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High-performance computing

Licensed software in Slurm (Comsol)

The Slurm workload manager can handle licensed software by assigning available licenses to jobs at scheduling time. If licenses are not available, jobs are kept pending until specified licenses become available, rather than failing at runtime due to a lack of available licenses. This can be particularly useful for software that only has a few licenses. For example, for the Comsol software, MPCDF currently maintains only two licenses for each Comsol module for batch use. In order to use this feature, you need to add the `-L, --licenses` option to the batch job scripts with a comma-separated list of required license names. To find out which licenses the `mph` comsol file requires, you can check it in the comsol GUI or simply run the `mphlicenses` command after loading the comsol module on HPC *Cobra* or *Raven* systems:

```
~> module load comsol/6.2
~> mphlicenses test_file.mph
comsol_nonlinearstructmaterialsbatch@lserv,\
comsol_comsolbatch@lserv,\
comsol_structuralmechanicsbatch@lserv,\
comsol_clusternode@lserv,\
comsol_comsoluser@lserv

# note, there are no linebreaks in the actual
# output, added here for layout reasons only
```

The complete Slurm #SBATCH directive to run this comsol test_file on the clusters then reads

```
#SBATCH -L \
  comsol_nonlinearstructmaterialsbatch@lserv,\
  comsol_comsolbatch@lserv,\
  comsol_structuralmechanicsbatch@lserv,\
  comsol_clusternode@lserv,\
  comsol_comsoluser@lserv

# note, there must be no linebreaks in the actual
# script, added here for layout reasons only
```

In order to get a list of all available comsol licenses on HPC systems, run the command:

```
scontrol show licenses
```

Mykola Petrov

HPC Software News

Improved workflow for multimer predictions with AlphaFold2 on *Raven*

AlphaFold2 (AF2) is an artificial-intelligence program released by Google DeepMind which performs predictions of protein structure based on the sequence of amino acids. AF2 has been provided by MPCDF since summer 2021 on *Raven* and on several institute clusters, and is regularly updated and customized to achieve optimal performance on the MPCDF systems.

Initially, the prediction of the structure of single proteins (monomers) has been a main application of AF2, however more recently the users' focus shifted towards predicting protein-protein complexes (multimers). As the prediction of multimers is considerably more expensive than most monomer cases, users sometimes hit the 24-hour job time limit on *Raven* with the original AF2 program, which internally loops over multiple models and random seeds.

To overcome this limitation, MPCDF has refactored the internal double loop over the models and predictions into individual Slurm jobs. In particular, individual Slurm array jobs are now used for each model, each array containing a configurable number of tasks calculating individual predictions using individual random seeds. As a result, each individual prediction task now has a maximum wall clock time of 24 hours.

On *Raven*, run `module help alphafold/2.3.2-2024` to get fur-

[*]Editors: Dr. Renate Dohmen & Dr. Markus Rampp, MPCDF

ther instructions. For multimer cases, copy, adapt and run the script `submit_alphafold_jobs.sh` to submit the job-array-based predictions. Users are encouraged to approach us via the helpdesk with their feedback, which is valuable to further improve this service.

Klaus Reuter

New version of Intel oneAPI with deprecation of ifort compiler

Intel oneAPI version 2024.0 has been installed on *Raven* and other HPC clusters recently. With this installation, we drop the `.x` suffix and the patch-level version from the compiler module name. Thus, the Intel compiler module is now called `intel/2024.0`. Bugfixes provided by Intel incrementing the patch level number will be installed under the hood without further notification. Run `module show intel/2024.0` in order to see which exact compiler version is present. The corresponding MPI module is `impi/2021.11`, and the latest MKL module is `mkl/2024.0`. As announced previously[1], MPCDF, starting with `intel/2024.0`, is using `ifx` as the default Intel Fortran compiler, together with its MPI wrapper `mpiifx`. The "classic" Fortran compiler `ifort` is still present, but is now formally tagged as deprecated by Intel.

Tobias Melson

CUDA modules on *Raven*

MPCDF offers various CUDA modules on *Raven*. It depends on the desired compiler, which of these modules should be picked. If an application code is compiled with the GNU compiler (`gcc/11` or `gcc/12`), the CUDA modules `cuda/*` are suitable. In case the code is compiled with the Nvidia compiler (`nvhpcsdk/23`), the matching CUDA modules are named `cuda/*-nvhpcsdk` (note the suffix here). The following table lists the compatible CUDA modules for the recent GNU and Nvidia compilers:

```
Compiler:   Compatible CUDA modules

gcc/11:     cuda/11.4,cuda/11.6
gcc/12:     cuda/12.1,cuda/12.2
nvhpcsdk/23:cuda/11.8-nvhpcsdk,cuda/12.3-nvhpcsdk
```

As announced previously[2], CUDA-aware OpenMPI (`openmpi_gpu/4.1`) is available after having loaded one valid combination of compiler and CUDA modules.

Tobias Melson, Tilman Dannert

New AMD-GPU ELPA release

The ELPA library[3] provides highly optimized, scalable solvers for generalized and standard, dense symmetric (Hermitian) eigenproblems. Since 2022, the ELPA library supports AMD GPUs and on Europe's first pre-exascale system *LUMI* (CSC, Finland) ELPA was successfully employed for solving huge standard eigenvalue problems with a matrix size of up to 3.2 million (leading dimension) on more than 8000 AMD MI250x GPUs. In preparation for the new HPC system *Viper* at the MPCDF we have released a new version 2024.03.001 of the ELPA library which has been further extensively optimized for AMD GPUs. Among others, support of the GPU-to-GPU collective communications library RCCL (the equivalent to Nvidia's NCCL library) has been implemented. In addition, the GPU implementation of the routines for the generalized eigenvalue problem has been reworked and speedups of up to a factor of 10 have been achieved. The latest version of ELPA is available to all users as a pre-built software package in the module environment of the MPCDF software stack.

Andreas Marek

Kubernetes in the HPC-Cloud

Containers have been widely adopted as a way to develop, distribute, and deploy applications. Kubernetes provides a framework to run containerized applications in a reliable and scalable fashion. Kubernetes is based on cluster management technology developed at Google (cf. Verma, Abhishek, et al.: "Large-scale cluster management at Google with Borg", Proceedings of the tenth European conference on computer systems, 2015[4]) and donated to the Linux Foundation in 2015. It has enjoyed wide adoption since.

At MPCDF projects can deploy Kubernetes clusters hosted in the HPC-Cloud based on an OpenStack Heat Orchestration Template[5] as provided by the MPCDF Cloud enabling team[6]. The team maintains two templates: one for a small and simple cluster aimed at projects that wish to test and evaluate Kubernetes, and the second providing a production-grade cluster aimed at projects looking to deploy their services and applications using Kubernetes.

[1]https://docs.mpcdf.mpg.de/bnb/214.html#intel-oneapi-transition-from-ifort-to-ifx
[2]https://docs.mpcdf.mpg.de/bnb/214.html#cuda-aware-openmpi-on-raven
[3]https://elpa.mpcdf.mpg.de
[4]https://dl.acm.org/doi/abs/10.1145/2741948.2741964
[5]https://docs.openstack.org/heat/latest/template_guide/hot_guide.html
[6]https://gitlab.mpcdf.mpg.de/mpcdf/cloud/kubernetes/
[7]https://kubernetes.io/docs/reference/kubectl/

Usage

The canonical way to control a Kubernetes cluster is with `kubectl`[7]. The credentials required to connect to the cluster are provided on the control plane nodes set up by the template. The most important feature is that users define desired states for pods executing their containers and any peripheral resources in configuration files.

Many software projects publish the configuration states required to run their products using `Helm`[8], the package manager for Kubernetes. Helm charts define the desired state of many interacting Kubernetes components. Users can configure charts by setting desired values of chart variables defining the specific features of their deployment.

In productive deployments, it is imperative to store and track the configuration files of the services orchestrated in Kubernetes. This can be accomplished, for example, using GitLab. In addition, GitLab offers integrations for Kubernetes that deploy the state defined in the configuration files stored in a repository to Kubernetes as defined in the GitLab CI/CD pipelines. Taking advantage of this feature of GitLab provides a concise way to manage applications for teams of administrators and developers.

Function

Kubernetes is best suited for orchestrating long-running services that are implemented as many inter-dependent microservices. It is also possible to run applications on a schedule, or execute single commands in their containers.

Deploying a web service

Here is a configuration file you can apply with `kubectl create -f <filename>.yaml`

```
---
apiVersion: apps/v1
kind: Deployment
metadata:
  name: svc-demo-deployment
  labels:
    app: svc-demo-app
spec:
  replicas: 2
  selector:
    matchLabels:
      app: svc-demo-app
  template:
    metadata:
      labels:
        app: svc-demo-app
    spec:
      containers:
      - name: svc-demo-container
        image: jmalloc/echo-server
        ports:
        - containerPort: 8080
---
apiVersion: v1
kind: Service
metadata:
  name: svc-demo
spec:
  selector:
    app: svc-demo-app
  type: LoadBalancer
  ports:
  - port: 80
    targetPort: 8080
    protocol: TCP
```

The first section defines a deployment with a container image that runs the application, in this case a server that parrots your HTTP requests. The second section defines a service, exposing the application using a load balancer. Now running `kubectl get all` will give you:

```
NAME
READY   STATUS    RESTARTS   AGE
pod/svc-demo-deployment-587b7c9974-4z5wn
1/1     Running   0          66s
pod/svc-demo-deployment-587b7c9974-lz7pp
1/1     Running   0          66s

NAME                 TYPE           CLUSTER-IP
EXTERNAL-IP      PORT(S)        AGE
service/svc-demo     LoadBalancer   10.101.113.187
XXX.XXX.XXX.XXX  80:32260/TCP   66s

NAME                                      READY
UP-TO-DATE   AVAILABLE   AGE
deployment.apps/svc-demo-deployment   2/2
2            2           66s

NAME
DESIRED   CURRENT   READY   AGE
replicaset.apps/svc-demo-deployment-587b7c9974
2         2         2       66s
```

You can see two pods running the application and the service making the application available at `http://XXX.XXX.XXX.XXX:80`. The application can be removed with `kubectl delete -f <filename>.yaml`.

Existing applications

Kubernetes on the HPC-Cloud is already used at MPCDF to host a number of prominent applications, for example MoveApps[9], NOMAD[10], or GlycoSHIELD[11].

Frank Berghaus

[8]https://helm.sh
[9]https://www.moveapps.org/
[10]https://nomad-lab.eu/nomad-lab/
[11]https://dioscuri-biophysics.pages.mpcdf.de/glycoshield-md/

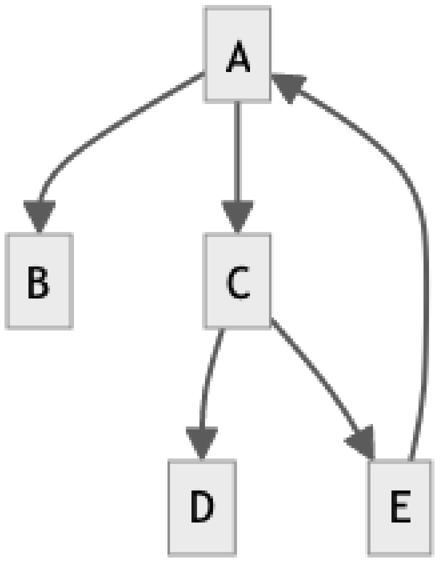
GitLab: Graphs & Diagrams

In addition to classic Git functionality, MPCDF's GitLab instance offers a wide range of capabilities around code organisation and project management. In many of these scopes, for example Wiki pages or issues, the user can enter formatted text in Markdown format. After saving, GitLab will render the Markdown annotations which results in a nicely formatted human readable document. Beside standard Markdown annotations, GitLab integrates out-of-the-box libraries for rendering graph structures and diagrams in Markdown texts. In this article, the creation of graphs and diagrams with the help of the Mermaid library is introduced.

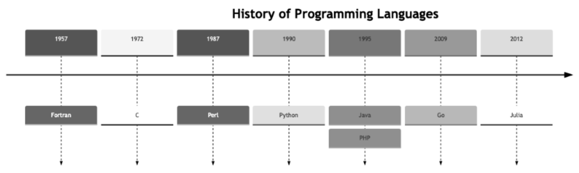
Inside any Markdown-formatted document in GitLab, the following code fragment encapsulates a Mermaid sub document:

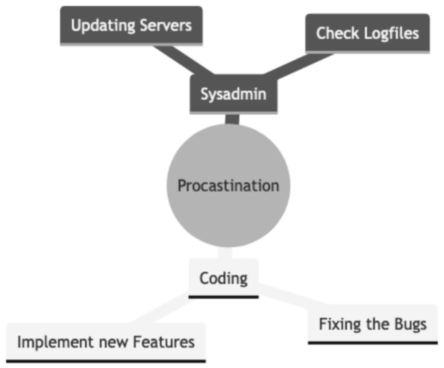
~~~
```mermaid
graph TD
    A --> B
    A --> C
    C --> D
    C --> E
    E --> A
```
~~~

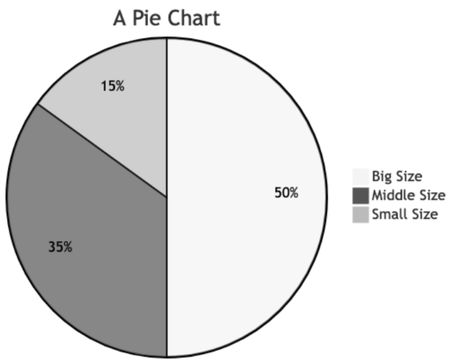
After saving the Markdown document, GitLab would create the following graph from the code above:

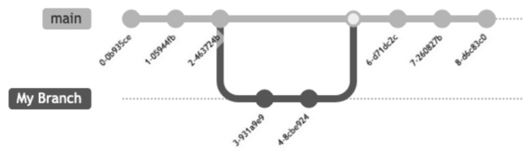


The Mermaid library supports different types of graphs and diagrams. The image below shows some examples, top to bottom: a timeline, a mindmap, a pie chart and - maybe particularly relevant for GitLab users - a Git graph, showing the branch and commit structure of a Git repository:









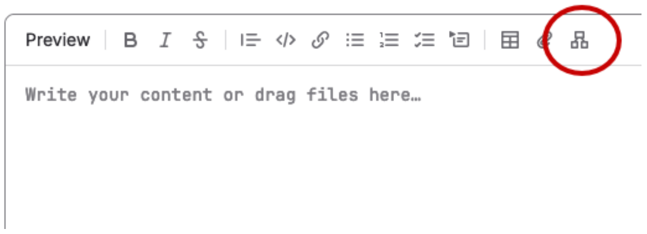
The Markdown and Mermaid code of the examples examples can be found here[12]. Further information about supported graph and diagram types can be found in the Mermaid Documentation[13].

Alternatives

In the same way GitLab supports the Mermaid library, also PlantUML[14] for UML diagrams and Kroki[15] are

[12]https://gitlab.mpcdf.mpg.de/thomz/graphs-and-diagrams
[13]https://mermaid.js.org/intro/
[14]https://plantuml.com/en/
[15]https://kroki.io/

supported. And if you don't want to dive into another descriptive language, GitLab allows you to insert manually drawn diagrams via the external service draw.io[16]. You can find this function as "Insert or edit diagram" button in the Markdown editor (red circle):



Thomas Zastrow

LLMs meet MPCDF

Figure 1: A GPT4 interpretation of Max Planck using LLMs at the MPCDF

The term "Large Language Model" (LLM), has been part of public discourse since at least the end of 2022, following the release of OpenAI's ChatGPT. The general-purpose capabilities of these large AI models to process and store unstructured data have ignited a wave of new applications, also in the world of science (cf. *The Impact of Large Language Models on Scientific Discovery: a Preliminary Study using GPT-4*. Microsoft Research[17]). However, most state-of-the-art models are provided by major tech companies and are accessible only through paid APIs. This paywall, along with the requirement to transfer research data to third parties, often hinders the use of so-called "closed" LLMs. In contrast, "open" LLMs, which can be downloaded and used on-premise, are rapidly narrowing the gap in capabilities compared to their closed counterparts (cf. *Open LLM Leaderboard*. Hugging Face[18]). However, the immense size and complexity of LLMs require significant computational resources and pose technical challenges for less experienced users, both in terms of operation and training.

Given the computational resources and expertise at the MPCDF, an increasing number of scientists from the Max Planck Society are seeking our advice and support on utilizing LLMs. The inquiries come from a wide range of scientific domains, from natural sciences to the humanities, underscoring the broad impact these models have on the scientific community. The AI group at the MPCDF is actively enhancing its expertise in large language models and expanding its support for various use cases. To this end, we have created the "LLMs Meet MPCDF" GitLab repository[19], where we start offering examples and guidance on deploying and fine-tuning LLMs on our HPC systems. For now we showcase how to set up an inference server for open models with TGI[20], and how to supervise-fine-tune a 70B Llama2 model by means of FSDP[21].

If you have unaddressed use cases or projects involving LLMs, please don't hesitate to reach out to us, we would be more than happy to hear from and collaborate with you.

David Carreto Fidalgo, Andreas Marek

[16] https://draw.io
[17] https://arxiv.org/pdf/2311.07361.pdf
[18] https://huggingface.co/spaces/HuggingFaceH4/open_llm_leaderboard
[19] https://gitlab.mpcdf.mpg.de/dcfidalgo/llms-meet-mpcdf
[20] https://github.com/huggingface/text-generation-inference
[21] https://pytorch.org/tutorials/intermediate/FSDP_tutorial.html

News & Events

Introduction to MPCDF services

The next issue of our semi-annual online course "Introduction to MPCDF services" will be held on April 25th, 14:00-16:30 via Zoom. Topics comprise login, file systems, HPC systems, the Slurm batch system, and the MPCDF services remote visualization, Jupyter notebooks and datashare, together with a concluding question & answer session. Basic knowledge of Linux is required. No registration is required, just connect at the time of the workshop via the zoom link[22].

Meet MPCDF

The next editions of our monthly online-seminar series "Meet MPCDF" are scheduled for

- May 2nd, 15:30 "CMake - Cross-supercomputer Make" by Vedran Miletic (MPCDF)
- June 6th, tba

All announcements and material can be found on our training webpage[23].

We encourage our users to propose further topics of their interest, e.g. in the fields of high-performance computing, data management, artificial intelligence or high-performance data analytics. Please send an E-mail to training@mpcdf.mpg.de[24].

Tilman Dannert

[22] https://mpcdf-mpg-de.zoom-x.de/j/69488919156?pwd=T256S1dXSjhXcU1hNGhZNExkeVVsQT09
[23] https://www.mpcdf.mpg.de/services/training
[24] mailto:training@mpcdf.mpg.de