Contributing to the Reproducibility of R-matrix Data Fits

For SG49

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R-matrix nuclear data fits (as in any model)

- The R-matrix method searches for fits to data by varying:
- R-matrix parameters:
 - R-matrix pole energies
 - Reduced-width amplitudes in each channel for each pole
- Data adjustment parameters:
 - Normalization of experimental data sets (e.g. an EXFOR subentry)
 + Chi-squared contributions if normalizations determined by experiment
 - Energy scaling of experimental data sets (e.g. an EXFOR subentry)
 + Chi-squared contributions if energy scale determined by experiment
 - (or by generalized least squares)
 - Sometimes within a subentry these have their own adjustments: excitation functions for a given scattering ; or angular distributions for a given incident energy
- All these parameters and adjustments are part of the fit & covariance



All parameters and adjustments part of the fit

- All these numerical values should be saved from each search.
 Not just R-matrix parameters
- Then easy to replicate old work, to build on others work, etc.
- Many of us want to save the full covariance matrix of our fits, thus including the correlations between the fitted parameters and the fitted data adjustments.
 - Roberto Capote, for example, is sensitive to any missing correlations in data evaluations. Doro Wiarda wants to save these in SAMMY too.
- So far GNDS or ENDF6 files save only the R-matrix parameters. Full covariances are not yet specifiable in GNDS.
- I am now including the data adjustment information in the computerCodes / inputDecks parts of the GNDS format.
- Should become standard practice.





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