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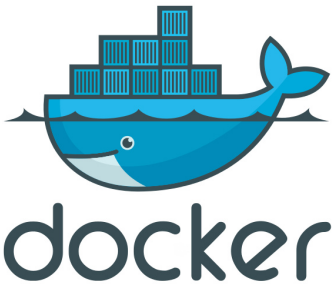

Using Trilinos from Containers & Interactive Environments

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U.S. DEPARTMENT OF ENERGY | National Nuclear Security Administration

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Doing science in HPC

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Typical workflow from the first idea to the final performance tests:

1) Idea & Algorithm design

- Rapid development (Matlab, Python, C++)
- Quick experiments on small data sets

2) Implementation

- Final parallelized implementation in C++ (using Trilinos)
- Algorithmic optimizations & Performance optimizations

3) Performance studies on HPC clusters

- Final performance studies on HPC clusters with large datasets
- Produce results for scientific paper

Doing science in HPC

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What are the challenges?

1) Idea & Algorithm design

- Focus on algorithms and mathematics
- Need for rapid development tools and programming languages

2) Implementation

- Error-prone reimplementation and parallelization of algorithms using Trilinos
- Expert knowledge for best results necessary (Trilinos, etc.)

3) Performance studies on HPC clusters

- Make your algorithms work on all HPC platforms

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New technologies and tools

What is docker?

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Docker is a software containerization platform.

- New concepts for *organizing*, *developing*, *testing* and *shipping* software
- Maintain one general software/development environment independent of underlying host OS or hardware
- **Focus on the applications!**

More information: `https://docs.docker.com/install/`

What is jupyter?

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Jupyter is an interactive computing environment.

- Support for many language kernels including Python, Julia, R, C++
- Ideal tool for interactive tutorials
- Jupyter notebooks for documenting and organizing scientific experiments

Jupyter usage scenarios

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- Document your ideas, algorithms, experiments and results in notebooks
- Use functionality from existing C++ libraries in your notebooks
- Extend the functionality by writing new classes and functions live in your notebook
- Gain better insight into legacy code and complex algorithms by adding advanced debugging statements
- Optimize your algorithms in an interactive way

Example

`AutoWhiteBalancingLiveDemo.html`

What jupyter is and what it is NOT

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Jupyter

- helps you minimizing the effort for porting the Jupyter C++ implementation to the final implementation.
- helps you developing algorithms and gaining in-depth insight.
- helps you organizing your ideas, experiments and results.

Jupyter does not

- make porting the experimental C++ code to final C++ code superfluous.
- help you writing clean code and unit tests.
- help you organizing your notebooks. You still need a systematic way of storing your notebooks in order to quickly find results from a specific experiment. Use a version controlling system!

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New technologies in context of Trilinos

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How can docker and jupyter help?

1) Idea & Algorithm design

- Use C++ with Cling and Jupyter as rapid prototyping environment?

2) Implementation

- Improve your Trilinos knowledge with Jupyter Trilinos tutorials
- Manage your development environment with docker

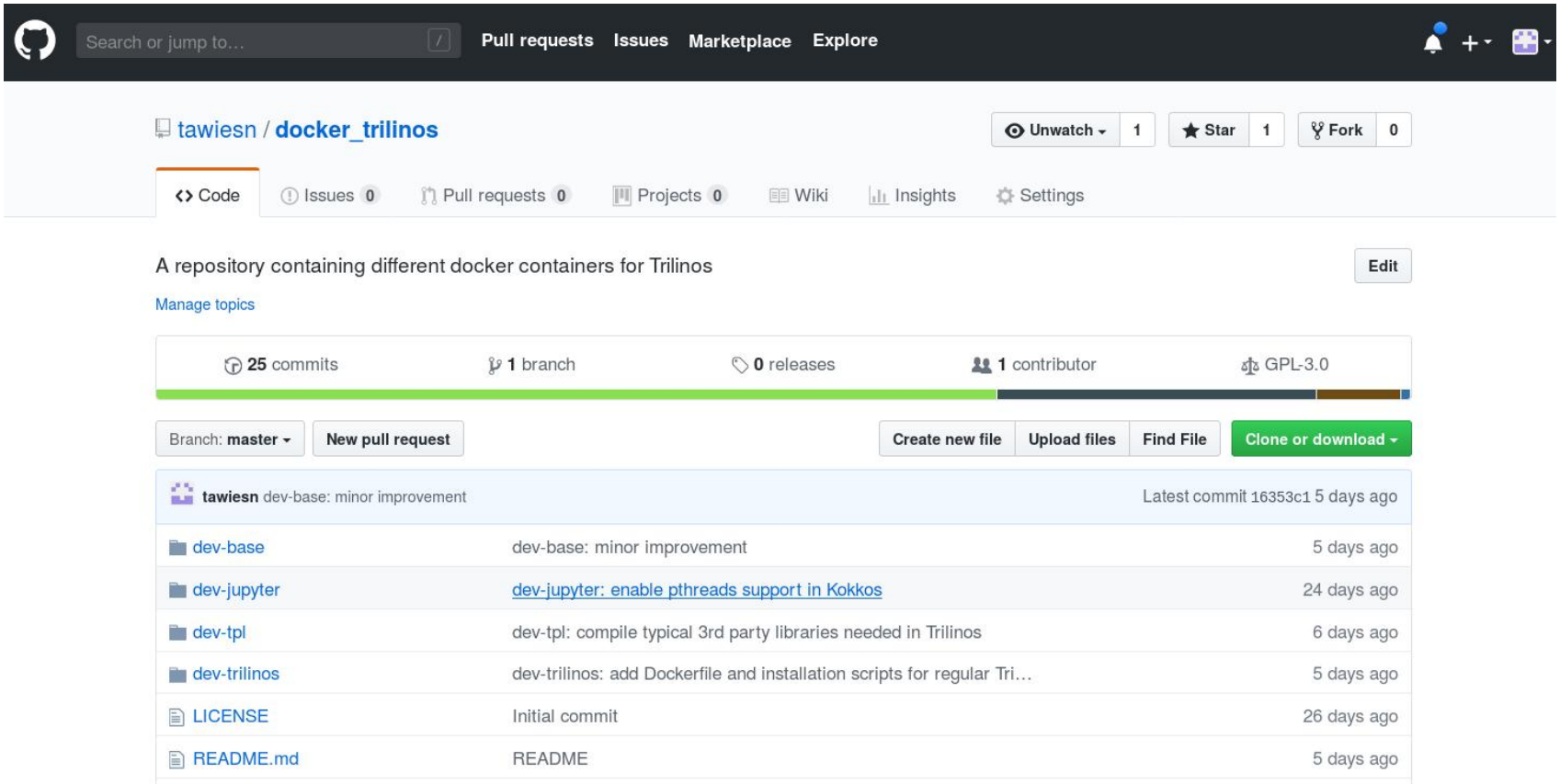
3) Performance studies on HPC clusters

- Manage your development environment with docker

github repository

Check out the github repository

`https://github.com/tawiesn/docker_trilinos`



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Docker for Trilinos

Trilinos docker container

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The dev-trilinos docker container

- Classical docker container based on CentOS 7 (Redhat compatible)
- Contains a clone of the public Trilinos repository
- Builds some core Trilinos packages using gcc with OpenMPI support
- **Meant as an example for your own Trilinos container** that can be used to link your application against
- Use it as **standardized development platform** that can also be used on **HPC clusters**, e.g. via the Shifter project (`https://github.com/NERSC/shifter`)

More information here: `https://github.com/tawiesn/docker_trilinos/blob/master/README.md`

How to create your own Trilinos container for your application

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- Clone the `https://github.com/tawiesn/docker_trilinos` repository
- Follow the instructions to build all dependencies. For details see `https://github.com/tawiesn/docker_trilinos/blob/master/installation_dev_trilinos.md`
- Create a copy of the dev-trilinos folder and rename it, e.g. my-dev-trilinos
- Edit the my-dev-trilinos/do-configure file and enable all Trilinos features that you need
- If you need a specific Trilinos version for your application you might adapt the git clone statement in the my-dev-trilinos/Dockerfile

How to create your own application docker container

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- Build your my-dev-trilinos docker container
- Create a new folder, e.g. my-application
- Create a new Dockerfile in you my-application folder
- Edit the my-application/Dockerfile and make sure you derive your docker container from the my-dev-trilinos folder.
- Copy the sources and build scripts into the docker container. Use the dev-trilinos/Dockerfile for some inspiration.

Benefit

Your Dockerfiles contain all necessary commands to compile and install your Trilinos libraries and application.

- Put your Dockerfiles under version control
- Set up nightly builds for the Docker container to track changes and detect compilation issues as soon as they pop up

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Jupyter and Trilinos

Trilinos jupyter notebooks

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The dev-jupyter docker container

- Docker container based on CentOS 7 (Redhat compatible) with clang installation and cling extensions
- Contains a clone of the public Trilinos repository
- **Meant for tutorials and algorithmic experiments**
- Find a small set of basic Trilinos tutorial notebooks here: `https://github.com/tawiesn/trilinos-notebooks`
- Limitations:
  - No OpenMPI support at the moment (can be added)
  - Some instabilities when running parallel Kokkos kernels (needs to be investigated)

More information here: `https://github.com/tawiesn/docker_trilinos/blob/master/README.md`

Basic Trilinos Jupyter mini tutorials

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Repository

`https://github.com/tawiesn/trilinos-notebooks`

1) Epetra tutorial

Apply power method to tridiagonal matrix

2) Belos tutorial

Solve linear equation with GMRES w/wo ILUt

3) Tpetra tutorial

Create Tpetra vector and access data

4) Kokkos tutorial

Some basic examples for parallel kernels and Kokkos views

Questions?

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For more information check out the repositories:

Docker container

`https://github.com/tawiesn/docker_trilinos`

Jupyter notebooks

`https://github.com/tawiesn/trilinos-notebooks`