Progress of the SES-HPC Project

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Introduction

- Less progress than intended due to new cluster
  - Documents are a LOT of work
  - But also chance to do some things right from beginning

- Multiple construction sites
  - Matlab best practice
  - Cluster website
  - Publicity
  - Miscellaneous

- New colleague: started in-person consulting

Outline

- Introduction

- Construction Sites:
  - **Matlab Best Practice**
  - Cluster Website
  - Publicity
  - Miscellaneous

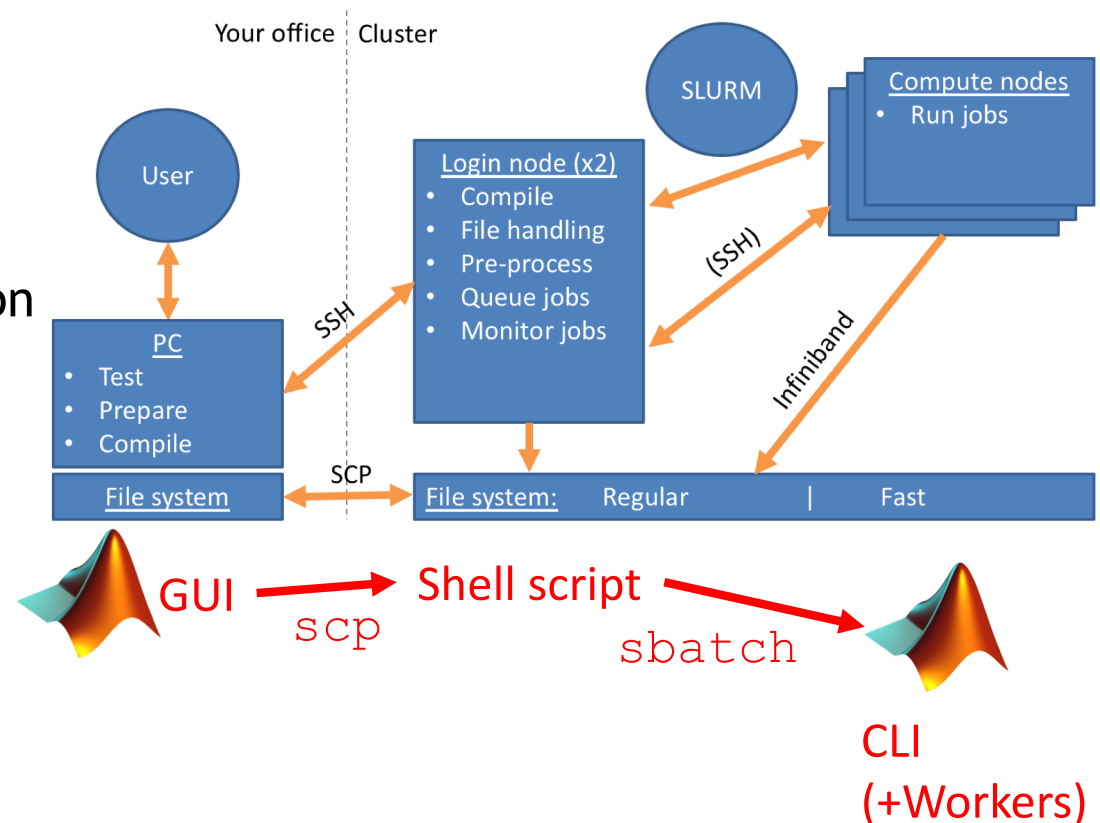- Outlook

Matlab Best Practice

- Started "bastelcode" in my free time
  - CFD problem
  - Intended as typical use case
    - LES matrix filled
    - LES solver
    - Not too complex, not too simple
  - Initially Numpy
    - Ported to Matlab
    - Currently: Fortran
  - Also: software engineering use case

Matlab Best Practice

- When porting code to Matlab, learned lots of interesting stuff
  - Using Matlab on cluster
  - Parallel features
  - (parallel) debugging
  - Performance measurement
- Idea:
  - Workshop
  - State clearly: "this is not a tutorial"
  - Share my results
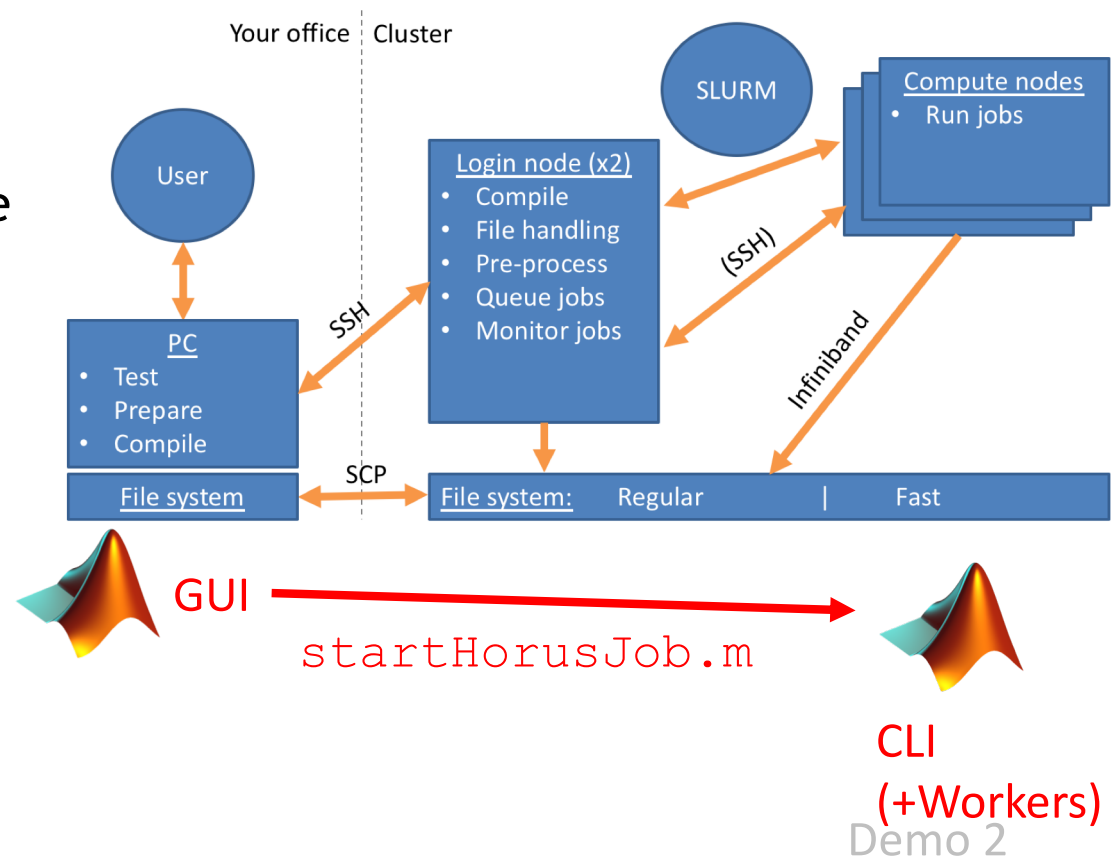 - Invite others to present their work

Using Matlab: Scenarios

- **Scenario 1:** local Matlab client
  - Run locally for debugging
  - Send jobs to cluster manually

+ No one disturbs you

+ Works without internet connection

+ Local parpool possible → no wait times

+ Job script flexibility

- Heterogenous systems, toolboxes
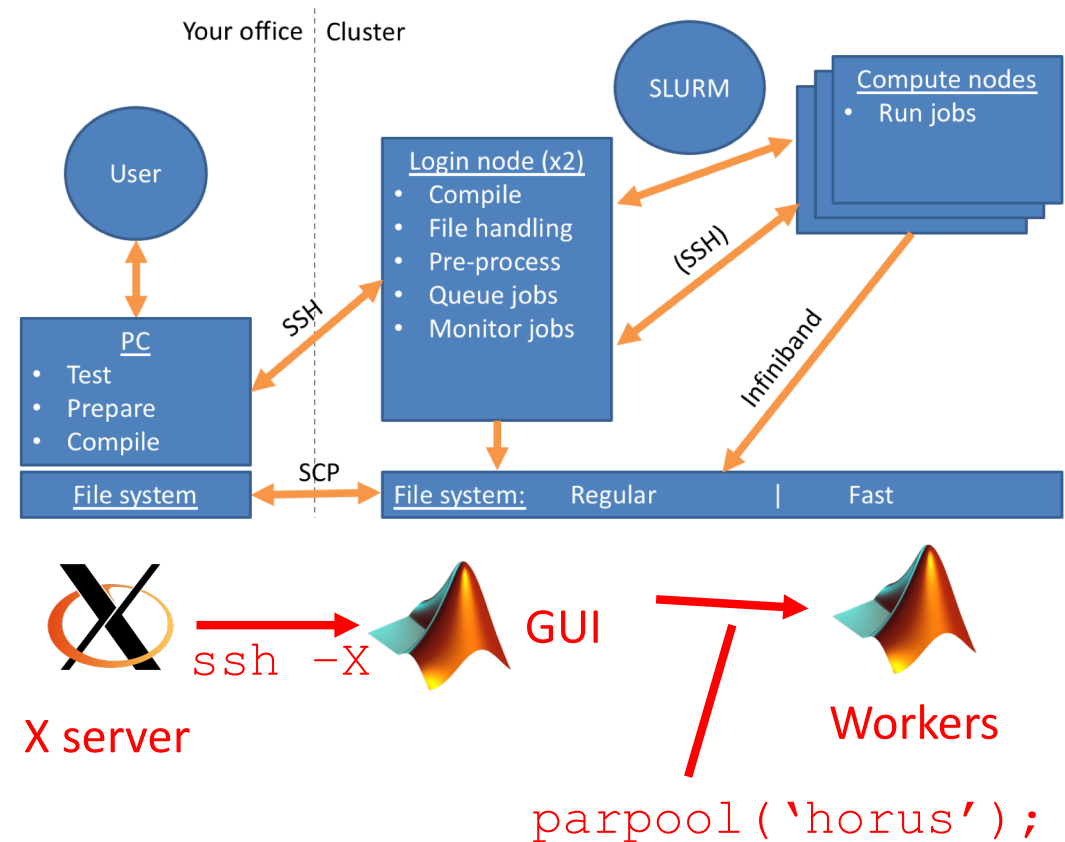- Requires separate file synchronization
- No direct job queueing or monitoring

Using Matlab: Scenarios

- **Scenario 1b:** local Matlab, auto-generate script
  - Provided by Nelles group
  - To be added to cluster website

+ Like regular job script

+ Easier to use

+ Handles file synchronization...

- Custom solution (may break)

- No direct job queueing or monitoring

- ... depending on your files

Your office | Cluster

User

PC
- Test
- Prepare
- Compile

File system

SSH

SCP

Login node (x2)
- Compile
- File handling
- Pre-process
- Queue jobs
- Monitor jobs

SLURM

Compute nodes
- Run jobs

(SSH)

Infiniband

File system: Regular | Fast

GUI   startHorusJob.m
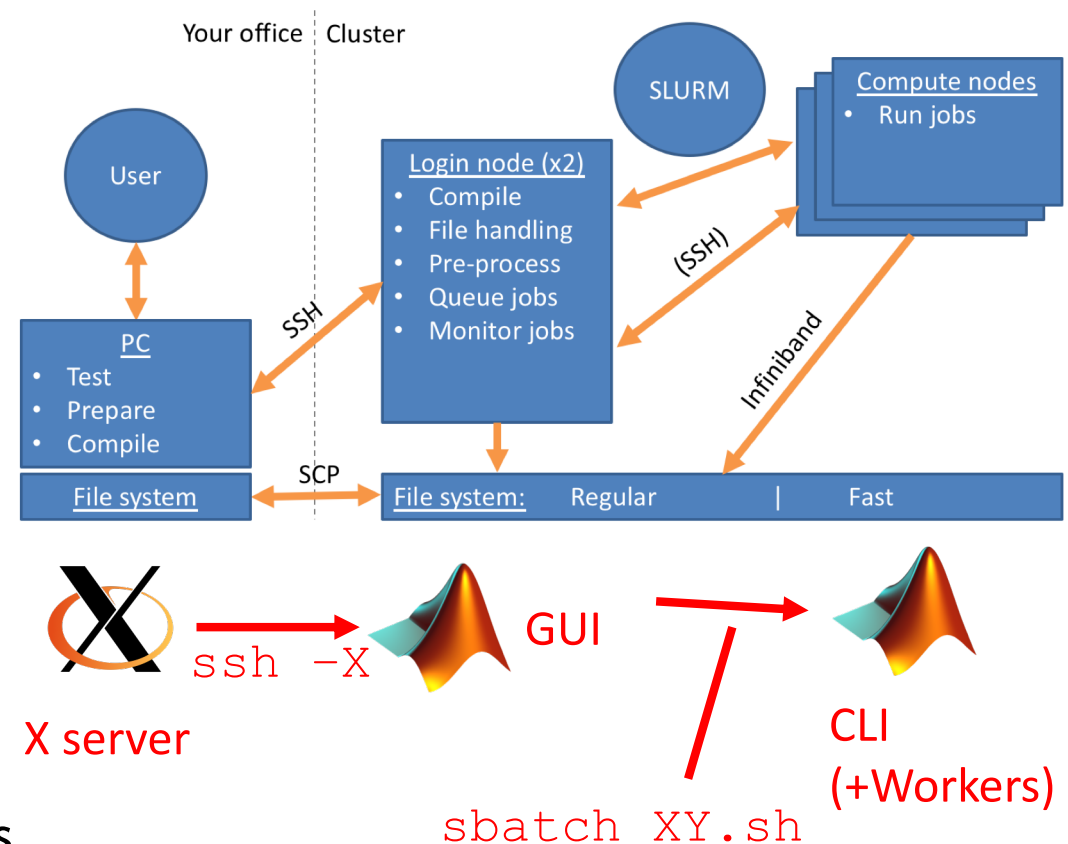
CLI (+Workers)

Demo 2

Using Matlab: Scenarios

- **Scenario 2:** Matlab on login node
  - Pools created with cluster profile
  - **DO NOT RUN JOBS ON FRONTEND**

+ Needs no Matlab license

+ Start workers on node(s)

+ Same architecture as run

+ Interactive possible (`pmode`)

+ Start job from within Matlab

- Ugly interface
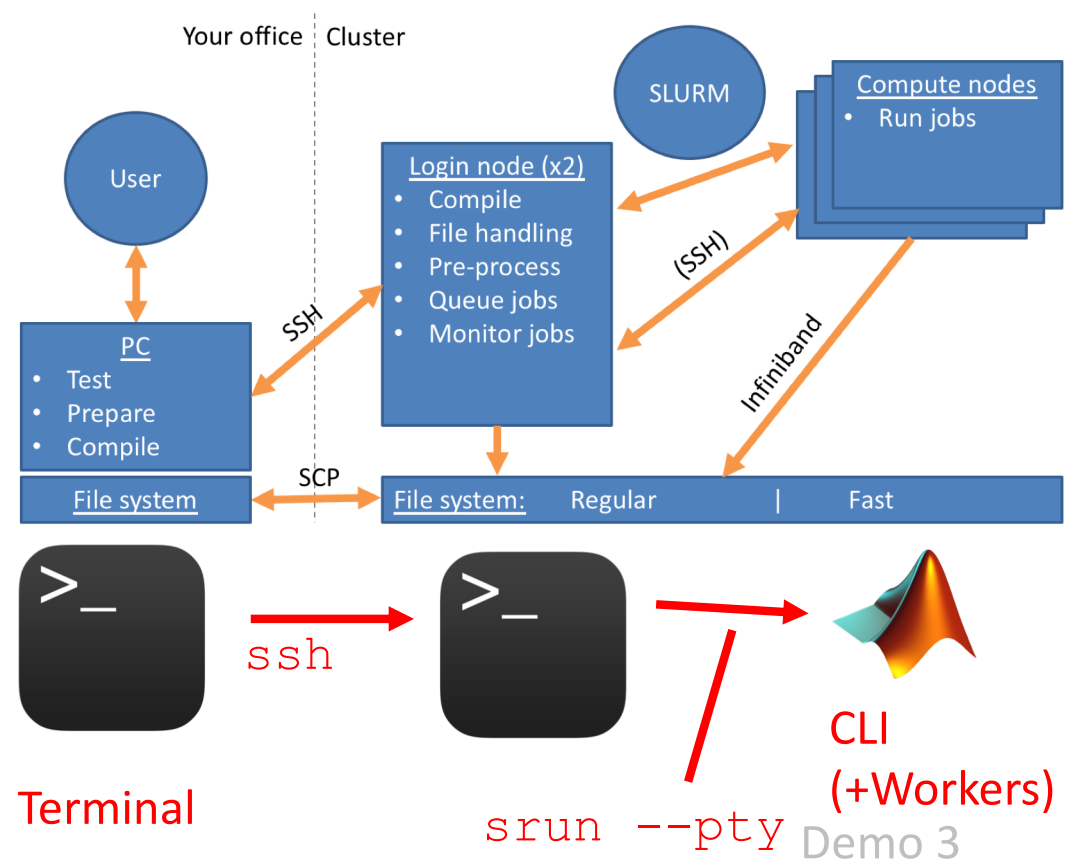- Sometimes wonky connection
- Sometimes wonky MPI

Using Matlab: Scenarios

- **Scenario 2b:** Matlab on login node, manual or generated job script
  - Combination of scenario 1 and 2

+ Combines advantages

+ Uses local pool (on compute nodes)

+ Should allow more than 12 workers (could not test)

- Also combines disadvantages
- Currently no auto-generation script (but easy to adapt)
- Cannot use Run button or breakpoints

Using Matlab: Scenarios

- **Scenario 3:** Matlab in interactive job on compute node
    - CLI Matlab (breakpoints theoretically possible) + workers
    - Edit M files with separate editor

+ Compute resources reserved for you

+ Exact same architecture as run

+ Completely interactive

+ Starts quickly, (re-)runs quickly (once job started)

- Initial job wait time
- Job dies if connection lost
- Only CLI

Your office | Cluster

SLURM

User

Login node (x2)
- Compile
- File handling
- Pre-process
- Queue jobs
- Monitor jobs

Compute nodes
- Run jobs

(SSH)

SSH

Infiniband

PC
- Test
- Prepare
- Compile

SCP

File system

File system: Regular | Fast

Terminal

`ssh`

`srun --pty`

CLI (+Workers)

Demo 3

Matlab Best Practice

- Matlab Best Practice Guide basically writes itself

- Sideproduct: "Using Matlab on Cluster" course

- Initially worried about time spent on dev work
  - Paid off big time

- Attendees reported they did not know 50 % of what I said on average

Matlab Best Practice

- Workshop "Forum Part" Results
  - Immediately found users of same toolboxes on different sides of Uni
  - Typical Tier 3 problem: either too small for cluster or so large that they have existing solutions for their problems
  - Was hoping for more synergy

- Synergy found
  - Automatic queuing script from one institute
    - Overhauled, currently in beta, will be offered for download

- Still too little attendance
  - Most users came because I personally asked them

Outline

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- Construction Sites:
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  - **Cluster Website**
  - Publicity
  - Miscellaneous

- Outlook

Cluster Website

- Cluster Website

  - Starting to gain traction

  - New users get "Welcome" email pointing them to "Getting Started" section of website

  - Users starting to report actually using website

  - Cluster now has auto-generated Message of the Day

Cluster Website

- Course entry WP mask
  - Sort upcoming/past automatically
  - Download links to materials
  - Integrate into HPC Calendar

- Include HPC Calendar on website
  - Still technical problems
  - But possible in principle
  - Add courses automatically, mark as local

Cluster Website

- Stepchild: "FAQ" section

  – Nothing to put in it

  – Not intended for "frequently" asked questions to begin with

  – Needed: section for "stuff that fits on no other page"
    - Separate from guides

  – Will try "Blog" next

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Publicity

- Cannot advertise only to HPC community
  - But there is no other community to advertise to

- Mitigation:
  - Advertise very broadly
    - University press office offers counseling
  - Create community
    - Scientific computing
    - Draw interest with courses (e.g. C++)
    - Idea: "SciComp Stammtisch"
      - Thanks for café idea

Publicity

- Discussion with press office
  - Would have happened with new cluster anyway

- They want "testimonials" from users
  - Attended courses
  - Got in-person counseling

- Asked for corner facts
  - "Layman's terms" stuff

- Idea: only for increasing visibility

Outline

- Introduction

- Construction Sites:
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  - Publicity
  - **Miscellaneous**

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Miscellaneous

- Started looking into HPC Wiki
  - Identified areas where our content would help
  - Very impressed with login process

- Since I am getting a crash course in "How to buy a cluster"
  - Develop best practice guide from notes
  - HPC wiki – admin section?

- Course lecturer checklist
  - Anyone interested in sharing?

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- **Outlook**

Outlook

- Programming Introduction Courses
  - Thanks, Anja!
  - Use chance to advertise us beyond HPC community

- ZIMT about to launch Gitlab hosting service
  - Already using it as a beta tester

- Go through tickets of 5+ years, identify trends
  - Already identified issue: environment modules
    - Chance to make everything better with new cluster

Outlook

- Next workshop goal: scientific software engineering
  - Version control
  - Data flow
  - Documentation
  - Important: differences to

- Background: community is forming to establish job of "Research Software Engineer"
  - de-rse.org (e.V.)
  - Initiated by DLR, much resonance DLR-internally
  - Internationally: UK, US:"Better Scientific Software" Sandia/Argonne

Thank you for your attention

Questions?