Visa and Singularity

16th September 2022

Singularity Containers

- Conventional Workflow

Singularity Containers

- Conventional Workflow

Computing environment

Install dependencies & application

```
> apt-get update
> apt-get install pkg-config
> ...
```

Binaries

```
> indexamajig -i files.lst ...
```

```
> crystfel
```

Process

GUI
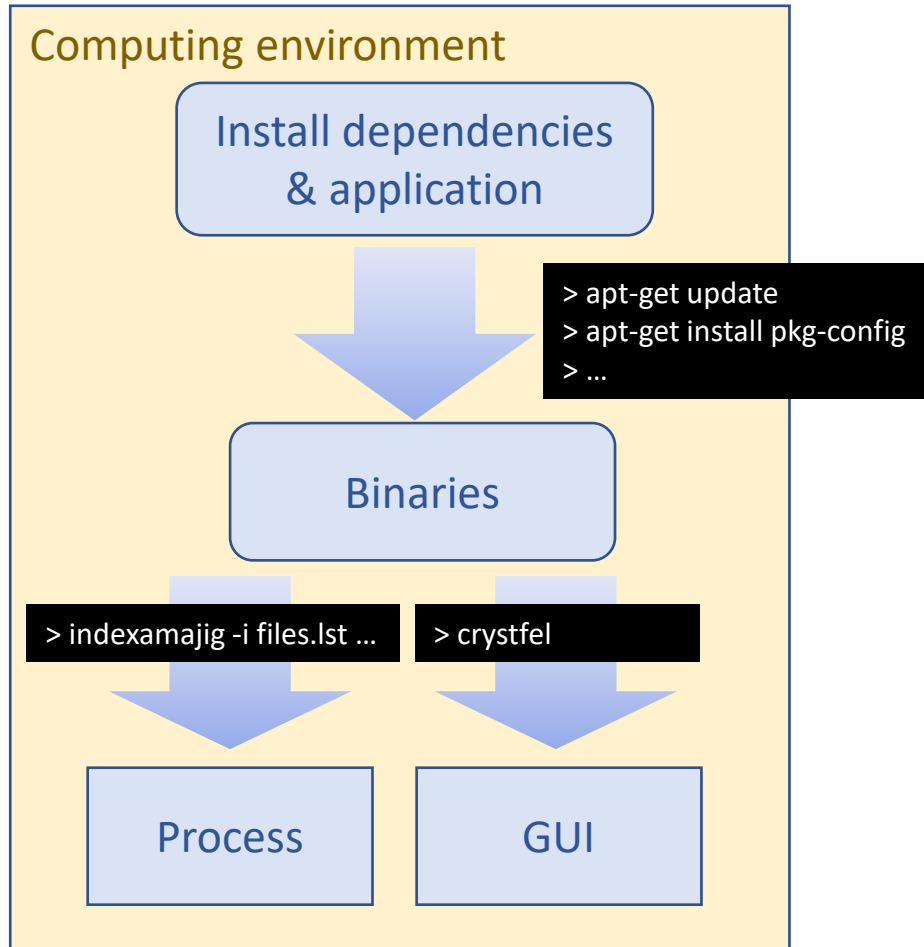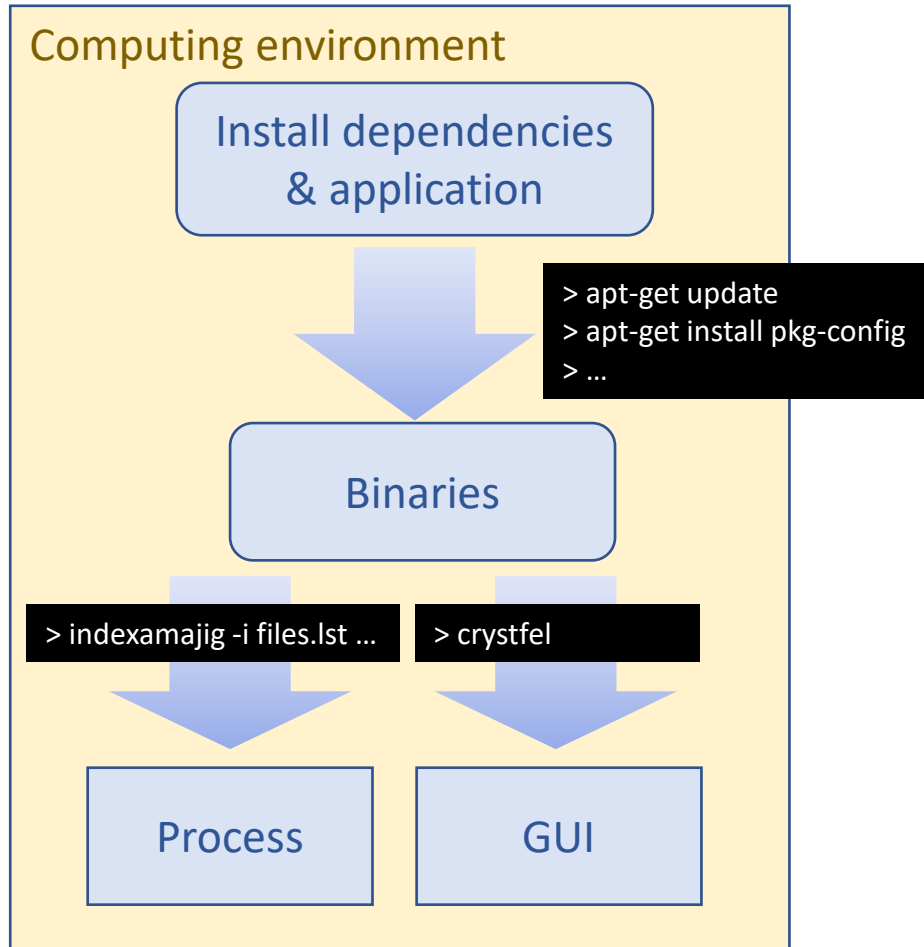
- Containerized Workflow

Computing environment (Singularity)

Pull container from registry

```
> singularity pull
docker://gitlab.desy.de:5555/silvan.schoen/crys
tfel/crystfel:latest
```

Container Image

```
> singularity exec indexamajig -i ...
```

```
> singularity exec crystfel
```

Containerized Environment

Process

GUI

```
> --bind /path/to/data
```

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Singularity Containers

Pros:

- No installation, all dependencies are met within the container allready

- Reproducibility

- No elevated rights necessary

- Concerning Visa:
  - independency on pre-configure Visa-images from the facility
  - Full control of application and used versions

- Container commands are fully Slurm supported

Contras:

- Container needs to be build/available

- Additional syntax needed

- Additional paths need to be mounted

- Slurm does not work from within the container

Containerized Application

Simplified Container workflow:

- Configure config file

- Run installation script

- Run application with container
  behind the scenes

Containerized Application

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- Configure config file

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- Run application with container behind the scenes
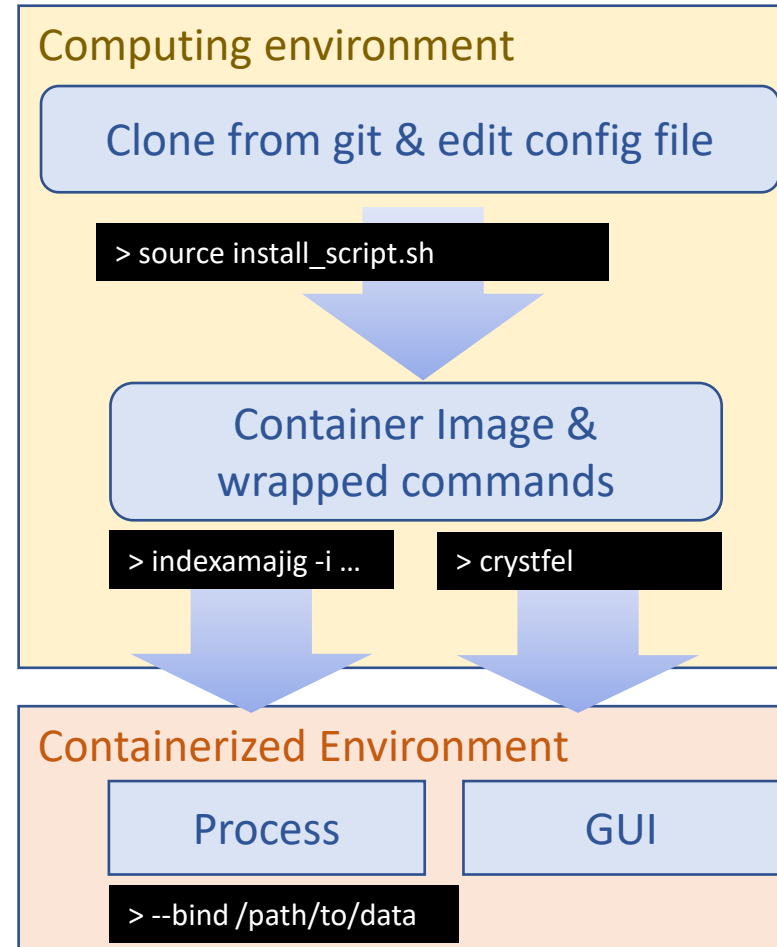
Computing environment

Clone from git & edit config file

> source install_script.sh

Container Image &
wrapped commands

> indexamajig -i ...   > crystfel

Containerized Environment

Process   GUI

> --bind /path/to/data

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Containerized Application

Simplified Container workflow:

- Configure config file
- Run installation script
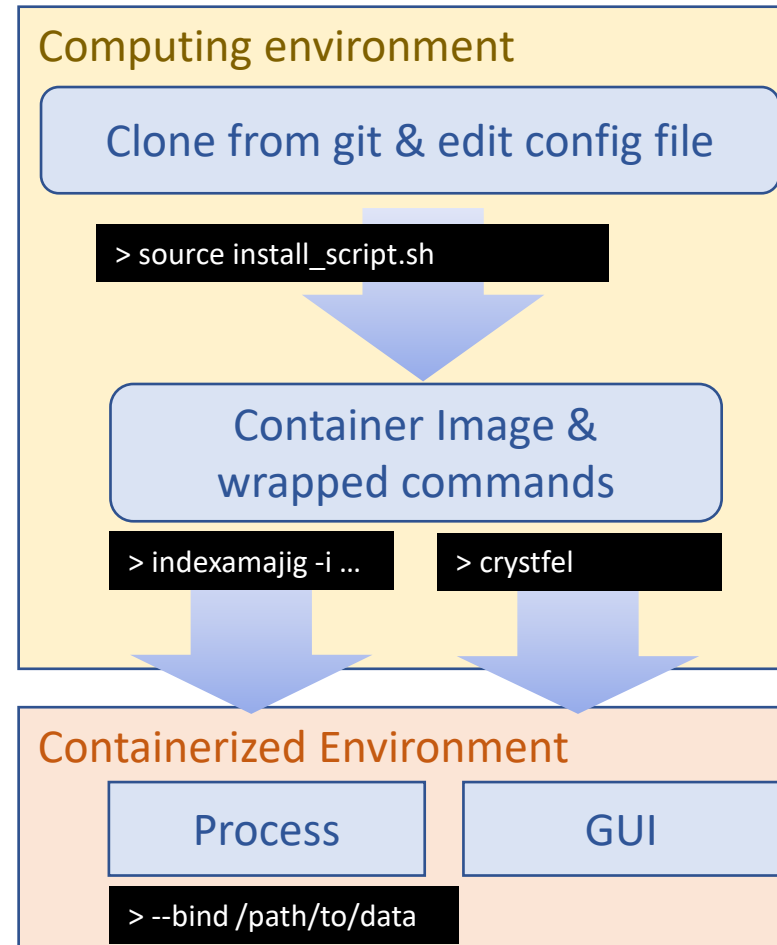- Run application with container behind the scenes

Computing environment

Clone from git & edit config file

```
> source install_script.sh
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Container Image & wrapped commands

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```
```
> crystfel
```

Containerized Environment

Process

GUI

```
> --bind /path/to/data
```

Config file:

```bash
#!/bin/bash
myregistry="gitlab.desy.de:5555/thomas.white/crystfel"
myimage="crystfel"
mytag="test"

# add commands that need to call Slurm commands (f.e. GUIs)
slurm_supported_commands=(
    crystfel
)

# add a slurm supporting container shell
slurm_shell=true

# other commands available through the container
mycommands=(
    indexamajig
)

# add data directories to the container
bind_directories=(
    /path/to/data
)

# define needed keyword arguments from singularity
singularity_kwargs=(
    --bind
)
```
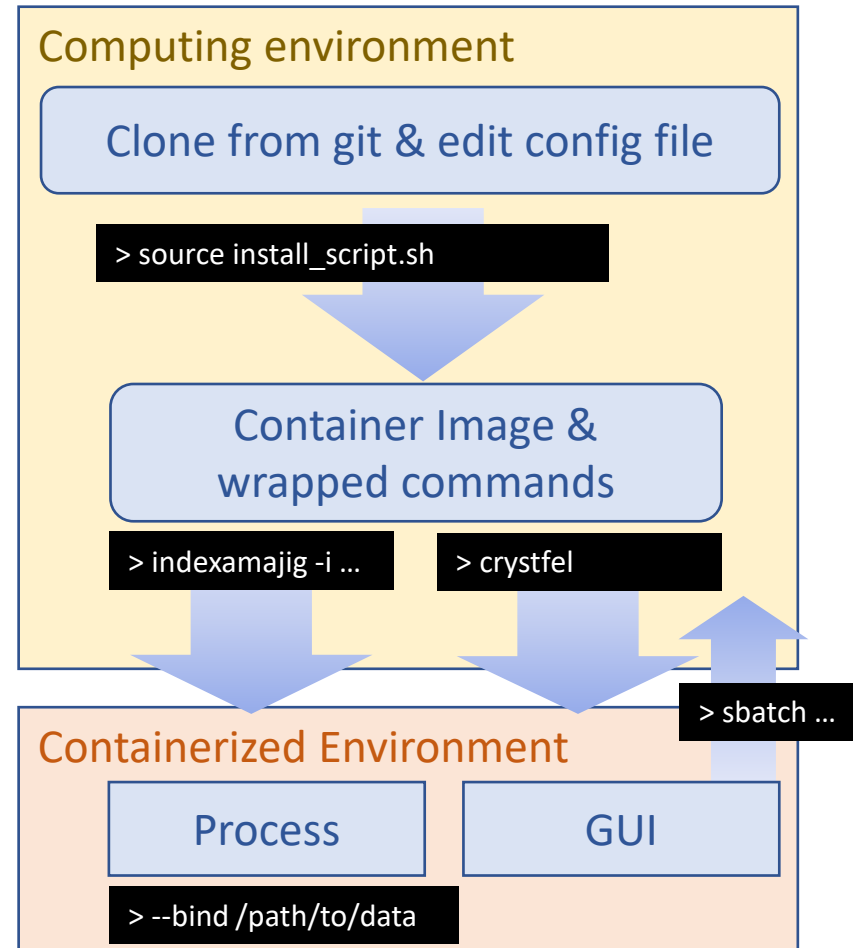
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Containerized Application

Simplified Container workflow:

- Configure config file
- Run installation script
- Run application with container behind the scenes
- Supports running Slurm commands from within the container

Computing environment

Clone from git & edit config file

> source install_script.sh

Container Image & wrapped commands

> indexamajig -i ...   > crystfel

Containerized Environment

Process   GUI

> sbatch ...

> --bind /path/to/data

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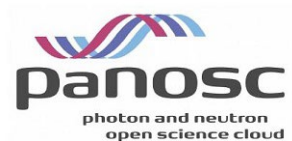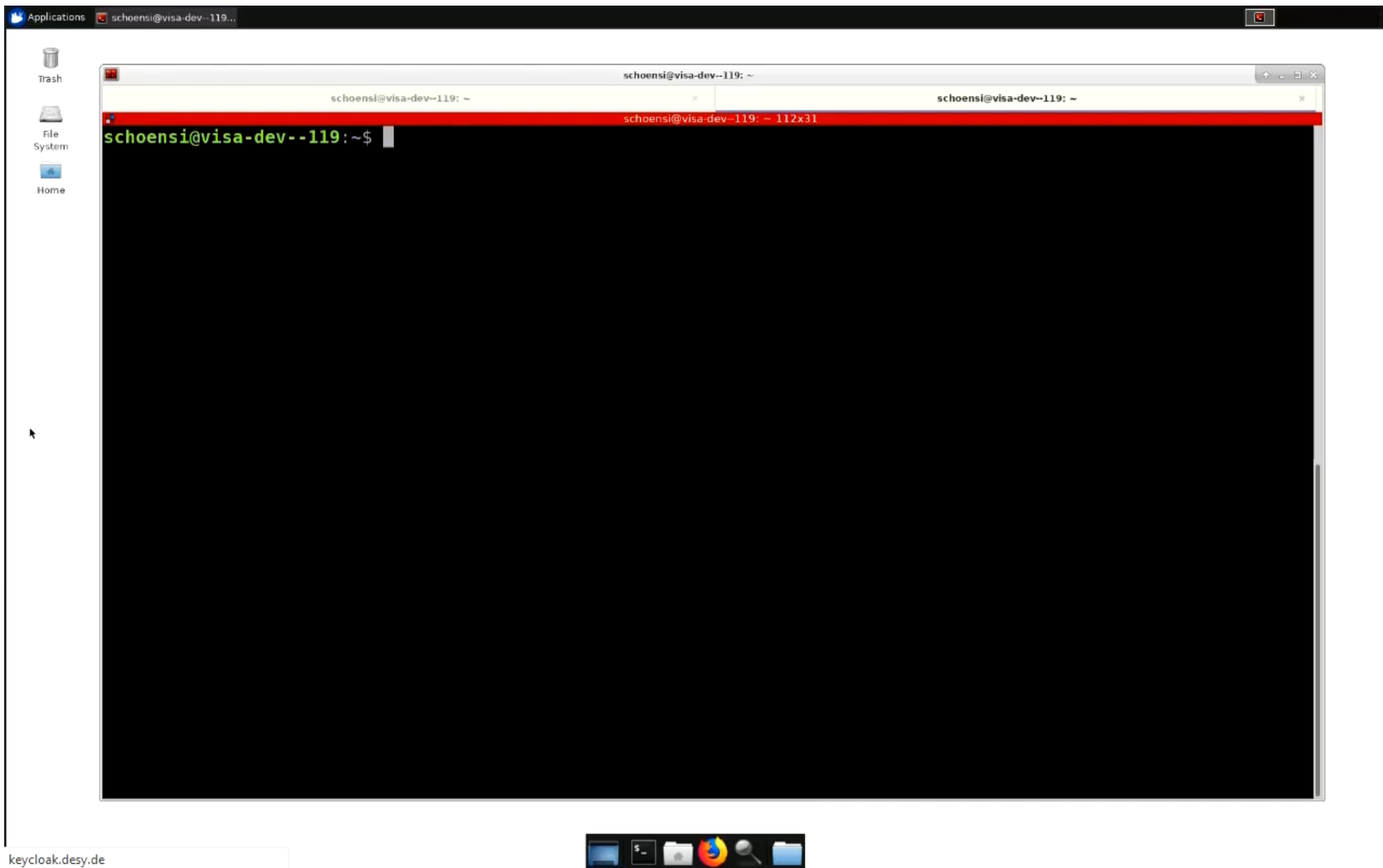
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Demo