Surrogate models for Quantum many-body systems

Recent Progress in Many-Body Theories(RPMBT22)@Tsukuba, Sept. 23-27, 2024

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RIKEN Nishina Center

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Why **surrogate models** matter ?

Condensed matter physics, Quantum Chemistry, Nuclear Physics, *etc.*

share issues on…

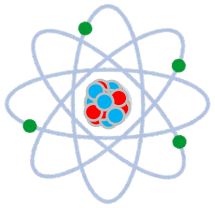
- **exponential growth of the size of Hilbert space**
- repeating **simulations under tons of different params** for **quantifying uncertainties/inverse problem** (*e.g. nuclear force*)

surrogate models, emulators, reduced order models, …

you may call them in different ways

Difference between nuclei and other systems

Quantum chemistry:



"99 > % of energy of a molecule in equilibrium

is explained within Hartree-Fock level"

(i.e., single Slater determinant)

rest 1 % is called **correlation energy**

Møller – Plesset (MP a.k.a MBPT)

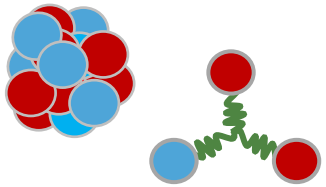
Coupled Cluster Single and Double (CCSD)

CCSD + Triple (CCSDT)

Full Configuration interaction (Full-CI)

accurate but heavy

Nuclear physics:



Interaction is highly non-perturbative & uncertain

many channels, **three-nucleon force**,...

^{56}Ni under modern Nuclear Force (Chiral EFT)

HF = - 302.716 MeV

HF + MP2 + MP3 = -473.089 MeV
(MP2 = -152.533, MP3 = -17.716)

~~How dare people say perturbation theory !!~~

c.f. Energy (Exp.) = -483.996 MeV

Nuclear landscape

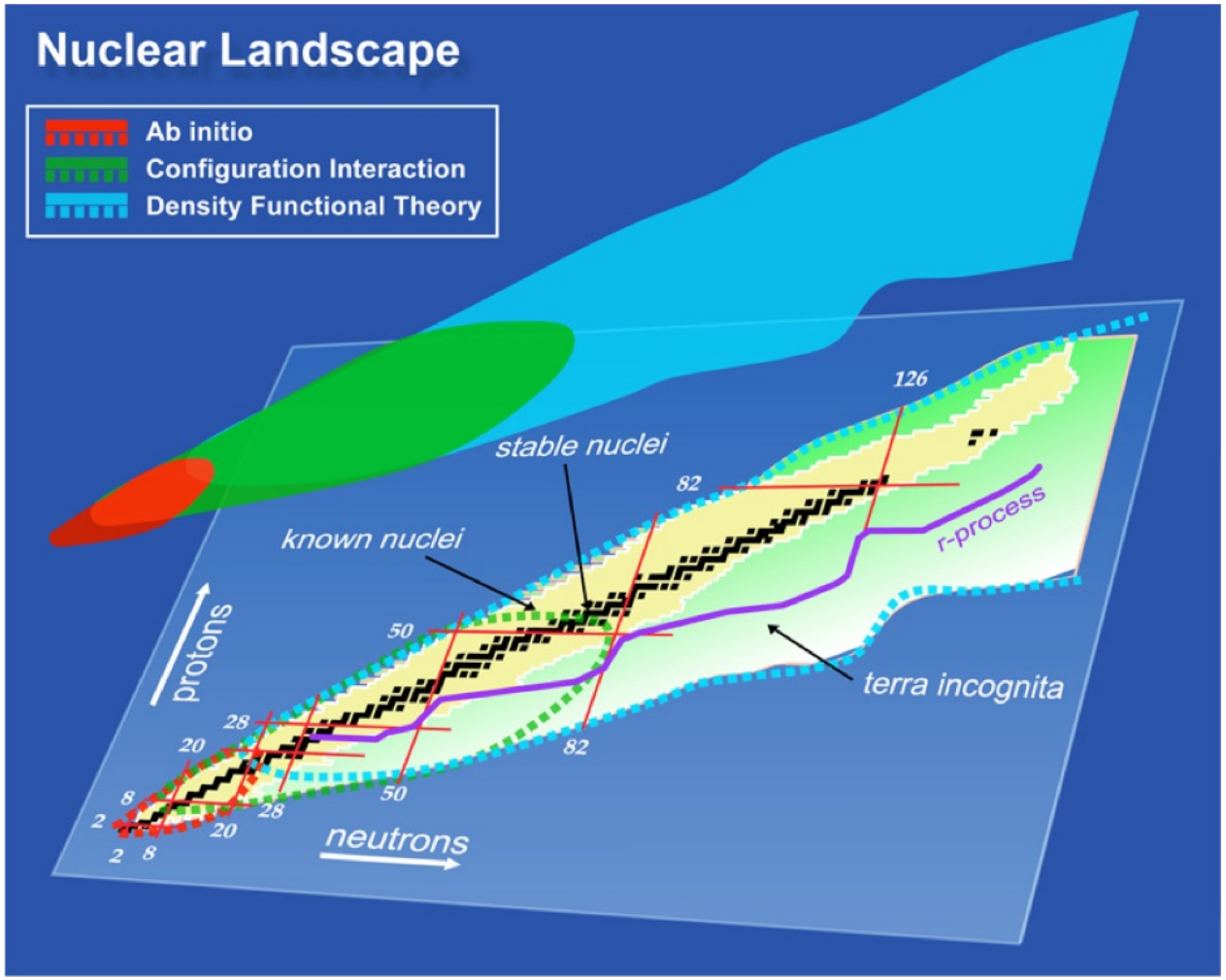


Fig. from UNEDF

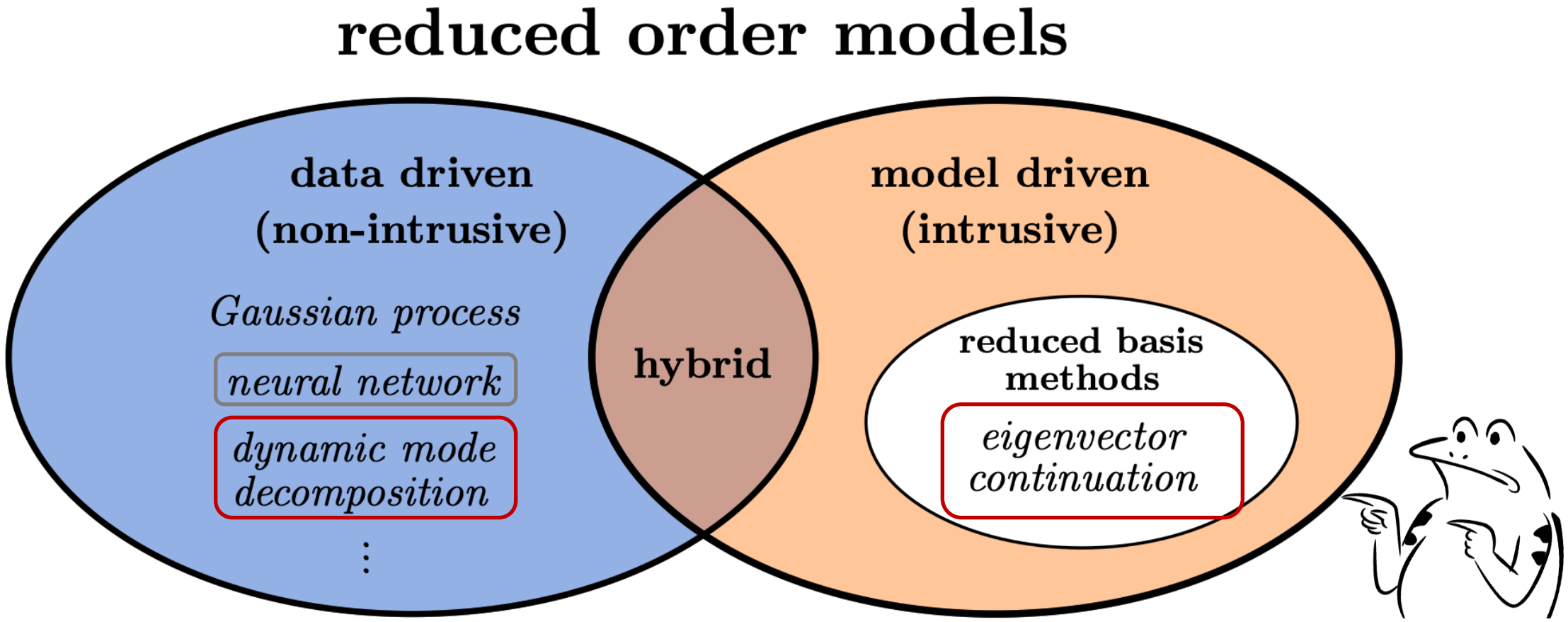
"Terra incognita" in nuclear physics

- unstable nuclei (e.g. r-process path)
- superheavy nuclei
- etc.

The scope of Ab initio and CI is gradually expanding, but still limited

The connection between EDF and nuclear force is unclear

Reduced order models/surrogate models



T. Duguet et al., Rev. Mod. Phys. 96, 031002 (2024)

Pioneering work in nuclear physics community

In 2018, a seminal paper is published: Eigenvector Continuation (EC)

PHYSICAL REVIEW LETTERS **121,** 032501 (2018)

Featured in Physics

Eigenvector Continuation with Subspace Learning

Dillon Frame,[1,2] Rongzheng He,[1,2] Ilse Ipsen,[3] Daniel Lee,[4] Dean Lee,[1,2] and Ermal Rrapaj[5]

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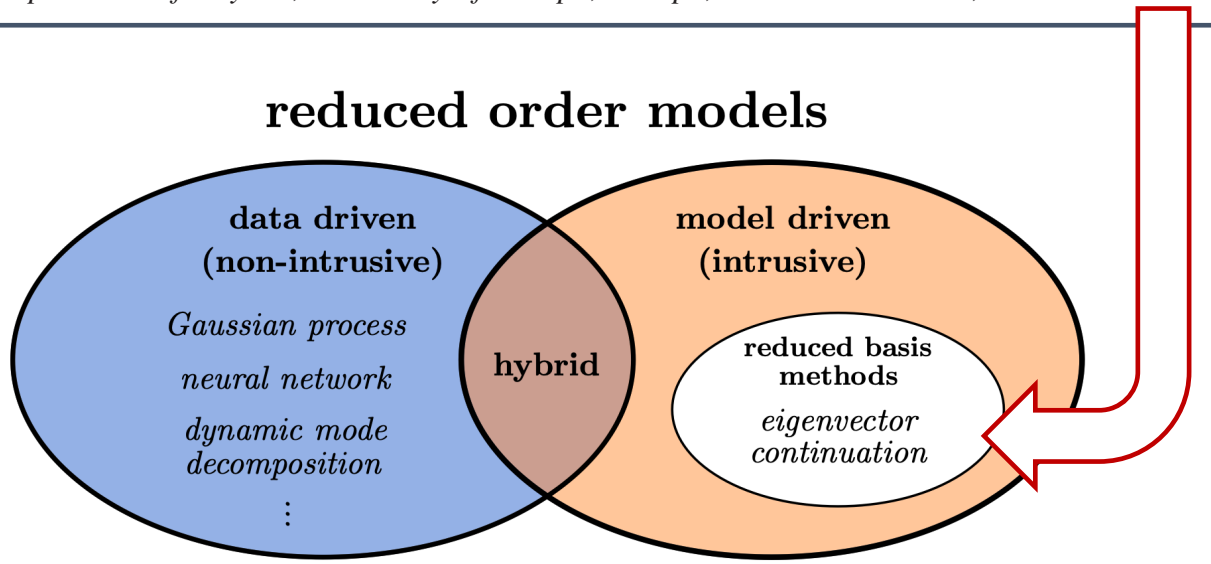
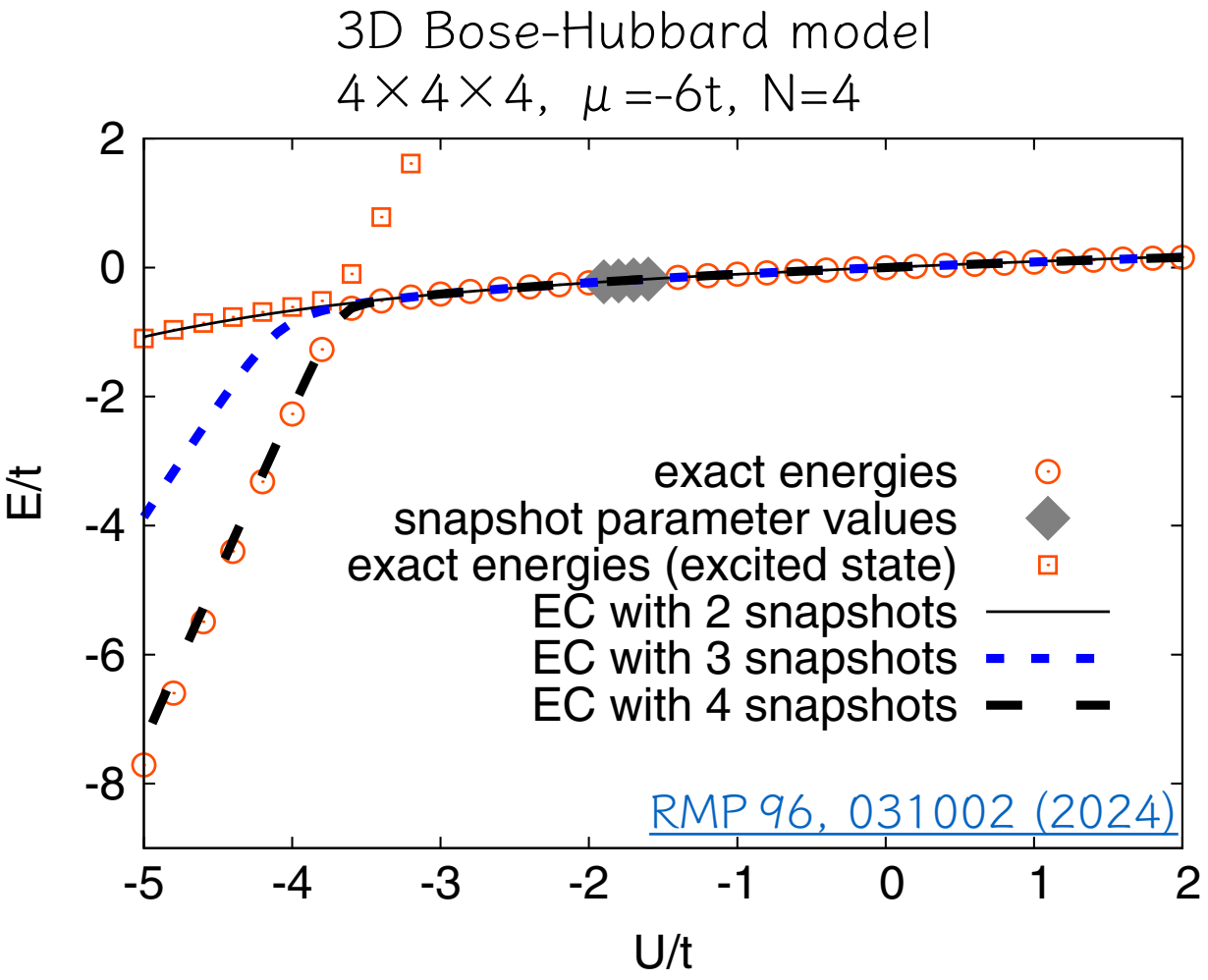
[4]*School of Engineering and Applied Science, University of Pennsylvania, Philadelphia, Pennsylvania 19104, USA*

[5]*Department of Physics, University of Guelph, Guelph, Ontario N1G 2W1, Canada*



T. Duguet et al., Rev. Mod. Phys. 96, 031002 (2024)

Eigenvector continuation (EC) in a nutshell



1. Suppose you have *exact eigenstates* at some points (taking **snapshots**)

2. Span the wavefunction by the samples and solve generalized eigen val. prob.

$$\tilde{H}\vec{v} = \lambda N\vec{v},$$
$$\tilde{H}_{i,j} = \langle\psi(\vec{c}_i)|H(\vec{c}_\odot)|\psi(\vec{c}_j)\rangle,$$
$$N_{i,j} = \langle\psi(\vec{c}_i)|\psi(\vec{c}_j)\rangle.$$

$$E(\vec{c}_\odot) \simeq \lambda, \quad |\psi(\vec{c}_\odot)\rangle \simeq \sum_{i=1}^{N_s} v_i|\psi(\vec{c}_i)\rangle \equiv |\psi_{EC}(\vec{c}_\odot)\rangle.$$

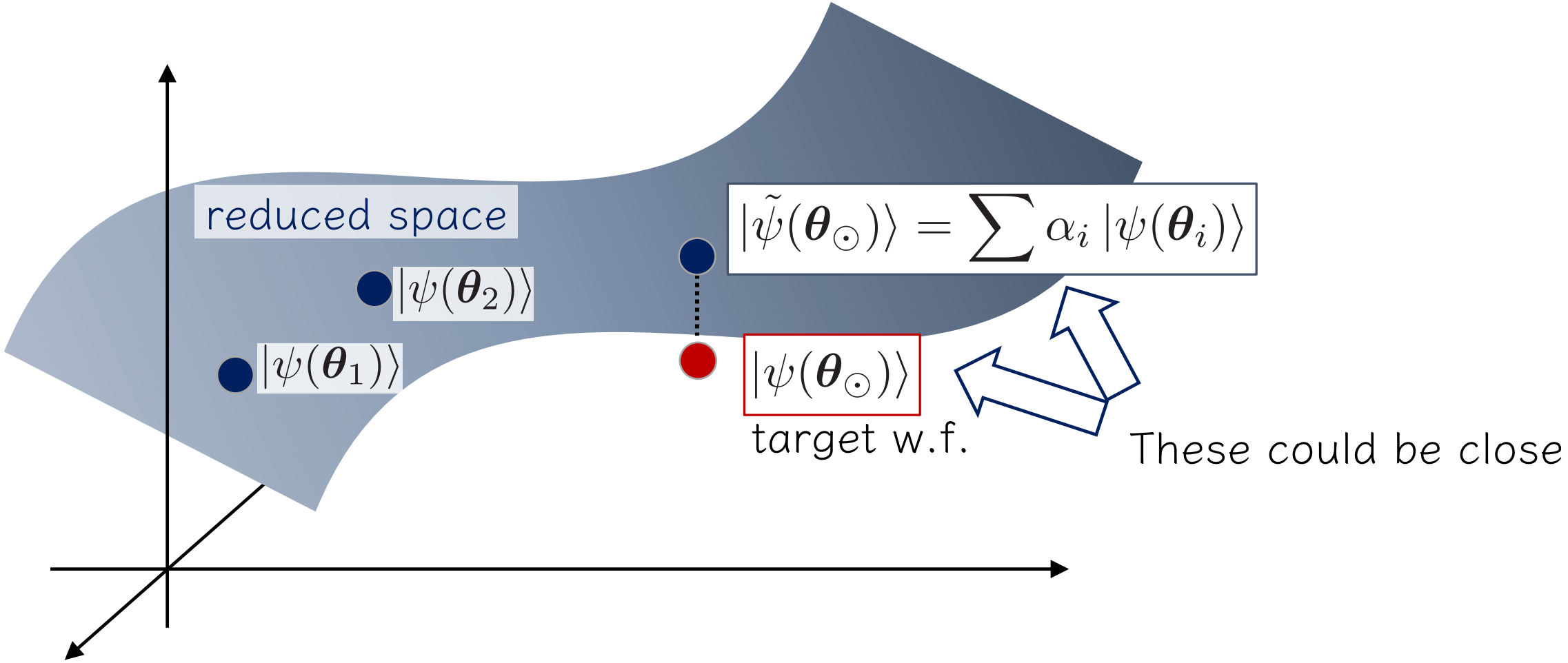
⇑ *several snapshots are enough to express eigenstates elsewhere*

That have been proven in other quantum many-body systems

How could it be?

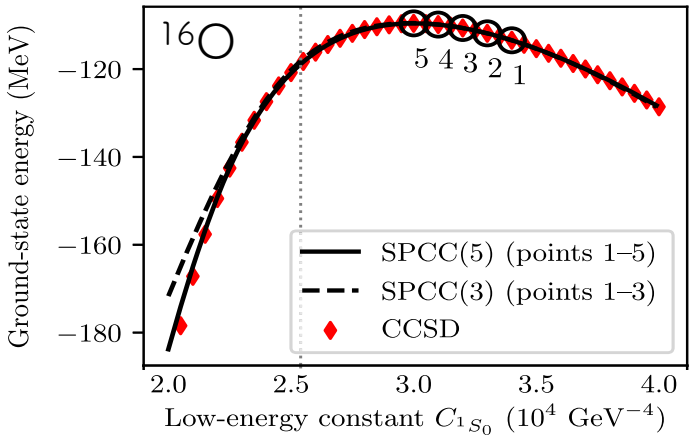
Wavefunctions/eigen states are obviously **not arbitrary** in the Hilbert space

Your snapshots and target eigenstates may live on a certain subspace



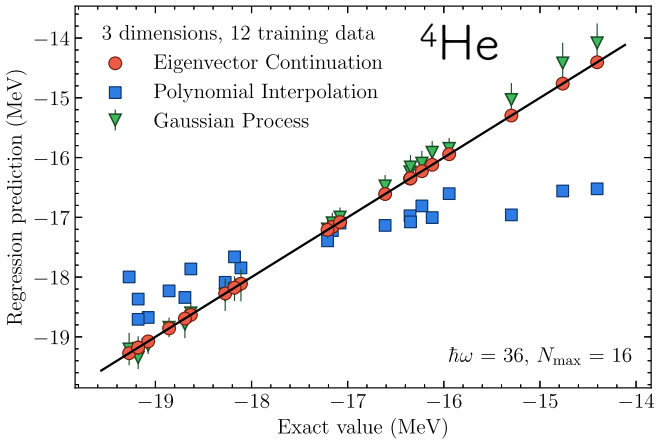
Incomplete list of EC applications

Coupled cluster



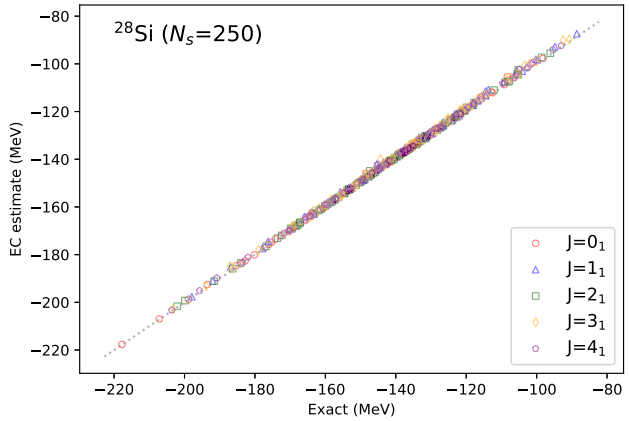
PRL 123, 252501 (2019)

No-core shell model (Full-CI)



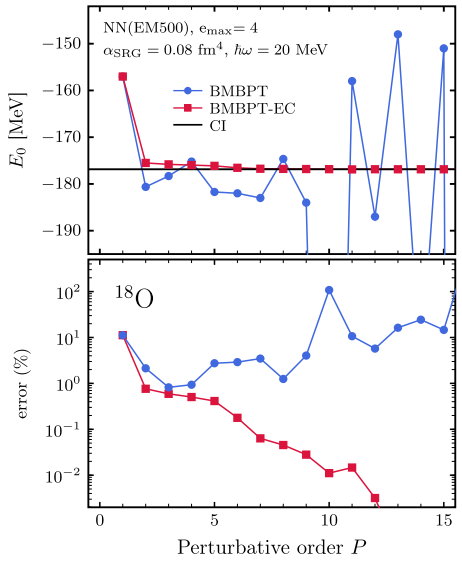
PLB 810, 135814 (2020)

Valence CI



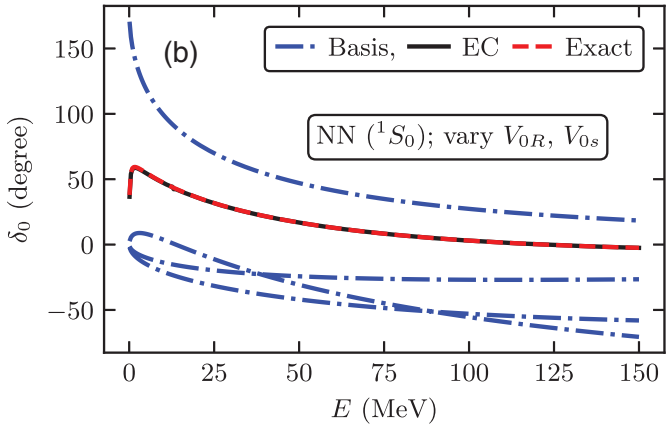
SY and N.Shimizu, PTEP 2022 053D02 (2022)

Bogoliubov-MBPT



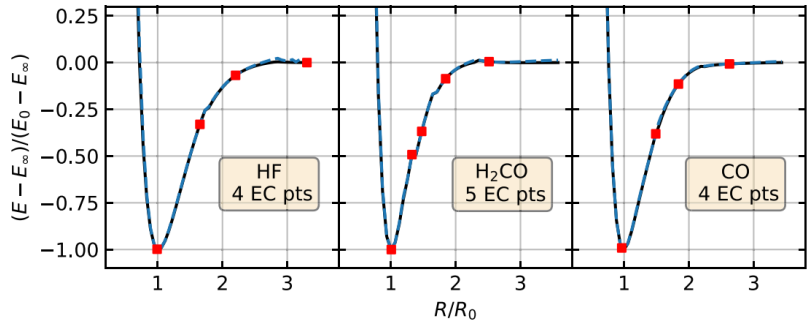
PRC 101, 041302(R)(2020)

Scattering phase shifts



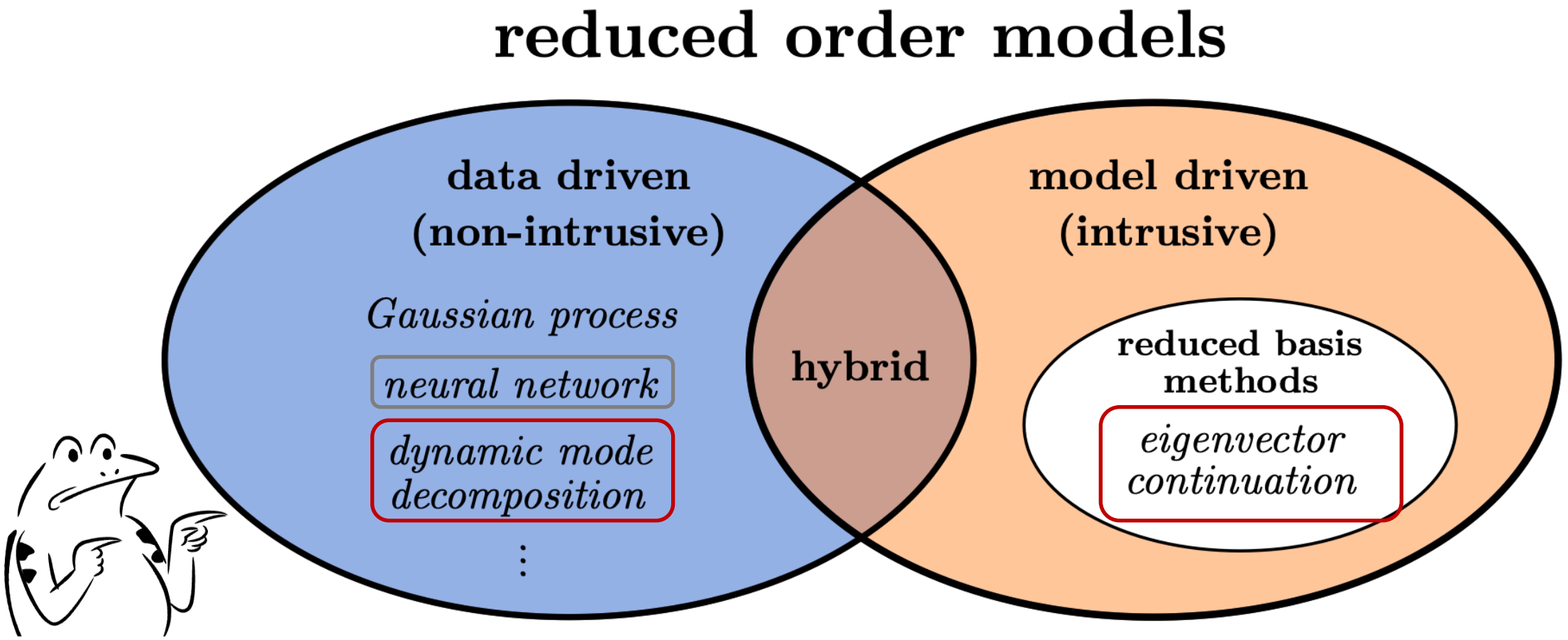
PLB 809, 135719 (2020)

Chemistry



Electron. Struct. 5 (2023) 045007

Data driven approaches



T. Duguet et al., Rev. Mod. Phys. 96, 031002 (2024)

Dynamic Mode Decomposition (DMD)

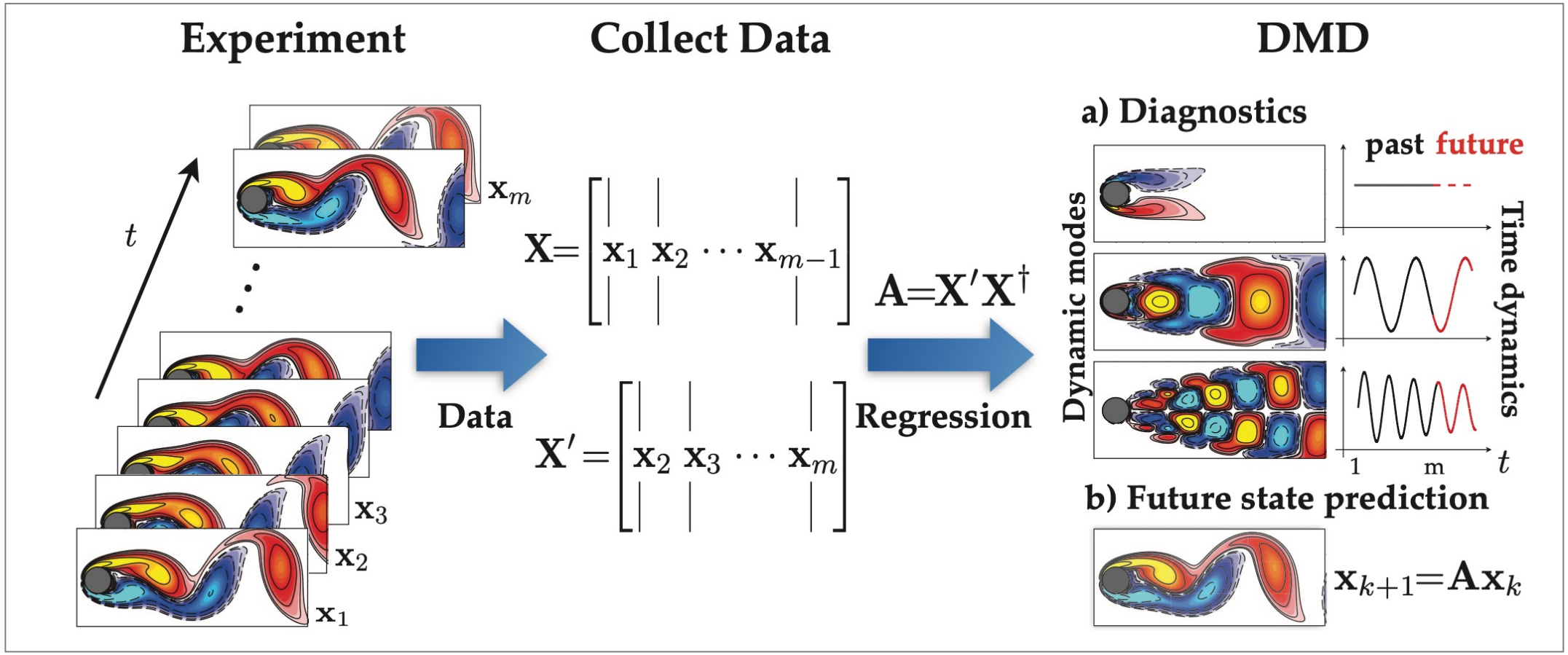


Fig 1.1 from Kutz et al., "Dynamic Mode Decomposition" SIAM

- various modes are decomposed into "dynamical modes"
- one can reconstruct original snapshots (and make predictions)

DMD algorithms

1. $$\boldsymbol{X} \equiv \underset{D\times N}{\begin{pmatrix} | & & | \\ \boldsymbol{x}_1 & \cdots & \boldsymbol{x}_N \\ | & & | \end{pmatrix}}, \boldsymbol{Y} \equiv \underset{D\times N}{\begin{pmatrix} | & & | \\ \boldsymbol{x}_2 & \cdots & \boldsymbol{x}_{N+1} \\ | & & | \end{pmatrix}}$$

$$\boldsymbol{Y} = \boldsymbol{F}(\boldsymbol{X}) \Rightarrow \boldsymbol{Y} \approx \boldsymbol{A}\boldsymbol{X}$$

D (dimension of many-body operator) > 10^7
N (# of snapshots) ~ 10 – 10^3?

approximating non-linear map F by linear map A

2. SVD of X $\quad \boldsymbol{X} = \boldsymbol{U}\boldsymbol{\Sigma}\boldsymbol{V}^* \rightarrow$ truncated SVD $\boldsymbol{X} \approx \boldsymbol{U}_r\boldsymbol{\Sigma}_r\boldsymbol{V}_r^\dagger$

3. Compute the matrix A using Moore-Penrose pseudo-inverse of X

$$\mathbf{A} \approx \mathbf{Y}\mathbf{X}^+ = Y\left(\mathbf{V}_r\boldsymbol{\Sigma}_r^{-1}\mathbf{U}_r^\dagger\right)$$

4. Obtain the time evolution linear map in a latent space

$$\tilde{\mathbf{A}} = \mathbf{U}_\mathbf{r}^\dagger\mathbf{A}\mathbf{U}_\mathbf{r} \approx \mathbf{U}_\mathbf{r}^\dagger\mathbf{Y}\mathbf{V}_\mathbf{r}\boldsymbol{\Sigma}_\mathbf{r}^{-1}$$

encoder

$$\mathbf{A} = \mathbf{U}_\mathbf{r}\tilde{\mathbf{A}}\mathbf{U}_\mathbf{r}^\dagger$$

decoder

k-time step forward can be done in the latent space

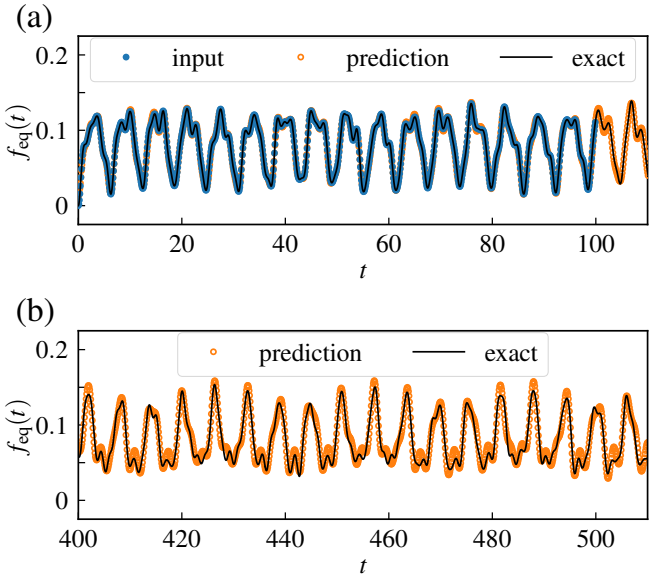
applications to quantum many-body systems

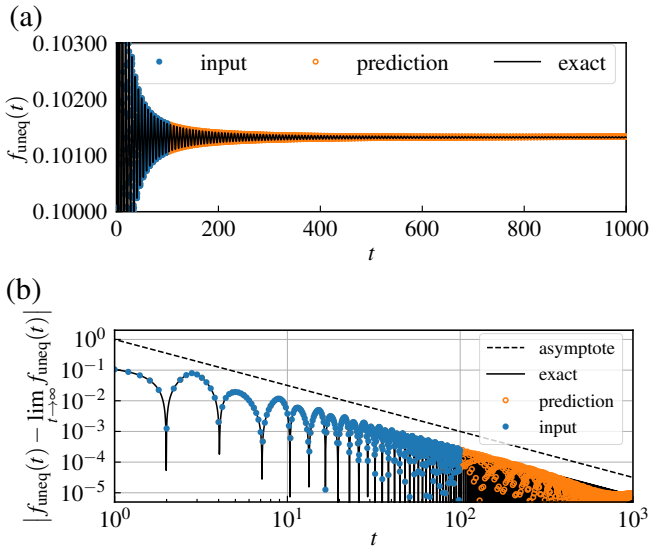
Spin system

transverse-field Ising model

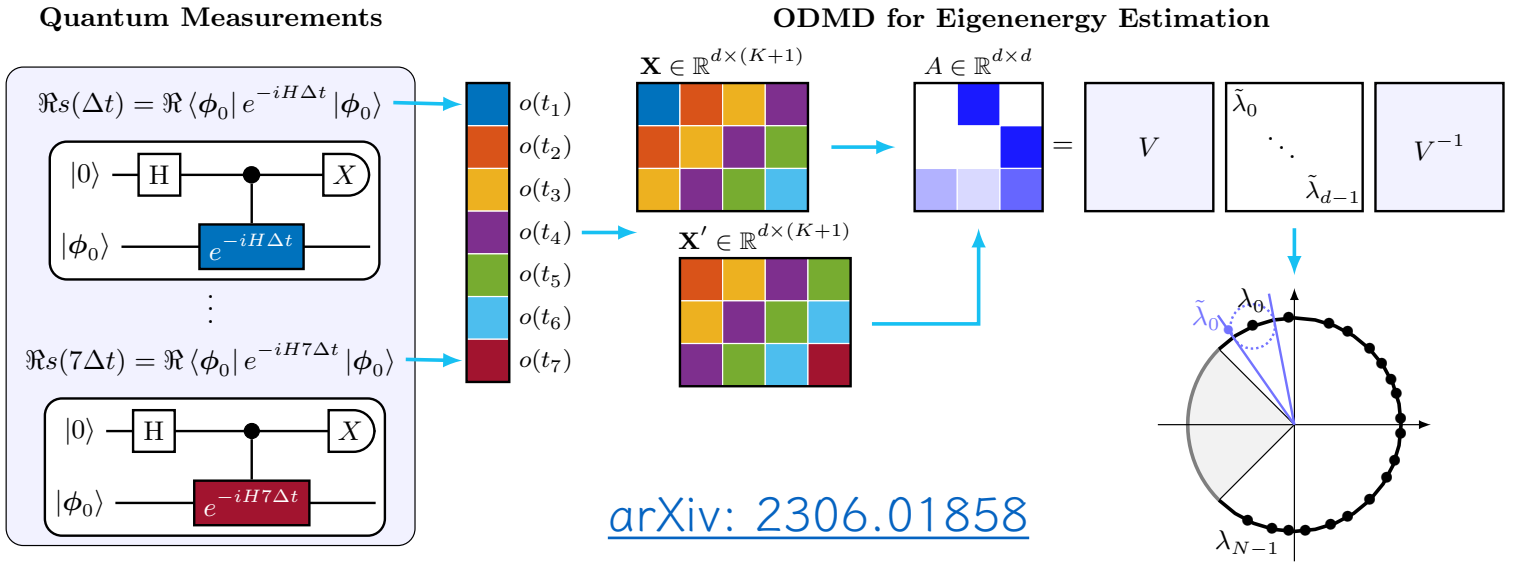
$$H = -J \sum_{\langle i,j \rangle} S_i^z S_j^z - \Gamma \sum_i S_i^x,$$

arXiv: 2403.19947





Quantum computing



arXiv: 2306.01858

In-medium Similarity Renormalization Group (IMSRG)

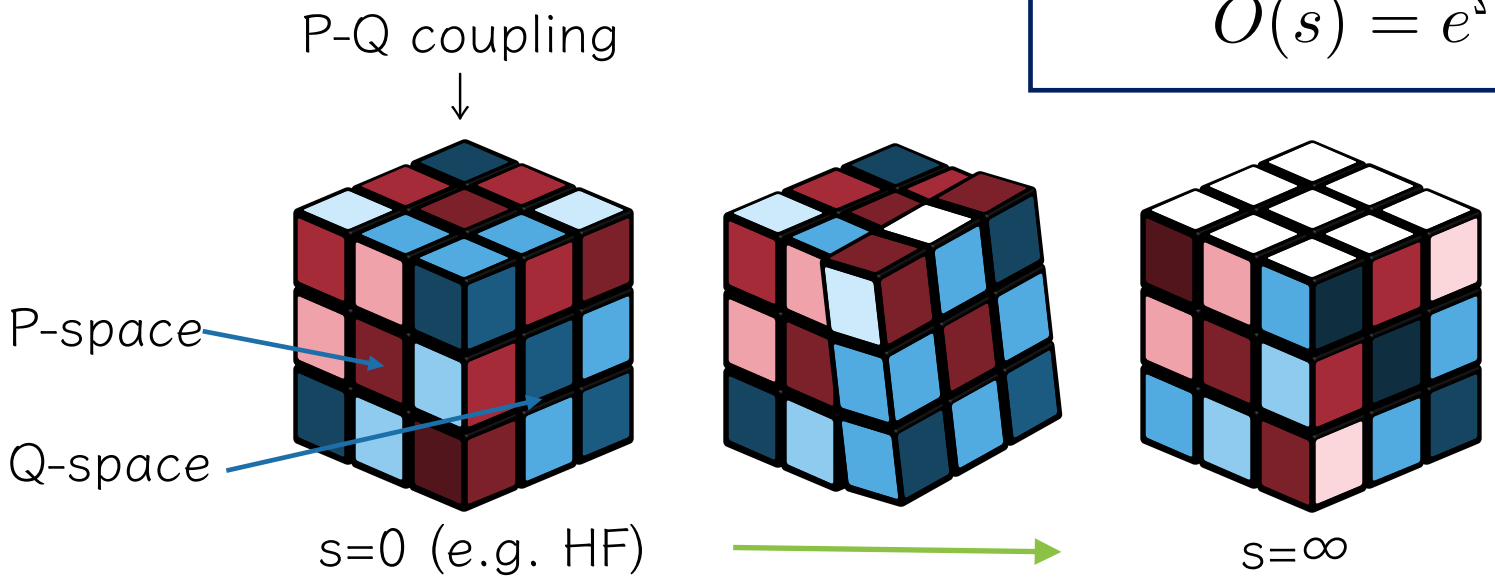
IMSRGflow:

K. Tsukiyama, S. K. Bogner, and A. Schwenk, PRL **106**, 222502 (2011), PRC **85**, 061304 (2012).
S.R.Stroberg et al., Annu. Rev. Nucl. Part. Sci. 2019. 69:307–362 (2019)
T.D.Morris et al., PRC 92, 034331 (2015)

$$\frac{dH(s)}{ds} = [\eta(s), H(s)]$$

Magnus formulation $U(s) = e^{\Omega(s)}$

$$O(s) = e^{\Omega(s)} O(0) e^{-\Omega(s)}$$



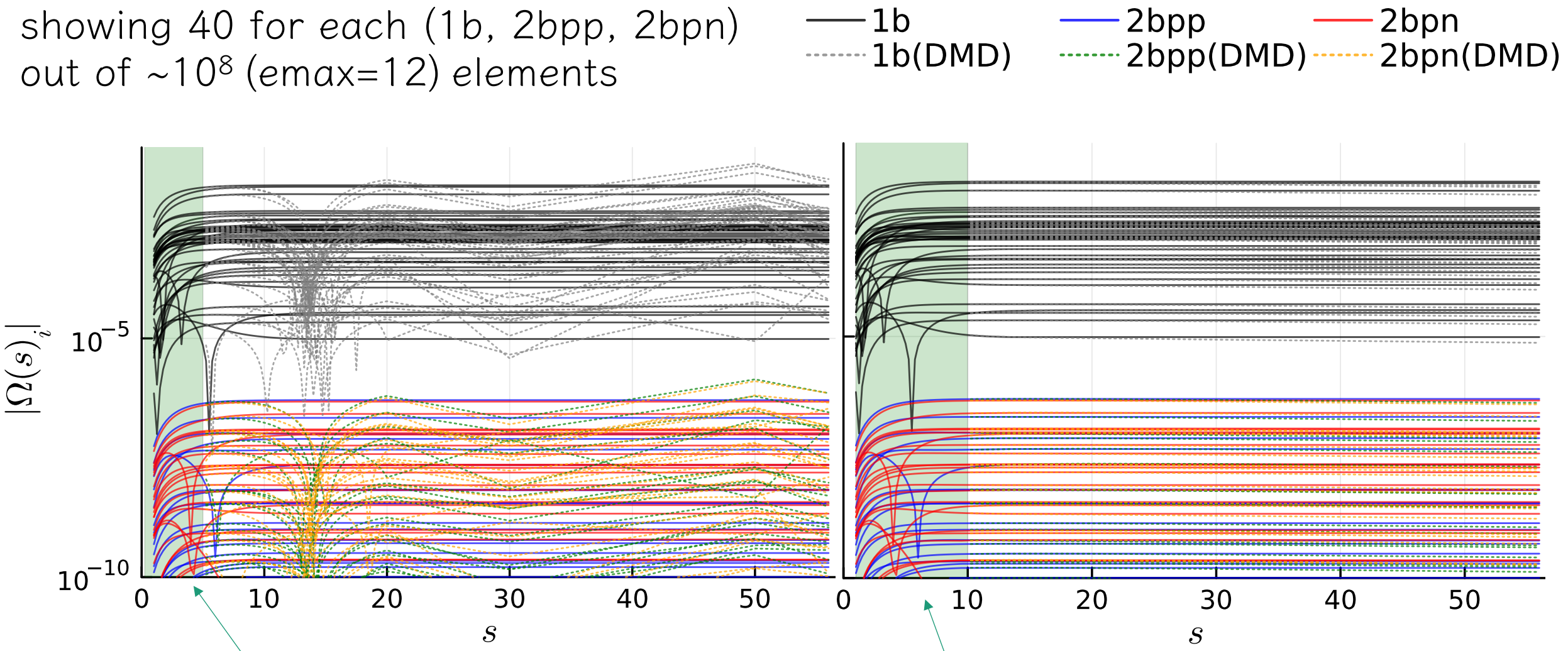
(P, Q) = (hole, particle), (valence, others), etc.

c.f. T.Miyagi's talk, afternoon

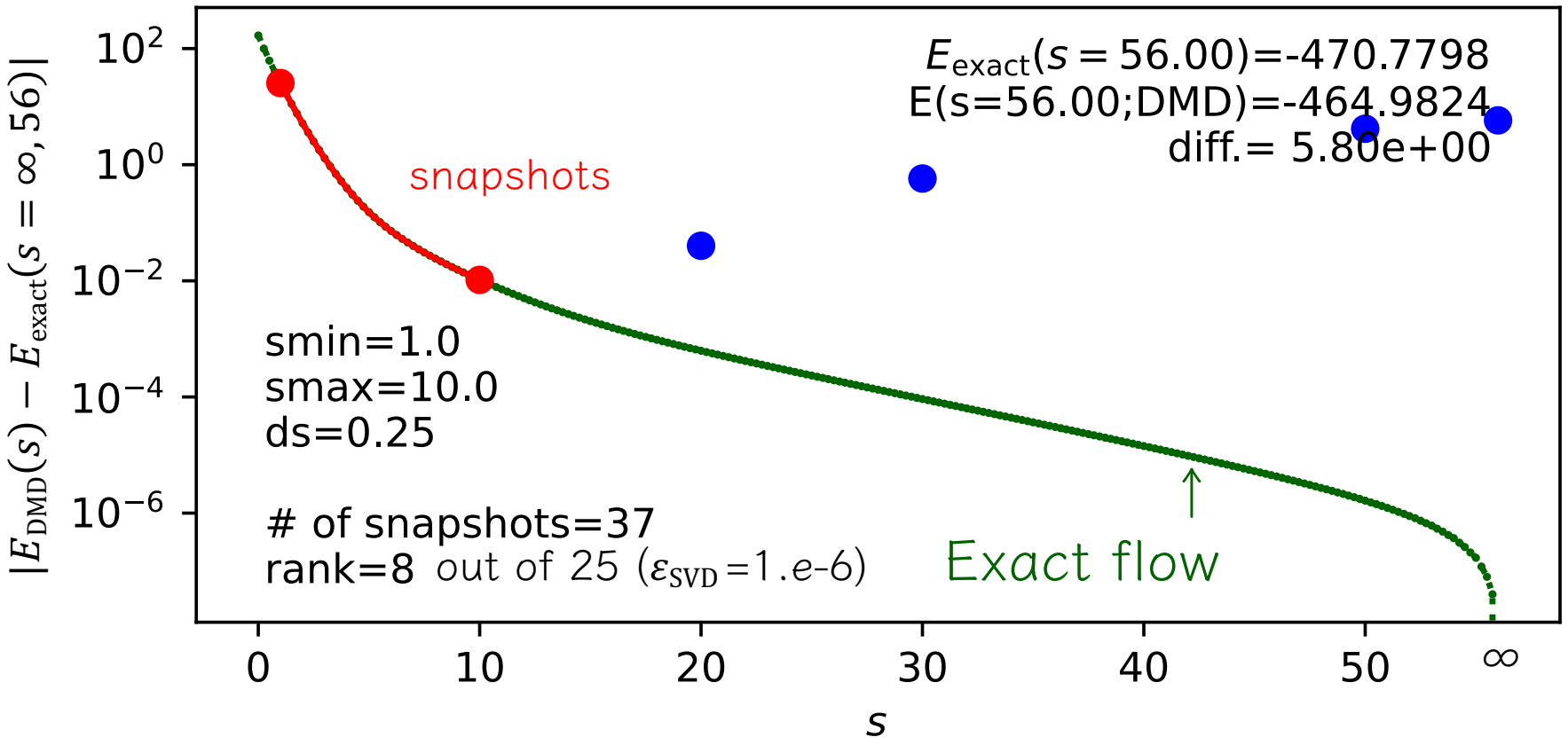
flow of Magnus operators

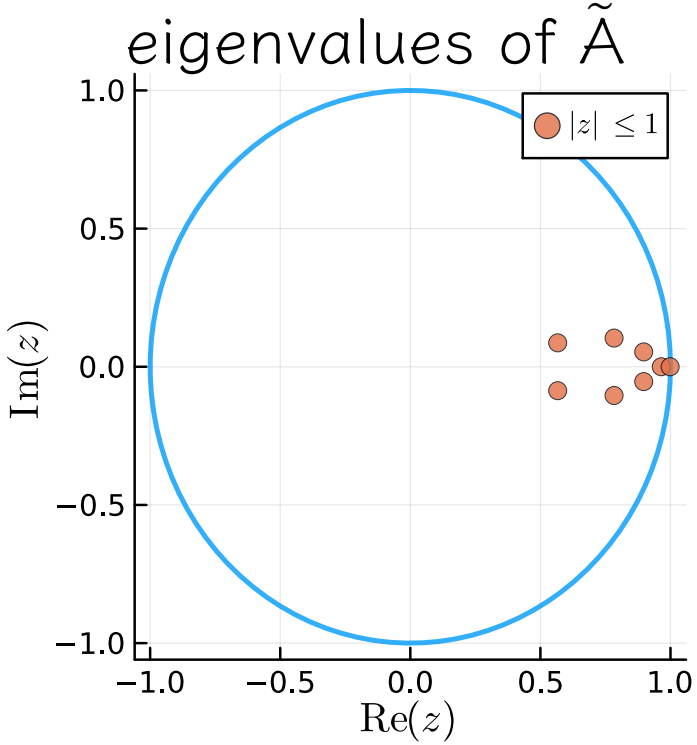
^{56}Ni under N3LO + 3NF(lnl)

showing 40 for *each* (1b, 2bpp, 2bpn)
out of ~10^8 (*emax*=12) *elements*



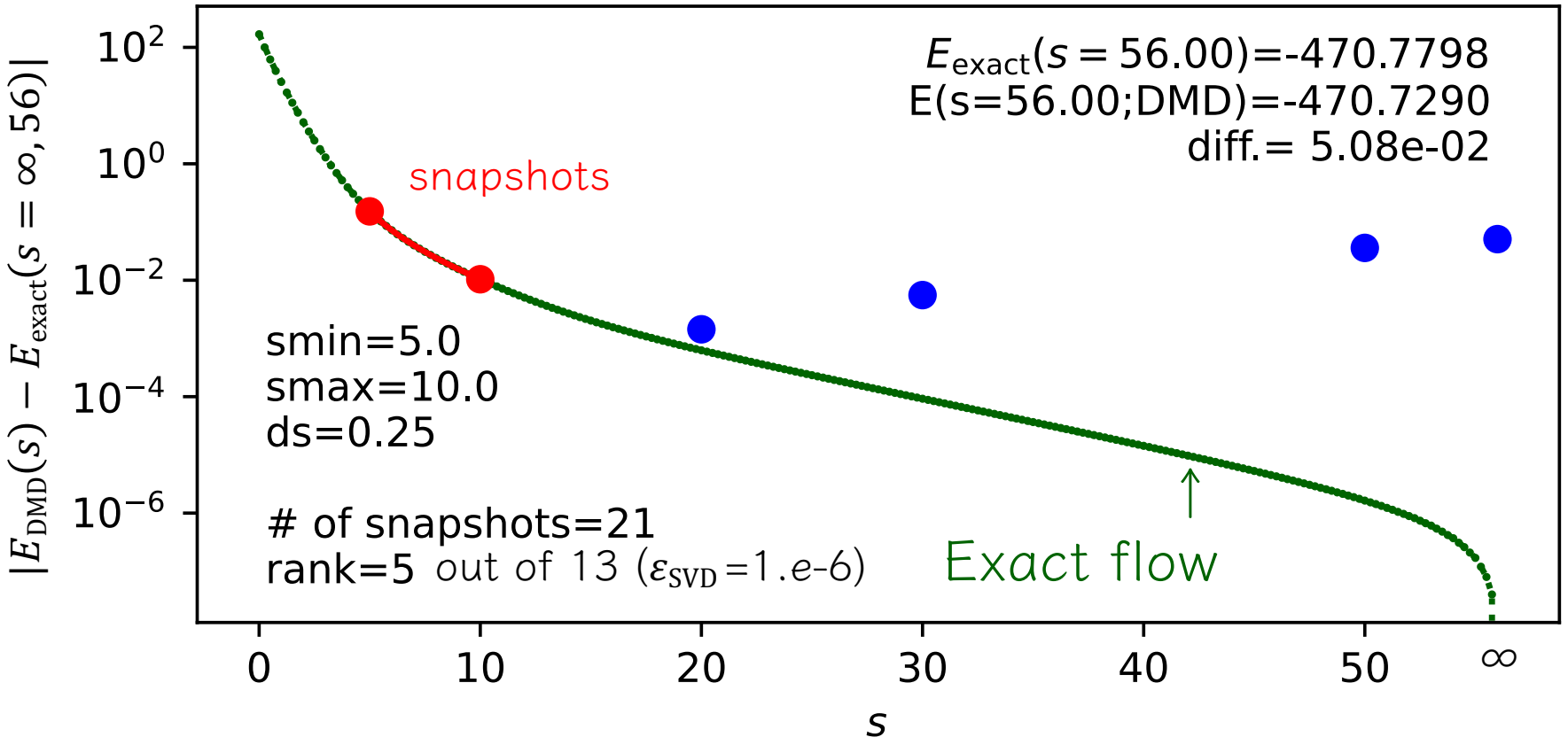
Errors on energy estimation

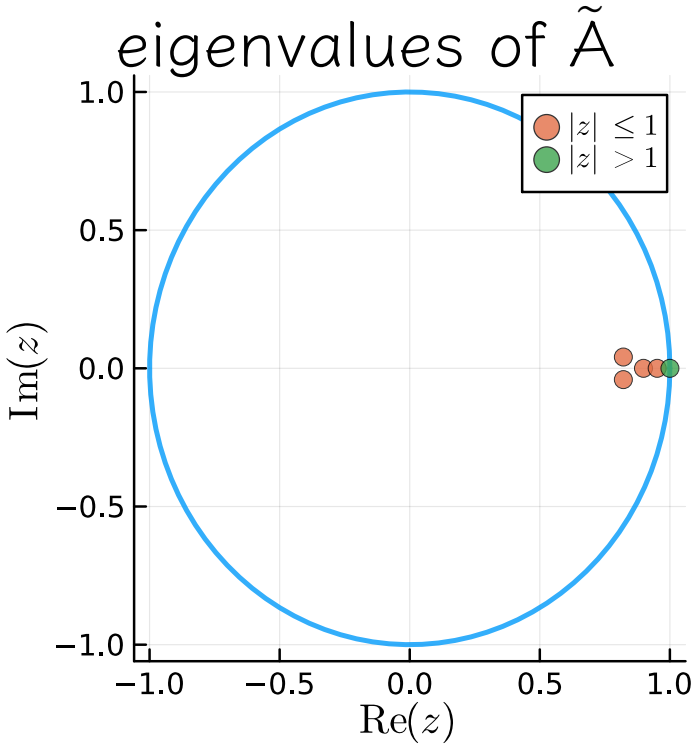




DMD predictions (blue circles ●) are obviously wrong

Errors on energy estimation discarding small s data...

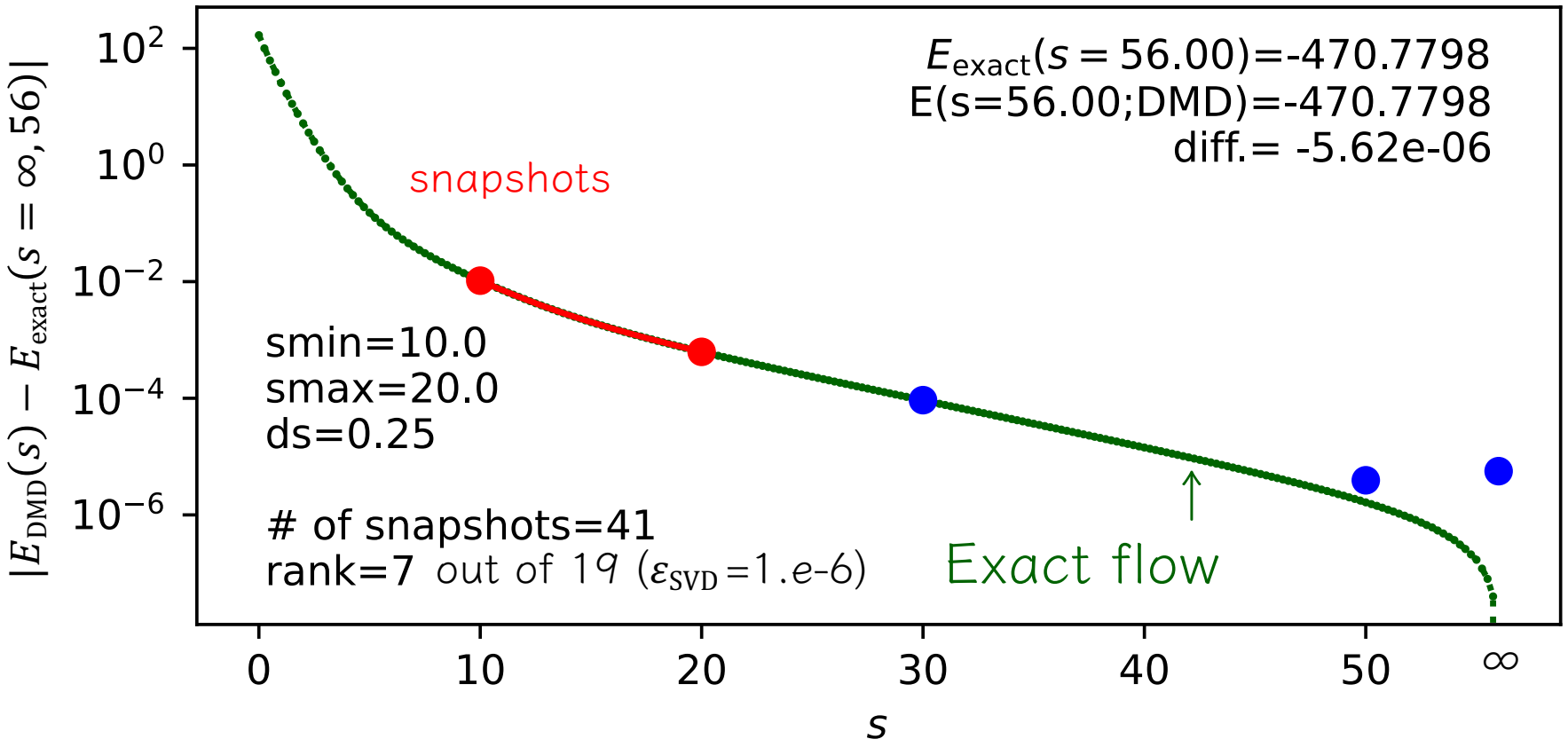


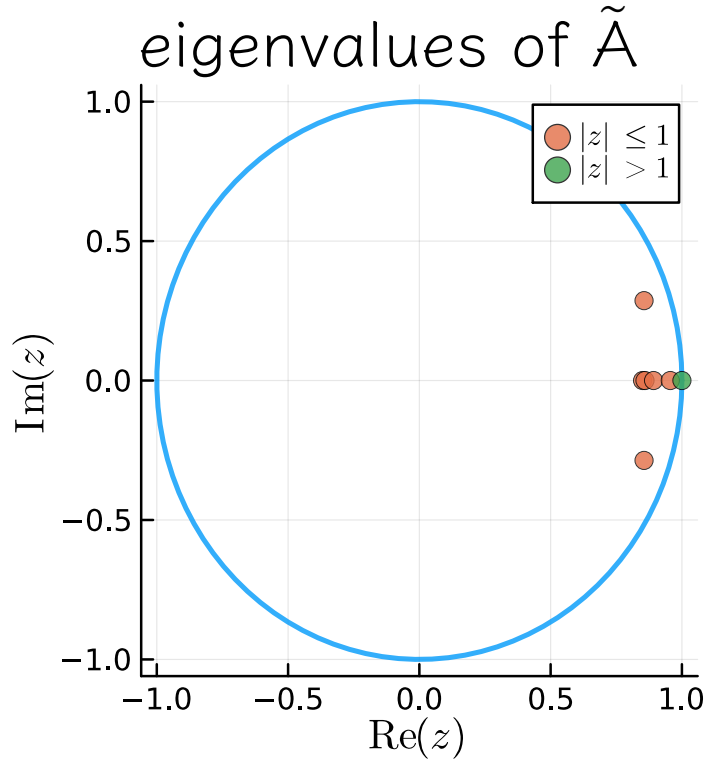


slightly improved but ...

→ non-linear nature of IM-SRG seen in smaller s region
may not be well captured by DMD (single linear operator)

Errors on energy estimation feeding more larger s data...





we got even better results, but...

it is nontrivial to take snapshots from where to where

DMD + IMSRG

PROS:

low-rank nature, cost on emulator is negligible → X 3~5 speedup

DMD can learn (at least) "linear" part of quantum dynamics

CONS:

c.f. ML approach, IMSRG-Net(PINNs)
SY PhysRevC.108.044303 (2023)

accumulation of errors from imperfect linear map

no a priori knowledge where to stop high-fidelity calculations

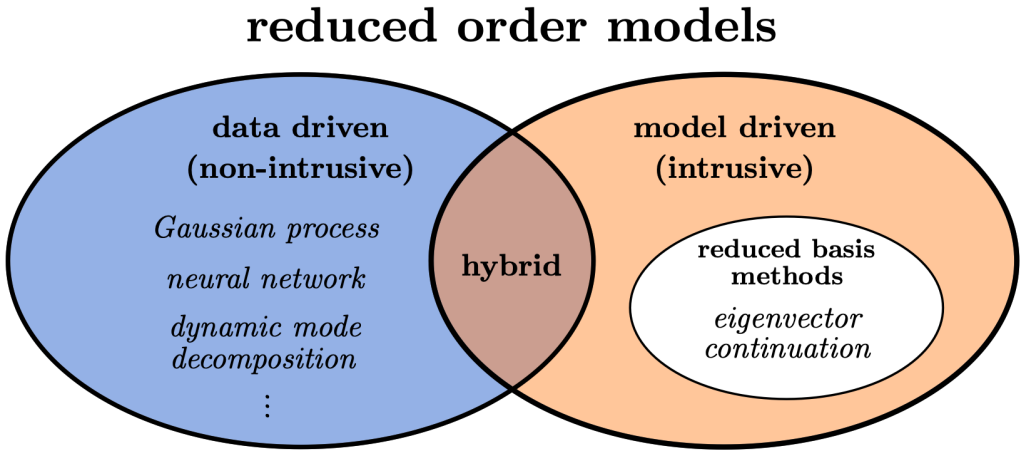
If an emulator is fast enough, you can make a diagnostic on emulator by e.g., looking at credible intervals of emulator predictions

Summary

Surrogate models/Emulators matter!!

- Eigenvector continuation

- Dynamic Mode Decomposition



T. Duguet et al., Rev. Mod. Phys. 96, 031002 (2024)

Emulators for IM-SRG

DMD & Neural Network (For the latter, see appendix)

Both work fine for "linear" part of the IM-SRG flow,
They are complementary. Next step will be to learn non-linear part

Related talks on emulators in nuclear physics :
Hinohara-san@Tsukuba, Xilin Zhang@MSU/FRIB

NuclearToolkit.jl: Julia package for structure calculations

SY, Journal of Open Source Software, 7(79), 4694,(2022)

v.0.4.2 (Mar. 2024)

- ChiEFTint ~ 9,000 lines
  - NN potential, Entem-Machleidt(N3LO), EMN(N4LO)
  - SRG in momentum space (NN-only)
  - read 3NFs by NuHamil code (T. Miyagi@Tsukuba)
  - etc.

- HartreeFock ~ 3,500 lines
  - spherical HF
  - Møller-Plesset (a.k.a MBPT)
  - Normal ordering (including TNO/ENO)

- IM-SRG ~ 3,000 lines

  IMSRG &VS-IMSRG (only scaler ones for now)
  emulator for Magnus-IMSRG(2) with Dynamic Mode Decomposition (DMD)

- ShellModel.jl ~8,700 lines

  eigenvector continuation SY and N.Shimizu PTEP 2022 053D02

EC: shell model emulator

SY and N.Shimizu, PTEP 2022 053D02 (2022)

Example:

$$\tilde{H}\vec{v} = \lambda N\vec{v},$$
$$\tilde{H}_{i,j} = \langle\psi(\vec{c}_i)|H(\vec{c}_\odot)|\psi(\vec{c}_j)\rangle,$$
$$N_{i,j} = \langle\psi(\vec{c}_i)|\psi(\vec{c}_j)\rangle.$$

$$E(\vec{c}_\odot) \simeq \lambda,$$
$$|\psi(\vec{c}_\odot)\rangle \simeq \sum_{i=1}^{N_s} v_i|\psi(\vec{c}_i)\rangle \equiv |\psi_{EC}(\vec{c}_\odot)\rangle.$$

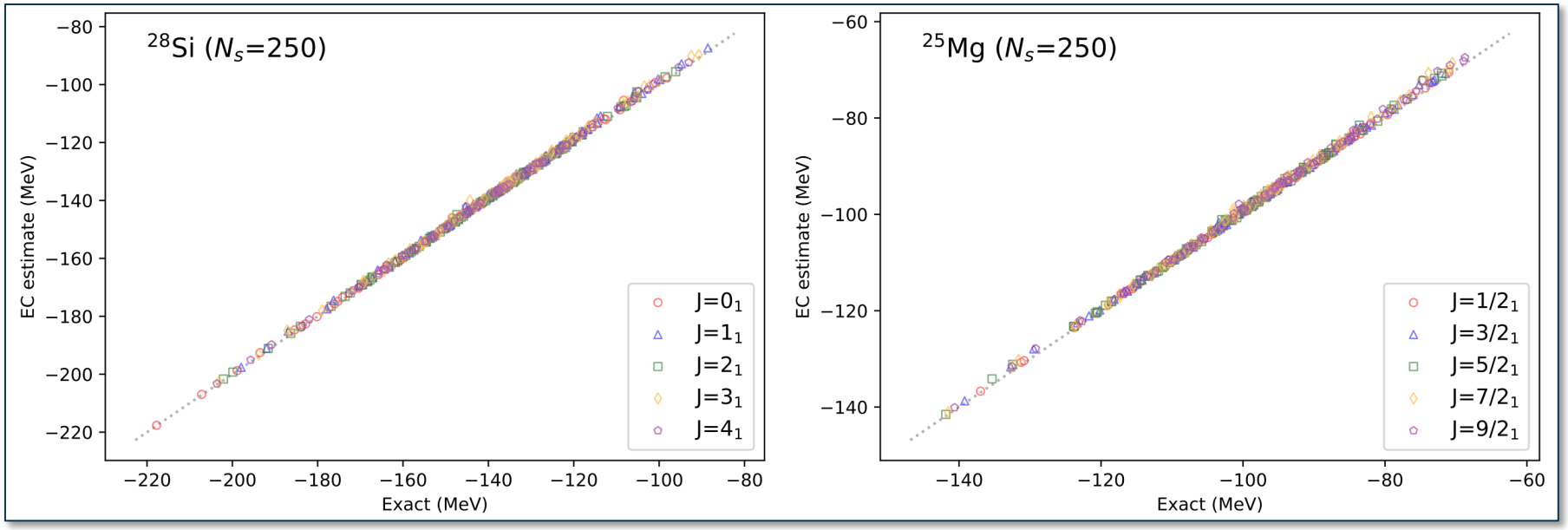
sd-shell (^{16}O core + 0d5/0d3/1s1 valence orbits)

parameters: 66 (3 SPEs & 63 TBMEs, w/ isospin)

target nuclei: ^{25}Mg (vp=4,vn=5), ^{28}Si (vp=vn=6, dim. ~ 90,000)

sampling 5 states for given total J at 50 (random) different points (5×50=250 samples) **around USDB**

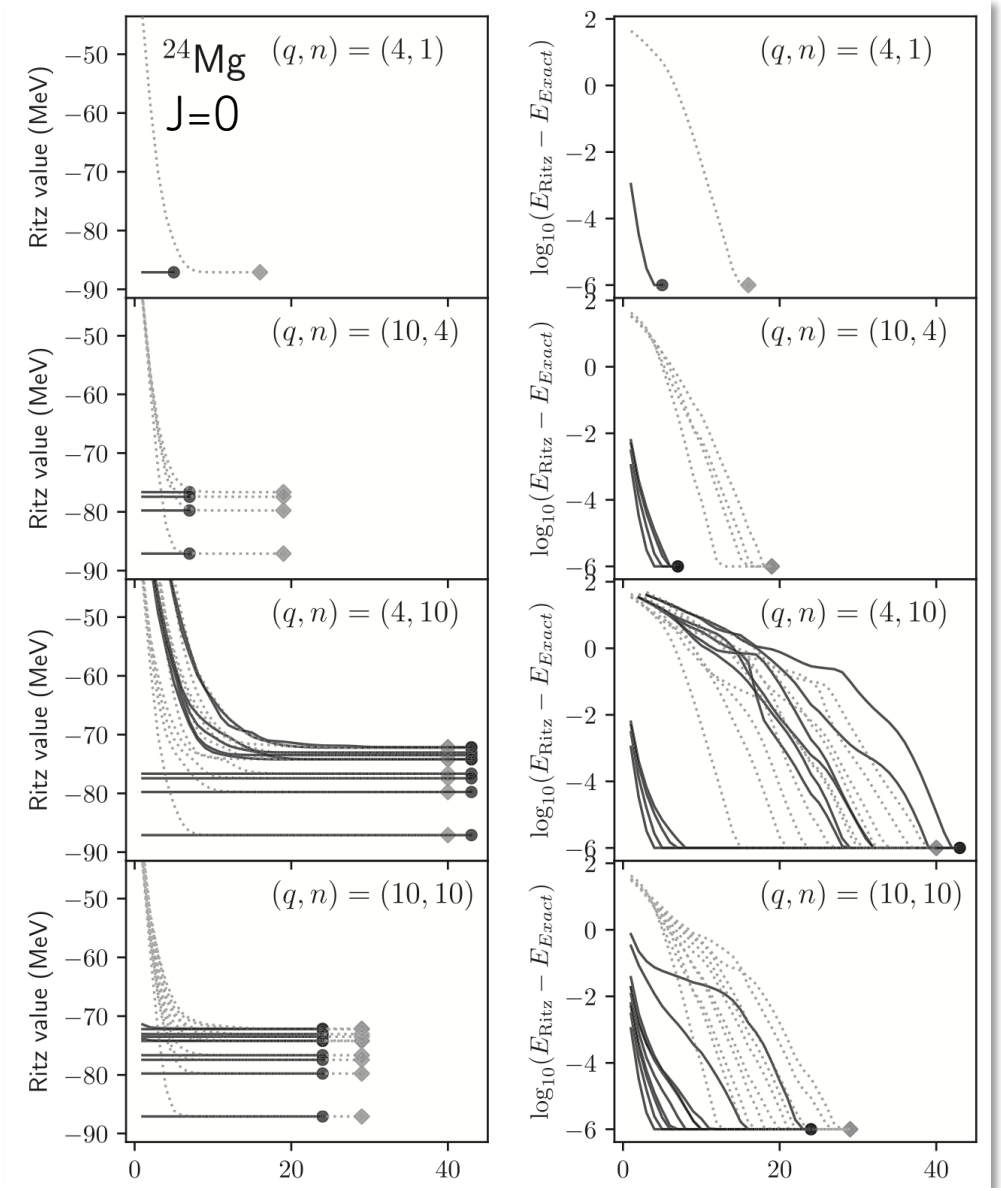
"validation" for 100 random parameters



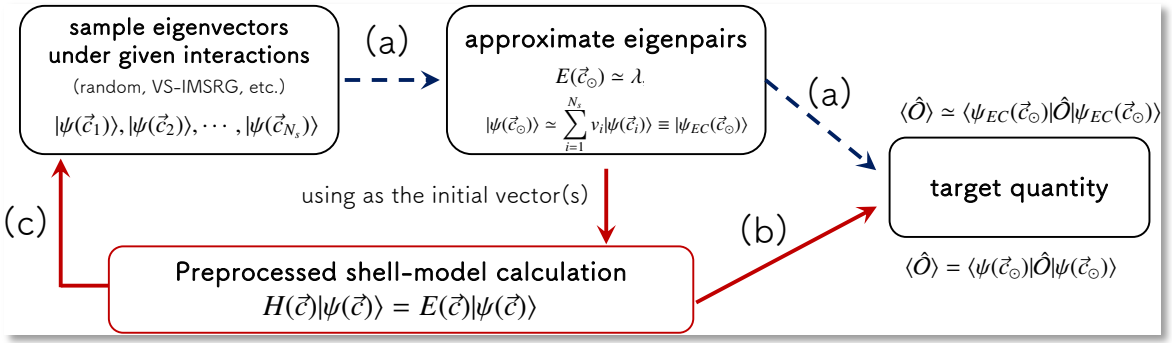
EC approximates energies within a few percent accuracy

EC: As a Lanczos preprocessor

SY and N.Shimizu, PTEP 2022 053D02 (2022)



Number of H operation during the (block) Lanczos method



q: size of initial "block" vector

n: # of excited states of interest

dotted: initialized by random vectors

solid: initialized by EC eigenvectors

Starting from better initial guess,
# of manipulation could be reduced!!

Exception => (q, n) = (4,10)

since the emulator is trained with 5 lowest states,
such emulator do not have much info. on higher states

converged results are obtained at ●/◆

EC: To feed more samples...

SY and N.Shimizu, PTEP 2022 053D02 (2022)

Sampling itself is not easy ...

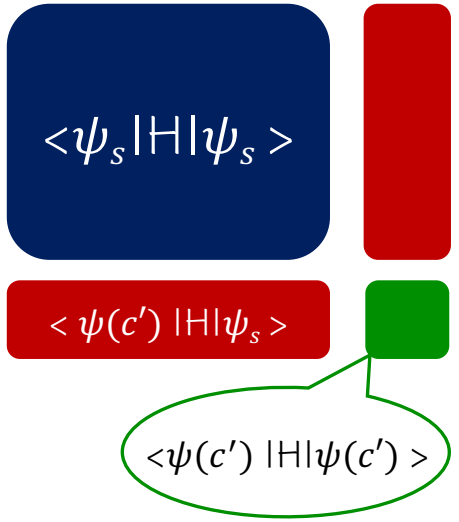
$$\tilde{H}\vec{v} = \lambda N\vec{v},$$
$$\tilde{H}_{i,j} = \langle\psi(\vec{c}_i)|H(\vec{c}_\odot)|\psi(\vec{c}_j)\rangle, \quad \leftarrow \text{most time-consuming part}$$
$$N_{i,j} = \langle\psi(\vec{c}_i)|\psi(\vec{c}_j)\rangle.$$

- You don't need to explicitly calculate $H(C_\odot)|\psi(cj)>$ for each parameter $C_\odot$ to evaluate H-tilde above:

all you need is 1&2-body transition densities

$$\tilde{H}_{i,j} = \sum_k \underbrace{h_k^{(1)}}_{\text{SPEs}} \times \overline{\text{OBTD}_k}^{\,i,j} + \sum_k \underbrace{V_J(abcd)_k}_{\text{TBMEs}} \times \overline{\text{TBTD}_k}^{\,i,j},$$

s: sampled w.f.s



- If you want to increase sample number (for better accuracy),

  prepare new sample (green) and calc. overlap (transition densities)

  between new w.f. and previous samples (red)

First attempt to apply DMD to IMSRG

Jacob Davison, Ph.D. dissertation, MSU, 2023:

"Theoretical and computational improvements to the in-medium similarity renormalization group"

$$H(s) = \mathcal{U}(s)H(0) = \{\Phi \exp(\Omega t)\Phi^{\dagger}\}H(0)$$

"DMD emulation will treat H(s) as a one-dimensional vector" chapter7

chapter8

sensitivity analysis

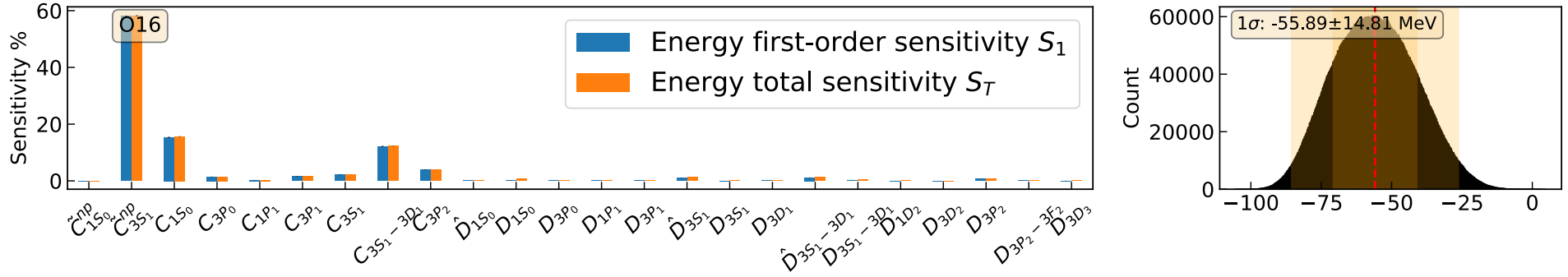
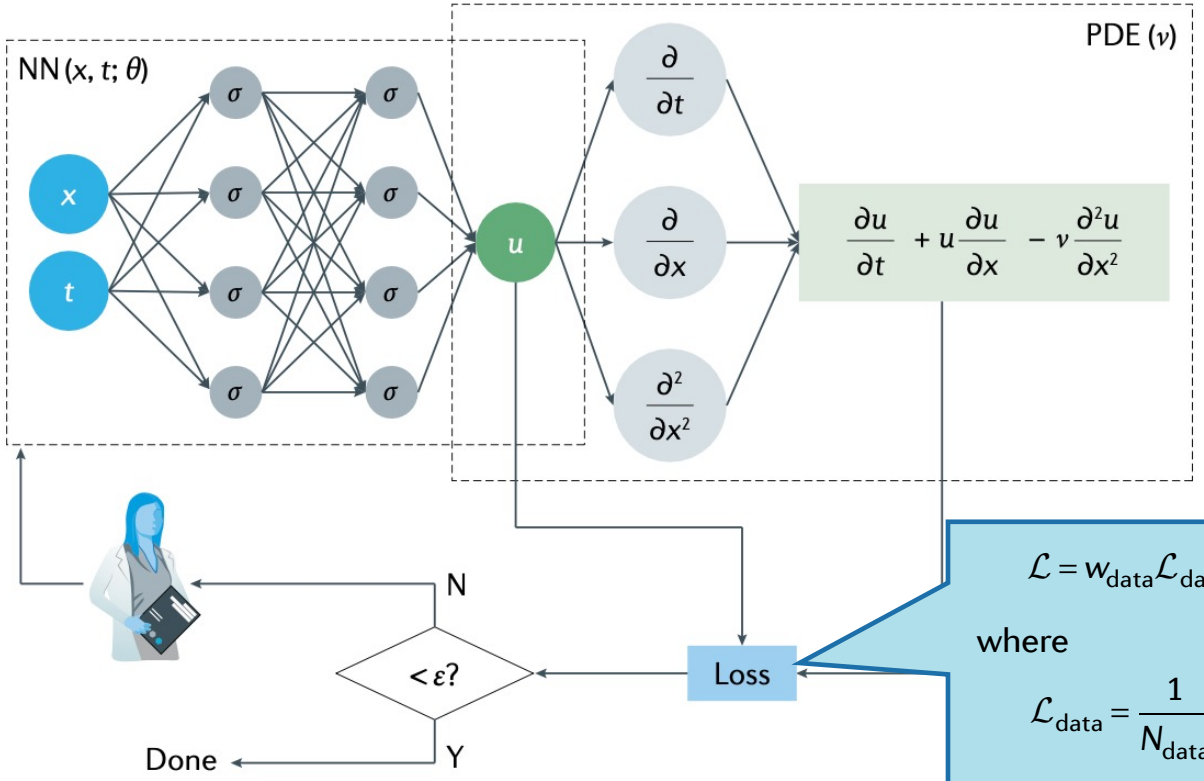


Figure 8.1 First-order and total sensitivity of the IMSRG(2) ground-state energy for ^{16}O energy to variation of the LECs around the standard N^{3}LO(500) interaction of Entem and Machleidt [4]. The left panel contains the sensitivity information per LEC. The right panel plots the total variance in the energy. The shaded region in the variance plot represents the 1σ and 2σ range.

ML example: Physics-Informed Neural Networks (PINNs)

Burgers eq. : $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2}$

Ref: Nature Reviews Physics 3, 422–440 (2021)



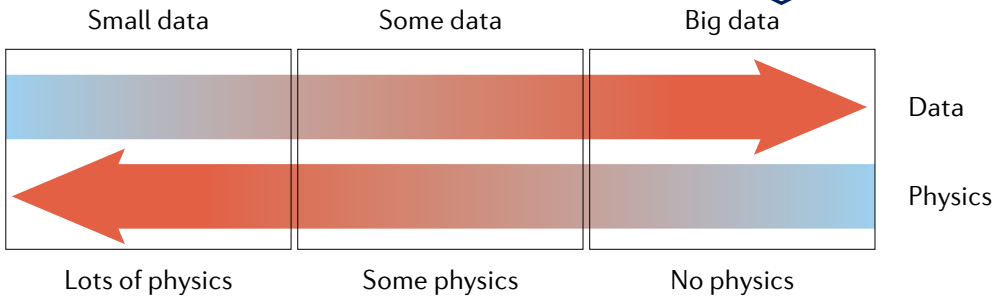
$$\mathcal{L} = w_{\text{data}}\mathcal{L}_{\text{data}} + w_{\text{PDE}}\mathcal{L}_{\text{PDE}},$$

where

$$\mathcal{L}_{\text{data}} = \frac{1}{N_{\text{data}}}\sum_{i=1}^{N_{\text{data}}}(u(x_i, t_i) - u_i)^2 \quad \text{and}$$

$$\mathcal{L}_{\text{PDE}} = \frac{1}{N_{\text{PDE}}}\sum_{j=1}^{N_{\text{PDE}}}\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2}\right)^2 |_{(x_j, t_j)}.$$

e.g. Large Language Model

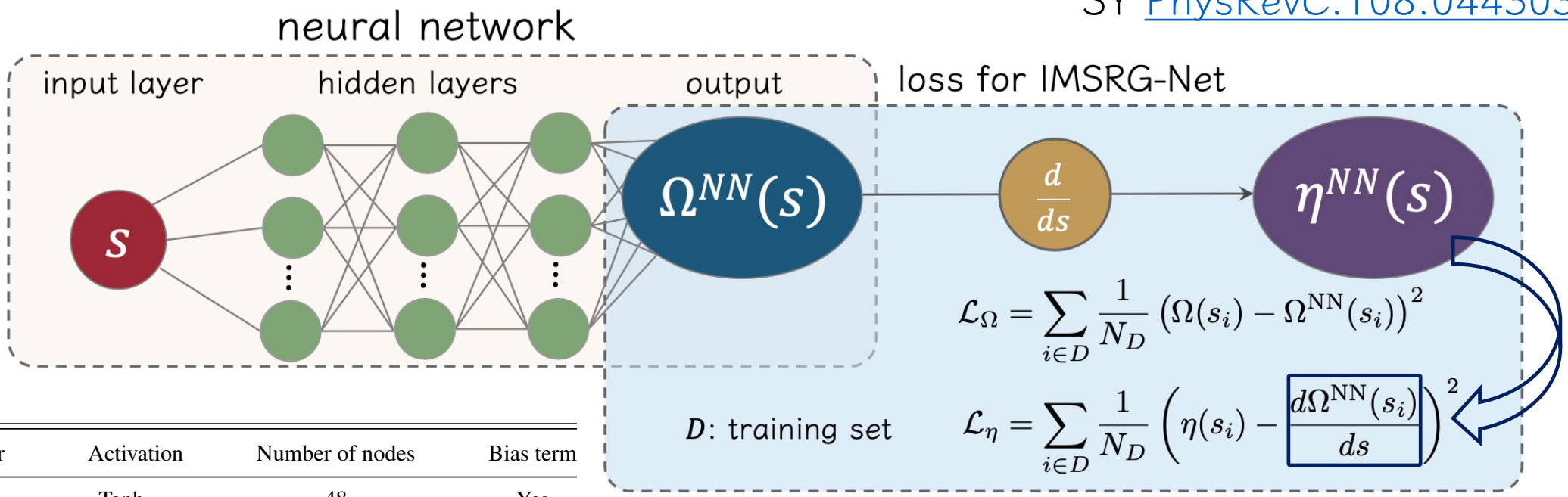


high-fidelity model calculations

"natural" expectation: you want neural networks approximating $u(x,t)$ respecting underlying equation and boundary conditions, but…

IMSRG-Net: PINN-based solver for IMSRG

SY PhysRevC.108.044303 (2023)



Layer	Activation	Number of nodes	Bias term
hl-0	Tanh	48	Yes
hl-1	Softplus	48	Yes
hl-2	Softplus	16	Yes
Output	Identity	Dim. Ω vector	No

$$\frac{d\Omega}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} ad_\Omega^{(k)}(\eta),$$

$$ad_\Omega^{(k)}(\eta) = \left[\Omega, ad_\Omega^{(k-1)}(\eta)\right],$$

$$ad_\Omega^{(0)}(\eta) = \eta,$$ taking leading term

neural network part is simple Affine layers

and trained to minimize the sum of loss terms $\mathcal{L} = \mathcal{L}_\Omega + \lambda_\eta \mathcal{L}_\eta$

$\lambda_\eta = 100$