Parallel Computing for Nucleon-Nucleus Scattering

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\( \sigma(n+A \rightarrow X_i) \) at energy \( E_{\text{projectile}} \)

**Computational Workflow**

1. **Target** \( A = (N,Z) \)
2. **UNEDF:** \( V_{NN}, V_{NNN}, \ldots \)
3. **\( V_{\text{eff}} \) for scattering**
4. **Structure Model**
   - Methods: HF, DFT, RPA, CI, CC, ...
   - Ground state
   - Excited states
   - Continuum states
   -\( \{|\alpha\rangle\} \)
5. **Transitions Code**
6. **Folding Code**
7. **Transition Potentials** \( V_{\alpha\alpha'}(r) \)
   - (Later: density-dependent & non-local)
8. **Coupled Channels**
   - Code: \( \text{FRESCO} \)
   - Global optical potentials
   - Elastic S-matrix elements
   - Elastic production
9. **Hauser-Feshbach**
   - \( \text{decays} \)
   - \( \text{chains} \)
   - Delayed emissions
10. **Partial Fusion Theory**
    - \( V_{\text{optical}} \)
    - Elastic production
    - Inelastic production
    - Prompt particle emissions
11. **Compound production**
12. **Deliverables**
    - Residues \( (N',Z') \)
    - Compound emission
    - Preequilibrium emission
    - Global optical potentials
13. **Reaction work here**
14. **SciDAC/2 Project**
15. **KEY:**
   - **Code Modules**
   - UNEDF Ab-initio Input
   - User Inputs/Outputs
   - Exchanged Data
   - Future research
16. **Future research**
Coupled Channels Sets

- Coupled Channels Set
  - For each total spin $J$ and parity $\pi$
  - For each target spin state $I$
  - For partial wave combination $| (ls)j, I, J \pi >$

- Solve coupled second-order differential equations
  - Each $J \pi$ set is independent $\iff$ parallel computations
  - No exchange: local couplings (so far)
  - With exchange and/or transfers: nonlocal couplings (iteration, or basis expansion)
Complexity Estimates

- RPA $^{90}$Zr states up to 10, 30, 60 MeV
  - Core states: # 19, 279, 7216
  - Partial wave sets: # 97, 1281, 43487

- Spreading of RPA states should be tested:
  - Estimate: 30000 core states, 500 000 partial waves
  - Scaling as $N^3$, so now ~ 6 000 000 hours.
Methods and Options

- Coupling matrices take up the space:
  - N*N full matrices for each radius!
  - Need parallel methods for data generation & flow on multi-threaded nodes
- Basis expansion methods, for non-local couplings
  - R-matrix methods have been tested (M functions/channel)
  - NM-square square matrix to solve:
    - Linear equations for single energy, otherwise full diagonalisation needed
    - Conjugate-gradient methods usable for single energy
- Replace N coupled 2nd-order equations by 2N-parameter non-linear search optimisation (suggested recently)
  - Derivatives from reverse-direction adjoint solutions
  - Need best quadratic search methods
  - Find: convergence not also reliable.
- Simplified methods for main contributions
  - Parallel computation of just two-step contributions from ‘doorway states’.