Coupled-Channels Scattering Solutions using the R-matrix Method

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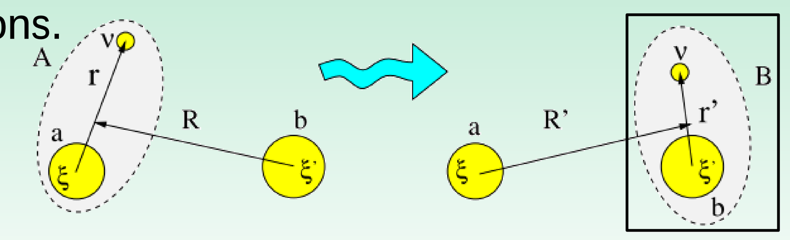
Motivation

The calculable R-matrix method was developed as an efficient method for finding solutions to the Schrödinger equation. Previous to the method's use, solutions were found using direct integration methods. These methods, while accurate, are computationally intensive and time consuming, especially in more complicated reactions. Integration techniques become especially inefficient with the calculation of non-local potentials or coupled channels, thus providing a motive for a more efficient method. The R-matrix method instead uses linear algebra techniques which provides a much more elegant solution with greatly improve efficiency. The benefits of the method are especially apparent when calculating solutions to coupled channels reactions.



Theory

Use of the R-matrix method will be demonstrated through its application to coupled channel scattering reactions. In a coupled-channels scattering problem, the goal is to calculate solutions to the radial Schrödinger equation for a projectile nucleon interacting with a target, which, because of target excitation, consists of a coupled-channel problem.

$$\left[-\frac{\hbar^2}{2\mu_c}\left(\frac{d^2}{dr^2}-\frac{l_c(l_c+1)}{r^2}\right)+V_c(r)+E_c-E\right]u_{c(c_0)}(r)+\sum_{c'}\int_0^\infty W_{cc'}(r,r')u_{c'(c_0)}(r')dr'=0$$

The R-matrix method divides the problem between an internal and external region at an arbitrary point. The internal region, where the R-matrix method is applied, is calculated over a finite number of basis functions using the Lagrange mesh method. The problem becomes a linear algebra problem with matrix elements:

$$C_{ci,c'i'} = <\varphi_i|T_c+\mathcal{L}_c+E_c-E|\varphi_{i'}>\delta_{cc'} + <\varphi_i|V_{cc'}|\varphi_{i'}>$$

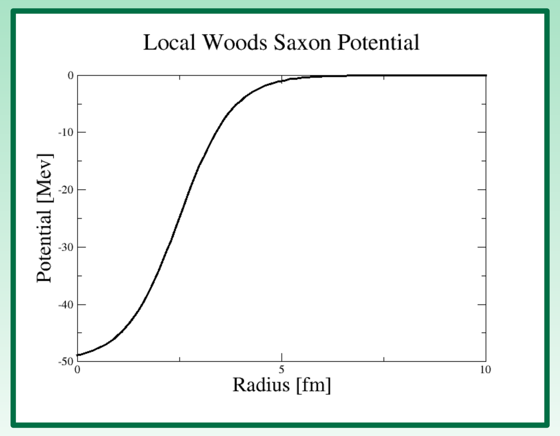
In the exterior region, the asymptotic behavior of the wavefunction can be modeled using the collision matrix for the system and Coulomb functions.[1]

$$u_{c,ext} = v_c^{-1/2}(I_c(k_c r)\delta_{cc_0} - U_{cc_0}O_c(k_c r))$$

Inputs

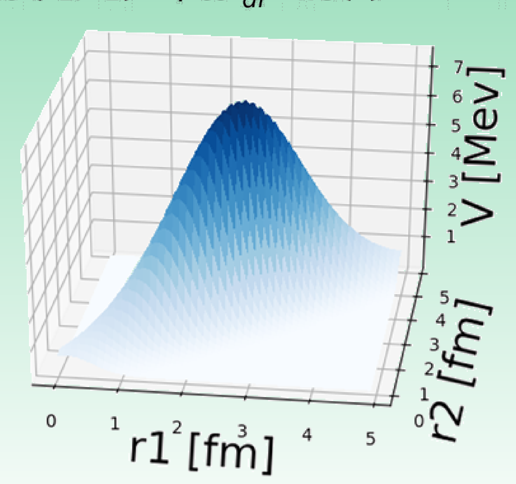
Input to the program includes important physical parameters such as the energy (E) of incoming nucleon and excitation energies (Ec), angular momentum values in each channel (l), and reduced mass of projectile-target system (mu).

Also included are the potential parameters used for the projectile's Hamiltonian (V(r)). The potentials can be local or nonlocal. The usual shape for the potential is a Woods-Saxon: $V_{WS}(r) = \frac{-V_0}{1+e^{\frac{r-R}{a}}}$



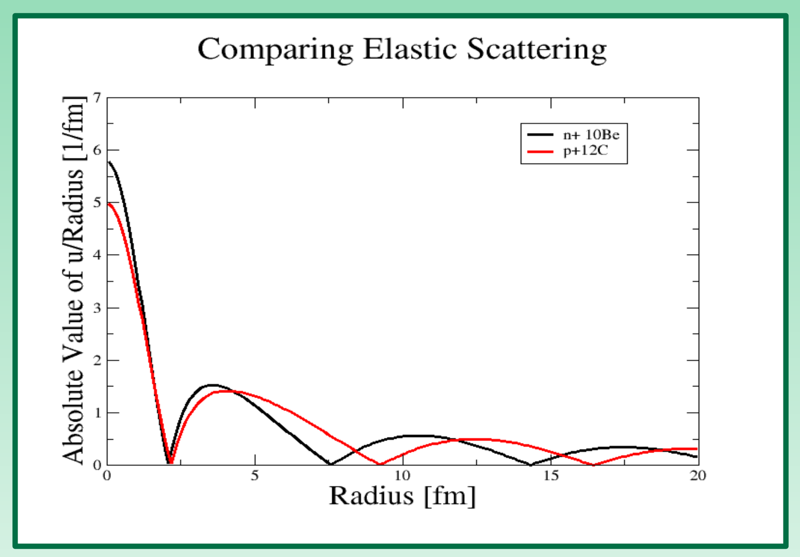
Also included are non-local Couplings between the channels:

$$V_{cc'}(r_1,r_2) = \beta_{cc'}\frac{d}{d\bar{r}}V_{WS}(\bar{r})\, e^{-\left(\frac{r_1-r_2}{\beta_{nl}}\right)^2}$$



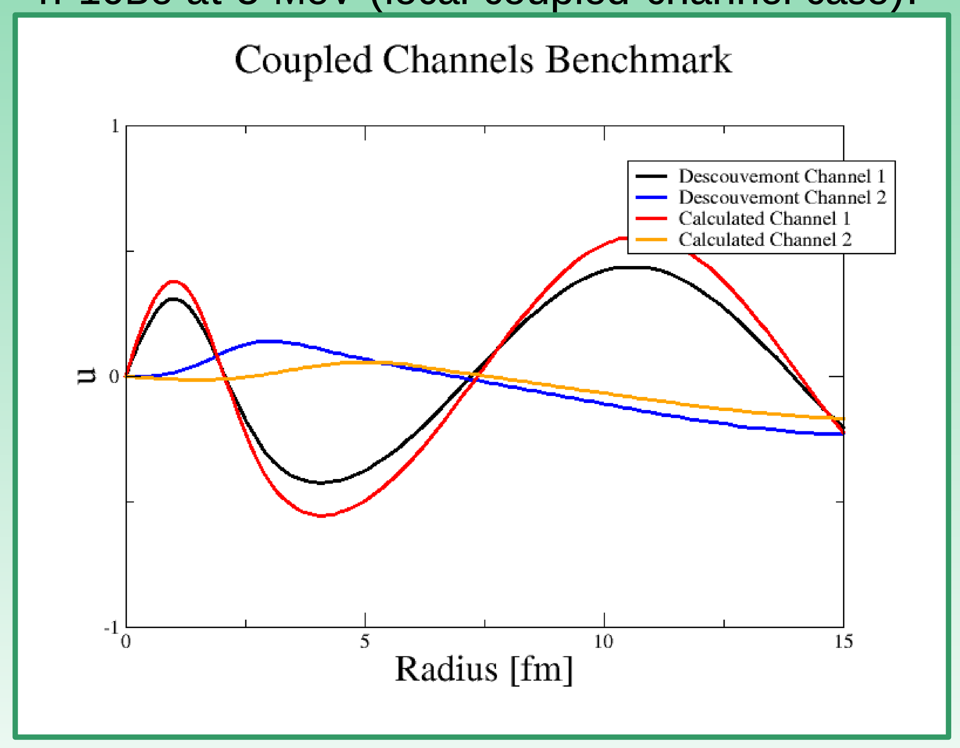
Preliminary Results

Single-channel wavefunctions for elastic scattering: black n+^{10}Be E=5 MeV , p+^{12}C both at 5 MeV.

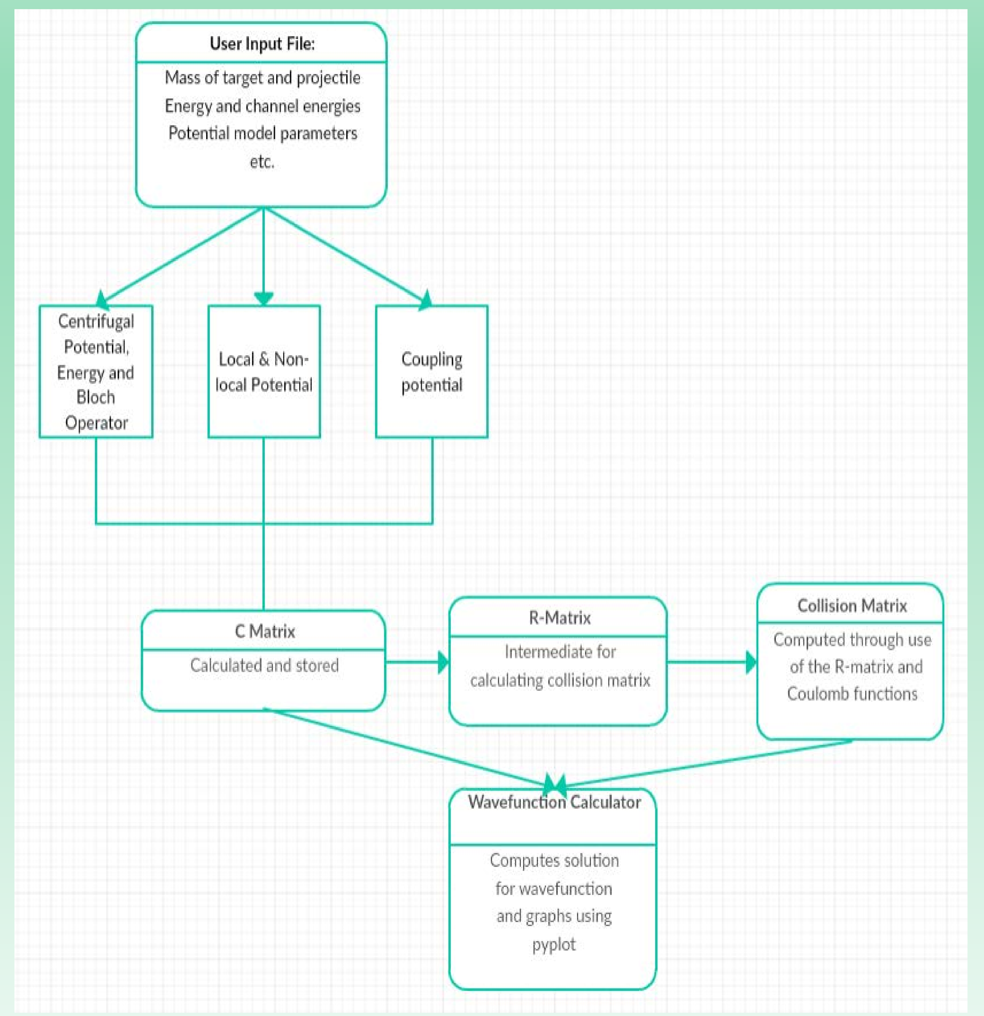


- Short-distance differences due to Coulomb repulsion
- Wavefunction also acquires different phase for large R

Benchmarking with code from [3]:
n-10Be at 5 MeV (local coupled-channel case).



Control Flow

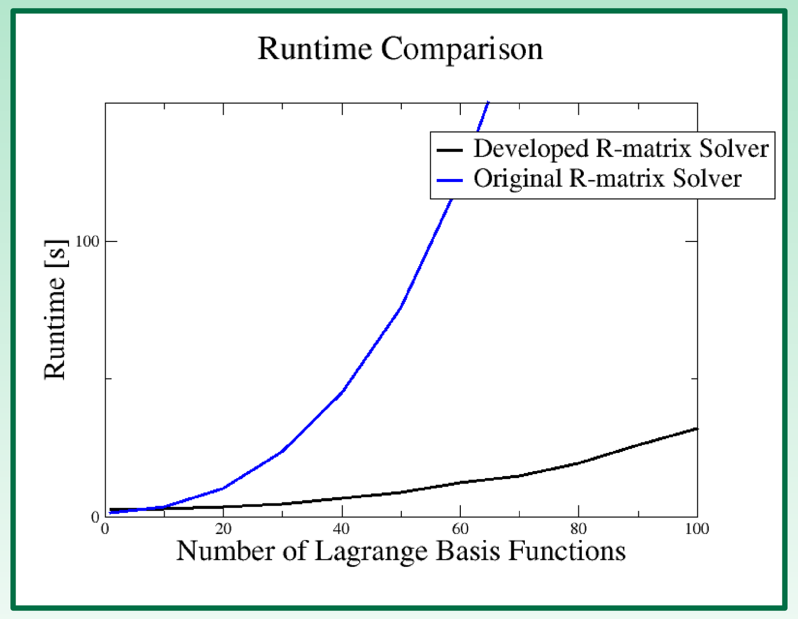


Code Design

Coupled channels R-matrix solver:

- Written in Python
- Started from single-channel solver
- Generalized to two channels
- Included coupling between channels
- modular approach

Optimization:
Efficient matrix element calculations
Matrices calculated once and stored at the top



References

[1]:Descouvemont, P., & Baye, D. (2010). *Rep. on Prog. in Phys.*, *73*(3), 036301.
[2]:Nunes, F. M., Thompson, I. J., & Johnson, R. C. (1996). *Nucl.Phys. A*, *596*(2), 171–186.
[3]:Descouvemont, P. (2016). *Computer Physics Communications*, *200*, 199–219.

Future Improvements

After more testing ensures the accuracy of the developed coupled channels solution, there are many opportunities for future work:

- Generalization for arbitrary number of channels
- Include parallel programming techniques.
- Expand the solver to calculate for three-body problems.

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