Towards reproductible science using Feel++

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Feel++ is a Finite Element method Embedded Language written in C++ [1] to solve partial differential equations using standard Galerkin methods. Feel++ provides a mathematical kernel that encompasses a broad range of numerical methods such as (i) arbitrary order continuous and discontinuous Galerkin methods in 1D, 2D, and 3D, (ii) domain decomposition methods, (iii) fictitious domain methods, (iv) level-set methods and (v) reduced-order methods.

In recent years, our group emphasis reproducibility as one of the main pillars of the Feel++ development strategy. Our goal is to be able to document, publish, version, compare simulation results alongside with our versioned programming and runtime environment evolving in time. In this talk, we would like to present our framework to facilitate reproducible science. We start with the container technologies, Docker and Singularity, that we use to provide Continuous Integration (CI), Continuous Delivery (CD) and Continuous Deployment (CD) for Feel++ and its associated projects. The Feel++ containers comprise a complete programming and runtime environment, from pre to post-processing, which usually is complicated to set up. We continue with a benchmark framework which allows creating versioned descriptions of test cases or benchmarks. These descriptions are stored in a database for easy post-processing (convergence analysis, scalability, runtime environment) by using queries for cloud and HPC resources for advanced and non-expert users from the scientific community. Then we describe how we publish the simulation results online in web pages displaying the simulation set-up, the model, inputs, outputs, performances as well as embedded 2D and 3D visualization. Finally, we demonstrate our reproducibility framework on the pilot applications, Eye2brain and Hifimagnet, of the EU H2020 E-INFRA MSO4SC project[2] as well as of the Feel++ toolboxes.

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References

[1] http://www.feelpp.org

[2] http://mso4sc.eu/