Parallel Computing for Nucleon-Nucleus Scattering

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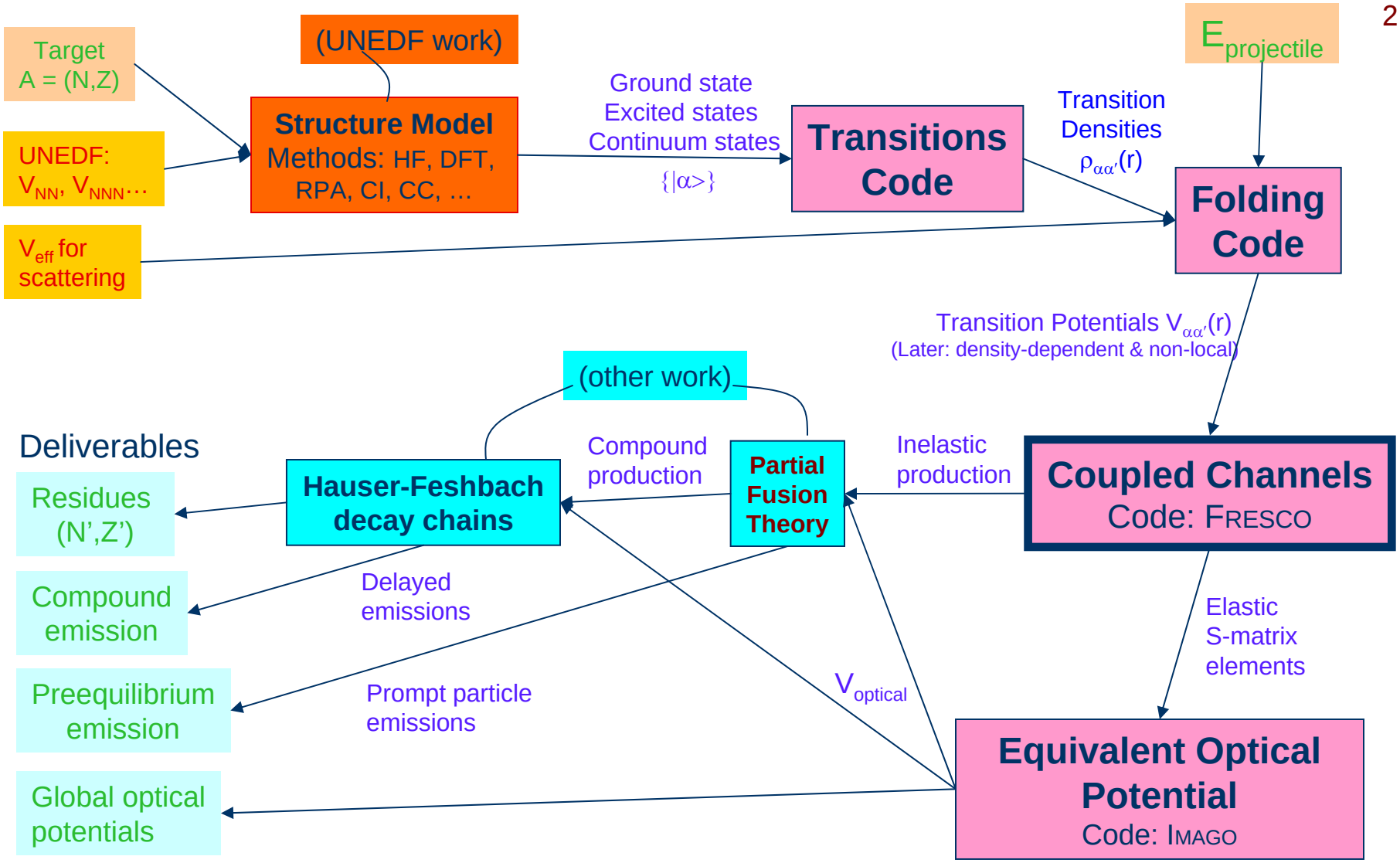

KEY:
Code Modules
UNEDF Ab-initio Input
User Inputs/Outputs
Exchanged Data
Future research

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

Computational Workflow

Reaction work here

SciDAC/2 Project

Coupled Channels Sets

- Coupled Channels Set
  - For each total spin J and parity π
  - For each target spin state I
  - For partial wave combination | (Is)j, I, Jπ >
- Solve coupled second-order differential equations
  - Each Jπ set is independent $\Leftarrow$ 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’.