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

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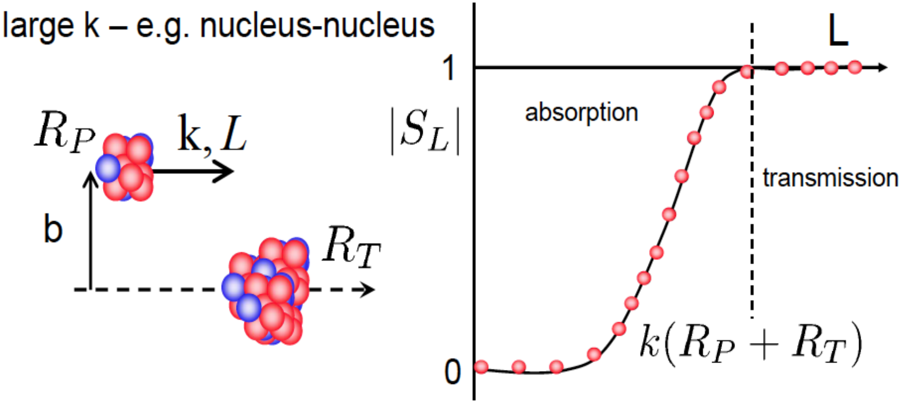
$$V_{nl}u(r) = \int_0^\infty V(r, r')u(r')dr' \quad (2)$$

- 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
R_P
k, L
b
R_T
1
$|S_L|$
absorption
L
transmission
$k(R_P + R_T)$
0

The R-matrix method[1]

- 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

[1] P Descouvemont and D Baye. "The R-matrix theory". In: *Reports on Progress in Physics* 73.3 (2010), p. 036301. DOI: 10.1088/0034-4885/73/3/036301.

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- 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
- 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 problem is reduced to matrix calculations

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

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

The Lagrange basis

Lagrange functions:

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

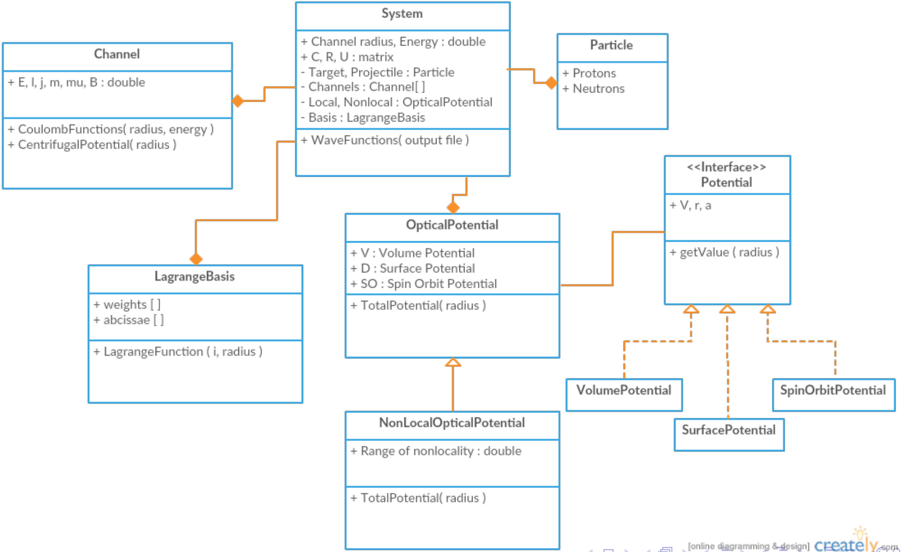
where x_i are the roots of $P_N(2x-1)$
From the Gauss-Legendre quadrature rule:

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

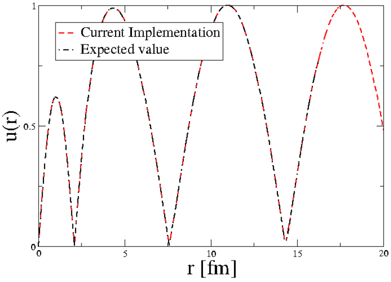
$$\langle\varphi_i|V(r)|\varphi_j\rangle \approx V(ax_i)\delta_{ij} \tag{9}$$

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

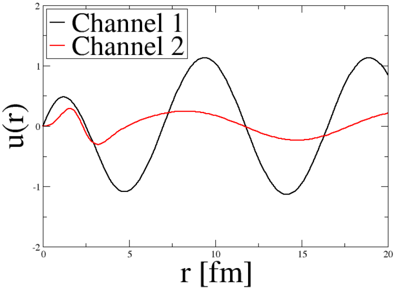
Program structure (C++)



Results

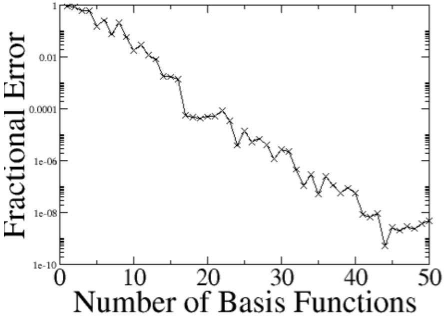


(a) n+^{10}Be elastic scattering at 10 MeV overlaid with expected results for single channel case.

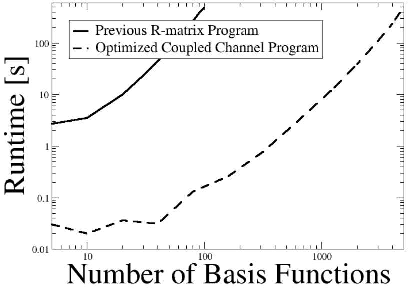


(b) n+^{10}Be elastic scattering at 10 MeV output including $I = 0^+$ and $I = 2^+$ ($E_c = 3.368$ MeV) channels

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

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

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