1. QuakeCoRE/NSC/UC Software Team

The QuakeCoRE/NSC/UC software team has been established in recognition of importance of developing computational capability for the QuakeCoRE research community. 2.0FTE is funded by QuakeCoRE, 0.5FTE by NSC, and 2.5FTE by UC.

Our role is not only limited to software development (see other posters at this meeting for examples of those), and we often provide workshops and training to the QuakeCoRE research community, in order to enable computational capabilities to be fully utilized.

We are happy to collaborate with the QuakeCoRE research community to develop and offer high-quality SW training programmes.

2. Past/Current Training Offerings

Software Carpentry

An international initiative helping researchers to increase research productivity by acquiring basic research computing skills. Usually 3–4 segments (such as Unix shell, Python (or R), Git, SQL) delivered in two full days. The training material for these segments were carefully selected and designed to help researchers to automate repetitive works, reproduce the experiment and analysis with a structured code and collaborate with other researchers more effectively.

QuakeCoRE’s Sung Bae is a certified Software Carpentry instructor, and QuakeCoRE and NeSI co-hosted this event in 2016 and contributed to UC ResBaz 2017 where Software Carpentry was a core programme.

Using NeSI HPC Resources

New Zealand eScience Infrastructure (NeSI) is the national provider of high-performance computing (HPC) resources, and QuakeCoRE-NeSI partnership has proved to be very productive. QuakeCoRE has repeatedly secured large computing allocation and has produced significant research output by utilizing the HPC resource in the areas of ground motion simulation and the seismic response of infrastructure. We have been providing informal training on request that covers how to remotely access the HPC facility and submit/monitor the computational job. We plan to offer a revised workshop once NeSI’s new Cray cluster becomes operational in early 2018.

OpenSees

Training workshops for the open-source finite element platform for seismic response analysis of infrastructure, OpenSees, were held in 2016 and 2017 in both Christchurch and Auckland. These workshops were intended to provide a general introduction to working with OpenSees for structural and geotechnical applications. The content ranged from introductory topics such as a step-by-step anatomy of an OpenSees model file, to advanced topics such as carrying out IDA and MSA in parallel on HPC resources.

Now that a critical mass of OpenSees users has been established within QuakeCoRE, it’s anticipated that future OpenSees training workshops will be delivered in alternating years, with a workshop or short course on a computational analysis topic of choice in the intermediate years.

ParaView

Scientific visualization is very important for research scientific discovery and also to communicate research with other researchers and general public. ParaView is an open-source 3D visualization software with virtually unlimited feature sets. Our workshop in 2017 provided a gentle introduction to ParaView basics through small examples followed by a session where each participant can attempt to display their own research data with the instructor’s help.

Applications of ParaView, so far, with QuakeCoRE have focused on visualisation of HPC results (e.g. Figure 5), but we are working with researchers currently on visualisation of post-earthquake recovery.

Git

As the extent of deep collaborations within QuakeCoRE increases, the importance of collaborative software development becomes increasingly important. Git is the most commonly adopted development platform for software collaboration.

This 2017 workshop demonstrated, in a hands-on environment, the importance of git for version-control in collaborative software projects. It was a two-hour session that covered terminology, branching, git workflow, selective commits/merges, merge conflict resolutions and forking. This workshop was aimed for people who have used git before and wanting to increase their git proficiency.

3. Suggestions for Future Training Programmes

In order to provide the greatest value to the QuakeCoRE community, we are interested in your suggestions for future training/workshops that can be developed (or repeated) in the context of our goal to enable QuakeCoRE researchers to fully utilize computational capabilities.

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Figure 1: Software Team personnel
Figure 2: Software Carpentry @ UC June 2016
Figure 3: NeSI’s new Cray XC50
Figure 4: First OpenSees training workshop @ UC June 2016
Figure 5: Visualisation of simulations of the 2016 Mw7.8 Kaikoura earthquake using Paraview
Figure 6: Git logic for version control