

PACE Project Management Plan

Title		Version	Date
PACE: Proper Analysis of Coherent Excitations		1.4	29/11/20
Duration	Approved Budget	Project Type	
01/10/18 – 31/12/22	£1.25M (excluding existing ISIS staff effort)	Internal	
Project Manager	Sponsor	Department	
Toby Perring	ISIS Management Committee	ISIS	

1 Project Description

PACE (Proper Analysis of Coherent Excitations) is a software project to provide an integrated visualisation, simulation and fitting environment, on massively parallel and distributed computing, which interfaces to experimental data and materials modelling codes. PACE will:

- perform virtual experiments before and during the beam time to make most effective use of neutron beam;
- enable quantitative analysis of the full set of data collected during the experiment with proper account of instrument resolution;
- lower the barrier for users to analyse their data, so increasing the number and quality of publications, and reducing the time between experiment and publication.

In essence, the PACE deliverables are the parallel computing implementations and integration of proven data analysis packages and modelling codes in use on the Excitations Group instruments, together with parallelisation and interfacing to third party modelling codes. In more detail, PACE consists of refactoring the HORACE data analysis and visualisation framework, the TOBYFIT fitting and resolution function convolution package (both developed at ISIS), the parallelisation of the third party modelling package SpinW (spin waves), the parallel computation of scattering functions for single crystals and powders from the output from CASTEP (lattice vibrations), and the development of a generic interface to other materials modelling codes.

PACE does not include the creation of new modelling codes. Visualisation of functions of one and two dimensions in the style of HORACE will be implemented, but more sophisticated visualisation will use pre-existing packages e.g. sliceomatic in HORACE or graphics from Mantid or other sources. The STFC Scientific Computing Department (SCD) will provide and maintain the computing hardware on which users will run PACE – christened Data Analysis as a Service (DAaaS), which is a separate and fully funded project.

2 Project Organisation

2.1 Project roles and responsibilities

Following the STFC Project Management Framework, the roles and responsibilities are as follows:

Project Customer: Philip King (ISIS Spectroscopy and Support Division head, on behalf of the ISIS Management Committee)

The role of the Customer is:

- Approving the final Project Management Plan and Project Brief in consultation with the Project Manager or Sponsor
- Approving any other documentation as agreed
- Keeping the Project Manager or Sponsor informed of changes, if any, in their requirements
- Taking responsibility for any contribution to the project by the Customer's organisation

Project Sponsor: Russell Ewings (ISIS Excitations and Polarised Neutrons Group leader)

The role of the Sponsor is:

- Chairing the Project Board
- Providing the senior management ownership of the project
- Ensuring that the project is actively managed and meets its objectives
- Ensuring the benefits of the project to STFC as defined in the Business Case, are realised

Principal Investigator: Toby Perring (ISIS Scientific Computing Lead and Programme Manager)

The Principal investigator (or equivalently Project Scientist) is responsible for the scientific success of the project.

Project Manager: Toby Perring

The Project manager is responsible for delivering the project to specification, on time and within budget. In smaller projects, the Project Scientist may also be the Project Manager.

Previous experience with the HORACE code, which forms the template of PACE, is that close scientific engagement is important to ensure the success of the project. The agile approach to software development has been selected for PACE, in which the internal running of the project splits the roles of a Project Manager between the Product Owner and Scrum Master. The ISIS Project Management Office will assist in the creation of monthly project reports and finance documentation.

Project Board: Chair: Project Sponsor

Reporting: Project Manager, Project Scientist

Members:

Philip King (Project Customer) (ISIS Spectroscopy and Support Division)

Lamar Moore (ISIS Scientific Software Group Leader)

Gordon Brown (SCD Facilities Programme & Head of Ada Lovelace Division)

Stephen Hayden (Bristol University)

Jon Taylor (Head of ESS Data Management and Software Center)

Ray Osborn (Argonne National Laboratory)

The Project Board is responsible for advising the Project Sponsor and Project Customer on the delivery of the project, performing both an oversight and top-level management function on behalf of the ISIS Management. The board is chaired by the Project Sponsor, and therefore has authority to make cost, scope and schedule decisions.

In the case of PACE the role of the Project Board is advisory rather than binding. A small project on the scale of PACE would not normally have a Project Board. However, PACE is an unusual project for an ISIS science group because it is a software project beyond the scale of the single developer model with which scientific software has generally been developed within an ISIS group. PACE is also a flagship project across two STFC departments (ISIS and Scientific Computing Department) that may act as a model for future projects. Accordingly, ISIS management considers it valuable to have an advisory and oversight board with representation from both departments and external advisors.

2.2 Project Reporting

The Project Manager will prepare monthly reports for the Project Sponsor (ISIS Excitations Group leader) and the Customer (ISIS Spectroscopy and Support Division Head and ISIS Management Committee) via the ISIS Project Management Office. The reports include a progress report, financial report, and updated risk register and communications plans.

The Project Board will meet twice a year, with ad hoc meetings in between as required. The Project Manager will prepare a six-monthly progress report as well the financial report, and updated risk register and communications plans for the Board meetings.

2.3 Organisation within the PACE development team

Between the key milestones at the end of the investigating/piloting, design, build, and release phases, the project will be organised using the Scrum methodology for agile programming. Objectives will be set on a two-weekly cycle, with daily 'scrums' (15 minute stand-up meetings). This model is well suited to the situation when there are unpredictable challenges in a software project. In the case of PACE this will be especially true in the investigation/pilot phase and the User Collaborative Development phases. In the former, the biggest risk areas, different methodologies, and existing open source applications that PACE may exploit need to be investigated. In the agile development phase, PACE will be developed in response to the feedback from instrument scientists and users from experience on the Group spectrometers.

Using Scrum terminology, the Product Owner will be Toby Perring, with the responsibility of setting the overall priorities and vision. The role of Scrum Master (removing obstructions to the ability of the team to deliver and to take responsibility for day-to-day oversight) will initially be taken by a contractor with prior experience of this approach and of architectural design in a parallel computing environment. It is important to get this role filled at the beginning, hence the choice of a contractor.

During this period one of the software engineers who is recruited onto PACE will be trained into the role of Scrum Master and take over when the contract ends.

3 Objectives and Deliverables

PACE is a software project with several interacting but distinct components that need to be created. The key deliverables are as follows:

- 1) Optimisation of the current HORACE data analysis and visualisation framework by
 - Parallelisation for multiple core computers and distributed computing, operating on the Data Analysis as a Service (DAaaS) and SCARF high performance computing services at STFC;
 - Provision of file-backed operations so that datasets larger than the available memory can be processed.

- 2) Optimisation and extension of the current TOBYFIT resolution convolution and least-squares fitting application by
 - Production of a parallelised version of for parallel computing, operating on DAaaS and SCARF, using the framework developed above in (1).
 - Extension of the formalism to use Monte Carlo simulations of the primary spectrometer from McStas for greater accuracy of the resolution model for neutron guides.

- 3) Parallelisation of SpinW (spin wave modelling and scattering cross-section computation).
 - Formally this activity is now a separately funded project; however its results are integral to the use of PACE with multiple modelling codes.

- 4) Computation of scattering function for single crystals and powders from *ab initio* determination of phonons using CASTEP and from other codes that output force constant matrices.
 - This utility is now named Euphonic.

- 5) Development of an Application Programming Interface (API) to third party modelling codes so that they can be interfaced to the HORACE framework and the TOBYFIT resolution convolution application. Integration of SpinW and CASTEP into the framework using the API.

- 6) Construction of a GUI based 'workbench' for managing analysis of data with refinement of parameters in resolution broadened models for scattering i.e. GUI interface to TOBYFIT.

- 7) Mantid based manipulation and GUI based visualisation of powder data that accesses the modelling and resolution convolution/fitting capabilities of PACE.

- 8) PACE will be handed over for routine operation on the instruments and first formal release for users at end of the project.

The Project Brief gives more explanation and background to each of these deliverables in Section 3.1. These higher level objectives are broken down into milestones in Section 4.2 (Timeline and milestones).

4 Project Schedule

Appendix 1 contains a Gantt chart for the project schedule.

4.1 Breakdown into sub-projects

The core of the development is split into three subprojects, namely framework (objective 1), optimisation and resolution (objective 2), and modelling and interfacing with simulation codes (objectives 3-5). SpinW (spin wave modelling) and McPhase (crystal fields, intermultiplet transitions and spin waves) will now be parallelised by a project funded by the Ada Lovelace Centres at STFC, working in collaboration with the European Spallation Source. Direct responsibility of the PACE team will be to interface with SpinW. The development of codes to compute phonon cross-sections efficiently from CASTEP and other phonon codes will be done within PACE.

In addition to software engineers working on the above, a post doctoral research associate (PDRA) with experience of neutron scattering and writing data analysis programs is employed to investigate and prototype methods for resolution convolution that go beyond the current TOBYFIT formalism. The PDRA will also act as the scientific 'glue' between the sub-projects on a day-to-day basis to ensure the scientific coherency of PACE for users. The PDRA will participate in scientific projects, and will be under the supervision of Toby Perring.

Overall scientific vision and priority setting will be performed by the Project Scientist, Toby Perring (original author of HORACE and TOBYFIT).

Each of the three sub-projects will have a scientific lead from the ISIS Excitations group who will be an integral part of the PACE development team:

- Framework: Alex Buts (primary code developer for HORACE)
- Optimisation and resolution: Greg Tucker (PACE PDRA), with input from Toby Perring. With the imminent departure of Greg Tucker in December 2020 and the recruitment of STFC staff onto the project in Autumn 2020, the skills profile of the replacement are under review.
- Modelling and interfacing with 3rd party code: David Voneshen (experimental measurement of lattice dynamics), Keith Refson (lead developer of CASTEP), Duc Le (spin waves)

In addition, there are two other smaller subprojects:

- GUI development for workbench operation of PACE in the final six months
- Interaction with Mantid for powder analysis: ISIS Excitations group champion: Duc Le

4.2 Timeline and milestones

As of the date of this updated Project Management Plan, a good understanding of the architectural design for the framework has been achieved. The decision has been taken, on the basis of piloting studies of Matlab-to-Python interactions, to provide both a Matlab and Python user interface. The updated project plan (Appendix 1) accounts for this change, and the corresponding merging of the originally separate Matlab and Python deliverables is detailed below.

Although not strictly coincident across the three subprojects (framework, optimisation and resolution, and interaction with 3rd party modelling), there are three broad phases:

Pilot and design phase

Deliverables:

D1. A design will be created for

- the framework (**D1a**), detailed as (**D1a1**) parallelization framework infrastructure and implementation in it of principal operations (gen_sqw, cut, symmetrize); (**D1a2**) redesign of the SQW object to permit use with the new interfaces. Additional work is needed for (**D1d**) a continuous integration build and test system to validate the changes, and (**D1e**) a parallel job management system for the targeted clusters.
- optimisation (**D1b**) and resolution (**D1c**), which are the design phases of deliverables **D5** and **D6** below. They are included here as to integrate their design with **D1a** above. The design also includes (**D1c1/2**) improved representation of the instrument information.

D2. Design interfaces to 3rd party phonon modelling codes (**D2a**), and generic interface to other 3rd party modelling codes and user provided Matlab, Python and compiled C++ (**D2b**).

D3: Revision of project plan and re-evaluation of project priorities in the light of better estimates of the time to complete the various work packages and availability of effort.

Main build phase

The goal at the end of the main build phase is to have a release version for use on the ISIS Excitations Group instruments. The framework will have sufficient features and functionality for use by instrument scientists to provide feedback for the User Collaborative Development phase. The framework will have a Matlab and Python interface very similar to HORACE, and will accept user functions for scattering models or fit functions that are Matlab, Python or compiled C++ functions. The Matlab interface to PACE will endeavour to be backwards compatible with existing HORACE scripts and functions.

Deliverables:

D4: Matlab user operation optimization and generic basic interfaces to modelling codes (Matlab, Python or compiled C++) that conform to the PACE framework API, with at least the same functionality as the current HORACE.

- Operating on hardware platforms:
 - o DAaaS using multicore and distributed computing (**D4a0** – parallel framework implementation).
 - o Single node computers (Windows, Linux, MacOS).
- Using the parallel framework to optimize principal operations (**D4a1/2**)
- Use compiled MATLAB to provide license-free operation when used with a non-MATLAB interface (**D4a3**)
- Will be able to (**D4a4**) handle data sets at least as large current datasets (0.5TB .sqw files) by file-backed operation where only sub-sets (pages) of the file-backed data are held in memory for processing.
- Use appropriate MATLAB new classes to allow interfacing with Python, in a new SQW object class (**D4a5**). The classes will be integrated with the new instrument information classes designed above in **D1a2**.

D5: Generic parameter optimisation framework with plug-in capability for fit functions that conform to the PACE framework API (i.e user functions or 3rd party codes).

D6: TOBYFIT resolution convolution function for the optimisation framework:

- Parallelization: Able to run on as many nodes as the available DAaaS and Scarf hardware permits.
- extend to hybrid McStas/analytic.
- $S(Q,\omega)$ models must conform to the PACE framework API.

D7: Application (now named Euphonic) to compute $S(Q,\omega)$ from dynamical force constant matrix output from CASTEP, GULP, phonopy (written in Python & C++ only, i.e. no Matlab). Interfaced to the PACE framework API.

D8: Interfacing of parallelised SpinW into the PACE framework API.

D9: Generic projections (spherical, cylindrical, user-provided) implemented.

D10: Python port of the Matlab interface created in **D4-D8**. This is split into (**D10a**) interface design and (**D10b**) interface implementation.

*Note: the previous Python user interface deliverables **D10-D14** were essentially identical to the Matlab user interface **D4-D8**. They were subsequently merged into **D4-D8**; however, the delay in starting the Python interface has made it desirable to re-include them as a separate, but simpler, single task.*

The following remaining deliverables have been left with their original numbering for ease of cross-referencing with the previous project plan. Deliverable tags D11-14 are not currently used.

D15: Optimised interfaces to specific 3rd party modelling codes will be written as determined to be necessary from user feedback.

D16: Generic APIs for user Matlab, Python, and compiled C++ codes to framework

GUI build (final 6 months)

The GUI workbench will only be written towards the end of the develop-in-use period to capture proven analysis strategies and workflows from operation of PACE by instrument scientists and users.

D17: Interactive workbench to for managing analysis of data with refinement of parameters in resolution broadened models for scattering.

Interface to Mantid (Project duration)

Throughout the build phase an interface will be maintained between the main PACE data objects to primary Mantid workspaces, in particular to the MDworkspace and to the Mantid Mslice extension for powders. The level of interoperability and code sharing will be regularly reviewed.

User Collaborative Development phase

The software will be developed in release cycles of 2-3 months with continuous feedback from instrument scientists and users, once an initial working product has been developed. This is an essential part of the later construction phase, as reshaping the framework and the functionality of the modelling and resolution convolution sub-projects with the feedback from real-world use is what makes genuinely valuable software. It is during this period that analysis strategies will be developed as the capabilities and opportunities of PACE become fully understood by the developers and users, and which will feed into the GUI workbench design.

Apart from optimisation of slower parts of the code, agile inclusion of new functionality, additional features that are desirable include implementation of alternative resolution convolution strategies, and interfaces to specific 3rd party codes according to user requests.

Project close

Documentation for users on how to use PACE will be continually created and updated during the course of the project. Shortly after the project completion a teaching workshop will be held for users of PACE.

D18: Project close-out report.

D19: Web documentation describing how to use PACE completed.

5 Finance

The cost of the project is almost entirely staff, with consumable costs of approximately £10K per annum being found as required from the ISIS Spectroscopy and Support Division budget. The table below gives the costs on a quarterly basis in units of £1k. The total cost excluding ISIS staff is £1.46M, and with ISIS staff is £1.72M. Full details with a quarterly breakdown are given in Appendix 2.

The staff breakdown is as follows:

- Three software engineers with experience of parallel programming in C++ and python are required, employed in the STFC Scientific Computing Department, broadly one for each of the sub-projects of framework, optimisation and resolution, and interfacing with modelling codes. The Senior developer role is Band E/F, the other two at Band D/E and the PDRA at Band D/E.
- Two contractors have been recruited for a total of 15 months. Their roles are being taken by two new recruits above (Senior and Junior developers).
- For the final 6 months a specialist GUI designer and builder will be recruited to construct the interactive workbench for managing analysis of data with refinement of parameters in resolution broadened models for scattering.
- A PDRA with previous neutron scattering and data analysis coding experience will be employed.
- Dominik Jochym (Scientific Computing Department) will spend a fraction of his time on PACE as the local supervisor of the developer of interfaces to 3rd party codes. In addition, Keith Refson will spend approximately 10% of his time on PACE.

6 Resources

The allocated costs of the project are entirely staff. However, PACE is a capital project because it delivers a product, namely a software application for data analysis.

In addition to the capitalised staff effort recruited onto the project, there will be effort from existing ISIS Excitations Group staff. The major component will be Alex Buts who maintains and develops HORACE, who is expected to contribute 50% of his effort using HORACE to prototype idea and a source of expertise to the developers of PACE in the design. Following a change of his responsibilities within ISIS, Toby Perring will contribute 25% as overall scientific leader and Project Manager, but will no longer be contributing development effort. In addition Duc Le, David Vonshen and Keith Refson will spend 10% each of their time as scientific leads and contributors to their respective sub-projects.

7 Procurement Plan

ISIS is providing full funding for the project. This amount is already accounted for in the budgeting of ISIS.

The contractor effort was recruited via Digital Outcomes and Specialists, a procurement framework for the public sector to acquire development services.

8 Risk Management

The separate Risk Register document details the project risks, and will be updated during the course of the project. It will be reviewed regularly as part of the project reporting to the Project Customer (Section 2.2).

The major risks are the difficulty in recruiting software engineering staff on fixed term contracts, and staff leaving before the end of their fixed term contracts as the end looms. The two remaining software engineers to be recruited will now be recruited on open-ended contracts, with the prospect of working on other scientific computing projects once PACE formally is completed.

9 Stakeholder Communication

PACE is a software project on behalf of the ISIS Excitations and Polarised Neutrons Group, for the benefit of the scientific output of the Group and users of the instruments operated by the Group. In addition to these and the Project Customer (ISIS Spectroscopy and Support Division and ISIS Management Committee), there are a number of other stakeholders. These include the ISIS Computing Group, the Mantid project, STFC Scientific Computing Department and European Spallation Source.

The separate document Communications Plan lists the stakeholders and details the formal and ad hoc communications that are expected to take place. In general these will be in the form of regular formal meetings with the project manager and/or project sponsor, together with ad hoc meetings with the project manager. In the case of the users, the communication will largely be when users are on site for experiments, although the Neutron and Muon Science and User Meeting (NMSUM) is a good venue for a formal update. The purpose of the Communications Plan is to ensure that the project properly responds to the needs of the stakeholders as well as to inform them about progress on PACE. The plan will be updated during the course of the project. It will be reviewed regularly as part of the project reporting to the Project Customer (Section 2.2).

10 Monitoring and Reporting

The reporting will be monthly to the Project Sponsor (ISIS Excitations Group leader) and the Customer (ISIS Spectroscopy and Support Division Head and ISIS Management Committee), and biannually to the Project Board. See Section 2.2.

In addition, a technical design document for expert review will be created at the end of the framework design phases.

11 Quality Plan

11.1 Software development

PACE will use a software repository with version control. Code will have appropriate unit and systems tests to ensure that the multi-developer application is robust to code additions and changes. Code reviews may be implemented before checking developments into the code trunk, but it is important particularly during the early stages not to slow down piloting and prototyping by too rigid and slow a management process. A Jenkins build server will be used to build and test nightly versions of the code for the supported operating systems.

11.2 Project documentation and change control

Project documentation, technical review reports, and meeting minutes will be stored on the ISIS projects Sharepoint site. A link will be created so that the external members of the Project Board has access to the documentation at all times.

Changes that affect the agreed cost, time, risk and specification will need Project Board approval. The project manager can approve changes that affect the sub-projects but do not affect the overall cost, time, risk and specification.

Appendix 1. Project Gantt charts

1. Current chart, Data Analysis
2. Current chart, Fitting and Resolution and Modelling Code Interfaces
3. Current chart, Miscellaneous tasks

STFC Project Management Plan





