

Compute wave functions in multichannel collisions with non-local potentials using the R-matrix method

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Research Question

Previous project:

A program to compute wave functions of neutrons and protons in nuclear scattering problems involving **non-local potentials**

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

Motivation

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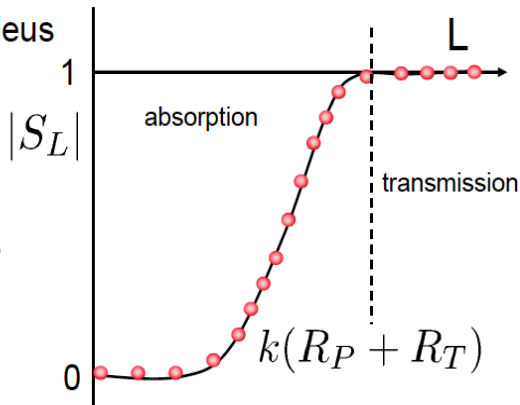
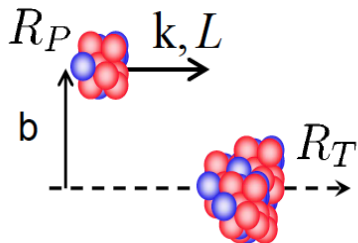
$$V_{nl}u(r) = \int_0^{\infty} V(r, r')u(r')dr' \quad (2)$$

- During collisions, nuclei can enter multiple **channels**, or states.
 - ▶ To account for these, we must introduce coupling into our potential

$$V(r)u_c(r) = \sum_{c'} V_{cc'}(r)u_{c'}(r) \quad (3)$$

Motivation

large k – e.g. nucleus-nucleus



The R-matrix method¹

- First, divide the problem into two regions, internal and external, at the **channel radius**, a
 - ▶ We ignore nuclear forces in the external region so that $u^{ext}(r)$ is solved analytically

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- We then relate $u^{int}(r)$ with $u^{ext}(r)$

$$\sum_{c'} [(T_c + \mathcal{L}_c + E_c - E)\delta_{cc'} + V_{cc'}] u_{c'}^{int} = \mathcal{L}_c u_c^{ext}$$

(Bloch-Schrodinger Eq.)

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The R-matrix method

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- The problem is reduced to matrix calculations

$$R_{cc'}(E) = \frac{\hbar^2}{2\sqrt{\mu_c \mu_{c'} a}} \sum_{i,i'=1}^N \varphi_i(a) (C^{-1})_{ci,c'i'} \varphi_{i'}(a) \quad (5)$$

$$C_{ci,c'i'} = \langle \varphi_i | T_c + \mathcal{L}_c + E_c - E | \varphi_{i'} \rangle \delta_{cc'} + \langle \varphi_i | V_{cc'} | \varphi_{i'} \rangle \quad (6)$$

The Lagrange basis

Lagrange functions:

$$\varphi_i(r) = (-1)^{N+i} \left(\frac{r}{ax_i}\right) \sqrt{ax_i(1-x_i)} \frac{P_N(2r/a-1)}{r-ax_i} \quad (7)$$

where x_i are the roots of $P_N(2x-1)$

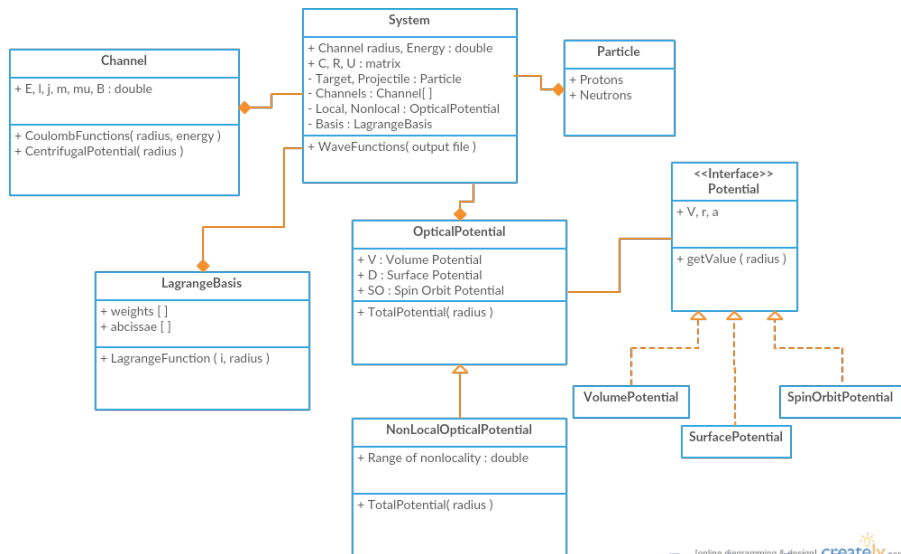
From the Gauss-Legendre quadrature rule:

$$\langle \varphi_i | \varphi_j \rangle = \int_0^a \varphi_i(r) \varphi_j(r) dr \approx \delta_{ij} \quad (8)$$

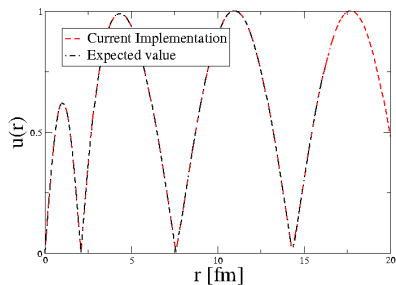
$$\langle \varphi_i | V(r) | \varphi_j \rangle \approx V(ax_i) \delta_{ij} \quad (9)$$

$$\langle \varphi_i | W(r, r') | \varphi_j \rangle \approx a \sqrt{\lambda_i \lambda_j} W(ax_i, ax_j) \quad (10)$$

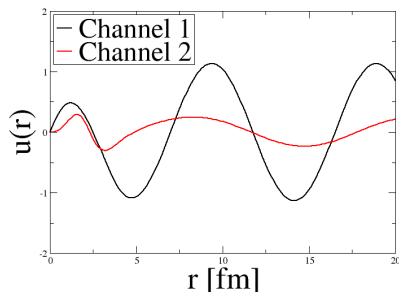
Program structure (C++)



Results

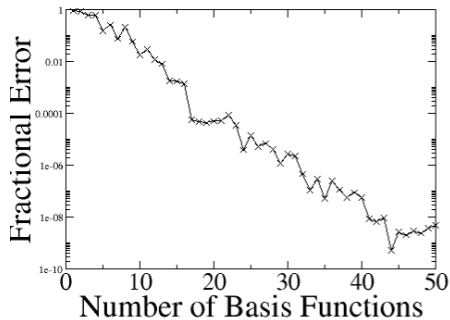


(a) $n+^{10}\text{Be}$ elastic scattering at 10 MeV overlaid with expected results for single channel case.

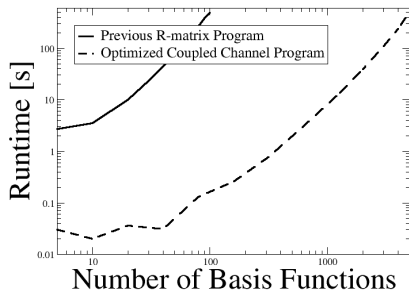


(b) $n+^{10}\text{Be}$ elastic scattering at 10 MeV output including $l = 0^+$ and $l = 2^+$ ($E_c = 3.368$ MeV) channels

Results



(a) Plot showing convergence to accurate results with number of Lagrange functions in basis expansion



(b) Time analysis showing 10^3 speedup from original program (Python)

Advantages, Limitations, & Future work

Advantages

- Fast program, accounts for arbitrary number of channels, MPI implementation

Limitations

- Current bug with normalization
- Does not handle closed channels

Future work

- Applying the program in Uncertainty Quantification problems
- Using the program to fit predictions to experimental data

Acknowledgements



Advanced Computational
Research Experience for Students

$$\mathcal{L}_c = \frac{\hbar^2}{2\mu_c} \delta(r - a) \left(\frac{d}{dr} - \frac{B_c}{r} \right) \quad (\text{Bloch operator})$$

$$u_c(a) = \sum_{c'} \sqrt{\frac{\mu_c}{\mu_{c'}}} R_{cc'} [a u'_{c'}(a) - B_{c'} u_{c'}(a)] \quad (\text{R-matrix})$$