APAC EOT PROGRAM
PROJECT LEADER REPORT

JANUARY TO JUNE 2005

Project Title.

QPSF Education, Outreach and Training (EOT) Project

This report also refers to the following document:

APAC EOT Program
QPSF Plan for the CS&E Courseware Project
Visualisation and grid technologies via the access grid

Herein Referred to as "***QPSF EOT plan***"

Name of Project Leader

Dr J. Young (QUT)

Major Achievements
(Briefly describe any major achievements that have happened in the period. Reference any publications, publicity etc or relevant URL's. Each achievement should be about 1 paragraph).

In this reporting period, efforts relating to the APAC-II QPSF EOT Project were directed at

1. ongoing review of existing materials
2. continuing liaison and planning with relevant QPSF EOT personnel in the form of regular cross-institutional meetings and information sharing
3. initial development of core materials for introductory courseware modules in HPC, Problem Solving Environments (PSEs) and visualisation

These were foreshadowed in the previous report and in the June 2005 milestones given in the *QPSF EOT plan*.

Module Development

MultiMATLAB
Students in scientific computing are doing less programming in Fortran and C while at the same time, many students are now very familiar with MATLAB. MultiMATLAB is a system that enables one to run MATLAB in parallel on computational clusters and thus provides a suitable environment for students to learn parallel programming techniques. It allows students to focus on parallel programming issues. A Web-based module (including exercises) for using MultiMATLAB has been prepared and will be available on the APAC Repository by 9/SEPT/05. This module has been trialed with students and the completed module represents about 6 to 8 hours of lecture material.

Thinking Parallel
This module contains newly developed core materials for an introductory module on "thinking parallel." – an early preparatory unit for parallel programming classes. About 6-8 hours of lecture material has been developed, and an initial draft of this material has been delivered to u/g science and selected p/g students. A zip file containing a draft of this material will be available on the APAC-II EOT repository no later than 09/SEPT/05.

Introduction to Computational Structural Analysis
This module introduces the subject of computational structural analysis to postgraduates and practicing engineers (subsequent modules will equip the student with advanced computational modeling and analysis of civil structures). The module has been completed and placed on the APAC EOT repository. It represents about 8 hrs of lecture material and it is an introductory module that provides the background and understanding necessary for students to move onto more advanced and computationally intensive subjects. For example, the module introduces students to the non-linear behavior exhibited by structures before they fail.

Other activities

Further revision work (in the form of software evaluation and development of revised T&L materials) has been undertaken regarding core materials for an introductory module on CFD. An initial version (v-0.1) of this module was uploaded to the EOT-repository in January 2005, and was based on the Fluent/Gambit CFD PSE (Fluent Inc.) for student exercises. In the current version of this module, we have based student activities around the recently released FloWizard CFD PSE (also by Fluent.Inc). FloWizard is far easier to learn for first-time or casual CFD users, and allows student learning activities to focus on key CFD concepts such as grid refinement rather than the details of driving the software. FloWizard also has advanced collaboration features, and these will be incorporated into student activities in a future version of this module. An initial draft of the revised material has recently been presented to u/g engineering and selected p/g students, and a zip file containing the revised material will be available on the APAC-II EOT repository later this year after instructor and student feedback has been reviewed and incorporated into the revised draft.

Additional work has also progressed on a number of other modules relating to HPC, PSEs and visualisation. These include introductory modules on OpenMP and MPI, a module on visualizing 2D data using the MATLAB PSE, computational fracture mechanics, particle systems and a module on advanced visualisation of vector fields. Some of the material just mentioned has been presented in various contexts, but requires further development and is not suitable for uploading to the EOT repository at this stage. Other material is under development. However, it is expected that initial drafts of most of these modules will be available on the EOT repository in late 2005.

Progress against the AIMS
(Describe what progress has been made with any of the AIM described in the project plan. Mention only those that are relevant to this period).

The aim of the QPSF EOT plan is to create core educational materials on advanced visualisation, HPC, PSEs and grid technologies. The core materials developed by QPSF are specifically targeted to inform research and other students about new technologies that are driving science and engineering, and to introduce them to scientific visualisation, high performance computing and available APAC grid and HPC facilities, commonly used PSEs (such as MATLAB), and data visualisation/ mining applications.

See the points given above in *Module Development* and *Other Activities* above for specific progress against the aims.

Progress against the Milestones
(Insert the text for the milestone and add a description of the progress against the milestone).

The main focus of the QPSF program is the development of targeted modules as outlined in the Revised Milestones of our previous report. This includes development in a range of areas including *MultiMATLAB*, *Thinking Parallel*, *computational structural analysis*, *computational fracture mechanics*, *shared and distributed memory programming* and *visualisation of 2D datasets* (using MATLAB). Excellent progress has been made against these targets with initial versions of the first three topics completed and the expectation is that the remaining modules will be completed by the end of the year.

Thus, outcomes from work performed to date, as previously described in this report, are consistent with the planned milestones. An initial draft of a new module on *Thinking Parallel* has been completed and will be available in September. Work on the *shared and distributed memory programming* modules listed above has been completed, and initial drafts of these modules will be uploaded to the EOT repository at end of 2005. Educational materials on using *MultiMATLAB* and *computational structural analysis* has been developed and delivered to students in Semester 1, 2005. The *computational structural analysis* is available on the APAC EOT repository while the *MultiMATLAB* module will be available in September.

In addition, refinement of the existing module concerning *Introduction to CFD* has been done, and a revised draft of materials will also be uploaded to the repository later this year.

Project Team
(Indicate any significant changes to the resources: eg (1) new or removed institution, groups, key people; (2) major change to the efts of key people.
Note: Any changes to personnel should detail the person's name, institution and time allocation as per your original proposal. Indicate any additional equipment that has been used during the last quarter. This equipment should be reflected in the financial statement submitted by the partners).

No changes at this time.

Proposed Changes to the Plan
(List any changes that are proposed for the plan. If there are significant changes to the plan, a revised plan must be submitted to the EOT Manager. This includes changes to the names of key people or addition/deletion of sub-projects tasks.
Note: We expect that most plans will have changed since they were approved and therefore expect revised plans to be submitted with this report).

At this stage, the planned efforts for the next reporting period do not expect to substantially depart in spirit from those outlined in the *QPSF EOT plan*. The main focus will continue to be on materials development, early testing and initial delivery. The specific work proposals and milestones for module development in the next six months is detailed in the section *Revised Milestones* below.

Revised Milestones
(A set of milestones should be included even if there are no changes to the plans. Milestones must be included for the next period (6 months). Additions/changes can be made to the milestones for the remainder of the period.)

During the next 6 months, the milestones are as follows:

1. Existing Module Refinement
Work in the next 6 months will continue to refine the material in existing versions of modules uploaded to the EOT repository into a more useable form. This refinement may include the production of instructor notes (e.g. to accompany the *Curves and Surfaces* module in the repository), the development of more extensive range of assessment materials, and/or the removal of any copyright material inhibiting open distribution.

2. New Module Development
Work will continue on the development of initial drafts of introductory modules relating to core concepts in HPC and PSEs. We expect to trial the delivery of these materials in student-facing settings in the first instance.

The development of initial drafts for the modules listed below will be targeted for completion in the next 6 to 12 months. Our target is to have, at the end of the next reporting period, an advanced draft of materials suitable for uploading to the EOT repository for three or four of the modules listed below:

(i) an introductory module on *shared memory parallel programming* using OpenMP which is a natural continuation of the recently developed *Thinking Parallel* module.

(ii) a continuation of the module described in (i) above for *distributed memory programming* using MPI – with a hands-on emphasis using simple, clear coding examples.

(iii) *visualizing 2D data* using the MATLAB PSE, which will complement other MATLAB-based modules being developed at UQ and QUT.

(iv) a module on *advanced visualisation of vector fields*

(v) a module on *particles systems*

(vi) a module on *computational fracture mechanics*

If time and other constraints permit, work will commence on a number of other possible modules and activities, as follows.

(vii) A series of workshop lectures on *finite volume methods* was developed and presented by Prof. Ian Turner, QUT at the APAC summer school in Jan 2005. Work will be undertaken using this material so as to incorporate feedback from the initial presentation, and to create separate modules that will be suitable for presentation in a series of sessions over the AG.

(viii) The *computational fluid dynamics PSE FloWizard* allows limited collaboration features that are suitable for use by geographically dispersed teams working on different aspects of a common engineering design problem. It is proposed that a case study involving collaboration via Access Grid between two or more geographically dispersed teams be developed using FloWizard. An appropriate academic within QUT would be required to assist with the academic content required for this project, and informal agreement from Dr R. Brown (Engineering) as been obtained. It is envisaged that Dr Brown's academic contacts at other APAC institutions with Access Grid facilities will be contacted with a view to collaboration. This case study would be a natural continuation of other modules being developed by QUT.

(ix) More readily available HPC resources means that the use of suitably configurable CFD software for design optimization (as opposed to just flow prediction) is increasingly feasible. With this in mind, it is proposed that a case study in flow device design optimization be developed using the nimrod and Fluent/Gambit/FloWizard software suites. Our initial development of this *CFD case study* will be informed by the experiences of an initial trial of this concept, recently conducted by VPAC. Initial contact with the relevant VPAC personnel has been made, and ongoing collaboration with VPAC is envisaged for this project. This case study would be a natural continuation of other modules being developed at QUT.

(x) The emerging area of Multi-Disciplinary Optimisation (MDO), especially in the context of digital or virtual product design, is becoming increasingly important in engineering and other cross-disciplinary research activities. The development of an introductory module on MDO would be both timely and potentially useful to APAC partners.

(xi) Other modules on Advanced Visualisation Techniques (e.g. volume visualisation).

(xii) An introductory module or presentation on e-Research from the researcher perspective would be timely and potentially useful to APAC researchers. This relatively new term is fairly familiar to administrators, policy makers and senior academics, but less well understood by the wider research community, especially early career academics and postgraduate students.

The proposed modules given in (vii)-(xii) above represent possible extension activities for the next reporting period in 2005 but they are more likely to inform our development work during 2006.

Finally, if it is feasible and if time allows, we would like to trial the delivery of module(s) or part thereof over the AG between QPSF and other APAC institutions(s) to selected groups of students or staff at each site.

Signature

Print Name: Joseph Young

Date: 25-AUG-2005