

```

username@login:/CRESTA_BENCH/applications/GROMACS> perl ../../bench/jube bench-Cray-XC30-ARCHER.xml
-----
Benchmark-Suite: starting at Wed Oct  8 15:09:52 2014
-----
jube version 1.1p18
-----
OPTIONS: start                = 1
-----
OPTIONS: verbose              = 0
OPTIONS: Benchmark XML-file   = bench-Cray-XC30-ARCHER.xml
OPTIONS: Compile XML-file     = $PWD/compile.xml
OPTIONS: benchlogfile         = $PWD/benchlog/benchlog_1.log
OPTIONS: configdir            = $PWD
OPTIONS: platformdir          = /CRESTA_BENCH/bench/./platform
-----
--> processing benchmark-Cray-XC30-ARCHER.xml ...
--> processing $PWD/compile.xml
--> processing $PWD/prep.xml
--> processing $PWD/execute.xml
--> processing /CRESTA_BENCH/bench/./platform/platform.xml ...
scanning benchmarks for GROMACS on Cray-XC30-ARCHER:
  methanol
  -> generating run step $platform
      1: 128 nodes 24 tasks 1 threads
      1: [timesteps->100][account->xyz][time_limit->00:05:00]
          -> compile step $platform (Cray-XC30-ARCHER)
          -> prepare step methanol (Cray-XC30-ARCHER)
          -> execute step $platform (Cray-XC30-ARCHER)
          -> submit job command: qsub cray_qsub.job
      2: 256 nodes 24 tasks 1 threads
      1: [timesteps->100][account->xyz][time_limit->00:05:00]
          -> compile step $platform (Cray-XC30-ARCHER)
          -> prepare step methanol (Cray-XC30-ARCHER)
          -> execute step $platform (Cray-XC30-ARCHER)
          -> submit job command: qsub cray_qsub.job
-----
JUBE: used id:                1
-----
Benchmark-Suite: ending at Wed Oct  8 15:16:00 2014
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BENCHMARK SUITE

The principle of co-design lies at the very heart of all work undertaken in the CRESTA project. Our co-design vehicles are a set of scientific applications, which drive the research. These applications have now been collected in a Benchmark Suite, which is available for public use.

The benchmarking framework

The Benchmark Suite collates the co-design vehicles in a unified framework that is designed to automate compilation, execution, results gathering and verification for supported platforms in a user-friendly manner. The execution step allows the user to select from a specified range of test cases for each application, exposing different performance and scalability behaviours. Results are gathered in comprehensive logs and their correctness is automatically verified.

Customising the CRESTA Benchmark Suite

The Benchmark Suite is deliberately designed to be customisable and expandable. Both the platforms that are supported and the test cases that can be run can easily be adapted to suit the user's specific needs. The release of the Benchmark Suite contains documentation that explains the steps necessary for customisation.

Aim of the CRESTA Benchmark Suite

The co-design vehicles drive CRESTA's Exascale research. The target test cases provided with the Suite are representative of the type of scientific problems that will require Exascale resources in the future and have motivated the research agenda from the start of the project. The aim of the Benchmark Suite is to make the co-design vehicles available to a wider community in order to support, and potentially inspire, the on-going Exascale research effort.

The availability to the HPC community, together with the user-friendly design, promotes the Suite's continued development and growth long beyond the lifetime of the CRESTA project.

The principle of co-design lies at the very heart of all work undertaken in the CRESTA project.





EPCC
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Edinburgh, Scotland
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About EPCC
The University of Edinburgh is one of the world's leading research universities. Through its supercomputer centre, EPCC, it is the project coordinator of the CRESTA project. EPCC manages a collection of HPC systems including ARCHER, the UK's national high-end computing system. EPCC coordinated the development of the benchmark suite, together with the application partners: The European Centre for Medium-Range Weather Forecasts (ECMWF); Kungliga Tekniska Högskolan (KTH); Åbo Akademi University (ABO) and University College London (UCL).



Collaborative Research into Exascale Systemware, Tools & Applications
cresta-project.eu

About CRESTA
CRESTA (Collaborative Research into Exascale Systemware, Tools & Applications) is a collaborative research effort funded by the European Union exploring how to meet the exaflop challenge. The project has two integrated strands: one focused on enabling a key set of co-design applications for exascale, the other focused on building and exploring systemware for exascale platforms.

Contents of the Benchmark Suite

The Benchmark Suite consists of five key co-design applications from a broad range of scientific areas and addressing current societal challenges.

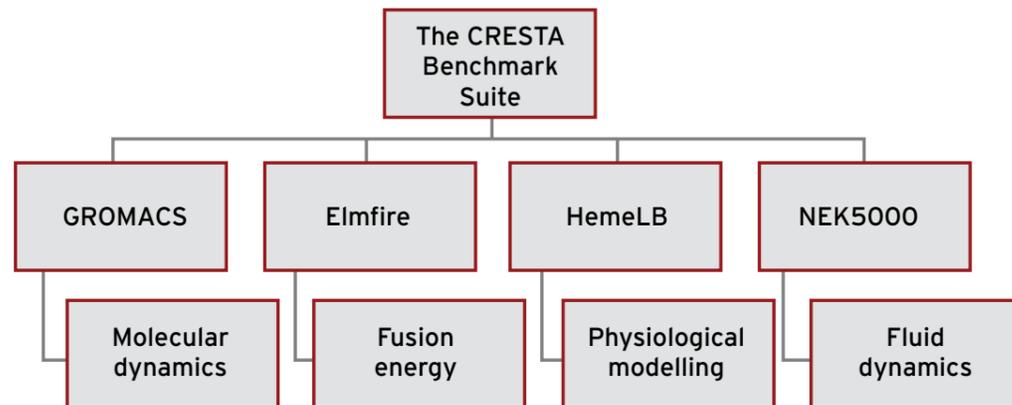


Figure 1 shows a graphical representation of the contents of the benchmark suite. The benchmark suite consists of 4 co-design applications.

Obtaining the CRESTA Benchmark Suite

The CRESTA Benchmark Suite can be downloaded from the CRESTA project website as a single archive:

<http://www.cresta-project.eu/cresta-co-design/software>

We are keen to receive community feedback on the Benchmark Suite; new test cases for the applications and platform support contributions will be considered as well. Please email info@cresta-project.eu with any questions or comments.



HemeLB Test Cases

The CRESTA Benchmark Suite contains three test cases for HemeLB, a code designed as a specialised predictive tool for fluid flows in complex geometries. Its main focus is on simulating blood flow in parts of the cerebral arterial network.

The three test cases are 'bifurcation 50um', 'bifurcation 40um' and 'cowTestVel_Large'. The two bifurcation test cases are based on a 3D rotational angiography scan of an anonymous patient with a cerebral aneurysm being treated at the National Hospital for Neurology and Neurosurgery. The simulations are of the region around the bifurcation of the internal carotid artery's bifurcation into the anterior cerebral artery and the middle cerebral artery. The third test case is a simulation of all the major arteries of the brain, particularly focusing on the circle of Willis.

