AI/Machine Learning for Extrapolations of No-Core Shell Model Results

James P. Vary, Iowa State University

"Feed-forward ANNs can be viewed as universal non-linear function approximators [Hornik 1989 & 1991]. Moreover, ANNs can find solution when algorithmic methods are computationally intensive or do not exist. For this reason, ANNs are considered a more powerful modeling method for mapping complex nonlinear input-output problems."

"Training/testing data" supplied by ab initio NCSM results obtained on Leadership-Class supercomputers

↓

ANN

↓

Predictions of exact NCSM results in the continuum limit

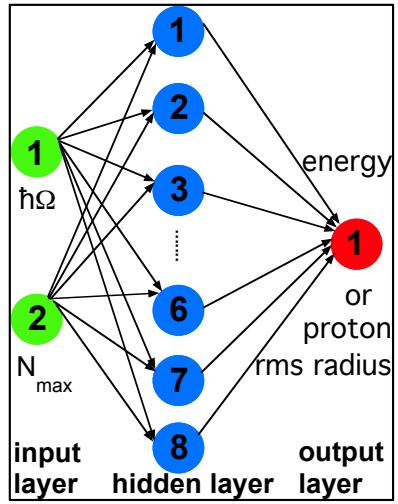
G.A. Negoita, G.R. Luecke, J.P. Vary, P. Maris, A.M. Shirokov, I.J. Shin, Y. Kim, E.G. Ng and C. Yang, in Proceedings of the Ninth International Conference on Computational Logics, Algebras, Programming, Tools, and Benchmarking COMPUTATION TOOLS 2018; arXiv: 1803.03215

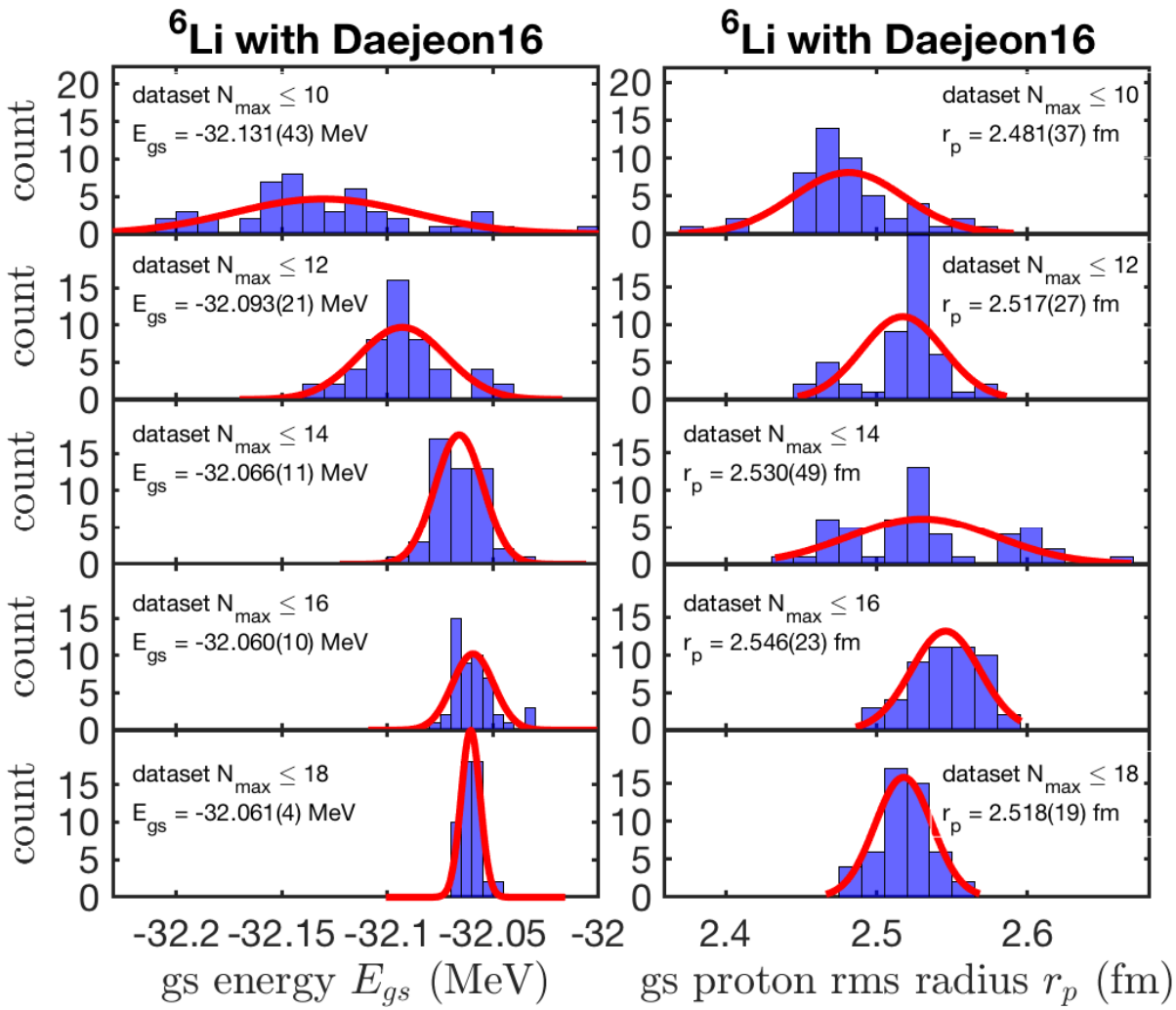
G.A. Negoita, J.P. Vary, G.R. Luecke, P. Maris, A.M. Shirokov, I.J. Shin, Y. Kim, E.G. Ng, C. Yang, M. Lockner and G.M. Prabhu, Phys. Rev. C 99, 054308 (2019); arXiv: 1810.04009

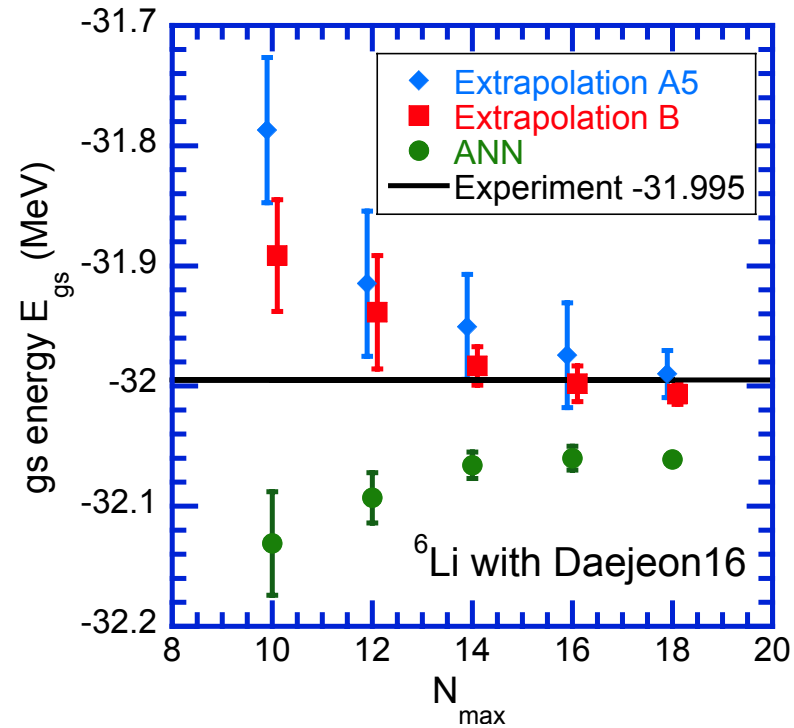
M. Lockner, et al., in preparation

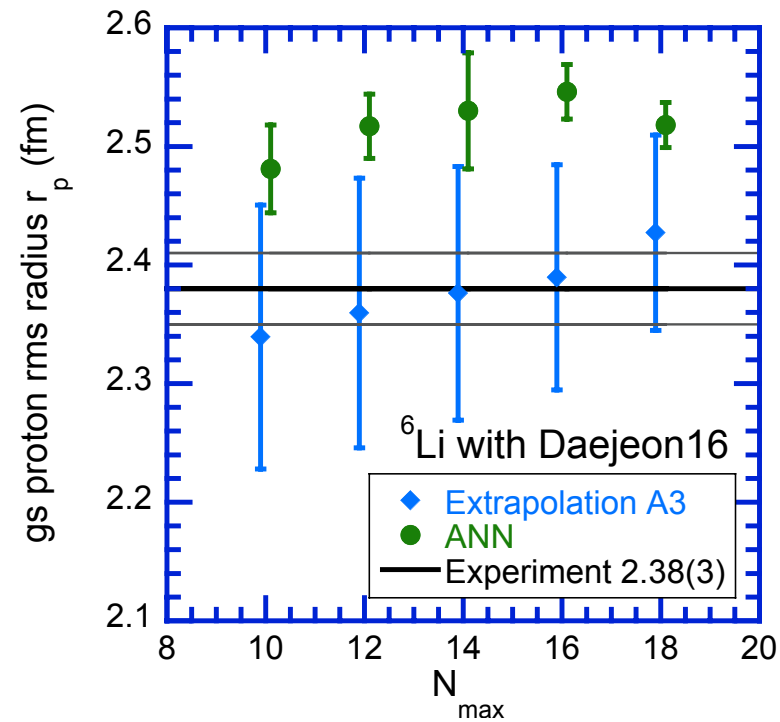
R. McCarty, et al., in preparation

"Deep Learning: Extrapolation Tool for Ab Initio Nuclear Theory," G.A. Negoita, et al., PRC 99, 054308 (2019); arXiv:1810.04009

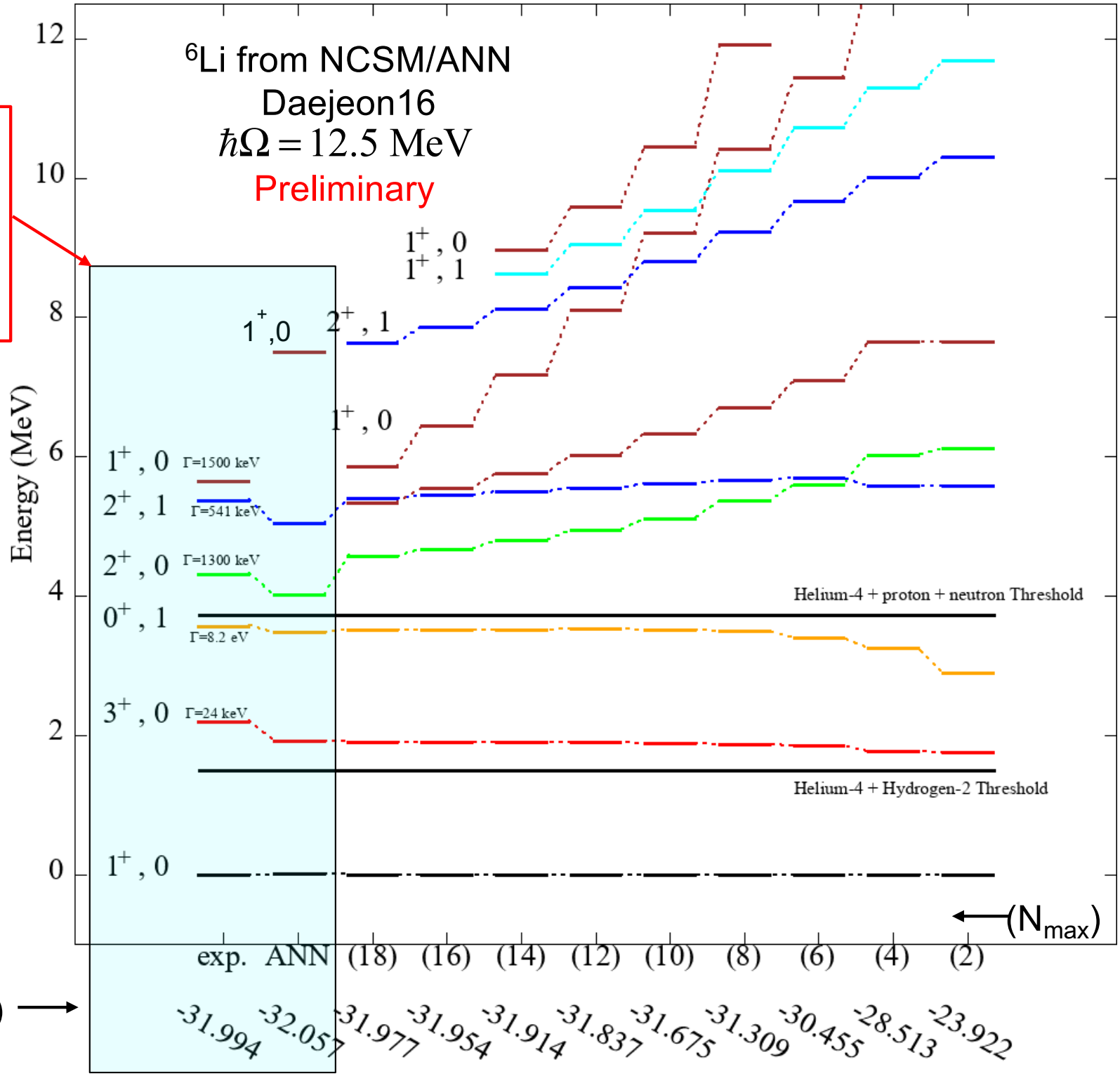




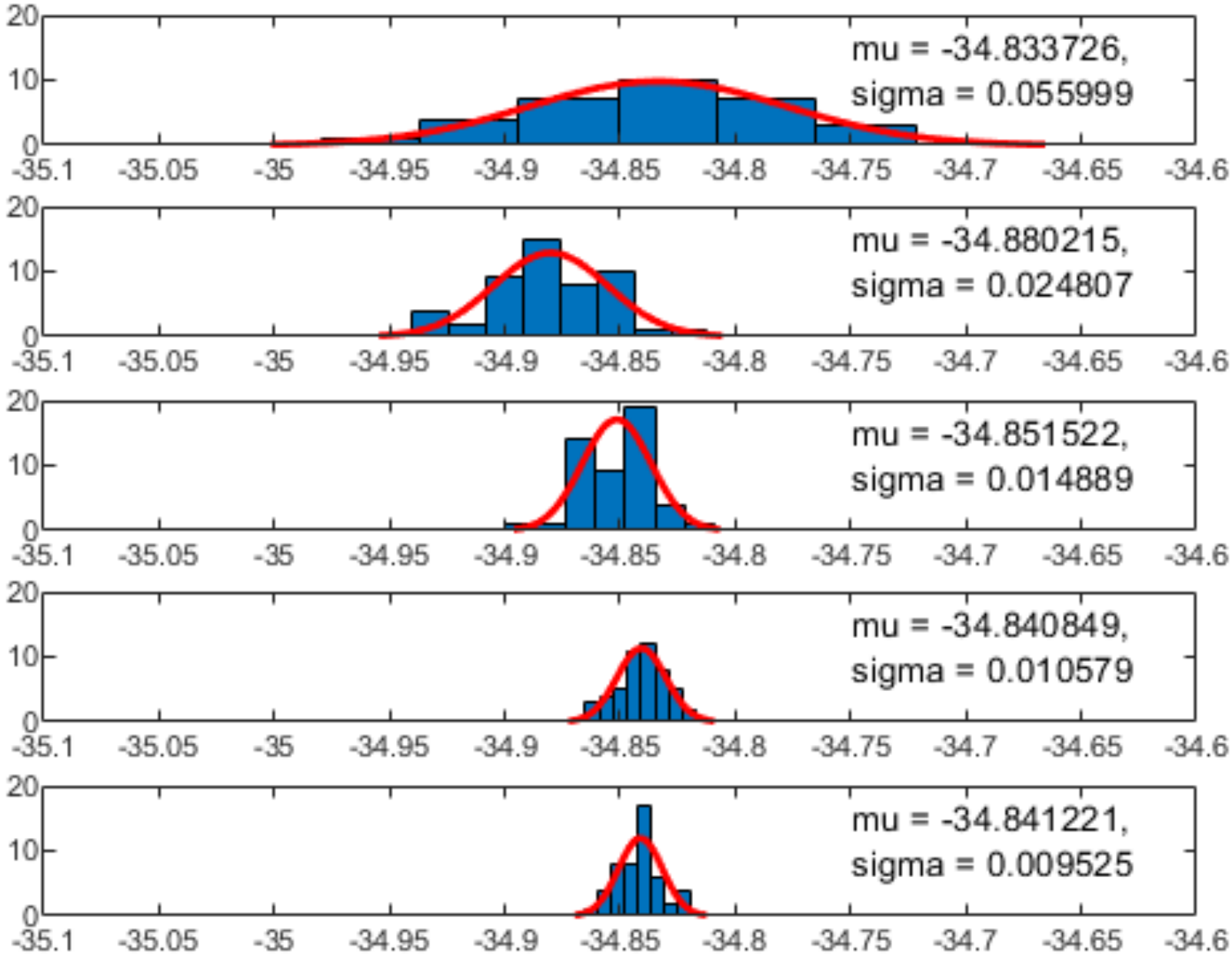




New ANN appl.
to excited states
incl. resonances
R. McCarty, et al.,
in preparation



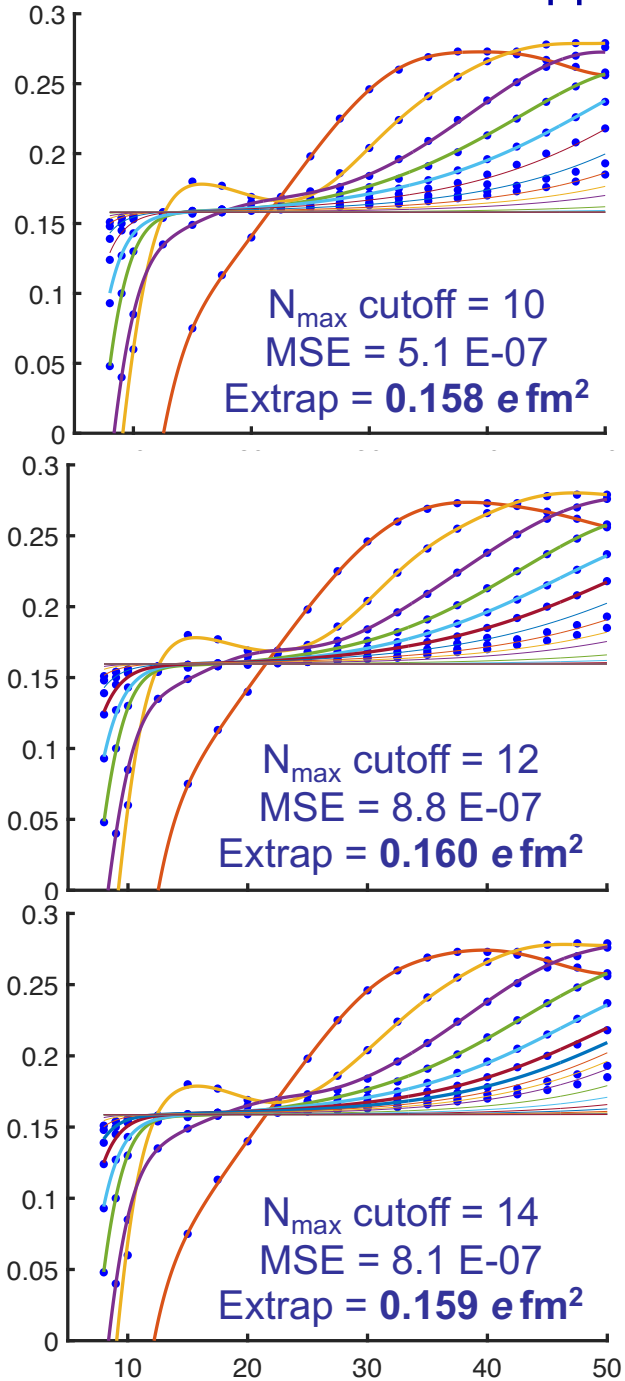
^{7}Li from NCSM/ANN second excited state (7/2$^-$)
Daejeon16, $\hbar\Omega = 12.5$ MeV
Preliminary

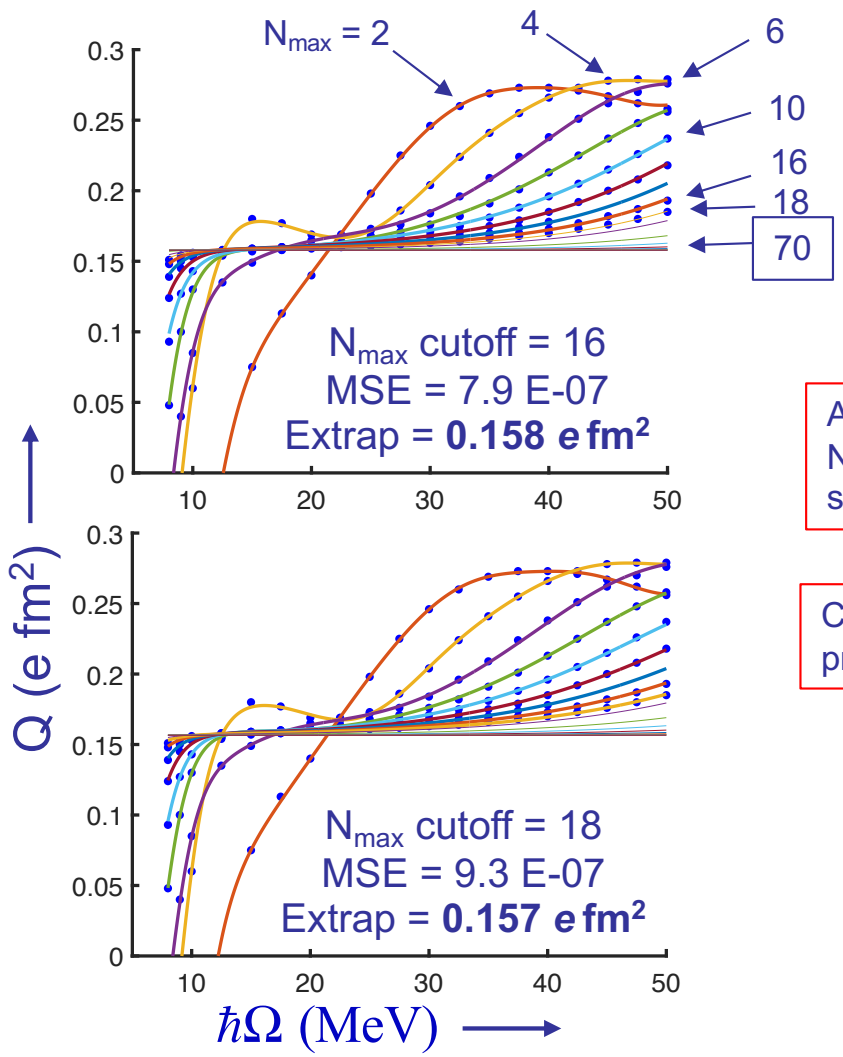


M. Lockner, et al., in preparation

Initial application to the ^{6}Li ground state quadrupole moment

"Best in Class"





ANN predictions for N_{max} = 20, 25, . . . 65, 70 shown in all graphs

Converged sequence of ANN predictions: Q = 0.157(2) *e* fm²

M. Lockner, et al., in preparation

Machine Learning – Issues & Challenges

- **Discovering the best ML approach: a research project in its own right**
- **Opening the black box: from application success to physics insights**
- **Gaining trust in ML results: uncertainty quantification, benchmarking**
- **Quantifying network bias: model studies, multiple approaches - GP vs NN**
- **Sharing "expensive" simulated data sets: a community resource**
- **Limited computational resources: ML-friendly architectures**
- **Trained workforce considerations: career path, sustainability**
- **Sharing experiences: improving exchanges with private sector**

Funding Sources

DOE NP Division

DOE NP/ASCR Divisions (SciDAC/UNEDF SciDAC/NUCLEI)

DOE ASCR Division INCITE Awards on Leadership Class Supercomputers

DOE ASCR Division NERSC Annual Awards