

# UPDATES ON PANDAROOT IN DOCKER

AND SINGULARITY FOR HPC SYSTEMS

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# THE GOAL

Use PandaRoot on any machine (with docker or Singularity) without installing FairSoft/FairRoot. Avoid dependency/compiler hell.

- MC Data Generation on HPC
- Analysis on Workstation
- Software Development

Advantage: easy setup and clean separation from host system.

**A bit has changed since my last presentation.**

You want to run PandaRoot

PandaRoot: built upon ↓

FairRoot: requires ↓

FairSoft: provides ↓

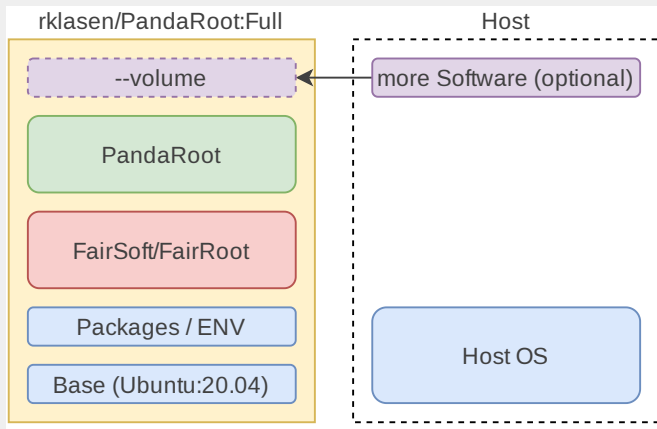
External Packages (ROOT etc.)

And of course some installed packages. Which means for a new user, all these packages had to be downloaded and compiled.

**How can we package this for ease-of-use?**

# POSSIBLE LAYOUTS 1: ALL-INCLUSIVE (NOT YET READY)

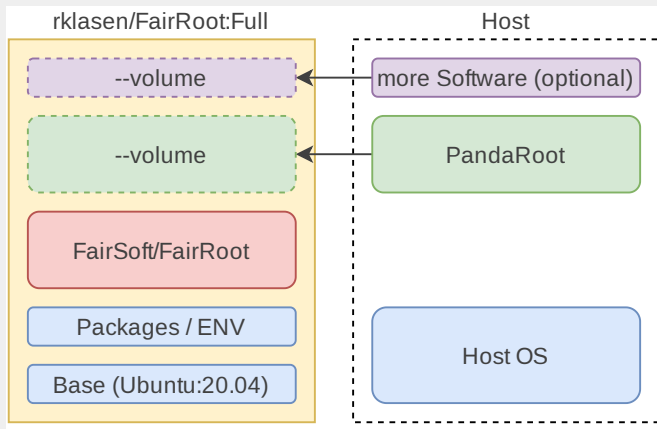
Complete PandaRoot installation with all necessary packages, ready to go.



**Con:** Large Image Size (May run into issues on HPC systems)

## POSSIBLE LAYOUTS 2: FAIRSOFT/FAIRROOT FULL (READY)

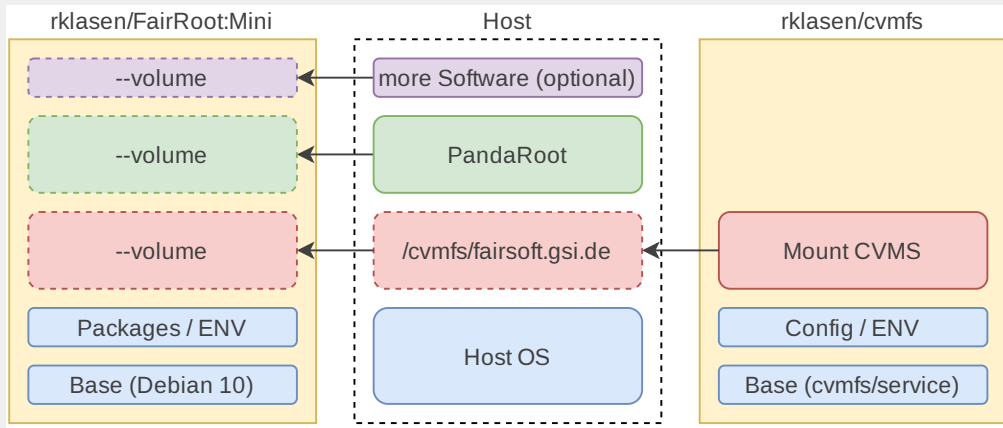
Includes FairSoft/FairRoot but needs external PandaRoot source directory.



Good for code development, this is what I'm using right now.

## POSSIBLE LAYOUTS 3: EXTERNAL EVERYTHING (READY)

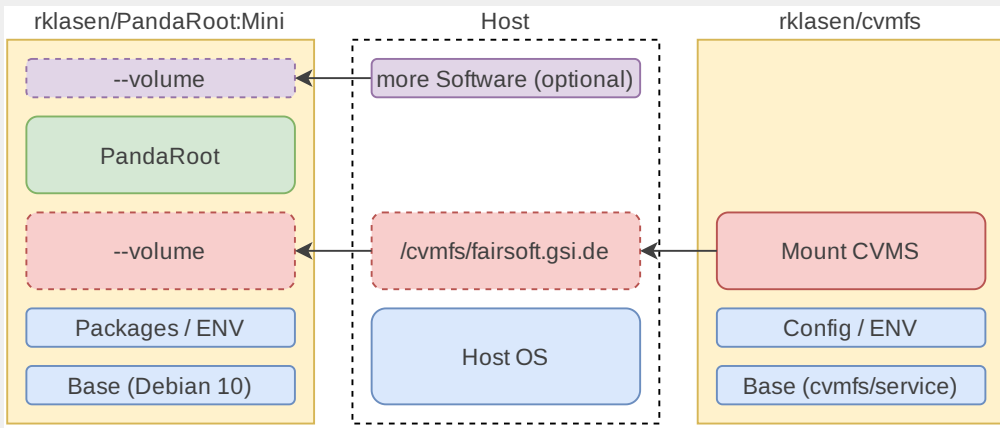
Sandbox ready for PandaRoot, but doesn't include FairRoot/FairSoft or PandaRoot



**Pro:** Use auto builds from GSI. **Bonus:** Mount CVMFS via another container!

# POSSIBLE LAYOUTS 4: EXTERNAL FAIRROOT/FAIRROOT

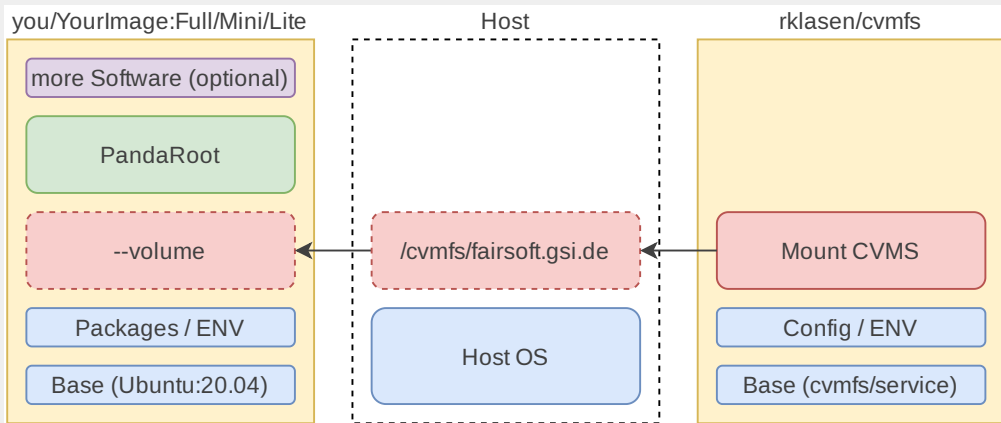
Includes PandaRoot, needs external FairSoft/FairRoot.



Best suited for HPC systems, `/cvmfs/fairsoft.gsi.de/` is already there.

# POSSIBLE LAYOUTS 5: A-LA-CARTE (UP TO YOU :)

You desired software+PandaRoot, baked into a ready-to-go image



Use PandaRoot:Mini/Full as base image for your custom image.



## LAYOUT 3: MOUNT GSI CVMFS VIA CONTAINER

- Idea: Mount GSI's cvmfs (which provides FairSoft/FairRoot) and compile only PandaRoot yourself.
- On cluster systems, this mount is (probably) already there
- For best system-separation, mount cvmfs via docker container

### Mount cvmfs

```
docker run -d --name cvmfs --privileged --cap-add SYS_ADMIN \\
--device /dev/fuse --volume /cvmfs:/cvmfs:shared rklasen/cvmfs
```

You should now have a new directory on your **host**:

```
/cvmfs/fairsoft.gsi.de/
```

## LAYOUT 3: USE HOST CVMFS IN PANDAROOT CONTAINER

PandaRoot-Mini requires external PandaRoot code and /cvmfs/ mount. The image is build and uploaded to Docker Hub. You can pull and run it with:

Pass to FairRoot:mini Docker container:

```
docker run -it -v $(HOME)/PandaRoot:/mnt/work/PandaRoot \\  
-v /cvmfs:/cvmfs rklasen/fairroot:mini
```

In there, you can build and run PandaRoot.

See: <https://git.panda.gsi.de/PandaRootGroup/PandaRoot/-/blob/dev/docs/Docker/Dockerfile-Mini>.

## ON HPC SYSTEM: CONVERT TO SINGULARITY

I'll use Himster2 as example here. You can't run Docker containers, but you *can* run Singularity containers. So, on your workstation:

### Convert Docker to Singularity

```
singularity build fairroot-mini.sif \<\  
docker://rklasen/fairroot:mini
```

And copy the resulting file to your user home on Himster2. Clone PandaRoot to your home and make sure it's really at

~/PandaRoot/

So that it can be used by the Singularity container.

## ON HPC SYSTEM: RUN CONTAINER

On Himster2 (and probably other HPC systems) cvmfs is provided for you, so you only need to run this image (and not rklasen/cvmfs):

```
module load tools/Singularity
singularity exec fairroot-mini.sif bash
```

In that container, you can compile PandaRoot as usual. All needed packages are installed and all environment variables are set. This can also be done in job submission scripts with sbatch:

```
singularity exec fairroot-mini.sif root -l -q myMacro.C
```

## LAYOUT 4: PANDAROOT COMPLETE

If you don't need to change PandaRoot source code and instead only run it, a complete PandaRoot image will be ready shortly. It will include pre-compiled PandaRoot, using hosts `/cvmfs/` mount for FairSoft/FairRoot:

```
docker run --it -v /cvmfs:/cvmfs rklasen/pandaroot:mini \\  
root -l -q myMacro.C
```

And on Himster2:

```
module load tools/Singularity  
singularity exec pandaroot-mini.sif root -l -q myMacro.C
```

## JOIN THE DISCUSSION

TODO: Automate Docker builds in GitLab (Dockerfiles are already there).

You can find the documentation at:

### GitLab Documentation

<https://git.panda.gsi.de/PandaRootGroup/PandaRoot/-/tree/dev/docs/Docker>

If you have a different requirement or can help, please open a GitLab issue.

**THANKS FOR YOUR ATTENTION!**