Chapter 7

Conclusions and summary

In this report, the optimization of the coupled channels algorithm, as implemented in the Nijmegen DYNA program package,[1] has been studied. Coupled channels can be used to solve inelastic scattering problems, or to construct distorted waves that can be used in a variational reactive scattering calculation, the main purpose of DYNA.

The optimization consists of two steps. The coupled channels algorithm uses a NAG library routine to solve numerically a system of second order differential equations, with given initial conditions. In the first step, the use of this routine was optimized. This resulted in two formulae [Eqs. (4.6) and (4.7)], to calculate the optimal step size and tolerance parameter settings for this NAG routine. With these formulae, it is possible to use the NAG routine to solve the differential equations up to a certain accuracy with the least computing effort. This resulted in a reduction of computing time with about 30%.

The second step involved the design of a new algorithm to solve the coupled channels equation. The idea is to use a locally optimal basis set to propagate the CC equation. To achieve this, several partial algorithms had to be designed. The first algorithm is neccessary to calculate the optimal division of the total integration interval in steps, in which one local basis is used. The calculation of each basis requires evaluation and diagonalization of a large potential matrix, which is very time consuming. If the steps are too small, the calculation of the basis sets takes very much time. But on the other hand, if the steps are too large, the basis is not optimal over the whole step any more, which also gives rise to more computing effort.

The second algorithm is used to solve the CC equations over one step, in the local basis, and then transform the results into the final basis. The last algorithm that has been developed, is used to combine the results of the different steps.

From tests, it can be concluded that this new method is particularly efficient when high-accuracy results are required. The new quasi-adiabatic method is about 50% faster than the old method. The scaling of computing time with accuracy is also more favorable. This means that the growth in computing time when more accurate results are required, is less than with the old method.

The two optimizations together give a reduction in computing time of about a factor three. Furthermore the new method only requires a minimal number of parameters to describe the desired accuracy in the propagation. The values for all the other parameters are determined automatically. This new method has been implemented as a black box routine in the DYNA program package. The user only has to supply two parameters to describe the propagation of the coupled channels equation.