PSTGF: time-independent R-Matrix atomic electron-impact code.

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Abstract

stgf is a community code employed for outer-region R-matrix calculations, describing electron-impact collisional processes. It is widely recognised that the original version of stgf was written by M. J. Seaton in 1983, but through constant refinement over the next decades by worldwide contributors has evolved into its current form that more reflects modern coding practice and current computer architectures. Despite its current wide acceptance, it was never formally published.

Therefore, we present an updated high-performance parallel version of pstgf, that balances the requirements of small university clusters, yet can exploit the computational power of cutting edge supercomputers. There are many improvements over the original stgf, but most noticeably, the full introduction of MQDT options that provide subsequent integration with ICFT (Intermediate Coupling Frame Transformation) codes, and for either Breit–Pauli/DARC (Dirac Atomic R-matrix Codes), better load balancing, high levels of vectorisation and simplified output. Semantically, the program is full fortran 90 in conjunction with MPI (Message Passing Interface) though has CUDA fortran options for the most numerically intensive code sections.

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**PROGRAM SUMMARY/NEW VERSION PROGRAM SUMMARY**

**Program Title:** RMATRIX-PSTGF  
**Licensing provisions:** GNU General Public License  
**Programming language:** Fortran90

**Does the new version supersede the previous version?:** Yes  
**Reasons for the new version:** Higher-efficiency of parallelisation, load balancing, and optimised memory usage.  
**Summary of revisions:** Numerov method for Coulomb functions [1]. Quantum defect theory [2].

**Nature of problem**(approx. 50-250 words):  
The R-matrix outer region code, PSTGF directly calculates various electron-impact driven processes such as excitation and ionisation, or provides K-matrices for input for subsequent ICFT, differential or magnetic sub-level codes. As the problem size increases, there is an associated increase in the input/output, the numerical computation and unbalanced workload, especially in electron-impact energies where the number of open-channels is equivalent to the number of closed. The code has been significantly modified to address these issues.

PSTGF interfaces the R-matrix inner region with the outer region, with the R-matrix acting as intermediary between the two regions. The outer region expresses an electron moving in the multi-pole expansion of the target and predominantly employs Coulomb functions, perturbed or otherwise to achieve this. This is a computationally expensive task, as the R-matrix must be formed for every energy point of every partial wave.

**Solution method**(approx. 50-250 words):  
An approach that permutes both the partial wave and energy of the incident electron has been implemented. In this version, each processor does not calculate the same incident energy point for each partial wave, but rather distributes all energy points across all processors. This achieves better load-balancing of the work between cores and avoids the case where an overloaded single processor has to always calculate in the energy range where there are approximately the same number of half-open or half-closed channels, which is numerically intensive.

**Additional comments**(approx. 50-250 words):  
Dimension parameters used to define arrays and matrices within PSTGF (PARAM file) have been removed, all array dimensions are dynamically allocatable based upon the H.DAT file and set to the exact dimension. A CUDA subroutine for matrix multiplications using...
GPUs has been included, it can be activated or deactivated commenting this module in the source.

References

[1] M. J. Seaton, Coulomb functions for attractive and repulsive potentials and for positive and negative energies, Comp. Phys. Comm. 146 (2) (2002) 225–249. doi:https://doi.org/10.1016/S0010-4655(02)00275-8.

[2] M. J. Seaton, Quantum defect theory, Rep. Prog. Phys. 46 (2) (1983) 167. doi:https://doi.org/10.1088/0034-4885/46/2/002.

1. Introduction

Time-independent R-matrix theory [3] is a powerful formalism that may used to calculate first order collisional processes: electron-impact excitation, ionisation, photoionisation, dielectronic recombination, radiative recombination for atoms and their associated ion stages. In its simplest form, R-matrix theory splits the collisional problem into two distinct regions: an inner and outer region. The inner region is defined by the radial extent of the most diffuse orbital from the nucleus. This is sufficient to encompass the charge cloud of the target, though mathematically this R-matrix radius may be extended further, though at a computational cost. The inner region represents target atom/ion plus incident/outgoing electron, and is treated as \( N + 1 \) electron many body problem, with all the interactions taken in account between indistinguishable particles, including exchange and correlation. We calculate a complete set of eigenfunctions representing both the bound and continuum spectrum. One of the strengths of the R-matrix approach is that as we achieve a complete description of the system in the inner region that is independent of the incident electron energy, therefore only requiring one diagonalisation of \( N+1 \) Hamiltonian, for a range of electron-impact energies. The set of codes used for the calculations in the inner region were published in [4, 5, 6, 7] and although they form a foundation for this work, they are not the subject of present paper.

In the outer region, the formalism is quite different, the problem is treated as a single electron moving in a multipole expansion of the target. In FSTGF this single electron, which is moving in the potential created by the remaining electrons, is considered to be at a distance that correlation effects would be minimal, and are
therefore are not included. Comparatively, in this region the physics simplifies but its range may extend to large distances due to the long-range effect of Coulomb-like potentials. To extract collision strengths, we must be at distances from the nucleus where the wave function has returned to well-known asymptotic forms, a distance several orders of magnitude larger than the R-matrix inner-region radius.

The key of R-matrix method is the connection of the wave function at the boundary between the inner and outer regions, as this interface determines the phase shifts, consequently the S matrices, and finally the collision strengths. Greater details about R-matrix method are given in [3].

pstgf is the most common atomic outer-region program used to perform the calculations in the outer region for electron-impact excitation processes. As well as directly calculating electron-impact excitation collision strengths, it is the progenitor code for subsequent ICFT, LS, jK and jj differential codes, as well as magnetic sub-level work. It has the capabilities to be interfaced with the molecular suite of R-matrix codes.

pstgf is a community code, employed by the majority of R-matrix groups around the world, many of whom have made contributions and improvements over the decades. In present work, we build upon this to provide new sustainable version, that will address future problems that inevitably will be larger in scale.

Below, are some notable additions to the code have been carried out over the years, that due to the original code not being formally published may have been overlooked. These include the extension to neutral atoms [8], the ICFT (Intermediate Frame Transformation) by Griffin and co-workers [9], and the first systematic parallelisation of the serial code by T. W. Gorczyca [10] and D. M. Mitnik (2002, unpublished), using the MPI protocol. This version tried to balance the work-load by distributing the impact-electron energy distribution across the whole energy range for each processor, and remains effective when the number of processors is significantly less the number of energy points. However, in the intervening years, the number of cores available to researchers has increased to the point where each processor only carries out 1-3 energy points per partial wave. This spurs some of the work presented later in this paper.

Subsequently, this parallel pstgf version was improved in efficiency. In this new version, pstgf was restructured in terms of its memory usage. At every point in the calculation, memory is assessed and if not required deallocated, before the next section reducing the memory footprint of the code by half. Additionally, the H.DAT input file was split into individual partial waves H.DATXXX files, that ensured that thousands of processors no longer needed to read a single file, competing against each other, but could concurrently read 40-100 files in smaller
groups of processors. Where possible, the LAPACK routines for matrix-matrix and matrix-vector multiplies where employed, especially if an optimised-vendor supplied library was available. Specific routines that considered the multipole perturbation of the non-perturbed results were heavily loop unrolled and refactored to ensure the greatest degree of vectorisation. However, even these improvements need further consideration if we are to progress routinely to systems involving Hamiltonian matrices in excess of 100 000 by 100 000 and involving over 10 000 channels. In this paper, we describe how to address these problems, ranging from removing the last vestiges of fortran 77 legacy code (COMMON blocks, hard-dimension arrays), to introducing GPU enabled sections for future hardware compatibility.

2. Glossary of terms

- **Target state**: eigenfunction of the Hamiltonian of the target, \( N \)-electron system. It can be labelled with quantum numbers appropriate to the coupling scheme employed. Usually the electronic orbitals are calculated by other specialised packages, for example autostructure \[11\], MCHF \[12\], GRASP \[13, 14\], or CIV3 \[15\]. R-matrix inner region codes use these orbitals to calculate the target energies and eigenfunctions.

- **Partial wave** \( J\pi \) or \( LS\pi \): symmetry of the initial system target state plus incoming electron, the quantum numbers are conserved. Each Hamiltonian representing a partial wave is calculated independently of every other partial wave. The total cross section is then the sum of the partial cross sections for all possible values of \( J/L \), from zero to infinity, all possible couplings of \( S \) (LS coupling case), and \( \pi \), even and odd.
  
  For practical reasons, we have used for present work the notation of the relativistic coupling \( J\pi \), but the whole procedure is equivalent for the non-relativistic case, and is achieved by just substituting the indexes \( J\pi \) for \( LS\pi \).

- **Channel**: In the inner region, it is an eigenfunction of the Hamiltonian for the \( N + 1 \)-electron system. They are orthogonal to each other. The channels conserve the quantum numbers of the total angular momentum \( J \) and parity \( \pi \), in the case we are working in level-resolved, relativistic \( J\pi \) coupling; or orbital angular momentum \( L \), total spin \( S \) and parity \( \pi \) in the case we are working in term-resolved non-relativistic \( LS \) coupling. Hence, channels are associated to the partial waves. Channels can be:
– Open: a channel is classified as open when the energy of the incident electron exceeds the energy between an initial term/level and a final term/level. In this case, a transition may be produced, the final population of the channel will be larger than zero. It has an oscillatory asymptotic form.

– Closed: A channel is classified as closed when the incident electron energy is less than the energy between and initial term/level and a final term/level. In this case, the transition is energetically impossible. It has an exponentially decaying asymptotic form.

• Phase shift $\delta_{J_\pi}$: phase shift of the wave function in the asymptotic region with respect to the case of a pure Coulomb potential, in the case of ion target; or constant potential, in the case of neutral target. Transition matrices, and in consequence cross sections, may be determined in terms of the phase shifts.

• Transitions matrix $T_{i f}^{J_\pi}$, from initial state $i$ to final state $f$: transition amplitudes. Its module square $|T_{i f}|^2$ is the transition probability from the initial target state $i$ to the final one $f$. The calculation of the transition matrix is particular and independent for each partial wave. $|T_{i f}|^2 = \sum_{J_\pi} |T_{i f}^{J_\pi}|^2$

• Collision strength $\Omega(i - f)$, from initial state $i$ to final state $f$. Dimensionless version of the cross sections, see [3] for details. $\Omega(i - f) = \sum_{J_\pi} \Omega^{J_\pi}(i - f)$

• $R$-matrix $R^{J_\pi}$: A matrix $(n_{channels} \times n_{channels})$ which connects the wave functions of the channels between the inner and the outer region. This matrix is the key to calculate the phase shifts, and with them the transition matrices, collision strengths and cross sections. See [3] for theory details.

3. Overview

$\texttt{pstgf}$ v1.1 beta 2019 is an upgrade of the previous working version v0.87.\footnote{http://connorb.freeshell.org} The program is implemented in Fortran90 language, parallelised with the message passing interface (MPI) protocol, and with optional CUDA features for further optimisations. $\texttt{pstgf}$ reads as input the target state eigen-energies, the channels associated with each target state for each partial wave, and the surface amplitudes...
(acquired from the matrix diagonalisation) for each partial wave. All this information is encapsulated in the $H.DATXXX$ file. PSTGF enforces the continuity of the radial wave function and its first derivative between the inner and outer regions via the $R$ matrix. The main goal is the solution of the Schrödinger equation for one electron under the potential created by the multipole expansion potential of the others, as a single particle model, neglecting the electron exchange. This may be expressed as

$$\left[ -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + \frac{2z}{r} + \epsilon_n \right] F^{J\pi}_n = \sum_{m=1}^{N} U^{J\pi}_{nm} F^{J\pi}_m,$$  \tag{1}$$

with $n$ from 1 to $N$, number of channels in the partial wave $J\pi$, $r$ is the radial coordinate, $l$ is the orbital angular momentum, which depends on the partial wave $J\pi$, $V = \frac{2z}{r}$ the potential in the outer region; $z = Z - N_e$ is the effective charge. $\epsilon_n = E - \epsilon_n$ is the channel reduced energy, being $E$ the impact energy of the projectile, and $\epsilon_n$ the excitation energy of the individual target level, hence $\epsilon_n > 0$ determines an open channel, while $\epsilon_n < 0$ a closed one. $F_n$ is the radial wave function, and $U_{nm}$ is the long-range multipole expansion.

Once equation (1) has been solved, the radial wave function $F_n$ is calculated from the asymptotic region to the interface between the inner and outer regions $r_0$, then we have to match the solution with that from the inner region to fulfil its continuity. This is achieved by the $R$ matrix, which performs the unitary transformation among the channels to fulfil the continuity of the radial function and its first derivative

$$F_n(r_0) = \sum_{m=1}^{N} R_{nm} \left( r_0 \frac{dF_m}{dr} \bigg|_{r=r_0} - b F_m \right),$$  \tag{2}$$

$b$ is defined by the boundary conditions in the inner region, as the value of the logarithmic derivative of the radial wave function in the interface between inner and outer region. This is usually chosen to be zero.

The surface amplitudes $w_{nk}$ are defined as follows

$$w_{nk} = \sum_{j=1}^{n_c} c_{njk} u_{nj}(r_0),$$  \tag{3}$$

where $u_{nj}(r_0)$ are the reduced surface amplitudes in the inner region; and $c_{njk}$ coefficients obtained from the $N + 1$ Hamiltonian diagonalisation. The summation extends to the size of the continuum basis for each orbital $n_c$. $n$ extends over the
number of channels, while \( k \) the second index is over the Hamiltonian matrix size. The \( R \) matrix itself can be defined as follows.

\[
R_{nm} = \frac{1}{2r_0} \sum_{k=1}^{M} w_{nk} w_{km} (E_k - E),
\]

(4)

where the \( E_k \) are the R-matrix poles or eigenvalues of the \( N + 1 \) system. This expression was traditionally the part of the calculation which took the most of the time, but now has been highly optimised using the CUDA programming techniques for GPU (Graphical Processing Units). For further mathematical details we refer to [16, 17, 3].

Note in equation (1) that the reduced energy \( \epsilon_n \), greater or lower than zero, will determine the character of the channel, open or closed, so a different asymptotic behaviour, see Section [2]. The relative number of open and closed channels for a value of the impact energy will be relevant in terms of the computation, we designate as \( n_o \) the number of open channels and \( n_c \) the number of closed channels. Equation (1) varies slightly if written in a different coupling scheme ie. Dirac R-matrix calculations replace \( l \) with \( \kappa \). Equation (1) has to be solved for all the values of the impact energy \( E \) and the complete set of partial waves \( J\pi \), usually several thousands of times. For ions, the collision strengths versus the impact energy present narrow Rydberg resonance structures and as a consequence the grid of the impact energies has to be quite fine to delineate them.

Use of \textsc{pstgf} assumes that the eigen-energies and eigen-functions in the inner region have been previously calculated, so we know all the channel energies \( E_n \) and coefficients \( w_{nk} \) for all the partial waves. This can be done with several methods and software packages; some examples are RMATRX [5], DARC [6, 7], or BSR [18]. All the information about the channels in the inner region \( (E_n \text{ and } w_{nk}) \) is stored in a set of generic binary files \textsc{H.DATXXX}. These may be concatenated into a single \textsc{H.DAT} file, used by previous versions of the code, though for good optimisation we would advise against this. Ideally, the inner region has diagonalised every Hamiltonian concurrently and the Hamiltonians are already in this \textsc{H.DATXXX} form. \textsc{pstgf} requires as input the values of the wave functions of all the channels at the boundary of the inner region \( r_0 \) for all the partial waves. With this initial conditions, \textsc{pstgf} expands the wave function in terms of equation (1) from \( r_0 \) up to a certain asymptotic limit \( r_1 \), in which the wave function can be replaced by its analytic form, of a Coulomb function in case of a charged target, or a spherical Bessel function in case of the neutral target. From this point onwards, the wave function \( F^{J\pi}_{n} \) just follows its analytical asymptotic solution.
face between the inner and outer region $r_0$, we have to impose the continuity of
the wave function and its first derivative.

The main calculation is distributed in two nested iterative loops. The first loop
runs over partial waves $LS\pi$ or $J\pi$, \texttt{pstgf} has input options (\texttt{dstgf}) to calculate
all the partial waves stored in \texttt{H.DATXXX} files or to restrict the calculation to a
subset of them. To obtain the final collision strengths $\Omega$, \texttt{pstgf} has to sum up
all the contributing partial ones $\Omega_{J\pi}$, obtained for each partial wave. The second
loop concerns the impact energies $E$, this loop runs over a set of $NE$ discrete
values of the scaled energy $E_k$. This grid should be fine enough to delineate fine
Rydberg resonance structure, and therefore requires a minimum several thousand
energy points. The loop in energy is the one which is parallelised, the energy
array \{\textit{E}_k\} is split among the processors \textit{nproc}, so each processor is assigned a set
of \textit{nproce} = $NE/nproc$ energies to calculate. For an optimum performance, the
number of energies should be an even divisor of \textit{nproc}, if this is not the case, then
\texttt{pstgf} will add additional points to enforce this.

The first step in the calculation is to determine which channels are open and
which ones are closed, so their asymptotic behaviour is set as boundary condition
to the equation (1). Then, \texttt{pstgf} performs a Numerov method to propagate the
coupled radial wave functions $F_{nm}^{J\pi}$ from the boundary of the inner region $r_0$ and
the asymptotic limit $r_1$. An overview of the operating mode of \texttt{pstgf} is as follows:

1. Read standard input: energy grid \textit{E}, partial waves $J\pi$ to be processed, other
calculation parameters.
2. Read information about the target \texttt{H.DAT}, $J\pi$ independent.
3. Start loop in $J\pi$.
4. Read information about the partial wave $J\pi$ \texttt{H.DAT}.
5. Start loop in \textit{E}. Parallel, split all the \textit{E} values in all the processors.
6. Calculate partial $\Omega_{J\pi}$ for each energy.
7. End loop in \textit{E}.
8. End loop in $J\pi$.
9. Add up the partial $\Omega_{J\pi}$ for all partial waves, add the top-up up to $J \rightarrow \infty$,
and get the total $\Omega(E)$.
10. Write output to file \textit{OMEGA}.

4. Computational details

As computer hardware capabilities have improved, more complicated systems
have been undertaken, resulting in increasing number of symmetries and more
channels being calculated by \texttt{PSTGF}, which revealed some implementation issues. The first problem detected was the large time differences based upon different incident electron energies. The key understanding in this issue concerns the number of open and closed channels \( n_o, n_c \). It was detected that when both were approximately equal \( n_o \sim n_c \), the computation time increases dramatically in comparison to the cases where either only a few channels were open, or all channels were open. Therefore, in the input array of impact energies \( E_k \), there is a distinction between what we call “fast energies” and “slow energies”. Usually all the partial waves include channel energies up to a certain threshold \( E_{\text{max}} \), common for all partial waves. Up to now, for a fixed impact energy, all the partial waves will have a similar number of open and closed channels. In other words, if an energy is ‘fast’ or ‘slow’ for an individual partial wave, most probably, it will have the same character for all of them. However, computationally the bottleneck lays in the energies around those with half the channels being closed and the other half open. In previous v0.87 version, the energy array to be calculated by each processor was independent of the partial wave, and all the processors worked on the same energies for each and every partial wave. When the number of processors increases that gave rise to some of the processors only had a small number of slow energies, or even none, while other processors had to work considerably harder for several slow energies for all the partial waves. Hence, the time distribution among the processors was very different and the fastest ones remained idle for large parts of the calculation, while waiting for the few slow ones. This problem is maximised when the number of processors increases, so there are less energies per processor to proceed. In new version v1.1, we fix this issue and improve the time balancing by having the energy grid different for each partial wave, so the amount of fast energies and slow energies calculated by each processor is evenly distributed. Figure 1 shows a diagram of this energy distribution to the processors, in the left picture (v0.87) each processor works only an energy array for all partial waves, while in the right picture (v1.1) each processor works all the energies.

In v0.87 all the processors worked the same energies for all the partial waves, and the output was split into several \texttt{OMEGAXXXX} files, \texttt{XXXX} being the index of the processor, from 0000 to 9999. Each processor was assigned a unique output file, containing unique calculated energies which via a post-processing code, sorted and collated each file into a single universal \texttt{OMEGA} file of ascending incident energy values. In v1.1 all processors calculate all energies, but never consecutive energies for the same partial wave. This mitigates the issue of the ‘slow’ and ‘fast’ energies, as no individual processor is assigned the half-closed/half-open channel energy for all partial waves, this now becomes shared among all proces-
Figure 1: Colour online. Diagram of energies and symmetries worked by each processor. Left: v0.87; right v1.1. \( E_i \) represents the energy array to be processed by processor \( P_i \) in the partial wave \( J_\pi \). The oval represents the partial wave where the processor \( P_i \) starts calculating.

As consequence, each \textit{OMEGAXXXX} will not contain a converged collision strength at each energy point, in fact each \textit{OMEGAXXXX} file now containing every energy only has meaning when summed over the respective energy points in all files. Consequently, the \textit{OMEGA} output file can not be split, and therefore the partial collision strengths are added up inside \textsc{pstgf} using the MPI routine \texttt{mpi\_reduce}, and a single \textit{OMEGA} output file is produced.

A second lack of efficiency of previous versions to v0.87 was the reading of the input file \textit{H.DAT}. If the number of partial waves and channels increases, the size of the \textit{H.DAT} file can reach several gigabytes. In previous versions of \textsc{pstgf}, this single file had to be read by all the processors each time they started the calculation for a new partial wave. It was usual when the program was started, that all the processors attempted to read the same large file at the same time, inevitably leading to some processors blocking others, wasting computing time. Version v0.87 had already implemented the possibility to work beyond a single large \textit{H.DAT} file, by splitting the monolithic single \textit{H.DAT} into several smaller \textit{H.DATXXX} files, being XXX the label of the partial wave, from 000 to 999. Then for each partial wave, the processor must read just the individual \textit{H.DATXXX} which contains the information about it, and not the whole \textit{H.DAT} file, with several records of irrelevant information. Nevertheless, it was still a blocking issue when all the processors attempted to read the same file for the same partial wave, especially at the starting of the calculation. As mentioned above we solve this problem changing the order that the processors work the partial waves. In v1.1 all the processors carry-out all the same partial waves, but with the difference being, not in the same order. This implementation avoids all the processors reading from the same file at the same time, so these reading waiting queues are minimised.

Finally, other programming semantic improvements have been performed. All common blocks have been removed and replaced by \texttt{module}, so the programming style is clearly \texttt{fortran90}. All the statically dimensioned arrays and matrices have
been removed, previously enforced through a parameter file (PARAM). Now, all arrays/matrices are designated allocatable and their scope is dynamically assigned based upon the values read from the H.DATXXX files. With this change, PSTGF does not suffer from unexpected segmentation faults, due to a badly user defined variable in the PARAM file. In addition, the memory usage is minimised to the essential required. The calls to auxiliary routines from libraries LAPACK and BLAS has been strategically modified in order to take advantage of their optimisation. Another change carried out in the subroutines that contain the most load of work for PSTGF, is to split the memory in an strategic efficient way to work at cache level, with faster access.

5. CUDA optimisations for PSTGF

As the processor speed of individual CPUs has remained largely stagnant for the last decade, one option to maintain greater scalability of existing codes is to interface with the power of GPUs (graphical processing units). Cuda fortran combined with Nvidia GPUs is one of the simplest ways to seamlessly harness the

![Figure 2: Colour online. Half of the symmetric R-matrix is calculated by 10 matrix multiplies, and then symmetrised for the full result. We optimise the memory usage of the GPU, by allowing several mpi tasks to access the GPU simultaneously. In the figure, the blue, red and green blocks are representative of a particular matrix multiply but for different energies and partial waves, and hence different R-matrices.](image)
power of MPI and the GPUs. GPU usage is ideally suited to dense matrix multiplies, and the initialisation of the R-matrix falls into this category. As illustrated in the Figure 5, the R-matrix can be calculated in a single matrix multiplication, but this would exhaust the total memory of the GPU by a single processor. A more optimal use involves separating the R-matrix formation into ten smaller matrix multiplies, essentially pipelining them, one after another. The collective result from these 10 matrix multiplies, can be then symmetrised to provide the full result. This greatly reduces the consumption of memory on the GPU and allows more MPI tasks to concurrently access it. The different coloured blocks, and the respective positioning in the resulting R-matrix is given in Figure 5, and corresponds to 3 different R-matrix matrices, at 3 different energies, being carried out concurrently. Actual matrix multiplies are further optimised by padding the larger matrices with zeros to ensure that the matrices fall on optimal, divisible by 32 or 64 boundaries.

Traditionally, for medium to small cases the most time-consuming aspect of the code was the formation of the R-matrix itself (subroutine RINIT). Test cases for neutral Fe, show that for 7261 channels and a Hamiltonian size of 106 661 takes 14 – 18 secs per R-matrix formation and achieves a factor of 80 – 100 speed-up over existing code.

6. Code Structure

6.1. Input files

6.1.1. Standard input

File dstgf, mandatory, ASCII.
Structured in namelist blocks, and optionally additional parameters.

- namelist stgf General calculation parameters, mandatory.
  - iprint Integer from -2 to 3, moderates level of standard output (routf). Default = -2. Mainly used for debugging, a value of -2 will print to standard output the minimum essential information, while a value of 3 will print the maximum available information to the standard output file, with associated increase in the file size.
  - ipert Integer from 0 to 4. To include the long-range multipole potentials. = 0, default. Omit the long-range multipole potentials. = 1, 2 Omit long-range multipole potentials for closed channels when
their asymptotic tail extends outside the asymptotic limit $r_1$.

= 3, 4 Include all the long-range multipole potentials, consider the contribution from $r_1$ to infinity.

= 1, 3 Perturbation for the $T$ matrix.

= 2, 4 Perturbation for the $K$ matrix.

See QDT-variable section for more details.

– **pert** Character(3). Activates the perturbation, variable *ipert* automatically. Useful if QDT is not activated.

  = "YES" or = "yes" Activate perturbation, set *ipert*= 4.

  Otherwise, default, not activate perturbation, set *ipert* to its default value (0).

  This variable should not be included in the namelist if *ipert* is set manually.

– **ac** Real positive. Default = $1.E - 5$. Accuracy/tolerance required for some numeric subroutines.

– **imesh** Integer, negative or from 1 to 3. Mandatory, no default value. Define the energy mesh,

  = 1 For fixed linear grid of incremental energies.

  = 2 For fixed non-linear grid based upon effective quantum number (not recommended).

  = 3 Read directly the energy mesh from standard input. See below.

  = $-2S + 1$ To chose appropriate mesh for a case of spin $S$ (not recommended).

See namelist *imesh1, imesh2, imesh3* for details.

– **iopt1** Integer = 1, 2, -1, -2, 10, 11. Defines the partial waves $S \pi \sigma$ or $J\pi$ to be calculated.

  = 1 default. Calculate all the symmetries stored in the $H.DATXXX$ files.

  = 2 Specify directly in the standard input (dstgf) the symmetries to be calculated. See below format *additional variables*.

  = -1, -2 As options = 1, 2 but treat target levels as degenerate, specify the degenerate levels after namelist, see below *additional variables* and *nastd* parameter.

  = 10, 11 For JAJOM, obsolete and not implemented in parallel code.

– **minlt, maxlt** Case iopt1= 1, Operate only the symmetries which fulfil $L, 2J \geq \text{minlt}$ and $L, 2J \leq \text{maxlt}$. 
Default \( \text{minlt} = -1, \text{maxlt} = 1000 \). Do all the symmetries. Irrelevant if \( \text{i0pt1} = 2 \).

- \text{irdec} Integer = 0, 1, 2. For radiative decays.
  - 0, default, no radiative decays are calculated.
  - > 0 radiative decays are calculated for excitation and DR if activated (see variable \text{nrmert} > 0).
  - 1, no QDT, Bell and Seaton radiative decays.
  - 2, if MQDT activated, Hickman-Robicheaux radiative decays.

- \text{lr glam} Integer. For high-\( L \) top-up.
  - Negative default, no top-up.
  - Positive, perform top-up from the highest calculated partial wave up to infinity.
  - If top-up is activated then the partial waves must be calculated in ascending order by all the processors, so the efficiency is reduced. It is recommended to use the top-up option in a single calculation including only the two last partial waves.

- \text{lcb e} Integer. For dipole top-up.
  - Default same value as \text{lr glam}. Not recommended to modify.

- \text{itop} Integer. Controls the non-dipole top-up over degenerate states.
  - -1 default, interpolate between degenerate and non-degenerate limits when energy ratio exceeds \( 2L \).
  - Other case, interpolate between degenerate and non-degenerate limits when energy ratio exceeds the \( J \) ratio.
  - Not necessary if \text{i0pt1} positive. Not recommended to modify.

- \text{elas} Character(3). If elastic collision strength should be written to output file.
  - "YES" or "yes" Write elastic transitions to \text{OMEGA} file.
  - Otherwise, default. Do not.
  - If the target is neutral, the elastic collision strengths are written by default, unless directly specified not to.

- \text{iprkm} Integer from 0 to 4. Print \text{K} matrixes in optional output file \text{KMAT.DAT}. For ICFT method.
  - 0 Default, no write \text{K} matrix.
  - 1 Each processor writes a sequential file \text{KMAT.DATXXXX} file with the physical \text{K} matrix elements, being XXXX the processor number.
  - 2 Write unphysical \text{K} matrix to \text{KMATLS} file. Not implemented in
parallel code.
= 3 For input of post-processing differential cross sections. Removed from code.
= 4 Each processor writes unphysical \( K \) matrixes to \( KMTLS.YYY.XXXX \) files, if QDT is not activated, or \( S \) matrixes to \( SMTLS.YYY.XXXX \) files, if QDT is activated, prepared as input for ICFT code. \( YYY \) is the number of symmetry, and \( XXXX \) the number of processor. Not recommended to use this option, ICFT code is not prepared for present implementation of \( \text{pstgf} \). To work in ICFT formalism, use previous v0.87 version.

- \( \text{idip} \) Integer. If = 1 then write the dipole line strengths \( S \) to output file \( \text{STRENGTH.DAT} \).
  If = 0, default, do not write the line strengths.

- \( \text{nomwrt} \) Integer. Output management.
  If > 0, default +\text{Large}(1). Collision strengths \( \Omega \) for first \( \text{nomwrt} \) transitions are written to output file \( \text{OMEGA/U} \) as upper triangle row-wise.
  If < 0 Collision strengths \( \Omega \) for first -\text{nomwrt} transitions are written to output file \( \text{OMEGA/U} \) as upper triangle column-wise.
  If = 0 No \( \Omega \) are written.

- \( \text{bigge} \) Integer. If > 0 print the infinite energy limit of the \( \Omega \) for dipole transitions, see [19] for details.
  If = 0, default, do not.

- \( \text{isgpt} \) Integer. If > 0 then write partial-wave cross sections to output file \( \text{SIGPW.DAT} \).
  If = 0, default, do not.

- \( \text{itrmn}, \text{itrmx} \) If \( \text{isgpt} \neq 0 \) then write in output file the partial-wave cross sections from transition \( \text{itrmn} \) to transition \( \text{itrmx} \) and also the sum of these partial wave cross sections for each \( J\pi \) partial wave.

- \( \text{print} \) Character(6). If ="FORM" or ="form", default, then write the \( \Omega \) to the final output \( \text{OMEGA file ASCII formatted} \).
  Otherwise, write the \( \Omega \) to the file \( \text{OMEGAU binary unformatted} \).

- \( \text{mzmeg} \) Integer, default \( \text{Large}(1)/2E20 \) (no scratch files to open). Mega-words of memory available to store in memory the \( \text{omem} \) array, containing all the open-channels collision strengths for all energies. If the size of \( \text{omem} \) is larger than \( \text{mzmeg} \times 8 \times 2^{20} \) bytes, then a scratch file
must be opened to store the array in hard disk. Warning, one scratch file is opened by each processor, if the number of processor is large, the hard disk can be exhausted.

- \( mzfts \) Integer, default = 3201. Number of spatial grid points of the outer region, to perform the Numerov integration.

- MQDT variables
  - \( iqdt \) Integer. Controls the MQDT operation. 
    If = 0, default, then no QDT operation is performed. 
    If = 1 then full MQDT, all channels treated as open, it uses unphysical K/S matrixes. 
    If = 2 then work with unphysical K matrixes rather than S ones. 
    If \( iqdt > 0 \) then higher dipole perturbing potentials will be included in terms of variable \( ipert \).
  - \( imode \) Integer. Controls read and write of unphysical matrix when MQDT is activated. 
    If = 0, default, then calculate the unphysical matrix and write it to output file JBIN. 
    If = 1 then read the unphysical matrix from file JBIN. Solution on a newly defined energy mesh obtained solely by interpolation of the previous coarse mesh data read. 
    If = −1 then single pass operation. It is performed a full solution on a coarse mesh and an interpolative solution on a fine mesh.
  - \( ijb \) In Integer. If = 0, default, do not write JBIN file in case \( imode=0 \).
  - \( lmx \) Integer. If perturbations are activated, largest perturbing multipole. Default = 2, quadrupole.
  - \( ieq \) Integer. Controls how often the unphysical K or S matrix is updated. 
    If > 0 then K or S matrix is updated at \( ieq \) linearly spaced energies across the total energy range defined by the input energy mesh. 
    If < 0, default = −1, then K or S matrix is updated at every \( |ieq| \)th point of the mesh, fine for constant step in a previously calculated coarser energy mesh (\( imode=1 \)), not so good (inefficient) for constant step in effective quantum number.
  - \( qetest \) Floating point, default = 1.\( E − 7 \) scaled Rydberg. The K or S matrix is only re-interpolated when the total energy has changed by
more than the \textsc{qetest} value since the last time. It gives a small time saving when using a very fine mesh.

- \textsc{fnumin} Floating point, default = 0.0. The effective quantum number below which the closed channel is omitted when iqd= 1, 2.

- \textsc{fnuhyb} Floating point, default = −1.0. The effective quantum number below which the closed channel is a $\Theta$ function rather than $S$ and $C$ ones, when iqd= 1, 2.

- \textsc{iomsw} Integer, MQDT. If = 1, default, then full MQDT, it omits closed channels with $n < l + 0.1$.
  - If = 0 then MQDT: keep (with $a = −a$, \textsc{iomit}(ichan)= −1 in subroutine SC when $a < 0$).
  - If = −1 then hybrid: use $\Theta$ functions for $\nu < \textsc{fnuhyb}$ and $\nu < l$, otherwise operate as in case \textsc{iomsw}= 0.

- \textsc{lfrtsw} Integer, default −1 for ions and 5 for neutrals. Value of $L$ or $2J$ above which negative $\textsc{ipert}$ is allowed.

- \textsc{iccint} Integer. Whether to include closed-closed channels perturbing integrals in both MQDT or non-MQDT operations.
  - If = 1, default, include them.
  - If = 0 not included.

- \textsc{intpq} Integer. Use internal calculation subroutine.
  - If = 0, default, use CORINT subroutine for closed channel MQDT $S$ and $C$ integrals.
  - If = 1 use $\Theta$ function subroutines to generate $Q$ integrals.

- **namlst mesh1** Mandatory if imesh=1. Otherwise not present.

  - \textsc{mxe} Integer, number of electron-impact energies.
  - \textsc{e0} Floating point. First $z$-scaled energy of the grid.
  - \textsc{eincr} Floating point. Energy increment, step.
  - \textsc{qnmax} Floating point, default = −1.0. If iqd= 0 no MQDT except Gailitis average for $n > \textsc{qnmax}$.
– **ABVTHR** Floating point, default = −1.0 for ions or 1.E-3 for neutrals. Drop energies from the grid within \( ABVTHR \) \( z \)-scaled Rydberg above the first excitation threshold. If negative, do not drop any energy.

– **BELTHR** Floating point, default = −1.0 for ions or 1.E-3 for neutrals. Drop energies from the grid within \( BELTHR \) \( z \)-scaled Rydberg below the first excitation threshold. If negative, do not drop any energy.

For an optimum performance \( MXE \) must be an even multiplier of the number of processors. This condition is sometimes difficult to fulfil if \( ABVTHR \) or \( BELTHR \) are used, so energies are dropped from the grid. This happens commonly in the case of neutrals.

- **NAMELIST MESH2** Mandatory if \( IMESH=2 \) or negative, otherwise not present. This option is not yet implemented in PSTGF.

- **NAMELIST MESH3** Mandatory if \( IMESH=3 \). Otherwise not present.

  – **MXE** Integer, number of electron-impact energies.

- Additional variables not sorted as namelist, mandatory for determined values of the variables in namelist \( STGF \), see above.

  – Case \( IOPT1=2 \). After the namelist \( STGF \), a list of 3 integers of user supplied length, denoting the partial wave symmetries to be calculated. These symmetries should be present in the H.DATXXX passing files. Each shortlist denotes \( 2S + 1 \ L \ \pi \) of the partial wave. If \( 2S + 1 = 0 \) then the second integer is interpreted as \( 2J \). \( \pi \) must value 1, for even terms or levels, or −1 for odd terms or levels. If a shortlist −1 −1 −1 or an END-OF-FILE indicates end of symmetry list.

  – Case \( IOPT1=−1,−2 \). In this case the target term or level energies are treated as degenerate, and the number of degenerate terms or levels for each target energy must be read in.

One integer \( NASTD \) is expected after namelist \( STGF \), number of degenerated energies. Afterwards a shortlist of \( NASTD \) additional integers, number of degenerated terms or levels for each energy. In the case \( IOPT1=2 \) the list of partial-wave symmetries is specified after the shortlist of the degeneration of the energies.
– Case imesh= 3. After the namelist mesh3, expected a total of mxe floating point numbers, electron-impact \( z \)-scaled energies in Rydberg, sorted from smallest to largest. For an optimum performance, mxe should be an even multiplier of the number of processors.

6.1.2. H.DAT

Mandatory, binary.

Binary output from the inner region codes, used as input for the outer region codes.

It can be presented in three different ways. \texttt{pstrgf} inquires which one is present in the following order, if several types are present, just the first one inquired as positive is used, the remaining ones are just ignored:

1. Several H.DATXXX files, starting by H.DAT000 (recommended). H.DAT000 contains the information about the target and at least the first \( J_\pi \) or \( LS_\pi \) partial wave. Each H.DATXXX file contains information about the channels of one (recommended) or several partial waves. In the case the number of H.DATXXX files is the same than the number of lines in the sizeH.dat file and the sorting of the XXX indexes agrees with the sorting of partial waves in sizeH.dat (see 6.1.3) the performance will be optimum.

2. One single H.DAT file. The single file contains the information about the target and the channels of all the partial waves calculated in the inner region. \texttt{pstrgf} will still work, but its performance will be not optimum due to all the processors will have to read the same large file for all the symmetries.

3. One single DSTGH.DAT file. For inner region calculations with the old version DARC code, now obsolete. The option is kept just to allow the code work for older calculations, but it is not recommended for new work.

6.1.3. sizeH.dat

Optional, nevertheless highly recommended, ASCII.

All the codes that work the inner region and provide H.DAT files are able to provide an auxiliary formatted sizeH.dat file. There are two kinds of sizeH.dat files readable by \texttt{pstrgf}. It inquires if they exist in the following order:

1. \texttt{sizeH.dat} for \( LS_\pi \) or \( J_\pi \) coupling.

2. \texttt{sizeBP.dat} for \( J_\pi \) coupling only.

If both files exist, only \texttt{sizeH.dat} is read by \texttt{pstrgf} and \texttt{sizeBP.dat} is ignored. sizeH.dat contains the basic information about each partial wave: \( 2S + 1, L, \pi, \ldots \)
number of channels, number of continuum basis \( \times \) number of channels, number of eigenvalues for the \( N + 1 \) Hamiltonian. If \( 2S + 1 = 0 \) then \textsc{pstgf} assumes that partial waves are presented in \( J\pi \) coupling and \( J = 2L \). The number of lines in the file is interpreted by \textsc{pstgf} as the number of partial waves stored in the \textit{H.DATXXX} files (see \[\text{[6.1.2]}\]). The best performance is reached if there is exactly one partial wave per \textit{H.DATXXX} file and the sorting of the XXX indexes agrees with the sorting of partial waves in \textit{sizeH.dat}.

\textit{sizeBP.dat} file works the same way as \textit{sizeH.dat} file but it has no value of \( S \) stored, it assumes always \( J\pi \) coupling.

If no \textit{sizeH.dat} or \textit{sizeBP.dat} files are found or they have different number of lines than the number of \textit{H.DATXXX} files, then a preliminary read of the \textit{H.DATXXX} files has to be carried out in order to let the program know in which file is stored which partial wave, and that will take some time if the files are large. A correctly formatted \textit{sizeH.dat} will help a good performance of \textsc{pstgf}.

\textbf{6.1.4. DBUT}

File to store the Buttle correction. It works only for old versions of inner-region codes, currently the Buttle correction is integrated in \textit{H.DATXXX} files.

\textbf{6.2. Output files}

\textbf{6.2.1. Standard output}

File \textit{routf} from processor 0 and \textit{routfgXXX} from other processors, being \( XXX \) the processor number, ASCII. Standard output, execution information, warnings and errors. If the calculation finished OK, with no errors, then the standard output files from processors different to 0 will have no additional information, and they can be removed to save space in the hard disk.

\textbf{6.2.2. OMEGA/U}

Final results, binary or ASCII depending on input variable \textsc{print}.

One single file, if in the standard input the variable \textsc{print} is specified as \textquotedblleft FORM\textquotedblright; then output will be formatted in an \textit{OMEGA} file, any other value and it will be unformatted with sequential access in an \textit{OMEGA/U} file.

In any of the formats it contain the following information:

- First record: nuclear charge and number of electrons of the target.

- Second record: Number of target terms or levels, number of impact energies and number of transitions stored, \textsc{nomwrt}, or between all the target levels, it can also contain elastic transitions if variable \textsc{elas} is set to \textquotedblleft YES\textquotedblright;
Third record: Array containing the $LS\pi$ or $J\pi$ of each target term or level.

Forth record: Array containing the term or level excitation energies of the target in Rydberg scaled units with respect to the ground state energy.

Following records: Impact energy in Rydberg and array with the $\Omega$ values for the collision strengths for that energy. The $\Omega(i - j)$ matrix is stored as the upper triangle by rows or columns depending of the sign of the variable NOMWRT.

6.2.3. SIGPW.DAT

XXXX: index of processor.
Partial wave transition amplitudes, to calculate partial cross sections. If ISGPT = 1.

6.2.4. JBINLS.DAT

XXXX: index of processor.
Channel information to input in STGICF. If IPRKM = 4.

6.2.5. SMTLS.YYY.XXX

XXXX: index of processor; YYY: index of symmetry.
Unphysical S matrix, to be used as input for STGICF. If IPRKM = 4 and QDT is active.

6.2.6. KMTLS.YYY.XXX

XXXX: index of processor; YYY: index of symmetry.
Unphysical K matrix, to be used as input for STGICF. If IPRKM = 4 and QDT is not active. These two files should be used with care, as the output is sorted by each processor in terms of its local energy grid. ICFT code does not work with present implementation of PSTGF, so these files can not be used unless PSTGICF is updated in a consistent way of current PSTGF version.

6.2.7. OMEGDR

Dielectronic recombination cross sections. If NDRMET > 0. PSTGF is not the appropriate code to use to calculate DR. The radiation-damped code PSTGFDAMP should be used instead.

6.3. STRENGTH.DAT

E1 collision strengths between all target terms or levels, if IDIP = 1.
6.3.1. TERM.DAT

Information about the target terms or level: $2S + 1$, $L$, $\pi$ and $E$. If $\text{iprkm}=4$.

6.4. Scratch files

6.4.1. SCRATCH1

File to store the $\text{oem}$ array if its dimension is larger than $\text{mzmeg} \times 10^6$. In this case a scratch file is opened and the array $\text{oem}$ is stored on the hard disk. One file is opened by each processor, if the number of processors is large, caution must be taken to ensure that hard disk is not unexpectedly filled.

The best practice is not to modify the default value of $\text{mzmeg}$ to ensure that no scratch files are open. There is also a reduction the input and output time.

7. Test cases

We have used v1.1 to calculate the electron-impact excitation of the ion $\text{Ni}^{3+}$, for 42 $J\pi$ partial waves, with a maximum of 1818 channels per partial wave and 10
Figure 4: Total time of each processor Ni^{3+}. The horizontal lines mark the total calculation time (maximum).
Figure 5: Total time of each processor Fe neutral. The horizontal lines mark the total calculation time (maximum).
energies per processor. We compare the computation time with the version v0.87. Figure 4 shows the real nature of the problem, how the calculation time is very different for each value of the impact energy. The difference between the named slow and fast energies is self-evident, reaching in the worst cases a factor ten. The most of the calculation time will be spent in energies around the 150 index.

Figure 4 illustrates the workload unbalance versus processor time. When some processors have to calculate a larger number of slow energies, other processors do not. In the slowest cases, the relative difference in the processing time can reach a 20%, this is unused processing time. In contrast, twisting the distribution of energy points and forcing all processors to work all energies, the workload balancing is greatly improved reducing the overall processing time by approximately 15%, and the maximum processor waiting time to less than one half. Both curves in figure 4 have the same area, but curve for v1.1 is flatter and its maximum (total calculation time) is a 15% smaller.

This difference is more evident in a more extreme calculation case. Figure 5 shows a calculation case for neutral Fe, with 10 partial waves and number of channels between 6943 and 7102. In this case we perform the calculation in the most extreme case, one processor per energy, and equal number of partial waves than energies, so each processor works only one symmetry in each energy. The unequal workload balance is more extreme in this case, reaching a comparative factor of 4 in the worst case. The effect of the twisting of the energies and symmetries leads to a reduction of a factor 1/2 in the computing time.

8. Example of input

We show an example the ASCII standard input (dstgf) for the case of electron-impact excitation of ion Ge$^{2+}$, 30-electron system plus projectile.

For the inner region calculation, we carried out 42 relativistic partial waves, with $J = \frac{1}{2}$ to $20\frac{1}{2}$, even and odd parity. From the inner region, 42 $H.DATXXX$ files were produced and one sizeBP.dat of length 42 lines, transcribing the partial wave symmetry associated with $H.DATXXX$ file. section 6.1.3.

We calculate in the outer region the collision strengths for the first 40 partial waves, from the first excitation threshold of the ion ($0.56 \text{Ry} = 0.14z^2$) to twice the ionisation limit ($5.0 \text{Ry} = 1.25z^2$), with a fine energy mesh of $10^{-5}z^2$.

```verbatim
&STGF IMESH=1 IQDT=0 IPRINT=-2 IOPT1=2 LRGLAM=-1 &END
&MESH1 MXE=120000 E0=0.1300 EINCR=0.00001 &END
0 1 0
0 1 1
```
With this input we will perform the calculation of the first 40 partial waves specified in sizeBP.dat file and no top-up, with the full balancing efficiency of \texttt{pstmt}, distributing read files in the different processors and doing the efficient energy split in processors and partial waves.

In order to use this efficient split, we are forced to deactivate the top-up procedure, through setting \texttt{LRGLAM} to negative. As a second step we perform the high-\textit{J} top-up, in this case it is necessary that all processors calculate the collision strengths for the same energies at least for the two last partial waves. Hence, to perform the top-up, we carry out a second calculation including just these two last partial waves. In this second calculation, we do not take advantage of the efficiency improvements of v1.1-2018, but it is a small calculation, so the loss in user time is minimal.

\begin{verbatim}
&STGF IMESH=1 IQDT=0 IPRINT=-2 IOPT1=2 LRGLAM=43 &END
&MESH1 MXE=120000 E0=0.1300 EINCR=0.00001 &END
  0  41  0
  0  41  1
-1 -1 -1
\end{verbatim}

This time, we set the top-up variable \texttt{LRGLAM} to the value of $2J$ of the first partial wave to be topped-up = 41. With the simple post-processing tool OMADD, we can add-up the two \texttt{OMEGA} files from the two calculations.

\section*{9. Future work}

All these improvements in the implementation have been applied to the undamped version of \texttt{pstmt}. Nevertheless, they do not modify the physics of the problem. As a consequence all these modifications can be integrated within the radiationally damped version \texttt{pstmt} with a similar increase of efficiency.

Likewise, it would be necessary to modify the ICFT code \texttt{psract} to allow for the reading of the files containing the $K$ and $S$ in a consistent way with current version of \texttt{pstmt}.

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