Calculating electron impact excitation of iron peak elements on HPCx using parallel R-matrix codes

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One of the major outstanding problems in atomic physics is the accurate calculation of collision data for low ionization stages of iron peak elements such as iron, cobalt and nickel. This data is urgently required in the analysis of observations by the Hubble Space Telescope of gaseous nebulae (Figure 1) and in the analysis of laboratory spectra from, for example, laser-plasma interactions and tokamaks.

There are two main difficulties which arise from open d-shells in the target states of these ions. Firstly, a large Configuration Interaction (CI) expansion is required to adequately represent electron correlation effects within the target ion, and secondly, the open d shells give rise to a large number of target states, and in turn to hundreds, or even thousands of closely coupled channels. In addition, in order to resolve low-lying Rydberg resonances, calculations must be carried out over a very fine energy mesh.

These difficulties have necessitated a major redevelopment of the standard scalar R-matrix codes to produce the parallel PRMAT codes that are currently being used for calculations on HPCx. The latest optimised eigensolvers from the Scalapack library have been incorporated in order to address the computational bottleneck associated with diagonalizing large Hamiltonian matrices (of order 10000) in parallel. The PRMAT codes scale well and are able to exploit the high-end computing resources available on HPCx.

These codes have been applied sucessfully in LS coupling to study electron collisions with FeII, FeIII and FeIV, where comparison with previous work demonstrates the importance of including additional correlation effects and coupled channels and the need for using a sufficiently fine energy mesh. Typical results are shown in figure 2, where complex resonance structure can be seen.

Other computational innovations based on the R-matrix method and using HPCx facilities include the development of computer codes to study multiphoton ionisation in super-intense laser fields and the development of a 2-dimensional R-matrix propagator to study electron impact excitation and ionisation at intermediate energies.

Further information:
www.hpcx.ac.uk/research/atomic/prmat.html

Figure 1: Orion Nebula, NGC 1976, photographed from the Hubble telescope. Forbidden transitions of Fe ions are observed, for example in FeII.

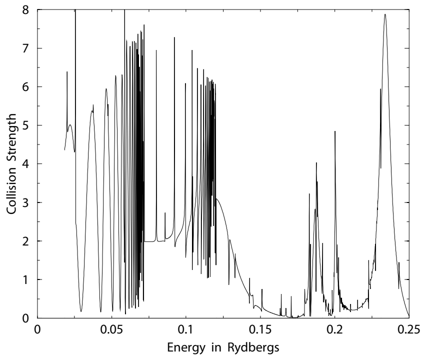

Figure 2: Typical collision strength results for electron impact excitation of FeII, illustrating the complex resonance structure that has to be resolved.

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there is significant work developing new grids, boundary datasets, and testing of numerical solvers. It is envisaged production runs of the new high resolution model will start later in the year.

The figure shows how the representation of the ocean will change with HiGEM model compared to our current climate model (HadCM3). Shown are the ocean depths around Australia, red and oranges indicate deep ocean, blue and green shallow ocean, with white regions land. The increased horizontal resolution of HiGEM gives a much better representation of the coastlines, allows more islands, and a more accurate representation of the width of straits and channels. In this region this will allow a better representation of the passage of water through Indonesia which was poor in HadCM3 but known to be important for the global circulation of the ocean.

Other benefits of increased resolution in the ocean will include dramatic improvement in the representation of the gulf stream and the North Atlantic current. Increased resolution in the atmosphere will result in much more realistic low pressure systems and storm tracks across the North Atlantic. It is known that both the gulf stream and the storm tracks play an important role in the ocean's thermohaline circulation which releases a huge amount of heat into the North Atlantic and so warms Northern Europe. The fidelity of the simulations produced by HiGEM will provide better assessments of the likelihood of a collapse of the thermohaline circulation, a possibility that is currently receiving much public attention in the film 'The day after tomorrow'

Further information:
www.higem.nerc.ac.uk