Containers for portable, productive and performant scientific computing

Jack S. Hale* Lizao Li[†] Chris N. Richardson[‡] Garth N. Wells[§]

Abstract

Containers are an emerging technology that hold promise for improving productivity and code portability in scientific computing. We examine Linux container technology for the distribution of a non-trivial scientific computing software stack and its execution on a spectrum of platforms from laptop computers through to high performance computing (HPC) systems. We show on a workstation and a leadership-class HPC system that when deployed appropriately there are no performance penalties running scientific programs inside containers. For Python code run on large parallel computers, the run time is reduced inside a container due to faster library imports. The software distribution approach and data that we present will help developers and users decide on whether container technology is appropriate for them. We also provide guidance for the vendors of HPC systems that rely on proprietary libraries for performance on what they can do to make containers work seamlessly and without performance penalty.

1 Introduction

Traditionally, scientific and engineering software libraries had few dependencies and were developed by small groups in a stable and well-established language, such as Fortran 77 or C. In contrast, many modern scientific libraries have numerous dependencies and are developed by multiple groups and developers in various (and increasingly often multiple) languages, e.g. C++, C, Fortran, Python, R. In modern scientific software libraries, key tasks are commonly delegated to specialised, high-performance libraries, and these form the dependencies of higher-level libraries. These lower-level libraries will in turn themselves typically have dependencies. The introduction of dependencies, which usually differ in their level of maintenance, standards compliance and build system quality, brings significant challenges for users installing scientific libraries, and for portability of scientific libraries to different platforms.

Introducing high-quality, specialised software dependencies into a library can allow small research teams to produce novel, sophisticated and high performance programs

*Research Unit in Engineering Science, Faculty of Science, Technology and Communication, University of Luxembourg, 6 rue Richard Codenhove-Kalergi, L-1359, Luxembourg (`jack.hale@uni.lu`, `http://orcid.org/0000-0001-7216-861X`)

[†]School of Mathematics, University of Minnesota, Minneapolis, Minnesota, 55455, United States. (`lzlarryli@gmail.com`, `http://orcid.org/0000-0001-7056-3368`)

[‡]BP Institute, University of Cambridge, Madingley Road, Cambridge CB3 0EZ, United Kingdom (`cnr12@cam.ac.uk`, `http://orcid.org/0000-0003-3137-1392`)

[§]Department of Engineering, University of Cambridge, Trumpington Street, Cambridge CB2 1PZ, United Kingdom (`gnw20@cam.ac.uk`, `http://orcid.org/0000-0001-5291-7951`)

with fewer errors and reduced development time, and without being expert in the implementation of all underlying operations. However, effective distribution of complex software packages and their dependencies, both within a research group and to the wider community, is challenging and time consuming. It is difficult to justify the researcher time required to support the deployment of software on esoteric, wide-ranging and sometimes poorly maintained platforms, from laptops to high performance computing facilities, through to cloud computing infrastructures. Moreover, the necessary expertise and range of test systems is not generally available in research teams for actively supporting a wide range of platforms.

Motivated by the difficulties in distributing modern high performance software to a wide range of users and developers, we address the use of Linux containers as an approach to portable deployment of scientific software libraries, from laptop computer to supercomputer, with no noticeable performance penalty. We describe a container-based approach that we have developed for both users and developers of a collection of widely used scientific libraries from the FEniCS Project (`https://fenicsproject.org`), an open-source finite element method (FEM) toolkit for solving partial differential equations. We use a common image for the FEniCS libraries in tutorials for new users (running on their own computers) through to high performance, parallel simulations. The focus of this work is the ease and simplicity with which containers can be used to dependably share and deploy scientific software stacks, without performance penalty, across a range of platforms. We want to share our experiences to aid the developers of other scientific libraries in deciding whether to adopt containers to support the distribution of their software.

To demonstrate the performance characteristics of container-based approaches for scientific applications, we present a range of performance data on different systems comparing native and containerised performance. In particular, we address running on HPC systems that require system-specific vendor libraries for performance. We also touch upon what steps vendors of HPC systems, which often depend on proprietary libraries for performance (most notably Message Passing Interface (MPI) libraries), can take to support the deployment of container technologies on HPC systems.

Containers have already received some attention in the academic literature. Boettiger [9] focused on scientific reproducibility by using containers as a stable framework to propagate software stacks between generations and teams of researchers. Apaolaza et al. [7] used Docker [2] to package and execute a complex video processing workflow, with an accompanying blog post by Haines and Jay [14] containing specifics on using Zenodo (`https://zenodo.org`) to archive software with a permanent Digital Object Identifier (DOI). Di Tommaso et al. [10] and Gerlach et al. [13] examined the use of containers to ease the portability challenge of complex data analysis workflows, where multiple containers (each containing its own complex software environment) are chained together. Di Tommaso et al. [10] also compared the performance of some commonly used genetics analysis software running natively and inside a container. Seo et al. [24] compared the performance of containers and virtual machines for non-scientific software stacks deployed in the cloud. Macdonnell and Lu [19] benchmarked the performance of the VMWare virtualisation platform for a variety of common scientific computing tasks. The overhead for compute-intensive tasks was around 6% and for IO tasks around 9%. Felter et al. [12] also looked at the performance differential of non-scientific software within virtualised and containerised environments. The performance studies published in the literature [10, 12, 24] found negligible differences between container and native performance, as long as the container is setup and used appropriately, e.g. using data mounts for I/O intensive tasks [12] and not setting up many containers for individual tasks with run times on the order of container setup time (typically fractions of a second) [10].

The focus of this paper differs from previous studies in two ways. Firstly, instead of concentrating on how containers aid scientific reproducibility [7, 9, 14], we consider how containers can be used to ease the difficulty of sharing and distributing scientific code to developers and end-users on a wide range of computing platforms. Secondly, unlike previous studies [10, 12, 24] that showed performance parity between containerised and native *shared* memory parallel software, we consider performance of software using *distributed* memory parallel programming models (e.g. MPI). MPI forms the backbone of modern HPC systems and modern scientific computing codes in the physical sciences, so for containers to be accepted by the community the performance characteristics on distributed memory machines must be demonstrated.

2 Background: Linux containers

We give a brief overview of containers by comparison with traditional virtual-machine based virtualisation, a technology which many researchers in the scientific computing community are already familiar with, an we provide a simple example of configuring a container. Our objective is not to provide an in-depth review of the technology behind Linux containers; we refer the reader to the white-paper [11] for a detailed discussion of a container runtime and security model.

2.1 Technology

Containers are, on the surface at least, similar to traditional virtualisation technologies, e.g. VMWare, QEMU, Hyper-V, Xen, in that they allow multiple isolated applications to run on a single host computer. Traditional virtualisation involves running an entire guest operating system (OS) within an isolated environment, with the kernel of the guest OS communicating with the host via a complete set of virtualised devices (CPU, disk, memory, etc.). In contrast, Linux containers share the underlying kernel of the host and isolate the processes running within it from all other processes running on the underlying host operating system. Instead of virtualising the hardware, containers virtualise the operating system itself [20].

While the end effect of both traditional virtualisation and containers are similar, namely, an isolated, distinct and portable computing environment, the means by which they achieve this results in a very different experience for the end-user. Traditional virtual machines load an entire guest operating system into memory. Each guest OS might take up gigabytes of storage space on the host, and require a significant fraction of system resources just to run, even before doing any work. Furthermore, starting up each guest OS usually takes on the order of minutes. Because containers share the existing host kernel, they can utilise most of the dependencies and features of the host. If a container does not execute anything, it uses little to no system resources. Running thousands of containers on one host is possible. To start a new container, the host just has to start new processes that are suitably isolated from its own. This means that startup times are similar to that of a native application.

We wish to note the distinction between an image and a container. An image is an immutable file that contains a description of a complete computing environment (libraries, executables, default networking configuration, default initialisation, and more) that can be used by a runtime (e.g., Docker) to create a container. A container is a runtime instantiation of a particular image. It is possible to have many containers based on the same image. Each new container can re-use the data stored in an image without duplication, just storing the differences in a layered file system. We want to emphasise that the image format and container runtime are mutually exclusive entities. Currently, by far the most popular container runtime is Docker [2]. However, we show performance results in this paper using the Docker, rkt [4] and Shifter [5] runtimes, each of which uses a different approach to instantiate containers from the same image. The recently formed Open Container Initiative [3] seeks to standardise image formats and container runtimes across vendors so that images and containers are portable between the different runtime platforms.

In summary, containers can initially be viewed as a lightweight counterpart to traditional virtualisation technology. Traditional virtualisation still has some advantages over containers, such as a time-proven security model. Containers, by virtue of sharing the host OS kernel directly, cannot run images designed for another OS. So if a user wishes to run Linux images in a container on macOS, then they must still use a virtual machine to host an OS with a Linux kernel.

2.2 Elementary demonstration

To provide an simple exposition of the use of images and containers with the Docker runtime, we show how to write a `Dockerfile`, build an image from it, and finally how to launch a container from the created image.

Simply put, a `Dockerfile` file is a sequence of some Docker-specific directives and shell script commands that prescribe the entire build process and runtime configuration of a software environment. An attractive feature of `Dockerfile` files is that they unambiguously describe the configuration and build process behind an image.

An example of a simple `Dockerfile` that builds an Ubuntu 16.04-based image with with SciPy installed from the system package manager might be:

```
FROM ubuntu:16.04
USER root
RUN apt-get -y update && \
    apt-get -y upgrade && \
    apt-get -y install python-scipy && \
    rm -rf /var/lib/apt/lists/* /tmp/* /var/tmp/*
```

Running `docker build .` in the same directory as the `Dockerfile` will build and package the result into an image with a unique mathematical hash, e.g. `d366b85a7fdb`. The image can be given an easy to remember name using `docker tag d366b85a7fdb scipy-image`. Using

```
docker run -ti scipy-image python
```

an interactive Python terminal session will appear and the SciPy module will be available. The above methodology can be extended to package and distribute complex scientific software stacks with the benefit of working with a well-defined environment. We have only shown three `Dockerfile` directives (`FROM`, `USER` and `RUN`) in the above example, many more are discussed in the Docker documentation at `https://docker.com`.

A strength of both the Open Container Initiative and Docker image formats is the layered file system. Taking the above `Dockerfile` as an example, the directive `FROM ubuntu:16.04` instructs the build to start with the official Ubuntu Docker image as the first layer. This first layer is often called a base image. Many other base images are available in registries, for example at Dockerhub (`https://hub.docker.com`) and Quay (`https://quay.io`). Every subsequent directive (here, `USER` and `RUN`) creates a new layer that only stores the difference between itself and the previous layer. Each layer is associated with a unique mathematical hash. This simple but elegant construct has multiple beneficial effects. First, if we build stages of a software pipeline in separate images with each `FROM` the same base image (e.g. `ubuntu:16.04`), the end-user only needs to download the base image once and storage of the complete pipeline can be very compact. Secondly, on calling `docker run` to run the image in a new container, a new empty filesystem layer is created to store runtime changes made by the user. This operation is very lightweight, taking up only a few kilobytes of disk space in addition to the storage space required by the modification, and typically takes fractions of a second to run.

3 Distributing, sharing and reproducibility with scientific software

We now discuss some issues that open-source scientific software projects face when distributing code and supporting user installation, and how container runtimes and standardised image formats can help address these issues. Much of what we present is influenced by our first-hand experiences as developers of the open-source FEniCS Project ([18], `http://fenicsproject.org`).

3.1 Installation and complex software dependency trees

Users of scientific software run on a broad range of platforms, including Windows, macOS and a variety of Linux distributions, with their installations maintained to varying degrees. Moreover, users have different needs; from beginners wishing to run their first analysis, to advanced users wanting a specific version of a library or wanting to run on high-performance computing clusters, through to developers adding new features. The complex chain of dependencies that characterises many modern, user-level scientific libraries compounds the difficulties in supporting robust and appropriately configured installations. Supporting installation on all user platforms and meeting the needs of all users is beyond the resources of the vast majority of open-source scientific software projects.

Up until early 2015 the FEniCS Project supported an automated installation system called 'Dorsal'. Now deprecated, Dorsal was a somewhat successful attempt to build an entire FEniCS environment automatically on a variety of Unix-like operating systems. Notably absent was Windows support. As much as possible, Dorsal used binary software dependencies from distributions (packages), and then compiled (and where necessary patched) various other dependencies and FEniCS itself from source on the end-user's machine. In practice, this approach has a number of issues. There are a wide variety of Linux distributions and each is subtly different, which in practice means supporting even a small number of distributions reliably is a significant task requiring time and a range of test systems. Furthermore, even small customisations by a user to their underlying environment, like having a different version of a library or application in their `PATH`, could lead to a failure of the build.

Container runtimes, such as Docker, rkt and Shifter, largely abstract away the differences between the many operating systems that users run. The same image runs identically inside a container on almost any platform. Using container images, we now distribute an entire FEniCS environment that has proven to be reliable, and is simple and quick to run on wide variety of systems. The environment is reproducible, in that every image is associated with a mathematical hash that is unique to every specific realisation of a build. This has greatly simplified development and testing processes, and improved user experience. FEniCS users of the images have required very little support, and when support has been required is has become easier to provide as the environment in which a user is working is well-defined.

Containers complement, rather than replace, packaging and build systems such as apt, pip and EasyBuild. We make heavy use of both apt and pip when building the FEniCS images, with only judicious use of builds directly from source. The advantage of using these existing systems within a container environment is that the build system is completely isolated from the user's underlying system. In our experience, this leads to significantly fewer build failures. In addition, developers can choose the best build systems for the job at hand, rather than being limited by what system administrators have installed or what end-users are comfortable with.

3.2 Ease of launching a runtime environment

We want every new user of FEniCS to be able to reliably run it on almost any platform with a minimal number of commands. Once users have installed Docker on their platforms, they can start using FEniCS with the command:

```
docker run -ti quay.io/fenicsproject/stable
```

To share files from the host into the container environment the user can add the `-v` flag:

```
docker run -ti -v $(pwd):/home/fenics/shared quay.io/fenicsproject/stable
```

While the above commands are straightforward, many users and developers will want more control over the environment, e.g. persistent state and the ability to re-launch a container. However, the command line interface (CLI) to the Docker runtime has been designed with technical users in mind. Moving beyond the simplest interactions, the CLI is too low-level for typical scientific software users and developers, and especially for beginners. For example, launching an interactive Jupyter notebook [21] session requires knowledge of the `docker` command's networking features:

```
docker run -w /home/fenics/shared -v $(pwd):/home/fenics/shared -d \
  -p 127.0.0.1:8888:8888 quay.io/fenicsproject/stable \
  'jupyter-notebook --ip=0.0.0.0'
```

To make the use of the containers as easy as possible for users following typical workflows we have developed a lightweight wrapper script `fenicsproject` that sets up some common workflows, such as starting a Jupyter notebook session as described above:

```
fenicsproject notebook my-project
fenicsproject start my-project
```

This script has been used successfully for a number of FEniCS tutorials, with participants using the FEniCS Python interface via Jupyter notebooks on their own laptop computers. FEniCS developers are also using this script to quickly setup and build development branches of FEniCS in lightweight isolated environments.

For users who want to develop their own FEniCS container workflows using the `docker` command we provide extensive documentation [1] that targets common scientific computing use cases.

3.3 Deployment on high performance computing systems

One of the most appealing features of containers is the possibility of running the same image on a wide range of computing platforms, including HPC systems. However, a recurring challenge when moving to a new HPC machine is configuring and compiling a library with all its dependencies. A characteristic of HPC systems is that each is unique and the software environment changes over time as compilers and libraries are updated. Moreover, users and developers will typically work infrequently on HPC systems, with development and testing typically taking place on user machines before occasional execution of large-scale simulations on HPC systems. It is our experience that there are serious productivity barriers when moving from local development machines to HPC systems. We find that, particularly with infrequent HPC use, there is a high time cost in updating and rebuilding libraries, even for experienced developers. Due to the differences between HPC systems, there is also a significant time cost associated with moving from one HPC system to another. For experienced users, these issues lower productivity; the time to update a software stack on a HPC system can dwarf the wall clock run time. For less experienced users, these issues can seriously hamper accessibility. The appeal of containers is that a user's familiar local development environment can be reproduced with minimal effort and time on a HPC system.

Shifter [16] is a new open-source project at the National Energy Research Scientific Computing Centre (NERSC) that provides a runtime for container images, and is specifically suited to the security and performance challenges of HPC workflows. The Docker image format is one of a number of image formats supported by Shifter. Images are pulled ahead of running a job, by issuing the `shifterimg pull` command, which pulls an image from an image registry. The practical task of running a container using Shifter is then straightforward. For example:

```
shifter --image=docker:quay.io/fenicsproject/stable:2016.1.0r1 \
./demo_poisson
```

will run the command `./demo_poisson` inside a FEniCS container. In contrast to the Docker runtime, the Shifter images are run in read-only mode and the user's environment and home directory are automatically passed through to the container. When using the Docker runtime, users can store data inside a container using the layered file system, whereas with Shifter any user generated objects, e.g. executable files, must be stored outside of the container on the host system. We refer to Jacobsen and Canon [16] for further details.

When executing a program in parallel, MPI is typically used to communicate (pass messages) between processes. The MPI libraries included in the FEniCS image work adequately if a parallel job is run on a single compute node because modern MPI libraries do not use the network to pass messages when memory is shared. However, when a job is distributed across more than one compute node, communication takes place across a network and the standard MPI libraries in the container will not take advantage of the specialised high-performance networking hardware that characterises modern HPC systems. Thanks to the MPICH application binary interface (ABI) initiative [22], we can distribute an image linked against the Ubuntu MPICH library package, and change the linking of the libraries to the host ABI-compatible MPI implementation at runtime. We discuss this in more detail in the run time performance section.

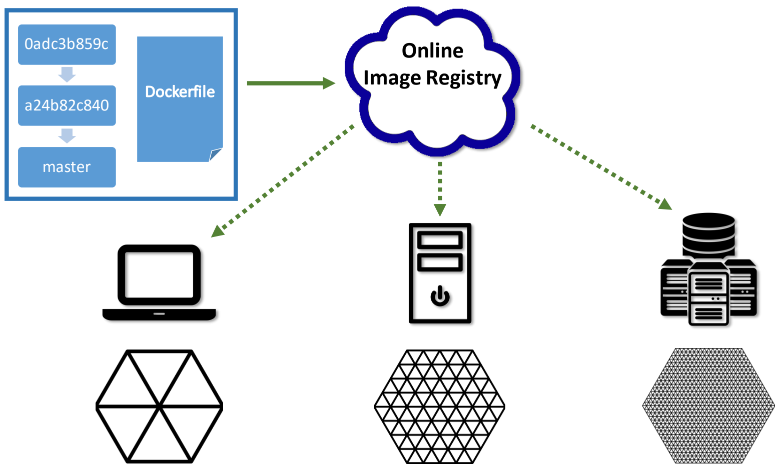


Figure 1: An image is defined by a Dockerfile, and is built locally or by a cloud-based service such as `https://quay.io`. The latter can also also act as a registry. An image is pulled from the registry and run on different platforms, for example solving smaller problems on a laptop, to large-scale problems on an HPC machine.

3.4 Provisioning and maintenance of images

To build the entire FEniCS software stack we maintain a collection of `Dockerfile` files under version control at `https://bitbucket.org/fenics-project/docker`. If a user wants to install their own pieces of software alongside FEniCS, they can create their own simple `Dockerfile` that begins with `FROM quay.io/fenicsproject/stable`. We also provision the images with scripts for users to update and build specific libraries within a container.

We use a cloud-based service (`https://quay.io`) to build and distribute FEniCS images. We have developed a hierarchy of images that allow re-use between various end-user containers, e.g. stable user, debug and developer images. On a commit to the repository where we store the `Dockerfile` files, a build command is executed automatically. When the build is finished, the images, in both Docker and Open Container Initiative-compatible formats, are ready and available publicly. We have found this workflow very reliable and requiring very little developer intervention. Making small configuration changes requires changing just one file and the steps used to build the container are automatic and transparent. The process from Dockerfile to deployment of an image on different systems is illustrated in Fig. 1.

4 Runtime performance studies

Performance is a critical factor in deciding whether or not containers are viable for scientific software. We address this point by presenting performance data for a range of representative simulations on a typical workstation, and tests and benchmarks on a leadership class HPC system. We pay special attention to use of system MPI libraries on the HPC system.

All necessary instructions, scripts and images, along with the raw data and plotting scripts from our own tests, are available in the supporting material [15].

4.1 FEniCS workstation performance

We compare the performance of a selection of tests running inside the FEniCS Project stable image, hosted at `quay.io/fenicsproject/stable:2016.1.0r1`, running within the Docker [2] and rkt [4] runtimes to a nearly identical version of FEniCS running on the same machine natively. In addition, we also run the same image with the Docker runtime inside a virtual machine (VM), which reflects the experience of macOS and Windows users where a lightweight Linux distribution must be virtualised to host Docker. The Docker virtual machine setup on macOS and Windows is transparent to the user and their experience is nearly identical to that of Docker users on Linux.

As far as possible, we create identical software stacks within the image and natively on the host. We use the Ubuntu 16.04 LTS Linux distribution as the base in both cases, and use as many core libraries from the distribution packages (e.g., MPICH, OpenBLAS, LAPACK) as possible. The test system is a 16-core Intel Xeon-based workstation ($2 \times$ E5-2670 (Sandy Bridge)) with 128GB of RAM. The relative differences in performance between each of the environments are of interest.

Within each environment we run a selection of single-process finite element method performance tests, that is, *without* using MPI. We briefly summarise these tests here: 'Poisson LU' solves a two-dimensional Poisson equation using LU decomposition, 'Poisson AMG' solves a three-dimensional Poisson equation using the conjugate gradient method preconditioned by algebraic multigrid, 'IO' reads in a large mesh file from the host and writes a solution back to a file on the host, and finally 'elasticity' solves a three-dimensional elasticity problem using the conjugate gradient method with an algebraic multigrid preconditioner. These tests are slightly modified versions of demos distributed with the FEniCS Project and are representative of the types of simulations that users might run. The test programs are implemented using the Python interface of FEniCS. FEniCS uses just-in-time (JIT) compilation from Python to generate loadable shared objects at runtime for operations that are model-specific, and these shared object libraries are cached as files. The run times reported below do not include the JIT compilation time, which is only incurred on the first run.

Figure 2 shows the run times for the four tests in the four environments. The *Docker*, *rkt* and *native* platforms provide nearly identical performance. This is no surprise given that the container runtimes leverage the same Linux kernel functionality. However, it does highlight that there are a variety of runtime systems to choose from, and choices can be made to suit particular system policies. The *VM* platform has up to a 15% performance penalty, slightly worse that the results of Macdonnell and Lu [19]. Other virtualisation environments may provide better results than the VirtualBox software we used in this work. We conclude that for these tests that there is no performance penalty when running inside a container.

4.2 FEniCS HPC performance tests using the Shifter runtime

FEniCS supports distributed memory parallelism (using MPI), and has been shown to scale to over 20,000 processes on HPC machines [23]. We have prepared a simple FEniCS test program which solves the Poisson equation using the conjugate gradient method with an algebraic multigrid preconditioner, and which also involves distributed mesh refinement and I/O. We use this to compare native and containerised performance. The test program is fairly representative of a typical user program. This test program is implemented in both the C++ and Python interfaces of FEniCS.

The tests in this section have been performed on *Edison*, a Cray XC30 system at

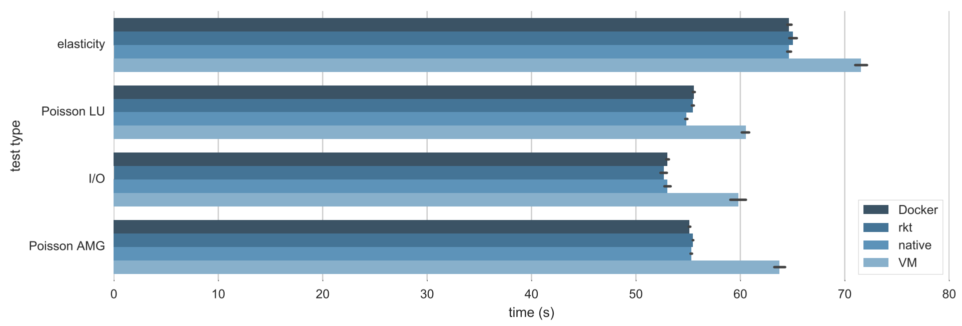


Figure 2: Performance of *Docker*, *rkt*, *native* and *VM* platforms running four different benchmark problems on a workstation. Shorter bars are better. *Docker*, *rkt* and *native* are very close, with performance differentials less than 1%. The extra overhead introduced by the *VM* virtualisation leads to a performance drop of around 15%. The error bars for five runs are shown in black.

NERSC. Edison has 24 cores per compute node (2 × E5-2695v2 (Ivy Bridge)). To use the system MPI libraries, we need the containerised application to load the Cray MPI libraries. We do this, as shown by Bahls [8], by adjusting the `LD_LIBRARY_PATH` environment variable on job submission and copying the required system libraries to a path that is accessible from within the container. This hinges on ABI compatibility of the container and system MPI libraries. The command

```
srun -n 192 shifter env LD_LIBRARY_PATH=$SCRATCH/hpc-mpich/lib \
  --image=docker:quay.io/fenicsproject/stable:2016.1.0r1 ./demo_poisson
```

uses the SLURM submission system MPI launcher to launch Shifter on 192 cores and adds the appropriate library path to the environment. The required libraries for using the system MPI are copied into `$SCRATCH/hpc-mpich/lib`, a location that is visible from within a running container. All other libraries are provided by the container, and are identical to those that we distribute to end-users for running on laptops and workstations. Note that with Shifter we execute the MPI `srun` command on the host and each process is a container.

To test performance we compare a native build of the FEniCS library and test application to a container build. The native build uses the Cray system modules as much as possible (gcc/4.9.3, cray-mpich/7.2.5, libsci/16.07.1, cray-tpsl/16.03.1, cray-petsc/3.6.1.0). The only FEniCS dependency compiled from source was SWIG, which is required when using the Python interface. For the C++ version of the container test, the test code was compiled inside the container on Edison by invoking an interactive Shifter session. For the Python version of the test, the JIT cache of shared objects was pre-generated and the reported run times do not include the JIT compilation time.

Wall clock run times for the C++ version of the test program on Edison are shown in Fig. 3 for between 24 and 192 processes. Performance inside the container when using the system MPI library (case (b) in Fig. 3) is comparable to or better than the native performance (case (a) in Fig. 3). When using the container MPICH library (case (c) in Fig. 3), the solver time increases dramatically for higher MPI process counts, highlighting the importance of loading the system MPI library for container programs.

Python has become increasingly popular in HPC, in particular as a 'driver' for programs written in compiled languages. There is however a serious performance problem

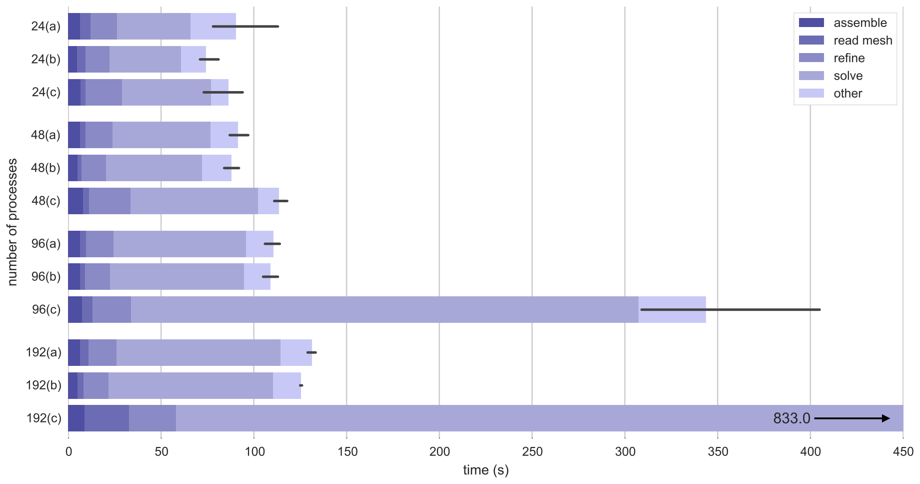


Figure 3: C++ FEniCS benchmark run times on *Edison* when: (a) run natively without containers; (b) run in Shifter with Cray MPI libraries; and (c) run in Shifter with the container MPI libraries. Tests were performed with with 24, 48, 96 and 192 MPI processes, with one MPI process per CPU core. Shorter bars are better. The x-axis is truncated for the 192(c) result. In each case, the time is shown for various compute operations. There is little difference between the run times for cases (a) and (b), which both use the system MPI library. Performance for (c) deteriorates rapidly when computing across compute nodes (Edison has 24 cores per compute node). Error bars for three runs are shown in black.

on HPC systems, which is often referred to as the 'Python import problem', see [17]. The Python `import` statement appears early in a Python program, and each process imports (loads) Python modules/code from disk into memory. Each imported module will itself typically import/load modules from disk. HPC filesystems are optimised for access to a few large files by many processes, but can be extremely slow when many processes access many small files, as happens when Python imports modules on each process. When running with 1000 processes we have observed on some systems that it can take over 30 minutes to import the Python modules required by the Python interface of FEniCS. Containers bypass this problem as the Python modules are included in the filesystem of the container image, which is mounted on each node as a single large file [16]. A small price is paid in memory usage per node.

To examine the improvement in Python import performance, Fig. 4 shows the run times for native and containerised (using the system MPI library) executions of the Python version of the test program. The key observation here is the large difference in total run time between the native (case (a)) and container (case (b)) executions of the program, with run time for the native case being significantly greater than the container case. This is due to the Python import time. Additionally, the native run time shows more variation, which is probably due to unpredictable contention on the file system. We also note that containers have an advantage for Python programs that employ just-in-time compilation since we can be sure that the necessary compilers and libraries are available on the compute nodes.

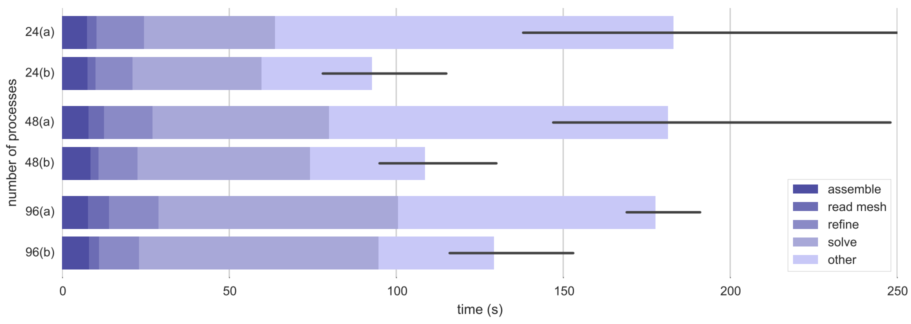


Figure 4: Python benchmark run times on *Edison* when: (a) run natively without containers; and (b) run inside Shifter with the system MPI library. Tests were performed with with 24, 48 and 96 MPI processes, with one MPI process per CPU core. Shorter bars are better. Each compute operation takes comparable time in each case, but the total run time is significantly greater and more variable when running natively because of the Python module import time. Error bars for three runs shown in black.

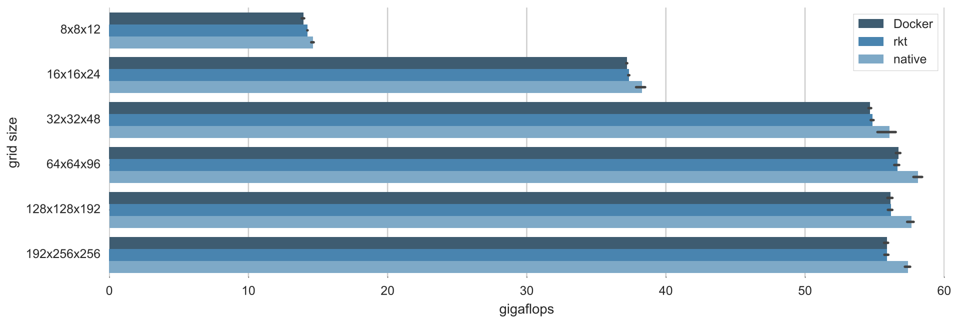
4.3 High-Performance Geometric Multigrid (HPGMG-FE) benchmark

HPGMG-FE is a new benchmark for ranking supercomputers [6]. It aims to provide a balanced measure of system performance characteristics that are important for modern scientific software on HPC systems. It is a useful test for container performance due its highly tuned implementation; any weakness in configuration or container performance issues become acute and immediately obvious. For optimal performance, the benchmark requires exploitation of a CPU-specific instruction set, namely the Advanced Vector Extensions (AVX).

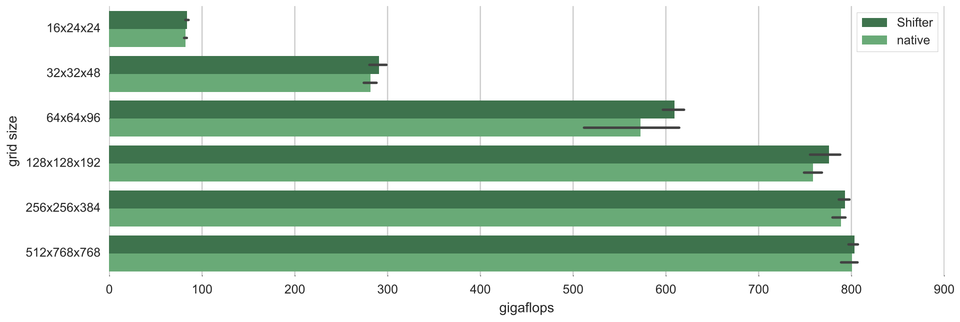
In the same way as our C++ benchmarks above, we have compiled HPGMG-FE both natively and in a container. In both cases, it is important to compile for the host architecture and to use the best optimisation flags available for the C compiler. Thus we ensure that features of the host CPU, such as the AVX instruction set, are activated. We make use of OpenBLAS, which dynamically selects at runtime the implementation that is appropriate for the CPU type. For workstation tests we execute the MPI `mpirun` command inside a container, whereas on Edison the MPI `srun` command is executed from outside the containers.

The performance results for the HPGMG-FE benchmark are shown in Fig. 5 using 16 cores on the Xeon workstation (Fig. 5a) and using 192 cores on Edison (Fig. 5b). On the workstation, the native compile outperforms the Docker and rkt containers by around 3%, while on Edison the Shifter container essentially matches the native performance at larger problem sizes. Both performance margins are in our view small enough to claim that the containers match the native performance of both systems.

This benchmark is an example of where a precompiled program or library inside a container might not be able to exploit hardware instructions that are specific to the host architecture and which may be critical for performance (vectorisation in this case). In such cases a container can be provisioned with the necessary scripts to build performance critical binaries on the host system. Such scripts are straightforward to develop and support as they are run inside the well-defined and controlled environment of the container.



(a) A 16-core Xeon workstation with the *Docker*, *rkt* and *native* platforms.



(b) Edison Cray-XC30 using 192 cores with the *native* and *Shifter* platforms.

Figure 5: HPGMG-FE performance on (a) Intel Xeon and (b) Cray XC30. Longer bars are better. This difference between the native and containerised performance is small. Error bars for five runs.

5 Conclusions

We have discussed some of the challenges in distributing scientific software and the role that containers can fulfil in addressing this issue. Images can provide a complete, stable, and consistent environment that can be easily distributed to end users, thereby avoiding the difficulties that end-users commonly face with deep dependency trees. Containers have the further advantage of largely abstracting away the host system, making it possible to deliver a common and consistent environment on many different platforms, be it laptop, workstation, cloud instance or supercomputer. We have shown through a selection of test problems (both representative and benchmark) using a common image that containers introduce no performance penalty; on the contrary it is our anecdotal experience that optimised images generally outperform native user installations as the container environment can be suitably optimised by the developers of a library. A production or development environment can be moved with ease and efficiency between platforms. This will improve productivity in the use of different systems for scientific computing.

We have shown performance data including tests on a Cray XC30 HPC system. The test data underlines the importance of using the native MPI library on HPC platforms to fully exploit the specialised interconnect. Loading the Cray MPI library from a container was made straightforward by the ABI compatibility between the Cray MPI library and the open-source MPICH library. We hope that our results will strengthen arguments for vendors to make their proprietary and specialised system libraries ABI compatible with open-source libraries, and to devise simple approaches to switching dynamically linked libraries. This will enhance the usability of HPC systems via containers without compromising performance. We also showed that containers provide a portable solution on HPC systems to the problem with languages that load a large number of small files on each process (the 'Python import problem'). Images also provide a robust solution to just-in-time compilation on HPC systems by encapsulating the necessary libraries and compilers, which are sometimes not available on HPC compute nodes.

We hope that the discussion and performance data in this work will assist researchers in scientific computing who are contemplating an investment in container technology. We believe that container technology can improve productivity and sharing in the scientific computing community, and in particular can dramatically improve the accessibility and usability of HPC systems.

Supplementary material

Supporting instructions, data, images and scripts are archived at [15].

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References

[1] FEniCS for Docker Containers, 2016. URL http://fenics-containers.rtfd.io.

[2] Docker, 2016. URL http://www.docker.com.

[3] Open Container Initiative, 2016. URL https://www.opencontainers.org.

[4] rkt, 2016. URL https://coreos.com/rkt/.

[5] Shifter, 2016. URL https://github.com/NERSC/shifter.

[6] M. F. Adams, J. Brown, J. Shalf, B. V. Straalen, E. Strohmaier, and S. Williams. HPGMG 1.0: A Benchmark for Ranking High Performance Computing Systems. Technical Report LBNL-6630E, Lawrence Berkeley National Laboratory, 2014. URL http://dx.doi.org/10.2172/1131029.

[7] A. Apaolaza, R. Haines, A. Aizpurua, A. Brown, M. Evans, S. Jolly, S. Harper, and C. Jay. ABC: Using Object Tracking to Automate Behavioural Coding. In *Proceedings of the 2016 CHI Conference Extended Abstracts on Human Factors in Computing Systems*, CHI EA '16, pages 2766–2773, New York, 2016. URL http://dx.doi.org/10.1145/2851581.2892483.

[8] D. Bahls. Evaluating Shifter for HPC Applications. In *Cray User Group Conference Proceedings*, 2016. URL https://cug.org/proceedings/cug2016_proceedings/includes/files/pap135-file2.pdf.

[9] C. Boettiger. An Introduction to Docker for Reproducible Research. *SIGOPS Oper. Syst. Rev.*, 49(1):71–79, 2015. URL http://dx.doi.org/10.1145/2723872.2723882.

[10] P. Di Tommaso, E. Palumbo, M. Chatzou, P. Prieto, M. L. Heuer, and C. Notredame. The impact of Docker containers on the performance of genomic pipelines. *PeerJ*, 3:e1273, 2015. URL http://dx.doi.org/10.7717/peerj.1273.

[11] Docker, Inc. Introduction to Container Security, 2015. URL https://d3oypxn00j2a10.cloudfront.net/assets/img/Docker%20Security/WP_Intro_to_container_security_03.20.2015.pdf.

[12] W. Felter, A. Ferreira, R. Rajamony, and J. Rubio. An updated performance comparison of virtual machines and Linux containers. In *Performance Analysis of Systems and Software (ISPASS), 2015 IEEE International Symposium on performance analysis of systems and software*, pages 171–172, 2015. URL http://dx.doi.org/10.1109/ISPASS.2015.7095802.

[13] W. Gerlach, W. Tang, K. Keegan, T. Harrison, A. Wilke, J. Bischof, M. D'Souza, S. Devoid, D. Murphy-Olson, N. Desai, and F. Meyer. Skyport: Container-based Execution Environment Management for Multi-cloud Scientific Workflows. In *Proceedings of the 5th International Workshop on Data-Intensive Computing in the Clouds*, DataCloud '14, pages 25–32, Piscataway, USA, 2014. IEEE Press. URL http://dx.doi.org/10.1109/DataCloud.2014.6.

[14] R. Haines and C. Jay. Reproducible Research: Citing your execution environment using Docker and a DOI, 2016. URL http://www.software.ac.uk/blog/2016-03-29-reproducible-research-citing-your-execution-environment-using-docker-and-doi.

[15] J. S. Hale, L. Li, C. N. Richardson, and G. N. Wells. Containers for portable, productive and performant scientific computing; supporting data and code, 2016. URL https://dx.doi.org/10.6084/m9.figshare.3570813.

[16] D. M. Jacobsen and R. S. Canon. Contain This, Unleashing Docker for HPC. In *Cray User Group Conference Proceedings*, April 2015. URL https://cug.org/proceedings/cug2015_proceedings/includes/files/pap157.pdf.

[17] N. Johnson. Python import scaling, 2014. URL https://www.archer.ac.uk/documentation/white-papers/dynamic-import/ARCHER_wp_dynamic-import.pdf.

[18] A. Logg, K.-A. Mardal, and G. N. Wells, editors. *Automated Solution of Differential Equations by the Finite Element Method*, volume 84 of *Lecture Notes in Computational Science and Engineering*. Springer, 2012. URL http://dx.doi.org/10.1007/978-3-642-23099-8.

[19] C. Macdonnell and P. Lu. Pragmatics of Virtual Machines for High-Performance Computing: A Quantitative Study of Basic Overheads. In *Proceedings of the 2007 High Performance Computing and Simulation Conference*, 2007. URL http://www.scs-europe.net/conf/ecms2007/ecms2007-cd/ecms2007/ecms2007%20pdf/hpc_1019.pdf.

[20] D. Merkel. Docker: Lightweight Linux Containers for Consistent Development and Deployment. *Linux Journal*, 2014(239), Mar. 2014. URL http://dl.acm.org/citation.cfm?id=2600241.

[21] F. Pérez and B. E. Granger. IPython: a system for interactive scientific computing. *Computing in Science and Engineering*, 9(3):21–29, 2007. URL http://dx.doi.org/10.1109/MCSE.2007.53.

[22] K. Raffenetti et al. MPICH ABI initiative, 2013. URL http://www.mpich.org/abi.

[23] C. Richardson and G. N. Wells. Parallel scaling of DOLFIN on ARCHER, 2015. URL https://dx.doi.org/10.6084/m9.figshare.1304537.

[24] K.-T. Seo, H.-S. Hwang, I.-Y. Moon, O.-Y. Kwon, and B.-J. Kim. Performance comparison analysis of Linux container and virtual machine for building cloud. *Advanced Science and Technology Letters*, 66:105–111, 2014. URL http://dx.doi.org/10.14257/astl.2014.66.25.