Workshop on Continuous Integration on High Performance Computing Platforms

Overview of the day with:

> Links to notes from discussion sessions
> Link to presentations

Summary/Take home messages

> Survey of current practice suggests lots of interest in this topic

> Some very sophisticated testing frameworks already set up in various locations.
- Buildbot used by Nektar++
- Singularity container at Cambridge
- Jenkins/Travis combination at UCL

> The choice of CI framework was deemed to be largely unimportant

> Build time is a real issue, especially as this needs to be done from scratch on HPC. Do you provide computer nodes to do this? Often not parallelisable so very wasteful.

> Module on HPC are tricky and often not standardised

> Often older linux platforms (>=RHEL6) with older libc 2.12 and custom versions of MPI

> No reason this cannot be done, Chris Richardson aims to to set some proof of concept on a Tier 2 system

The day started with an overview from the head of the new Research Computing Services at Imperial, which encompasess both HPC and the RSE team here at Imperial.

I then gave a short overview of my experience and motivation for putting together the workshop. My work focused on coupled simulation, which requires me to support users building and running a coupled simulation using OpenFOAM and LAMMPS together, as well as ensuring the shared CPL library which is my responsibility works as expected. In order to run on ARCHER at large scale,

Parallel testing
Conda deployment
Aprun and build issues with ARCHER
Lack of containers

The first talk was by Steven Lamerton, about the Software Engineering Support Centre (SESC) effort to provide a centralised Jenkins testing system focused on Collaborative Computational Projects (CCP). The CPPForge aims to be a centralised UK repository of best practice software, offering repository hosting, documentation, forums and training; with SESC extending this service to include build services and CI testing which is freely available to any project registered

with CCPForge (Also see this article on the SSI website). The Jenkins server is up and running, available provided your code is a CCP project.The next step will beto include future HPC integration and move towards including deployment on ARCHER.

The next talk was by Catherine Jones, outlining the STFC survey results. The key take home messages from this were that Travis was the most used CI, then Jenkins, with Linux the key operating system and provision of necessary compilers, shared libraries and then testing tools are key identified as very important.

This was then followed by a discussion of what would be best in a centralised service. The first thing which became apparent is the scope of interest here. Certainly even testing on HPC is not a solved problem and many issues emerged with this. The SESC service is available
Travis CI in parallel

The next session was by Chris Cantwell

Then Jeffrey Salmond and Krishna Kumar

The conclusion is that no framework is ideal, and that the choice of framework is not as important as doing something.
Deployment and building time is the major problem, in a virtual environment on HPC. Dedicated queue for this?

The final session included a presentation by Alin Elena and David Perez-Suarez. UCL have a system which selects between Travis for simple parallel jobs and moves to Jenkins for more complex and parallel deployment.

Session start	Session end	Title	Speaker
9:45:00	10:00:00	**Coffee and Registration**	
10:00:00	10:10:00	Introduction and plan for the day, Summary of Suggestions from sign-up form	Edward Smith (Imperial)
10:10:00	10:30:00	HPC and CI at Imperial	Spencer Sherwin (Imperial)
10:30:00	10:40:00	Challenges to Testing on HPC from my work on CPL library	Edward Smith (Imperial)
10:40:00	11:00:00	The SESC Build Service - CI for the UK computational science community	Steven Lamerton (STFC)
11:00	11:20:00	Results of the STFC CI survey	Catherine Jones (STFC)
11:20	11:50	Panel Guided Discussion -- what would be useful in a central service?	All above

11:50	12:50	**Lunch**	
12:50	13:10	Continuous Integration of Nektar++ with Buildbot	Chris Cantwell (Imperial)
13:10	13:30	HPC-CI infrastructure at Cambridge	Jeffrey Salmond and Krishna Kumar (Cambridge)
13:30	14:00	Brainstorming on the pros and cons of Travis, Buildbot, Jenkins, CircleCI, etc for HPC	All
14:00	14:15	Break	
14:15	14:30	Continuous Integration for DL_POLY_4	Alin Elena (STFC)
14:30	14:50	Overview of RSE and CI on HPC at UCL.	David Perez-Suarez (UCL)
14:50	15:50	Break off with group discussion session on key problems	All
15:50	16:00	Discussion of outcome summary document and close	Edward Smith (Imperial)