HiGEM1 on HPCx: High Resolution Global Environmental Modelling

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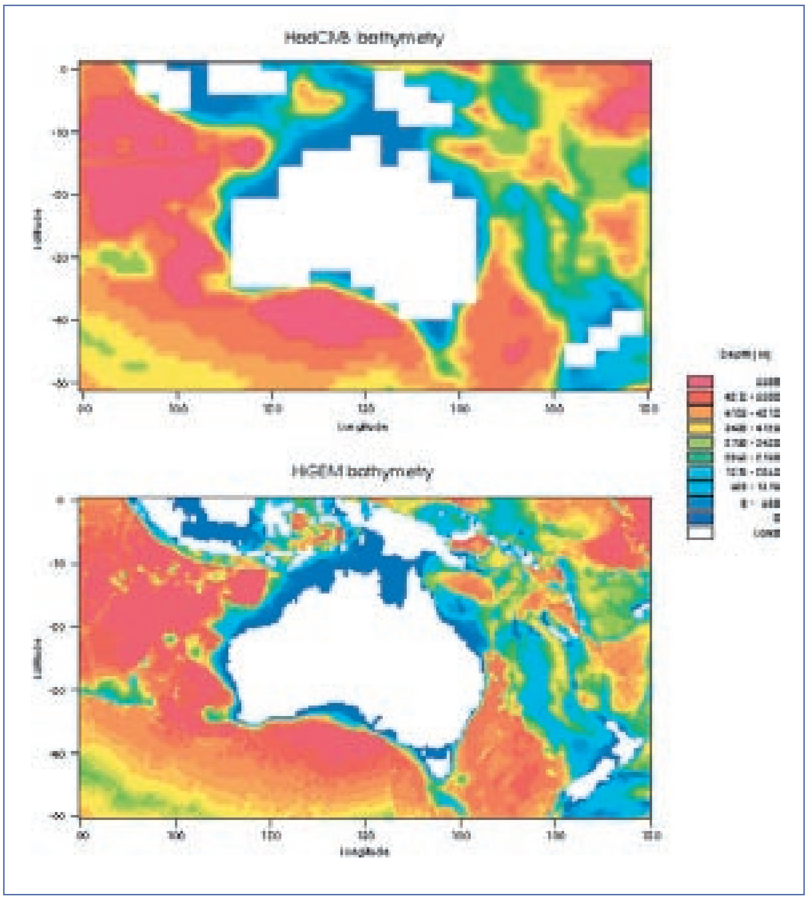

HiGEM is a national UK programme in 'Grand Challenge' high resolution modelling of the global environment between NERC and the Hadley Centre of the Met Office. In a three year programme (2004-2006), the new Met Office climate model will be taken to unprecedented resolutions. This will achieve a major advance in the fidelity of simulations of the global environment, and improve our understanding of mechanisms of climate variability and change on time scales of days to centuries.

To model the global environment requires representation of the atmosphere, ocean, ice, and land surface. To do this, the earth is divided into horizontal grid boxes, these are typically 300 km square for the atmosphere and 100 km square for the ocean. However at this resolution, many processes are not properly represented, or represented at all. For example: the impact of mountains on the atmosphere; small-scale eddies in the ocean that form in regions like the gulf stream; polynyas (large cracks in sea-ice) which are sites of intense exchange between the sea and the overlying atmosphere.

The goal of HIGEM is to simulate these processes much more accurately than has hitherto been possible. Initially the HiGEM model will have a resolution of 100 km in the atmosphere and 30 km in the ocean. Subsequently the resolution of the HiGEM model will be increased to 60 km in the atmosphere, and 15 km in the ocean. 100 years of model integration will be run so that important climate processes can be studied in detail. HPCx is the only academic computer in the UK that can provide the necessary computer power. Even so, this will be a very large capacity job on HPCx requiring some 5000 hours using 256-512 processors. The HiGEM model will also be run on the Earth Simulator in Japan as part of a closely related project.

The model code itself is based on the weather forecasting model of the Met Office. It solves forms of the Navier Stokes equations and simulates the many complex processes in the atmosphere, ocean, ice and land surface. The HiGEM model integrations will produce 10s of terabytes of output and an important aspect of project is to verify this output against the latest observational measurements. The complexity of the model and huge task in analysing the output requires a multidisciplinary consortium. The HiGEM consortium (listed below) brings together a wide range of expertise including:

• Hadley Centre: Provision of new Met Office Climate Model, expert advice on climate modelling.

• Centre for Global Atmospheric Modelling: Atmospheric processes, HPC expertise.

• British Antarctic Survey: Polar processes, modelling the cryosphere.

• Centre for Ecology and Hydrology: Land surface processes and modelling.

• Environmental Systems Science Centre : Clouds and radiation processes, model evaluation against satellite data.

• Southampton Oceanography Centre: Ocean processes and modelling, remote sensing.

• University of East Anglia: Ocean processes and modelling.

• British Atmospheric Data Centre: Data management.

During the start up phase of HiGEM, which is currently underway,

Continued opposite.

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.

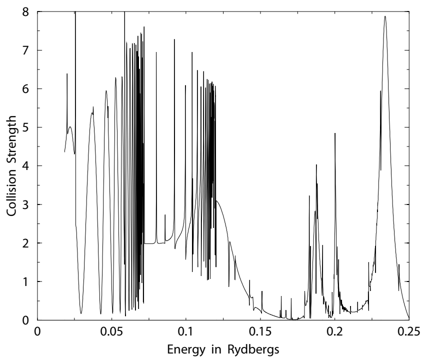

Figure 2: Typical collision strength results for electron impact excitation of FeII, illustrating the complex resonance structure that has to be resolved.

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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