

# GAP Docker containers for reproducible computational experiments (and more ...)

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Computational  
Discrete  
Mathematics

# What if ...

- 📌 You need to quickly get fully functional installation of GAP and packages, but ...
  - 📌 Some packages are not compiling on your computer
  - 📌 Some packages have complicated dependencies
  - 📌 Some may be only installed on a particular machine so you need network connection to access it
- 📌 But you want to:
  - 📌 Be able to take this with you to the journey
  - 📌 Share your experimental setup with collaborator
  - 📌 Provide environment for reproducing your experiment
  - 📌 Automate deployment on the cluster / in the cloud
  - 📌 Save time in a large-scale tests or experiments

# Ideas?

-  Virtual machines
-  VMWare, VirtualBox, ...
-  One more computer to maintain?
-  Eventually becomes outdated
-  Could automate installation scripts
-  Wouldn't it be nice to have something more lightweight?

# What is Docker?




- 📌 Solution for virtualisation
- 📌 Lightweight “containers” instead
- 📌 <https://www.docker.com>
- 📌 Documentation: <https://docs.docker.com/>
- 📌 For Linux, OS X, Windows, major cloud platforms, ...
- 📌 To get it, go to <https://www.docker.com/products/overview>
- 📌 Docker toolbox - for older versions of OS X and Windows:  
<https://www.docker.com/products/docker-toolbox>

# A simple example

- 📌 run Docker container for GAP and packages:
  - 📌 First, pull the container from the Docker Hub
  - 📌 Then run the `gap` command in this container
  - 📌 GAP options can be added after, e.g. `gap -A`
- 📌 See this container in
  - 📌 Docker Hub: <https://hub.docker.com/r/gapsystem/gap-docker/>
  - 📌 GitHub: <https://github.com/gap-system/gap-docker>
- 📌 Explore container's filesystem and GAP installation

```
docker pull gapsystem/gap-docker
docker run --rm -i -t gapsystem/gap-docker gap
```

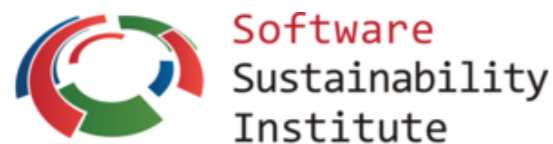
# More use cases in README.md




-  Using network
-  Mounting local folders
-  Let's see the demo

```
docker run -v /Users/alexk/dockermount:/work --rm -i -t gapsystem/gap-docker  
gap /work/homophony.g
```

# History of Docker support in GAP

- 📌 Hackday project at Collaborations Workshop 2015, with Sarah Mount (University of Wolverhampton), Devasena Inupakutika (Software Sustainability Institute), and myself
- 📌 Shortly after that joined by Sebastian Gutsche
- 📌 We have since established a pipeline of containers
- 📌 As alternative GAP distributions, they are usually updated shortly after the GAP release



 <a href="#">gapsystem/gap-docker</a> public   automated build	3 STARS	734 PULLS	<a href="#">&gt;</a> DETAILS
 <a href="#">gapsystem/gap-container</a> public   automated build	1 STARS	158 PULLS	<a href="#">&gt;</a> DETAILS
 <a href="#">gapsystem/gap-docker-base</a> public	1 STARS	119 PULLS	<a href="#">&gt;</a> DETAILS
 <a href="#">gapsystem/gap-docker-jupyter</a> public   automated build	1 STARS	70 PULLS	<a href="#">&gt;</a> DETAILS


# GAP Containers pipeline

























- 📌 Container for the core GAP system and only GAPDoc package
  - 📌 <https://hub.docker.com/r/gapsystem/gap-container/>
  - 📌 <https://github.com/gap-system/gap-container>
- 📌 Intermediate container for external software used by GAP packages.
- 📌 Needed to build gap-docker
  - 📌 <https://hub.docker.com/r/gapsystem/gap-docker-base/>
  - 📌 <https://github.com/gap-system/gap-docker-base>
- 📌 Container for GAP and all packages redistributed with GAP
  - 📌 <https://hub.docker.com/r/gapsystem/gap-docker/>
  - 📌 <https://github.com/gap-system/gap-docker>
- 📌 Container for the GAP Jupyter interface
  - 📌 <https://hub.docker.com/r/gapsystem/gap-docker-jupyter/>
  - 📌 <https://github.com/gap-system/gap-docker-jupyter>








# Use case: testing GAP packages using Travis CI

 <https://github.com/gap-system/gap-docker-pkg-tests>

 <https://travis-ci.org/gap-system/gap-docker-pkg-tests>

✓ # 23.1	 </> C	 PKG_NAME=ace	 3 min 1 sec
✗ # 23.2	 </> C	 PKG_NAME=alnuth	 2 min 56 sec
✗ # 23.3	 </> C	 PKG_NAME=anupq	 13 min 8 sec
✗ # 23.4	 </> C	 PKG_NAME=atlasrep	 9 min 43 sec
✓ # 23.5	 </> C	 PKG_NAME=automgrp	 3 min 28 sec
✓ # 23.6	 </> C	 PKG_NAME=browse	 4 min 55 sec
✓ # 23.7	 </> C	 PKG_NAME=circle	 2 min 54 sec
✓ # 23.8	 </> C	 PKG_NAME=cohomolo	 3 min 27 sec





# Reproducibility

-  Code inside new container
-  Code outside existing container
-  Recommend to read this Bill Mills' blog post:
  -  “Full Stack Science”
  -  <http://billmills.github.io/blog/full-stack>

# What's in the future?

- 📌 Reliable to “use as you go”
- 📌 Reasonable to expect to run not too old containers for a while
- 📌 Unclear (to me at least) how much it is reliable for long term preservation
- 📌 Docker's first release made in March 2013
- 📌 Popular and active project
- 📌 Docker Hub (<https://hub.docker.com/>) - free for public repositories
- 📌 If situation will change, the mindset will still stay

# Coding sprint at this workshop?

-  Installing and trying GAP Jupyter interface
-  Update for GAP 4.8.6
-  Help with issues on GitHub
-  Trying and testing