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Improving reproducibility of scientific software using Nix/NixOS: A case study on preCICE adapters and solvers

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Ensuring the reproducibility of scientific software is crucial for the advancement of research and the validation of scientific findings.

However, achieving reproducibility in software-intensive scientific projects is often challenging due to dependencies, system configurations and software environments.

In this paper, we present a possible solution for these challenges by utilizing Nix and NixOS.

Nix is a package manager and functional language that allows to mitigate these problems by guaranteeing that a package and all its dependencies can be built reproducibly as long as there is a build plan at the desired time.

NixOS is a purely functional Linux distribution, built on top of Nix that enables the build of reproducible systems including configuration files, packages and their dependencies.

We present a case study on improving the reproducibility of preCICE, an open-source coupling library, and some of its main adapters using Nix and NixOS.

Using this approach, we demonstrate how to create a reproducible and self-contained environment for preCICE and highlight the benefits of using Nix and NixOS for managing software and system configurations, resulting in improved reproducibility.

In addition, we compare the usability and reproducibility provided by Nix, in the context of preCICE, with two already established high-performance computing (HPC) solutions, Spack and EasyBuild.

This evaluation enables us to assess the advantages and disadvantages of employing Nix to improve reproducibility in scientific software development within an HPC context.

Slot length

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