

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

Joey Bonitati<sup>1,2</sup>, Benjamin Slimmer<sup>1,2</sup>, Weichuan Li<sup>1</sup>, Gregory Potel<sup>1</sup>, and Filomena Nunes<sup>1</sup>

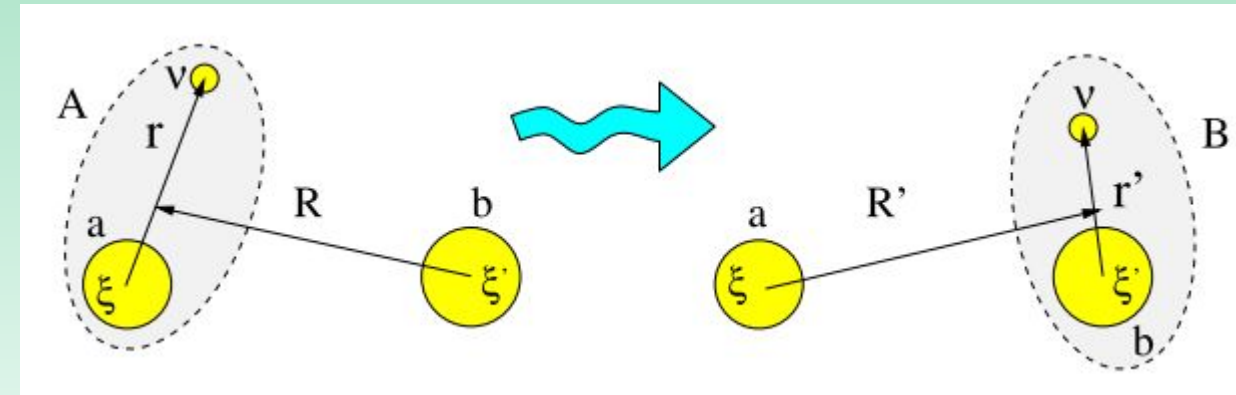
<sup>1</sup>National Superconducting Cyclotron Laboratory, Michigan State University, East Lansing, MI 48824, USA

<sup>2</sup>Clemson University, Clemson, SC 29632, USA,

## Motivation

To describe quantum properties and predict the positions of particles after collisions, we use wave functions. The wave functions for two-body nuclear collisions are also important input to understand more complicated three-body collisions, specifically nuclear transfer reactions [2].

Previous solutions to this problem have been computationally time-consuming. Since wave functions appear often in nuclear physics, there is a demand for faster methods for calculating them.



Nuclear potentials in reality are *nonlocal*, meaning the nuclear force on a particle at one point depends on the force on that particle at all other points. Most problems also involve multiple states, or *channels*. This introduces coupling into the equations.

## Theory [1]

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

The R-matrix method makes use of the assumption that nuclear forces are short-ranged. The problem is divided into two regions, internal and external, which are separated at the channel radius  $a$ . Nuclear forces are only considered in the internal region so that the wave function in the external region is calculated analytically.

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

First, we introduce the Bloch surface operator into the Schrödinger equation to relate the internal and external wave functions

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

$$u_c^{int}(r) = \sum_{j=1}^N c_{cj} \phi_j(r)$$

Next, we expand the partial wave functions over a finite basis (see Lagrange Mesh section)

$$R_{cc'} = \frac{\hbar^2}{2\sqrt{\mu_c \mu_{c'}}} \sum_{i,i'=1}^N \phi_i(a) (\mathbf{C}^{-1})_{ci,c'i'} \phi_{i'}(a)$$

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

By taking the operators from the Schrödinger equation on the basis functions, we calculate the R-matrix, which is used to compute the external wave functions. We can then compute the internal wave functions at all points.

$$u_{c(c_0)}^{int}(r) = \sum_{c'} \mathcal{L}_{c'} u_{c'(c_0)}^{ext}(a) \sum_{i,i'=1}^N \phi_i(r) (\mathbf{C}^{-1})_{ci,c'i'} \phi_{i'}(a)$$

## Lagrange Mesh

For the finite basis expansion required by the R-matrix method, we use the Lagrange functions defined here:

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

Gauss quadrature rules:

$$\langle \phi_i | \phi_j \rangle = \int_0^a \phi_i(r) \phi_j(r) dr \approx \delta_{ij}$$

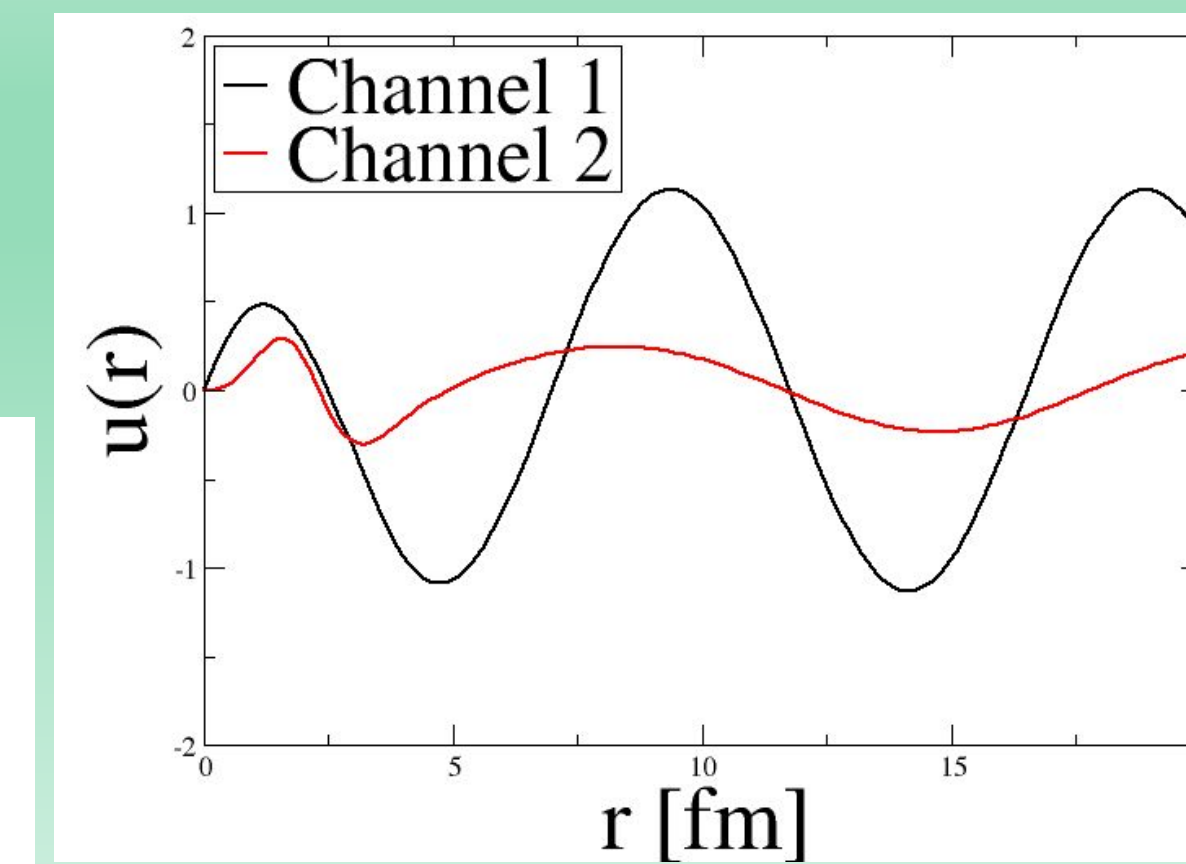
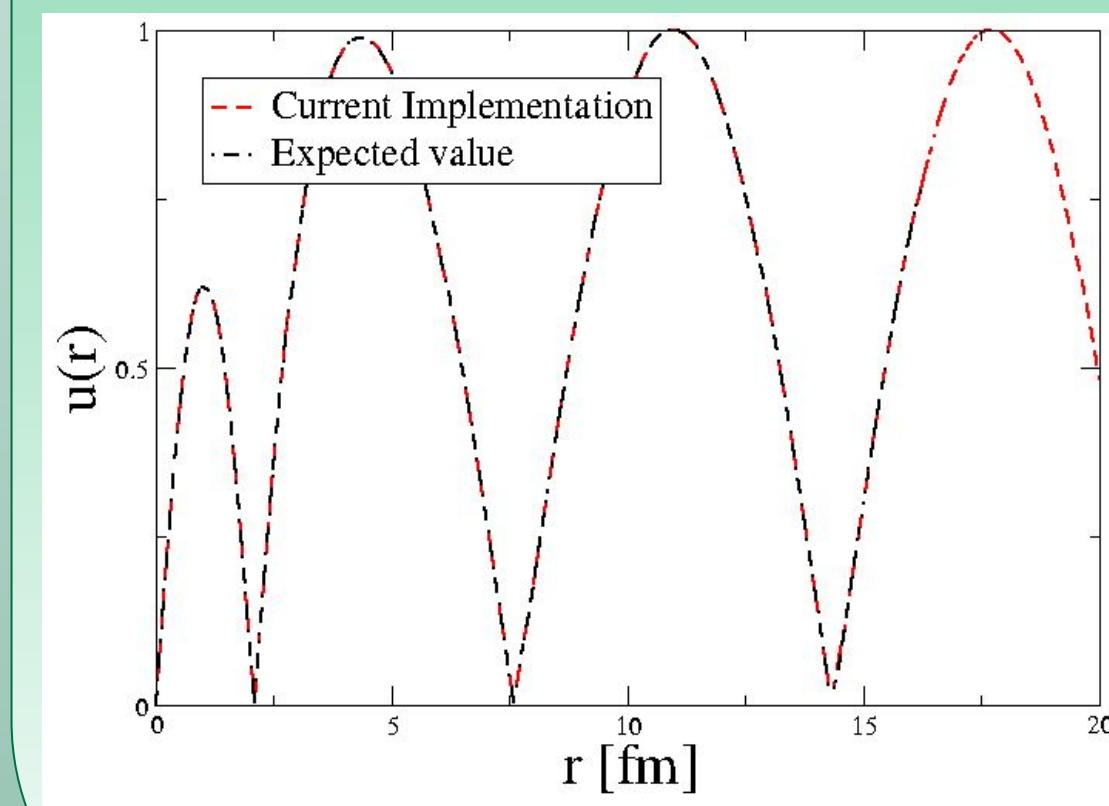
$$\langle \phi_i | V(r) | \phi_j \rangle \approx V(ax_i) \delta_{ij}$$

Due to the Gauss-Legendre quadrature rule, when evaluating the potentials on these functions, one only has to consider the value of the potentials at the mesh points,  $ax_i$ . This makes the R-matrix method **much faster** than other techniques which use direct integration [3].

$$\langle \phi_i | W(r, r') | \phi_j \rangle \approx a \sqrt{\lambda_i \lambda_j} W(ax_i, ax_j)$$

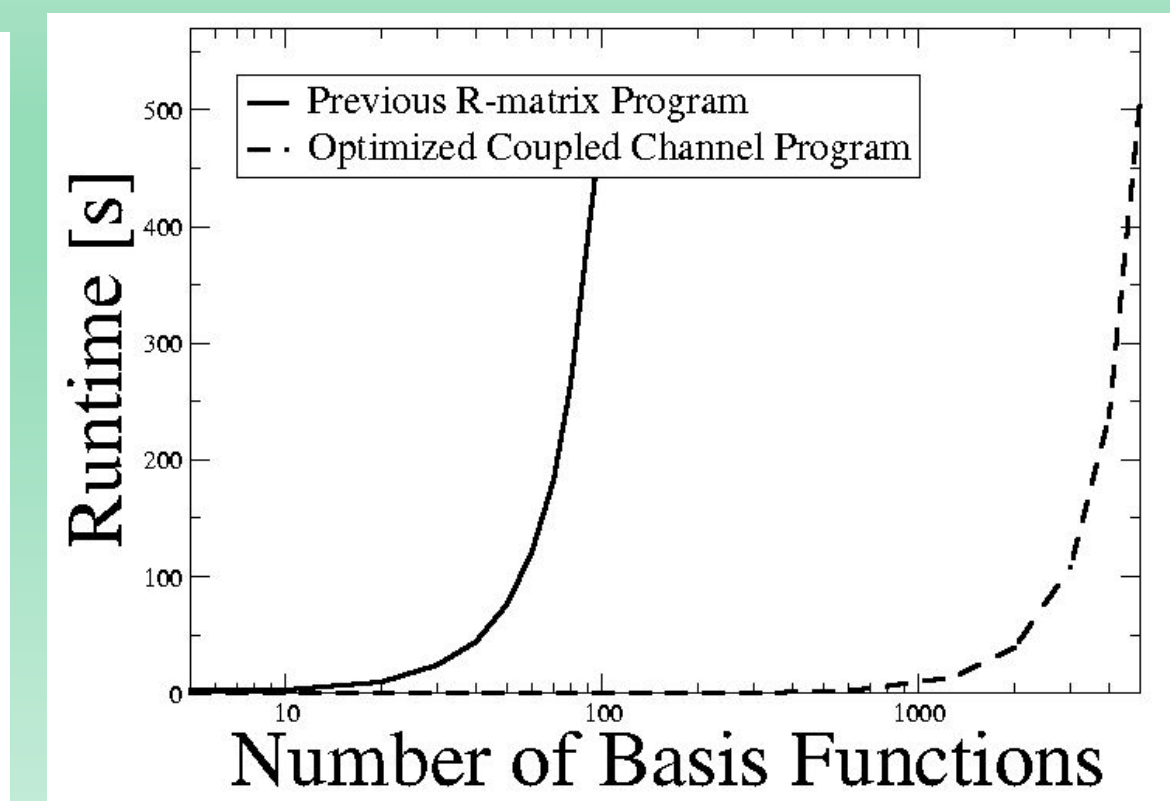
## Results

(below) Elastic scattering partial wave function for  $n+^{10}\text{Be}$  at  $E=10$  MeV, potential parameters from [4]. Absolute value overlaid with output of code from [1].



(above)  $n+^{10}\text{Be}$  at  $E=10$  MeV with potential parameters from [4]. Coupling of the entrance channel (1) with the excitation channel (2) can be observed.

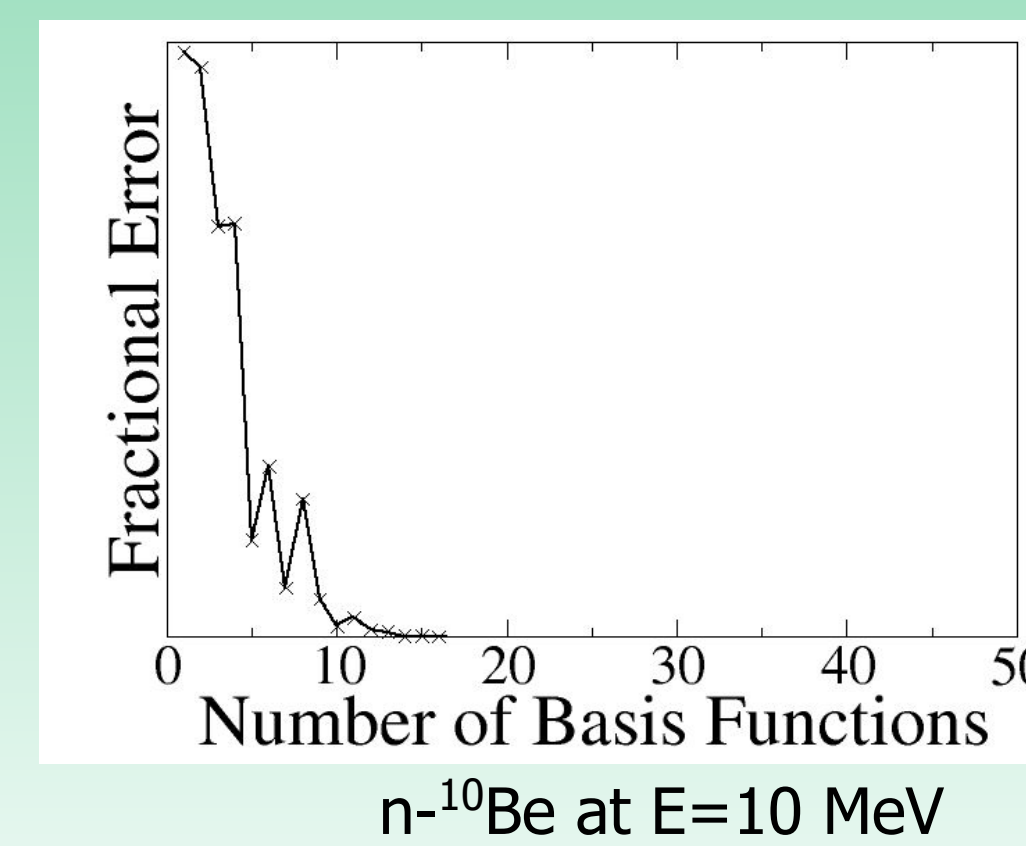
## Runtime analysis



Improvement of the order of  $\sim 10^3$  times from another implementation. Speed up partially due to the Armadillo C++ library [5] used for the matrix calculations. *Matrix Inversion* is the most time consuming step at high precision.

## Convergence with Number of Basis Functions

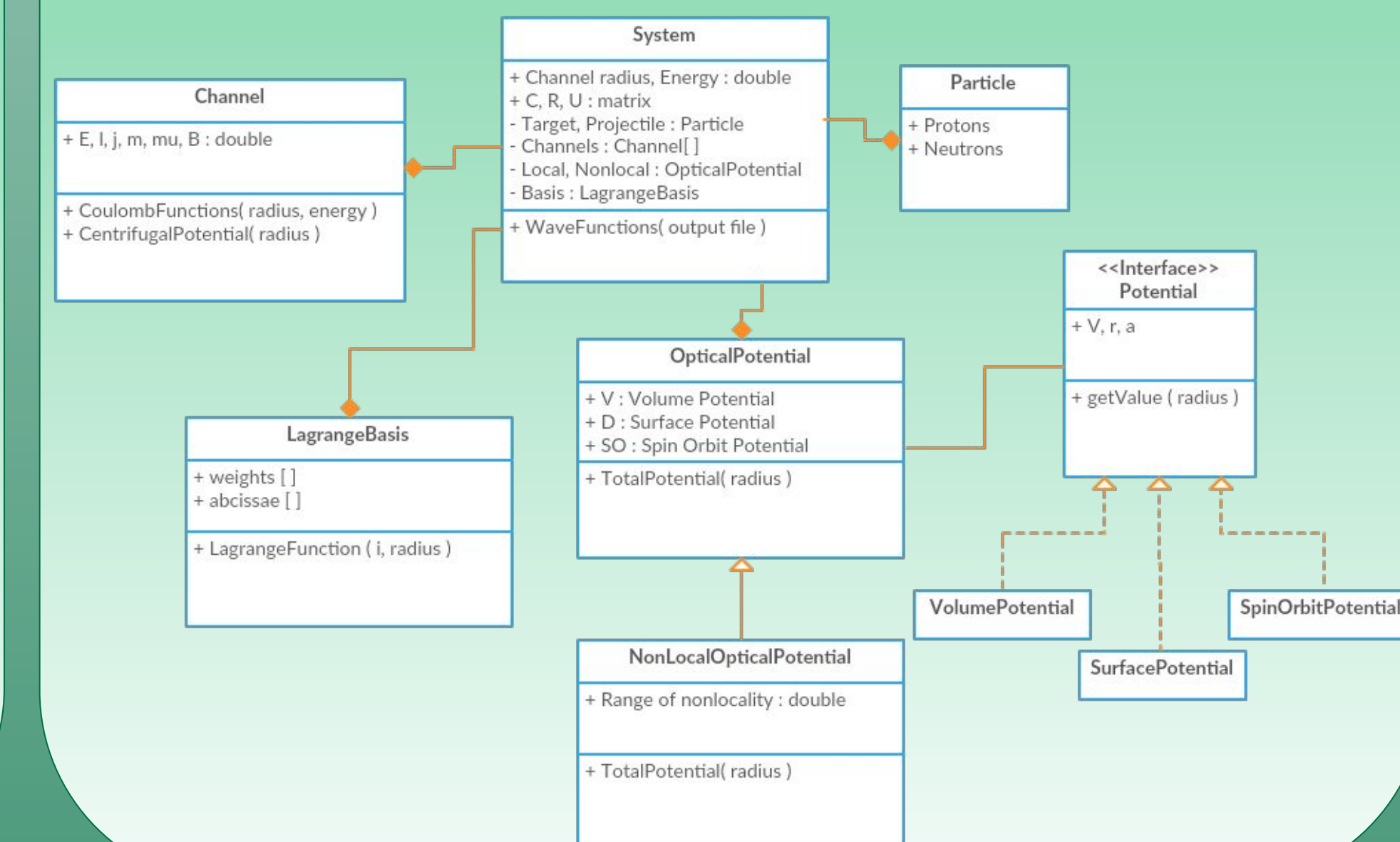
Fractional error of the modulus of the wavefunction at  $R=1.20$  fm including  $N$  Lagrange functions and the results obtained for  $N=300$



Convergence is obtained at  $N=15$ .

## Code Design

The program was written in C++ using Object-Oriented Programming techniques to increase modularity. An input file format was designed to make the program user-friendly.



## Advantages of the code

- $10^3$  times faster the predecessor code
- Handles an arbitrary number of channels
- Modular structure for easier future extensions
- Includes parallel processing (MPI)

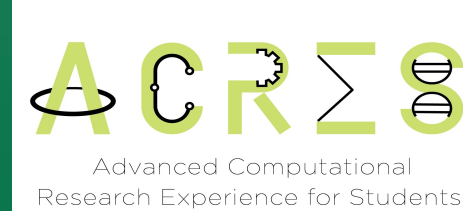
## References

- [1] P. Descouvemont and D. Baye. The r-matrix theory. Reports on Progress in Physics, 73(3):036301, 2010.
- [2] Joaquin Gomez Camacho and Antonio M. Moro. A pedestrian approach to the theory of transfer reactions: Application to weakly-bound and unbound exotic nuclei. The Euroschool on Exotic Beams, Vol. IV, pages 39–66, 2014.
- [3] M. Hesse, J. Roland, and D. Baye. Solving the resonating-group equation on a lagrange mesh. Nuclear Physics A, 709(1-4):184–200, 2002.
- [4] Nunes, F., Thompson, I., & Johnson, R. (1996). Core excitation in one neutron halo systems. Nuclear Physics A, 596(2), 171–186.
- [5] Conrad Sanderson and Ryan Curtin. Armadillo: a template-based C++ library for linear algebra. Journal of Open Source Software, Vol. 1, pp. 26, 2016.

## Future Research

There are many promising continuations to this research in R-matrix theory, including:

- Applying the program to compute wave functions in cases with many channels with High
- Extending the current implementation to include closed channels
- Using the program to fit predictions to experimental data
- Extending the R-matrix theory to three-body collisions
- Exploring Quantum Computing algorithms for the R-matrix method



This work was supported by NSF grant # 1560168 through the iCER ACRES REU program



The NSCL is funded in part by the National Science Foundation and Michigan State University.

