Parametric Matrix Models

Model Emulation, Model Discovery, and General Machine Learning

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Facility for Rare Isotope Beams
Michigan State University

Quantum Computing and Artificial Intelligence in Nuclear Physics
INPC 2025
May 15, 2025

STREAMLINE
SmarT Reduction and Emulation Applying Machine Learning In Nuclear Environments

INPC 2025
May 25-30, 2025
DCC, Daejeon, Korea

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Theory Alliance

Physics Equations

Vlasov-Poisson Equation:
$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{q}{m}\mathbf{E} \cdot \nabla_v f = 0$

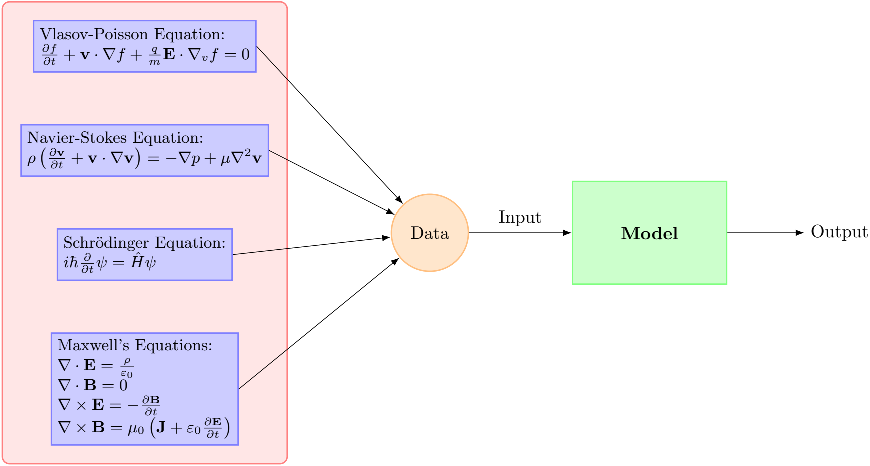
Navier-Stokes Equation:
$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v}\right) = -\nabla p + \mu \nabla^2 \mathbf{v}$

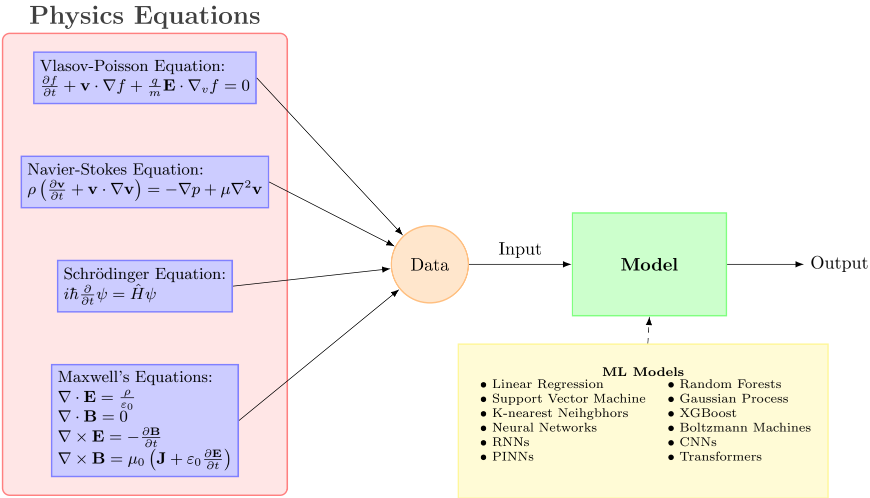
Schrödinger Equation:
$i\hbar \frac{\partial}{\partial t}\psi = \hat{H}\psi$

Maxwell's Equations:
$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$
$\nabla \cdot \mathbf{B} = 0$
$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$
$\nabla \times \mathbf{B} = \mu_0 \left(\mathbf{J} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t}\right)$

Data

Physics Equations





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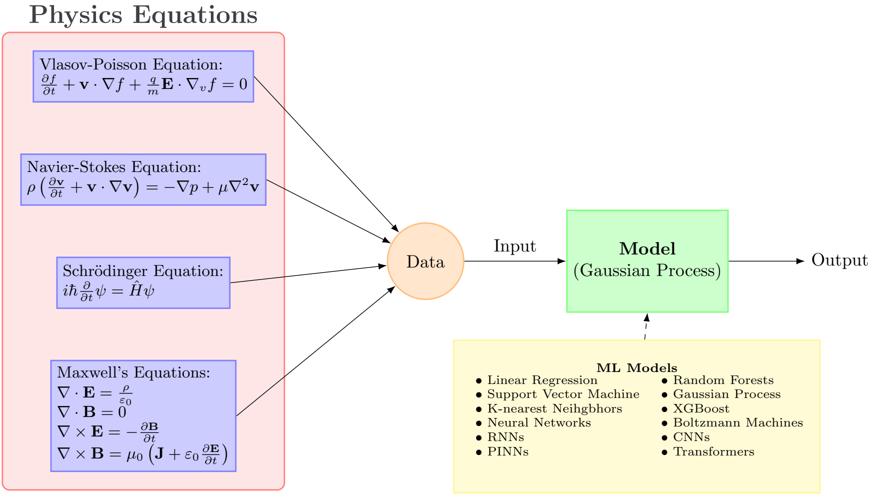
Data
Input
Model
Output
ML Models
• Linear Regression
• Support Vector Machine
• K-nearest Neihgbhors
• Neural Networks
• RNNs
• PINNs
• Random Forests
• Gaussian Process
• XGBoost
• Boltzmann Machines
• CNNs
• Transformers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Data
Input
Model
(Gaussian Process)
Output
ML Models
• Linear Regression
• Support Vector Machine
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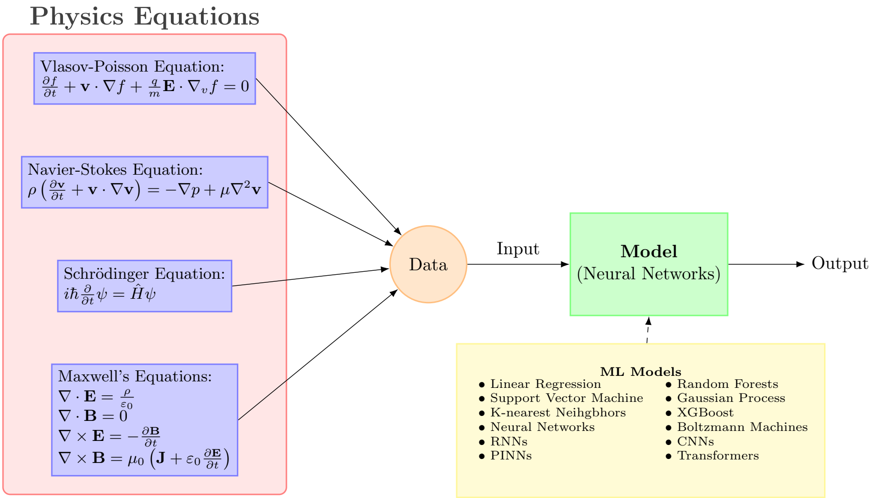
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Data
Input
Model
(Neural Networks)
Output
ML Models
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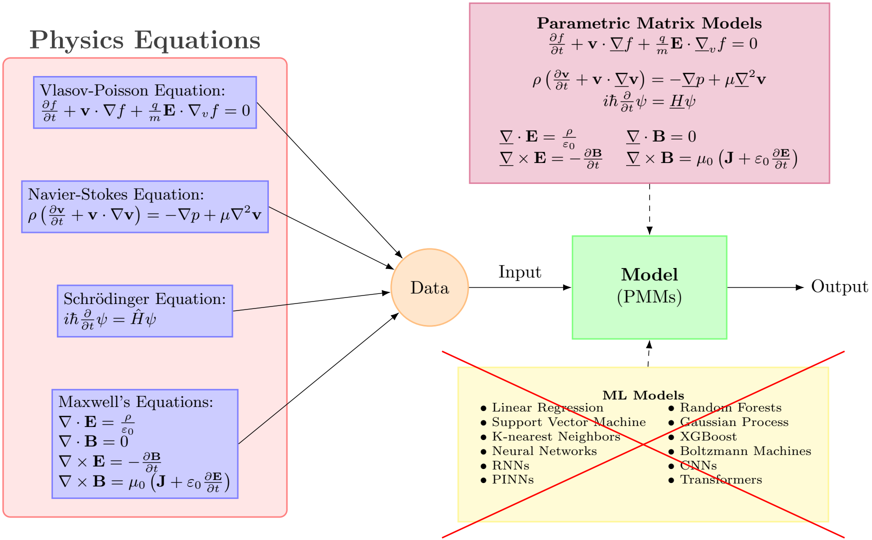
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Data
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Model
(PMMs)
Output
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Build-a-PMM$^{\mathrm{TM}}$

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Your Underlying Equations

$$\begin{cases} H(c) = H_0 + cH_1 \\ H(c)\,|\psi(c)\rangle = E(c)\,|\psi(c)\rangle \\ \langle\psi(c)|O|\psi(c)\rangle = f(c) \end{cases}$$

Build-a-PMM™

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Your PMM

$$\begin{cases} M(c) = \underline{M_0} + c\underline{M_1} \\ M(c)\,|\tilde{\psi}(c)\rangle = \tilde{E}(c)\,|\tilde{\psi}(c)\rangle \\ \langle\tilde{\psi}(c)|\underline{X}|\tilde{\psi}(c)\rangle = \tilde{f}(c) \end{cases}$$

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Okay it's not always *that* simple. . .

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Okay it's not always *that* simple. . .

Then fit to whatever data you have!

Example: Anharmonic Lipkin Model

$$H(\xi;\alpha) = (1-\xi)\hat{n} + \frac{2\xi}{S}\left(S^2 - {\hat{S}_x}^2\right) + \frac{\alpha}{2S}\hat{n}(\hat{n}+1)$$

$$\hat{n} = \left(S + \hat{S}_z\right)$$

Example: Anharmonic Lipkin Model

$$H_\alpha(\xi) = H_0 + \xi H_1$$

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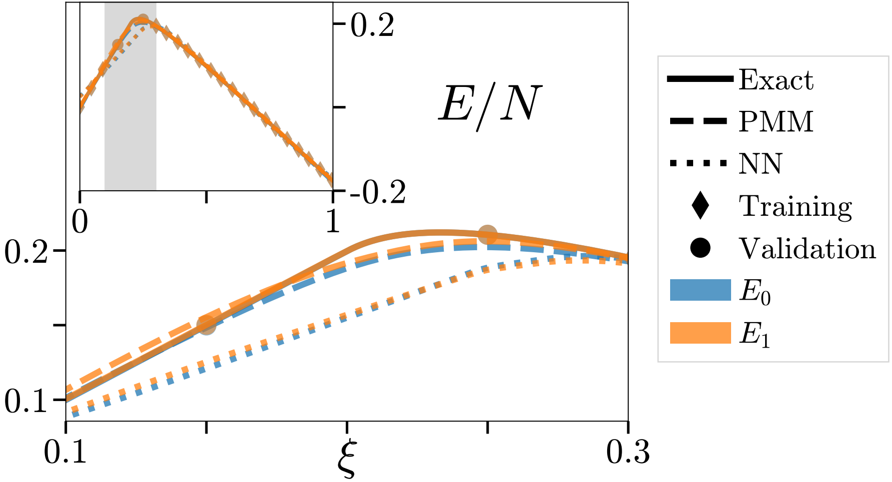

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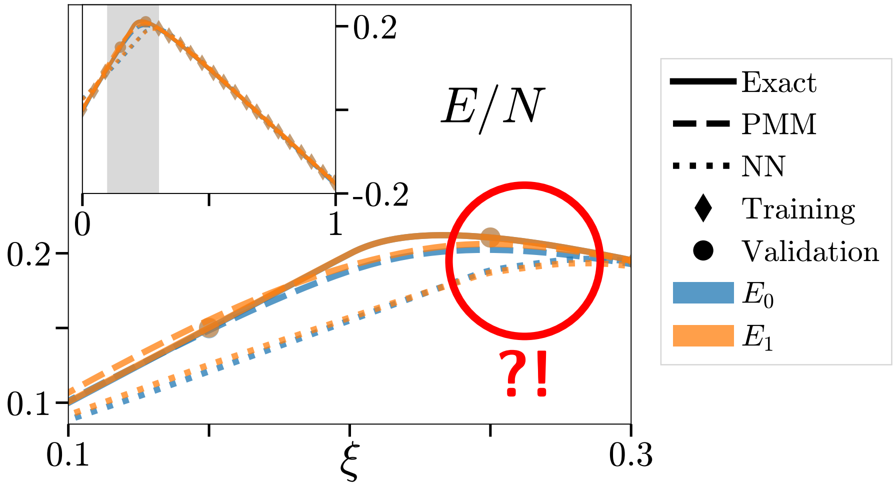

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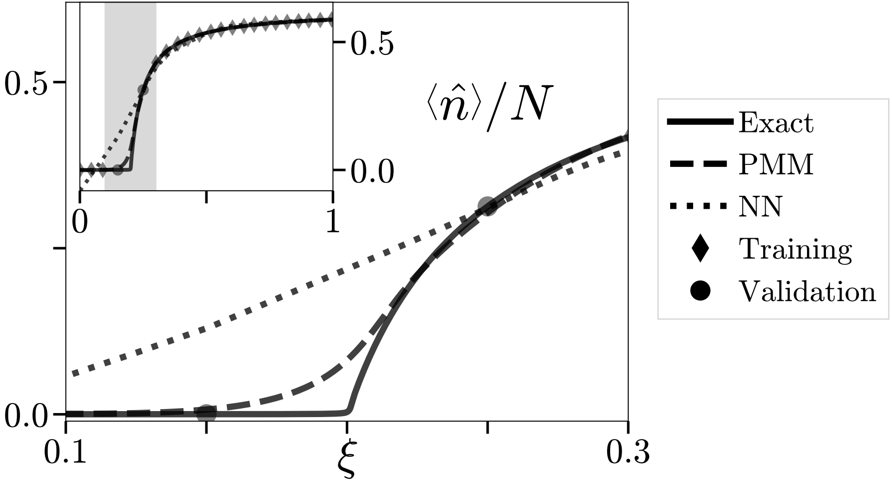

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$$\left\{\begin{matrix} H_\alpha(\xi) = H_0 + \xi H_1 \\ \langle E_0(\xi)|\hat{n}|E_0(\xi)\rangle \end{matrix}\right\} \sim \left\{\begin{matrix} M_\alpha(\xi) = \underline{M_0} + \xi \underline{M_1} \\ \left\langle \tilde{E}_0(\xi) \middle| \underline{X} \middle| \tilde{E}_0(\xi) \right\rangle \end{matrix}\right\}$$

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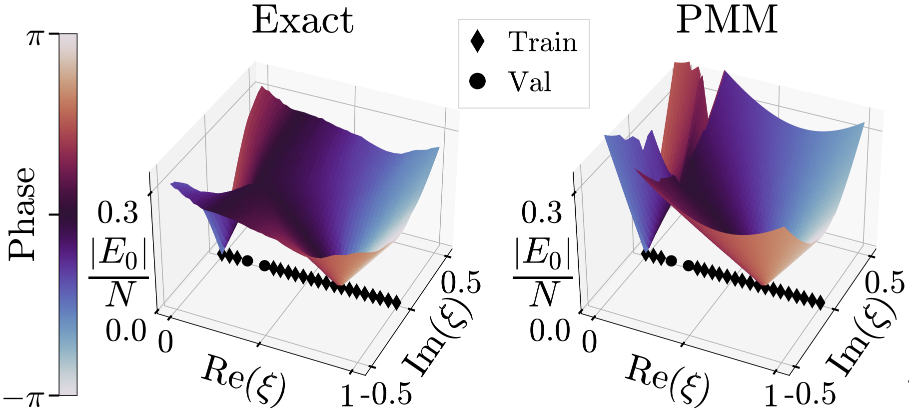

Time evolution on a quantum computer of a non-commuting Hamiltonian

$$H = H_0 + H_1 + \cdots + H_l$$

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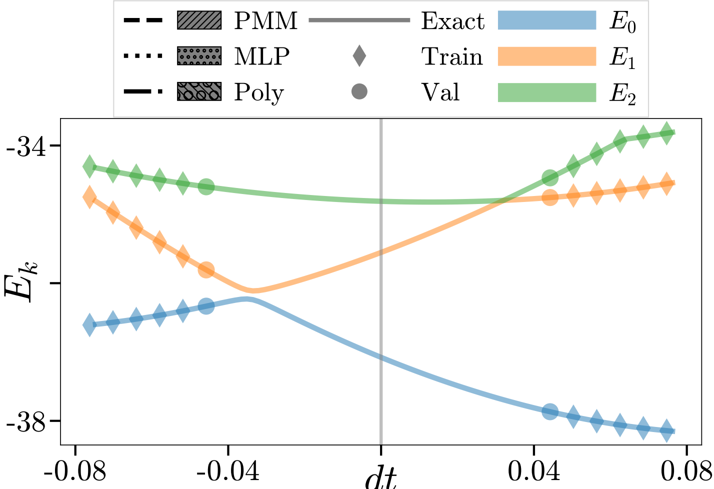
PMM

$$\tilde{U}(dt) = e^{-i\underline{M_0}dt} e^{-i\underline{M_1}dt} \cdots e^{-i\underline{M_l}dt}$$

1D Heisenberg Model with Dzyaloshinskii-Moriya Interaction

$$H = B\sum_{i}^{N} r_i\sigma_i^z + J\sum_{u\in\{x,y,z\}}\sum_{i}^{N}\sigma_i^u\sigma_{i+1}^u + D\sum_{i}^{N}\left(\sigma_i^x\sigma_{i+1}^y - \sigma_i^y\sigma_{i+1}^x\right)$$



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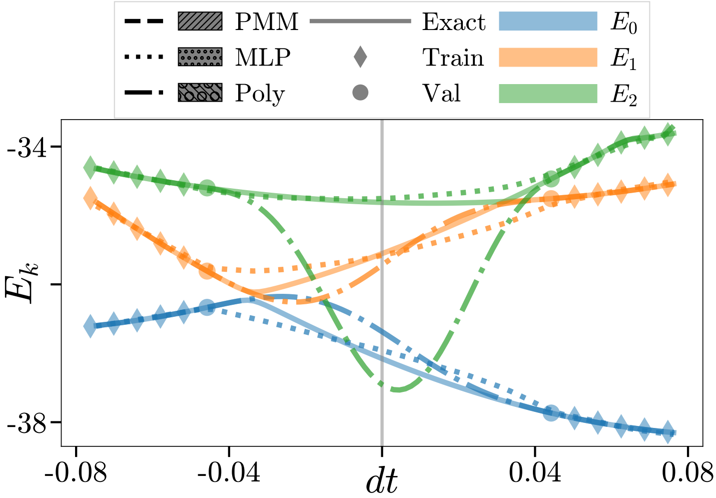

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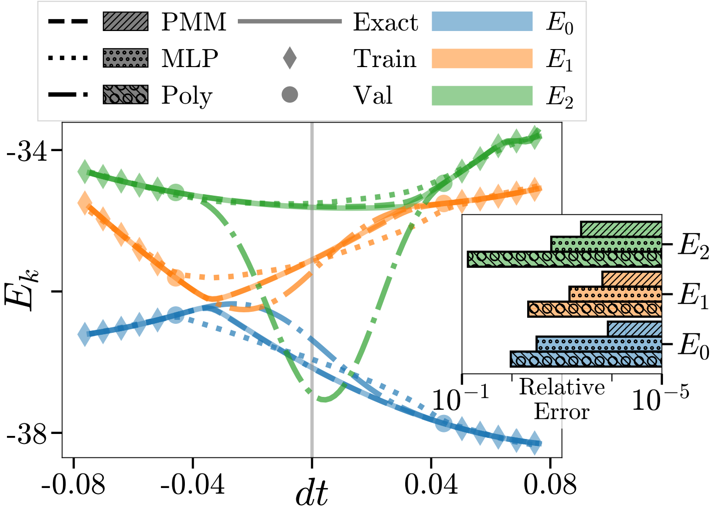

What else can we do with the eigensystem?

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Encode data: $\underline{M(\vec{x})}$

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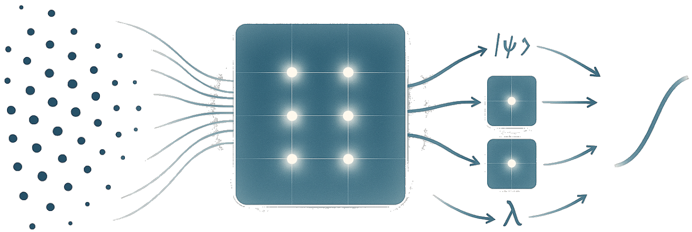
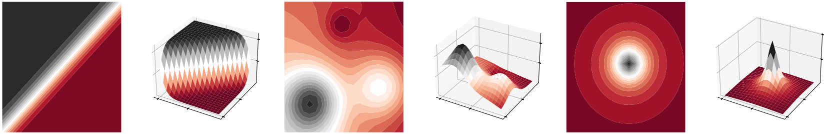
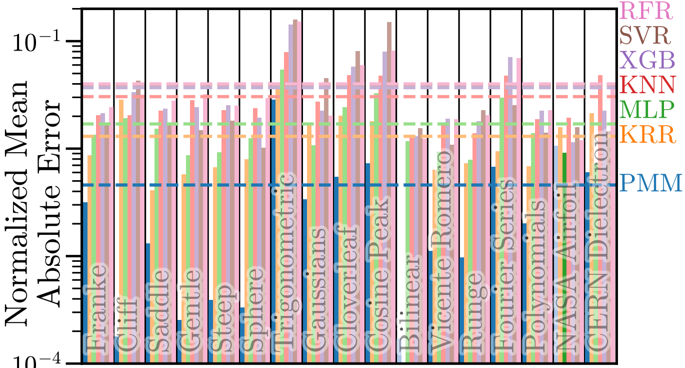
$$\underline{M(\vec{x})} \to V\Lambda V^\dagger$$

$$z_k = \underline{b_k} + \sum_{i\leq j}^{\bar{r}} \left|\langle V_i|\underline{O_{ijk}}|V_j\rangle\right|^2 - \frac{1}{2}\sum_{i\leq j}^{\bar{r}} \left|\left|\underline{O_{ijk}}\right|\right|_2^2$$

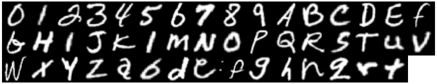


Regression




RFR
SVR
XGB
KNN
MLP
KRR
PMM
Normalized Mean Absolute Error
10^{-1}
10^{-4}
Franke
Cliff
Saddle
Gentle
Steep
Sphere
Trigonometric
Gaussians
Cloverleaf
Cosine Peak
Bilinear
Vicente Romero
Runge
Fourier Series
Polynomials
NASA Airfoil
CERN Dielectron

Classification



Dataset	Model	Acc.	`float`
MNIST Digits[55]	PMM†	97.38	4990
	ConvPMM	98.99	129 416
	DNN-2†[56]	96.5	∼ 311 650
	DNN-3†[56]	97.0	∼ 386 718
	DNN-5†[56]	97.2	∼ 575 050
	GECCO[57]	98.04	∼ 19 000
	CTM-250[58]	98.82	31 750
	CTM-8000[58]	99.4	527 250
	Eff.-CapsNet[59]	99.84	161 824
Fashion MNIST[60]	PMM†	88.58	16 744
	ConvPMM	90.89	278 280
	GECCO[57]	88.09	∼ 19 000
	CTM-250[58]	88.25	31 750
	CTM-8000[58]	91.5	527 250
	MLP†[61]	91.63	2 913 290
	VGG8B[61]	95.47	∼ 7 300 000
	F-T DARTS[62]	96.91	∼ 3 200 000
EMNIST Balanced[63]	PMM†	81.57	13 792
	ConvPMM	85.95	349 172
	CNN[64]	79.61	21 840
	CNN (S-FC)[64]	82.77	13 820
	CNN (S-FC)[64]	83.21	16 050
	HM2-BP†[65]	85.57	665 647

† non-convolutional

Ongoing Work

Two-Body Lattice Simulation

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$$H(c) = KE + V(\delta) + V_S(R_{\mathsf{wall}}) + cV_C(r)$$

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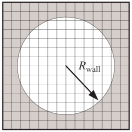

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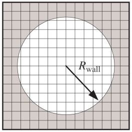

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  $H(c) = H_0 + cH_I$

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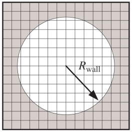

- Rewrite/Group: $H(c) = H_0 + cH_I$

- The training data set is motivated by what can be readily obtained from quantum Monte Carlo simulations.

$$\mathcal{M}_{ij}(t) = \langle \psi_i | e^{-H_0 t/2} O e^{-H_0 t/2} | \psi_j \rangle$$

- Where $O \in \{H_0, H_I, \rho\}$

Nonperturbative Ground State

Governing Equations

$$|\psi_k(t)\rangle = e^{-H_0 t/2}|\psi_k(0)\rangle$$
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PMM Equations

$$|\phi_k(t)\rangle = e^{-\underline{M_0} t/2}|\underline{\phi}_k(0)\rangle$$
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- Once PMM is trained on data only as a function of t, can it predict the ground-state energy of $H(c)$ and the expectation of ρ for any c?

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- Once PMM is trained on data only as a function of t, can it predict the ground-state energy of $H(c)$ and the expectation of ρ for any c?

$$M(c) = M_0 + c\,M_I, \qquad M(c) \xrightarrow{EVD} V\Lambda V^\dagger$$

Nonperturbative Ground State

Governing Equations

$$|\psi_k(t)\rangle = e^{-H_0 t/2}|\psi_k(0)\rangle$$
$$\mathcal{M}_{ij}(t) = \langle\psi_i(t)|O|\psi_j(t)\rangle$$
$$O \in \{H_0, H_I, \rho\}$$

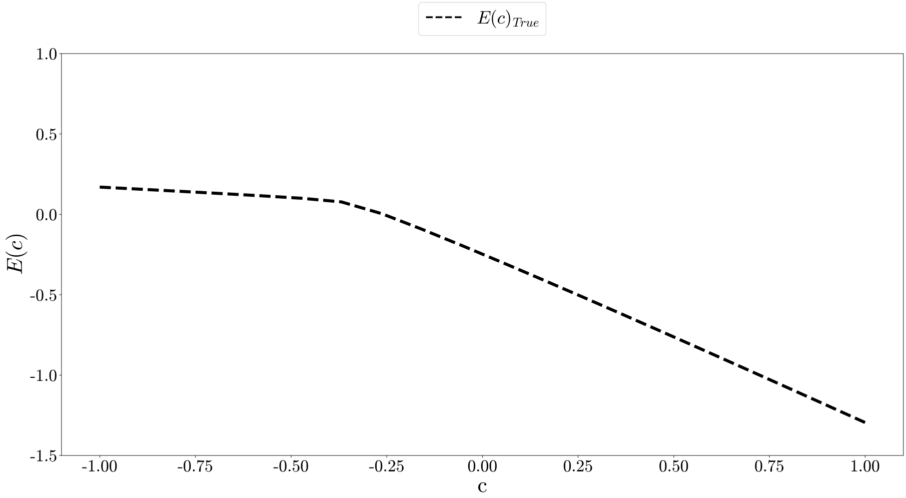
PMM Equations

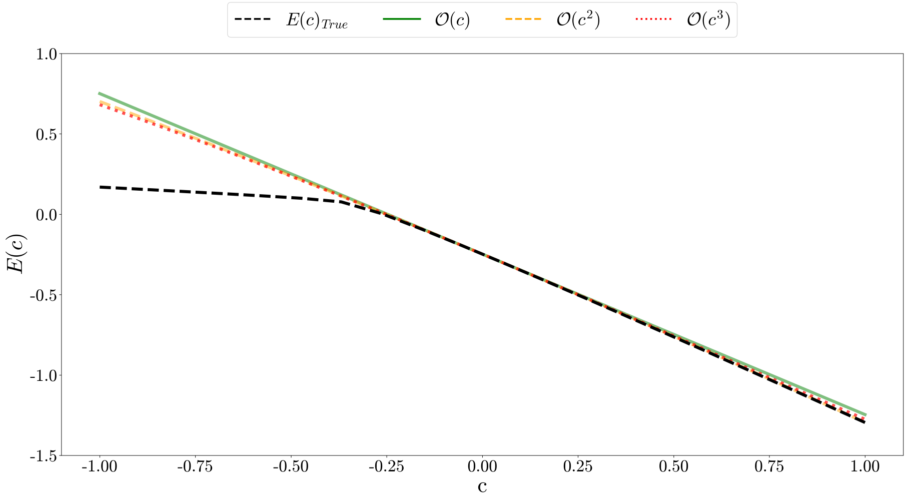
$$|\phi_k(t)\rangle = e^{-\underline{M_0} t/2}|\underline{\phi}_k(0)\rangle$$
$$\hat{\mathcal{M}}_{ij}(t) = \langle\phi_i(t)|\Delta|\phi_j(t)\rangle$$
$$\Delta \in \{\underline{M_0}, \underline{M_I}, \underline{p}\}$$

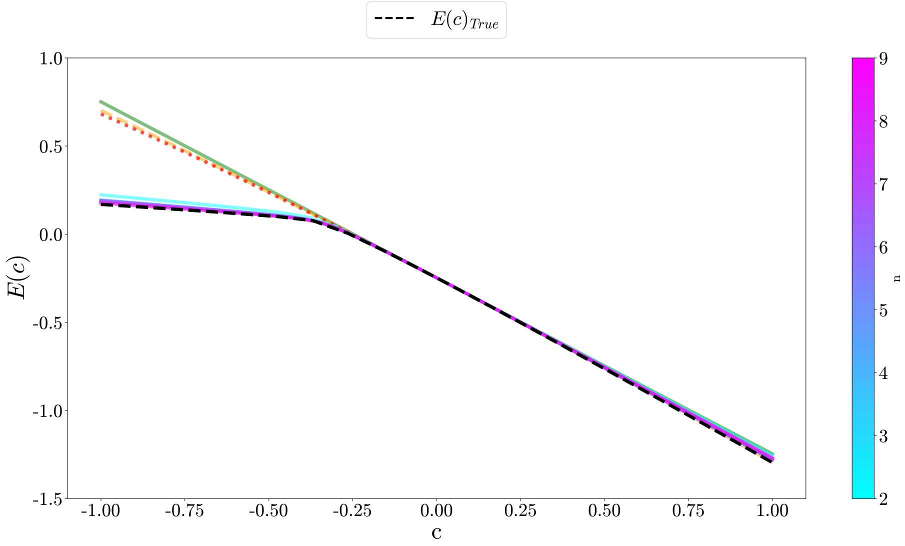
- Once PMM is trained on data only as a function of t, can it predict the ground-state energy of $H(c)$ and the expectation of ρ for any c?

$$M(c) = M_0 + c\,M_I, \qquad M(c) \xrightarrow{EVD} V\Lambda V^\dagger$$

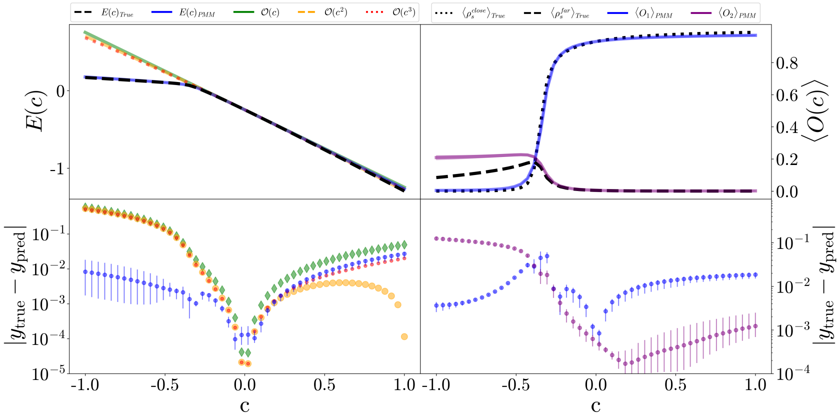
- Then calculate $E_0(c)$ and $\langle V_0(c)|\underline{p}|V_0(c)\rangle$.


$E(c)_{True}$
1.0
0.5
0.0
-0.5
-1.0
-1.5
$E(c)$
-1.00
-0.75
-0.50
-0.25
0.00
0.25
0.50
0.75
1.00
c

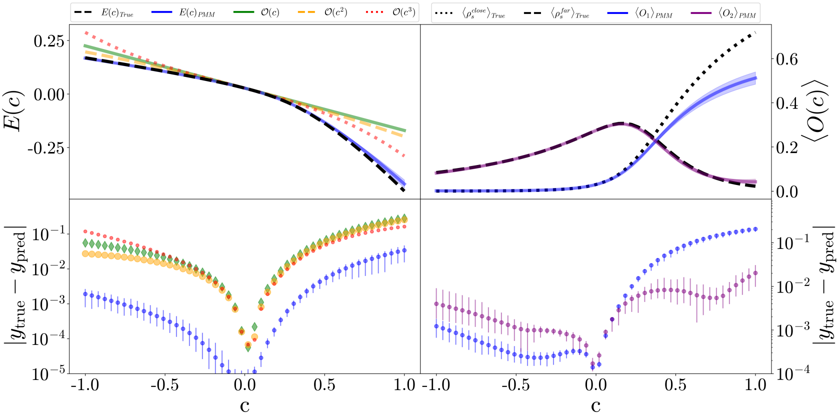

$E(c)_{True}$
$\mathcal{O}(c)$
$\mathcal{O}(c^2)$
$\mathcal{O}(c^3)$
1.0
0.5
0.0
-0.5
-1.0
-1.5
$E(c)$
-1.00
-0.75
-0.50
-0.25
0.00
0.25
0.50
0.75
1.00
c

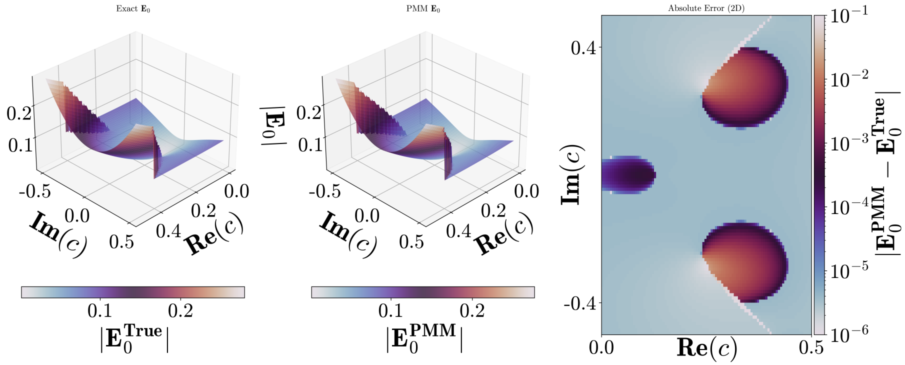


$E(c)_{True}$
$E(c)$
c
n
1.0
0.5
0.0
-0.5
-1.0
-1.5
-1.00
-0.75
-0.50
-0.25
0.00
0.25
0.50
0.75
1.00
2
3
4
5
6
7
8
9



$E(c)_{True}$
$E(c)_{PMM}$
$\mathcal{O}(c)$
$\mathcal{O}(c^2)$
$\mathcal{O}(c^3)$
$\langle\rho_s^{close}\rangle_{True}$
$\langle\rho_s^{far}\rangle_{True}$
$\langle O_1\rangle_{PMM}$
$\langle O_2\rangle_{PMM}$
$E(c)$
$\langle O(c)\rangle$
$|y_{\rm true} - y_{\rm pred}|$
c

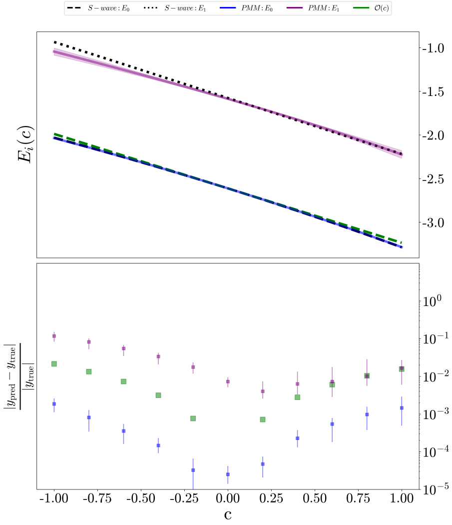

$E(c)_{True}$
$E(c)_{PMM}$
$\mathcal{O}(c)$
$\mathcal{O}(c^2)$
$\mathcal{O}(c^3)$
$\langle\rho_s^{close}\rangle_{True}$
$\langle\rho_s^{far}\rangle_{True}$
$\langle O_1\rangle_{PMM}$
$\langle O_2\rangle_{PMM}$
$E(c)$
$\langle O(c)\rangle$
$|y_{\rm true} - y_{\rm pred}|$
c



Exact $\mathbf{E}_0$
PMM $\mathbf{E}_0$
Absolute Error (2D)
$|\mathbf{E}_0|$
$\mathbf{Im}(c)$
$\mathbf{Re}(c)$
$|\mathbf{E}_0^{\mathbf{True}}|$
$|\mathbf{E}_0^{\mathbf{PMM}}|$
$|\mathbf{E}_0^{\mathbf{PMM}} - \mathbf{E}_0^{\mathbf{True}}|$

Spherical Well

Spherical Well



$$\begin{array}{c} H(c) = H_0 + cH_I \\ \Big\updownarrow ? \\ M(c) = M_0 + cM_1 \end{array}$$

$$\frac{d\rho_i}{dt} = Q^i_\mu \rho_\mu + R^i_{\mu\nu}\rho_\mu\rho_\nu + S^i_{\mu\nu\tau}\rho_\mu\rho_\nu\rho_\tau$$

$$\updownarrow ?$$

$$?$$

$$i\frac{d\Psi}{dt} = \left(T + V + g\left|\Psi\right|^2\right)\Psi$$

$$\Big\updownarrow \, ?$$

$$?$$

Typical Reduced Basis Method

$$\Psi \to P^\dagger \Psi \equiv \psi$$

Typical Reduced Basis Method

$$\Psi \to P^\dagger \Psi \equiv \psi$$

$$H \to P^\dagger H P \equiv M$$

Implicit Reduced Basis Method

$$\Psi \to P^\dagger \Psi \equiv \psi$$

$$H \to P^\dagger H P \equiv \underline{M}$$

Implicit Reduced Basis Method

$$\Psi \longrightarrow P^{\dagger}\Psi \equiv \psi$$

$$H \longrightarrow P^{\dagger}HP \equiv \underline{M}$$

$$H(c) = H_0 + cH_I$$

$$H(c) = H_0 + cH_I$$

$$\updownarrow$$

$$P^\dagger H(c) P = P^\dagger H_0 P + c P^\dagger H_I P$$

$$H(c) = H_0 + cH_I$$

$$\updownarrow$$

$$P^\dagger H(c) P = P^\dagger H_0 P + cP^\dagger H_I P$$

$$\updownarrow$$

$$M(c) = \underline{M_0} + c\underline{M_1}$$

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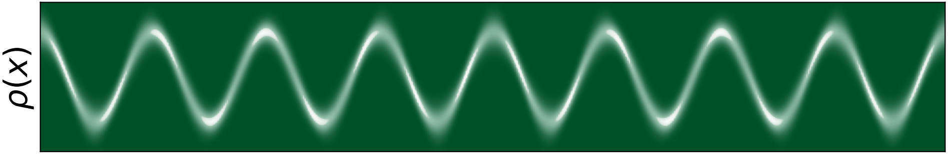
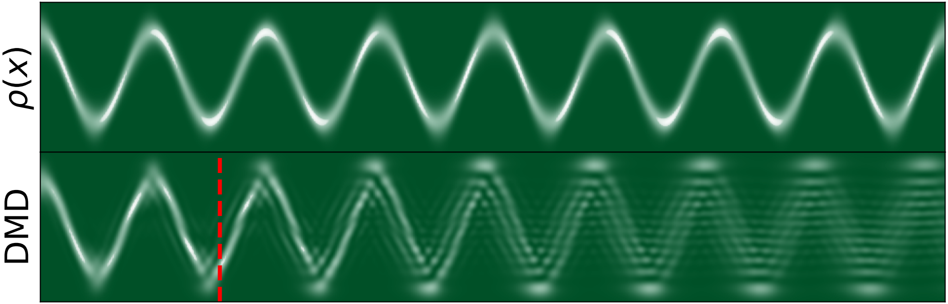
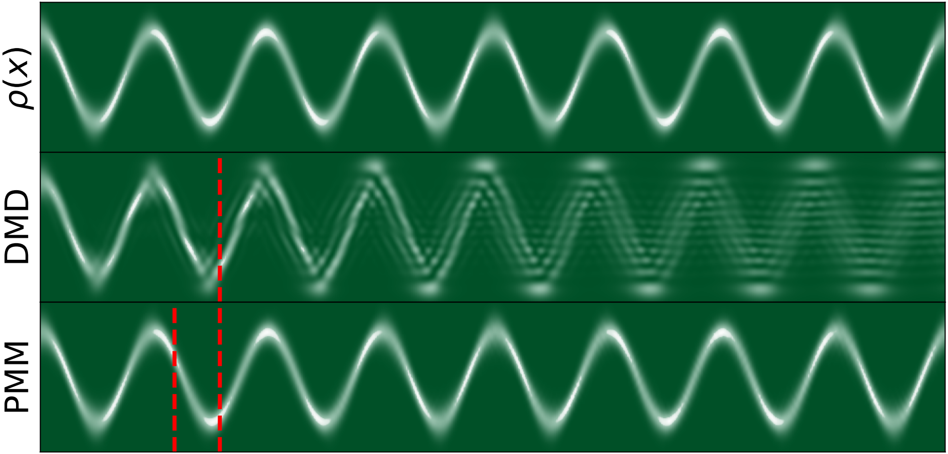
$$\updownarrow$$

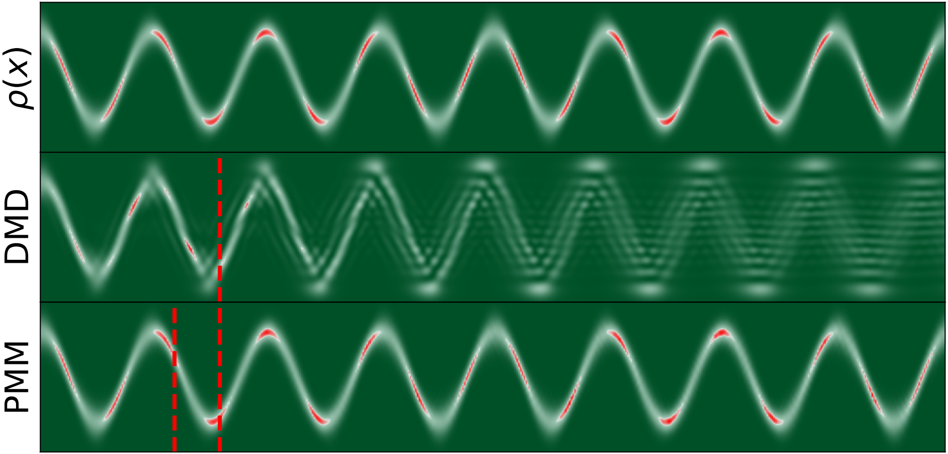
$$i\frac{d\psi_i}{dt} = \underline{T_{ij}}\psi_j + \underline{V_{ij}}\psi_j + g\underline{G_{ijkl}}\psi_j\psi_k\psi_l$$

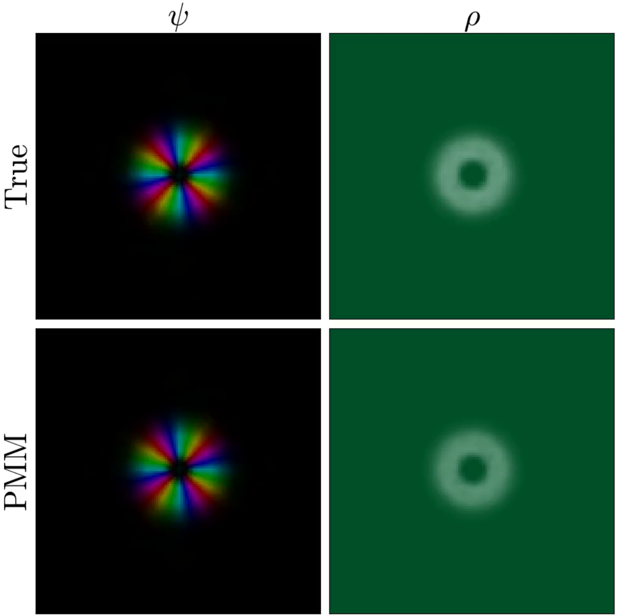

$\rho(x)$



$\rho(x)$
DMD


$\rho(x)$
DMD
PMM


ρ(x)
DMD
PMM


ψ
ρ
True
PMM

Equation-Free Methods

Equation-Free Methods

- **D**ynamic **M**ode **D**ecomposition

Equation-Free Methods

- **D**ynamic **M**ode **D**ecomposition
- **S**parse **I**dentification of **N**onlinear **Dy**namics

Equation-Free Methods

- **D**ynamic **M**ode **D**ecomposition
- **S**parse **I**dentification of **N**onlinear **Dy**namics
- Neural Operators

Equation-Free Methods

Equation-Full Methods

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Equation-Full Methods

- **P**roper **O**rthogonal **D**ecomposition

Equation-Free Methods

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- **S**parse **I**dentification of **N**onlinear **Dy**namics
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Equation-Full Methods

- **P**roper **O**rthogonal **D**ecomposition
- Eigenvector Continuation

Parametric Matrix Models

Equation-Free Methods

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Equation-Free Methods

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Equation-Informed Methods

Equation-Full Methods

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Parametric Matrix Models

Equation-Free Methods

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Equation-Informed Methods

***Implicit* Reduced Basis Methods**

Equation-Full Methods

- **P**roper **O**rthogonal **D**ecomposition
- Eigenvector Continuation

Thank You

Isn't this just Eigenvector Continuation?

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Eigenvector Continuation

Isn’t this just Eigenvector Continuation?

Eigenvector Continuation

Requires:

- Snapshots of full eigenvectors

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- The evaluation of $H(c)$

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Pros:

- Exponential convergence

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- Constructed rather than trained

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- Poor computational scaling

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$$H(c) = \frac{1}{2N}\sum_{i}^{N}(\sigma_i^z + c\sigma_i^x)$$

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Eigenvector Continuation

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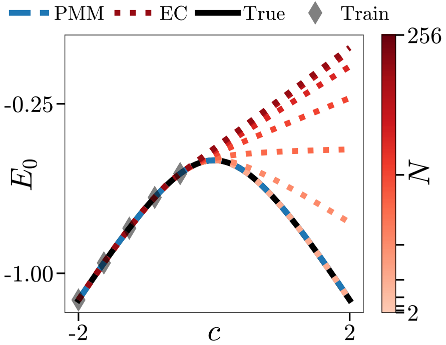
$$H(c) = \frac{1}{2N} \sum_{i}^{N} (\sigma_i^z + c\sigma_i^x)$$



$$i\frac{d\Psi}{dt} = \left(T + V + g\left|\Psi\right|^2\right)\Psi$$

$$\rho = \left|\Psi\right|^2$$

$$i\frac{d\Psi}{dt} = \left(T + V + g\left|\Psi\right|^2\right)\Psi$$

$$\rho = \left|\Psi\right|^2$$

$$\updownarrow$$

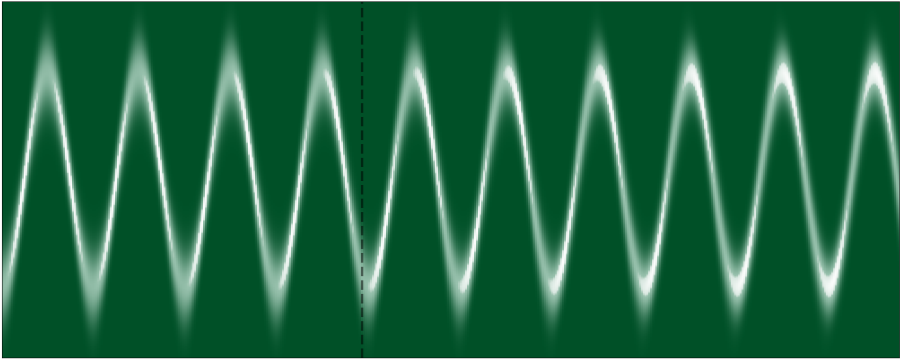
$$i\frac{d\psi_i}{dt} = \underline{T_{ij}}\psi_j + \underline{V_{ij}}\psi_j + g\underline{G_{ijkl}}\psi_j\psi_k\psi_l$$

$$q_i = \underline{F_{ijk}}\psi_j\psi_k$$

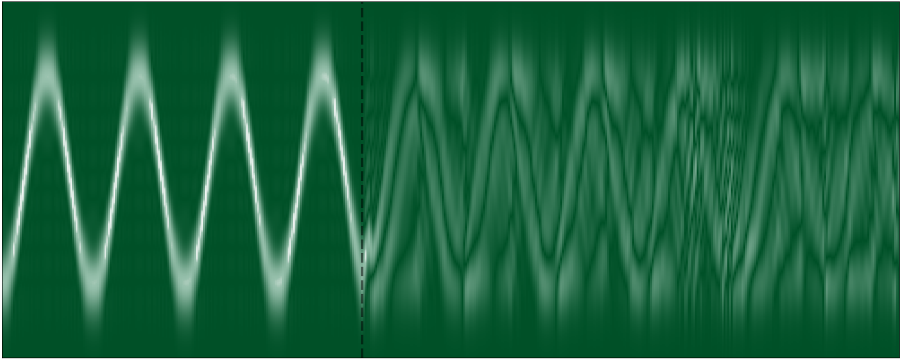
$$\psi(t=0) = \underline{\psi_0}$$

$$i\frac{d\Psi}{dt} = \left(\frac{p^2}{2\boxed{m}} + \boxed{a}\,x^2 + \boxed{g}\,|\Psi|^2\right)\Psi$$

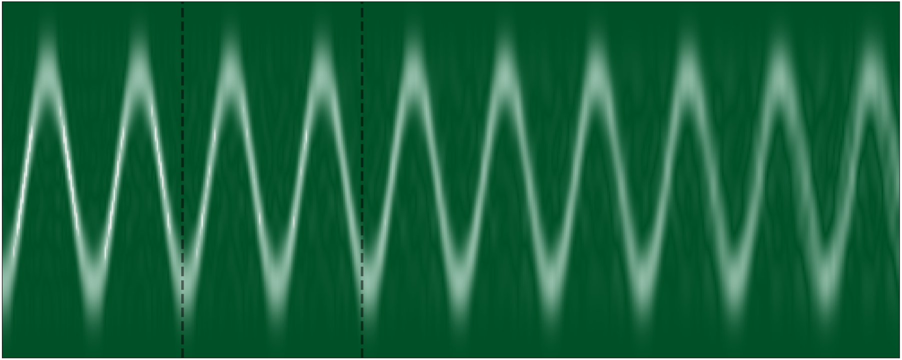
$$i\frac{d\Psi}{dt} = \left(\frac{p^2}{2\boxed{m}} + \boxed{a}x^2 + \boxed{g}\left|\Psi\right|^2\right)\Psi$$

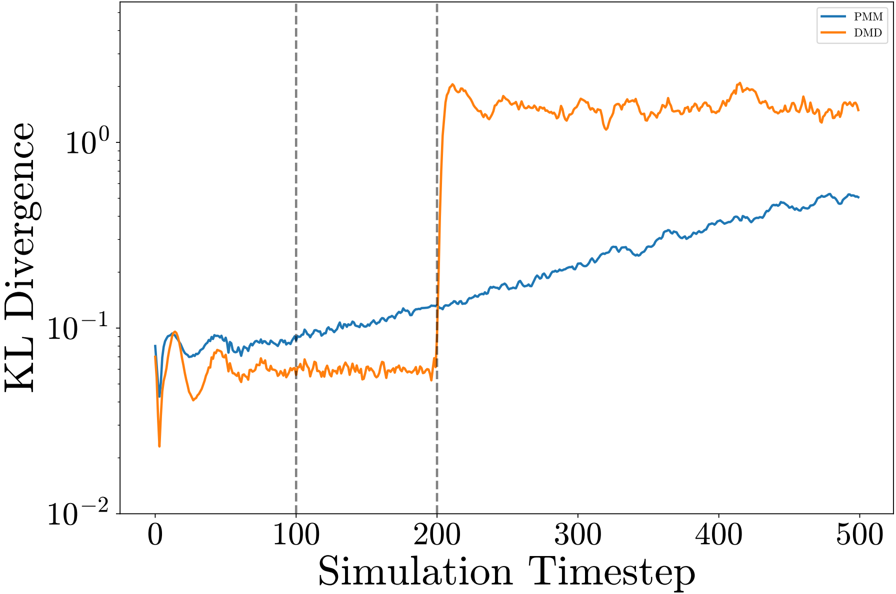


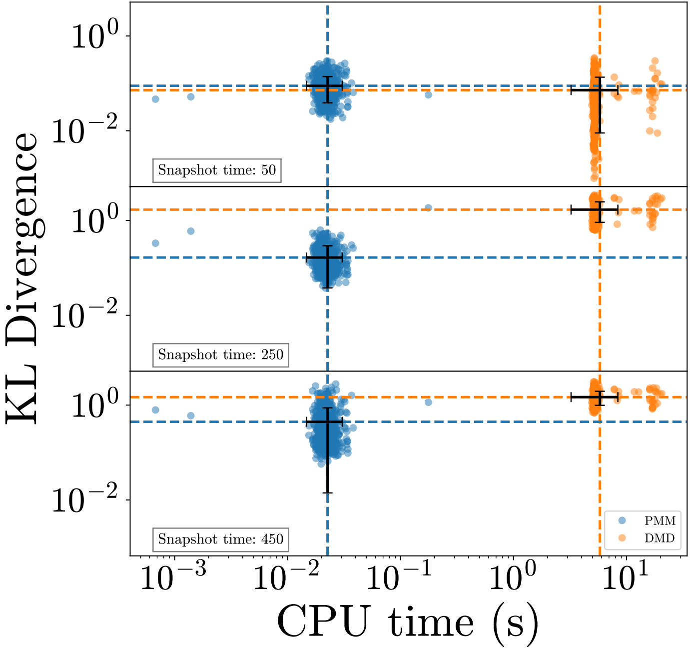
$$i\frac{d\Psi}{dt} = \left(\frac{p^2}{2\boxed{m}} + \boxed{a}\,x^2 + \boxed{g}\,|\Psi|^2\right)\Psi$$

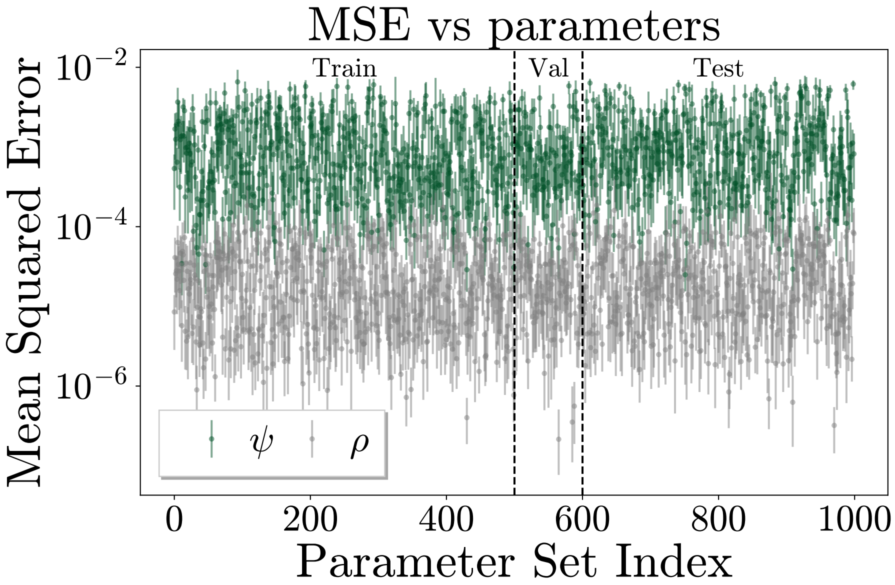


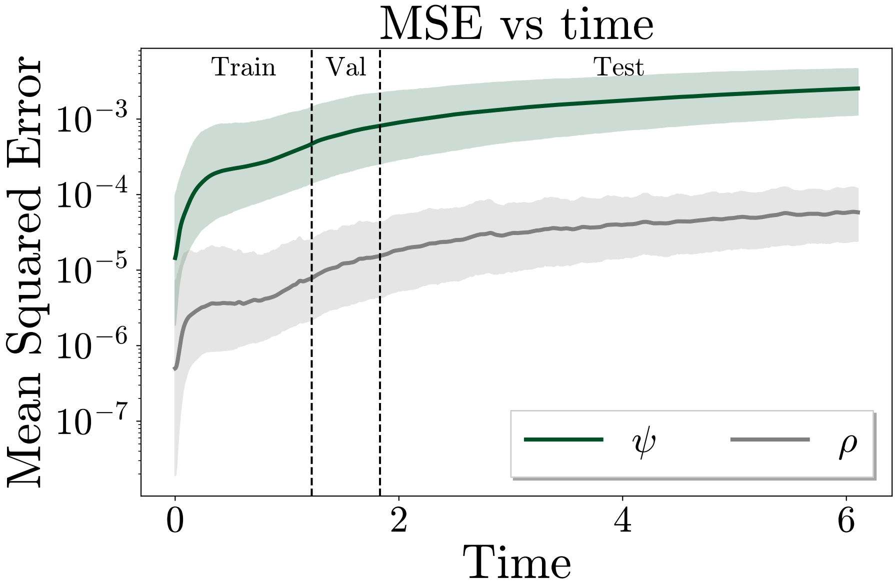
$$i\frac{d\Psi}{dt} = \left(\frac{p^2}{2\boxed{m}} + \boxed{a}\,x^2 + \boxed{g}\,|\Psi|^2\right)\Psi$$

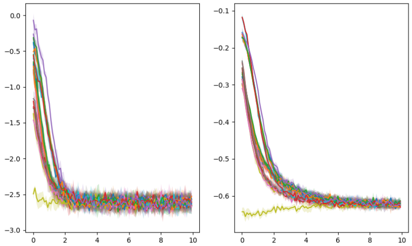


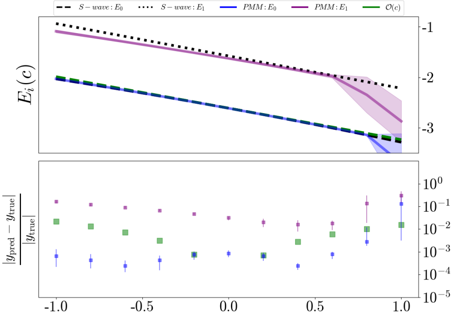

PMM
DMD
KL Divergence
10^{0}
10^{-1}
10^{-2}
0
100
200
300
400
500
Simulation Timestep


KL Divergence
10^0
10^{-2}
Snapshot time: 50
Snapshot time: 250
Snapshot time: 450
PMM
DMD
10^{-3}
10^{-2}
10^{-1}
10^0
10^1
CPU time (s)


MSE vs parameters
Mean Squared Error
10^{-2}
10^{-4}
10^{-6}
Train
Val
Test
ψ
ρ
0
200
400
600
800
1000
Parameter Set Index


MSE vs time
Mean Squared Error
Time
Train
Val
Test
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
0
2
4
6
ψ
ρ


0.0
−0.5
−1.0
−1.5
−2.0
−2.5
−3.0
0
2
4
6
8
10
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6


$S-wave: E_0$
$S-wave: E_1$
$PMM: E_0$
$PMM: E_1$
$\mathcal{O}(c)$
$E_i(c)$
-1
-2
-3
$\frac{|y_{\rm pred}-y_{\rm true}|}{|y_{\rm true}|}$
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
-1.0
-0.5
0.0
0.5
1.0