Enabling EASEY deployment of containerized applications for future HPC systems*

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Abstract. The upcoming exascale era will push the changes in computing architecture from classical CPU-based systems to hybrid GPU-heavy systems with much higher levels of complexity. While such clusters are expected to improve the performance of certain optimized HPC applications, it will also increase the difficulties for those users who have yet to adapt their codes or are starting from scratch with new programming paradigms. Since there are still no comprehensive automatic assistance mechanisms to enhance application performance on such systems, we are proposing a support framework for future HPC architectures, called EASEY (Enable exASclae for EverYone). The solution builds on a layered software architecture, which offers different mechanisms on each layer for different tasks of tuning. This enables users to adjust the parameters on each of the layers, thereby enhancing specific characteristics of their codes. We introduce the framework with a Charliecloud-based solution, showcasing the LULESH benchmark on the upper layers of our framework. Our approach can automatically deploy optimized container computations with negligible overhead and at the same time reduce the time a scientist needs to spent on manual job submission configurations.

Keywords: Auto-tuning · HPC · Container · Exascale.

1 Introduction

Observation, Simulation and Verification build the pillars of most of today’s HPC applications serving different goals of diverse scientific domains. Those applications have changed in the last decades and years, and they will and have to change again, driven by several factors. More applications, more scientists, more levels of detail, more data, more computing power, more on any contributing part. This more of everything needs to be satisfied by current and future computing systems, including not only computing power, storage and connectivity, but more and more also direct application support from computing centers.

* This is a preprint of a paper whose final and definite form will be published in the proceedings of the International Conference on Computational Science (ICCS) 2020 by Springer. Submitted February/2020.
This support is essential to execute a real high performance application with huge data sets in an efficient manner. This efficiency can have several objectives like time to solution or energy consumption. The latter will be the crucial factor to minimize to achieve an exascale system that serves the scientific community and does not stress our environment.

Computing efficiency in means of likely optimal usage of resources in an acceptable time to solution is heavily investigated from different sites. Many workflow management frameworks promise enhancements on data movement, deployment, management or reliability, like in SAGA, a grid based tool suit described in [11] or Pegasus, a scientific pipeline management system presented in [7]. The scalability of such frameworks is limited by the state-of-the-art service and bottlenecks are found inside and across of today’s supercomputing facilities.

Solutions to this challenge will not be found in one single place. Instead, it will be the most optimal interaction of exascale-ready services, hardware and applications. To support todays and future application developers, automatic assistant systems will be a key enabling mechanism, also shown by Benkner et al. in [2]. Computing systems will continue to develop and change faster than applications can be adapted to build likely optimal synergies between the application and the underlying system. Heterogeneity among also already connected centers increases the complexity.

Although scientist want to simulate, calculate, calibrate or compare data or observations always with the same application core, many hurdles slow down or stop those scientist to deploy on newer systems, since the effort to bring their application on new hardware or on new software stacks is too high in comparison to their actual work in their scientific domains. An astro physician wants to focus on the physic problems, not on how to deploy the code on a computing center.

This is supported by a survey from Geist and Reed in [9] who state, that the complexity of software needs to be reduced to reduce software development costs. This could also be solved if we can encourage application developers to include building bricks, which will adapt and optimize code or executions automatically, like proposed in our paper.

Therefore, new assistant systems are needed to make access to new supercomputing centers easier and possible also for unexperienced scientist. The complexity of those systems requires knowledge and support, which usually only the computing centers themselves can offer. Since their time is limited also the diversity of the applications might be limited.

This work introduces a framework to enable container applications based on Docker to be automatically transformed to Charliecloud container and executed on leading HPC systems. This transformation includes also the possibility to define mounting points for data. Charliecloud is considered the most secure container technology for supercomputers, since Singularity is not entirely free of breaches as reported in [6].

Within this paper we introduce the underlying technology and present the functionality of the framework, evaluated by a hydrodynamics stencil calculation benchmark. We show, that our approach adds automatically cluster dependent
Enabling scientists to focus on their actual work in their domain and remove all deployment overhead from their shoulders is the main goal of our approach. And while we reduce the necessary interaction between scientist and compute cluster, we also apply performance optimization on the fly. High performance systems need applications to adapt their technology to talk their language. We are able to add such optimizations while preparing the containerized application.

The architecture of the EASEY system is detailed in Figure 1 on page 4, integrated as two building bricks in the layered HPC architecture. On the upper Applications and Users layer the EASEY-client is mainly responsible for a functional build based on a Dockerfile and all information given by the user. The middleware on the local resource management layer takes care of the execution environment preparation, the data placement and the deployment to the local scheduler. The additional information service can be pulled for monitoring and status control of the execution through. The hardware layer of the compute cluster underneath remains not included in any optimization in this release of the framework (compare future work in Section 6).

2 EASEY Architecture

The client as the main service for any end-user prepares the basis of the execution environment by collecting all needed information to build a Charliecloud container. Therefore, the main information is given by the user with the Dockerfile. This file can also be pulled from an external source and needs to include all necessary steps to create the environment for the distinguished tasks. The client needs at some point root privileges to build the final container, hence, it needs to be deployed on a user’s system like a workstation or a virtual machine in a cloud environment.

As a first step, the Docker Service builds a docker image. Since HPC clusters can require local configurations, the Docker Service adds local dependencies to the Dockerfile. Therefore, the user needs to specify the target system in the build
command: `easey build Dockerfile --target cluster`, e.g. `easey build Dockerfile --target "lrz:supermuc-ng"`.

In addition for mpi-based applications, the actual mpi-version needs to match the system’s version. In the Dockerfile the user can specify the position where the cluster’s mpi-version needs to be integrated by including the line `###includeLocalmpi###`, which will be replaced by the client with the actual purge of all other mpi-versions and the compilation of the needed one. This should be done before the target application is compiled to include the right mpi libraries.

As a final step the later mounting point will be created as a folder inside the Docker image. The path was defined inside the configuration file (see Listing 1.2). Also specific requirements from the target system will be handled here, for example to include local libraries and functionalities inside the container (e.g. symlinks to special folders). Those requirements are known by the EASEY system and don’t need to be provided by the user.

In the same environment as the Docker Service the Build Service will transform the before created Docker image to a Charliecloud container archive. The service will call the Charliecloud command `ch-builder2tar` and specify the Docker image and the build location.

2.2 EASEY Middleware

The second building brick is the EASEY Middleware, which connects and acts with the resource manager and scheduler. The main tasks are job deployment, job management, data staging and creating the Charliecloud environment.

Thereby, a workflow is started including besides the before created Charliecloud container and configuration file, the local cluster storage and batch sys-
tem as well as the user specified external storage, if needed. A schematic view of the major steps is given in Figure 2 on page 5.

Starting with the user, the Dockerfile and the filled EASEY configuration file need to be included in a build call of the EASEY client, which is running on a user system with root privileges. Within this process a Docker container is built and transformed to a Charliecloud container, which again is packed in a tar-ball.

The EASEY middleware can be placed inside the target cluster or outside on a virtual machine for example. The framework will start the preparation of the submission based on the information given in the configuration. This can also include a data stage-in from external sources. To place data and later to submit a cluster job on behalf of the user, EASEY needs an authentication or delegation possibility on each contributing component. At this time of the development the only possibility included is access grants via public keys. This means in detail, if the EASEY middleware runs outside the cluster, that the public key of the host system needs to be added to the authorized keys inside the cluster. Thereby, EASEY can transfer data on the user’s storage inside the cluster.

Also the following job deployment needs a working communication from the middleware to the cluster submission node. The deployment based on the given configuration (see Listing 1.4) follows a well reinforced approach. The complete algorithm is shown in Algorithm 1.

Additionally to the already mentioned tasks the data folder is only created if at least one input or output file in specified. EASEY requires the user to place the output file after the computations inside this folder, mounted inside the Charliecloud container. For each input file, EASEY controls the transfer inside the data folder.

For the submission on the local batch system a batch file is required following also local specifications, known by EASEY. The resource allocation information is provided by the user in the configuration (number of nodes, ram, ...). For SLURM or PBS those are parsed into a valid form, other scheduler are not supported so far.
Algorithm 1 EASEY submission

Require: Charliecloud tar-ball
Require: EASEY configuration file
Require: User credentials

move tar-ball to cluster storage
extract tar-ball and create execution environment
if data in configuration then
    mkdir data_folder
end if
while input in configuration do
    transfer input[source] to data_folder
end while
create batch_file
for each deployment in configuration do
    parse to SLURM or PBS command in batch_file
end for
while execution in configuration do
    add command to batch_file
end while
submit batch_file to local scheduler and return jobID to EASEY

The actual computations follow after this prolog, described as executions by the user. For each the corresponding bash or mpi commands are also included. If data is required as input parameters, the user has to specify them relatively to the data folder, where they are placed.

Since the local job ID is known by the middleware the user can pull for the status of the job. In addition to pending, running, finished or failed, also error log and standard output is accessible, also at an intermediate state. After the job ended EASEY will transfer output files if specified.

This workflow includes all necessary steps to configure and run an originally Docker based application on a HPC cluster. Thereby, it saves time any scientist can use for actual work in their domain and removes any human overhead especially if such computations need to be deployed regularly. In the same time, it adds optimization mechanisms for the actual computing resource. In the following section, details on the user’s mandatory configuration are presented.

3 EASEY Configuration

Our approach requires a full and valid description of all essential and optional parts of the submission. Therefore we defined a json-based configuration file including all required information. This file needs to be provided by the user together with the application’s Dockerfile. The configuration consists of four main parts: job, data, deployment and execution.
Job Specification This part of the configuration can also be seen as mandatory meta data for a valid job management. The keys of the key-value pairs are presented in Listing 1.1.

An EASEY job needs to have an unique identifier, a hash which is determined by the system at the moment of submission, a user specified name and a mail address to contact the end-user if specified. Besides those, no further information is mandatory.

### Listing 1.1. Job Specification
```json
{  "job":{"name","id","mail",  "data":{ },  "deployment":{ },  "execution":{ }} }
```

Data Service Specification Our backend is able to fetch accessible data files via the protocols https, scp, ftp and gridftp. The latter is planned to be implemented in the next release. For the others already available only the path to the source and the protocol needs to be declared. If the data needs to be accessed on a different site, authentication with public-key mechanism is necessary. The input is declared as an array and can include several declarations of different input files.

The backend will place all input files in one folder, which will be mounted into the container on the relative position declared as path.

After the complete execution an output recommend as an archive can be also moved again to a defined destination. Also here a public key mechanism would be mandatory.

Deployment Service Specification The deployment service offers basic description possibilities to describe necessary resources for the execution.

As shown in the next section, within one deployment only one job is allocated. Therefore, each execution commands specified in Listing 1.4 will be run on the same allocation. The specifications regarding nodes, ram, tasks-per-node and clocktime will be translated into scheduler specific commands and need to be specified given in Listing 1.3.

### Listing 1.2. Data Specification
```json
"data":{"input":{  "source","protocol",  "user","auth"},  "output":{  "destination","protocol",  "user","auth"},  "mount":{"container-path"} }
```

### Listing 1.3. Deployment Specification
```json
"deployment":{"nodes",  "ram","cores-per-task",  "tasks-per-node","clocktime" }
```

### Listing 1.4. Execution Specification
```json
"execution":[{  "serial":{  "command"},  "mpi":{  "command","mpi-tasks"} }]```
Although there exist much more possible parameters, at this state of the framework only those are implemented, since all others are optional.

**Execution Service Specification** The main ingredients of HPC jobs are the actual commands. The execution consists of in principle unlimited serial or mpi commands. Those are executed in order of sequence given inside the execution array as shown in Listing 1.4. In all considered HPC jobs the only kinds of commands are bash (serial) or mpi-based commands.

A complete example is given in Listing 1.5 showing a practical description of the evaluated use case. The presented configuration will of course be adapted whenever necessary. However, the main goal is to stay as generic as possible to connect and enable as many combinations of applications on the one side and resource management systems on the other. The next section evaluates this approach regarding the computational and the human overhead.

### 4 Evaluation

The before presented framework builds the basis for further development. The main goal is to introduce auto-tuning on several layers. In this paper, we presented the EASEY client and middleware to support scientists deploying a Docker-based application on a HPC cluster without interacting with the local resource themselves.

This framework was tested on one of the fastest HPC systems in the world, the SuperMUC-NG, a general purpose system at the Leibniz Supercomputing Center in Garching, listed ninth in the Top500 list in November 2019 and has a peak performance of 26.87 Petaflops, computing on 305,856 Intel Xeon Platinum 8174 CPU cores, without any accelerators. All compute nodes of an island are connected with a fully non-blocking Intel Omnipath OPA network offering 100 Gbit/s, detailed in [3]. SuperMUC-NG uses SLURM as a system scheduler.

We used a Dockerimage for LULESH, the Livermore Unstructured Lagrangian Explicit Shock Hydrodynamics benchmark. It is a widely used proxy application for calculating the Sedov blast problem that highlights the performance characteristics of unstructured mesh applications. Details on the application and the physics are described by Karlin et al. in [13].

This benchmark in version 2.0.3 was ported by the MNM research team (Flinger et al., described in [8]) to DASH, a C++ template library for distributed data structures, supporting hierarchical locality for HPC and data-driven science. Adopting the Partitioned Global Address Space (PGAS) programming notion, DASH developed a template library that provides PGAS-like abstractions for important data containers and allows a developer to control and take advantage of the hierarchical data layout of global data structures. The authors in [8] showed, that DASH offers a performance advantages of up to 9%.

As described in Section 3 the EASEY client requires besides the Dockerfile the configuration specifying the deployment, data and execution parameters. Since

1 [https://www.lrz.de/english/](https://www.lrz.de/english/)
LULESH does not require any data, the json configuration shown in Listing 1.5 contains only job meta data, deployment and execution. Values, which are determined by EASEY, or which are not defined by the user (e.g. ram since there are no special memory requirements) are not set.

The command key for the actual execution includes the Charliecloud ch-run. With -b source/target data folders are bind into the container. Inside the container lulesh.dash the command /built/lulesh.dash -i 1000 -s 42 is executed. Together with the mpi-tasks LULESH is run with a cube size of 2.197 cells, a length of the cube mesh of 42 and in 1.000 iterations. The maximal runtime is given with 6 hours for the SLURM scheduler.

Listing 1.5. LULESH:DASH Execution Specification

```json
"job": {
  "name": "LULESH:DASH", "id": ",
  "mail": "hoeb@mnm-team.org",
  "deployment": {
    "nodes": "46", "ram": ","cores-per-task": "1",
    "tasks-per-node": "48", "clocktime": "06:00:00"
  },
  "execution": {
    "serial": {
      "command": "echo \"Starting LULESH:DASH\""
    },
    "mpi": {
      "command": "ch-run -b /lrz/sys/./lrz/sys -w lulesh.dash -- /built/lulesh -i 1000 -s 42",
      "mpi-tasks": "2197"
    },
    "serial": {
      "command": "echo \"Finished LULESH:DASH\"
    }
  }
}
```

This setup was used to run several execution of the original LULESH, the DASH LULESH and the DASH LULESH inside the Charliecloud container. As is can be seen in Figure 3 on page 10 the figure of merit (FOM) shows slightly higher values (higher is better) for DASH and Charliecloud runs, then for LULESH. The FOM values of Charliecloud are for all numbers of cores below the DASH version. This can be seen in detail in Figure 4 on page 10 where the FOM value is divided through the number of cores. Ideally we would see a horizontal line, however, the difference between this line and the measurements corresponds to the application.

Figure 3 on page 10 and Figure 4 on page 10 are based on preliminary results measured on SuperMUC-NG due to ongoing maintenance. The camera-ready version will include broader measurements.

Inside the container the application has access to the local optimized MPI version and the OmniPath network. This auto-tuning was performed by EASEY, which added the required parts to the user’s Dockerfile, before the Charliecloud container was built.
With the weak scaling in Figure 3 on page 10 we can show, that our approach scales as well as the manually compiled application without any container environment. Automatically enabling a container deployment on such a supercomputing cluster and in the same time applying local tuning possibilities show, that EASEY is a promising approach. It is also likely that such assistance systems will increase to number of users using those HPC systems and in the same time enabling them to include as much optimization as possible, without changing anything manually.

The time of scientists is limited and we want to enable physicians, chemists, engineers and all others to focus on their domain. They need to optimizes the application regarding the scientific outcome, while our framework takes care of the compute deployment. We also want to encourage more scientists not to be afraid of such huge systems. The learning curve is high, if someone wants to use a Top 10 supercomputer. However, with EASEY, there exists a solution to use a more and more common praxis: Docker container. General purpose systems like the SuperMUC-NG are made for general purpose applications. With the presented performance in this section, we can substantially offer an additional deployment approach on those systems, for everybody.

5 Related Work

The presented framework and its implementation bases on the development towards containerization and the abilities such encapsulated environments offer.

Charliecloud and Docker Priedhorsky and Randles from the Los Alamos National Laboratory introduced in 2017 in [15] a lightweight open source implementations of a container framework: Charliecloud. The authors followed their basic assumptions that the need for user-defined software stacks (UDSS) increases. Dependencies of application’s still need to be compiled on the actual target HPC systems since not all of them are available in the stack provided by the compute center. Todays and future users need particular dependencies and
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build requirements, and more over also portability and consistency to deploy applications on more than one system. This is offered by Charliecloud, which bases on Docker to build an UDSS image.

The advantage of Charliecloud lays in the usage of the user namespace, supporting non-privileged launch of containerized applications. Within this unprivileged user namespace also all other privileged namespaces are created without the requirement of root privileges. Therewith, any containerized application can be launched, without requiring privileged access to the host system, as described from Brayford et al. in [3]. In the same paper, the authors investigated the performance of Charliecloud scaling an AI framework up to 32 nodes. Their findings showed a similar, negligible overhead, although our performance analysis included more nodes. Concerning possible security issues the authors stated that Charliecloud is safe, since it only runs inside the non-privileged user namespace.

Docker, described by Merkel in [14] is considered an industry standard container to run an applications in an encapsulated environment. Nevertheless, since some containers require root privileges by default and others can not prevent privilege-escalation in all cases, as shown in [4], Docker is not considered a safe solution when deployed on shared host systems.

Charliecloud was also compared to other approaches like Shifter and Singularity. The Shifter framework also supports Docker images (and others, e.g. vmware or squashfs), shown by Gerhardt et al. in [10]. In contrast, it is directly tied into the batch system and its scalability and security outside the initial cluster is not shown so far.

Also Singularity was developed to be encapsulated into a non-privileged namespace, security issues have been detected, for example in [6], where users could escalate the given privileges. An example is detailed in [3].

Choosing the right container technology is crucial, especially regarding the security of the host and other users. Since Charliecloud is considered secure and shows promising scaling behavior, we choose this technology for our framework. Including Charliecloud in such a framework, only one related approach could be discovered so far.

**BEE** The authors of *Build and Execution Environment BEE* in [5] propose an execution framework which can, besides others, also deploy Charliecloud container on a HPC infrastructure. Their approach focuses on a variety of different cloud and cluster environments managed by the same authority. This broad approach tries to unify the execution of the same container. Compared to EASEY, which aims to auto-tune the performance for Petaflop-systems, it does not include any optimization to the underlying infrastructure.

*BEE* also includes a submission system for deployment of jobs, but deploys each single run command as one job. Our approach focuses on complex computations which might also include several steps within one job. Regarding the data service, no possibility is provided in *BEE* to connect to an external resource for data stage-in or -out.
We consider BEE as a valid approach to deploy the same container on many different technologies. However, we focus on auto tuning of adjusting screws to gain performance advantages, and our target infrastructures are high performance systems in the range of Petaflops and later Exaflops.

6 Conclusion

The presented architecture and its components are considered the starting point for further investigations. The heterogeneous landscape of computing and storage facilities need applicable and efficient solution for the next generation computing challenges. Exascale is only the next step as Petascale was a few years ago. We need to build assistent systems which can be adapted to the actual needs of different communities and enable those to run their application on more and more different and complex hardware systems.

To close the gap between application developers and resources owners, a close collaboration is needed. In fact, the presented solution for an efficient usage of containerized applications with Charliecloud is only the first part. We need to go deep in the systems, optimize the hardware usage on a node or even CPU, GPU and memory level and convince the scientific communities, that also their applications are able to scale up to such a level. Here, such an assistant system like EASEY, which automatically deploys optimized applications, will convince the communities and enable scientists to focus on their work.

Future Work As mentioned throughout this paper, this version of EASEY is the first step towards a comprehensive framework to enable easy access to future exascale systems. Our next steps focus on efficient data transfers, also including the model of data transfer nodes as investigated in the EU-funded project PROCESS and published in [12] and [1]. For this data access also the authentication mechanism need to be enhanced. The consecutive step will be to extent this framework to lower levels of the cluster’s architecture and provide assistance on deeper levels.

Acknowledgment The research leading to this paper has been supported by the PROCESS project, which has received funding from the European Unions Horizon 2020 research and innovation programme under grant agreement No 777533.

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