UNCERTAINTY QUANTIFICATION (UQ)

The purpose of this Editorial is to discuss the importance of including uncertainty estimates in papers involving theoretical calculations of physical quantities.

It is not unusual for manuscripts on theoretical work to be submitted without uncertainty estimates for numerical results. In contrast, papers presenting the results of laboratory measurements would usually not be considered acceptable for publication in *Physical Review A* without a detailed discussion of the uncertainties involved in the measurements….

The question is to what extent can the same high standards be applied to papers reporting the results of theoretical calculations…..There are many cases where it is indeed not practical to give a meaningful error estimate for a theoretical calculation….However, there is a broad class of papers where estimates of theoretical uncertainties can and should be made.

Papers presenting the results of theoretical calculations are expected to include uncertainty estimates for the calculations whenever practicable, and especially under the following circumstances:

1. If the authors claim high accuracy, or improvements on the accuracy of previous work.
2. If the primary motivation for the paper is to make comparisons with present or future high precision experimental measurements.
3. If the primary motivation is to provide interpolations or extrapolations of known experimental measurements.

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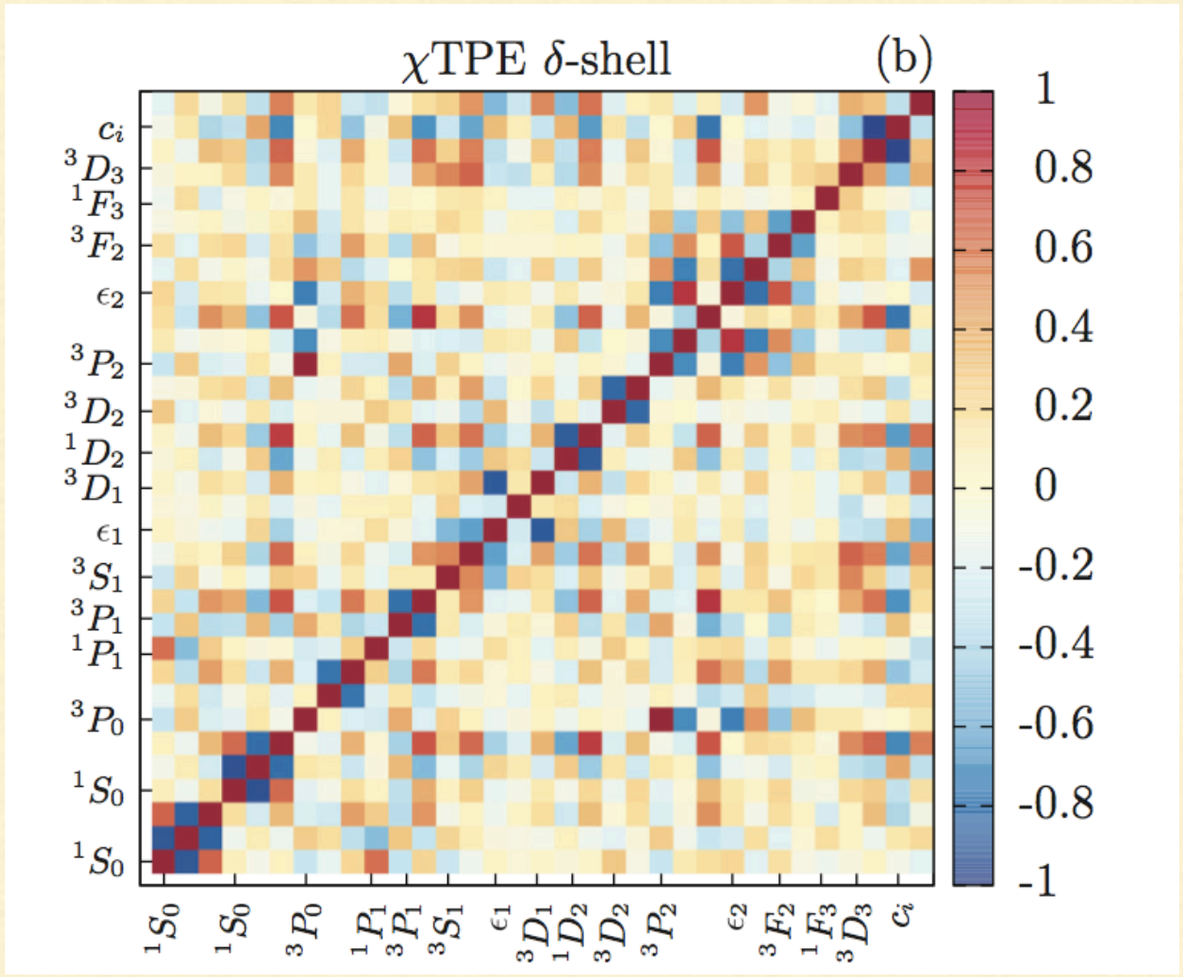
- NUCLEI, JET, TORUS, Lattice QCD for hadrons and light nuclei: confront experiment with precision theory
- Realizing full potential of such efforts requires quantification of theory uncertainties
- These arise from: starting Hamiltonian (H), computational/many-body technique, input parameters in H
- Multiple sources of theory uncertainty that connect to and correlate with one another in complicated ways
- Goal: ability to propagate uncertainties to predictions

EFTS HELP IDENTIFY AND QUANTIFY UNCERTAINTIES

Correlations between short-distance parameters ("LECs") in Chiral NN potential fit to data



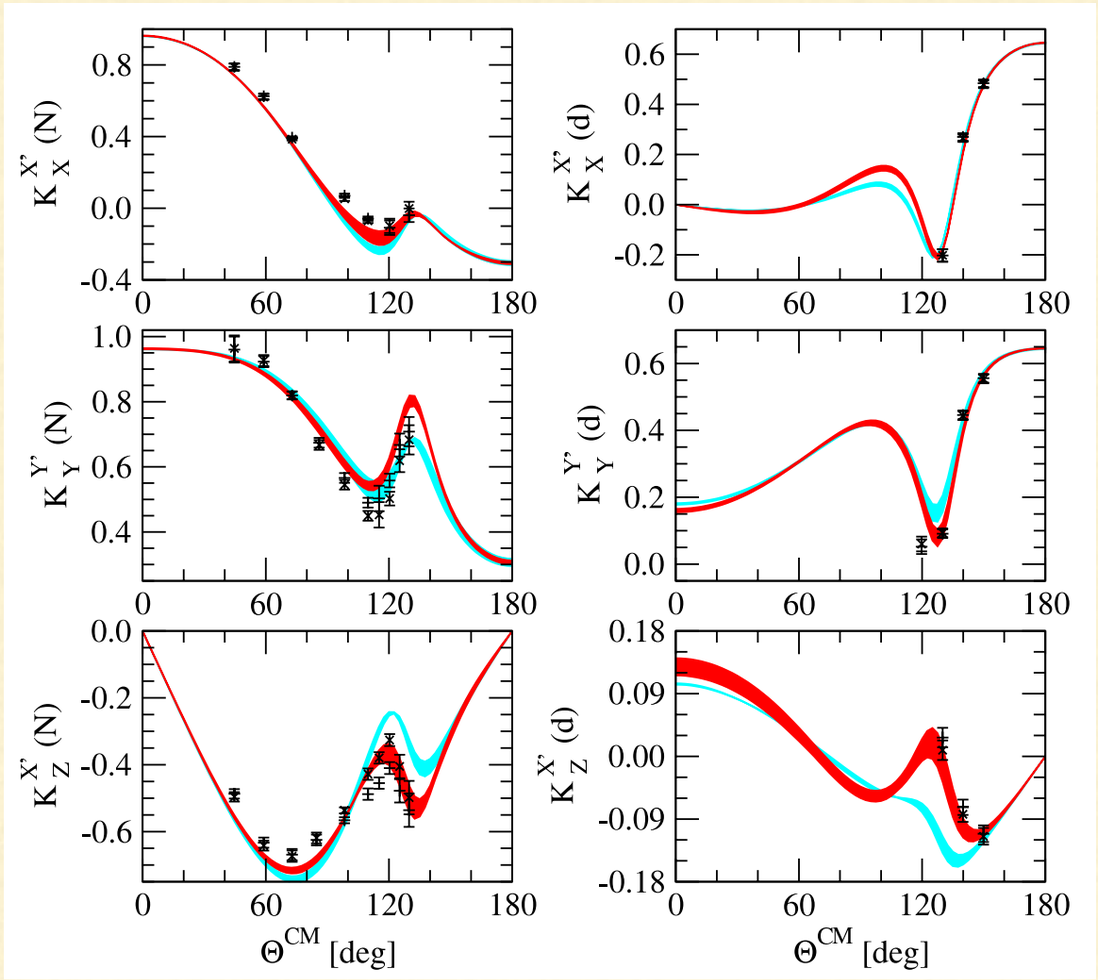
- Chiral NN and 3N potentials now the basis for many *ab initio* calculations
- State-of-the-art computational schemes for optimizing fits (e.g. POUNDERS)
- Can prune input data to obtain a statistical database
- Observed correlations between fitted parameters then propagated to predictions
- Uncertainty estimates due to omitted higher-order terms (still in its infancy)

Ongoing effort to move beyond naive least-squares fits

BUT: SO FAR THEORY UNCERTAINTIES USUALLY ONLY ACCOUNT FOR, AT BEST, ONE OR TWO OUT OF SEVERAL SOURCES

TOWARDS RIGOROUS THEORY UQ

Chiral EFT predictions for p-d spin observables with theory errors from cutoff variation



WHY DO BETTER?

- Goal 1: provide clear guidance on how to extract the EFT parameters
- Goal 2: facilitate tests of whether EFT is working as advertised

Overall: robust guidance regarding new measurements that refine and test the theory

SOME OUTSTANDING ISSUES:

- Analyze systematics of residuals: model selection for EFT testing?
- Bayesian priors + marginalization for higher-order terms? MCMC in high-dimensional space

NEEDS:

- INT program (2016). Topical Collaboration?
- Willingness to learn from, e.g. pQCD, cosmology, …, where similar issues arise
- Agreed-upon standards (a la PRA) for refereeing articles? Grants?

→ **Community commitment to work on these issues, and adopt best practices that emerge from broad discussion**