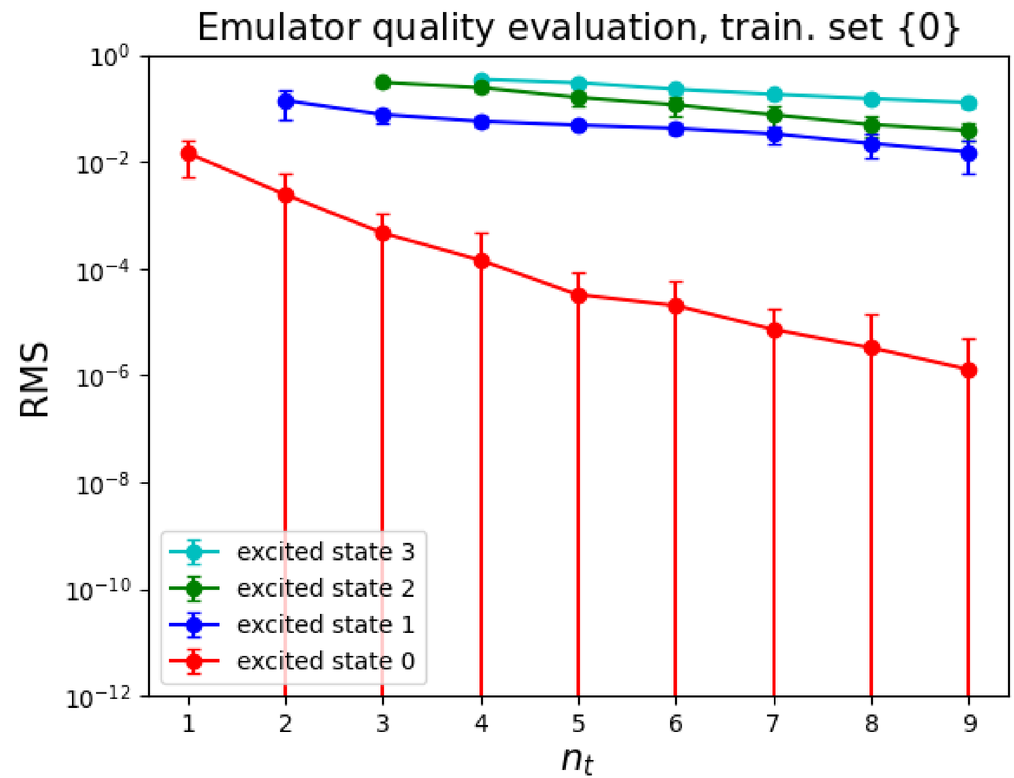
$$\mathrm{RMS}_a = \left(\sum_{\lambda \in \mathrm{TS}^{\mathrm{param.}}_{\mathrm{val.}}} \left(\frac{E_a^{\mathrm{emul.}}(\lambda) - E_a^{\mathrm{val.}}(\lambda)}{E_a^{\mathrm{val.}}(\lambda)} \right)^2 \right)^{1/2}$$

- Repeat N = 100 times

  $\longrightarrow$ Mean RMS, deviation

- Emulator trained on ground state

$$\mathrm{TS}_0^{\mathrm{ex.}} = \{0\}$$



Good overall reproduction of ground state

Not true for excited states

4 parameter GCM-EC random parameter training

- Regular rectangular mesh of $[\lambda_0 - 10, \lambda_0 + 10]^4$ with $4^4 = 256$ points

  $\rightarrow$ sketchy, should use **latin hypercube sampling**

- Random mesh partition into $\mathrm{TS}^{\mathrm{param.}}_{\mathrm{train.}}$ and $\mathrm{TS}^{\mathrm{param.}}_{\mathrm{val.}}$

  ⟶ $|\mathrm{TS}^{\mathrm{param.}}_{\mathrm{train.}}| = n_t$

- Emulator cost function

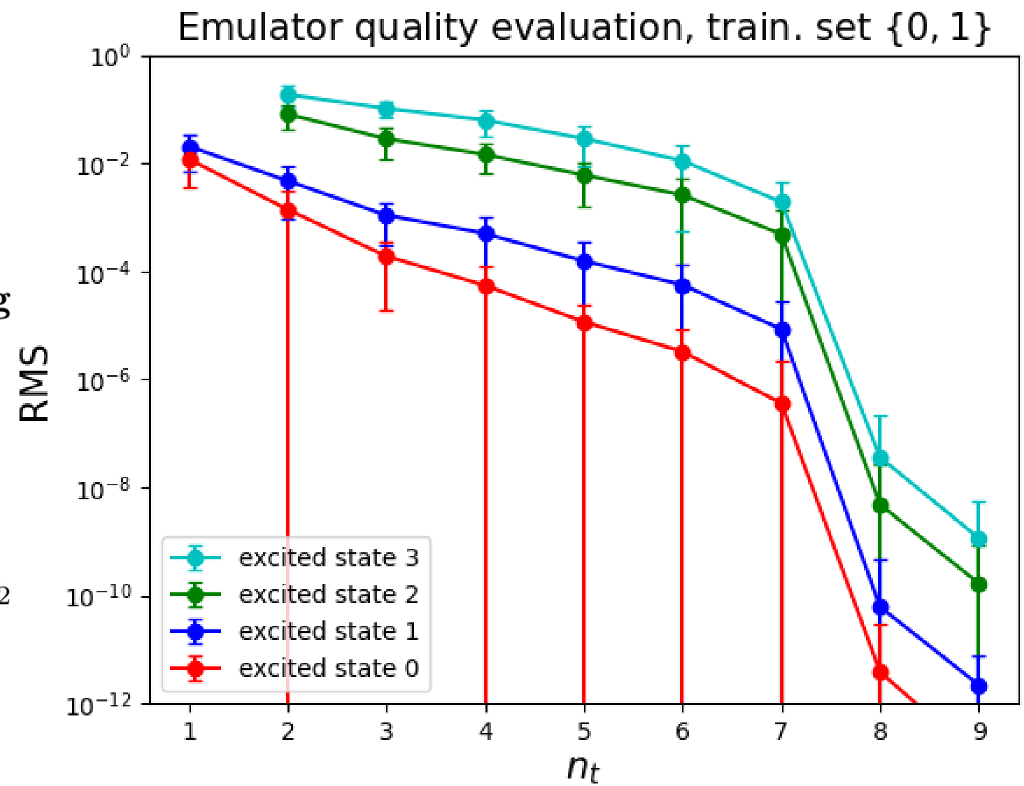
$$\mathrm{RMS}_a = \left(\sum_{\lambda \in \mathrm{TS}^{\mathrm{param.}}_{\mathrm{val.}}} \left(\frac{E_a^{\mathrm{emul.}}(\lambda) - E_a^{\mathrm{val.}}(\lambda)}{E_a^{\mathrm{val.}}(\lambda)} \right)^2 \right)^{1/2}$$

- Repeat N = 100 times

  ⟶ Mean RMS, deviation

- Emulator trained on ground state + excited state 1

$$\mathrm{TS}^{\mathrm{ex.}}_{01} = \{0, 1\}$$



Good overall reproduction of ground state

And first excited state

4 parameter GCM-EC random parameter training

- Regular rectangular mesh of $[\lambda_0 - 10, \lambda_0 + 10]^4$ with $4^4 = 256$ points

  $\rightarrow$ sketchy, should use **latin hypercube sampling**

- Random mesh partition into $\mathrm{TS}^{\text{param.}}_{\text{train.}}$ and $\mathrm{TS}^{\text{param.}}_{\text{val.}}$

  $\longrightarrow$ $|\mathrm{TS}^{\text{param.}}_{\text{train.}}| = n_t$

- Emulator cost function

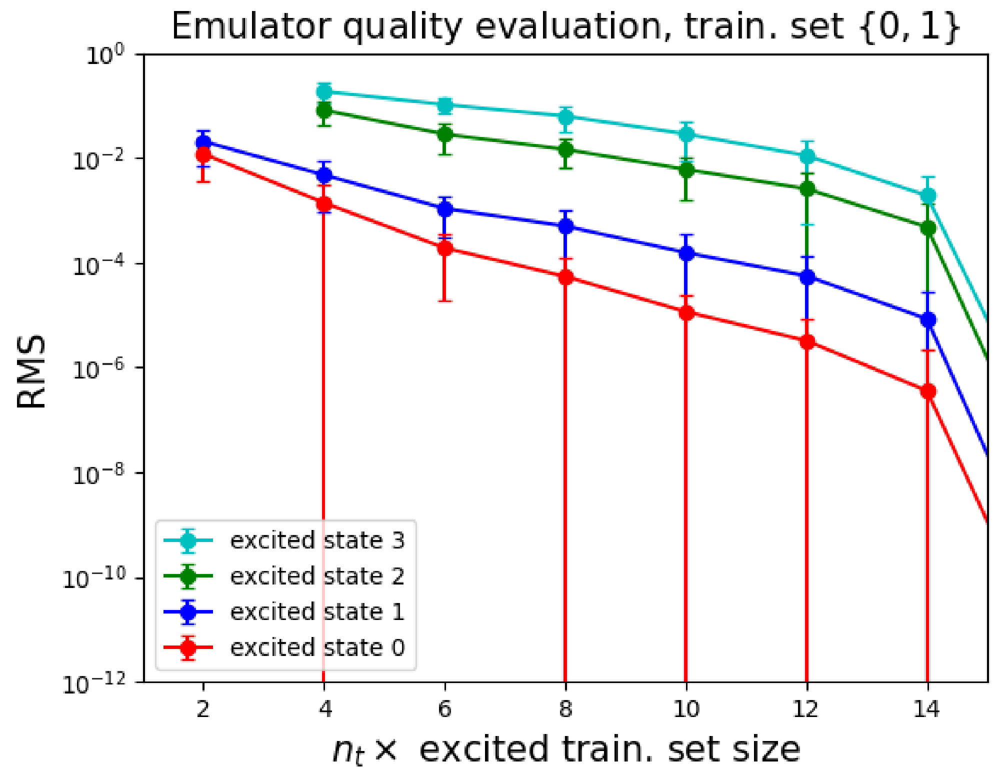
$$\mathrm{RMS}_a = \left(\sum_{\lambda \in \mathrm{TS}^{\text{param.}}_{\text{val.}}} \left(\frac{E_a^{\text{emul.}}(\lambda) - E_a^{\text{val.}}(\lambda)}{E_a^{\text{val.}}(\lambda)} \right)^2 \right)^{1/2}$$

- Repeat N = 100 times

  $\longrightarrow$ Mean RMS, deviation

- Emulator trained on ground state + excited state 1

$$\mathrm{TS}^{\text{ex.}}_{01} = \{0, 1\}$$



Good overall reproduction of ground state

And first excited state

Taking into account effective dimension

Conclusion & perspectives

- **Encouraging preliminary result**
  - → Absolute energies
  - → Excitation energies
  - → Radii
- **Quick generalisation to less trivial model**
  - → Ab initio
  - → More observables
- **Time complexity reduction**
  - → EC game-changing
  - → Application to sensitivity analysis and interaction fits in nuclear theory