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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