Emulators for nuclear physics

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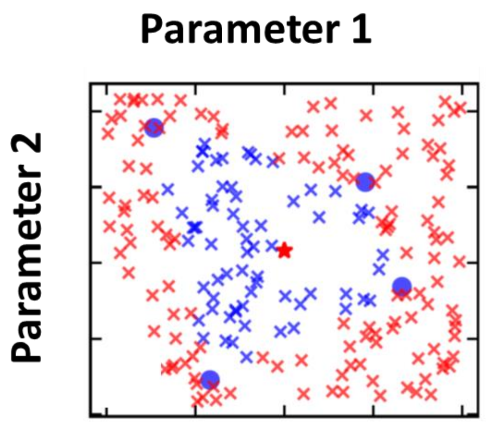
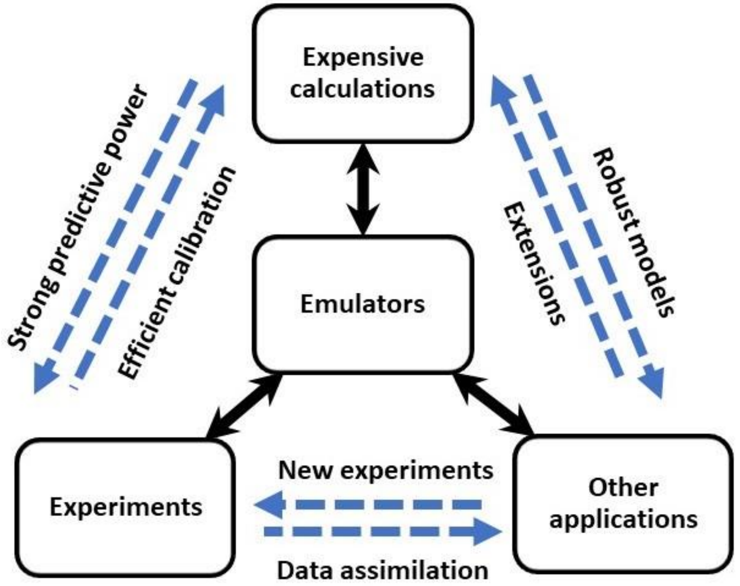
Emulators

D. Frame, et.al., (2018)
S. König, et.al., (2020)

- Fast interpolation and extrapolation of model predictions in its multi-dimensional parameters space
- Accuracy under control: from sub-percent to 10^{-12}
- Data-driven emulators (Gaussian process, artificial neural networks): physics blind
- Model-driven emulators (from the field of model order reduction): physics informed; eigenvector continuation/reduced basis method
- So far as we know, model-driven emulators have better accuracy and extrapolation capabilities
- Ongoing synergies between the two emulation strategies
- Efficient exploration of parameter space: sensitivity analysis, uncertainty quantification (UQ, calibrating chiral interactions, error propagations for large calculations), experimental design…
- Enabling difficult calculations by taking advantage of strong extrapolation capabilities (sign problem, continuum state calculations based on finite basis…)
- Better research workflow: efficiency (very easy to share emulators), closer and new connections between different studies → novel studies; new paradigm for open-access science



For nuclear coupled-cluster structure calculations: "about 1 Million sample in 16-dim space, 20 years calculation → 1 hour on a standard laptop."
A. Ekström and G. Hagen (2019)



Xilin Zhang and R.J. Furnstahl (2022)

Model-driven emulator developments

- The emulators are intrusive: the development requires physics knowledge
- Developed ones:
  - nuclear ground state and low-lying states, transitions
  - two-body realistic scatterings
  - simple three-body scattering

- Many more to be developed in the next decade:
  - realistic three-body continuum states
  - higher-body systems and nuclear matter
  - Emulators for traditional reaction modelings (e.g., CDCC and R-matrix fit)
  - response functions
  - for other problems with large eqn systems
  - emulation UQs
  - Unforeseen ones

- Their applications in nuclear and hadronic physics
- Their implementations in UQs
- Better research workflow
- Collaborations between emulator developers and high-fidelity calculation groups
- Synergy between data-driven and model-driven emulations

An (incomplete) list of works

- Discrete spectrum:
  - Dillon Frame et. al., Phys.Rev.Lett. 121 (2018) 3, 032501 [1711.07090]
  - S. König et. al. , Phys.Lett.B 810 (2020) 135814 [1909.08446]
  - Andreas Ekström and Gaute Hagen, Phys.Rev.Lett. 123 (2019) 25, 252501 [1910.02922]
  - P. Demol et.al., Phys.Rev.C 101 (2020) 4, 041302 [1911.12578]
  - Avik Sarkar and Dean Lee, Phys.Rev.Lett. 126 (2021) 3, 032501 [2004.07651]
  - Sota Yoshida and Noritaka Shimizu, PTEP 2022 (2022) 5, 053D02 [2105.08256]
  - Margarida Companys Franzke et. al., Phys.Lett.B 830 (2022) 137101 [2108.02824]
  - T. Djärv et.al., Phys.Rev.C 105 (2022) 1, 014005 [2108.13313]
  - Pablo Giuliani et. al., [2209.13039]
  - Nuwan Yapa and S. König, Phys.Rev.C 106 (2022) 1, 014309 [2201.08313]
  - Amy L. Anderson et. al., Phys.Rev.C 106 (2022) 3, L031302 [2206.14889]

- Introduction of model order reduction methods (many good references there):
  - J.A. Melendez et. al., J.Phys.G 49 (2022) 10, 102001 [2203.05528]
  - Edgard Bonilla et. al., [2203.05284]

- Continuum states:
  - R.J. Furnstahl et. al., Phys.Lett.B 809 (2020) 135719 [2007.03635]
  - Dong Bai and Zhongzhou Ren, Phys.Rev.C 103 (2021) 1, 014612 [2101.06336]
  - J.A. Melendez et.al., Phys.Lett.B 821 (2021) 136608 [2106.15608]
  - C. Drischler et.al., Phys.Lett.B 823 (2021) 136777 [2108.08269]
  - Xilin Zhang and R.J. Furnstahl, Phys.Rev.C 105 (2022) 6, 064004 [2110.04269]
  - Dong Bai, Phys.Rev.C 106 (2022) 2, 024611