PRISM Platform Proposal: Enhancing Configuration and Use of FEM Codes

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Overview The PRISM platform represents a set of groups developing open source software and tools for undertaking finite element analysis in a wide range of scientific fields. Applications such as Nektar++, Fluidity and PyFR present different interfaces to end users or developers but as with almost all advanced scientific applications, they require the setting of a number of configuration parameters to define the task to be undertaken by their users. In the case of complex codes, there can be large numbers of parameters that have a variety of constraints that affect what values can be selected under different usage scenarios or when running on different types of resources. There can also be challenges in managing the full pipeline of processes required to get from an initial geometry to defining and running a job. This project will build on the TemPSS (Templates and Profiles for Scientific Software) and Nekkloud tools, built as part of the EPSRC-funded libhpc (EP/I030239/1) and libhpc Stage II (EP/K038788/1) projects, to further assist users in addressing these challenges.

This project will bring together approaches developed as part of libhpc. It will build on early prototyping in TemPSS to represent constraints between parameters and initial trial development in Nekkloud to provide a console for generating meshes and Nektar++ input files from an initial geometry. The work will enhance the prototype meshing code in Nekkloud and develop a lightweight solution for highlighting parameter constraints to users. If time allows, we will also look to integrate another PRISM code, either Fluidity or PyFR, into a Nekkloud-style web-based tool. The outputs of this work also have the potential to feed into subsequent project work, in particular an advanced framework for developing a new and significantly more flexible approach to generic representation and handling of complex parameter constraints and configuration decisions that has recently been proposed to EPSRC.

Project objectives This work has four core objectives:

- **Enhancing the job pipeline** in Nekkloud to include meshing, enabling tasks to start with a geometry
- **Enhancing usability of TemPSS** by making it easier to formulate valid job configurations
- **Increasing user base** of Nektar++ by further lowering the barriers to setting up and running jobs
- **Promote collaboration and sharing** of techniques developed and demonstrated here within PRISM

This work will undertake further **prototyping** of approaches to represent parameter constraints within the existing TemPSS tree model that displays an application's configuration parameters to users as a tree-based structure. Constraint information will be made visible to TemPSS users when they build their profiles and will constrain the options available when selecting parameters for a task. The work will also take forward early prototype code in Nekkloud designed to demonstrate the potential to integrate with the NekMesh **mesh generation** utility in Nektar++. The outputs of this work will be extensions to TemPSS enabling developers to add parameter constraint information to an application template and meshing tooling fully integrated into the main release code for Nekkloud. This work will open up the capabilities of Nekkloud and TemPSS to a wider user group and demonstrate how they can run jobs more easily on cluster or cloud infrastructure without needing detailed technical knowledge of these platforms.

Alignment with PRISM strategy

Retention of key staff: This project will provide bridging of Dr Jeremy Cohen who has worked extensively with members of the PRISM platform for some time. He has significant knowledge and experience, developed over several years, of processes for simplifying access to complex scientific codes and computational infrastructure and has been involved in the development of a range of tools and services.

Longer-term research: This project will build on a strong research theme and a number of previous related EPSRC-funded projects. It will be of vital importance in continuing this research theme and the benefits it can bring to domain scientists and researchers.

Collaboration between PRISM members and groups: This project will provide a solution that is applicable to multiple codes across the PRISM platform. Through demonstrations and communication with the various groups within PRISM, the benefits of the tools used within this work will be highlighted to these groups with a view to extending the reach and usage of the tools over time.

Brief work plan This project will involve building on existing tools developed as part of the libhpc project to support the running of binary HPC applications. The key tasks and milestones are as follows:

- Extend TemPSS' HTML transform, for generating visual trees, with enhanced support for constraints
- Provide a user-friendly way to represent constraints and a developer interface to specify them
- Extend the interface to NekMesh with a complete meshing interface within Nekkloud
- (Advanced objective) Investigate the addition of Fluidity or PyFR into a Nekkloud-style interface