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Containers in HPC

Bob Dröge

Team HPC

Center for Information Technology

university of groningen

HPC @ RUG: Peregrine

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Peregrine nodes

	CPU	Memory	Internal disk	Network	Accelerator
159 Regular nodes	2x Intel Xeon E5 2680v3: 24 cores @ 2.5 GHz	128 GB	1 TB	56 Gbps Infiniband + 10 Gbps ethernet	-
48 Regular nodes extra	2x Intel Xeon E5 2680v4: 28 cores @ 2.4 GHz	128 GB	1 TB	56 Gbps Infiniband + 10 Gbps ethernet	
6 GPU nodes	2x Intel Xeon E5 2680v3: 24 cores @ 2.5 GHz	128 GB	1 TB	56 Gbps Infiniband, 10 Gbps ethernet	2x Nvidia K40
7 Big memory nodes	4x Intel Xeon E7 4860v2: 48 cores @ 2.6 GHz	1024 or 2048 GB	1 TB	56 Gbps Infiniband, 10 Gbps ethernet	-

5640 CPU cores,
34560 CUDA cores

Shared storage: >600 TB

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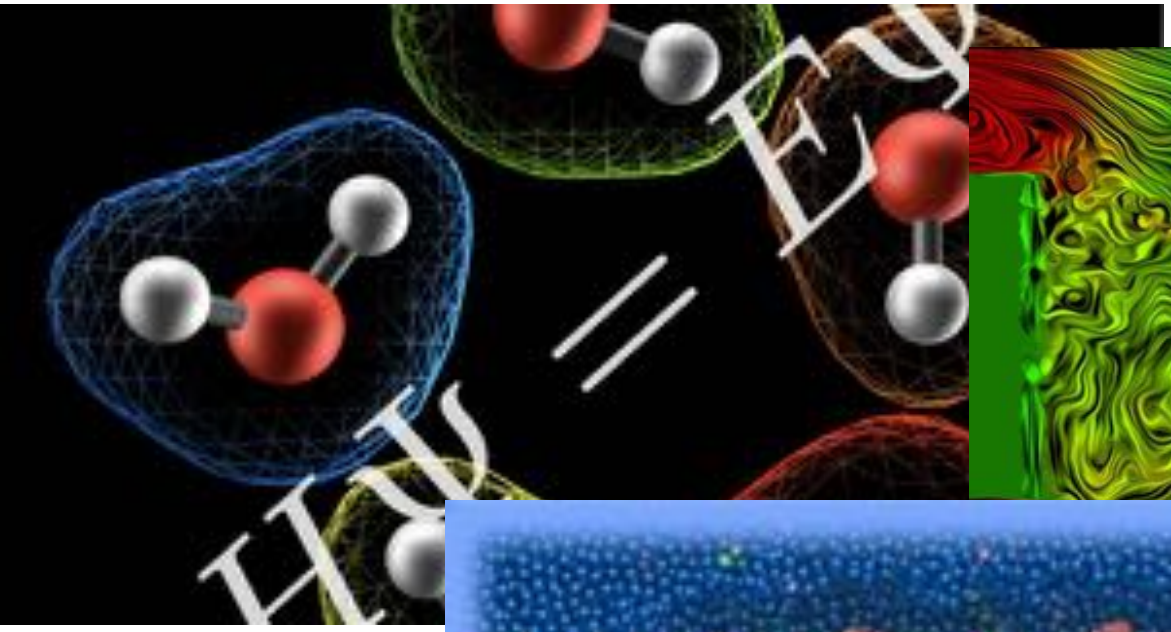
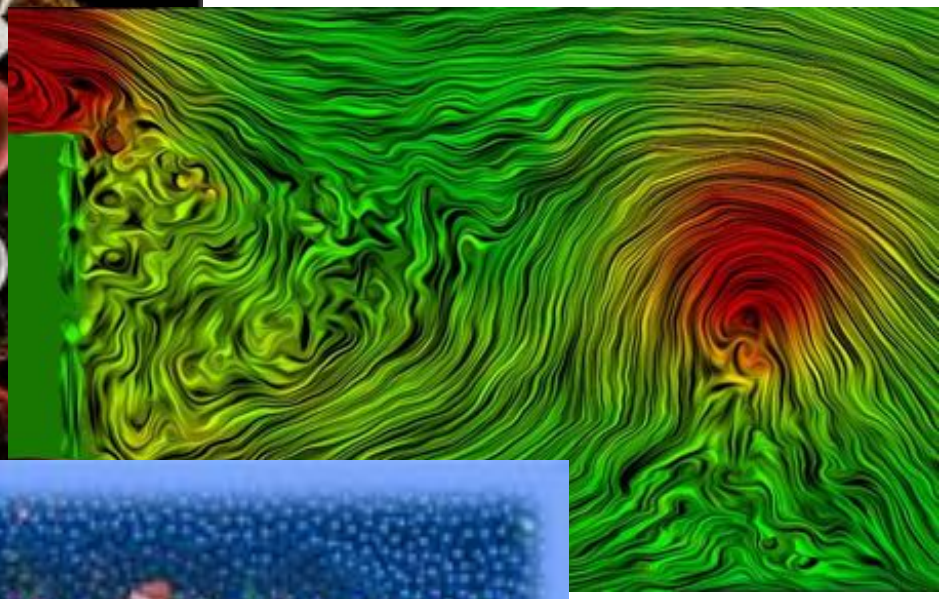
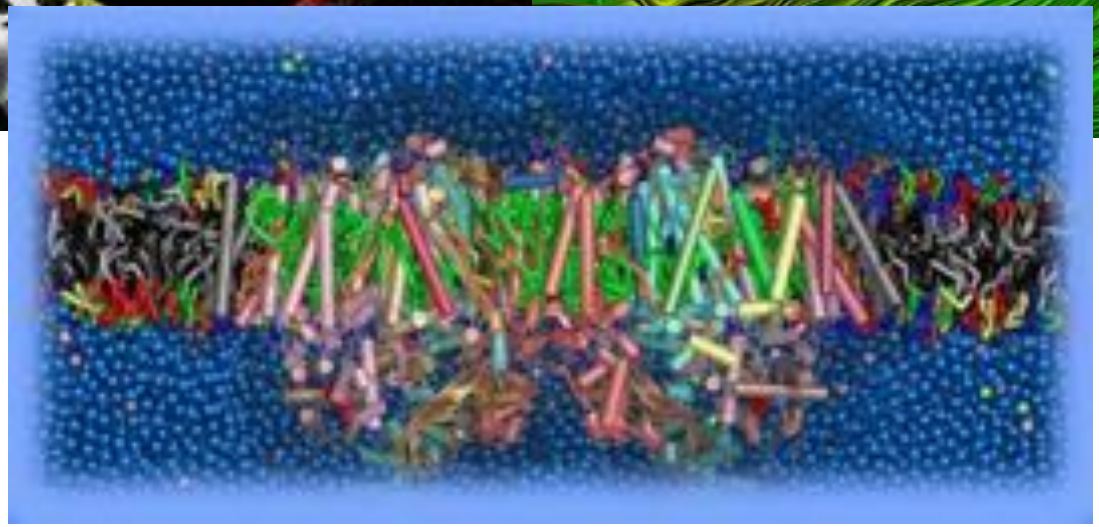
Simulation



Theoretical Chemistry
- Faraji



Computational Fluid Dynamics
- Veldman



Molecular Dynamics - Marrink

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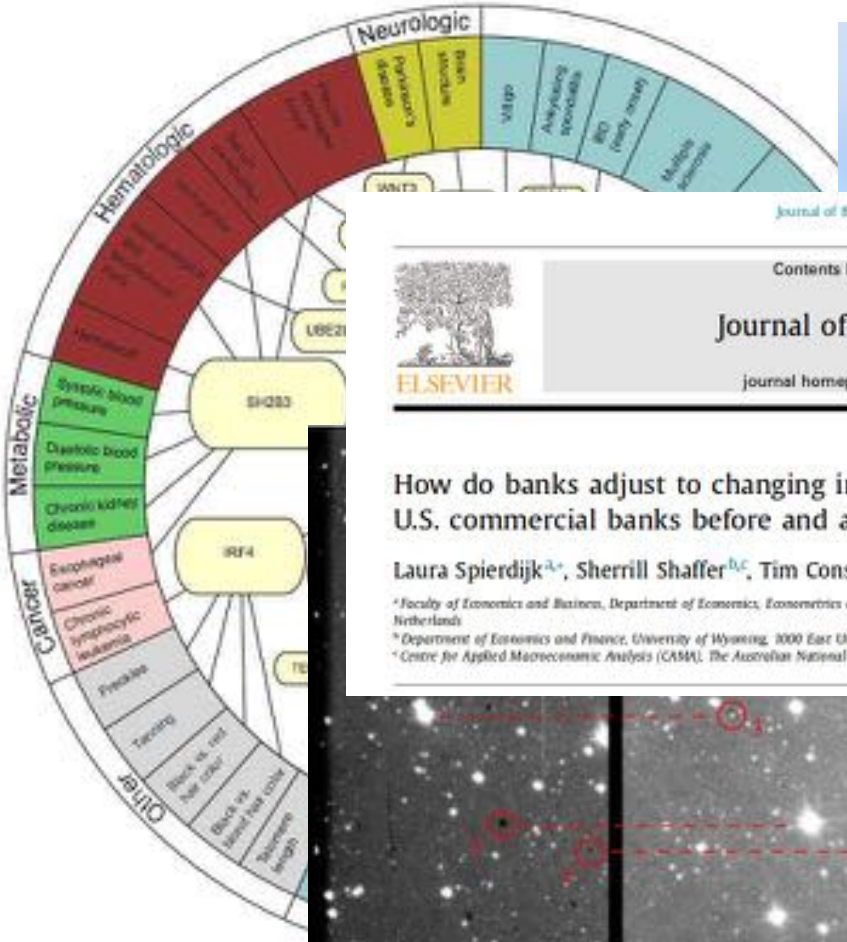
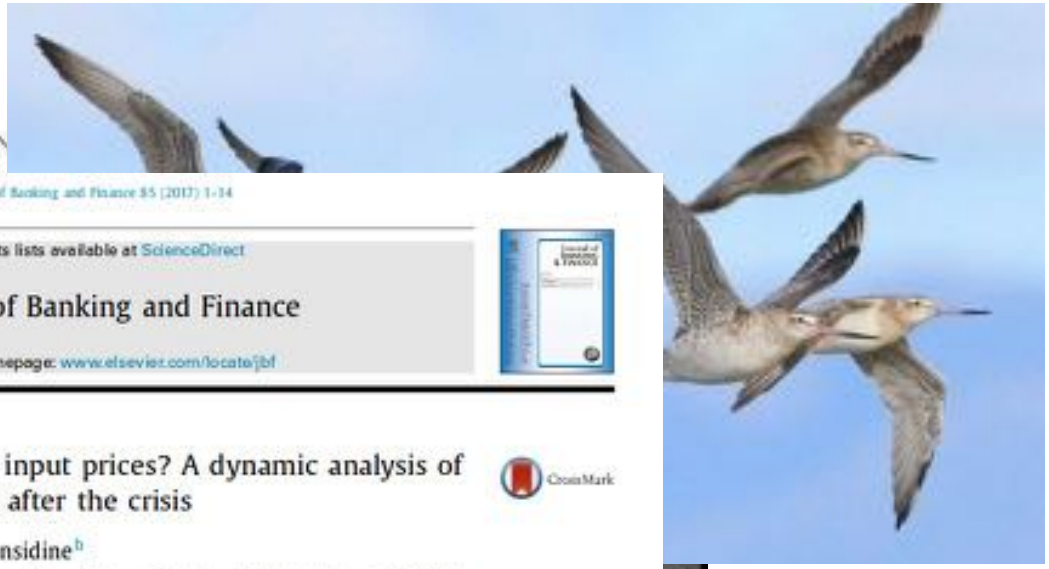
Data analysis



Genetics
- Wijmenga



Journal of Banking and Finance 85 (2017) 1–14

Contents lists available at ScienceDirect

Journal of Banking and Finance

journal homepage: www.elsevier.com/locate/jbf

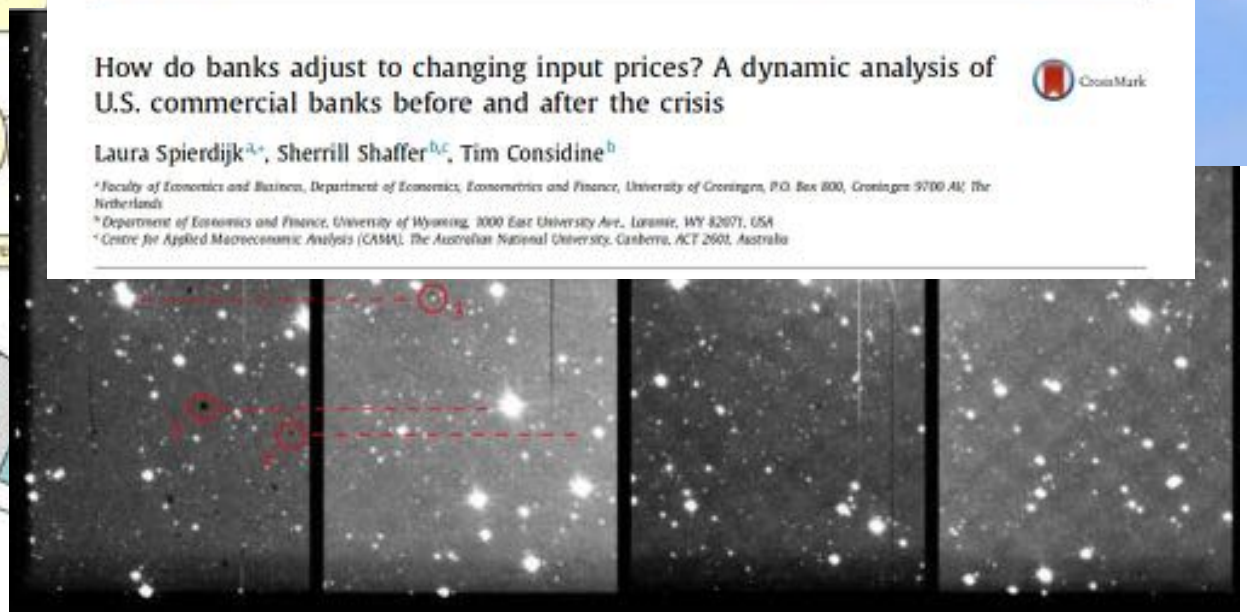
ELSEVIER

How do banks adjust to changing input prices? A dynamic analysis of U.S. commercial banks before and after the crisis

Laura Spierdijk[a,*], Sherrill Shaffer[b,c], Tim Considine[b]

[a] Faculty of Economics and Business, Department of Economics, Econometrics and Finance, University of Groningen, P.O. Box 800, Groningen 9700 AV, The Netherlands
[b] Department of Economics and Finance, University of Wyoming, 3000 East University Ave., Laramie, WY 82071, USA
[c] Centre for Applied Macroeconomic Analysis (CAMA), The Australian National University, Canberra, ACT 2601, Australia

Ecology
- Piersma



Astronomy - Valentijn

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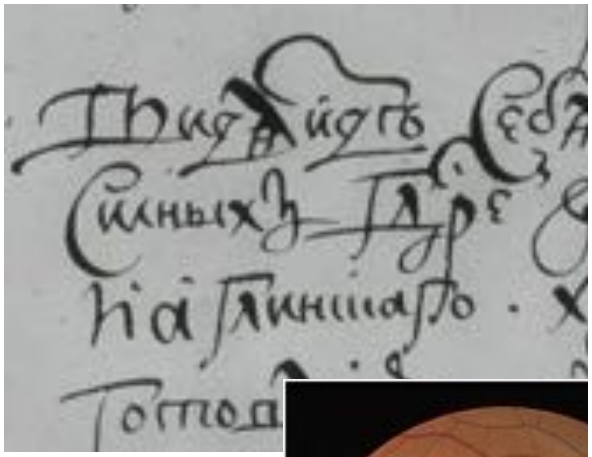
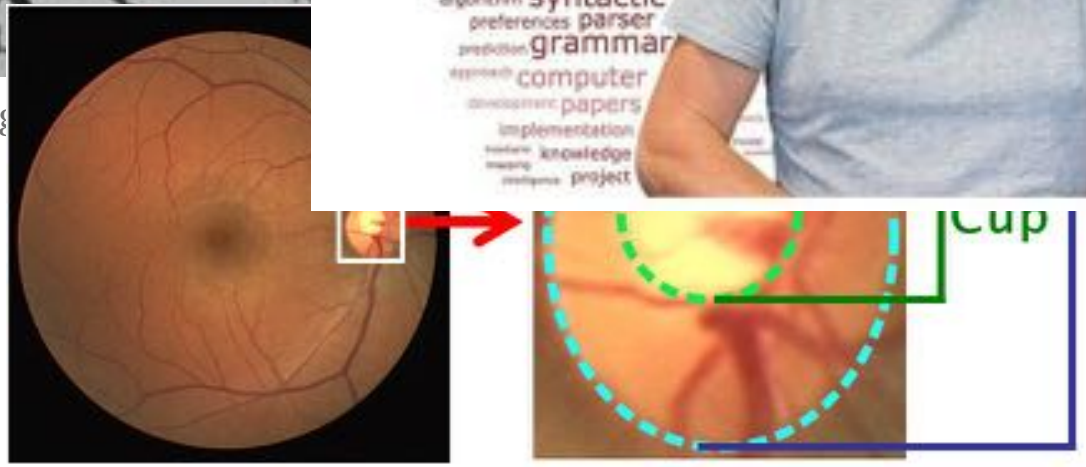
Machine learning



Artificial Intelli
- Schomaker

Natural language processing
- Van Noord



Ophthalmology / Intelligent Systems - Jansonius, Petkov

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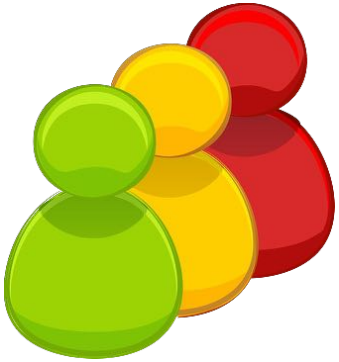
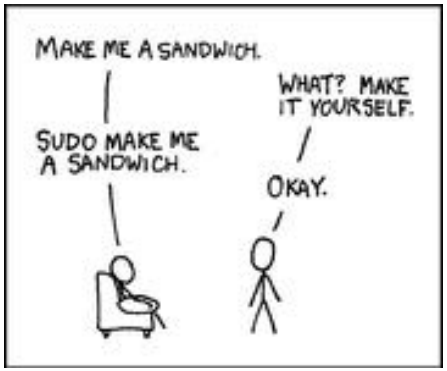
Peregrine environment



~750 users

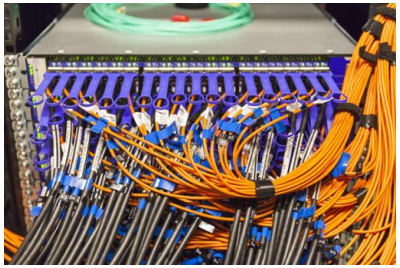
```
#!/bin/bash
#SBATCH --job-name=R_job
#SBATCH --time=00:01:00
#SBATCH --cpus-per-task=1
#SBATCH --mem=1000
#SBATCH --partition=short

module load R/3.3.1-foss-2016a
module list
Rscript myscript.r
```

Batch scheduler: job scripts



No special privileges (e.g. sudo)

Special hardware:



Lustre®

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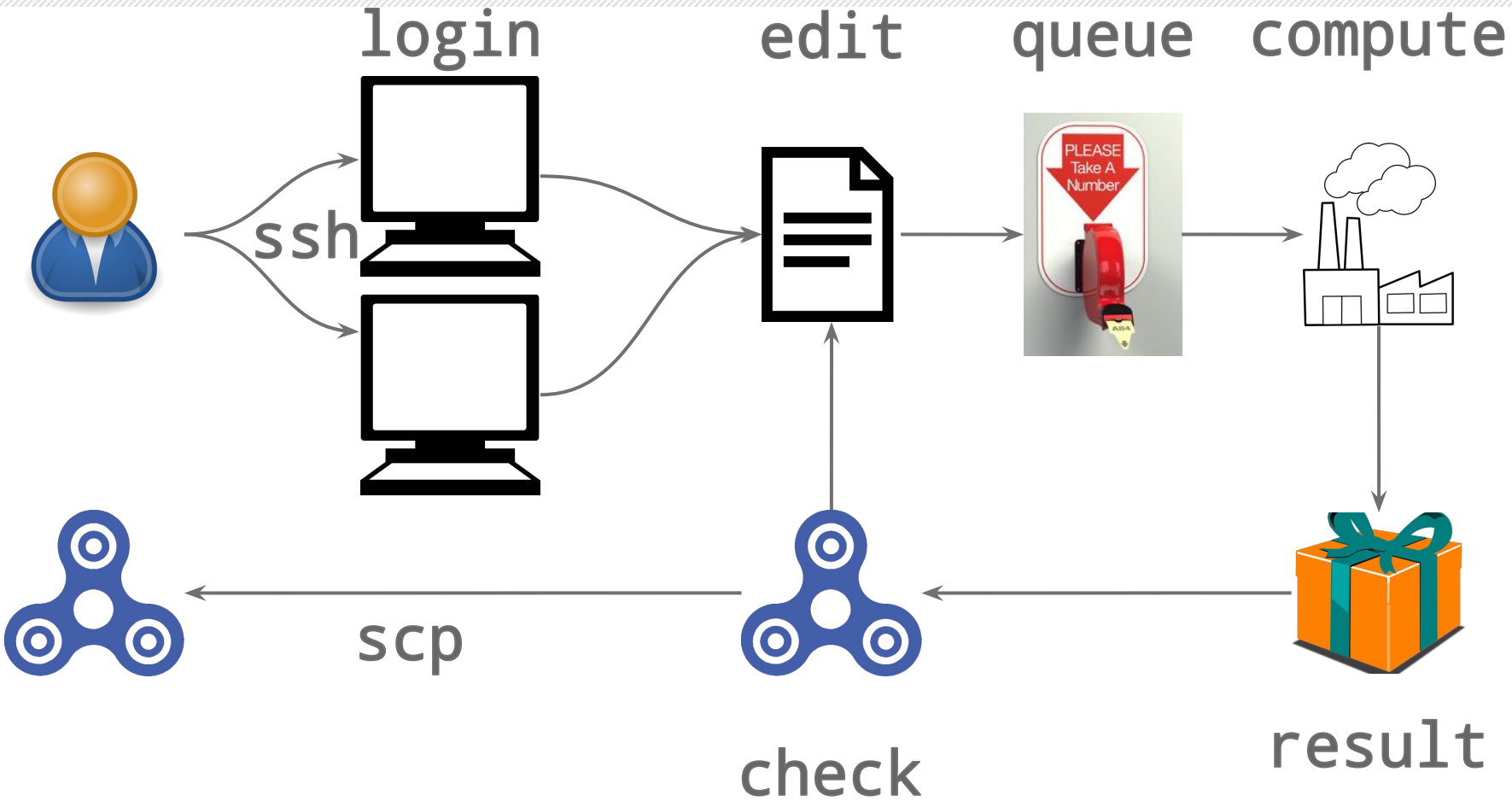
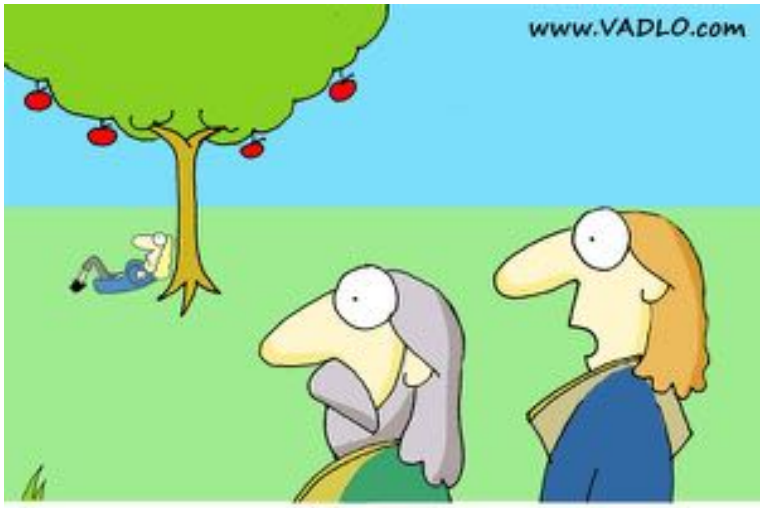
Typical workflow



Requirements scientific software

- Reproducibility
- Mobility
- High performance
  - Use the special hardware
  - Scalable
- Easy to install and (re)use in different environments
  - Talk by Kenneth Hoste @ FOSDEM 2018: https://fosdem.org/2018/schedule/event/how_to_make_package_managers_cry/



"Reviewers have asked him to reproduce the experiment."

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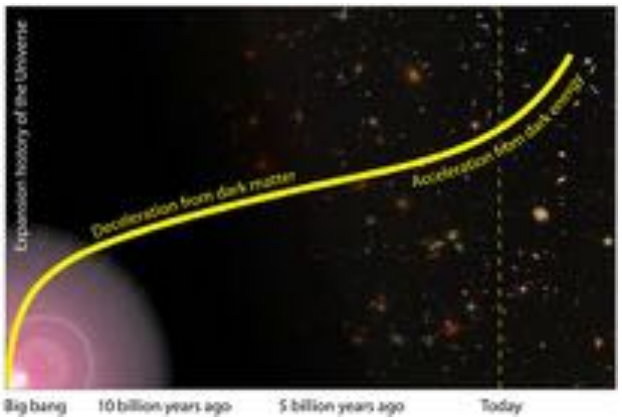
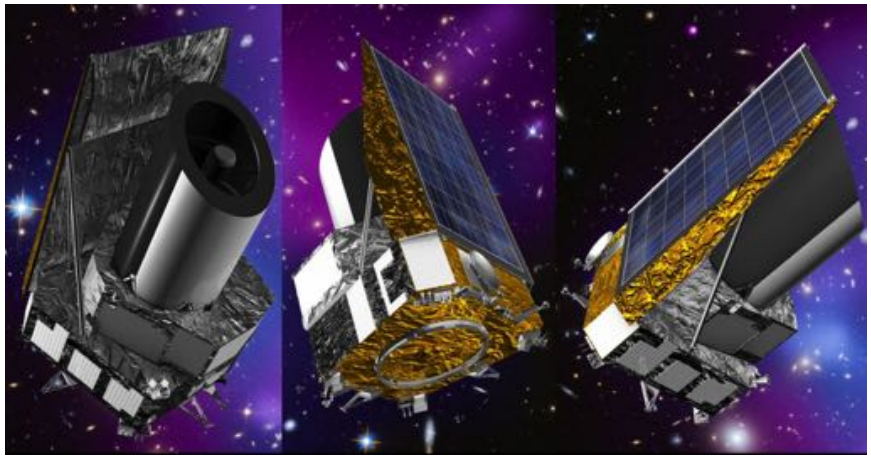
Extreme example: Euclid

- ESA space mission to map the Dark Universe
  - Satellite will be launched in 2021
- Why is the expansion of the universe accelerating?
- Understand the source of it: dark energy





euclid consortium

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Euclid: data processing

- ~100GB of compressed detector data per day
- Data gets distributed over 9 Science Data Centers
- Different resources across SDCs:
  - Hardware
  - Operating system
  - Scheduling systems
  - Storage technology
  - Shared / dedicated

- All pipelines must be able to run at all SDCs (!)
  - How to do this?

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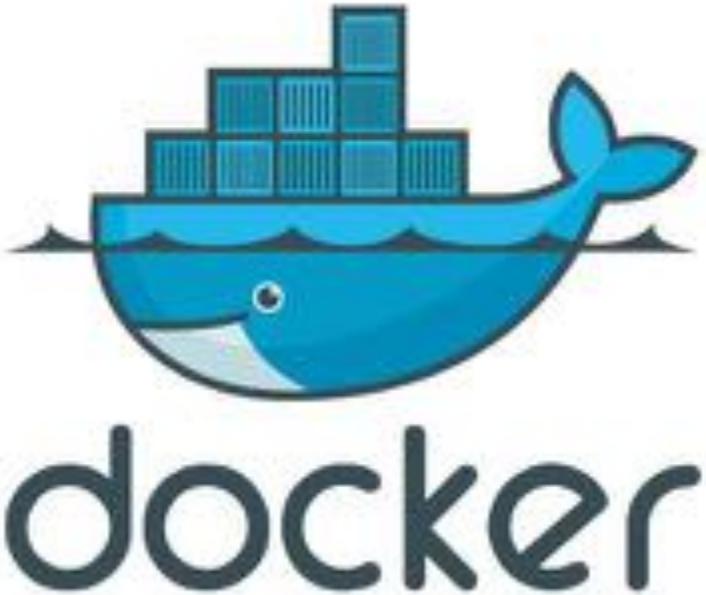
Docker!



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Docker?

- Almost does it all, but…

- Designed for network service virtualization
- Requires a daemon on all the compute nodes
- Only root can start/stop containers
  - Security concerns for shared environments
- No integration with scheduler

- Not really suitable for HPC
  (yet? See https://www.youtube.com/watch?v=JokQgRoCW54)

HPC containers: additional wishes

- No daemon
- Secure
- Scalable
- Works with:
  - scheduling systems
  - special hardware
  - MPI
  - shared environments
  - older kernels
- Run Docker images

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Singularity

Reproducibility

Mobility

Freedom

Security

"A container for HPC"

http://singularity.lbl.gov/

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Singularity

- Easy to install and configure
- Easy to run/use:
  - no daemons
  - no root
  - works with scheduling systems and existing resource contexts (e.g. cgroups)
- **User outside container == user inside container**
- Access to host resources
- MPI support

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Singularity: container formats

- SquashFS
- ext3 image
- Unix directory
- (Compressed) tarballs

- Supported URIs:
  - **docker://**
  - shub://

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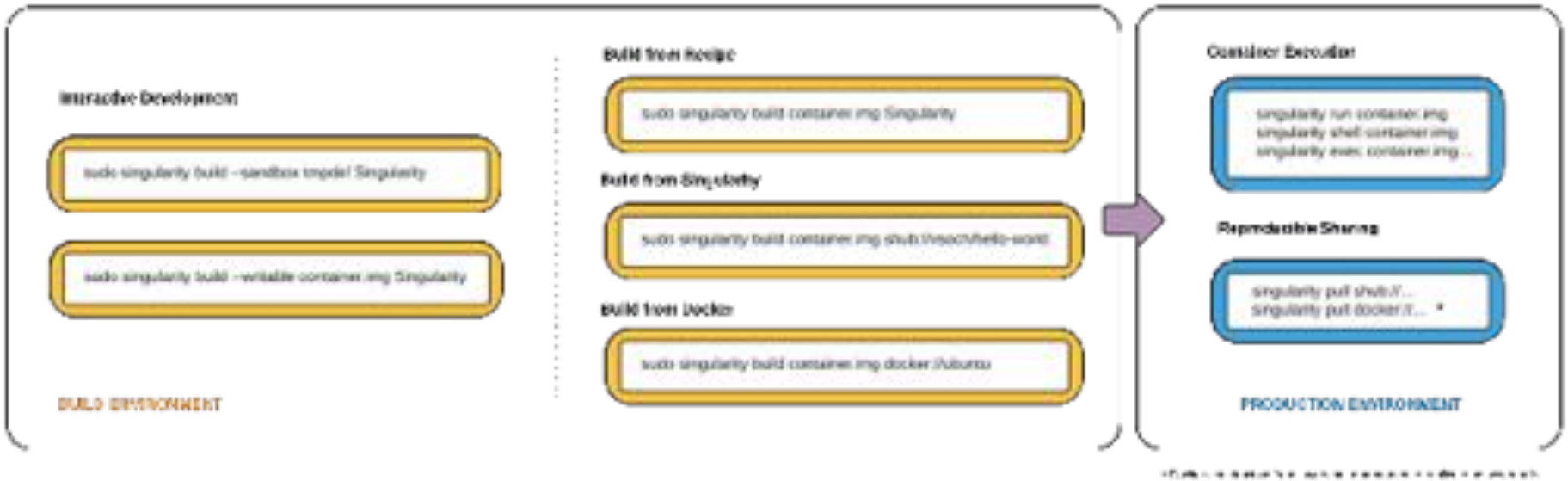
Singularity workflow



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Singularity hub

https://singularity-hub.org

Build, view, share, deploy, visualize

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Singularity demo

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Other HPC container solutions

- Many other solutions out there
- Most of them have some Docker connection

- Shifter https://www.nersc.gov/research-and-development/user-defined-images/
- CharlieCloud https://hpc.github.io/charliecloud/
- udocker https://github.com/indigo-dc/udocker

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udocker

- Simple tool written in Python
- Mimics subset of Docker functionalities
- No root privileges required to install or run it
- No Docker required
- Docker-like command-line interface
- Works with GPU and MPI
- Runs on older and newer operating systems
- Root user emulation using PRoot

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udocker demo

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Still some drawbacks...

- Size of (HPC) containers
- Dependency on host kernel
  - and partly on its supported container software
- Portability vs performance

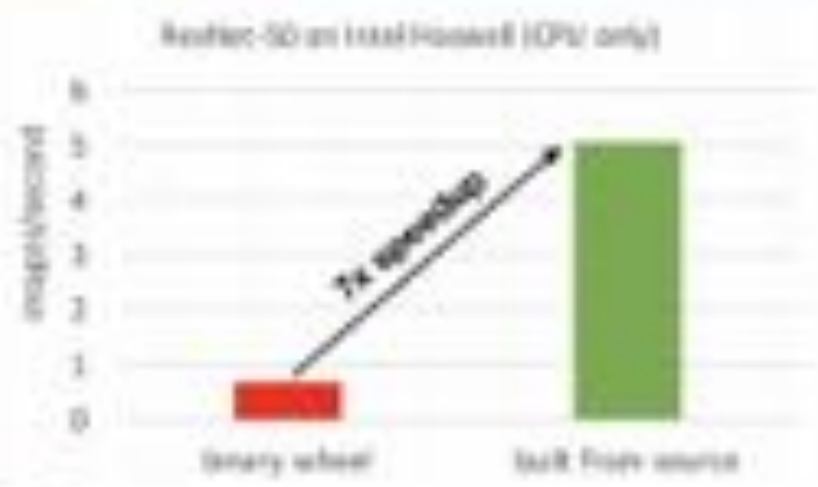

Image source: The State of Containers in Scientific Computing
https://fosdem.org/2018/schedule/event/containers_scientific/attachments/slides/2408/export/events/attachments/containers_scientific/slides/2408/The_State_of_Containers_in_Scientific_Computing.pdf

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Questions