

UNEDF and the Optical Potential

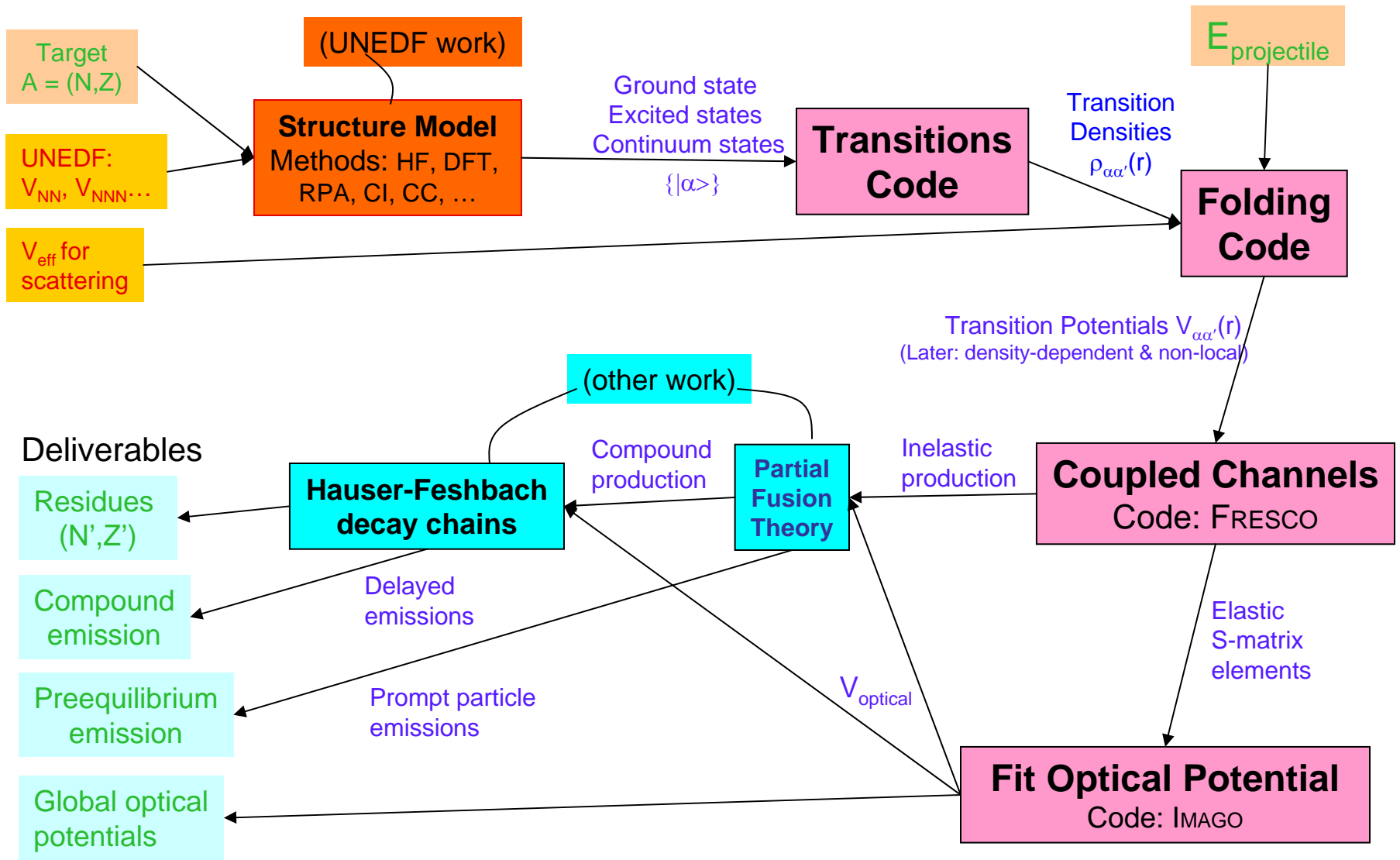
Progress and Plans



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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 $E_{\text{projectile}}$
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 \sim 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 $\sim 10^{11}$ levels up to 30 MeV: **No.**
- We can still learn from type-3 calculations (RPA)
 - Only $\sim 50\%$ 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 $90\text{Zr}(a, a')90\text{Zr}^*$ 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 $^1\text{H}(^{11}\text{Li}, ^9\text{Li})^3\text{H}$ 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



Related Topics in the Last Year

- Jutta Escher:
 - Using inelastic cross sections for surrogate reactions
- Ian Thompson:
 - Multi-step transfer reactions: $^{11}\text{Li}(p,t)$
- Ian Thompson and Neil Summers:
 - Breakup of deformed cluster systems: $^{11}\text{Be}^*$
- 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 $^1\text{H}(^7\text{Li}, ^9\text{Li})^3\text{H}$ 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

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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)