Combined-Multicore Parallelism for the UK electron-atom scattering Inner Region R-matrix codes on HECToR

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ABSTRACT: *Electron collisions with atoms were among the earliest problems studied using quantum mechanics. However, the accurate computation of much of the data required in astrophysics, plasma and optical physics still presents huge computational challenges, even on the latest generation of high-performance computer architectures, such as the Cray XE series. A suite of programs based on the 'R-matrix' ab initio approach to variational solution of the many-electron Schrodinger equation has been developed and has enabled much accurate scattering data to be produced. However, current and future calculations will require substantial increases in both the numbers of channels and scattering energies involved. An earlier dCSE report concentrated on optimization of PFARM (http://www.hector.ac.uk/cse/distributedcse/reports/prmat/), the program suite's high-scaling energy-dependent 'outer region' code. We now address the scattering energy independent 'inner region' in which intricate configuration interaction Hamiltonian and multipole matrices for the many-electron system are constructed (and diagonalized). Radial integrals and angular couplings are calculate separately then combined together. Serial, and in certain cases OpenMP-paralellized codes, have been extended to full many-node parallelism using a mixture of (a) mixed-mode MPI plus OpenMP techniques, and (b) pure MPI with intra-node shared memory segments and object-oriented Fortran 2003. Both methods take full advantage of the multicore nature of modern architectures. The three 'construction' codes now scale across multiple HECToR nodes. We have also developed two utility packages in object-oriented Fortran 2003: a shared memory segment package (with associated semaphores, intra- and inter- (virtual) node communicators etc) and a parallel I/O package adapted using asynchronous MPI-IO from an existing serial double-buffered direct access package: this allows independent parallel reading and writing combined with straightforward access to non-contiguous selections from large amounts of stored data. These utility packages are of course particularly suited to the R-matrix codes but are also of general interest.*

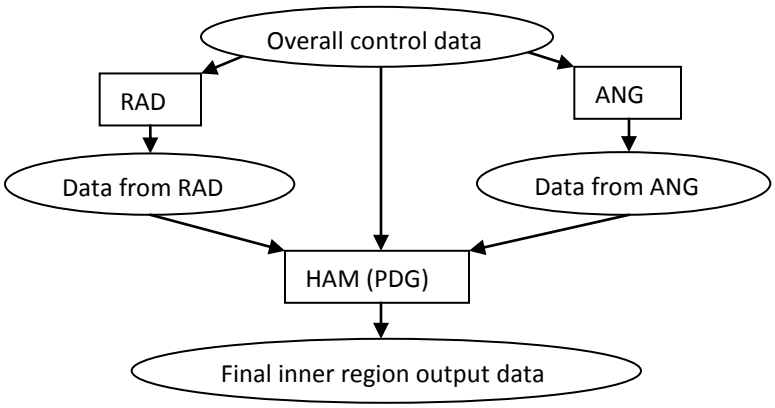
KEYWORDS: atomic physics, electron-atom scattering, R-matrix, configuration interaction, spherical tensor algebra, surfacing coefficients, Hamiltonian matrices, parallel computing, multicore systems, mixed-mode, shared memory segments, asynchronous parallel I/O, passive one-sided communication, object-oriented Fortran 2003, CCPForge.

1. Introduction

Electron-atom (ion) scattering data are essential in the analysis of important physical phenomena in many scientific and technological areas. These include the understanding of atmospheric processes, diagnostics of impurities in fusion plasmas (including JET and the new ITER project), interpretation of astrophysical data, the development of environmentally safer alternatives to replace mercury vapour lighting and investigations of laser-produced plasmas (such as for next-generation nanolithography tools). In addition, the HiPER project (http://www.hiper-laser.org) for laser-ignited fusion, with associated experiments in laboratory astrophysics, opacity measurements, laser-excited hollow atoms and atoms in strong magnetic fields will stimulate detailed calculations of atomic scattering data. Despite the importance of these applications little accurate collision (theoretical or experimental) data is available for many complex atoms and ions. Also of current (global) interest are electron-atom (ion) interactions in laser fields: multiphoton ionization, high intensity ultrafast processes followed by field-assisted recombination and scattering, harmonic generation and coherent control. In the UK, ab initio code to treat these laser field processes for atoms and molecules is being developed by, for example, the UK-RAMP consortium, supported by Collaborative Computational Project CCPQ (formerly CCP2) [1].

PRMAT [2] is a suite of programs based on the 'R-matrix' ab initio approach to variational solution of the many-electron Schrödinger equation for electron-atom and electron-ion scattering [3]. Relativistic extensions have been developed and the codes have enabled much accurate scattering data to be produced. The package has been used to calculate electron collision data for astrophysical applications (such as: the interstellar medium, planetary atmospheres) with, for example, various ions of Fe and Ni and neutral O, plus other applications such as plasma modelling and fusion reactor impurities (for example ions of Sn, Co, and in progress, W). In R-matrix calculations configuration space is divided into two regions by a sphere centred on and containing the atomic or molecular 'target'. Inside the sphere an all-electron configuration interaction (CI) calculation is performed to construct and diagonalize the full (energy-independent) Hamiltonian for each scattering symmetry within the finite volume in readiness for energy-dependent 'R-matrices' to be constructed on the boundary. The massively parallel outer region code PFARM was the subject of an earlier dCSE project [4]. The current project is focussed on the inner region codes, specifically the non-relativistic inner region codes comprising 3 or 4 standalone modules as shown below. The codes are used on HECToR by UK-RAMP and the 'Atoms for Astrophysics' project in particular.

Figure 1. Program flow for the inner region codes:



The RAD module calculates 1- and 2-electron direct and exchange radial Hamiltonian integrals plus multipole integrals for all the radial bound and continuum orbitals involved in the calculation: if the whole system comprises N+1 electrons (N-electron targets) then the wavefunctions will include antisymmetrized coupled products of N 'bound' orbitals (including 'pseudo-orbitals') and 1 continuum

orbital, plus certain antisymmetrized coupled products of N+1 bound orbitals: the continuum orbitals do not vanish at the sphere boundary radius. The ANG module calculates angular couplings for the diverse open- and closed-channel CI target state plus continuum orbital combinations and the 'N+1' product couplings: this is the most complicated module and a more detailed description is given in section 4. HAM essentially gathers together the diverse radial integrals and angular couplings required for each non-relativistic 'LSπ' (orbital and spin angular momentum, parity) scattering symmetry to form the N-electron target states and the N+1-electron scattering Hamiltonian matrices, plus N-electron multipole and, if required, N+1-electron dipole matrix elements. The Hamiltonians are then diagonalized and the eigenvalues, eigenvector boundary amplitudes and associated dipole matrices are output, either to the PFARM (or serial FARM [5]) code or to codes which modify and recouple the output for relativistic ('Jπ') calculations, or to the UK-RAMP multiphoton codes.

At the start of the project the package had become separated into two or three effective packages. For scattering calculations, radial continuum functions, orthogonal to the input bound orbitals, with fixed sphere radius boundary conditions were generated on a numerical grid (the 'traditional' method [2, 3]). RAD, ANG and HAM were serial codes (ANG included some OpenMP directives). The diagonalization was either performed serially with Lapack inside HAM, or for complex atoms with open d-shells a separate program PDG read output from HAM and performed it using ScaLapack. The N+1-electron dipole matrices were not required. For the UK-RAMP multiphoton codes, the RAD, ANG and HAM codes were needed to generate 'start-up' data for the TDRM [6] and RMT [7] laser-atom codes. The full dipole matrices were required. The radial continuum orbitals were generated from sets of B-splines, with the knot points chosen to form an appropriate radial grid. These functions obey arbitrary boundary conditions at the boundary radius, allowing the multiphoton calculation to proceed without certain disruptive (in this case) correcting factors [3] needed for the fixed boundary condition functions. In general ~100 (up to 200) B-splines are needed for each orbital angular momentum *l* (B-spline expansions are also used to fit to the input bound orbitals), compared to, say, 20 or 30 traditional continuum orbitals for each *l*. This RAD code was parallelized with OpenMP by H van der Hart (Queen's University Belfast), while HAM was purely serial: the 'targets' treated so far in this context are relatively less complex with open p-shells.

It was desired by the user communities to bring the packages back together as a single package maintained on CCPForge [8], so that future optimization and extensions would apply across the scientific applications. It was also desired to extend the RAD parallelization, parallelize HAM to allow for more ambitious calculations (both for complex atoms and for future applications and extensions for which the fixed boundary condition basis would be troublesome), and most importantly, parallelize the ANG code as this was becoming a major bottleneck for complex calculations despite a highly sophisticated procedure for dealing with the spherical tensor algebra [9].

2. dCSE personnel, objectives and outcomes.

The original application, sent in by the authors with backing from Dr M P Scott and Professor H V van der Hart of Queen's University Belfast, asked for 18 months of effort shared between AGS and CJN for an ambitious plan to achieve the above aims and to explore new coding that would make full use of the XE6 32-multicore many-node HECToR architecture (and hence comparable and future multicore HPC systems, also local multicore few-node systems). The plan was to explore both mixed-mode OpenMP/MPI coding and the use of IPC shared memory segments to utilize the multicore structure in a pure MPI context. The parallelization also implied use of parallel I/O between the internal region codes, with more standard/portable final output. Since the ANG code is the most mathematically complex, requiring an expert in theoretical atomic physics (and many-electron angular couplings) as well as in

numerical analysis and HPC, this would be handled by CJN, employing Fortran 2003 objects and structures to simplify the relation between the high-level coding and the theory while maintain high performance and future-proofing the code (as in his contribution to the previous dCSE project [4]). AGS would handle RAD developments, while HAM developments would be shared. The project was awarded 12 months' effort with instructions to attempt the full plan. Owing to commitments to the expanding PRACE [10] network, the final effort breakdown was around 0.7 (CJN) to 0.3 (AGS) and CJN has handled both ANG and the main development of HAM. Due to complications with compilers and other matters to be described below, a further concession was that during the project, the intra-node parallelization of RAD would be via OpenMP and that of ANG and subsequently HAM via MPI with shared memory segments. Summary outcomes are given here with more details and performance data in the following sections.

RAD objectives:

1. Combine the B-spline and 'traditional' continuum function generation with a single interface to produce a single RAD code for all applications.
2. Extend the OpenMP multicore parallelism to the bound orbitals and the general scheme to the 'traditional' continuum functions. Provide an option to use System V shared memory and pure MPI. (The OpenMP-produced data will produce results that can be used to assess the accuracy and performance of the System V MPI implementation).
3. Introduce a higher level task-management parallelism and MPI communicators over the *l* variables (for generation and integral combinations) and distinct bound or open (continuum) sections, with associated memory distribution. Use the 'xstream' parallel I/O library to keep track of parallel data and to write final data.

Objective 1 has been completed: RAD is now a single code with options for traditional and B-spline orbitals. The OpenMP code in objective 2 has been made more efficient as will be seen in the next section. This effort was concentrated on the B-spline code as for all the test cases so far the traditional RAD code takes much less time to run, the B-spline code having more 'orbitals' and 'grid' points, but it has also improved calculation of the traditional integrals. The 'shm' shared memory segment module developed for ANG was tested and verified independently (section 4). Since the application of OpenMP in RAD is computationally fairly straightforward and efficient, based on parallelizing certain important inner loops in both construction of orbitals and in subsequently performing the integrals (thus relatively few 'threadprivate' variables are needed in the Fortran 95 module-based code), replacing OpenMP with the shm module remains an option but was not prioritized.

The MPI introduction in objective 3 has been completed by distributing work over outer loops in the two halves of the code: the loops are essentially orbital indices {*n*, *l* expansion label and angular momentum} in the first half, and loops over 4 sets of orbital indices in the second half. This was not trivial as the orbitals generated in the first half of RAD are required by all loops in the second half which performs the integrals, thus some broadcasting is required. In fact, intermediate 'legacy' files storing the orbitals have been removed as modern systems have more than enough memory to cope with the data: using 'shm' to store this data is obvious follow-up work, to cope with future extremely large orbital bases. At the close of the project, the final output from RAD is being upgraded to allow data to be written using the new 'pfilehand' module developed for ANG (as part of CJN's 'xstream' package of custom I/O modules, see [4]).

ANG objectives:

1. Modification of the OpenMP code to improve scaling and performance, ideally simplifying the 'threadprivate' and binding requirements, with rigorous testing of the (relatively complex) OpenMP

structure to ensure strict compliance with OpenMP rules on HECToR. Incorporate the parallel 'xstream' I/O library to keep track of written data.

2. Incorporate the SMP parallelism into other sections of the code. Reproduce the parallelism using the System V module.
3. Introduce overseeing task-management MPI communicators into the outer loops over basic symmetries and 'open' and 'closed' sections of the code, with associated memory distribution.
4. At all stages, carefully comment and annotate the code. Give clear descriptions of the modular (and sub-modular) structure. While this will not directly contribute to output from performance benchmarks, it is essential for the long life and future enhancement of the code, and for the planned post-project) official CPC write-up (and hence enhanced user base). The availability of the code will be as for RAD, on the 4.5 (9 real) months timescale, with the code to be available on CCPForge.

The ANG code at the start of the project included OpenMP directives in the two places identified as needing parallelism: the initial construction of 'surfacing coefficients' and the subsequent 'bound-bound' coupling evaluation (these terms are explained in the detailed description in section 4) and had worked reasonably well in few-thread parallel on the IBM Power-series HPCx service (giving correct results). However on HECToR the code as written either failed to run or gave obviously incorrect results on all the compilers with OpenMP switched on. Race conditions were causing severe problems and examination of the code showed that the OpenMP was not strictly correct and standards-conforming: the IBM implementation was compensating for the errors. Some time was spent at the start of the project correcting more obvious errors, but the combination of Fortran 95 code structure, many 'threadprivate' variables and large numbers of out-of-scope variables made analysis difficult: the parallelism required for the code is coarse-grained over high level loops calling many subroutines. Owing to CJN's personal situation (he is retired and freelance, working from New Zealand and unable to travel, with HECToR access fast enough to work but not fast enough to allow full remote use of TotalView and similar tools), it was decided to suspend work on the OpenMP code and concentrate on MPI and shm. It is likely that a tool such as Intel Parallel Inspector [11] would be able to shed light on this problem and this remains as follow-up work for DL staff. However a practical reason for concentrating on the MPI approach is that many current and most envisaged calculations will certainly require more than one node to run in an acceptable time on batch-queue resourced systems such as HECToR.

The MPI/shm approach has turned out to be a great success and the new ANG code and the two utility packages shm and pfilehand will, we hope, turn out to be lasting legacies of this project. The shm package was developed to allow each shared memory segment to be a Fortran 2003 object accessed via pointer components. The package is described in more detail in section 4 and includes appropriate semaphores, barriers and routines to attach and detach from the segments. The iso_c_binding components and associated C routines are at a low level within the package so external access is kept to strict Fortran. This access is particularly appropriate for ANG and the Fortran 2003 shm package is complementary to the MPI-1 and Fortran-95 compatible modules previously developed for HECToR and the CASTEP code [12]: an academic paper describing the two modules and their performance is in preparation. In ANG, shm is used to store tables of 'surfacing coefficients' calculated in parallel (section 4).

'pfilehand' is a double-buffered parallel I/O module using asynchronous MPI-IO calls with indexing records reserved for minimal information for locating bulk data and allowing subsequent parallel reading to be completely independent of the communicators used to perform the parallel writing. It is again accessed as Fortran 2003 objects and is used in the main ANG code to write the final data which is calculated in parallel using MPI: this parallelism has been extended to all the various ANG routines, though the bound-bound coupling remains the most time-consuming. The pfilehand module was developed from an older set of serial filehand routines for direct access files used throughout the R-matrix codes and is therefore particularly suited to these codes (and others which use serial filehand). However, pfilehand is relatively easy to use and should be of general interest, competitive with more general

packages. It is used in ANG in combination with parallelized outer loops over coupling indices to calculate the required couplings from the surfacing coefficients. The new parallel ANG code has been tested for scaling up to 256 cores so far, from an initial serial code, and the shm and pfilehand modules are available as standalone packages with test runs. They are being made available on CCPforge [8] and we aim to publish them.

We note that the Fortran 2003 code requires a standards-conforming Fortran 2003 compiler. The Nag 5.3.rc5 compiler has the functionality required, as does the recent IBM compiler xlf13 (as tested on a Power7 machine). Tests of the packages have shown up bugs in the pgi compiler which are being fixed piecemeal with ongoing releases, and in the Cray compiler. Cray have requested and received a 'beta' version of the ANG code to use as part of their validation test suite for compiler upgrades. We thank the HECToR helpdesk for facilitating access to the compiler experts. We await the Cray Fortran 2003 compiler in particular, as our tests confirm that this is the best-performing compiler for the serial versions of the PRMAT codes and the parallel RAD code on HECToR. The ANG code is carefully commented and detailed notes link the routines to the main theory [9]. These will be supplemented by the planned publication document. The availability time for the code was underestimated for the reasons described here, however it is now available for users and feedback.

HAM objectives:

1. MPI sub-task communicators looping over *LSπ* scattering symmetries and classification of matrix elements (open-open, open-closed and closed-closed, both Hamiltonian and dipole elements). Arrange Hamiltonian output data files sympathetically to be picked up in parallel by PDG. Distribute the dipole data for different symmetry combinations.
2. Introduce OpenMP/System V parallelism into the construction of the matrix elements.
3. Adapt the routines for recalculating the dipole matrices (from the eigenvector coefficients after Hamiltonian diagonalization) and other eigenfunction data for the field-atom work so' that they appear as an option in the parallel PDG code.

Parallel loops have been introduced over the matrix element formation routines, with pfilehand used to pick up ANG data (and RAD data as an option), with shm introduced and used where needed. The 'xstream' routines developed as part of the previous dCSE have been introduced in the handling of the final data so that 'traditional' binary output or PFARM- and PDG-preferred XDR output may be chosen automatically. The HAM code is now a single parallel code for both scattering and multiphoton applications. At the time of writing, the code is undergoing an extremely thorough set of validation tests, which we considered to be of primary importance so that the parallel code could be delivered to users. We will update this report with full scaling data once these tests have been completed. The final work on the dipole matrix elements, replicating HAM routines for post-diagonalization treatment explicitly in PDG, will be performed subsequently as an upgrade to the released code.

3. Detail: RAD

In this section we show some performance results for the modifications made to RAD. We first consider the OpenMP code. Our main modification was to re-order loops in the second half of the code that calculate 2-electron exchange integrals over four orbitals and an inter-electronic potential term $\{r_<^k/r_>^{(k+1)}\}$ ($r_<$ is the lesser or r_1 and r_2). The algorithmic set-up of the code is such that where possible the inner integral is stored for a particular combination of orbitals to avoid recalculation, however the orbital index ordering for the exchange integrals ran counter to this and much unnecessary recalculation was being done. The loop reordering was performed while maintaining the 'correct' expected ordering for the writing to the output files. In addition, the integrals were in many cases written individually to the serial

filehand output buffers: while the buffering mechanism in filehand compensated to a reasonable extent, this has been rearranged so that filehand routines can be called less frequently for arrays of integrals. We also collapsed some inner loops and put in an option to move the OpenMP loop up one level, hopefully to reduce OpenMP overheads. Results are shown for an oxygen test case using 180 B-spline functions per angular momentum. We compare original and revised code execution time for up to 32 threads using gnu, pgi and cray compilers (at –O3 level, -fast for pgi).

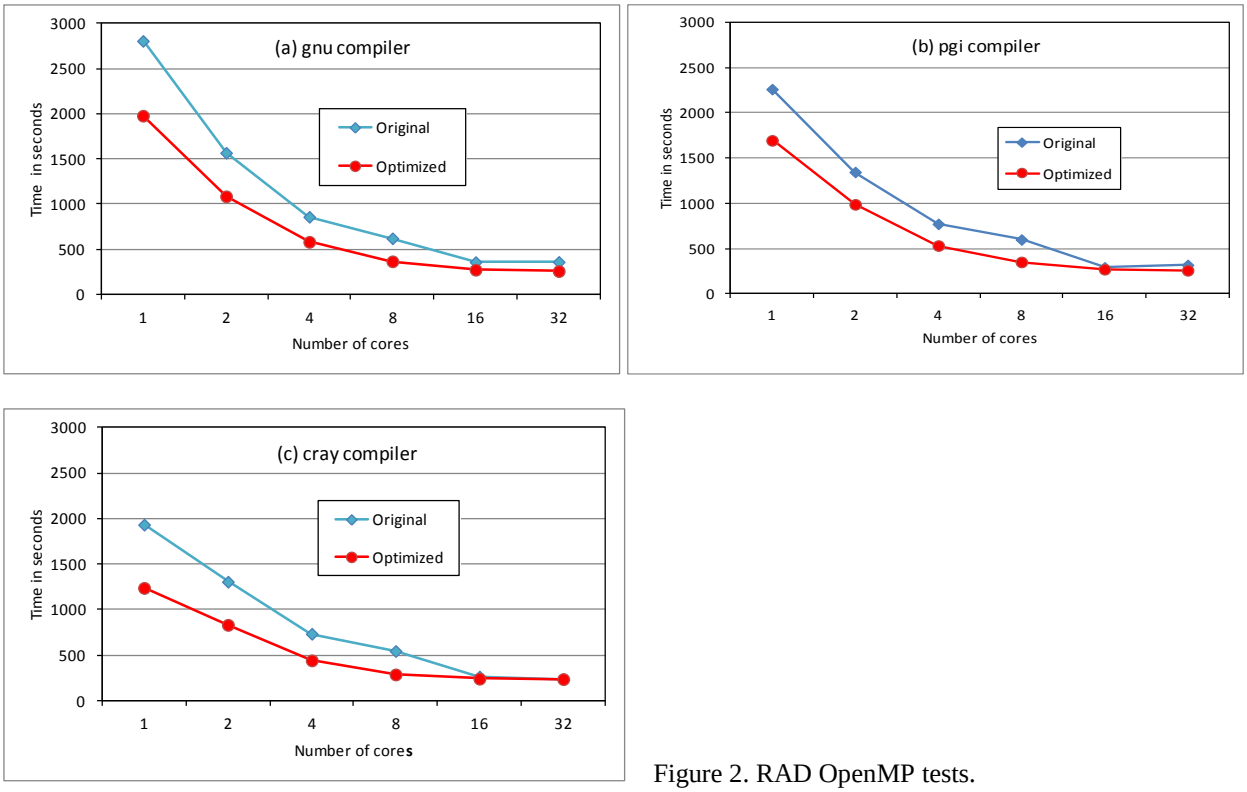


Figure 2. RAD OpenMP tests.

The loop reordering provides substantial serial optimization. Above 8 cores, the storage option slows down the scaling. We are checking returning the OpenMP loop to its previous position for 16 and 32 cores (ie so that less data needs to be held in memory). The cray compiler is much better suited to HECToR for this code, though this may not be the case on other platforms. Note that all tests were performed on a full node (ie the few-thread runs had access to all the memory on the node if required, etc).

The results above include the writing (and re-reading) of sets of orbitals to temporary files. This approach has traditionally been used in the serial code in order to minimize memory overheads on former memory-limited architectures. However, the latest HPC architectures such as Hector, provide relatively generous memory provisions (32GB) per node, and therefore this out-of-core storage approach has been replaced with on-core (memory) storage in the new parallel code. We now consider preliminary results (for the optimized code) using the cray compiler following the introduction of the MPI communications. The main code developments for implementing this new level of parallelization in RAD involves (*i*) distributing input configurations to all MPI Tasks at the start of the run, (*ii*) the replacement of temporary files with memory-based storage and (*iii*) a distribution of outer loop angular momentum *l* values amongst MPI tasks for both basis function and radial integral calculations. Note that this option not only allows for use of more than one node, but also can improve overall performance by determining optimal MPI task/ OpenMP thread combinations within a node.

The figure shows three cases, the pure OpenMP results for {8, 16, 32} threads already shown above, results for 8 OpenMP threads each for {1, 2, 4, 8, 16} MPI tasks (ie {1, 1, 1, 2, 4} nodes), and results for 16 OpenMP threads each for {2, 4, 8} MPI tasks (ie {1, 2, 4} nodes).

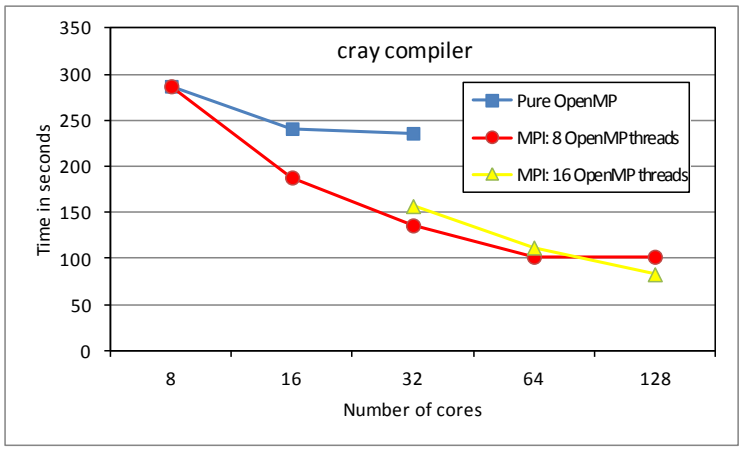


Figure 3. RAD mixed-mode tests.

It may be seen that for this oxygen test, the intermediate writing to disk did not significantly hold up performance (or its removal has compensated for any (minimal) overhead for 1 task introduced by the MPI code). The introduction of the MPI tasks, complementary to the OpenMP parallelization, has significantly improved the overall performance within one node, and the performance scales acceptably to two nodes.

The lack of scaling between 2 and 4 nodes for 8 threads per task may be explained as due to the test case: the outer loop parallelized with MPI has 8 independent (after appropriate preliminary data transfer) iterations. Thus we now show multi-node results for an expanded case (more realistic) with 16 independent outer loop iterations (note the linear horizontal scale for this figure). We have {4, 8, 12, 16} and {2, 4, 6, 8} MPI tasks respectively.

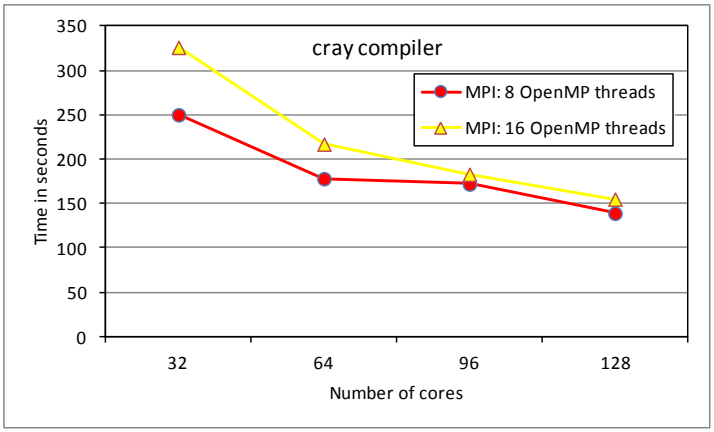


Figure 4. RAD mixed-mode tests (16 iter.)

While the 4-node run is now faster than the 2-node run, load-balancing of tasks to iterations is affecting the scaling. The iterations were assigned to tasks in round-robin fashion and while the overall time to completion was stable for repeated testing, the load-balancing between threads became progressively worse: from about 10% difference for 2 tasks, to some tasks taking nearly twice as long as others for 16 tasks. These timing differences reflect the different computational loads associated with different *l* values assigned to the different MPI tasks.

This load-balancing issue can be compensated for, for instance by a more careful allocation of tasks to particular loops by a code author (who can tell which loops are likely to be busier). We note that ~0.8 of the execution time is taken up by the second, integral evaluation, stage. Now that the MPI procedure is in place it is straightforward to collapse the two outer loops and assign the resulting single loop to MPI tasks, which will improve scaling for more than 2 nodes by statistical smoothing. The updated report will show improved timings. We will also introduce the passive RMA 'sgc' scaleable global counter (already part of pfilehand, see section 4) to balance out the work among tasks: RAD provides a useful comparison test for the two approaches (section 6). As things stand, the performance and scalability of RAD has been substantially improved, the use of MPI allowing the OpenMP operations to be performed with the optimum number of threads, usually 8 on HECToR.

4. Detail: ANG

In this section we give more substantial detail on the background to the code and the new packages, finishing with some performance figures.

4.1: Background

The R-matrix formalism ([3] and references) was developed by Wigner and Eisenbud to treat proton and neutron collisions with nuclei. The idea was to treat these nuclear collisions as two separate collision problems according to whether the incident nucleon was external to the target nucleus and Coulomb forces mediated the interaction between the colliding particles or the incident nucleon was inside the target and the interaction was via short-range nuclear forces. Matching the inverse logarithmic derivatives of these two solutions at the boundary of the target nucleus produces a real matrix, the R-matrix, which can be used to compute cross sections, resonance parameters and other physical observables.

In the 1970s P G Burke extended this formalism to treat electron-atom collisions. In atomic systems the requirements of the Pauli exclusion principle dictate that if the incident electron is inside the charge cloud of the target atom or ion exchange effects are important and result in a complicated set of integro-differential equations describing the collision process. If, however, the incident electron is outside the charge cloud of the target a simpler non-exchange scattering problem must be solved. The adapted R-matrix formalism simplifies the computation necessary to treat the collision from first principles.

Following an initial (and widely used) package RMATRIX-1 [13] developed at Queen's University, Belfast, the RMATRX-II formalism was developed by P G Burke, V M Burke (of DL) and K M Dunseath ([9], referred to hence as BBD) to improve the efficiency of previous implementations of atomic R-matrix theory in order to tackle more complex electron configurations. As larger and more complex atomic systems were considered the limitations of the initial code had become apparent. In particular the calculation of the angular integrals necessary to derive Hamiltonian matrix elements became a computational bottleneck as the contribution of more deeply bound electron shells was considered. The number of configurations rises steeply as more shells are unfrozen and allowed to participate in the collision process. BBD published an improved algorithm for treating atomic collision in which a set of angular momentum transformation coefficients, termed surfacing coefficients, are derived that express the recoupling transformation of a pair of electrons in the target occupied shells to the top of the coupling tree where it may interact via the one- and two-electron integrals involved in the interaction. These coefficients involve fractional parentage coefficients (to allow for electron shell antisymmetry), Racah coefficients and kinematic factors (BBD). Given tables of these coefficients the angular integrals may be evaluated rapidly and efficiently. This program was written principally by V M Burke.

In ANG, electron configurations are divided into two sets: a unique set and an equivalent set. Members of the latter set have the same angular momentum properties as a member of the unique set and differ only in the radial wavefunctions they involve. Only the unique set need be treated in detail. Most internal files are read and written using the filehand subpackage. Fixed record length unformatted Fortran files are treated using double buffering via the filehand interface. Program dimensions were, in 1994, determined via preprocessing.

RMATRXII was subsequently updated by: (1) conversion to standard Fortran 90, then Fortran 95; the introduction of dynamic memory allocation and a reorganization into a modular structure. (2) Sparse matrix techniques and derived data types were introduced into key parts of ANG. (3) A range of minor algorithmic and programmatic improvements were implemented. (4) The ANG program was parallelized on IBM architecture using OpenMP but scaling beyond 4-5 threads deteriorated rapidly.

The ANG calculation involves the consideration of all possible couplings from a given set of electron configurations and the detailed angular momentum algebra needed to define an orthonormal LSπ-coupled basis set (or, following recoupling, a JKπ-coupled basis: for the meaning of K, see [3]). As mentioned above, the mathematical basis of RMATRXII/PRMAT inner region formalism, in particular ANG formalism, is detailed in BBD. Essentially, ANG proceeds in 2 stages. Firstly, the surfacing coefficients required are identified and then calculated until the appropriate surfacing coefficient table has been completed. Then the tables are used to form all the angular couplings required (continuum-continuum, continuum-bound, bound-bound for direct and exchange 1- and 2-electron Hamiltonian and multipole matrix elements). In the new code both stages are parallelized: the surfacing coefficient calculations are distributed, the coefficients are written to a shared memory segment which is then updated across SMP-nodes, then the second stage is parallelized over outer loops over coupling indices in each case (c-c, b-c, b-b etc) and output data is written in parallel.

4.2: ParAng

The ParAng code (ie the new ANG code) is parallelized using MPI and assumes an SMP architecture in which there one or more nodes and an arbitrary number of cores attached to each node. It is also assumed that there is sufficient memory associated with each node that a single copy of the essential surfacing tables may be kept in shared memory.

The program is written in pure Fortran 2003 and C for very low-level interactions with the system. The C is model independent (ILP32, LP64). MPI version 2.2 is assumed. POSIX C functions are also assumed. It is disappointing that as we approach 10 years from the publication of the Fortran 2003 standard vendors still have not produced compliant compiler and that the missing features severely limit the utility of those that have been implemented. On Hector only the Nag 5.3 compiler is close to compliance. The IBM xlf13 compiler is fully compliant.

4.2.1: ParAng Features:

- SMP analysis using POSIX system functions
- MPI communicator construction for intranode and internode communications
- IPC Shared Memory Segment storage of R-matrix surfacing tables
- Mutex locking of shared-memory operations using IPC semaphores
- Object-oriented scalable global counters controlling MPI parallel loops
- Generic linked-lists using polymorphic data for temporary storage
- MPI-IO output of results directly from task nodes to a single unformatted disk file using double buffering and asynchronous I/O

Here we will describe some of the salient aspects of each of these features but will not attempt a full user manual. i.e. the parallelization will be described but little if any attention well be given to the physics embodied in the code or the description of the physics input data. The overwhelming portion of the CPU time required to perform a calculation is required in the angbb section that performs angular integrals for bound-bound N- and N+1-electron systems. In ParAng all sections have been parallelized so that the entire calculation can be performed conveniently on a single computer system. Although the code is useful primarily for larger, more demanding calculations the code has been adapted to handle even small calculations where there are more tasks available than the number of iterations in the parallel loops.

4.2.2: IPC and the shm utility package

Fortran 2003 provides a standard for interoperability with C language code. This in turn gives access to system functions that cannot be called directly using Fortran. The Unix System V IPC system calls provide messages, semaphores and shared-memory. Although not portable these are universally available on unix-based systems. IPC shared-memory segments (sms) are used in the impich2 implementation of MPI. The use of this approach in a Fortran context has been pioneered by I J Bush and colleagues, including C Armstrong, of NAG Ltd. This approach is informative and allows the sms approach to fit in efficiently with MPI-1 formalism, and has been used successfully in the materials science code CASTEP [12], but it is in certain respects inconvenient for the present application. The routines in the ParAng code represent an entirely independent implementation.

The IPC library functions are all called from functions defined in the file ipc.c. The function get_key calls the function ftok to generate an IPC key. The resulting key is required to be unique within each system image and is generated, in this implementation, from an integer between 1 and 99 and a file path that must be input by the user. This path is arbitrary but must be such that a file pointed to by the path is statable by the user. The integers are managed within a list internal to the ParAng IPC routines. This keeps track of IPC keys in use. Keys are obtained by one task attached to each node and MPI broadcast to the remaining tasks. It is important to appreciate that IPC resources (shared-memory segments, semaphores) are limited system wide and can persist at the end of a user job. ParAng will call routines to delete these IPC objects at the end of a job. To allow for possible job crashes or the job running out of time the job script needs to call the functions ipcs and ipcrm to eliminate any IPC objects owned by the user. A shell script, segrm.sh, written by I J Bush is provided for this purpose (the HECToR system call /usr/bin/ipcclean may also be used).

The Fortran interface for shared-memory segments is contained in file shm.f90 and semaphore interface in sem.f90. These modules define shm and sem derived datatypes that contain the data pertinent to each object. For example the shm type is (so far) defined to be either integer or real data. The datatype holds the size of the data, a pointer to it and the segment IPC id. A set of type bound procedures define the operations that may be performed on the segment. Finally the derived-type is overloaded by the type constructor. The segments and mutex locks therefore are objects in the usual object-oriented programming sense. They may be created and destroyed as required. This is of great convenience in this program. The Fortran 2003 finalization options have not been used as this feature is missing from nearly all compilers.

We illustrate the shm object:

```
type  shm            ! shared memory segment type
   private
   integer(c_int)       :: keygen_id = -1 ! project id of segment
   integer(c_int)       :: id = -999      ! segment IPC id
```

```
    type(c_ptr)          :: shm_address          ! c-pointer to segment
    integer(c_int)       :: num_els       ! # datatype elements
    integer(c_int)       :: datatype      ! type of data
    integer, pointer    :: iptr(:)     ! integer fortran ptr to SMS
    real(wp), pointer   :: rptr(:)     ! real fortran ptr to SMS
  contains
    procedure :: attach => attach_sms
    procedure :: kid => getId
    procedure :: shmid => getShmid
    procedure :: detach => detach_sms
    procedure :: getiValue
    procedure :: getrValue
    generic   :: get => getiValue, getrValue
  end type shm

  interface shm
    procedure constructor
  end interface

contains
  function constructor (count, datatype, inproc, keypath, error)
  .......
```

The structure of the sem.f90 module mirrors that for shared-memory segments. Apart from creating and destroying mutex locks the allowed operations are start_crit and end_crit marking the start and finish of a critical section. The package comes with a test run routine and wrapper routines for users who do not wish to use the Fortran 2003 object structure are available, for example combining the constructor set-up with the attach routine, and for later access. In fact, in ANG, the routines angbb, angbc, angcc etc access the completed surfacing coefficient tables via an intermediate module, so as not to distort the appearance of the earlier code. The shared memory segment is accessed within the intermediate module using shm%get(<real or integer pointer array>).

It was found by trial and error that MPI routines could not be used reliably to determine the connectivity of an arbitrary SMP cluster. Fortunately the POSIX library function gethostname can be used to quickly and efficiently determine the number and names of the nodes participating in a given job. It is then straight-forward to associate MPI ranks (within the MPI_COMM_WORLD communicator, or a user-supplied communicator name for public variable LOCAL_MPI_COMM in the module file comm_mpi.f90 containing the majority of MPI calls) with each node. The gethostname function is called in the file host.c. The remaining analysis is performed by the module smp_analysis in file smp_analysis.f90. The 'proclist' defining the tasks associated with each node is broadcast. In ParAng we wish to use a segment across the whole SMP node to store the surfacing data, however the standalone package will allow developers with knowledge of task to core assignment to subdivide this, for example on HECToR into groups of 8 cores.

The final file in this group is comm_constructor.f90. As its name implies these routines set up MPI groups and communicators reflecting the SMP structure. There are communicators allowing data to be broadcast among the tasks corresponding to each node. A distinct communicator is required for communication between one designated task on each node. In general the tables contained on shared-memory segments will be partially filled by each node according to the cases assigned to the tasks of that node. To obtain complete usable tables it is necessary to combine the node-tables using an MPI_allreduce

sum. This uses the internode communicator. Routines in this module may be used to check these communication patterns.

To reiterate, shm is available as a standalone package with a test program. A more detailed description will be given in a paper in preparation that compares the two sms packages developed on the HECToR service, and when the code is published.

4.2.3: ParAng parallelization: SGC and generic Linked-Lists

The core of the parallelization is to designate some key program loops as parallel. An iteration of these loops is assigned to a single task. That task may be any task across the entire communicator. It is important to avoid a two-way communication in order to provide the next available iteration number to the idle task. We therefore use the MPI one-sided RMA (remote memory access) facility to pickup and update the counter value. This use of a global counter is ideal, as in the present case, where there is significant variability in the CPU time required to perform a single iteration. The examples in the MPICH package include a scalable global counter. Scaling is achieved by setting up a tree structure and obtaining the count by summing the nodes from the origin of the tree to a particular leaf. This tree structure is maintained on an RMA window and so is available to all cores. The example code was written in C. In ParAng it has been rewritten in Fortran 2003 and incorporated in a derived-type sgc. This counter type is provided with type-bound procedures and put in the form of an object that can be replicated as required. This facility is contained in the file sgc_mod.f90. The MPI standard allows the RMA window to be exposed on a single processor. This option has been adopted here.

One of the characteristic problems of this angular integral calculation is lack of a convenient means of estimating (a) the sizes of the various surfacing tables and (b) the amount of data that must be stored for processing by subsequent stages of the calculation. Thus initially the size of the shared-memory segments needed to hold the surfacing tables is unknown. To circumvent this problem we require each of the tasks to hold the surfacing data that it calculates in its own linked-list. At the end of the surfacing calculation the relevant sizes are known so the shared-memory segments can be constructed. Location tables are first calculated then tasks may pop data from their linked-list and once having obtained the mutex lock place their data in the node surfacing tables. The data to be stored in the linked-list consists of a header record for a particular configuration and electron shell followed by a number of data records comprising index and coefficient data. Each set is terminated by an end of data record. This is not easily accommodated in a traditional linked list. The object-oriented features of Fortran 2003 make this easy. An outline of such a list has been described by PGI consultant Mark Leair [14]. A derived link type is defined in file gLink_mod.f90. The internal details of this module are hidden. An unlimited polymorphic variable is used to hold the link data. The user interface to the link module is defined by an abstract list type defined in absList_mod.f90. Finally the user list data types are defined in the file surf_list_mod.f90. This defines a surfList type and derived data types sch, sc and eod. Each of these datatypes can be added to or popped from the list. The full list may be printed out. The entire list may be deleted. Once the data is placed into the shared-memory segments the memory may be retrieved by deleting the linked-list.

4.3: Parallel Filehand (pfh)

4.3.1: Introduction

The objective of this code is to obtain an efficient parallel implemention based on MPI-IO for use with distributed memory computers whilst preserving as far as possible the interface and functionality of the serial filehand code devised by V M Burke [9]. The essential features of serial filehand are a standard

interface to unformatted integer or real files using fixed length records and double buffering to improve performance.

In parallel filehand (pfh) the interface code is provided in the module pfilehand (pfilehand.f90). Using MPI-IO it is possible to provide non-blocking asynchronous I/O that was not available in standard Fortran prior to the 2003 standard. If is also possible to allow any of the tasks in the array to write directly to a single output file thereby avoiding potential network bottlenecks if designated I/O-nodes are used. As a trade-off we can avoid the need for synchronization and file-locking by allowing only a single task to write to each file record. An MPI global counter is used to assign records to each task. This implies that a file written in parallel will comprise sets of records, each set associated with a specific task. In order to read the information from this file in the usual serial order it is necessary to save the starting location for each parallel iteration. This additional location information is written to the index portion at the start of each filehand file. The index records have therefore been expanded to include the first 6 records by default rather than the first 2 records used by the serial filehand code. This index region may arbitrarily be extended by adding the optional variable 'rec_offset' to the end of the 'open_fhfile' argument list. This change requires some generalization of the serial filehand file in order to keep track of the index writing and reading. The MPI-IO code underpining pfh is contained in module file_io (file_io.f90). The data defining each pfh file is contained in a abstract data type fhf. Variables of this type are allocated and saved in an array ffiles to maintain the usual Fortran file philosophy.

4.3.2: pfilehand.f90

The concepts underlying the filehand and parallel filehand (pfh) packages should be kept in mind. The files are divided into fixed-length records. Positions within the files are defined in terms of the record-number and the position within the record. Records are defined to be either of integer-type or of working precision floating-point type. The type and length of each datum must be known in order to read back the file contents. The initial records of each file are of integer-type and are used to hold catalogues of the starting position for data items located on the remainder of the file.

In the serial case file I/O is provided by fortran standard random-access files. Double buffering is employed: a buffer is written when full or read in advance asynchronously (if the system allows this) to ongoing computation and use of data from the other buffer. In generalizing to a parallel package we use the MPI-IO package. Each task or core maintains it own file-pointer. It can therefore write directly and independently to a single disk file. Stream-io is used so that the entire file may be viewed as a single byte stream. Each file sector is associated with a particular core: there is therefore a 'core-path' (CP) of sectors associated with each task. Provided the starting position is known, a sequence of read operations along the CP will return the data written by that particular task. If the CPs were written in the course of a parallel loop, the data can be returned in serial order provided each starting position is recorded and also processed in serial order.

We now list a selection of pfh routines that may be encountered by the user (again, a full description will be included in the main package publication). The standalone package includes options for wrapper routines that will group related pfh routine calls together.

- **initda** initializes filehand: it is now a link to a routine in file_io.f90 that checks the compatibility of the system's MPI-IO and sets the buffer size (either default or supplied as an optional argument).
- **open_fhfile** corresponds to the filehand open routine. Arguments specify the file unit number (here used only as an id), the filename (arbitrarily limited to 50 characters) and the 'rtype'. The latter logical variable is true if the file is to hold real data, false if it is to hold integer data. The 7-character argument stats designates whether the file is new, old or scratch. This routine simply calls the MPI-IO routine to open the file and set up the file buffers and other information. We prefer not to overload the standard Fortran

function open – hence the name change to open_fhfile (open filehand file). Note also that the open is for read-write access - there is no need to close the file before reading records.

- **newfil** starts a new subfile at the next available record. The record number is returned. In pfh the record number is obtained from routine get_next_record_number.
- **catlog** finds the next available position on the file specified by the unit number. The position is returned as the catalog entry interpreted by routine lookup. The catalog array is built up for writing to the index records, for subsequent reading.
- **{i}read{a,b,c), {i{write{a,b,c} '**read' or 'write' individual data, or 1- or 2-dimensional arrays (ie copy to or from the buffer, initiate actual I/O in advance if required). There will be an option for these routines to be accessed via overloaded interfaces.
- **endw** terminates writing to a subfile started by newfil. Providing the current record contains data the remainder of the record is zeroed before writing the record to disk. This is executed by a single task.
- **writix** signals the start of writing to the file index. Set the index flag and set the file pointers to point to the index record and pointer.
- **endwx** signals the end to writing to the index. Resets the current record pointer and record number before switching the index flag off. This routine did not exist in serial filehand. Does not trigger any disk io.
- **readix** is called to set up intial reading of index and catalogue data.
- **lookup** returns the record number and file position corresponding to the provided catalogue entry.
- **pend** adds a parallel path end symbol into the buffer
- **wr_ploop** is a special pfh routine to write parallel location data to the index of a file. The routine also deallocates the arrays used to hold the data. We use a MPI reduce routine to collect the data from each task node if there are more than one node.
- **close_fhfile** Corresponds to filehand close routine. Calls the file_io routine close_mpi_file to close the file, clean up the buffers and the global counter associated with the file. Retrieves and prints the file statistics.

4.3.3 file_io.f90

This module contains routines making the MPI-IO calls central to the operation of pfh. These are ordinarily not user visible or called directly but are accessed via the wrapper functions in pfilehand. Conceptually each task writes a chain of records: the end of each record contains the record number of the next record in the chain. The data written by each task can therefore be retrieved by reading sequentially along each of the task chains, The records to be used are assigned by calling a file specific global counter, There is an offset of file_offset so that file_offset records at the start of each file are reserved for use as the file index. When executing a parallel loop we expect, in general, that each task will process a number of loop iterations. In order that the records can be read back in a sequential order it is necessary to know the disk location (record number and record pointer) where the data from each loop iteration begins. Routines are provided for saving these loop iteration locations. These are start_ploop, save_ploc and end_ploop. Up to 5 (by default) loops may be saved in this way. If the order in which the output of each loop is unimportant, then there is no need to retain this data. In the final package these and routine write_partial_buffers will be aliased or set up as links in the main pfilehand module as they are required outside the package.

- **open_mpi_file** This routine initializes the data of the fhf member that corresponds to a particular element of the ffiles array. This (unwieldy) scheme is meant to minimize storage requirements as only the elements corresponding to active files are allocated. The option of defining a 'file' object does not permit a Fortran-like naming scheme in which the file is identified by a unique file number. This routine also allocates the buffers to be used by the file. There are normally two buffers. In the case of real files these are supplemented by additional integer buffers to accommodate the writing of index records. This routine also calls the constructor for the global counter used to allocate records of the file.
- **write_mpi_record** This routine waits until the I/O-buffer is available. The buffers are then swapped so the old I/O-buffer becomes the current active buffer. A new record number is obtained and appended to the end of the IO-buffer. A non-blocking (asynchronous) write of the filled buffer to disk is then initiated. This routine is triggered when a task has filled its current active buffer of if the file is to be closed. In the latter

case all records containing data must be written to disk. In this case the unused portion of the buffer is zeroed before writing. It is assumed that index records are only written by node 0.

- **read_mpi_record** This will read one record of the file or from the file index if the index flag is set. It is assumed that consecutive records of a record chain will be read by default. In this case the read operation is performed using MPI-IO non-blocking reads and checks are performed to ensure that a record is available. The initial read at the start of a chain is necessarily blocking and is treated separately.
- **set_mpi_record** is used to reposition a file at the start of a (parallel) sub-file and perform a blocking read, after checking whether this is necessary, ie if the required next record is different from that written into the index. This allows reading to be independent of the communicator and sgc used to write the file. The blocking read is required if the pre-buffered data and previously initiated non-blocking read are out of sequence for the reading communicator and sgc.
- **close_mpi_file** must first write to disk any partially filled records. Once this is completed the file may be closed and the file buffers deleted. As part of the closure process the file counter is destroyed and the file statistics written.
- **get_mpi_stats** collects the total number of records written by all the tasks and also the maximum record number used by write_mpi_record. The latter determines the total size of the file. The routine is called by close_mpi_file.
- **get_next_record_number** calls the global counter to find the next available record number. This is declared public but would not normally be called externally.
- **del_record_ctr** destroys the global counter releasing RMA windows. Should not be called externally.

Parallel Loops

As the data on the file that is written during a parallel loop is not in the usual serial order we create a special location index that records the starting position of the data for each configuration in a particular parallel loop, The indices for each computing task are combined on task 0 to form a complete index, ploc(0:<#iterations>). Redundant tasks not needed to perform an iteration must skip the parallel loop. A count of these skips is recorded in ploc(<#iterations>).

- **start_ploop** is called prior to the execution of a parallel loop. It allocates arrays ploc on each core to hold iteration location data.
- **save_ploc** is called by each task when it starts a parallel loop iteration. It adds the current file location data to its copy of the location array ploc. Subsequent disk I/O by the task will be in the chain of records beginning at the stored location.
- **end_ploop** is called globally by all tasks on exiting from a parallel loop. The routine uses an MPI collective reduce call to combine the location lists of each task on task 0. The partial ploc indices on the cores are then deleted.
- **write_partial_buffers** At the end of a run in which multiple tasks are used write a pfh file there will partially filled buffers in memory on each core. This routine zeroes the unused portion of these buffers and writes them to disk. This routine must be called prior to closing a file that has been opened for writing. There is no need to call this routine before closing a file open for reading.

There are several issues. Firstly, the numbers that are appended to the end of each record are of type integer(MPI_OFFSET_KIND) and are likely to be 8-byte integers for most processors. These numbers are therefore handled using the transfer intrinsic function. Routines are called at the beginning of the run to check and print the sizes of the various numbers being used. This insures that the record sizes are consistent and can be read (perhaps with some adjustments) on other computers. Note that we have chosen to use different record lengths for integer files and real files. The objective has been to carry the data defining a particular filehand file around in a derived datatype. In order to follow Fortran practice and serial filehand we use a ‘unit number’ to identify operations on each file. This kind of labelling does not allow a simple definition of a file ‘object’.

A test run of pfh is provided by the file test_filehand.f90. This includes a parallel write of a set of data followed by an independent parallel read-back of the same data.

The particular advantage of serial and parallel filehand in the R-matrix codes is that the data produced by ANG is likely to be re-used many times in HAM in an unpredictable order. Hence the use of direct access files originally and now MPI-IO files to allow for the independent parallel writing and reading. The much larger capacity of modern machines to store data in memory may be taken account of by the choice of the buffer size, however the current and envisaged calculations are such that the package will remain a vital component of the R-matrix package. Each type of matrix element component calculated in ANG has two files associated with it: an integer file containing labels and indices and a real file containing the associated coefficients.

4.4 Tests of ParAng

We present results for 2 test cases, the oxygen case used for RAD tests, and a much larger case for Fe^{+} that cannot be run on HECToR with serial ANG. The iron test is of the order of calculations currently being run by users and at the lower end of planned calculations. The NAG compiler was used at –O3 level. In both cases the bulk of the execution time was taken up by routine 'angbb' which calculates 'bound-bound' angular couplings.

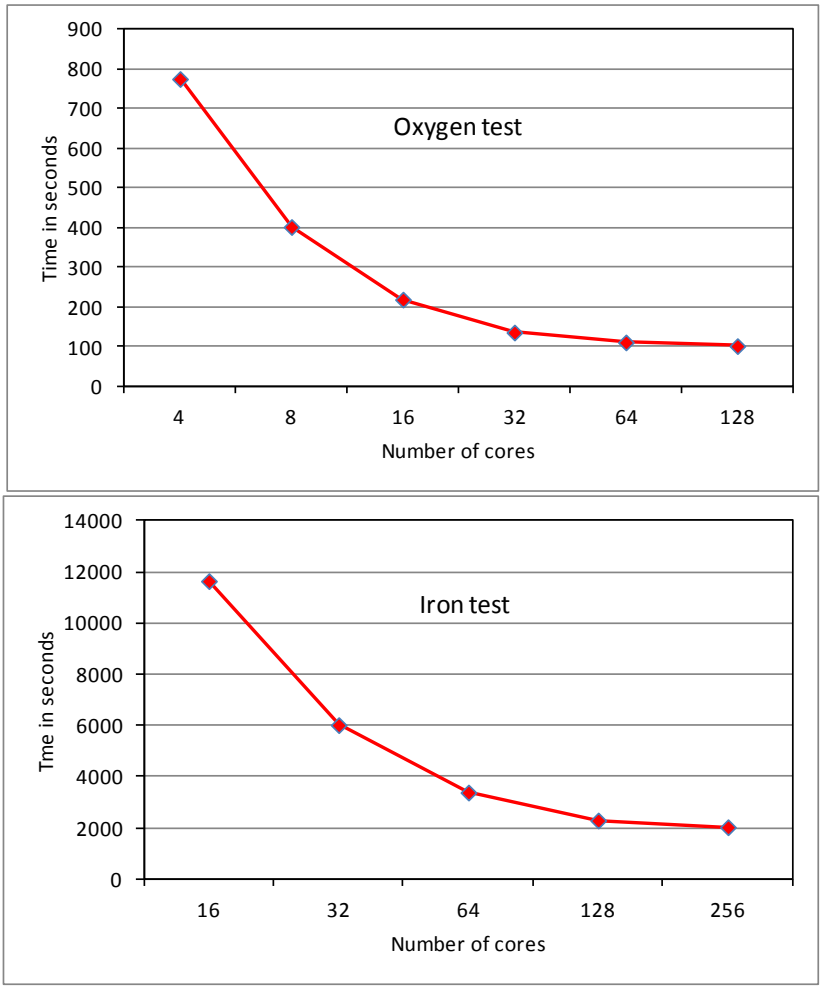


Figure 5. Tests of ParAng

The oxygen test scales extremely well to 32 cores, then scaling starts to drop off as MPI overhead becomes noticeable. We note that the original serial ANG code took, respectively: 1973s, 2152s and 1475s with gnu, pgi and cray compilers (-O3 level, -fast for pgi) as single jobs on a 32-core node. Thus we wait for the Fortran 2003-compliant cray compiler to be fully debugged as performance should improve considerably. The iron case scales extremely well to 64 cores and reasonably well with some MPI overhead noticeable at 128 cores. Scaling is tailing off at 256 cores. These results were obtained following some testing of varying the pfh buffer size, which had a noticeable effect for runs using more than 1 node: the default size was reset (increased from the serial filehand value) to produce the results. Repeats of tests showed some variation of up to about 5% in execution time for the 4 and 8 node Fe^+ runs, attributed to variations in the sgc procedure: this will be investigated (section 6). For an upgraded release, ParAng is currently being subjected to detailed parallel profiling to identify the main overhead bottlenecks and reduce them. However the current scaling at 256 cores is as good as for many other established quantum physics and chemistry codes on HECToR, and will improve for larger cases. Thus, apart from the new packages, we have transformed a serial code into a parallel code which should scale well to more than 256 cores for the complex atomic cases planned by the user community.

5. Detail: HAM

The HAM module performs the task of constructing the Hamiltonian matrix elements corresponding to a set of scattering symmetries. These matrix elements are written to disk files as input to PDG, or are diagonalized directly. The program stage also performs a number of subsidiary tasks: it constructs and diagonalizes target Hamiltonians; it forms asymptotic potential coefficients (multipole potential coefficients of the potential defining the scattering in the region where the incident electron and the target are distant from one another) and dipole coefficients used to calculated photoionization cross sections and in the multiphoton codes [6,7]. None of these tasks is particularly CPU-intensive. The core task of constructing Hamiltonian elements is, however, data intensive and we have incorporated the pfh code to cope with this.

The ‘ij’-th Hamiltonian matrix element is a linear combination of one-electron and two-electron radial integrals computed in RAD multiplied by coefficients computed in the ParAng code. For many R-matrix calculations the number of radial elements is not excessive and these elements may be read into memory and simply selected for use as required. For certain intermediate energy calculations this number may become sufficiently large that a more elaborate partitioning scheme must be employed. The new code ParHam allows radial elements to be read in using pfh. The angular coefficients and associated indices must be read from pfh parallel files.

The indices of the ANG files are read. The last block of data from each of these file sections is the location data providing the location on disk that corresponds to the start of a parallel path (a linked list of file records written by a single task). There is one set of locations for each parallel loop - and one location for each loop iteration. There are always two associated locations - the location in the integer file of the index information and the location in the real file of the coefficient information. This information is combined into a data object ‘ploc’ in the module plc_mod contained in file plc_mod.f90. Using type-bound procedures we associate the datatype and its methods to form an object (in the object-oriented sense) that is convenient to use throughout ParHam. Once the files are correctly positioned the ‘plc’ constructor is called to define the ploc object. The main method is the ‘ptr’ method that returns pointers to the data for a given parallel loop.

In the case of bound-bound matrix elements, treated in bb_ham.f90, it is necessary that two sets of parallel location data are returned. The loop that corresponds to the one used to write the parang file is

now read back in parallel using all available tasks. Tasks are assigned using the scalable global counter sgc exactly as was done in ParAng. The loop is initiated by selecting the ploc data according to the assigned loop iteration. The locations are converted to records and record offsets by calling the lookup utility from pfh. The files are then independently positioned by each task using set_mpi_record. The Hamiltonian element is then constructed. It is finally planted directly in the output file is the required position. bb_ham is used first to construct target Hamiltonians and later the bound-bound submatrix of the N+1-electron Hamiltonian.

The bound-continuum submatrix is constructed in a completely similar manner by the routine hambc contained in the file rdhmat.f90. Again the same loop over consfgurations used in ParAng is selected for parallelization. In this case only a single set of pointers are required for each parallel loop. In each of these modules there are routines for locating the radial integrals required for a given case. e.g. locbc for the bound-continuum two-electron radial integrals, loc1bc for the bound-continuum one-electron radial integrals.

The continuum-continuum parts are somewhat more involved as it is necessary to sum over the target eigenstates that are optionally computed at the first stage of the ParHam calculation. The full N+1 electron Hamiltonians are computed in stgmatf (non-exchange contribution) and stxmatf (exchange contribution). The corresponding ParAng files are read in routines in the module ang_ctl, file ang_ctl.f90. The files for the exchange data are read by rd_ang_data and those for direct data by rd_angd_data. Again ploc objects are used in the file positioning. In this case the angular data is read prior to performing the parallel loops. We have paid particular trouble to detect and print errors detected by the system and now exported by Fortran as syserr or ioerr, similarly the strings provided by MPI-II. Error halts are all via an error module which ensures that MPI is shut down cleanly.

Some of the output files, the H-file and the TARMOM-file, are intended for immediate use by follow-on R-Matrix programs (either FARM, PFARM, the relativistic recoupling codes or alternative programs). These files could be run on different computers than used for RAD, ParAng and ParHam. For this reason we have allowed for the possibility of a portable data representation for these files. Note that the external32 presentation defined in the MPI-2 standard is not available in mpich2. For this reason we have adopted the XDR representation defined by SUN for IPC as an option for output. This is a 32-bit representation which suffices for the present programs. Coding/Decoding routines are available as part of the standard library of effectively all computers. These are C-callable and therefore we have designed a standard Fortran interface, nxfiles.f90 (part of ‘xstream’, see [4]) that allows files to be written in either XDR or native representation. The XDR data is buffered for encoding and decoding in order to allow arbitrary buffer sizes to be used for both processes. This part of the calculation is performed by the routines in buf_mio.c. To simplify the options these files are written by MPI-IO explicit-offset C-callable routines. Files of matrix elements intended for the use in subsequent parallel calculations are output using pfilehand and the native representation.

As noted in section 2, ParHam is, at the time of writing, undergoing extensive validation and profiling tests. Scaling and performance data will be added in an update to this report.

6. Brief perspectives

Apart from the profiling and optimization already mentioned, ongoing verification tests and work to be performed as a result of user testing and feedback from real applications, there are some computational aspects that can be explored further. The RAD code provides a more straightforward opportunity for detailed investigation of the load-balancing of the sgc module. Conversely, given the efficiency of the

new RAD code, it may be possible to introduce some localized fine grain OpenMP into inner loops of ParAng, to reduce the overall number of MPI tasks while still making full use of the nodes. Similar possibilities will become apparent for ParHam. There are also possibilities for further development of pfh, including the introduction of shm as a user-invisible lower layer, most obviously to keep the indexing data as a shared memory segment (each task writes to a different location) and more ambitiously to make the main buffer arrays shm objects, to reduce communication overheads. This project has directly contributed to the upgrading of compilers towards correct Fortran 2003 compliance, and we aim to continue this encouragement and pressure, with the help of HECToR staff and successors on next-stage platforms.

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References

1. The UK-RAMP consortium is a 5-year EPSRC Software Development Call Grant shared between Queen's University Belfast, UCL, the Open University and STFC Daresbury Laboratory, commencing 1 October 2009 (EP/G055416/1, EP/G055475/1, EP/G055556/1, EP/G055599/1); CCPQ details at http://www.ccpq.ac.uk
2. A G Sunderland, C J Noble, V M Burke and P G Burke, Comput. Phys. Commun. 145 (2002) 311-340

3. P G Burke, 'R-matrix Theory of Atomic Collisions: Application to Atomic, Molecular and Optical Processes', Springer, 2011
4. 'Future-proof parallelism for electron scattering codes,' A G Sunderland, C J Noble and M Plummer, http://www.hector.ac.uk/cse/distributedcse/reports/prmat/
5. V M Burke and C J Noble, Comput. Phys. Commun. 85 (1995) 471-500; V M Burke, C J Noble, V Faro-Maza, A Maniopoulou and N S Scott, Comput. Phys. Commun. 180 (2009) 2450-2451
6. M A Lysaght, P G Burke and H W van der Hart, Phys. Rev. Lett. 101 (2008) 253001; Phys. Rev. A 79 (2009) 053411; A C Brown, S Hutchinson, M A Lysaght and H W van der Hart, Phys. Rev. Lett. 108 (2012) 063006
7. L R Moore, M A Lysaght, L A A Nikolopoulos, J S Parker, H W van der Hart and K T Taylor, J. Mod. Optics 58 (2011) 1132-1140; L R Moore, M A Lysaght, J S Parker, H W van der Hart and K T Taylor, Phys. Rev. A 84 (2011) 061404
8. http://ccpforge.cse.rl.ac.uk
9. P G Burke, V M Burke and K M Dunseath, J. Phys. B: At. Mol. Opt. Phys. 27 (1994) 5341
10. http://www.prace-project.eu
11. http://software.intel.com/en-us/articles/intel-parallel-inspector/
12. I J Bush, Technical Report HPCxTR0701 www.hpcx.ac.uk/research/hpc/technical_reports/HPCxTR0701.pdf , A Maniopoulou and C Armstrong, NAG HECToR Case Study CSE Report (2009) http://www.hector.ac.uk/cse/reports/castep_m.pdf
13. K A Berrington, W B Eissner and P H Norrington, Comput. Phys. Commun 92 (1995) 290-420 (this article subsumes earlier publications of the package)
14. http://www.pgroup.com/lit/articles/insider/v3n2a2.htm