Reliable Monte Carlo Inversion for Isotope Identification

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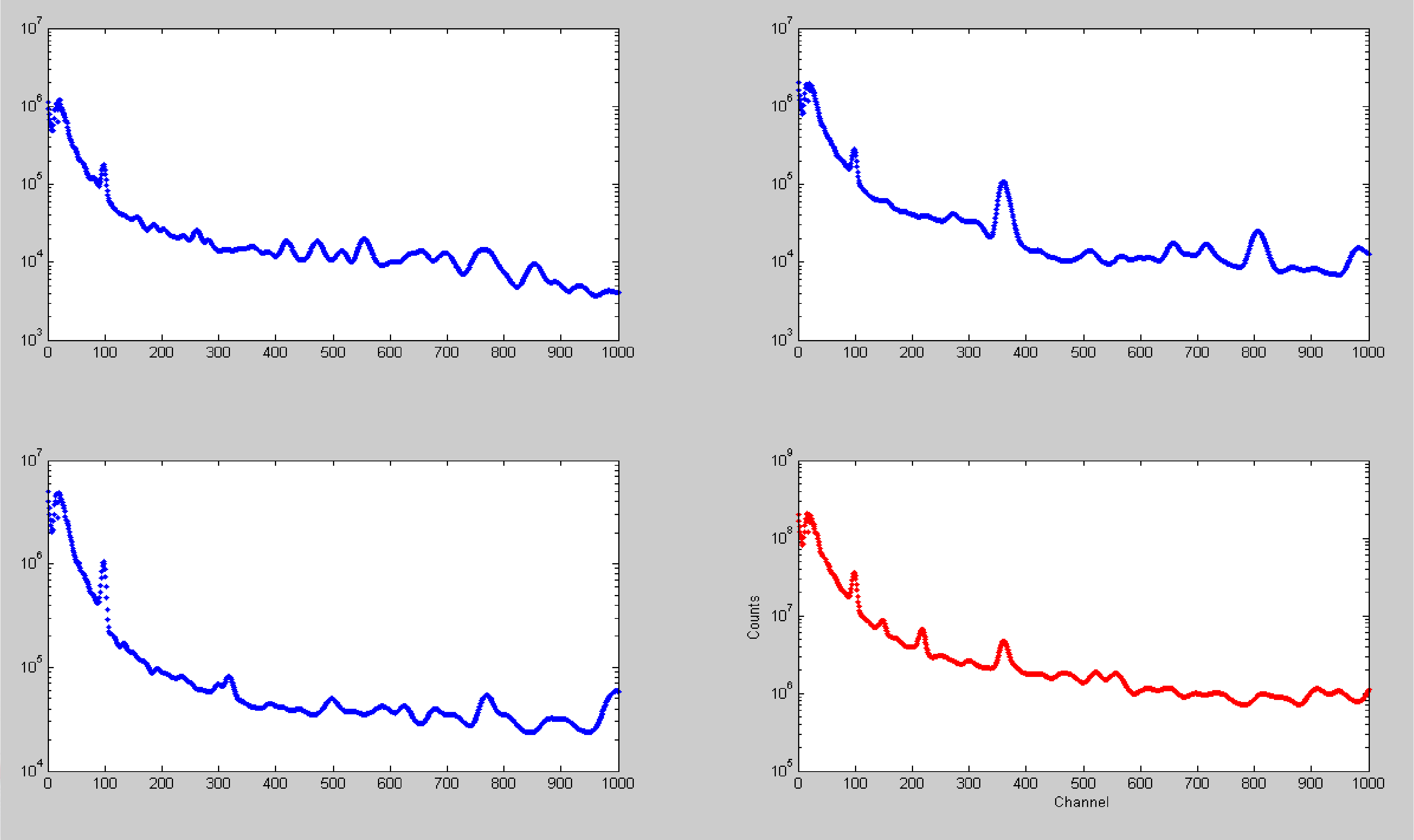
Relevance

- An efficient instrument for isotope identification is important for:
  - Many industrial applications
  - Reducing risk of illegally smuggled nuclear materials (Homeland Security)
    - Differentiate between threat and non-threat sources of radiation
    - Use low-to-intermediate resolution detectors

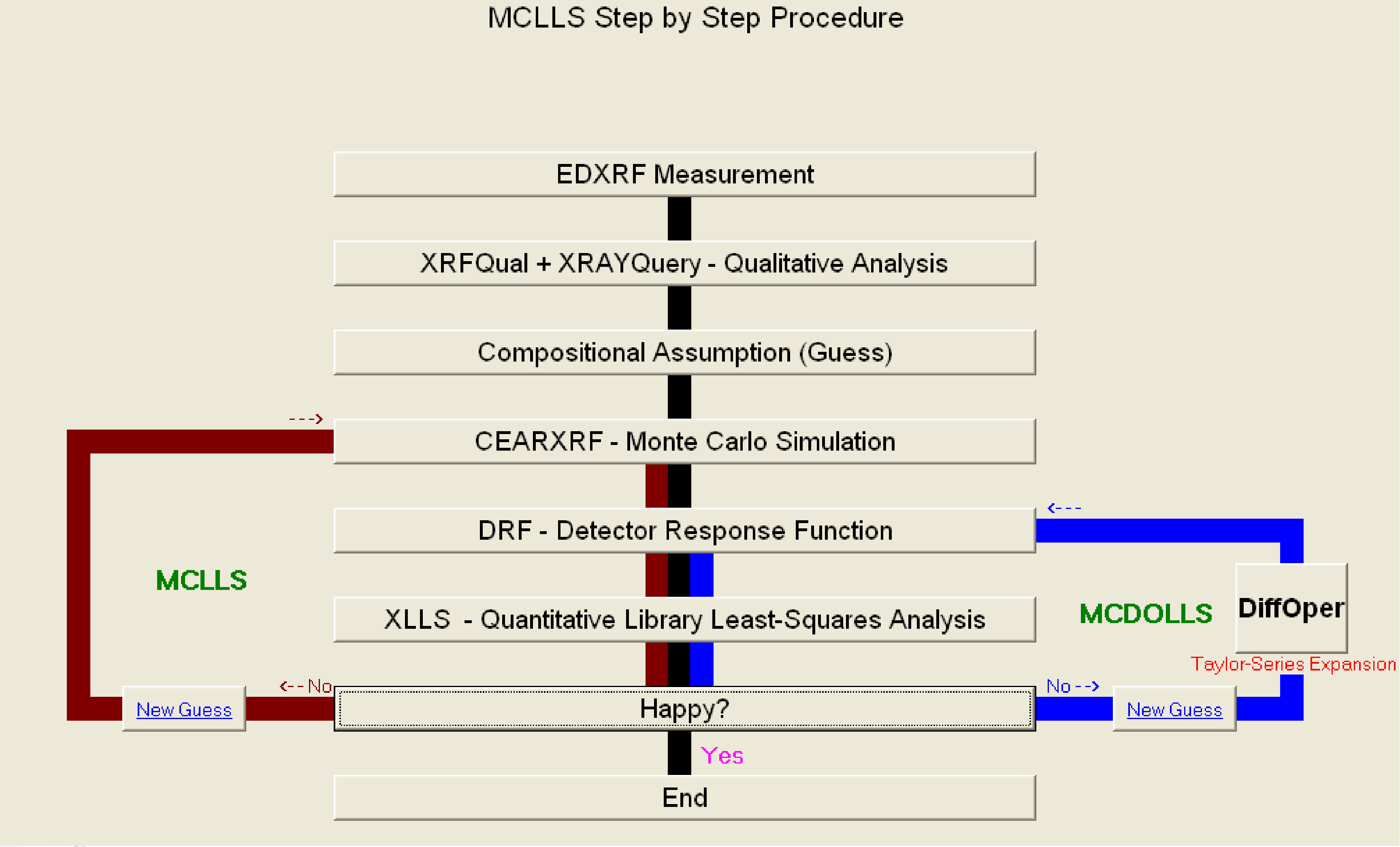
Current Approaches

- Region of Interest Monitoring
  - Specific regions in measured spectrum are monitored for elevated counting rates, e.g. photo peak-based identification
- Template Matching:
  - Entire measured spectrum is compared with pre-calculated library spectra for all identifiable isotopes, e.g. CEAR's library least-squares approach.

Monte Carlo Library Least-Squares (MCLLS)



MCLLS Procedure



Differential Operator

- Retain only first order derivatives

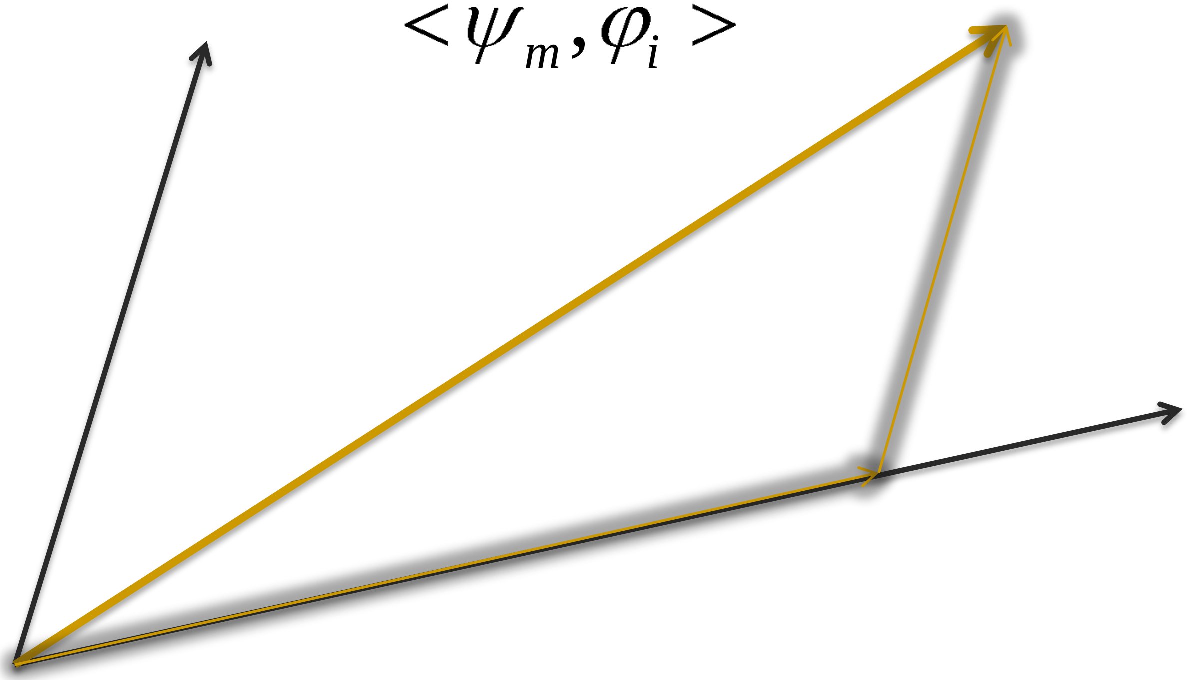
$$\vec{\psi}^{c} = \vec{\psi}_{0}^{c}(\vec{x}_{0}) + \sum_{i=1}^{N} \frac{\partial \psi^{c}}{\partial x_{i}} \quad x_{i} - x_{i0} \quad + \ldots$$

- If linearity assumption appropriate, no need to re-evaluate spectrum
- If moderately nonlinear, need for good initial guess
- If strongly nonlinear, likely will fail

Inversion?

- LS Inversion uses an inner product norm:

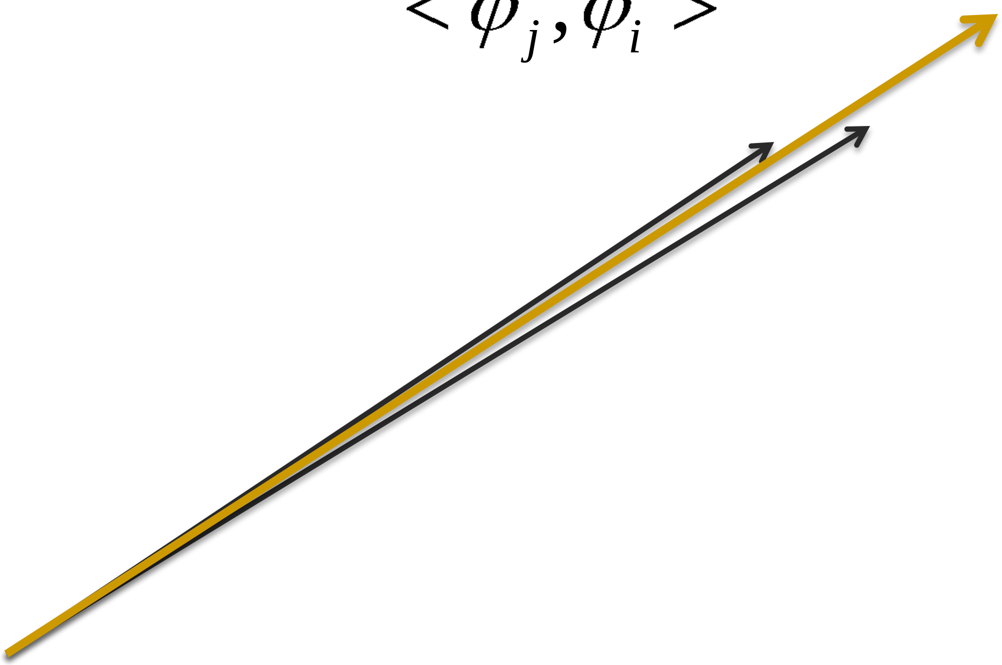
$$<\vec{\Psi}_m, \vec{\varphi}_i>$$



Inversion Challenges?

- When spectra are highly correlated

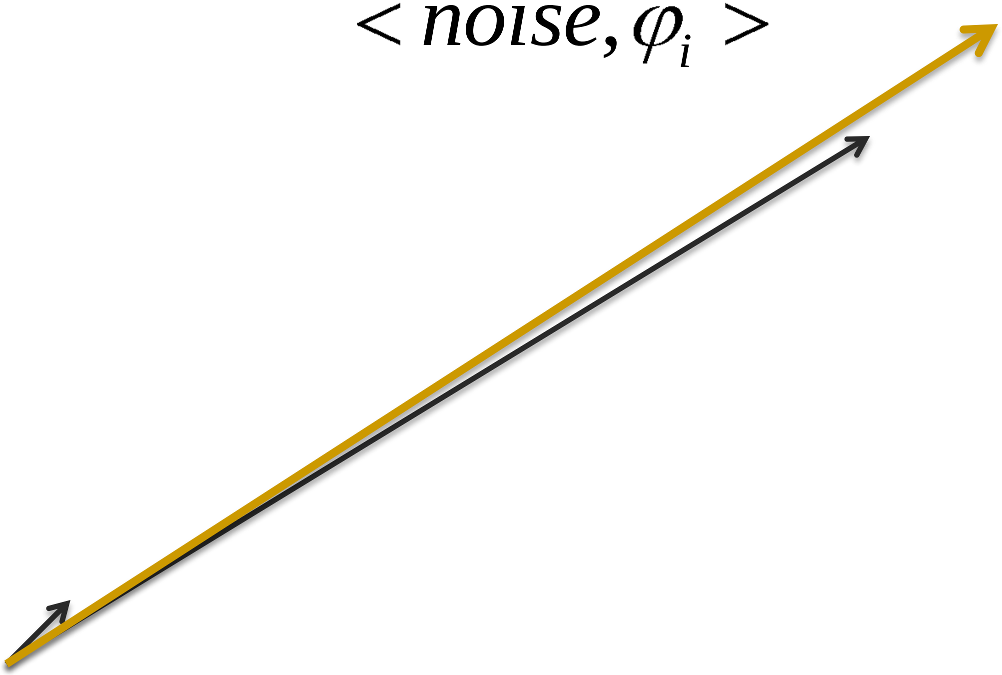
$$< \vec{\varphi}_j , \vec{\varphi}_i >$$



Inversion Challenges (Cont.)

- Or when one spectra overshadows another

$$< noise, \vec{\varphi}_i >$$



Need

- Feature-based identification, with ability to:
  - Identify the locations and widths of as many real peaks as possible.
  - Resolve closely spaced peaks.
  - Use entire spectrum.
  - Quantify trace elemental amounts with comparable accuracy to larger amounts
- Ability to calculate higher order derivatives (efficient sensitivity analysis)
- Ability to evaluate uncertainties due to ENDF cross-sections

1. Wavelet Decomposition

$$\mathbf{W}f(E,s)=\int_{-\infty}^{\infty} f(t)\Psi_{E,s}(t)\,dt$$

$$\Psi_{E,s}(t)=\frac{1}{\sqrt{s}}\Psi\left(\frac{t-E}{s}\right)$$

- Advantage over LS and other Fourier-Type expansions include:
  - identification of location of the peak and its scale

1. Wavelet Decomposition

- Spectral analysis tool initially presented in mid 80s, and have been successfully applied to wide range of engineering problems involving spectra exhibiting periodicity, large oscillatory behavior, and noise
- Recently applied to gamma ray spectroscopy problem for NaI detectors (Sullivan and Garner of LANL 2006-2007)

1. Wavelet-Based DOs

- Generate DOs for signature information obtained from WD
  - Instead of generating DOs for entire spectrum, only evaluate for the wavelet coefficients obtained via WD
  - This can be easily incorporated as a patch on the DRF step.

2. Regularization

- Historically, we noticed that correlations are unavoidable when more and more libraries are incorporated, a filtering technique is therefore required.
- Regularization keeps initial guesses for elemental composition unchanged if not enough information is available in measured spectrum, e.g. *Tikhonov* Regularization

$$\min_{x} \left\| \mathbf{W} \left(\psi^{m} - \psi^{c} \right) \right\|^{2} + \alpha^{2} \left\| x - x_{0} \right\|^{2}$$

3. Sensitivity/Uncertainty

- Considering the sizes of input (cross-sections, compositions, etc.) and output (spectra, fluxes, etc.) data streams involved in MCNP calculations, need for more efficient S/U analyses
- Propose to extend Efficient Subspace Methods developed for Deterministic Calculations to MCNP (Pending US Patent, and currently R&D supported by GEH for BWR applications)