

# CompBioMed Containerisation Meeting

29 March 2019 - Amsterdam

## Do containers *really* relieve the burden of installing scientific software?

Kenneth Hoste (HPC-UGent,  easybuild)  
(remote talk)

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# whoami

kenneth.hoste@ugent.be  
@boege1 (*GitHub, IRC, Slack*)  
@kehoste (*Twitter*)

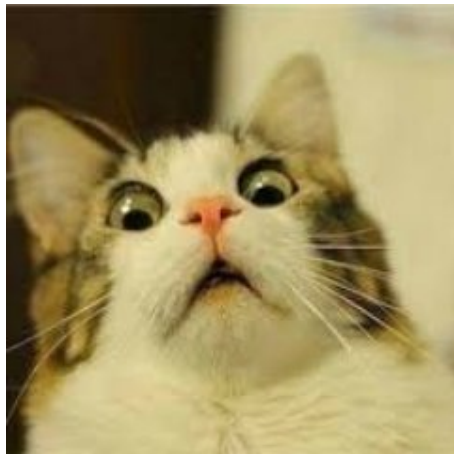
- Masters & PhD in Computer Science from Ghent University (Belgium)
- joined HPC-UGent team in October 2010
- main tasks: user support & training, *software installations*
- slowly also became  *easybuild* **lead developer & release manager**
- likes family, beer, loud music, FOSS, helping people, dad jokes, stickers, ...
- doesn't like CMake, SCons, Bazel, setuptools, software dependencies, ...

# Spoilers...

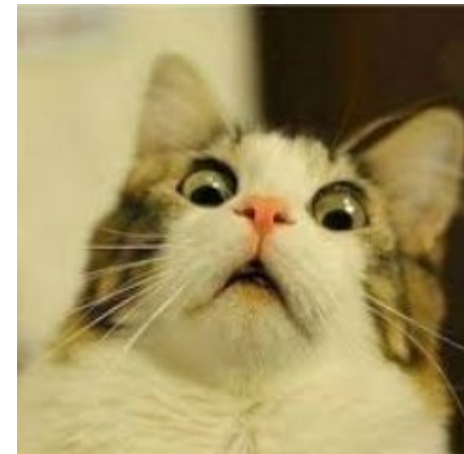
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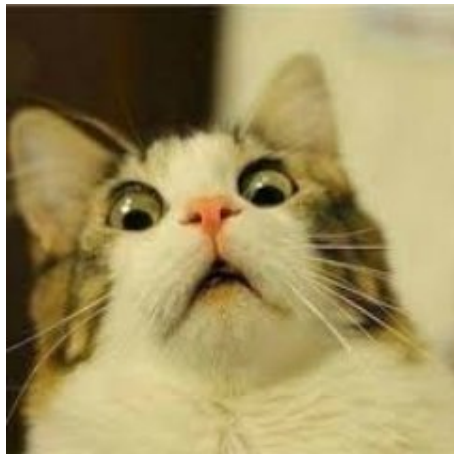


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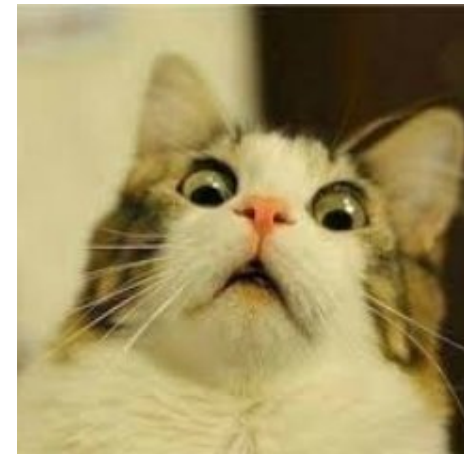


# Spoilers...

**Do containers *really* relieve the burden of installing scientific software?**



**No, not really.**  
*(not yet?)*



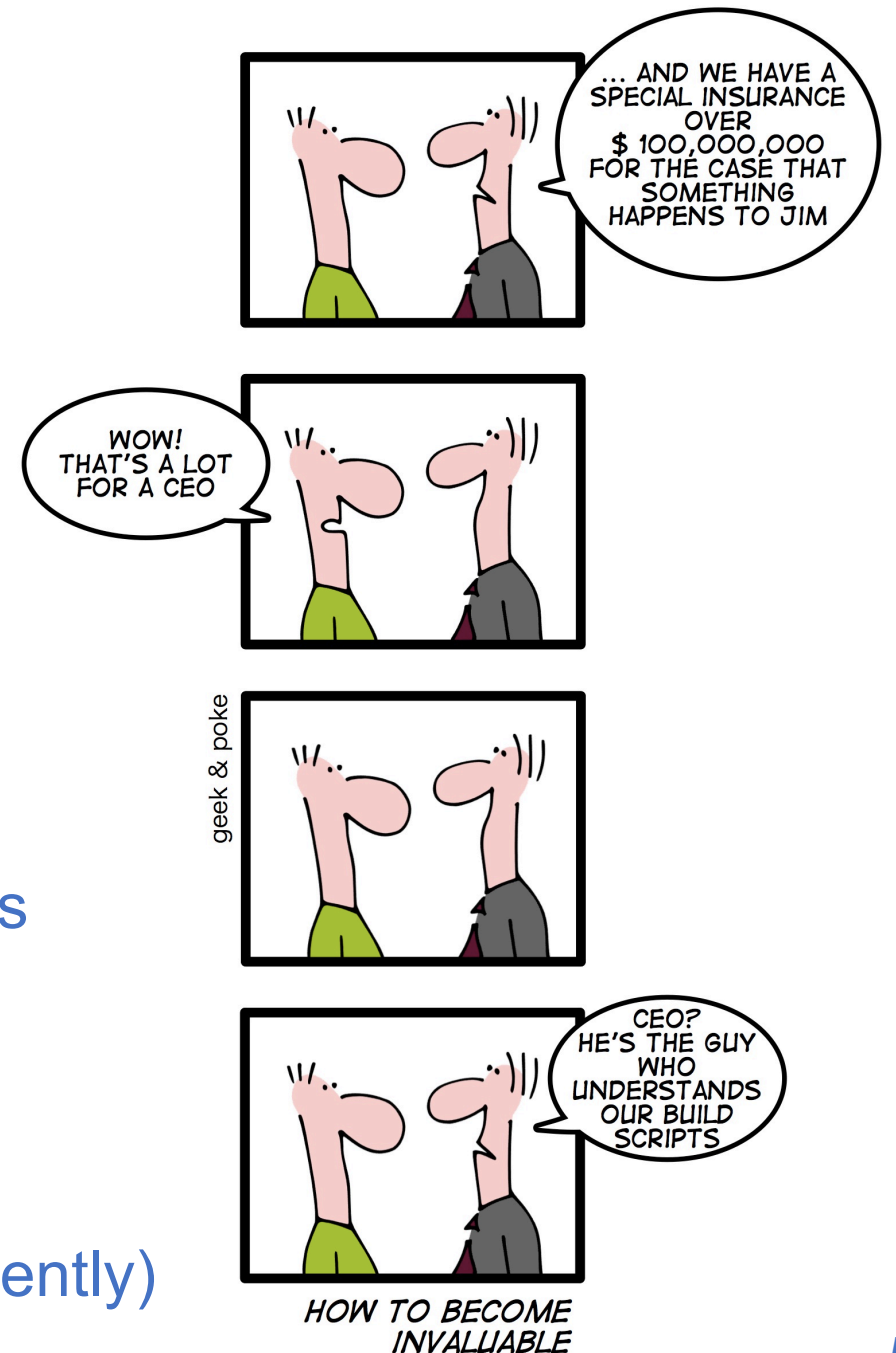
# Setting the stage

- The ubiquitous problem of getting scientific software installed
- A short look back at the "container revolution" in the HPC community
  - What happened, where are we now?
  - *Why* did it happen?
- Some concerns on using containers for scientific software on HPC systems
- A couple of ideas & possible solutions to improve current practice
- Q&A

# Getting scientific software installed

Installation of scientific software is a tremendous problem for HPC sites all around the world.

- ideally built from source (performance is key!)
- tedious, time-consuming, frustrating, sometimes simply not worth the (manual) effort...
- huge burden on researchers & HPC support teams
  - over 25% of support tickets at HPC-UGent, but consumes way more than 1/4th of support time...
- very little collaboration among HPC sites (until recently)



# Common issues with scientific software

**Researchers focus on the science behind the software they implement, and care little about software engineering, tools, build procedure, portability, ...**

**Scientists are (typically) not software developers or system administrators (nor should they be!)**

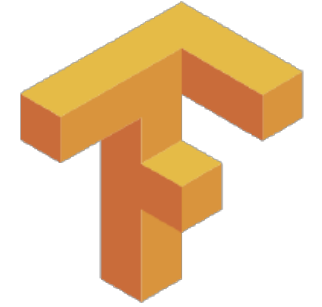
*“If we would know what we are doing, it would not be called ‘research’.”*

This results in:

- use of non-standard build systems (or broken ones)
- "creative" software versioning (or no versions at all)
- dependency hell on steroids
- interactive installation scripts
- hardcoded parameters (compilers, libraries, paths, ...)
- poor/outdated/missing/incorrect documentation



# Prime example: TensorFlow



popular open-source software for Deep Learning (<https://www.tensorflow.org>)

- auto-installs most dependencies, but not all...
- 'configure' script is a custom interactive script
  - silent configuration possible, but only if you *know* which `$TF_*` environment variables to set!
- uses **Bazel** (<http://bazel.io>) as build tool (there is was a contributed CMake alternative...)
  - *resets environment*, may result in unsetting important env. variables (e.g., `$PYTHONPATH`)
  - quite different from other build tools; e.g. to build TensorFlow:  

```
bazel build --config=opt //tensorflow/tools/pip_package:build_pip_package
```
  - `--config=opt`, `-c opt` and `-copt=...` all mean different things... 0\_o
- installation via 'pip install' of locally built Python wheel file (.whl)

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**No, that's not a typo...**

# How to make package managers cry



FOSDEM 2018

[https://archive.fosdem.org/2018/schedule/event/how\\_to\\_make\\_package\\_managers\\_cry](https://archive.fosdem.org/2018/schedule/event/how_to_make_package_managers_cry)

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- me **venting ~7 years of frustration** with getting scientific software installed
- TensorFlow & Bazel as main motivators
- **sarcastic tone for dramatic effect** (it worked!)
- lots of feedback (and ideas for an extended version of the talk), **clearly hit a nerve...**
- others discussing similar points:
  - *"Software disenchantment"*, blog post by Nikita Prokopov (Sept 2018)  
<http://tonsky.me/blog/disenchantment>
  - *"Don't package your libraries, write packageable libraries!"*, talk at CppCon 2018  
by Robert Schumacher (Microsoft) - <https://www.youtube.com/watch?v=sBP17HQAQjk>

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# What about existing software installation tools?

- package managers: *yum* (RPMs), *apt* (.deb), ...
- *Homebrew* (macOS), <http://brew.sh> ; *Linuxbrew*, <http://linuxbrew.sh>
- *Portage* (Gentoo), <http://wiki.gentoo.org/wiki/Project:Portage>
- *pkgsrc* (NetBSD & (a lot) more), <http://pkgsrc.org>

***None are well suited to scientific software and HPC systems in particular.***

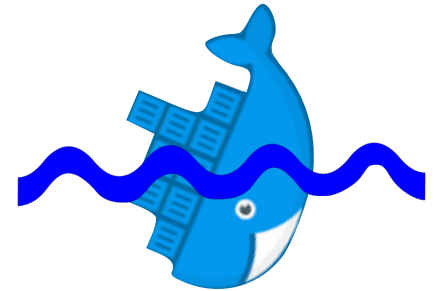
Common problems:

- usually poor support for old/multiple versions and/or to have builds side-by-side
- not flexible enough to deal with idiosyncrasies of scientific software
- little support for scientific software, non-GCC compilers, MPI, GPUs, ...

***Modern exceptions: conda, EasyBuild, Spack, Nix/Guix*** (different use cases)

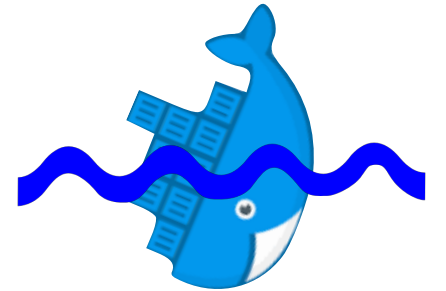
# The (HPC) container revolution

- **containers are an old idea that was revamped (again and again)**
  - chroot (1979), FreeBSD jails (2000), Solaris Containers (2004), LXC (2008), ...
- first became (really) popular in cloud environments, hyperscale
- hype took off with Docker in 2013
- buzz around **containers for HPC** started in 2015
- first Docker tried to convince the HPC community (& failed?)
- **Singularity** (LBNL, Sylabs) **started the revolution** in HPC (~2016)  
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# *Why* did the (HPC) container revolution start?

- **installing scientific software (correctly/efficiently) is becoming more complex**
  - dependency hell is getting worse (*fast*)
  - growing variety in target platforms (x86\_64, ARM, POWER, GPUs, ...)
  - specifically targeting host system is gaining importance for performance
- **scientists using/developing scientific software lack expertise in**
  - (sensible) software release management
  - picking the right tool for the job (tip: not a custom Perl script named 'configure')
  - diagnosing & fixing compilation/installation problems
- some popular programming languages & applications are not great examples...
- also, **people are lazy/impatient** (and StackOverflow doesn't always have an easy answer)

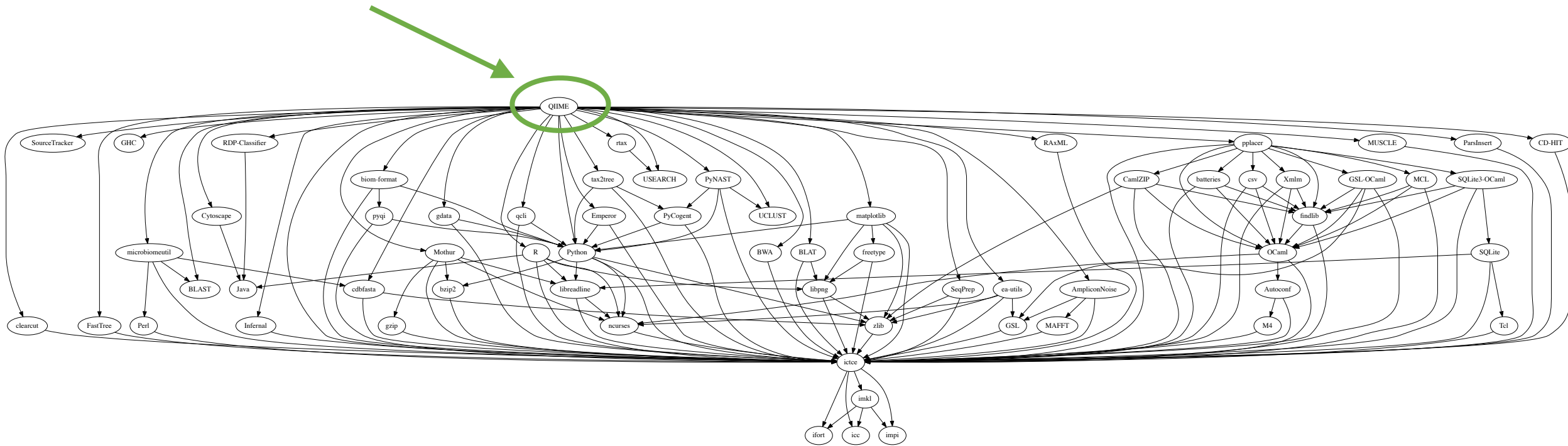
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# Dependency hell in scientific software

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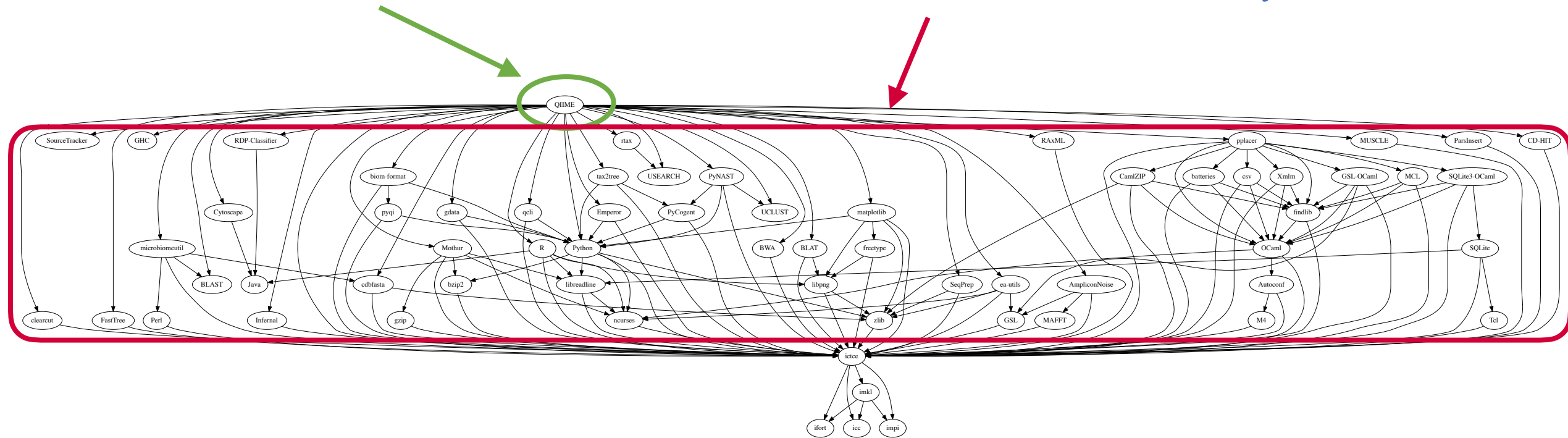


dependency graph for (old version) of QIIME (<http://qiime.org>)

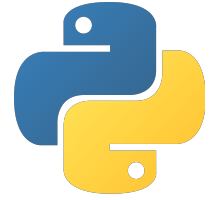
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most of the rest is a necessary evil

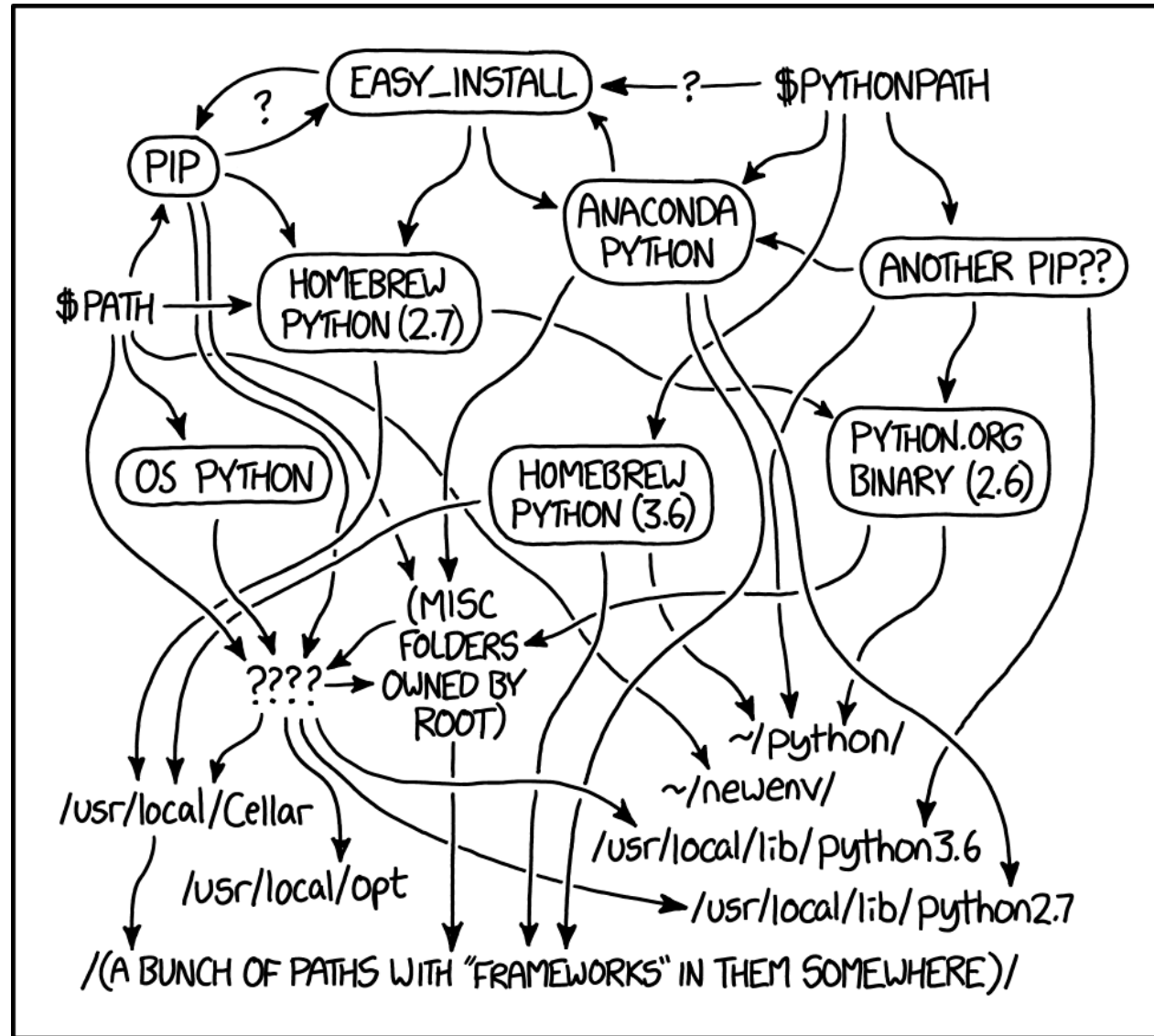


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the  
Python  
mess...

<https://xkcd.com/1987>



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THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

# Containers for HPC: buzzword bingo



(screenshot from Singularity website @ <https://www.sylabs.io/singularity>)

- simplicity
- "mobility of compute"
- "extreme mobility"
- Bring Your Own Environment (BYOE)
- "native" performance
- reproducibility
- easy integration with system resources & services
- security

So everything is rainbows & unicorns?



So everything is rainbows & unicorns?

**No, there's (still) some shit too...**



# Containers are a workaround, *not a solution...* (1/2)

- **container images are basically just a fancy set of binaries...**
  - they are most likely *not* built for the processor architecture of the host
  - ... which implies you may losing quite a bit of performance
  - containers built for x86\_64 will not work on ARM or POWER (and vice versa)
- **"native" performance really means "very little overhead"**
  - that's great, but it's also a *requirement* for success in HPC context...
  - there's a lot more to it in order to claim "native" performance (in my opinion)
- **integration with system resources & services is not a solved problem (yet)**
  - works great for some things (GPUs, resource managers like Slurm, ...)
  - still problematic for others (container/system MPI libraries need to be "in sync")




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# Containers are a workaround, *not a solution...* (2/2)

- **someone still needs to puzzle together the container image you need/want**
  - and hopefully in a way that is easy to tweak later...
  - ideally, the container is targeted to your host system in some way...
  - what if you want to update to more recent software versions?
- **we basically need a "containers on demand" service**
  - select the software (versions) you want
  - specify specs of your host system (processor, GPU, host libraries, ...)
  - click "Go!", wait for a while, download container image => happy computing!
- other unresolved issues/concerns: security, trust, transparency, ...
- **more work needed to make containers *truly* successful in HPC (beyond the hype)**

# Some ideas to improve current practice

- **raising awareness** that containers are not all pink fluffy unicorns and rainbows...
- more **standardisation**, less chaos
- documented (general) **best practices** for building container images
- **sharing *reproducible* container recipes** in an organised way
- **metadata** to capture specifics of target system for which containers were built  
+ accompanying tooling to query that metadata
- **leveraging established tools** like  *easybuild* for building containers images
- building container images as fancy sets of ***fat binaries*** (optimised for multiple targets)



<https://easybuilders.github.io/easybuild> - <https://easybuild.readthedocs.io>

- **framework for installing scientific software** (*built from source if possible*)
- strong focus on Linux & HPC systems (and hence also performance)
- **builds specifically for host architecture by default**
- implemented in Python 2, lead development by HPC-UGent
- available under GPLv2 license via PyPI, GitHub
- supports: different compilers & MPI libraries, > 1,600 different software packages
- **(experimental) support to generate (recipes for) Docker/Singularity containers**
- active & helpful worldwide community

# Supported software



[http://easybuild.readthedocs.io/en/latest/version-specific/Supported\\_software.html](http://easybuild.readthedocs.io/en/latest/version-specific/Supported_software.html)

- latest EasyBuild (v3.8.1) supports installing **over 1,643 different software packages**
  - preferably from source
  - including CP2K, NAMD, NWChem, OpenFOAM, TensorFlow, WRF, ...
  - also a lot of bioinformatics software is supported out of the box
  - + ~1,000 extensions: Python packages, R libraries, Perl modules, X11 libraries, ...
- diverse toolchain support:
  - compilers: GCC, Intel, Clang, PGI, IBM XL, Cray, CUDA
  - MPI libraries: OpenMPI, Intel MPI, MPICH, MPICH2, MVAPICH2, Cray MPI, ...
  - BLAS/LAPACK libraries: Intel MKL, OpenBLAS, ScaLAPACK, BLIS, Cray LibSci, ...

# Example output of using 'eb' command



```
$ eb TensorFlow-1.10.1-foss-2018b-Python-3.6.6.eb
== temporary log file in case of crash /tmp/eb-GyvPHx/easybuild-U1TkEI.log
== processing EasyBuild easyconfig TensorFlow-1.10.1-foss-2018b-Python-3.6.6.eb
== building and installing TensorFlow/1.10.1-foss-2018b-Python-3.6.6...
== fetching files...
== creating build dir, resetting environment...
== unpacking...
== patching...
== preparing...
== configuring...
== building...
== testing...
== installing...
== taking care of extensions...
== postprocessing...
== sanity checking...
== cleaning up...
== creating module...
== permissions...
== packaging...
== COMPLETED: Installation ended successfully
== Results of the build can be found in the log file /opt/easybuild/software/Tensor...
== Build succeeded for 1 out of 1
== Temporary log file(s) /tmp/eb-GyvPHx/easybuild-U1TkEI.log* have been removed.
== Temporary directory /tmp/eb-GyvPHx has been removed.
```

# What easybuild is *not*

- EasyBuild is not YABT (Yet Another Build Tool)

it does *not* replace build tools like `cmake` or `make`; it wraps around them

- it is not a replacement for your favourite package manager (`yum`, `apt-get`, ...)

it leverages some tools & libraries provided by the OS (`glibc`, `OpenSSL`, `libibverbs`, ...)

- it is not a magic solution to all your (software compilation/installation) problems...

you will still run into compiler errors (if nobody else has already taken care of it)

# What easybuild is

- a **uniform interface** that wraps around software installation procedures
- a huge **time-saver**, by automating tedious/boring/repetitive tasks
- a way to provide a **consistent software stack** to your users
- an **expert system** for software installation on HPC systems
- a **platform for collaboration** with HPC sites worldwide
- a way to **empower *users* to self-manage their software stack** on HPC systems
- a tool that can be leveraged for **building *optimised* container images**



# easybuild & containers: current status

- EasyBuild can generate a container recipes/images for a specific set of software
- the resulting recipe in turn leverages EasyBuild to install the requested software
- **fully automated building of optimised container images**
- both Docker & Singularity are supported
- current support is still experimental (needs more testing, has some rough edges)
- can be a starting point to tackle some of the raised concerns...
- for more information, see <https://easybuild.readthedocs.io/en/latest/Containers.html>

# Conclusions

- **Do containers really relieve the burden of installing scientific software?**
  - No, not really. Not yet.
- Containers for HPC systems are "booming business"
- ... but they are not all unicorns & rainbows!
- Open problems:
  - (truly) native performance by targeting host system better
  - sharing of reproducible/maintainable container recipes
  - leveraging established tools to build container images (from source)
  - tracking of metadata for transparency w.r.t. target system(s)

Do containers *really* relieve the burden of installing scientific software?

# Questions?

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(remote talk)

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