Emulators for Inverse Problems in Dense Matter Physics

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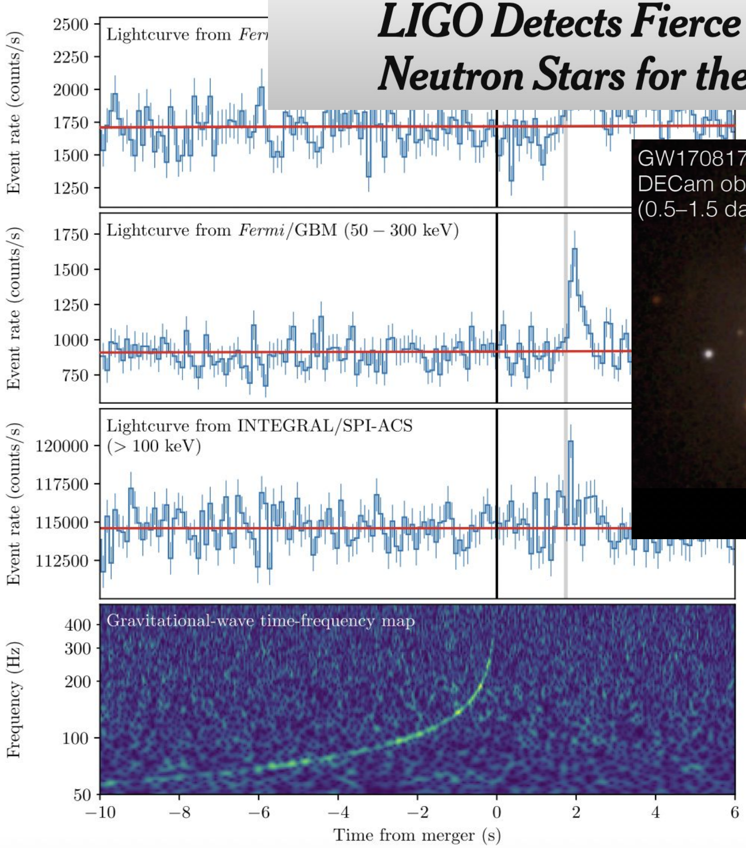
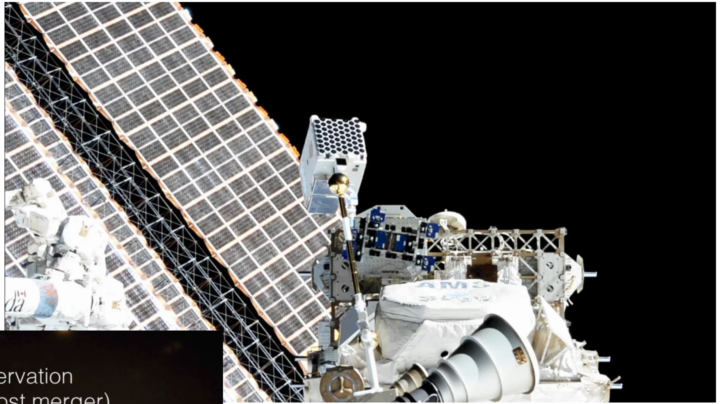
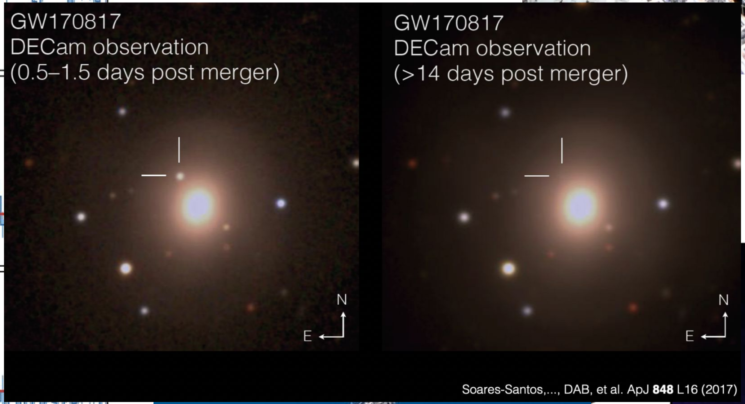
An explosion of NS observations!

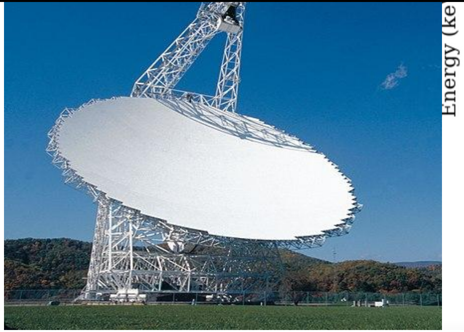
The New York Times

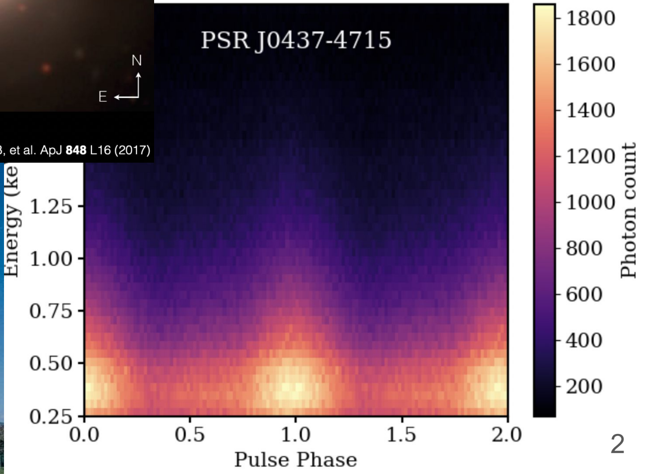
LIGO Detects Fierce Collision of Neutron Stars for the First Time





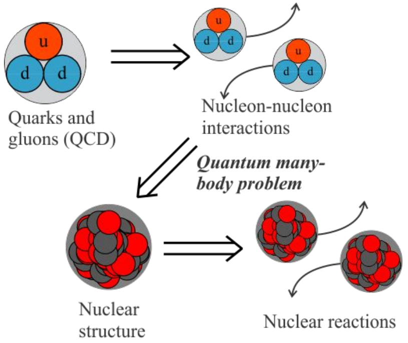


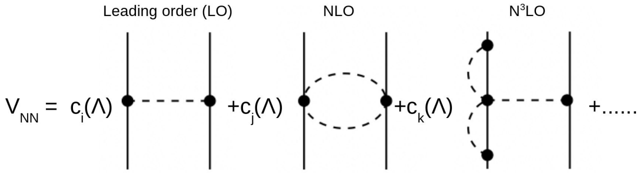




Dense matter physics in a nutshell

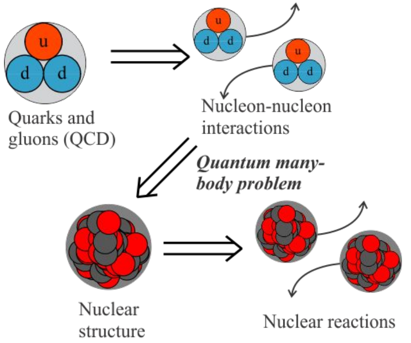
Model for interaction between particles

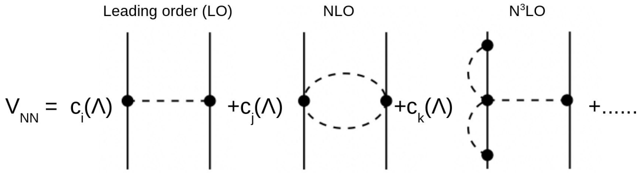


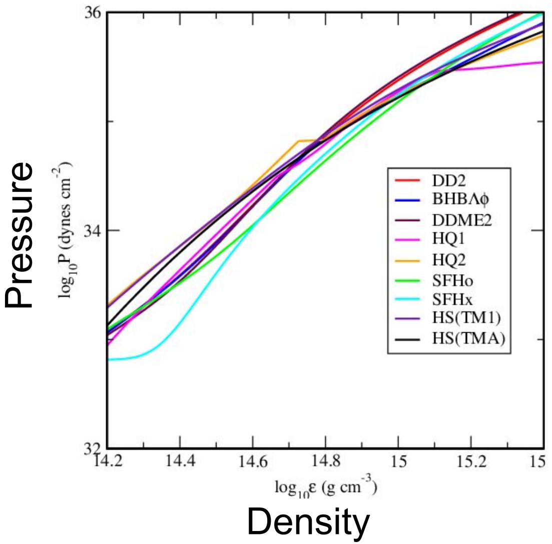


Dense matter physics in a nutshell

Model for interaction between particles $H|\psi\rangle = E|\psi\rangle$ The Equation of State







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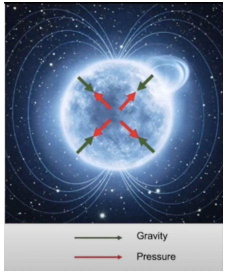
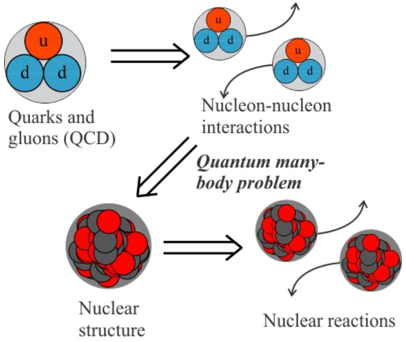
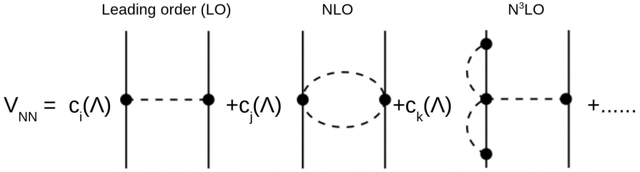


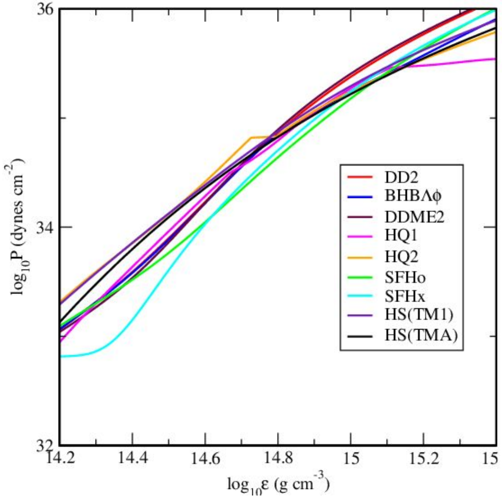
Tolman–Oppenheimer–Volkoff (TOV) equation

Model for interaction between particles $\;H|\psi\rangle = E|\psi\rangle\;$ The Equation of State $\;G^{\mu\nu} = \kappa T^{\mu\nu}\;$ Neutron star observables

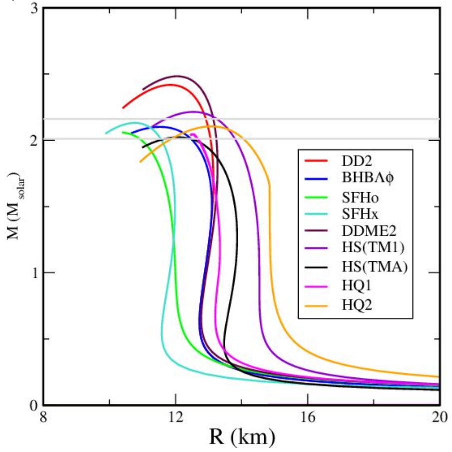




Pressure

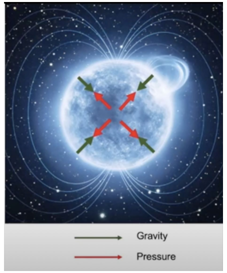


Density



Dense matter physics in a nutshell

Bayesian inference requires ~10^7 model evaluations



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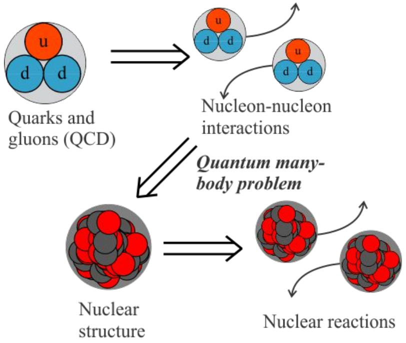
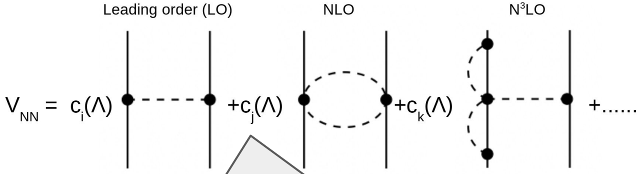
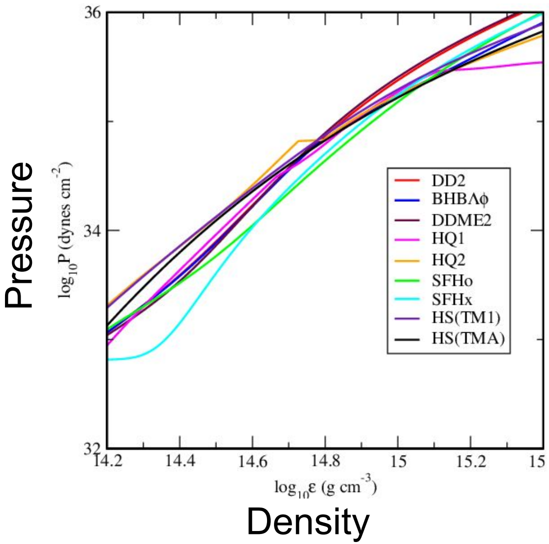
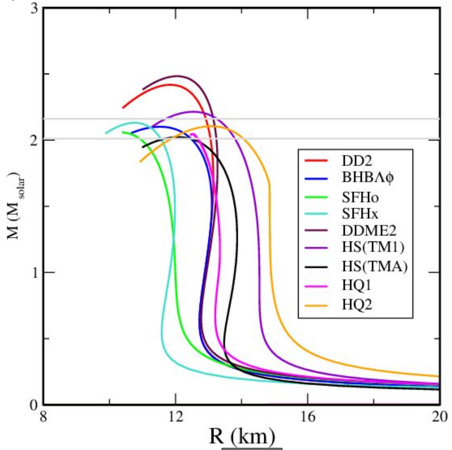




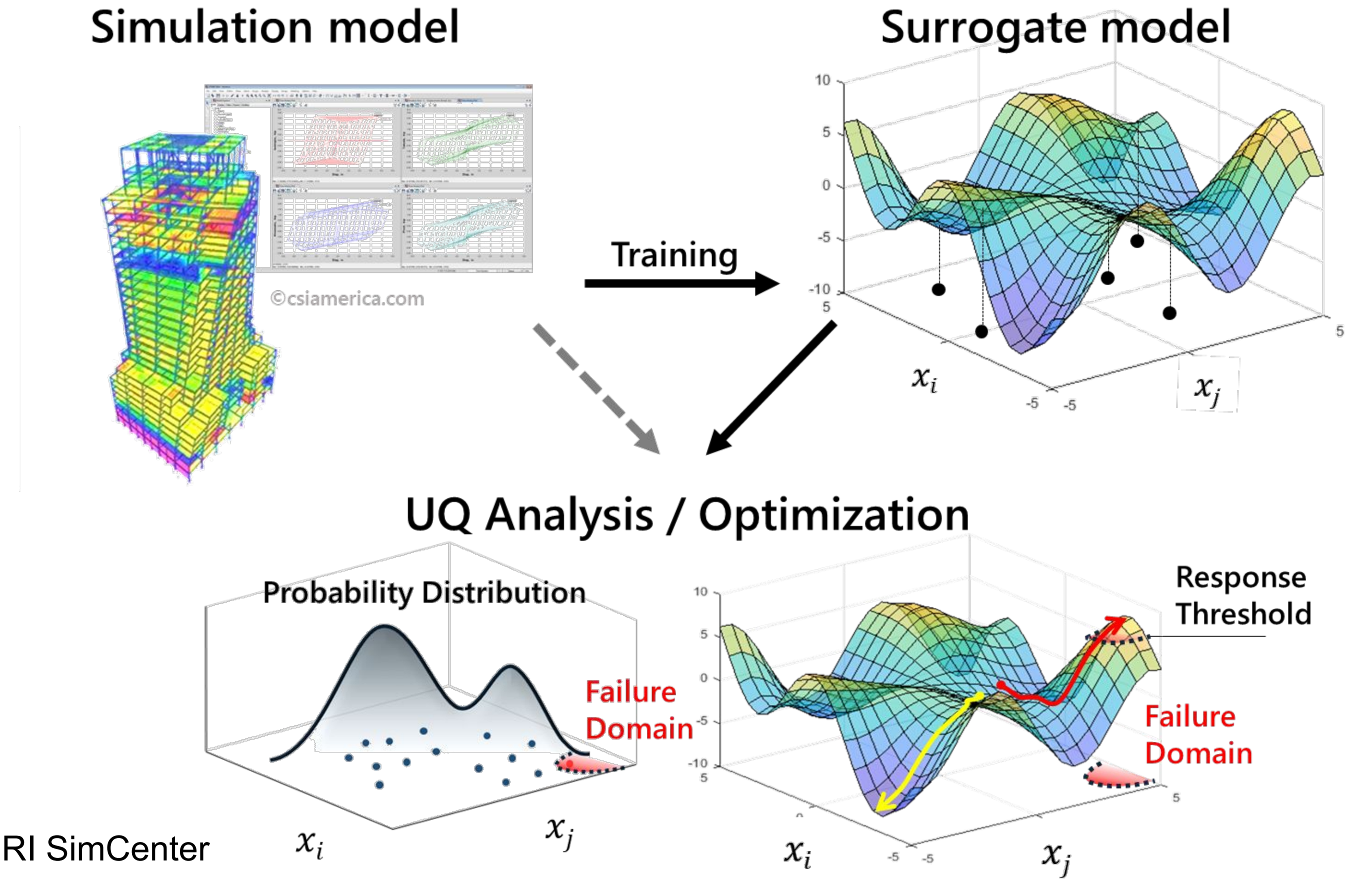




Bayesian Inference methods

The solution: Use emulators to accelerate calculations

Emulators mimic the behaviour of the full-scale model at a small fraction of its computational cost



Credits: NHERI SimCenter

Overall strategy

Quantum many-body methods
~1 million CPU hours
(scarce training data)

TOV equations
~5 seconds

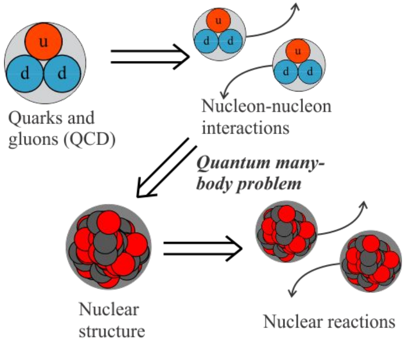
Model for interaction between particles

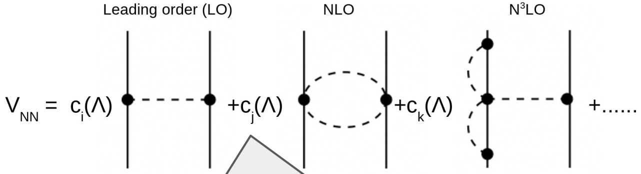
$H|\psi\rangle = E|\psi\rangle$

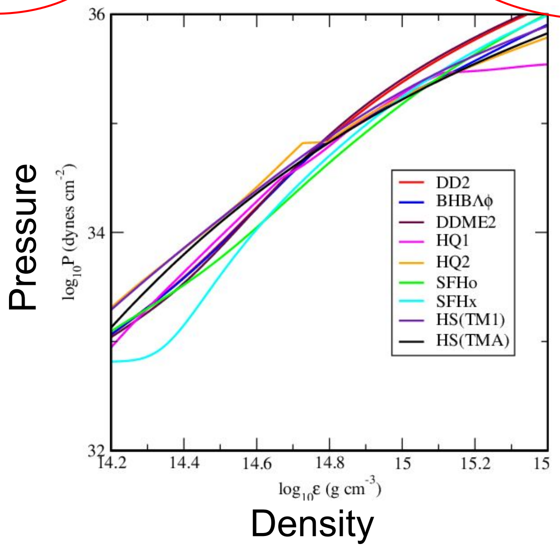
The Equation of State

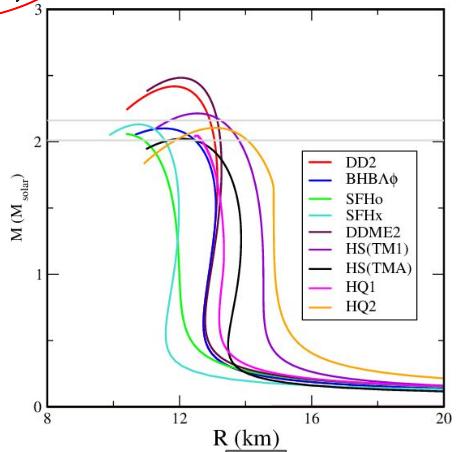
$G^{\mu\nu} = \kappa T^{\mu\nu}$

Neutron star observables









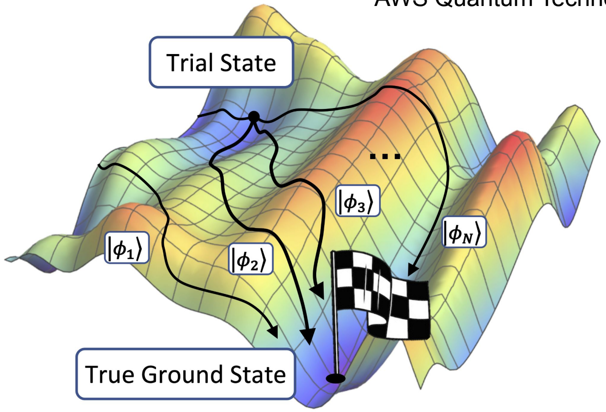
Bayesian Inference methods

Quantum Monte Carlo in a nutshell

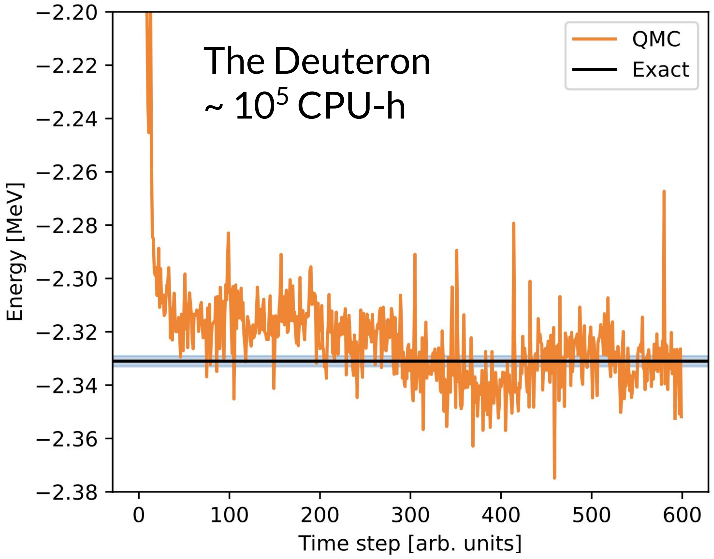
$$\lim_{\tau\to\infty} e^{-H\tau}|\Psi_T\rangle \to |\Psi_0\rangle$$

Trial wavefunction   True ground state

H(***a***) is the Hamiltonian

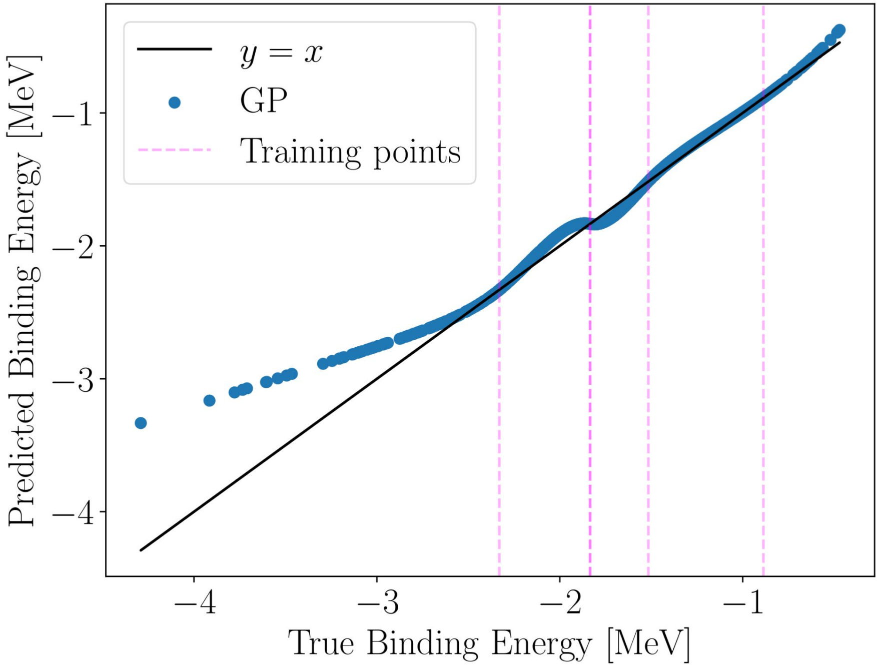


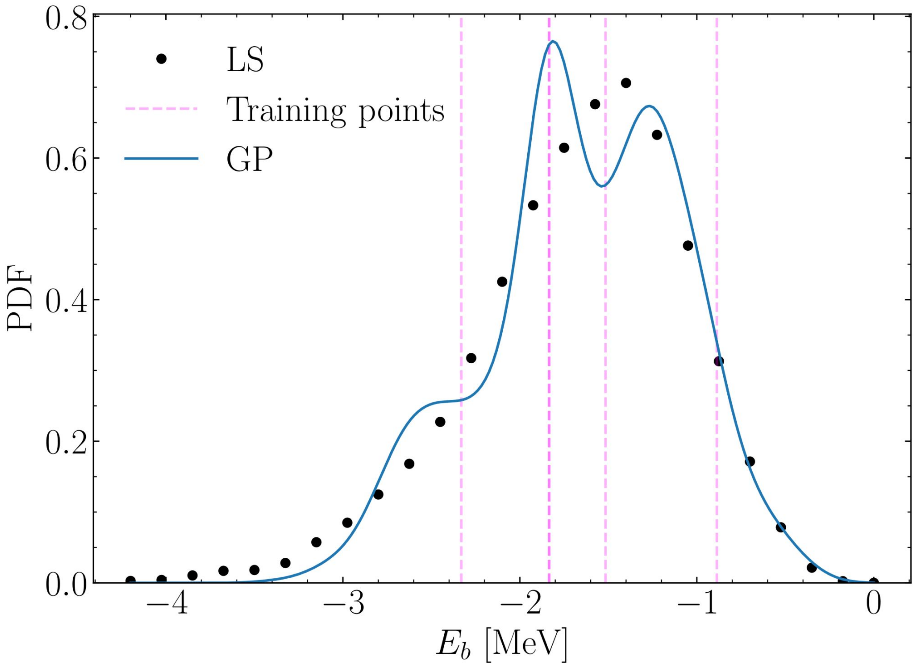
- Virtually exact method for strongly interacting many-body systems
- First step is the preparation of a trial wavefunction, i.e. our best guess for the true ground state
- The trial state is evolved in imaginary time. This is mathematically equivalent to the diffusion problem
- At infinite imaginary time, the system 'cools' to its true ground state



Emulators with scarce data: how about traditional ML?

- Goal: Build accurate surrogate models for QMC with ~5 - 10 training points
- The GP fails to accurately interpolate and extrapolate between training points



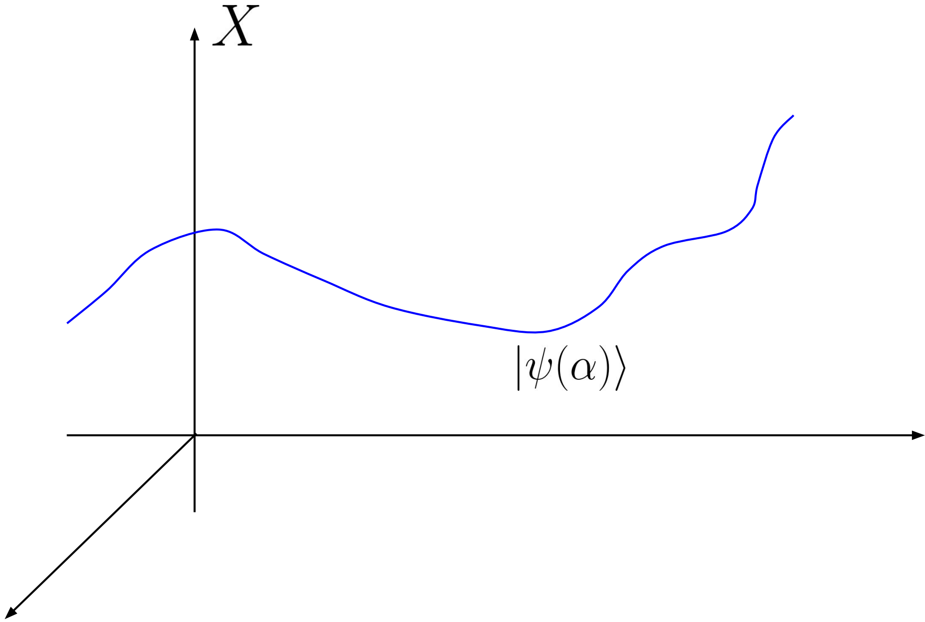


RS et al., arXiv:2404.11566

Emulators with scarce data: Reduced basis methods

- Start with the full Schrödinger equation

$$H|\psi\rangle = E|\psi\rangle$$



Emulators with scarce data: Reduced basis methods

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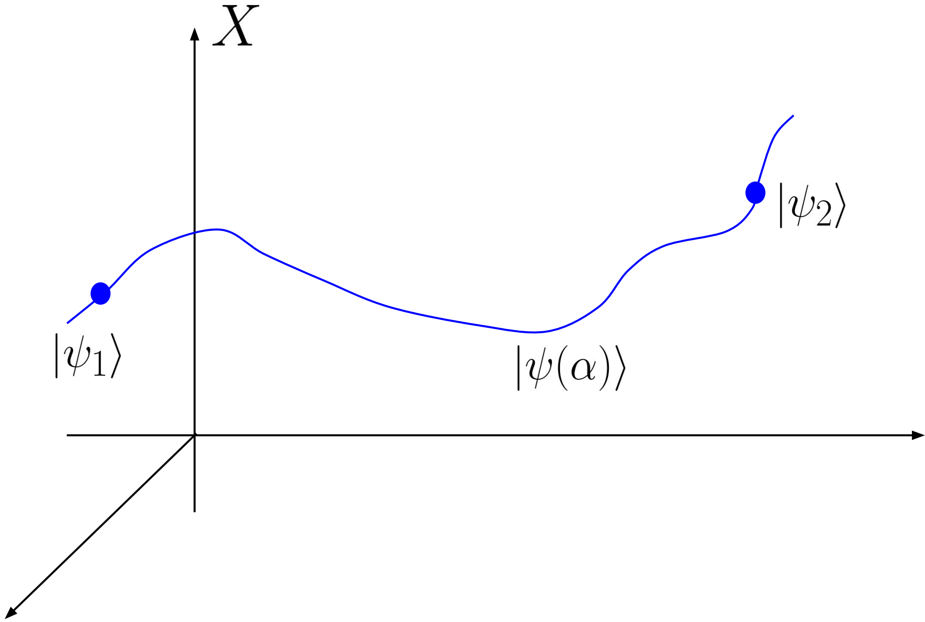
- Compute N training functions or ‘snapshots’ $|\psi_j\rangle$



Emulators with scarce data: Reduced basis methods

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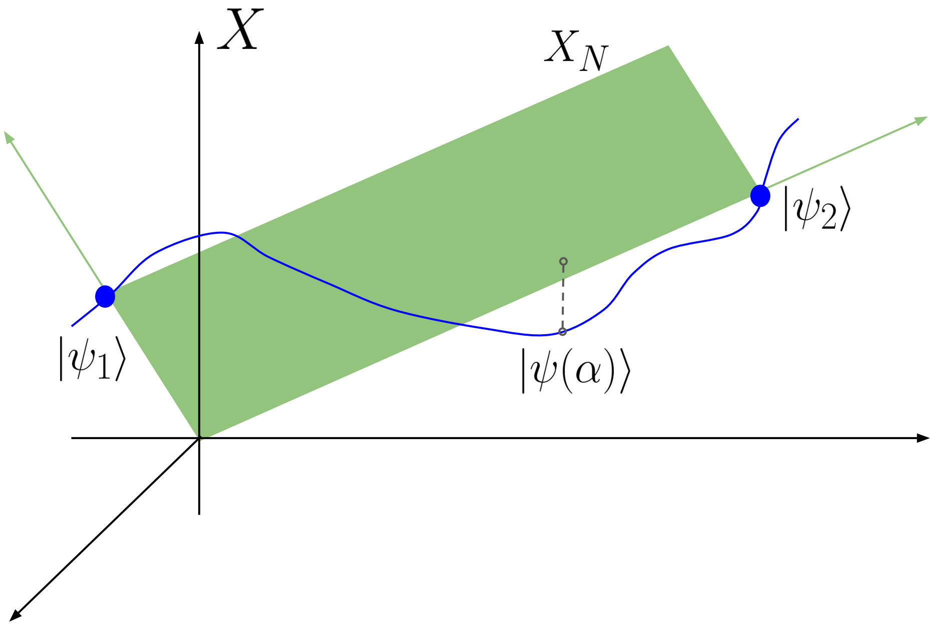
- Project the Hamiltonian into the reduced space spanned by $|\psi_j\rangle$

  Mathematically, this corresponds to computing the matrix

$$M_{ij} \equiv \langle\psi_i|H|\psi_j\rangle$$

Petrov-Galerkin projection method



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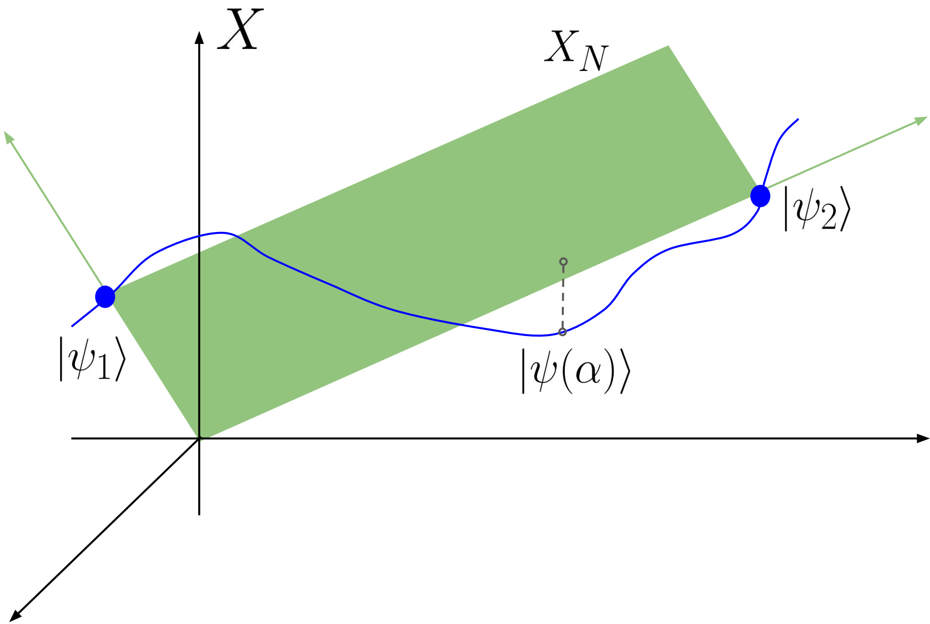
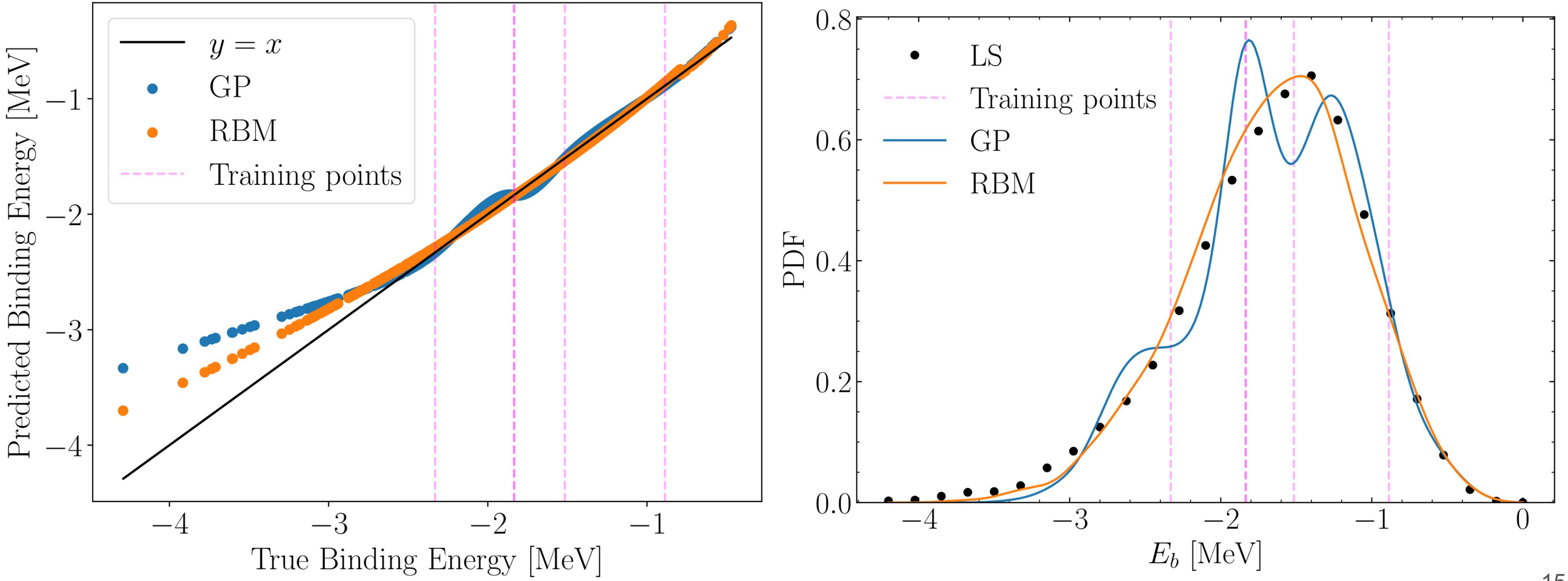


- For QMC, M_{ij} is dominated by stochastic noise and cannot be calculated. We therefore implemented a Petrov-Galerkin projection method for this problem:

$$\tilde{M}_{ij} = \langle\psi_i^T|H|\psi_j\rangle$$

Emulators with scarce data: Reduced basis methods

- The RBM outperforms the GP
- The RBM is capable of interpolating but fails to extrapolate away from training points



RS et al., arXiv:2404.11566

Emulators with scarce data: Hybrid models

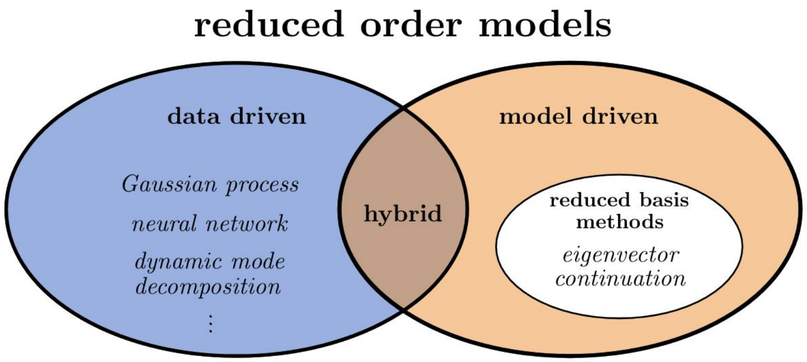
- Combine elements of RBMs with data-driven emulators

- We employ the recently proposed parametric matrix models

$$M(\vec{\alpha}) = M_0 + \sum_i \alpha_i M_i$$

- The form of the reduced subspace matrix is inspired by RBMs. However, we do not directly compute the projections, i.e. we do not compute the subspace matrix elements

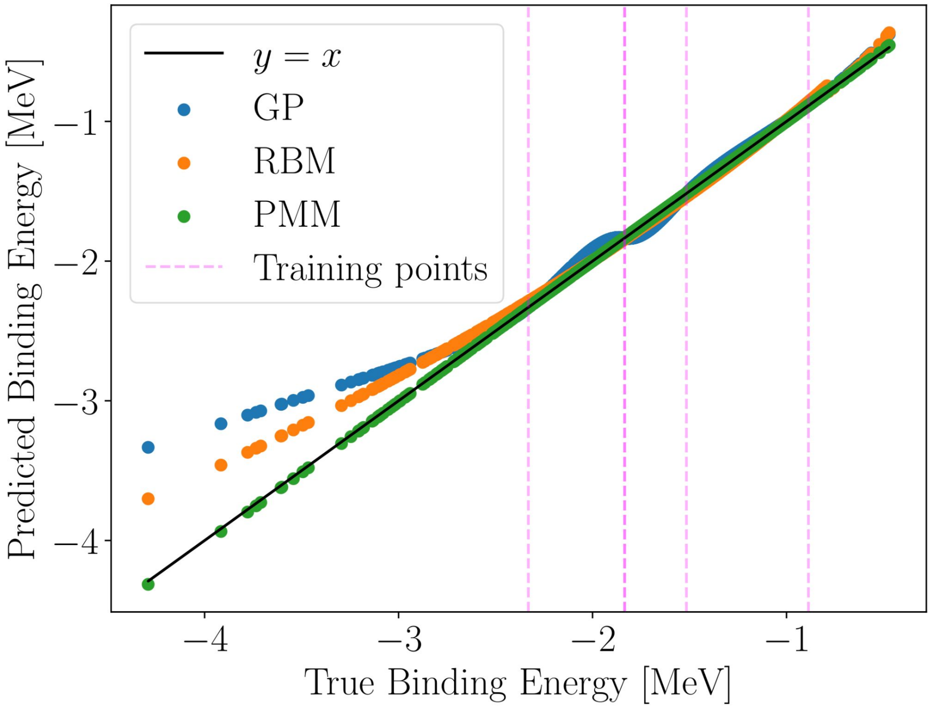
- Instead they are learned in some manner from the data

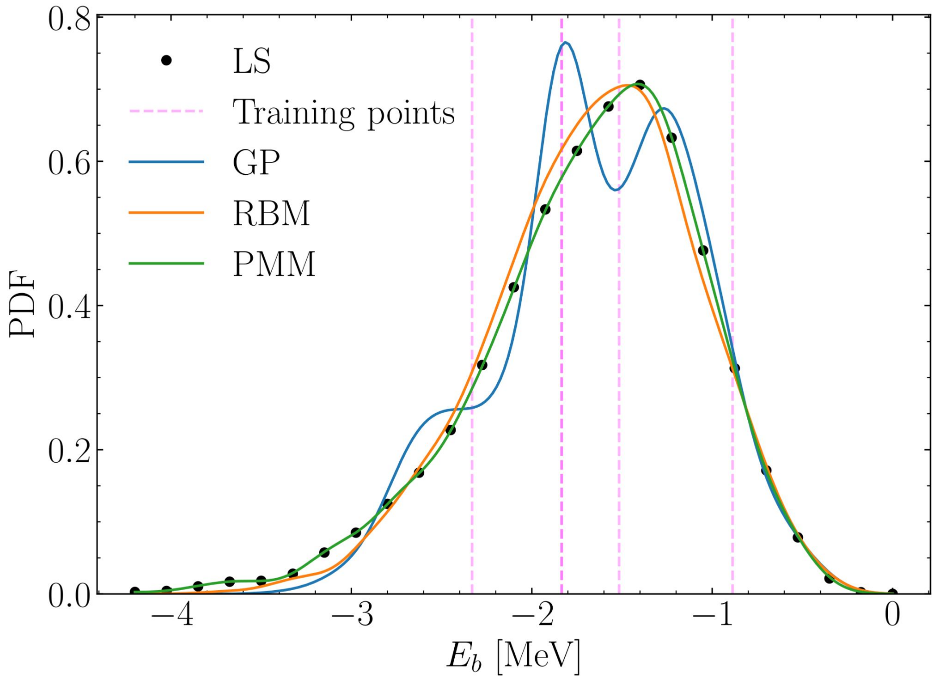


Duguet et al., arXiv:2310.19419

Emulators with scarce data: Hybrid models

- The PMM outperforms both the GP and RBM
- It interpolates well but also gives excellent results for extrapolation!





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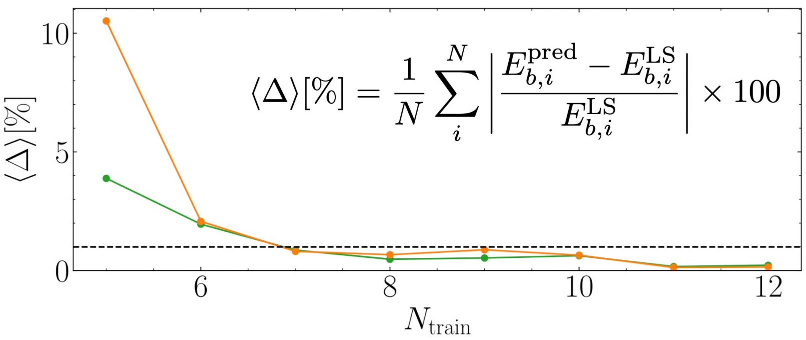
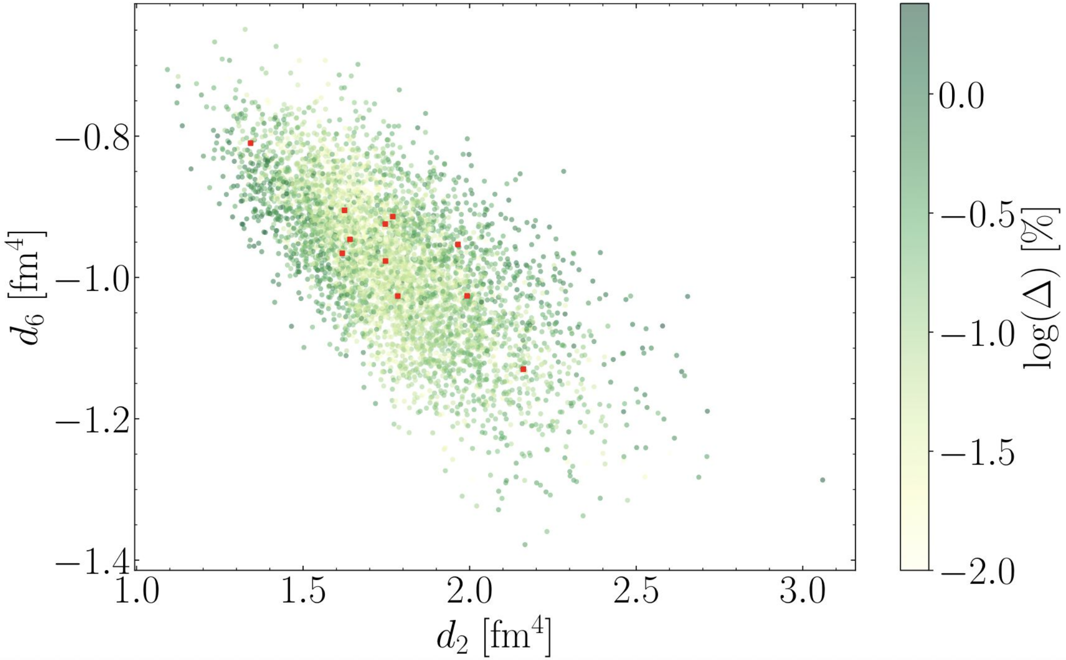




- We found that our PMM generalises very well to at least 4 - 5 dimensional parameter spaces.

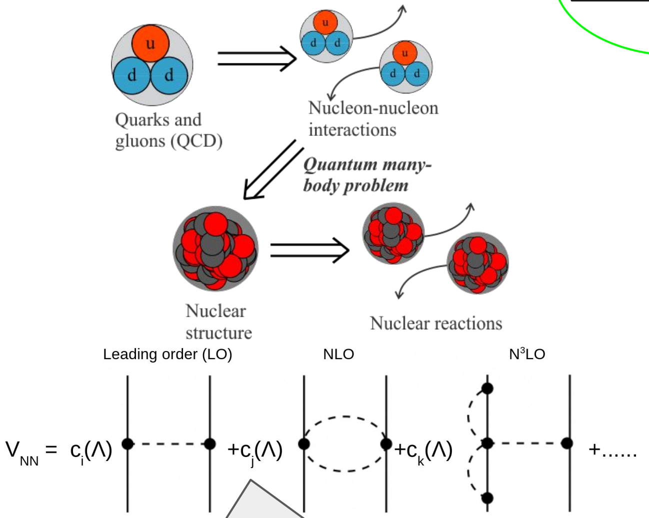
RS et al., arXiv:2404.11566

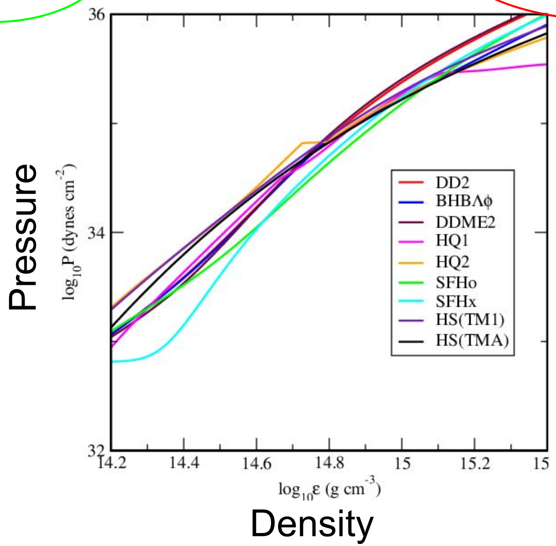
Overall strategy

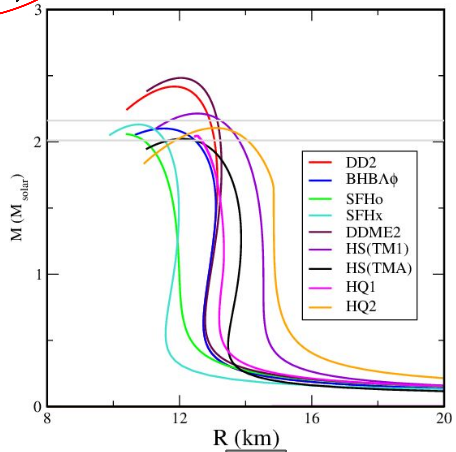
Speed-up factor ~ 10^7
Uncertainty ~ 0.1 %

TOV equations
~5 seconds

Model for interaction between particles → $H|\psi\rangle = E|\psi\rangle$ → The Equation of State → $G^{\mu\nu} = \kappa T^{\mu\nu}$ → Neutron star observables





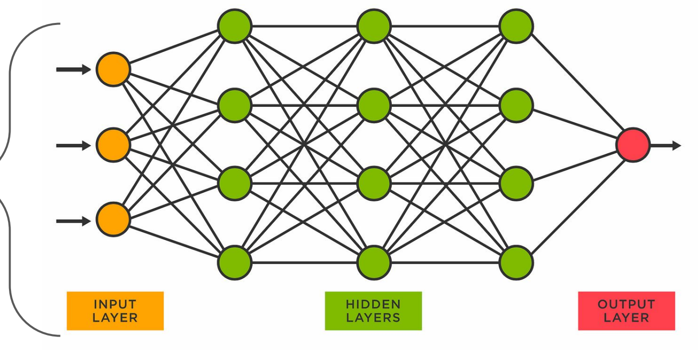


Bayesian Inference methods

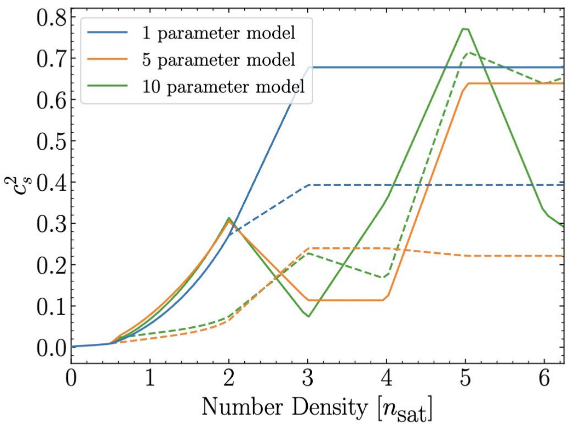
Multilayer Perceptrons for the TOV equations

Multilayer Perceptrons (MLP) are the simplest, dense, feedforward neural networks. We use the method of deep ensembles where we use a set of 100 MLPs

Equation of State parameters



(x100)



Reed, **RS**, et al., arXiv:2405.20558

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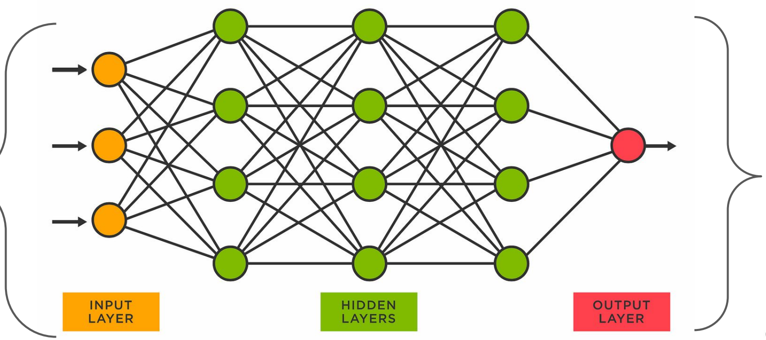
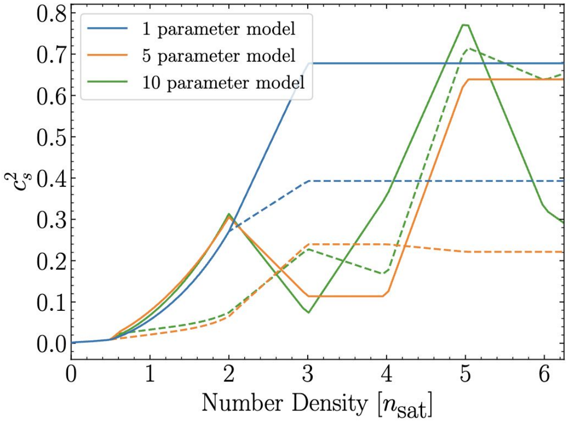
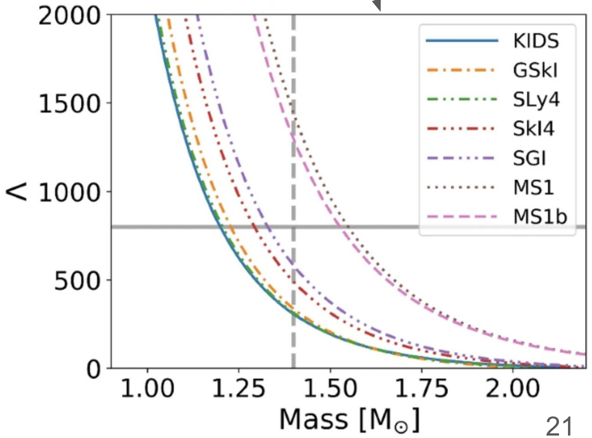


The neutron star tidal deformability

(x100)



We generated 200K samples, randomly split into training and test data



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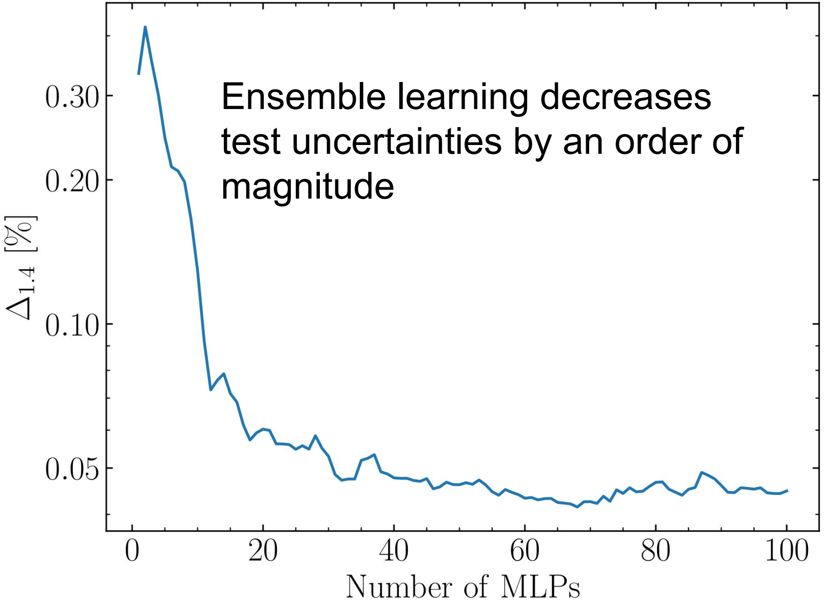
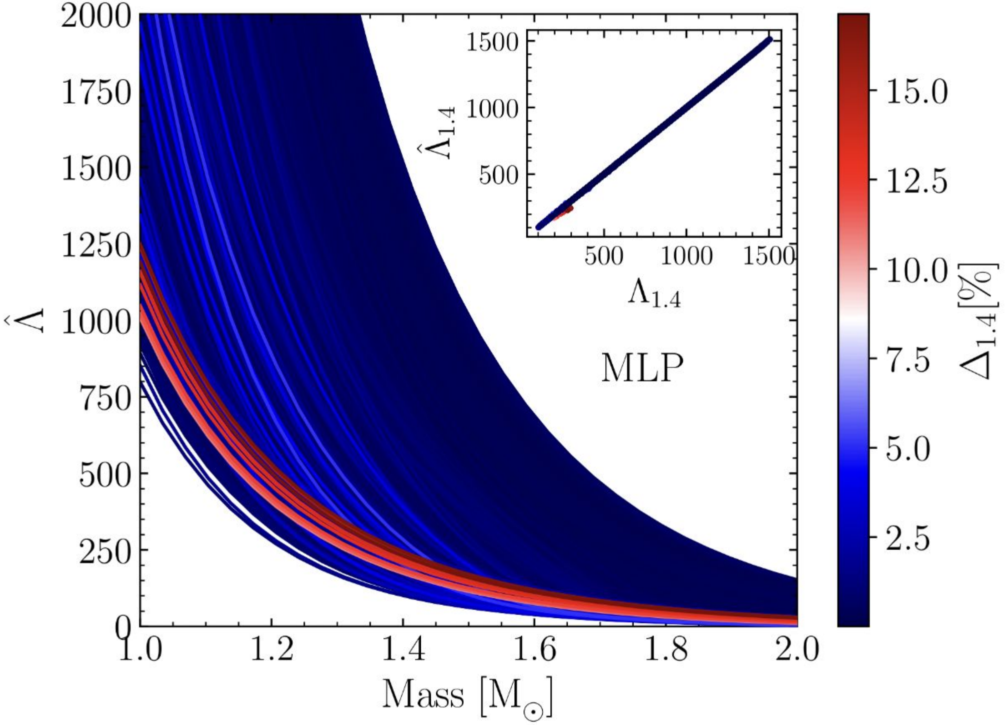


$$\Delta[\%] \equiv \left|\frac{\Lambda - \hat{\Lambda}}{\Lambda}\right| \times 100$$



- Average uncertainty on test samples is 0.04 %
- 0.01% of test samples are outliers (uncertainty > 10%)

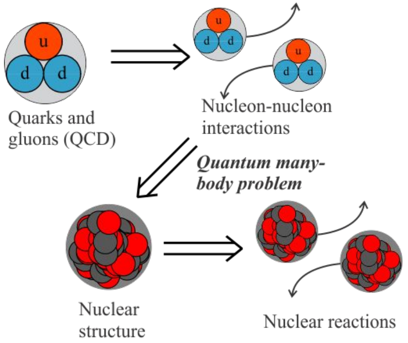
Reed, **RS**, et al., arXiv:2405.20558

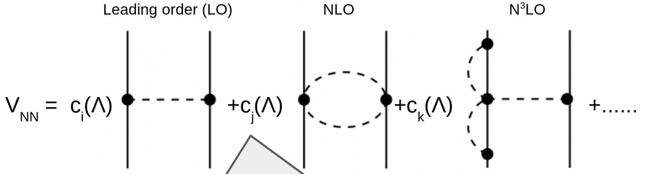
Summary

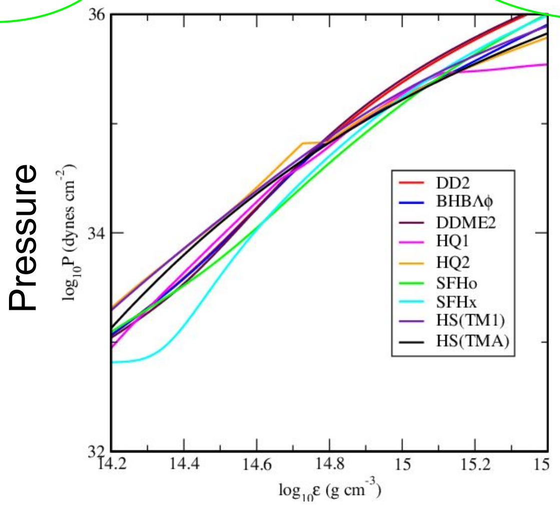
Speed-up factor ~ 10^7
Uncertainty ~ 0.1 %

Speed-up factor ~ 10^3
Uncertainty ~ 0.04 %

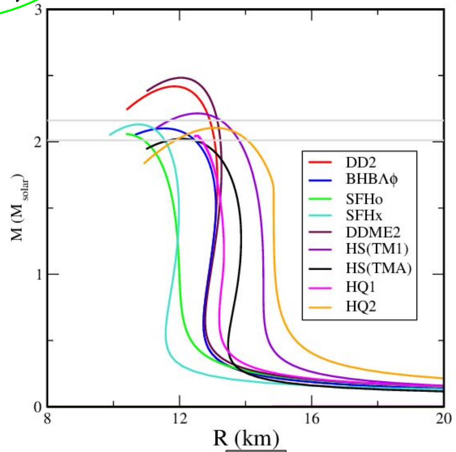
Model for interaction between particles → $H|\psi\rangle = E|\psi\rangle$ → The Equation of State → $G^{\mu\nu} = \kappa T^{\mu\nu}$ → Neutron star observables







(In Progress)



Bayesian Inference methods

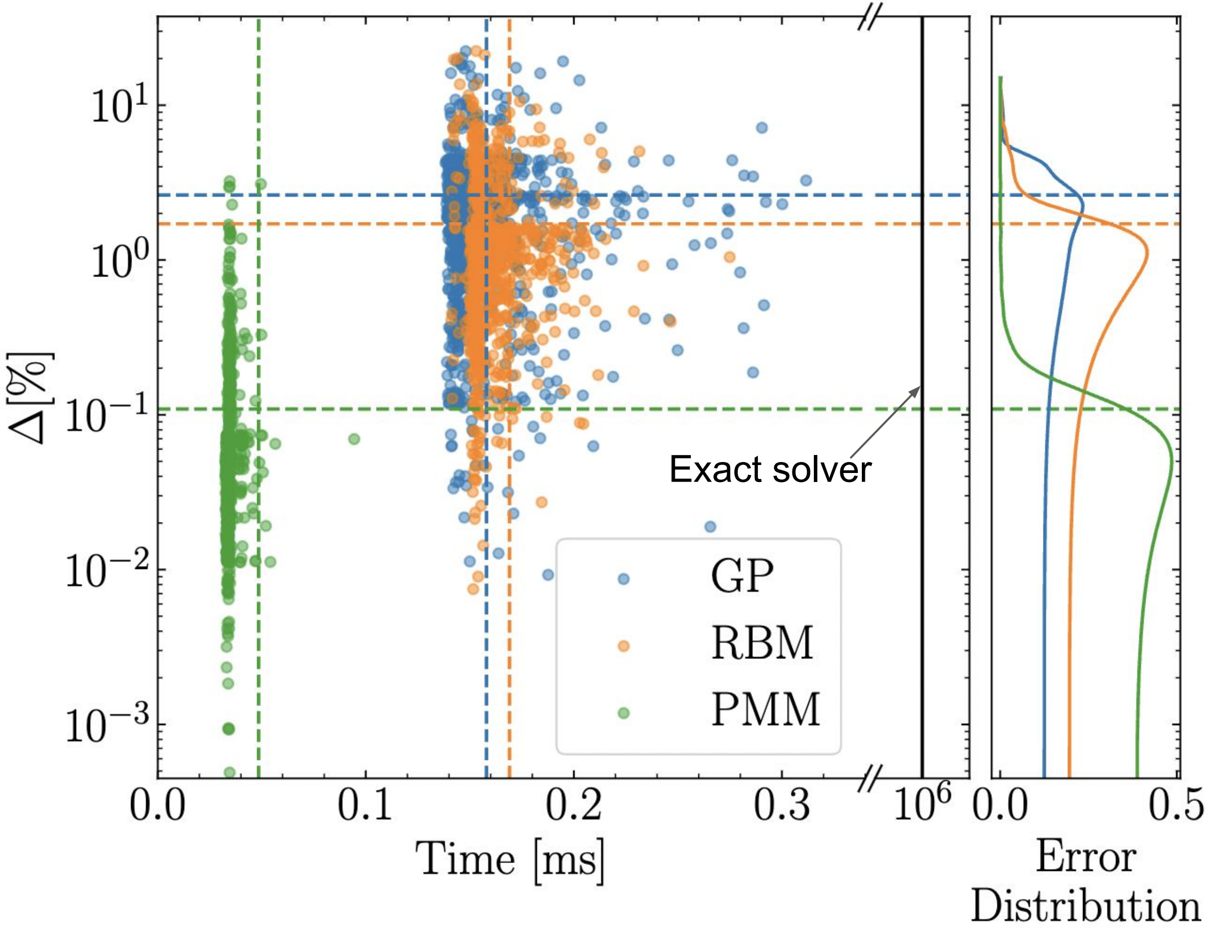
Acknowledgements

Collaborators:
Ingo Tews, Duncan Brown, Achim Schwenk, Stefano Gandolfi, Collin Capano, Soumi De, Cassandra Armstrong, Brendan Reed, Pablo Giuliani, Kyle Godbey, Andrew Deneris

Thank You!

Backup slides

The trade-off between speed and computational accuracy



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The tradeoff between speed and accuracy