UNEDF and the Optical Potential
Progress and Plans

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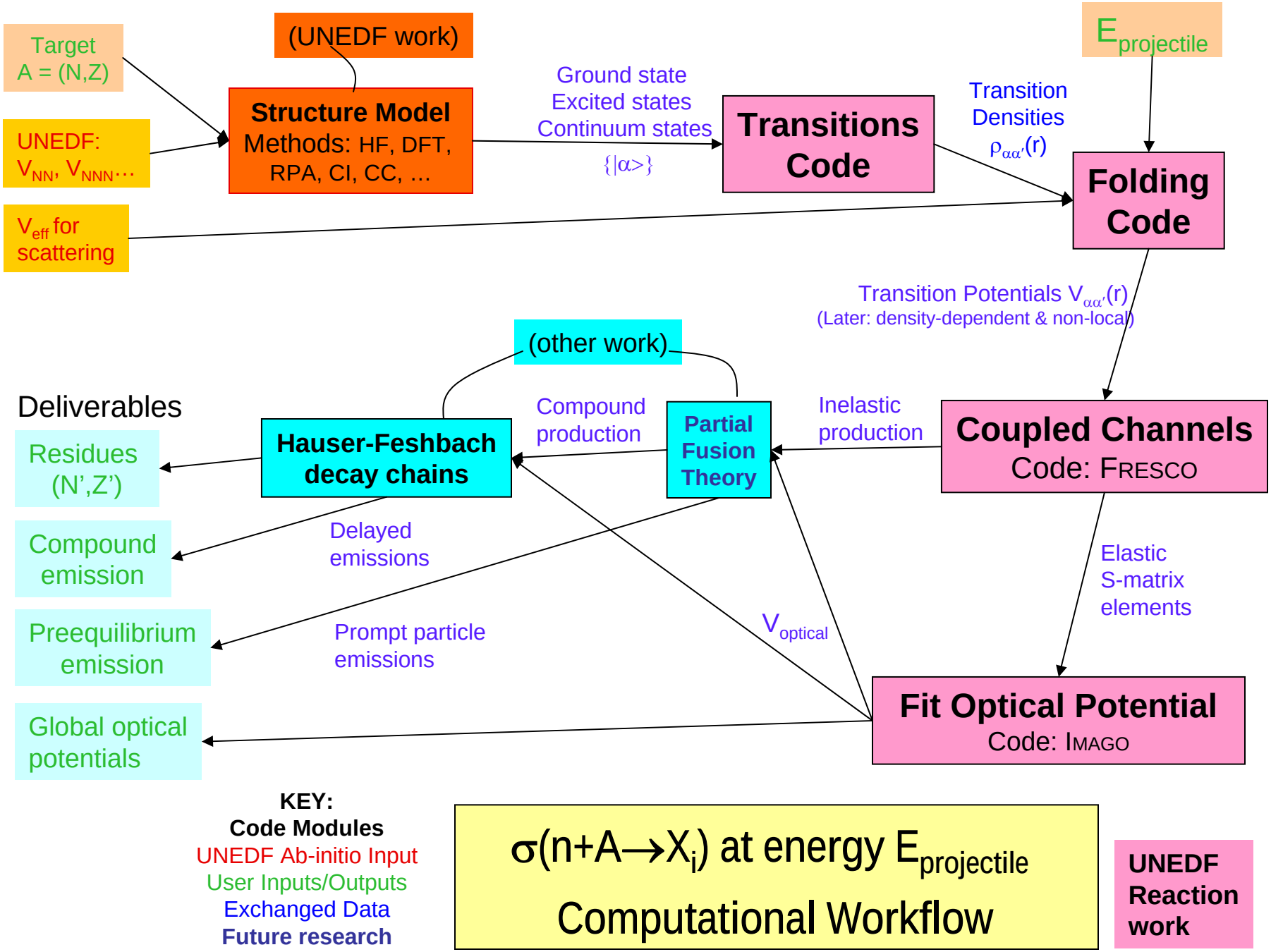
Target
A = (N,Z)
(UNEDF work)
UNEDF:
V_{NN}, V_{NNN}…
Structure Model
Methods: HF, DFT, RPA, CI, CC, …
Ground state
Excited states
Continuum states
{|α>}
Transitions Code
Transition Densities
$\rho_{\alpha\alpha'}(r)$
$E_{projectile}$
Folding Code
V_{eff} for scattering
Transition Potentials $V_{\alpha\alpha'}(r)$
(Later: density-dependent & non-local)
(other work)
Deliverables
Residues (N',Z')
Hauser-Feshbach decay chains
Compound production
Partial Fusion Theory
Inelastic production
Coupled Channels
Code: FRESCO
Compound emission
Delayed emissions
Elastic S-matrix elements
Preequilibrium emission
Prompt particle emissions
$V_{optical}$
Global optical potentials
Fit Optical Potential
Code: IMAGO
KEY:
Code Modules
UNEDF Ab-initio Input
User Inputs/Outputs
Exchanged Data
Future research
σ(n+A→X_i) at energy $E_{projectile}$
Computational Workflow
UNEDF Reaction work

Work Topics in the Last Year

- Gustavo Nobre (since May 08):
  - Energy-dependence of coupled-channels effects when using RPA models for (n,n') inelastic reactions.
- Jutta Escher and Marc Dupuis:
  - Look at significances of energy- and density-dependence of effective interactions
- Ian Thompson:
  - Testing non-linear methods for solving coupled equations

    Result: not competitive yet with usual matrix method; and sometimes fail to converge.
- Goran Arbanas:
  - Extracting Optical Potentials from S-matrix elements
- Marc Dupuis:
  - Using HF and RPA models for (n,n') inelastic reactions on spherical and deformed target.
  - DWBA on parallel computers: use realistic interactions (central, tensor and spin-orbit, density dependant, exact exchange term); huge number of target excited states (10^6 ph excitations ~ 2 hours on 40 processors).

Large Scale Computing in Reaction Theory

- General rule:
  - "Scattering calculation comparable in scale to the structure model used for the excited states"
  - Either need structure model, or invent your own (eg p-h levels)
- For example:
  1. GS density: 1-channel folding for elastic scattering : v. easy.
  2. Collective spectrum: 10 levels CC: done often.
  3. RPA spectrum: ^{90}Zr has 300 levels < 30 MeV, ^{208}Pb:1005 - now.
  4. 2nd-RPA: Expect 10^5 or 10^6 states: next challenge
  5. Real nucleus: ^{90}Zr has ~10^{11} levels up to 30 MeV: No.
- We can still learn from type-3 calculations (RPA)
  - Only ~50% of reaction σ, and undamped oscillations at low energy.
  - Will we be asked to do type-4 scattering (2nd RPA)?

HP Computing Questions:

1. Year-2 plan only started properly in May 2008.
   Now we apply methods to range of energies & nuclei.

2. HPC required for calculations beyond 3000 partial waves in CC set.

3. Computational issues are:
   (a) distributing coupling matrix form factors, or recalculating on the fly;
   (b) sharing the couplings on multi-threaded nodes.
   We believe LLNL has local expertise to help us with these issues.

4. Remaining part of Year-2 and Year-3? -- see next slides
   Could you sketch the work-plan for Years 4 and 5?

5. ”Showcase Physics”? Not in Year 2. Maybe in Year 3, when we
   (a) include all local couplings, and tested transfers.
   (b) have excited state spectrums and wfs from good structure models.

Publications

1. *Compound Nucleus Contributions to the Optical Potential*, I.J. Thompson, F.S. Dietrich, J.E. Escher and M. Dupuis, AIP Conference Series, **1005** (2008) 135
2. *Expressions for Form Factors for Inelastic Scattering and Charge Exchange in Plane-Wave, Distorted-Wave, and Coupled-Channels Reaction Formalisms*, F.S. Dietrich, LLNL report.
3. *Producing a compound nucleus via inelastic scattering: The 90Zr(a,a')90Zr* case, J. Escher and F.S. Dietrich,* LLNL Technical Report LLNL-TR-404300 (2008)
4. *Quantum preequilibrium multistep direct calculations for nucleon scattering on deformed nuclei: a microscopic approach*, Marc Dupuis, Ludovic Bonneau, and Toshihiko Kawano, AIP Conference Series, **1005** (2008) 154

Related:

1. *B(E1) Strengths from Coulomb Excitation of ^{11}Be*, N. C. Summers, S. D. Pain, J. C. Angélique, N. I. Ashwood, V. Bouchat, W. N. Catford, N. M. Clarke, N. Curtis, M. Freer, B. R. Fulton, F. Hanappe, M. Labiche, J. L. Lecouey, R.C. Lemmon, D. Mahboub, A. Ninane, G. Normand, F. M. Nunes, N. Soic, N. A. Orr, L. Stuttge, C. N. Timis, I. J. Thompson, J. S. Winfield and V. Ziman, Phys. Letts. B 650 (2007) 124
2. *Measurement of the Two-Halo Neutron Transfer Reaction ^{1}H(^{11}Li,^{9}Li)^{3}H at 3A MeV*, I. Tanihata, M. Alcorta, D. Bandyopadhyay, R. Bieri, L. Buchmann, B. Davids, N. Galinski, D. Howell, W. Mills, S. Mythili, R. Openshaw, E. Padilla-Rodal, G. Ruprecht, G. Sheffer, A. C. Shotter, M. Trinczek, P. Walden, H. Savajols, T. Roger, M. Caamano, W. Mittig, P. Roussel-Chomaz, R. Kanungo A. Gallant, M. Notani and G. Savard and I.J. Thompson, Phys. Rev. Lett. 100, 192502 (2008)
3. *Compound-Nuclear Reaction Cross Sections from Surrogate Measurements: Status and Challenges*, J. Escher, AIP Conference Proceedings 1005 (2008) 83
4. *Statistical Properties of Kawai-Kerman-McVoy T-matrix*, G. Arbanas, C. Bertulani, D. J. Dean, and A. K. Kerman, J. Escher, AIP Conference Proceedings 1005 (2008) 160

Work Plans for remaining 2008

- Gustavo Nobre and Frank Dietrich:
  - Implement couplings between excited states
  - Density dependence in folding transition densities
- Jutta Escher:
  - How to use DFT functional and mean field, but for scattering:
  - Find scheme for mapping effective interactions from nuclear interior at negative energies to nuclear surface at positive energies
- Ian Thompson and Neil Summers:
  - Plan parallelism for the couplings & wfs, eg for 10^5 eqns.
- Goran Arbanas:
  - Robust extraction of optical potentials
- Marc Dupuis:
  - Evaluation of compound nucleus emission from spherical nuclei
  - Extension of (n,n') calculations to other spherical and deformed targets.
  - Effect of collectivity in (n,n') reactions on deformed nuclei, eg ^{238}U and ^{232}Th.

Work Plans for 2009-

- Gustavo Nobre:
  - Test set of models from UNEDF for range of nuclei.
  - Using theory and programming developments for optical potentials.
- Jutta Escher:
  - Feeding inelastic (n,n') rates into Hauser-Feshbach decay schemes.
  - Extracting (n,2n) cross sections from RPA inelastic rates.
- Ian Thompson and Neil Summers:
  - Implement parallelism for couplings & wfs for eg 10^5 linear equations.
  - Coupled treatment of all ph pre-equilibrium couplings
  - Plan large-scale treatment of couplings to all ph+2p2h states
- Ian Thompson
  - Two-step transfer contributions to optical potential
- Goran Arbanas:
  - Using CC entrance channel wfs for (n,γ) captures
- Marc Dupuis:
  - energy shifts and damping widths from coupling to 2p2h.
  - improved (nn') calculations for deformed target: effect of the rotational bands
  - (n,n') (one-step) calculations with QRPA results

end

Maybe included: will ask

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Related Topics in the Last Year

- Jutta Escher:
  - Using inelastic cross sections for surrogate reactions
- Ian Thompson:
  - Multi-step transfer reactions: ^{11}Li(p,t)
- Ian Thompson and Neil Summers:
  - Breakup of deformed cluster systems: ^{11}Be*
- Goran Arbanas & Carlos Bertulani:
  - Statistical analysis for KKM method.
- Marc Dupuis:
  - Deformed Mean-field models with Gogny & Skryme forces

Related Publications

- *B(E1) Strengths from Coulomb Excitation of ^{11}Be*, N. C. Summers, S. D. Pain, J. C. Angélique, N. I. Ashwood, V. Bouchat, W. N. Catford, N. M. Clarke, N. Curtis, M. Freer, B. R. Fulton, F. Hanappe, M. Labiche, J. L. Lecouey, R.C. Lemmon, D. Mahboub, A. Ninane, G. Normand, F. M. Nunes, N. Soic, N. A. Orr, L. Stuttge, C. N. Timis, I. J. Thompson, J. S. Winfield and V. Ziman, Phys. Letts. B 650 (2007) 124
- *Measurement of the Two-Halo Neutron Transfer Reaction ^{1}H(^{11}Li,^{9}Li)^{3}H at 3A MeV*, I. Tanihata, M. Alcorta, D. Bandyopadhyay, R. Bieri, L. Buchmann, B. Davids, N. Galinski, D. Howell, W. Mills, S. Mythili, R. Openshaw, E. Padilla-Rodal, G. Ruprecht, G. Sheffer, A. C. Shotter, M. Trinczek, P. Walden, H. Savajols, T. Roger, M. Caamano, W. Mittig, P. Roussel-Chomaz, R. Kanungo A. Gallant, M. Notani and G. Savard and I.J. Thompson, Phys. Rev. Lett. 100, 192502 (2008)
- *Compound-Nuclear Reaction Cross Sections from Surrogate Measurements: Status and Challenges*, J. Escher, AIP Conference Proceedings 1005 (2008) 83
- *Statistical Properties of Kawai-Kerman-McVoy T-matrix*, G. Arbanas, C. Bertulani, D. J. Dean, and A. K. Kerman, J. Escher, AIP Conference Proceedings 1005 (2008) 160

Extra Slides

Future Work - Next Steps (Gustavo's list)

- Improve low-energy approach
- Analyze reactions involving ^{208}Pb: More States!
- Add couplings between excited states
- Investigate energy-dependence of off-diagonal potentials
- Investigate density dependence
- Use improved RPA model
- "Second RPA": states built from 2p2h (later years)
- Include couplings to transfer channels (later years)