Imperial College London

RCS RESEARCH COMPUTING SERVICE
Gateway to Discovery

Research Software Engineering

Summary of Work: Nektar++

Project details

References:	Nektar++/2019/1/1 and Nektar++/2019/2/1
Proposer:	Professor Spencer Sherwin, Department of Aeronautics (South Kensington)
Domain:	Computational Fluid Dynamics
Components:	Software engineering infrastructure

Project Overview

The goals of this project were to provide:

1. A comprehensive overview of the CI/CD State of the Art - addressed by Phase I
    - This considered the specific requirements of Nektar++ and informed the proposal for Phase II.
    - The wider expertise gained from this analysis formed the basis of the public project outputs detailed below and will continue to inform the practices of the RSE team going forward.
2. An implemented CI/CD solution for Nektar++ - addressed by Phase II
    - This forms a functionally complete replica of the previous system but providing additionally: fully reproducible Linux builds via Docker containers, configuration under an infrastructure-as-code approach, improved workload throughput and, improved GitLab integration.
    - The new system requires significantly less maintenance and supports trivial additional of new Linux distributions.
    - Documentation for the implemented solution has been written and incorporated into the main Nektar++ code base.

Project Timeline

Both phases were completed within the proposed budget without significant deviations in the planned work. Phase I was completed within the proposed timeframe. Phase II was extended to April 8th to incorporate a support period for use of the system in production and due to disruption caused by Covid-19.

- Phase I start – 12th August 2019
- Phase I finish – 30th September 2019
- Phase II start – 25th November 2019
- Phase II finish – 8th April 2020

Further Work

To further capitalise on the work up to this point there are several avenues that could be explored further.

- On-premise
    - Refinement of the provided system configuration could be made to improve the throughput of the system further. For instance, bottlenecks can be addressed by balancing the resources provided to different platforms.
    - Use of Kubernetes for executing Docker workloads. Deploying available execution hosts as a Kubernetes cluster may provide superior workload balancing and an integrated distributed caching mechanism. On-going work in ICT is exploring how to deploy a College Kubernetes service that could be used to replace the current execution infrastructure.
- Use of cloud services
    - It may be possible to replace the on-premise Windows and MacOS hosts with cloud hosted alternatives using the free tier of Azure Pipelines. Feasibility would depend on accessing Nektar++ dependencies on hosted runners and the quality of integration with GitLab that can be achieved.
    - Some work was carried out at the Research Software Reactor DevOps event to explore the possibility of using cloud resources to provide burst capacity. Whilst a system was successfully prototyped further work was required to make easy to deploy and configure. It should be possible to develop a simple system to launch and decommission cloud resources and provide cost estimates for use of such a system.

Project Outputs

Documents

- Original project proposal (link)
- Phase I implementation plan (link)
- End of Phase I report (link)

- Phase II implementation plan (link)

Code

- Merge requests against main Nektar repository
  - https://gitlab.nektar.info/nektar/nektar/-/merge_requests/1115 - fix for compiling on Windows 10
  - https://gitlab.nektar.info/nektar/nektar/-/merge_requests/1120 - CI configuration and Dockerfiles
  - https://gitlab.nektar.info/nektar/nektar/-/merge_requests/1125 - CI documentation
- Repositories
  - https://gitlab.nektar.info/ccaveayl/gitlab-server-services
  - https://gitlab.nektar.info/ccaveayl/project-settings-changer
- Prototypes
  - https://gitlab.nektar.info/ccaveayl/nektar/-/tree/devops-reactor - Configuration for running CI on Cloud Kubernetes instance.

Conference Talks

- Research Software London South East
- UKRI Cloud workshop

Other

- Informal feedback provided to STFC about the Anvil service
- Attendance at the Research Software Reactor DevOps event

Planned

- Blog post sharing insights from our comparison of different CI platforms
- Hackathon event leveraging expertise gained and aiming to provide a quick start guide for researchers to use CI