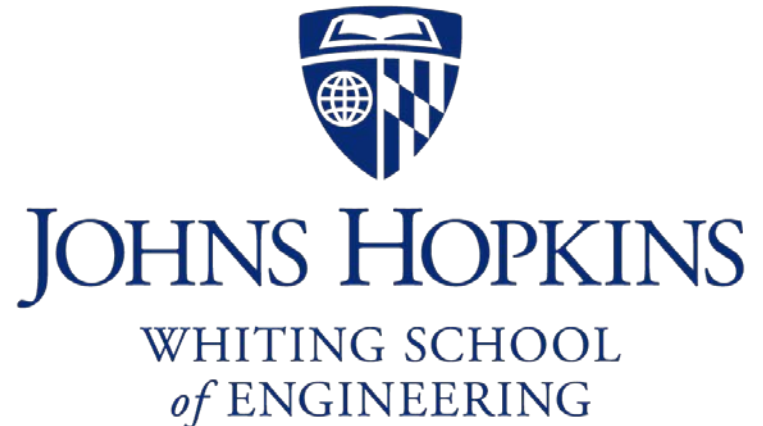


R.O.S.I.E.

The Rosetta Online Server that Includes Everyone

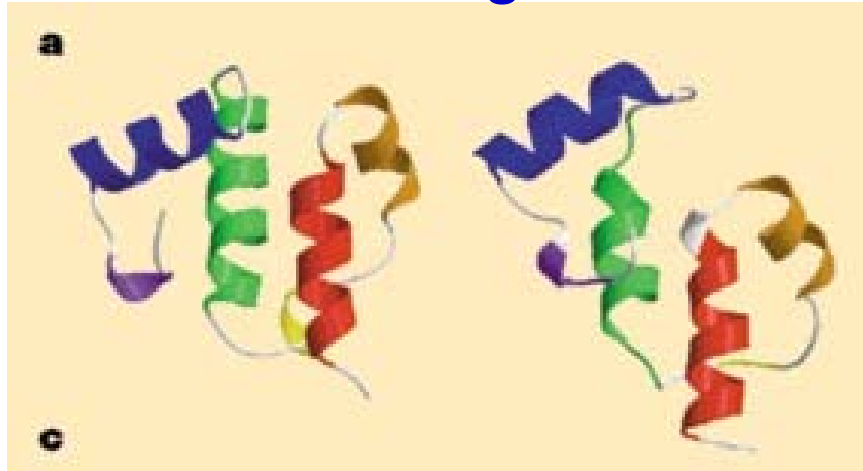
Jeffrey J. Gray, Rhiju Das, Sergey Lyskov

Johns Hopkins University, Stanford University, and the
Rosetta Commons



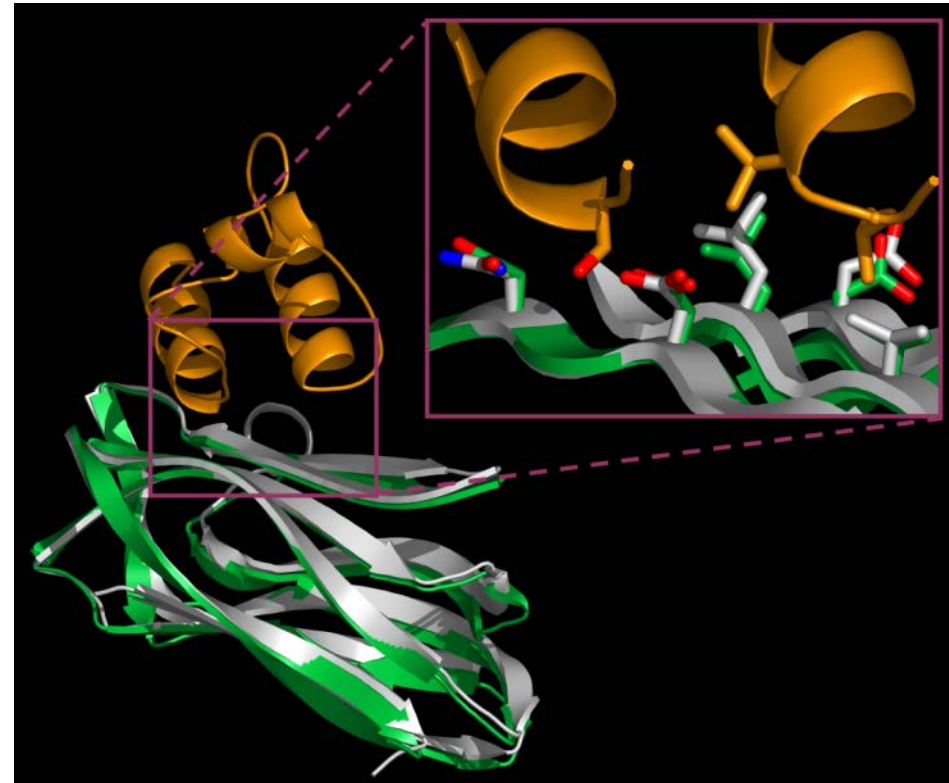
Protein Structure Prediction Milestones

Ab Initio Folding



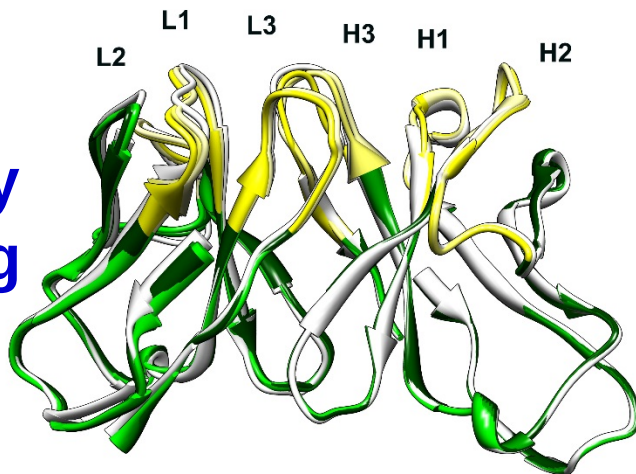
CASP3 / Baker *Nature* 2000

Protein-Protein Docking



Dockerin+Cohesin, CAPRI T12
Daily *et al.*
Proteins 2005

Antibody Modeling



AMA-II Ab09:L Sub-Ångström CDR H3 loop
Weitzner, Kuroda *et al.*
Proteins 2014

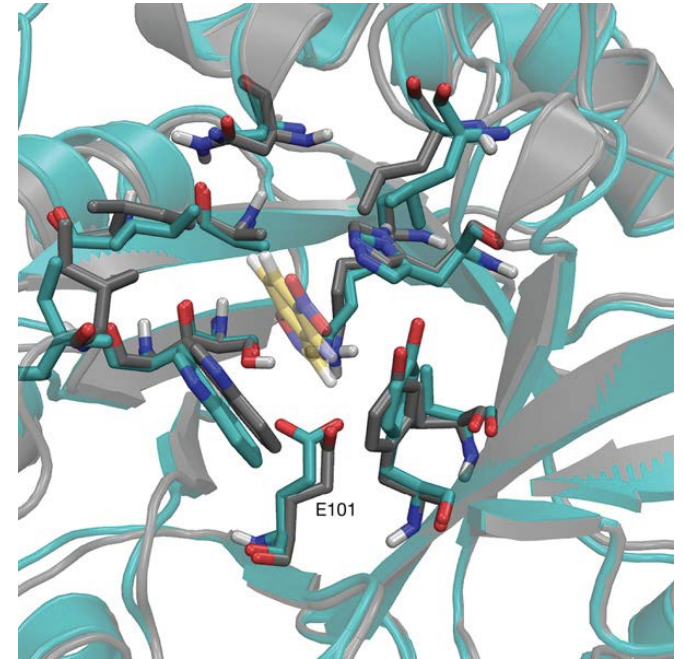
Protein Design Milestones

Designed New Fold

Top7
Kuhlman *et al.*
Science 2003



De Novo Enzyme

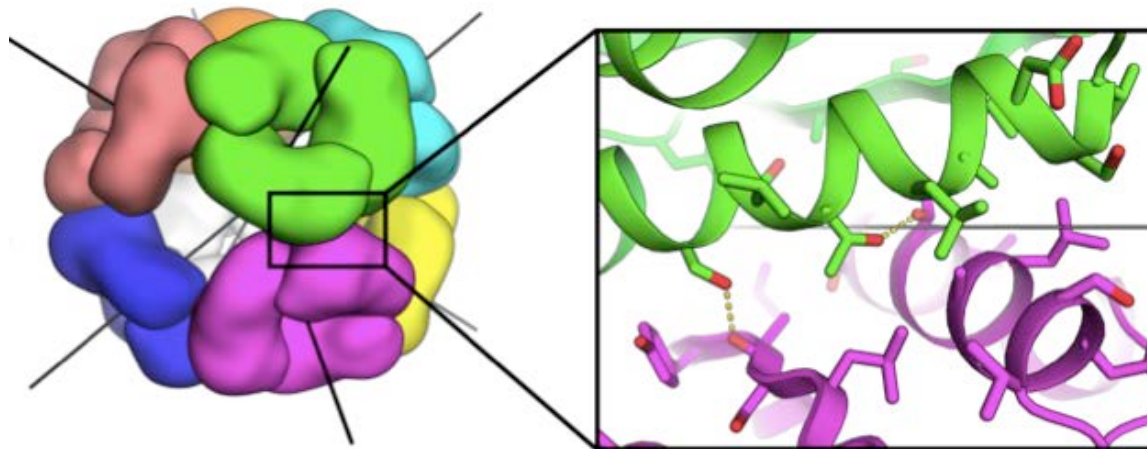
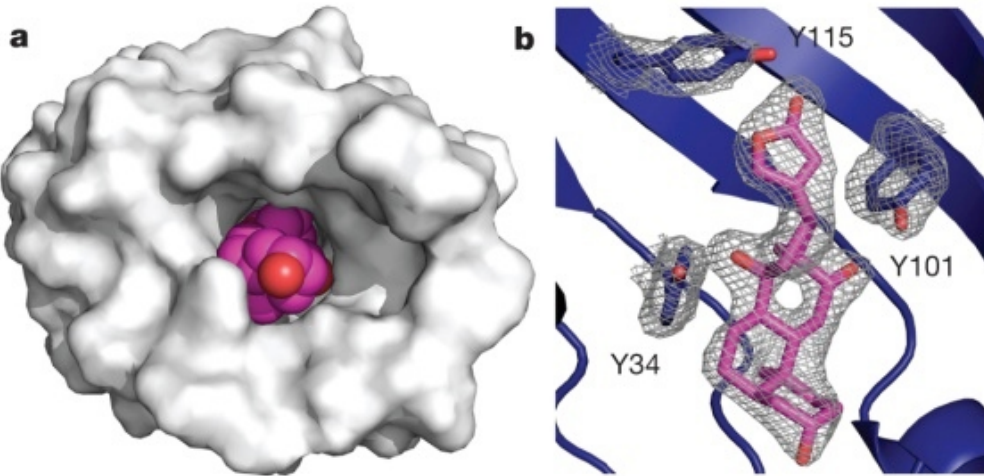


Kemp-elimination
Rothlisberger *et al.*
Nature 2008

Protein Design Milestones

$\mu\text{M} \rightarrow \text{pM}$ Small-Molecule Binders

Tinberg *et al.*, *Nature* 2013



Protein Cages

King *et al.*
Science 2012

40 Institutions/Labs
266 developers on GitHub
Annual conference
Thousands of licensees



Rosetta
Commons



TACC local network

- Extract job data to job image
- Generate key code for message ID
- Package scripts, config files, input
- r sync via ssh to stampede
- Start screen session via ssh

Stampede
HPC Cluster
(SLURM)

Gray Lab local network

TurboGears
Web server
rosie.graylab.jhu.edu

PostgreSQL
database

Back-end
Daemon
(Remote HPC)

Back-end
Daemon
(Condor)

GrayLab
HPC Cluster
(Condor)

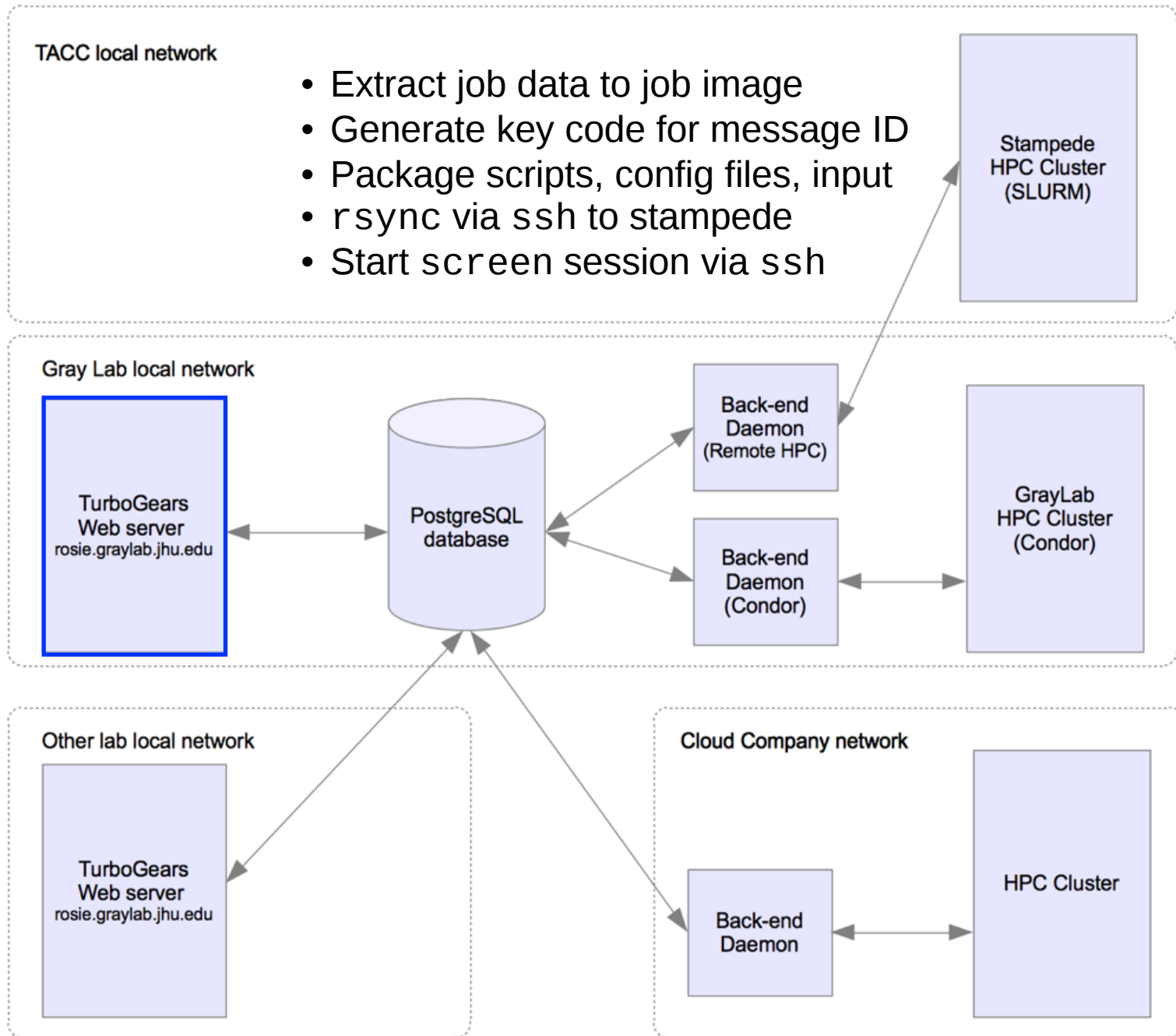
Other lab local network

TurboGears
Web server
rosie.graylab.jhu.edu

Cloud Company network

Back-end
Daemon

HPC Cluster



TACC local network

- Start job
- Sleep
- Check status and report to dB
- When finished, send output files

Stampede
HPC Cluster
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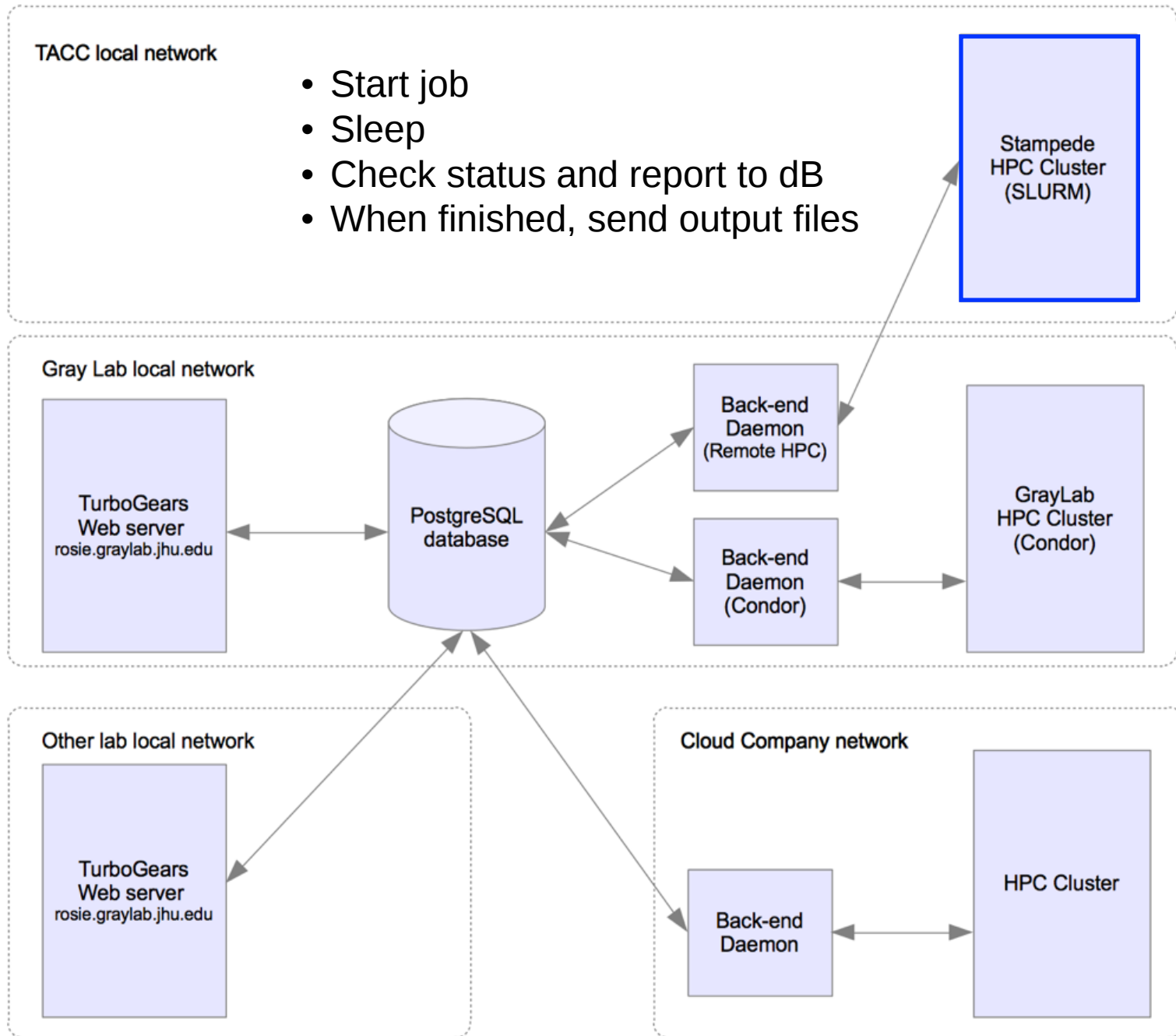
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TACC local network

- Sleep
- Check status message
- Extract job results → dB

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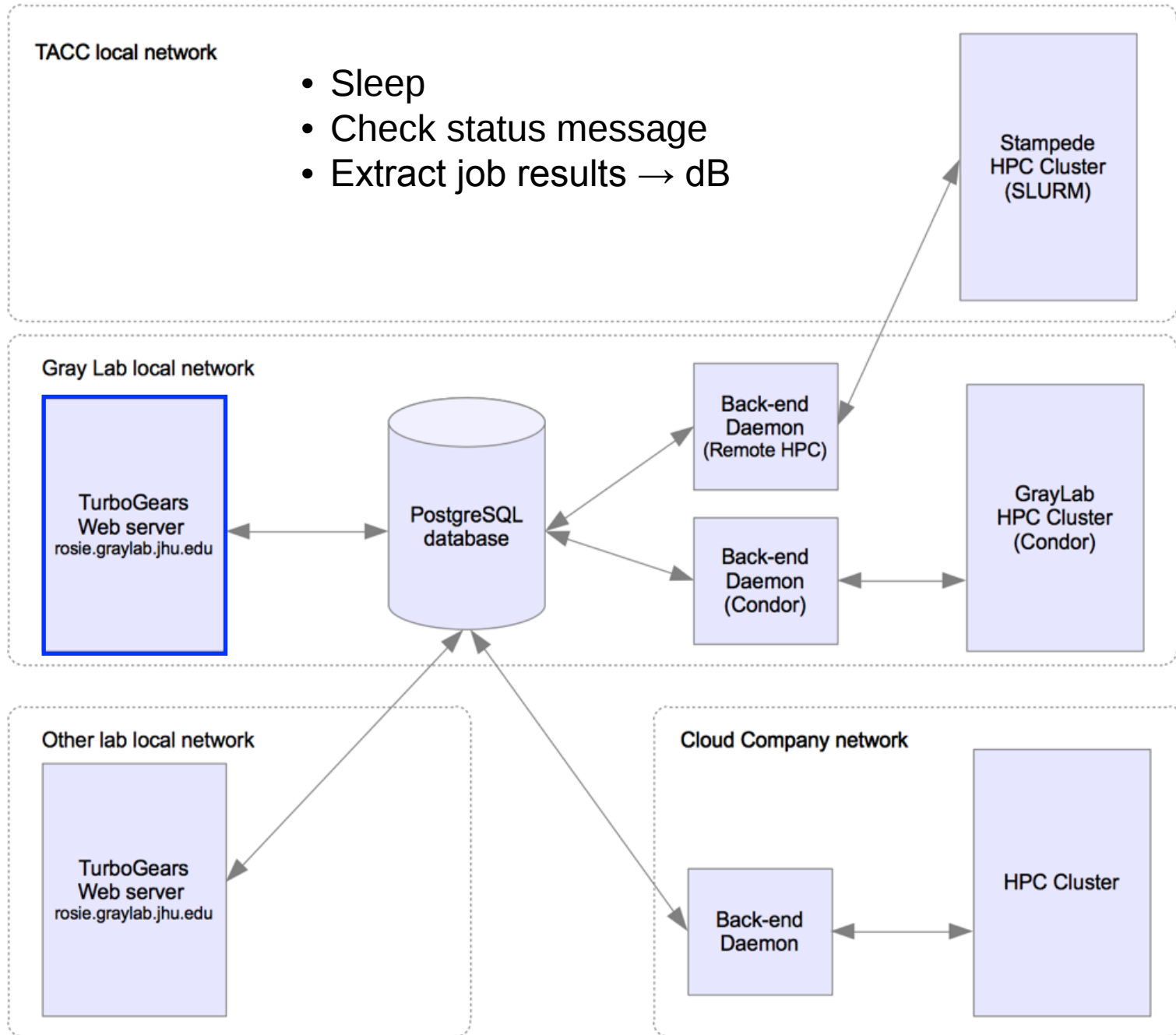
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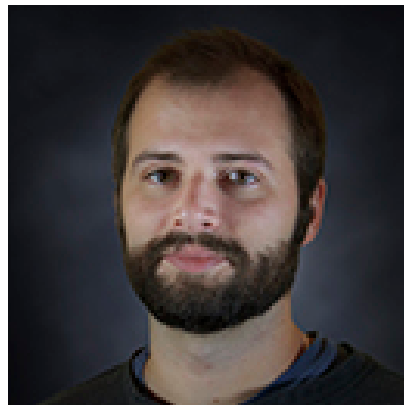
ECSS / Campus Champion

- Assisted in ROSIE deployment
- Installed Rosetta C++ executables and PyRosetta Python libraries in stampede module
- In progress: parallelizing code for the Intel PHI co-processors

Frank Willmore



Todd Evans



James McClure



(Show web pages)