VisRes-G: A Grid Computational Steering and Visualisation Tool for R-matrix Computations.

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Abstract

We describe the solution architecture of VisRes-G, a graphical tool for visualising and steering resonance analysis in atomic collision computations. VisRes-G is a comprehensive visual tool that facilitates the graphical display, manipulation and analysis of resonance data computed over the UKL2G. As the user interacts with the graph a collection of computation tasks are added to a task pool. A resource-task allocation component then attempts to match the tasks with available Grid resources, controls their execution across the L2G and returns the results to the graphical system. A major benefit of VisRes-G is that it enables the user to focus solely on physics without having to be aware of the computational resources being used.

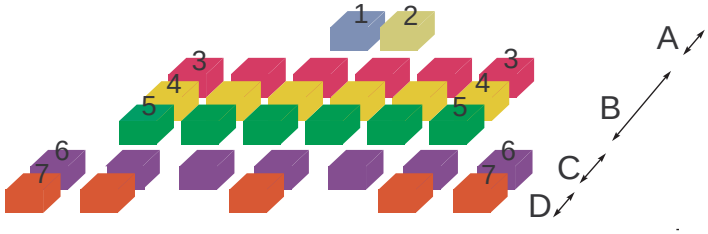

Fig. 1. The 2DRMP-G computation structure. Blocks A and B are independent of the collision energy and need only be performed once while blocks C and D are dependent on the collision energy and must be repeated hundreds of times.

1. Introduction

2DRMP-G, introduced at the e-Science All Hands Meeting 2003 [1], uses an R-matrix technique [2] to simulate the collision of an electron with a hydrogen-like atom or ion.

2DRMP-G's computation structure is illustrated in Figure 1. It consists of a sequence of seven solution steps that are developed as standalone implementations and is organized into four connected implementation blocks labeled A to D. Blocks A and B are independent of the incident electron energy and are performed only once. Solution steps 6 and 7 in blocks C and D, which involve manipulating large dense matrices and large systems of coupled second-order differential equations, are performed for each of the hundreds or thousands of electron collision energies. Each independent energy computation can typically take between 15 to 45 minutes depending on the problem being investigated and the resources used.

In [1] we focused on the grid solution architecture for blocks A and B. In this paper we describe VisRes-G, a graphical tool for visualising and steering the resonance analysis computations associated with blocks C and D.

VisRes-G, is a Grid enabled version of VisRes [3]. The software system is written in C, F77, OSF/Motif and Java and sits on top of Globus 2. The graphical interface is a comprehensive visual tool consisting of menu options and a multi-function tool-box which facilitates the graphical display, manipulation and analysis of resonance data computed over the UK L2G.

Before describing VisRes-G we set the scene by sketching the background to resonance analysis highlighting the benefit of computational steering.

2. Application Background

Electron collisions with atoms give rise to quasi-bound states with long lifetimes called resonances. In theoretical calculations resonances are revealed when the eigenphase sum, δ(E), rises rapidly by approximately π radians over a small range of collision energies. Resonance analysis is important in elucidating the collision process and in determining sensitive parameters against which theoretical computations and experimental results may be compared. However, the process is tedious and time consuming, particularly in regions where there is a dense accumulation of resonances.

First, since resonance positions are unknown at the outset of the computation, the randomly chosen scattering energies often provide an insufficient number of data points within the vicinity of the resonance to enable its characteristics accurately to be determined.

Second, since eigenphases are only known to modulo π, rapid changes in an eigenphase can result from the transition from one *arctan* branch to another and not from a resonance.

A graphical tool that can interactively steer the computation of eigenphases in the search for resonances is therefore of considerable value to the physicist.

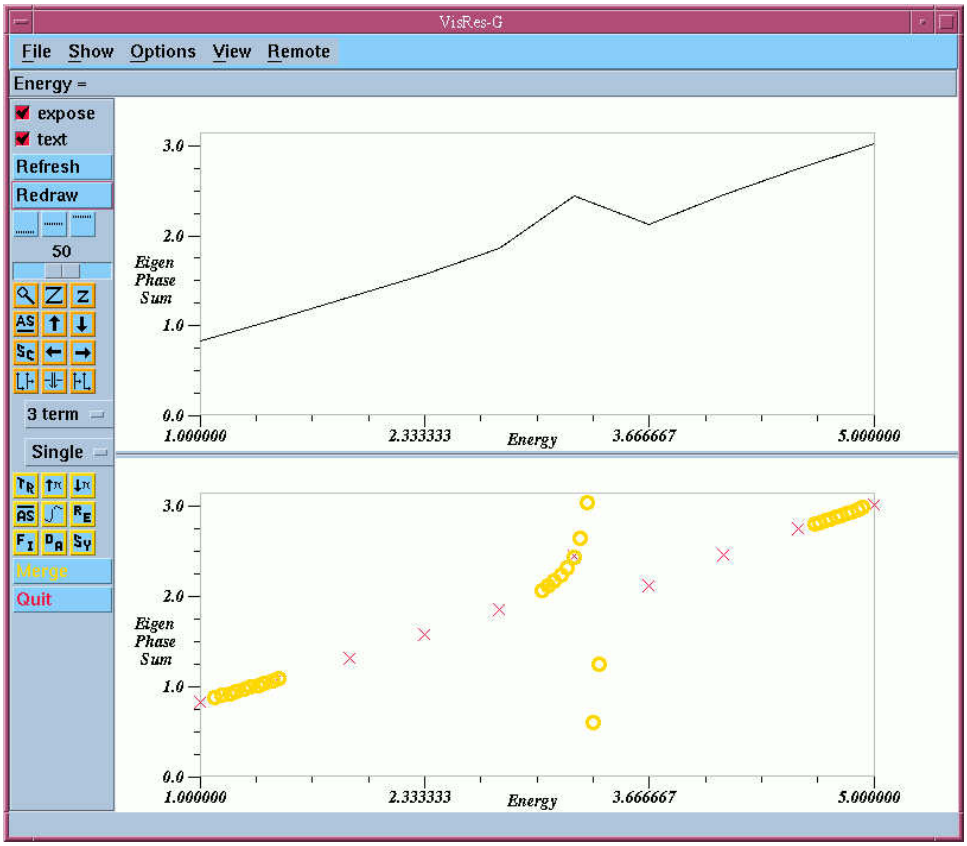

Figure 2. The initial eigenphase data returned to VisRes-G by 2DRMP-G is illustrated by the crosses. By clicking and dragging across the lower graph a new collection of Grid computations is initiated, collected and redisplayed in the form of the circles.

3. The VisRes-G User Interface

In this section we give a brief overview of the VisRes-G user interface.

First, as described in [1], 2DRMP-G is used to execute, using the UK L2G, the energy independent blocks A and B shown in Fig. 1.

VisRes-G is then be used to select and instigate the computation of eigenphases over an initial range of collision energies for blocks C and D. The output is automatically returned to VisRes-G and displayed on the user's workstation as illustrated by the ten crosses in Figure 2.

Through mouse interaction with the graph the user selects collections of points where extra data may be required, thereby steering the computation towards potential resonances. The

resulting eigenphase data is returned to VisRes-G and merged with the original data. For example, the data from three new collections of points are displayed as circles in Figure 2.

Further data can be generated in a similar fashion until the user is satisfied that all the necessary data has been computed. The position

rVis contains software to monitor the resources that are available in the grid and to allocate available tasks to available resources. The resource monitoring uses both national grid resource information and local historical information about resources in the grid environment. The local resource information

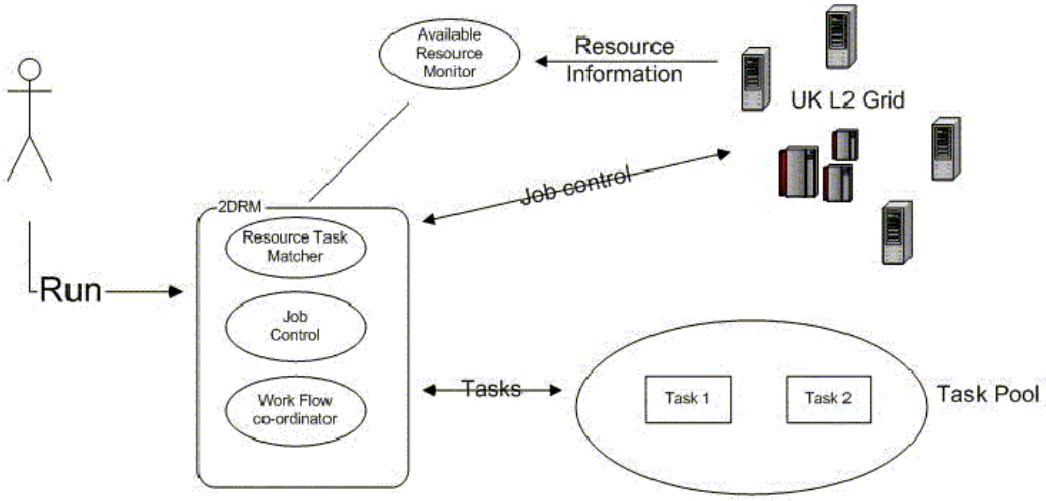

Figure 3.
VisRes-G uses rVis to monitor the resources that are available in the grid and dynamically to allocate waiting tasks to available resources.

and width of the resulting resonances can then be analysed using tool-box functions [2]. A major benefit of VisRes-G is that it enables the user to focus solely on steering the physics without having to be aware of the computational resources being used.

By using rVis, a Java program built on top of Globus 2, each requested energy computation from VisRes-G is farmed out to a suitable resource in the L2G.

4. The rVis Grid Architecture

The rVis component of VisRes is depicted by Fig 3. It uses the concept of a task pool to define the processing that is possible at any stage in its execution. Tasks are added to the task pool when the user clicks and drags across the VisRes window, each task corresponding to the computation of an eigenphase at a distinct energy. A work flow coordinator controls the execution by scheduling tasks to the task pool. A resource-task allocation component attempts to match tasks that are in the task pool with resources that are currently available in the computation grid.

can be updated in parallel to application execution. rVis uses this local database of available resources to determine whether it has permission to use a resource. It then tries to match waiting resources to available tasks in the task pool.

The job control component is used to control the execution of a task on a computational resource. Using Globus 2 its role is to package and transport the data that a task requires, to start job execution, to retrieve results, to detect and reschedule a task if execution fails and to log job submission details.

5. Concluding Remarks

In this paper we have sketched the functionality and grid architecture of VisRes-G a computational steering and visualisation tool for computing and analyzing resonances in electron atom collisions. This software is not R-matrix specific, and may be used in conjunction with any similar application.

The system has been tested using batch and interactive high performance and compute cluster resources within the National Grid Service and using interactive resources across

the L2G. Demonstrations of the system will be given at the Belfast e-Science Centre during the conference.

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