Effective interactions for reaction calculations? A first look at the effect of density dependence

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Nuclear Theory & Modeling Group

UNEDF Reaction Theory

Goal: Replace phenomenological input for reaction calculations by theoretically predicted quantities in order to enable reaction calculations for areas with little/no available systematics.

Strategy:

- Employ state-of-the-art nuclear theory input (e.g. nuclear structure input from DFT)
- Employ large-scale computational resources to minimize/eliminate those inputs that lump together physics that cannot be described properly with traditional tools (e.g.“channels”)

Practical approach:

- Implement a large-scale coupled-channels framework that is able to exploit the available (predicted) nuclear structure input.
- Develop/determine and test the ingredients that cannot be supplied by DFT.

Coupled-channels equations:

$$\left\{E - E_c^{\mathrm{ex}} + \frac{\hbar^2}{2\mu_c}\frac{d^2}{dr^2} - \frac{l_c(l_c+1)\hbar^2}{2\mu_c r^2} - V_{cc}^{\mathcal{J}}(r)\right\} u_c(r) = \sum_{c' \neq c} V_{cc'}^{\mathcal{J}}(r)\, u_{c'}(r),$$

The coupling potentials $V_{cc}^{J}(r)$ contain information on the structure of the target nucleus and on the effective NN interaction between the projectile (nucleon) and target nucleons, via terms of the type:

$$\frac{2}{\pi}\int_0^\infty dq\, q^2\, j_L(qr)\, v^{ST}(q)\, \rho_{LSJ}^{Tq,\mathrm{fi}}(q)$$

Transition densities for target states, obtained from a nuclear-structure calculation based on DFT results.

Effective NN interaction between a particle in the continuum and a nucleon in the target - to be determined!

Which effective interaction?

Coupling potentials require folding of effective interaction with transition densities (in r or q space):

$$\frac{2}{\pi}\int_0^\infty dq\, q^2\, j_L(qr)\, v^{ST}(q)\, \rho_{LSJ}^{Tq,\,\mathrm{fi}}(q)$$

It is not obvious which effective interaction to use for calculating the coupling potentials…..

Some of these issues have been considered in the context of the OMP….

….for the diagonal term.

The OMP is the potential the reproduces the observed elastic scattering cross section when used in a one-channel model.

Questions:

- **Which effective interaction?**
- **Should we use the same that was employed for the structure calculation?**
- **How do we account for the fact that one of the interacting particles is in the continuum?**
- **How do we connect with a Skyrme functional?**
- **Does it matter which (fitted) interaction we use?**
- **If so, can we identify constraints for selecting a good effective interaction?**

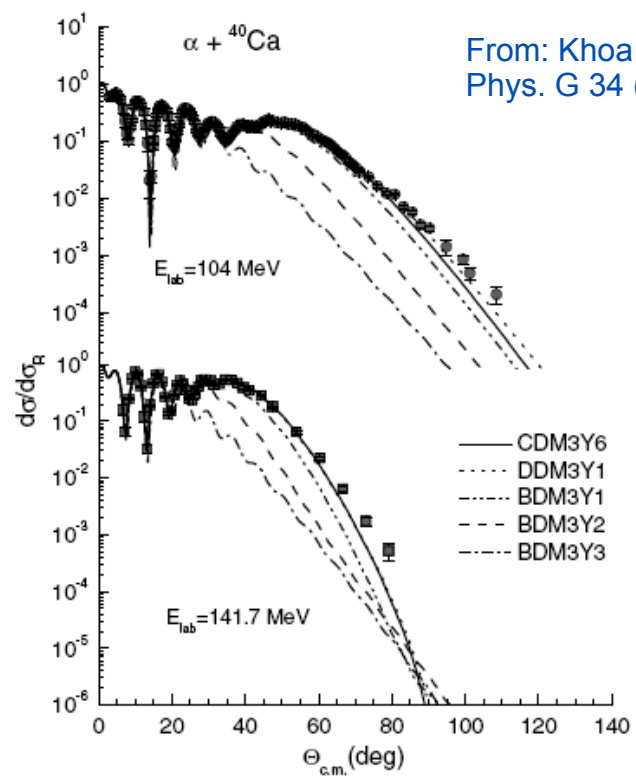
Which effective interaction? Insights from OMPs

Prior considerations in the context of the "standard" OMP:

- Single- and double-folding approach commonly used to determine the real portion of an optical potential for standard reaction calculations.
- **Density dependence** is important for describing inelastic α-nucleus scattering.
- **Energy dependence**: Phenomenological OMPs have been extrapolated to the E<0 region to calculate bound single-particle states.

These issues have NOT been studied in the context of coupled-channels calculations that explicitly include a very large number of channels.

OMP description of elastic scattering with OMPs obtained from folding with effective interactions with different density dependencies



Density dependence of the effective interaction

Constructing diagonal coupling potentials from effective interactions with/without density dependence:

- Effective nucleon-nucleon interaction:

$$V(E,\rho,r) = F(\rho)\, v(r)$$

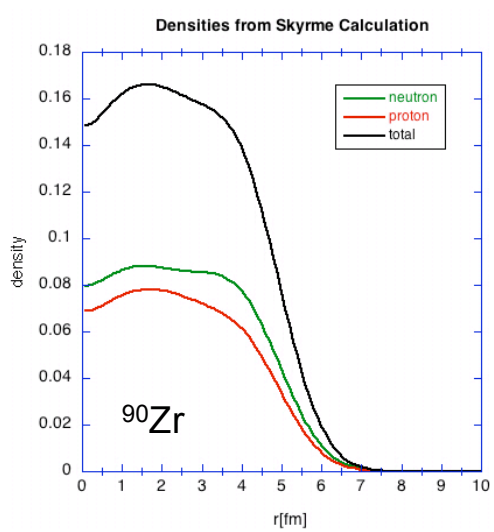
Where v is a M3Y interaction

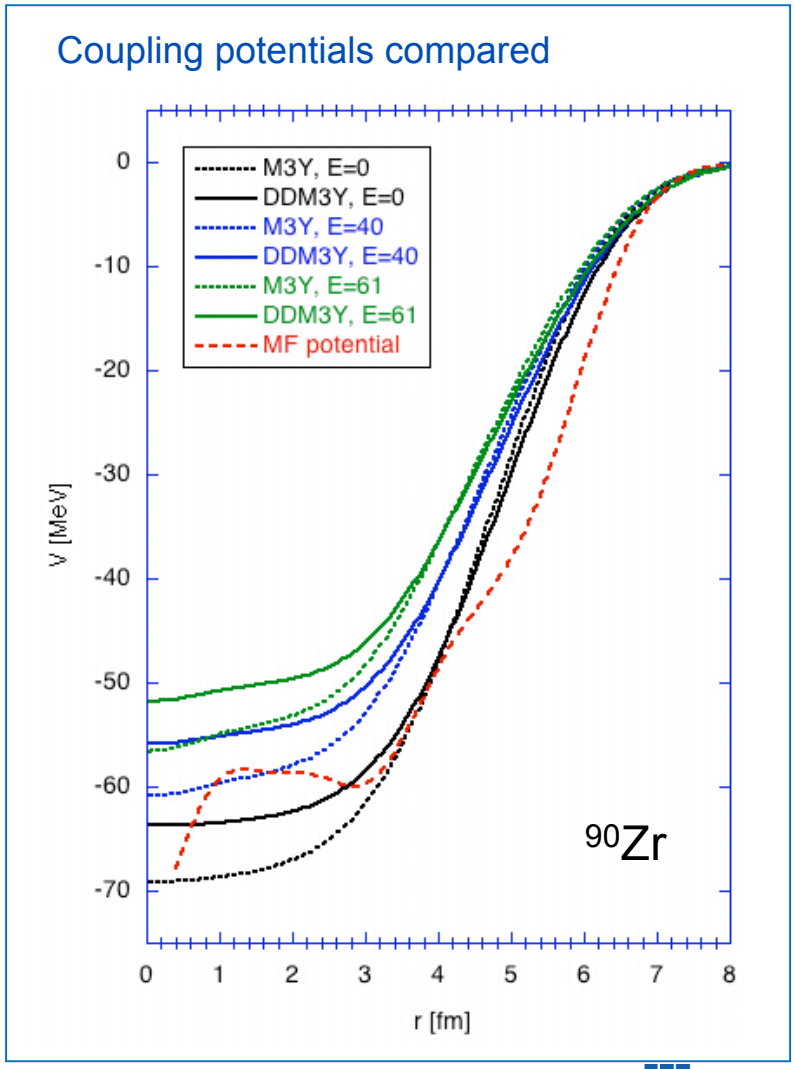
$v(r) = \Sigma_{i=1..3}\, G_i \exp(-\mu_i r)/(\mu_i r) + J_{00}$

$F(\rho) = C(1 + \alpha \exp(-\beta\rho))$

$J_{00} = -G_\delta(1-0.0005E/A)$

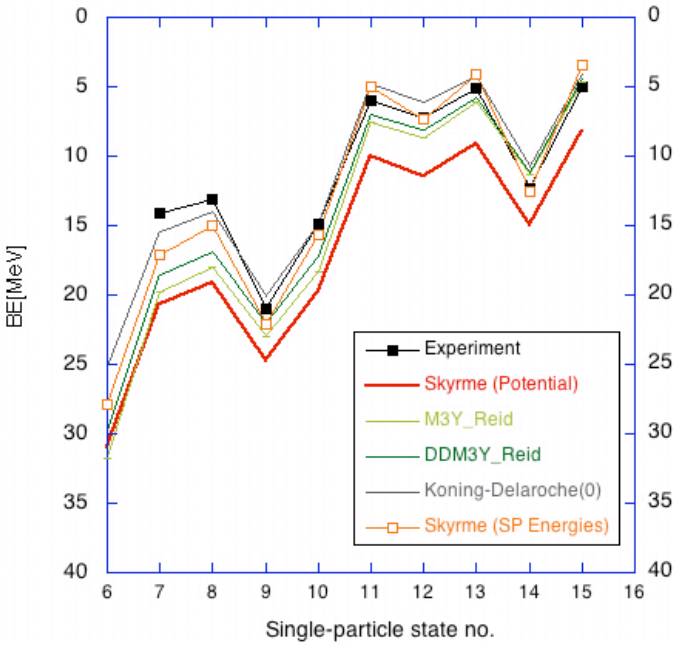
- Density from a Skyrme (SkM*) HF calculation

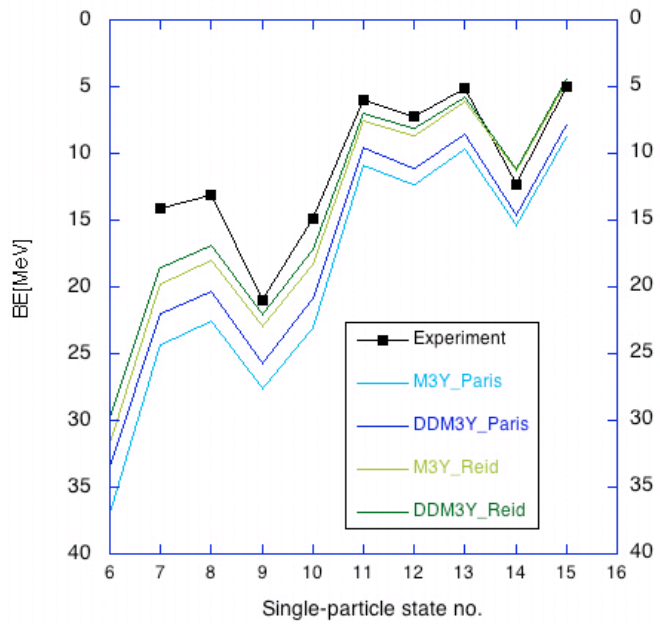




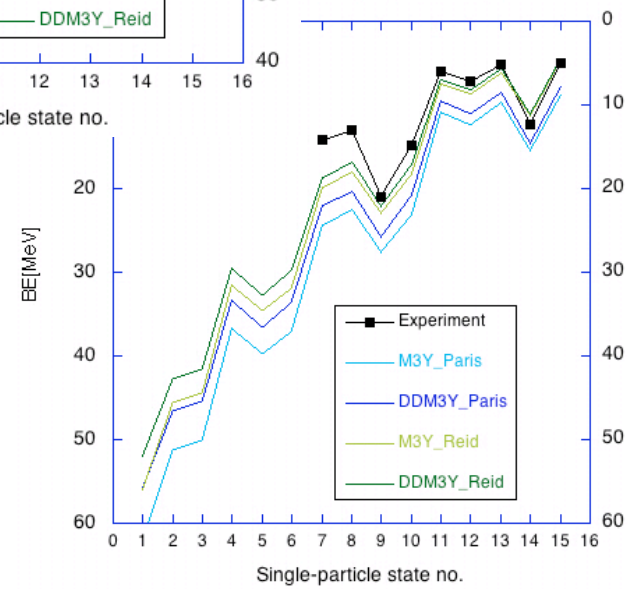
Constraints from single-particle energies?

Neutron single-particle states in ^{90}Zr





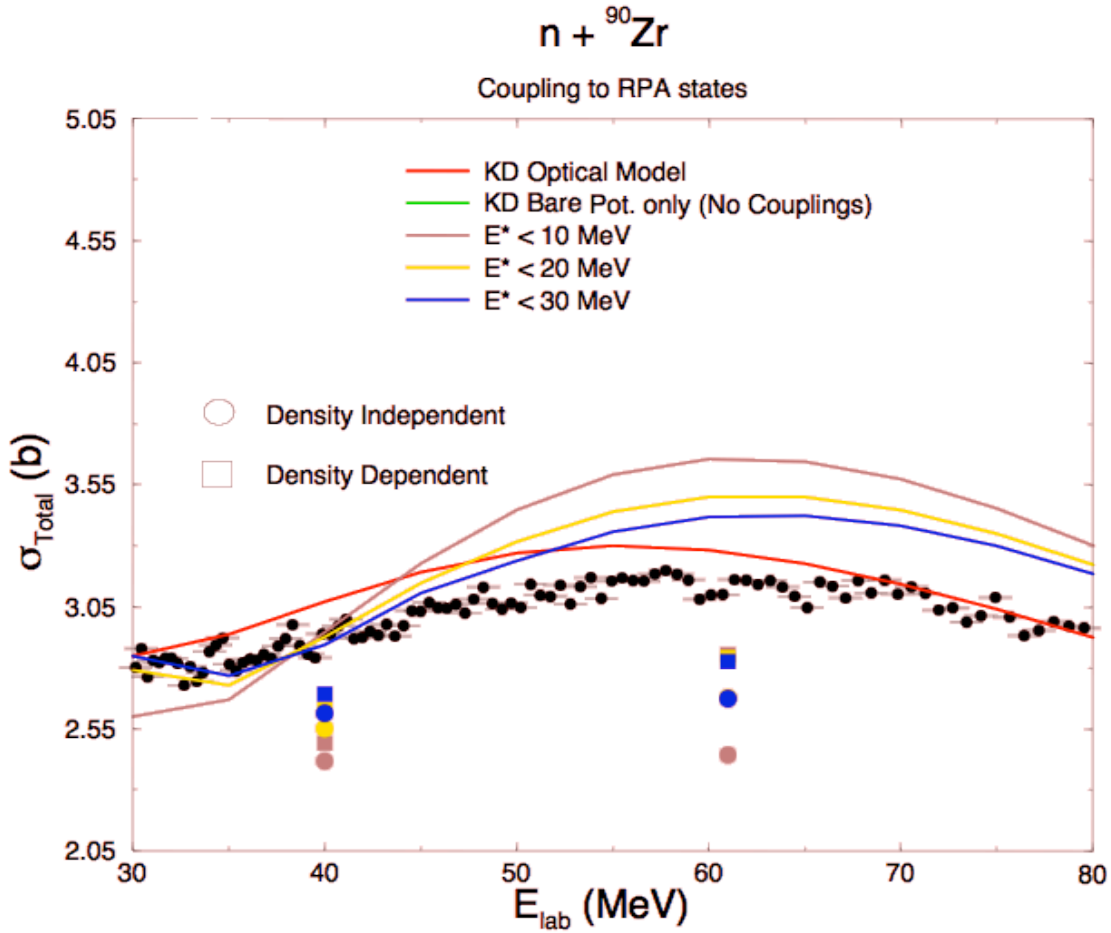
The folded (diagonal) coupling potential can be used to predict single-particle energies for bound orbitals. These can be compared to data and to DFT results.



Effects on coupled-channels results

Coupled-channels calculation of reaction cross section for n+^{90}Zr, employing different effective interactions in the diagonal coupling potential.

-> Results for density-dependent interaction improve agreement with data.



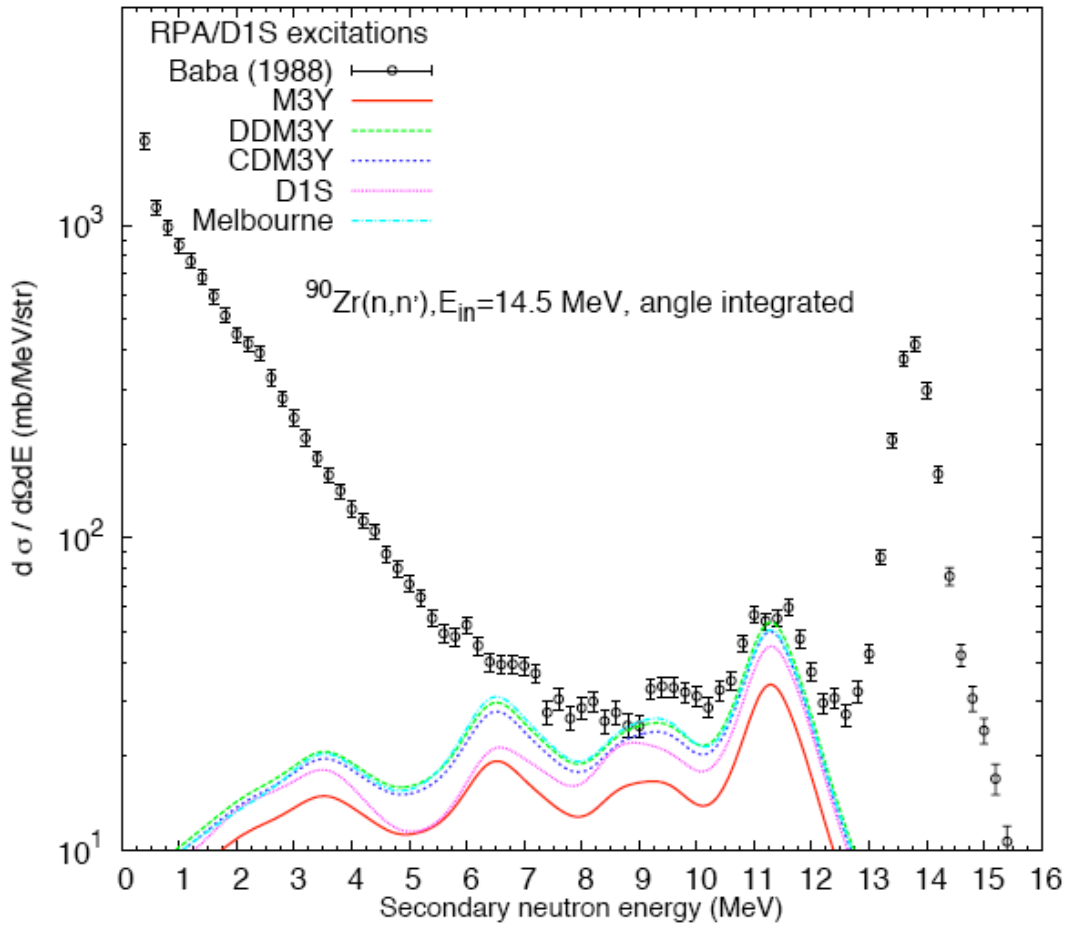
See also G. Nobre's presentation.

Effect on DWBA inelastic scattering results

DWBA calculation of inelastic n scattering cross section, employing different effective interactions in the (off-diagonal) transition potentials

-> Illustrates the impact of not having a definite prescription for selecting an effective interaction.

See also M. Dupuis' presentation.



Plan for Year 2 and Year 3

Determine effective interaction appropriate for reaction calculations

- Implement folding procedure for various candidate effective interactions (M3Y, DDM3Y, CDM3Yx, Gogny, Gogny at ρ=0, others) — Done for select cases. Others to be considered.
- Calculate the diagonal (c=c') potential and investigate effects of varying the effective forces with special emphasis on density and energy dependence — Started.
- Devise tests to constrain the coupling potentials and thus the effective interactions: — Started. Needs to be expanded.
  - Single-particle energies for the diagonal potential
  - Energy-dependence must satisfy the dispersion relation
  - Positions of doorway resonances, etc.
- Determine sensitivity of cross sections to choice of effective interaction — Started.
- Draw conclusions about the possibility of moving from an effective interaction for bound states to an interactions valid for positive energies — To be done.
- Recommend interaction(s) for reaction calculations (all couplings). — To be done.

APPENDIX

Effective nucleon-nucleon interaction

Effective nucleon-nucleon interaction - M3Y with ρ-dependence

$$V(E,\rho,r) = g(E)\, F(\rho)\, v(r)$$

where

$$v(r) = \Sigma_{i=1..3}\, G_i \exp(-\mu_i r)/(\mu_i r) + J_{00}$$

$$F(\rho) = C(1 + \alpha \exp(-\beta\rho) - \gamma\rho)$$

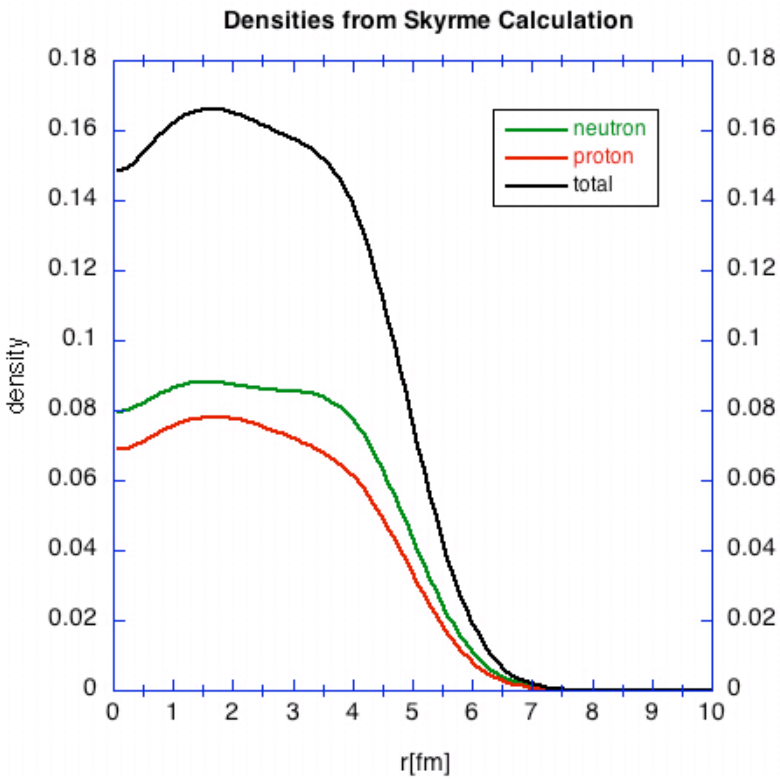
$$g(E) = 1 - k_p E$$

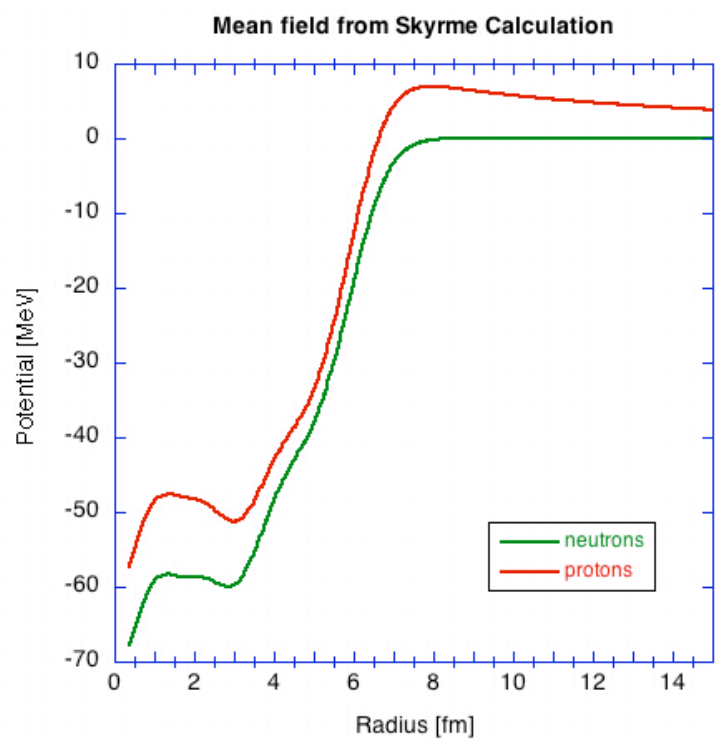
$$J_{00} = -G_\delta(1 - 0.0005E/A)$$

$F(\rho)(\gamma=0)$	Reid	Paris
C	0.2845	.2963
α	3.6391	3.7231
β [fm^3]	2.9605	3.7384

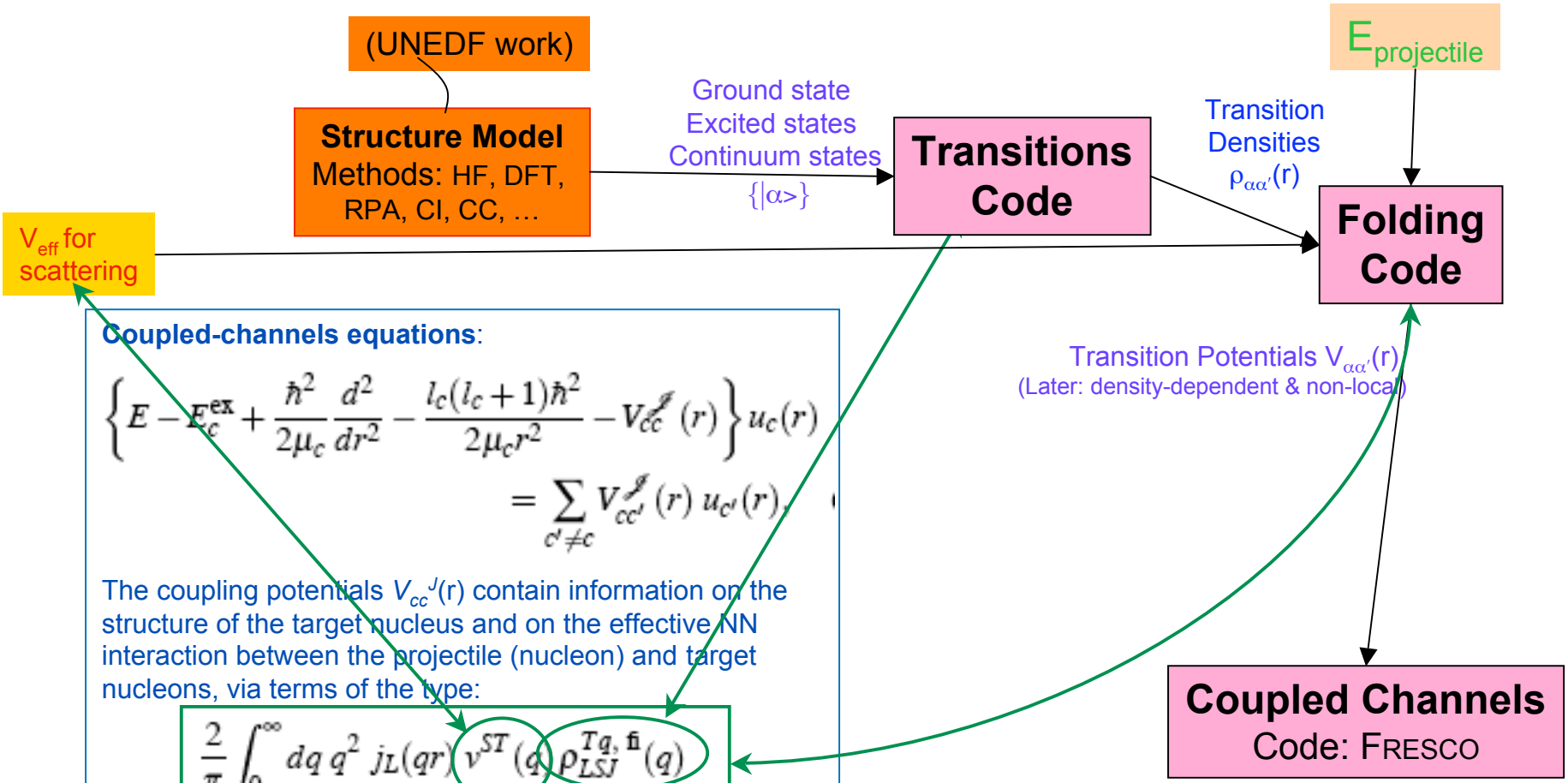
Coefficient	Reid	Paris
G_1 [MeV]	7999	11062
G_2 [MeV]	-2134	-2537.5
G_3 [MeV]	0	0
μ_1 [fm^{-1}]	4	4
μ_2 [fm^{-1}]	2.5	2.5
μ_3 [fm^{-1}]	0.7072	0.7072
G_δ[MeVfm^3]	-276	-592
k [MeV^{-1}]	0.002	0.003

Densities and mean field from Skyrme





In context…



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