Gesellschaft für wissenschaftliche Datenverarbeitung mbH Göttingen

AG-C

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HPC Usage Examples Repository

Complementing documentation for NHR, SCC et al.

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Overview

- freely accessible repository: hpc-usage-examples
- contains examples/know-how in regards to HPC usage, e.g.:
  - application specific know how, e.g. compilation etc.
  - example jobscripts for applications
  - scripts etc to compile/use GPU code on the clusters
  - domain specific examples in regards to run programs
  - . . .
- examples for all systems

Goals

- complement documentation
- cover all systems (SCC,EMMY,GRETE,KISSKI,. . .)
- working base for users and experts
- up-to-date with system changes
- create a common ground of understanding about systems/software usage (trust)

Motivation

Normal documentation rarely covers all aspects and is difficult to keep up-to-date:

- documentation is quite static
- huge effort to make good documentation
- gets outdated fast (compilation examples etc.)
- scope is limited in a dynamic system

Update easily

- repos are dynamic and easy to update
- experts are themselves using the repos
  - changes to the system affect experts, too
  - fixes have to applied anyway, updating the repo is then a no-brainer

Structure

- readme.md in the different sections
- system specific info are located in accordinlyg marked scripts and/or directories
- main structure (at the moment):
  - apps — different applications and benchmarks
  - dev — general development infos/examples for development, e.g. mpi
  - domains — science domain specific stuff
  - gpu — gpu related examples
  - performance-engineering — examples/info to improve software performance

Usage

- browse: https://gitlab-ce.gwdg.de/gwdg/hpc-usage-examples
- clone repo: git clone git@gitlab-ce.gwdg.de:gwdg/hpc-usage-examples.git

Regression testing

- ongoing effort to ensure system is working as expected
- context: systems unification
- goals:
  - identify issues as soon as possible
  - use automation to ensure tests are run
  - ensure consistent execution of tests
- approach/process:
  - run specific applications, e.g. gromacs, manually and/or regularily, to
    - test if specific software builds/runs after system updates
    - test if specific software builds/runs after config changes
- actual testbench will consist of multiple checks of different scale
- if a test breaks we know that there is an issue and can act

Relation to HPC-Usage-Examples

- the software/scripts for testing is taken from the *apps* folder
- the according scripts are executed unmodified under normal user rights
- if the software runs for the experts it should run for the users
- the user can trust standard software in the standard config works after updates

- Questions?