SciDAC Reaction Theory

Ian Thompson
Part of the UNEDF Strategy

Symmetry restoration
Multi-reference DFT (GCM)
Time dependent DFT (TDHFB)
QRPA

Excited States

Observables
excited states
decays
fission

Compound Nucleus
Reaction Theory

Ground State

Observables
global
properties

Effective Interaction

Expt

Coupled Channels
DWBA

Optical potentials

Expt
cross sections

Nuclear Density
Functional Theory
and Extensions

Ab Initio
Configuration Interaction

Excited
States

Compound Nucleus
Reaction Theory
1: UNEDF project: a national 5-year SciDAC collaboration

Target $A = (N,Z)$

**Structure Models**
- Methods: HF, DFT, RPA, CI, CC, ...
- $V_{NN}$, $V_{NNN}$...
- $V_{\text{eff}}$ for scattering

**Transition Density** [Nobre]
- Ground state
- Excited states
- Continuum states

**Transition Densities**

**Folding** [Escher, Nobre]

**Coupled Channels** [Thompson, Summers]
- Transition Potentials
- Inelastic production
- Optical Potentials [Arbanas]
- Two-step Optical Potential
- Elastic S-matrix elements

**Resonance Averaging** [Arbanas]

**Deliverables**
- Residues $(N',Z')$
- Compound emission
- Preequilibrium emission
- Global optical potentials

**Hauser-Feshbach decay chains** [Ormand]

**Partial Fusion Theory** [Thompson]

**Neutron escape** [Summers, Thompson]

**V_{optical}**

KEY:
- UNEDF Ab-initio Input
- User Inputs/Outputs
- Exchanged Data
- Related research
- UNEDF Reaction Work

Lawrence Livermore National Laboratory
LLNL-PRES-488272

UNEDF Meeting, June 2011
Promised Year-5 Deliverables

- Investigate reactions in light nuclei using NCSM with RGM:
  - Benchmark n-^8^He, and n-^9^Li scattering.
  - Investigate p-^7^Be and ^3^H+^4^He scattering and capture reactions.
  - Use two-, three-, and four-body transition densities for A=3,4 nuclei.
  - Development of three-body transition density calculation for A>4.
- Consistent nucleon-nucleus optical potentials within elastic and all inelastic and transfer.
- Fold QRPA transition densities with density-dependent and spin-orbit forces. Include effective masses, and direct charge-exchange.
- Calculate and investigate effects of exchange nonlocalities.
- Systematic generation of optical potentials for a wide range of near-spherical nuclei.
- First nucleon-nucleus calculations with deformed QRPA transition densities.
- Examine role of optical-potential L-dependences & non-localities in direct reaction calculations.
- Examine energy-dependence of eigensolutions in the expansion for the KKM theory
Delivered in Year-5 up to Q2

Funding Delays:
- LLNL reaction funding cut to 50% for Year-5, but not even that 50% all arrived.
- All received funding used for postdoc (Nobre) up to April 2011 + this meeting.

Deliverables:

Erich Ormand:
- Reactions in light nuclei using NCSM with RGM
  Implemented but not fully researched
- Effective masses for scattering
- Systematic generation of optical potentials for a wide range of near-spherical nuclei.

Spin-off for PhD topic at MSU:
- Examine role of optical-potential L-dependences & non-localities in direct reaction calculations.

Goran Arbanas:
- Examine energy-dependence of eigensolutions in the expansion for the KKM theory
  Not Implemented
- Consistent nucleon-nucleus optical potentials
- Fold QRPA transition densities with density-dependent, spin-orbit forces & charge exchange.
- First nucleon-nucleus calculations with deformed QRPA transition densities.
- Calculate and investigate effects of exchange nonlocalities.
Three Talks on Reaction Theory

Ian Thompson & Gustavo Nobre
- A Microscopic Reaction Model using Energy Density Functionals

Goran Arbanas
- Local Equivalent Potentials
- Statistical Models of Nuclear Reactions

Erich Ormand (for Petr Navratil & Sofia Quaglioni)
- Ab-initio Calculations of Light Ion Reactions:
  - Investigation of $^9$Be scattering & capture reactions
A Microscopic Reaction Model using Energy Density Functionals

Ian Thompson & Gustavo Nobre

PLS Directorate, Physics Division, Nuclear Physics Section

Prepared by LLNL under Contract DE-AC52-07NA27344
Outline of Coupled-Channels Calculations

- Mean-field HFB calculations using SLy4 Skryme functional
- Use (Q)RPA to find all levels $E^*$, with transition densities from the g.s.
- Structure calculations for $n,p + ^{40,48}\text{Ca}, ^{58}\text{Ni}, ^{90}\text{Zr}$ and $^{144}\text{Sm}$
- Fold transition densities with effective n-n interaction: Transition Potentials
- Couple to all excited states, $E^* < 10, 20, 30, 40$ MeV
- Find what fraction of $\sigma_R$ corresponds to inelastic couplings: more states, larger $\sigma_R$, until all open channels are coupled
- Couple to all pickup channels leading to deuteron formation
Inelastic Convergence

- Coupling to more states gives larger effect
- Convergence appears when all open channels are coupled

For reactions with protons as projectile, inelastic convergence is achieved with less couplings due to the Coulomb barrier.

\( \sigma_r / \sigma_{OM} = 38\% \)

\( \sigma_r / \sigma_{OM} = 39\% \)

\( \sigma_r / \sigma_{OM} = 41\% \)
Coupling Between Excited States

- Coupled-channel should (in principle) consider explicitly all possible couplings
- Different transferred angular momenta are possible for the same pair of states:
  \[ |J_i - J_f| \leq L \leq J_i + J_f \]
- Expressions for transition densities are much more complex and time consuming

<table>
<thead>
<tr>
<th></th>
<th># of Transitions (CPU time)</th>
<th>E* &lt; 10 MeV</th>
<th>E* &lt; 20 MeV</th>
<th>E* &lt; 30 MeV</th>
<th>E* &lt; 40 MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>From g.s. only</td>
<td></td>
<td>37 (13.9 s)</td>
<td>217 (26.1 s)</td>
<td>557 (49.7 s)</td>
<td>1037 (83.0 s)</td>
</tr>
<tr>
<td>L_{max} = 2</td>
<td></td>
<td>170 (29.5 s)</td>
<td>4825 (9 min)</td>
<td>28597 (53 min)</td>
<td>95371 (3 h)</td>
</tr>
<tr>
<td>L_{max} = 4</td>
<td></td>
<td>328 (55.0 s)</td>
<td>9774 (23 min)</td>
<td>60479 (2.26 h)</td>
<td>205292 (~ 8h)</td>
</tr>
</tbody>
</table>
Coupling Between Excited States

At not too low energies:

- Individual cross-sections change very little, except for some few states: up to 20%
- Overall sum of reaction over states remains the same
- Supports the concept of "doorway states"

G. P. A. Nobre et al.
Nonelastic Cross Sections for Different Reactions ($E_{\text{lab}} = 30$ MeV)

Inelastic + Transfer with non-orthogonality

Inelastic couplings only

Phenomenological Optical Model

Inelastic and pick-up channels account for all reaction cross sections
Comparison with Experimental Data

\[ p + ^{90}\text{Zr} \]

Total Reaction Cross-sections

- Optical Model
- CC to RPA states up to 10MeV
- CC to RPA states up to 20MeV
- CC to RPA states up to 30MeV
- CC to RPA states up to 40MeV
- CRC to (p,d,p) channel (W^*_{\alpha_{CC}})
- CRC + Non–Orthogonality

Good description of experimental data!

Inelastic and pick-up channels account for all reaction cross sections

Inelastic convergence when coupling up to all open channels
Comparison with Experimental Data

Inelastic and pick-up channels account for all reaction cross sections

Summary of Results at $E_{\text{lab}} = 30$ MeV

**Targets**

$^{40}\text{Ca}$, $^{48}\text{Ca}$, $^{58}\text{Ni}$, $^{90}\text{Zr}$, $^{144}\text{Sm}$

With all couplings, calculations agree with experimental data

$E_{\text{lab}} = 30$ MeV

$r_0 = 1.2$ fm

$\sigma_R/\pi(r_0 A^{1/3})^2$

- neutron as projectile
- proton as projectile

Phenomenological Optical Model
- Inelastic couplings only
- Inelastic + Transfer
- Inelastic + Transfer with non-orthogonality


Elastic Angular Distributions

- Provide complementary information on reaction mechanisms
- Are sensitive to the effective interaction used

![Graphs showing angular distributions](image)

- Density-dependent effective interaction:
  - Resulting coupling potentials improve large-angle behavior, still need improvements for small angles.
  - Work in progress to treat and then test UNEDF Skyrme functionals.

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Our approach predicts a variety of reaction observables.

Data provide constraints on the ingredients.
Promise Year-5-End Deliverables

- Investigate reactions in light nuclei using NCSM with RGM. Some of:
  - Benchmark n-\(^{8}\)He, and n-\(^{9}\)Li scattering.
  - Investigate \(^{3}\)H+\(^{4}\)He scattering and capture reactions.
  - Use two-, three-, and four-body transition densities for A=3,4 nuclei.
  - Development of three-body transition density calculation for A>4.

**LLNL nucleon-nucleus calculations:**

- Determine deuteron optical potentials, including deuteron breakup
- Folding of density-dependent, spin-orbit and charge-exchange forces
- Effects of Skyrmian effective masses in scattering

- **UNC collaboration:** generate & compare deformed-QRPA transition densities (?)
- **Support MSU student** on optical-potential L-dependences & non-localities in direct reaction calculations.

**Arbanas:**

- Examine energy-dependence of eigensolutions in the expansion for the KKM theory