Lecture 9: Cluster computing

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BIOST 561: Computational Skills For Biostatistics I

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Motivation

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In Lecture 8, you learned how to compute without `R`.

Today, you'll learn how to transfer those skills to computing on a cluster.

Examples from my research

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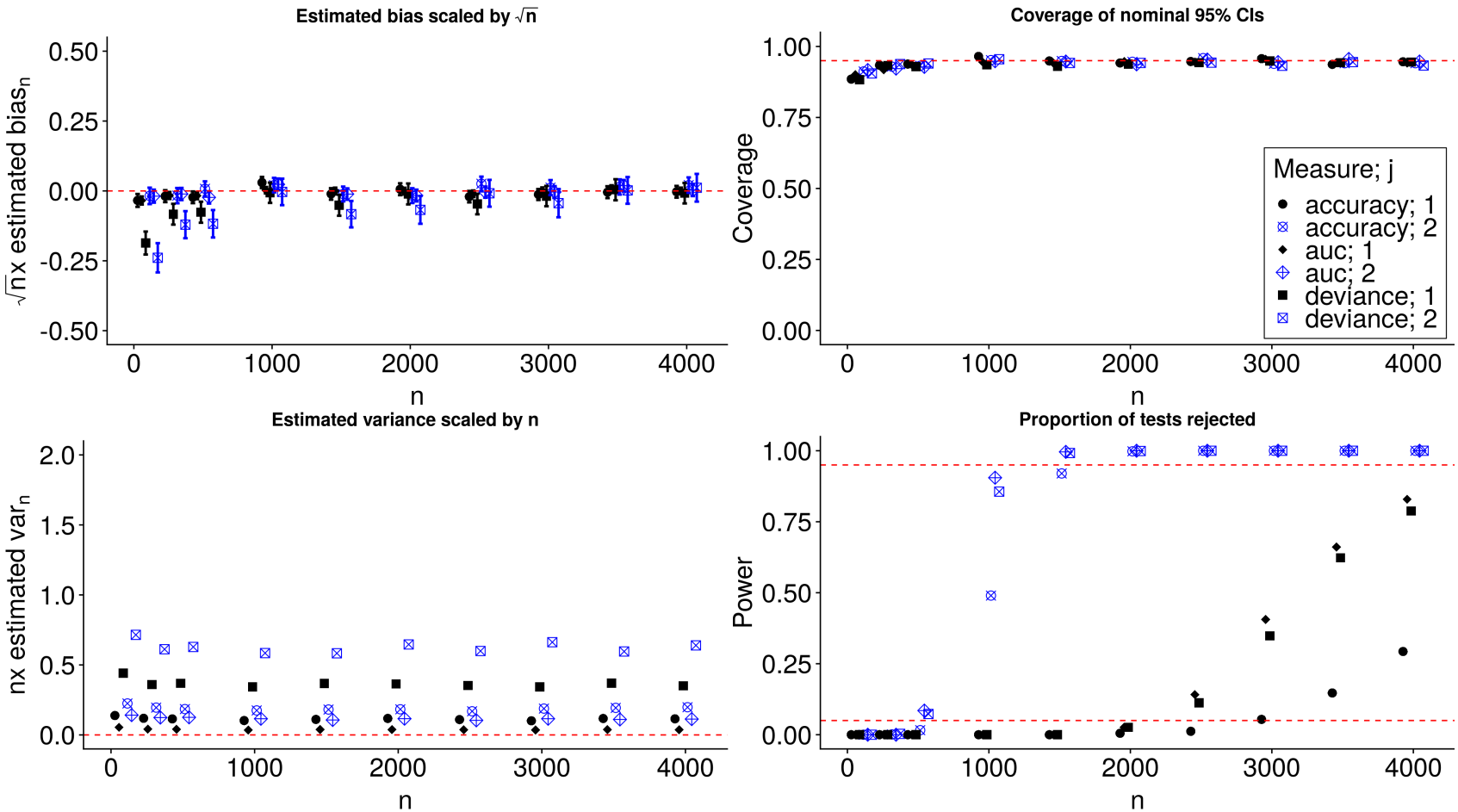

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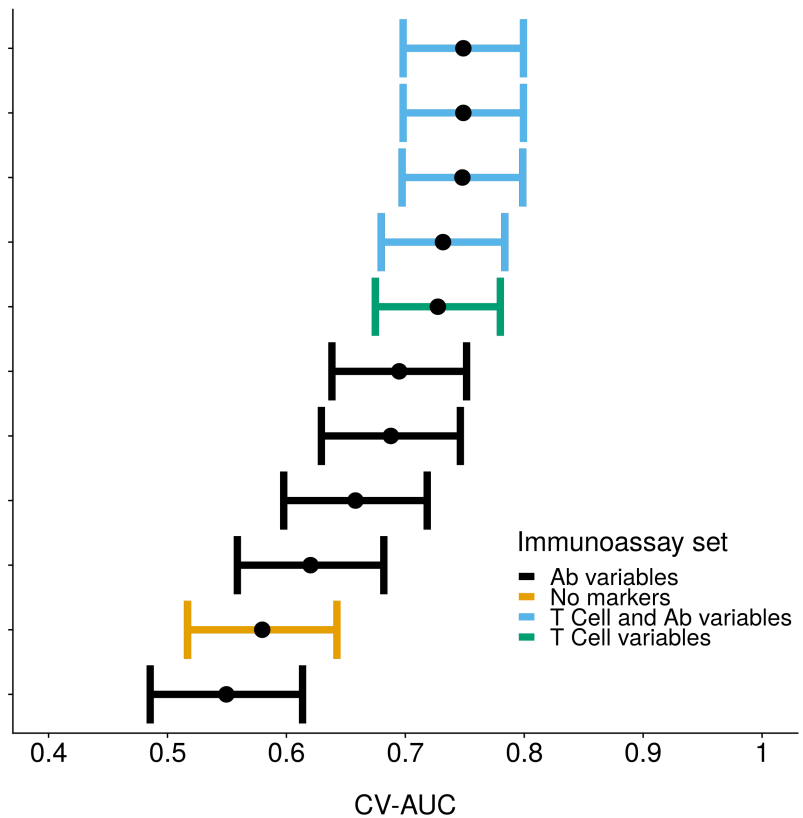
Assay combination	CV-AUC [95% CI]
IgG + IgA + IgG3 + T Cells	0.749 [0.698, 0.799]
IgG + IgA + T Cells	0.749 [0.698, 0.799]
All markers	0.748 [0.697, 0.799]
T Cells + Fx Ab	0.732 [0.680, 0.784]
T Cells	0.727 [0.675, 0.780]
IgG3	0.695 [0.638, 0.751]
IgG + IgA + IgG3	0.688 [0.629, 0.746]
IgG + IgA + IgG3 + Fx Ab	0.658 [0.598, 0.718]
IgG + IgA	0.620 [0.559, 0.682]
No markers	0.580 [0.517, 0.643]
Fx Ab	0.550 [0.485, 0.614]



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analyses without keeping an R session open (for the duration!) on my personal machine?

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*: we will discuss this further!

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Consider a sample of n observations generated iid according to

$$\begin{aligned} X &\sim N(0,1), \\ u &\sim N(0,1), \text{ independent of } X; \\ Y \mid X, u &= \beta_0 + \beta_1 X + \epsilon, \text{ where} \\ \epsilon &= |X| u. \end{aligned}$$

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We will use the cluster to do this!

Part I: coding for the cluster

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Today, I'll provide an alternative method (this should not always replace the simulator!).

Coding for the cluster: modular code

Modular code: each file has a single task

Coding for the cluster: modular code

Modular code: each file has a single task

Your turn!

Go to the `code` subdirectory. Then answer these questions **with a partner**:

1. what does `do_one` do? What are its arguments?
2. what does `generate_data` do? What are its arguments?
3. Write effective comments in each file so that **future you** understands each!

Coding for the cluster: modular code

Answers and Brian's comments (to be posted after class)

Coding for the cluster: setting the seed

Coding for the cluster: #! and executables

Coding for the cluster: saving output

Coding for the cluster: debugging

Coding for the cluster: compiling output

Part II: using the cluster

Using the cluster

Department resources for HPC*:

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- `cox`: 12-core computer

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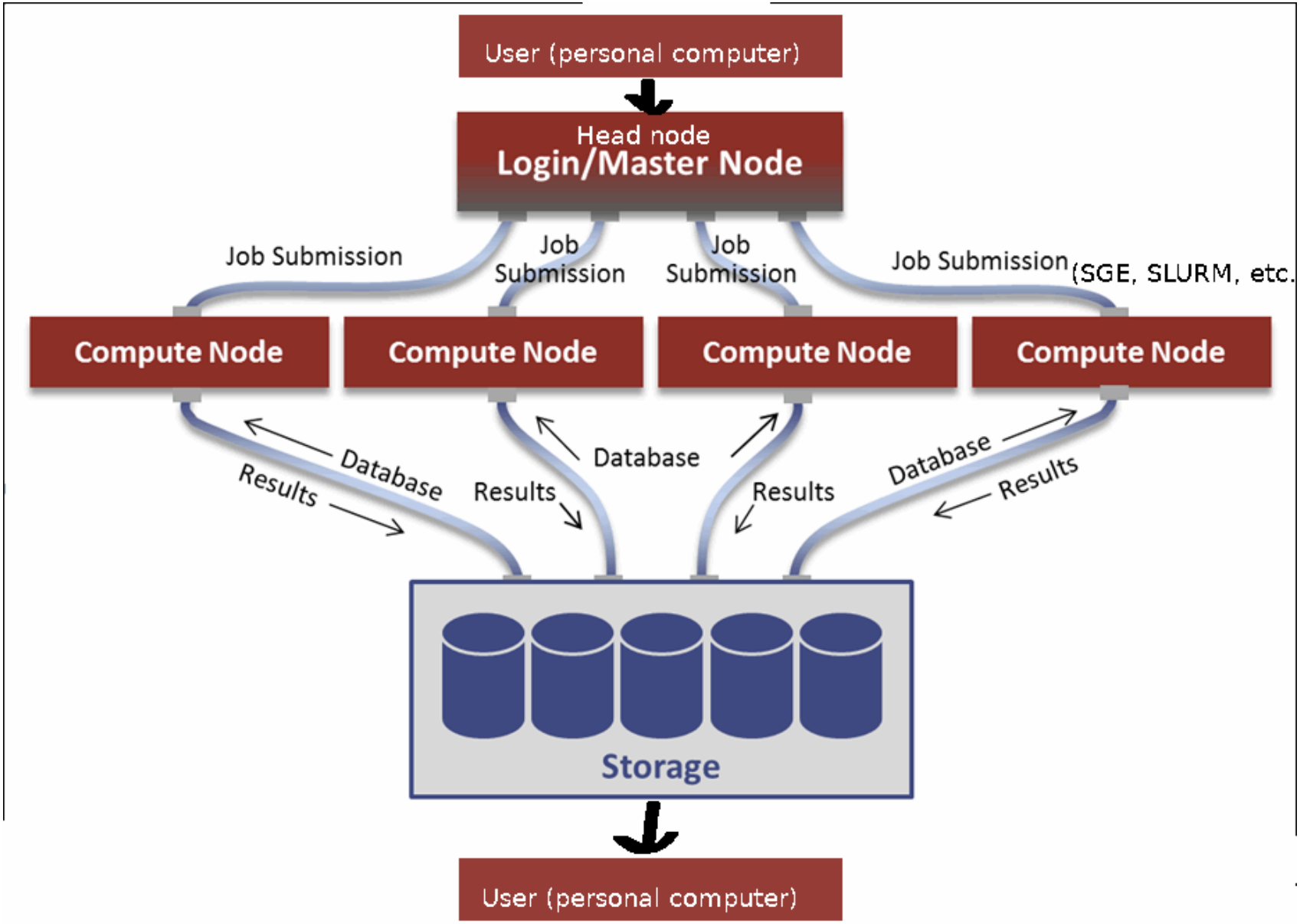
*other groups have similar resources, e.g.,

- `hyak` (managed by UW-IT)
- `pearson` (statistical genetics group only)
- `gizmo` (Fred Hutchinson Cancer Research Center only)
- Microsoft Azure, Amazon Web Services (AWS)

Using the cluster



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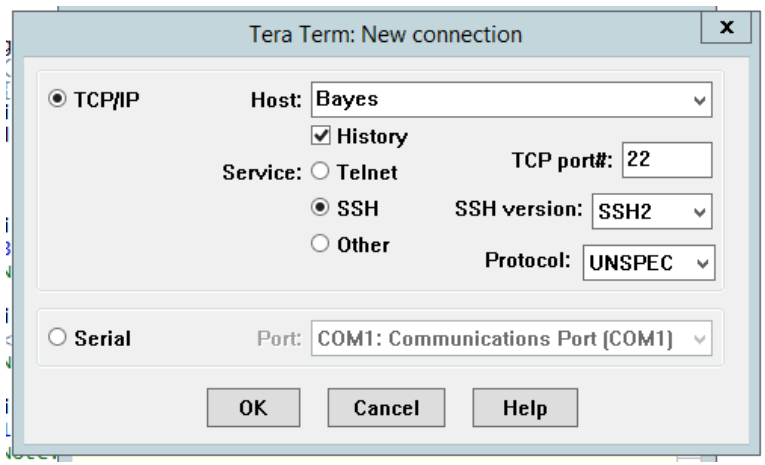
We'll practice good habits for being nice as we go along.

Using the cluster: logging in (Windows, incl. box)

1. Open TeraTerm [or your favorite secure shell (SSH) client]
2. Enter the address of your favorite cluster, e.g., `bayes.biostat.washington.edu`
3. Make sure that the "New connection" window is filled out as in the figure, except for "Host" (screenshot from box)
4. Click `OK`, enter your UW BIOST username and password when prompted (user and pass you use for box)



Using the cluster: logging in (Mac/Linux)

1. Open a Terminal window

2. Type `ssh mynetid@cluster.washington.edu`
   - replace `mynetid` with Your UW NetID, and
   - replace `cluster` with Your cluster, e.g., `bayes`

3. Enter password (same password as `box`) when prompted (the field will remain blank but your password will be received)

Using the cluster: logging in

Your turn! Take 2 minutes to complete this activity **by yourself** (if you don't have a computer, write down how you would do this).

1. Log into the cluster
2. What is the name of the directory that you are when you log in?
3. Create a directory called `robust_ses` in your `home` directory
4. Create a directory called `robust_ses` on **your** computer, under `biost561/lecture9`

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- navigation,
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are all used in exactly the same way!

Using the cluster: jobs

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Example job:

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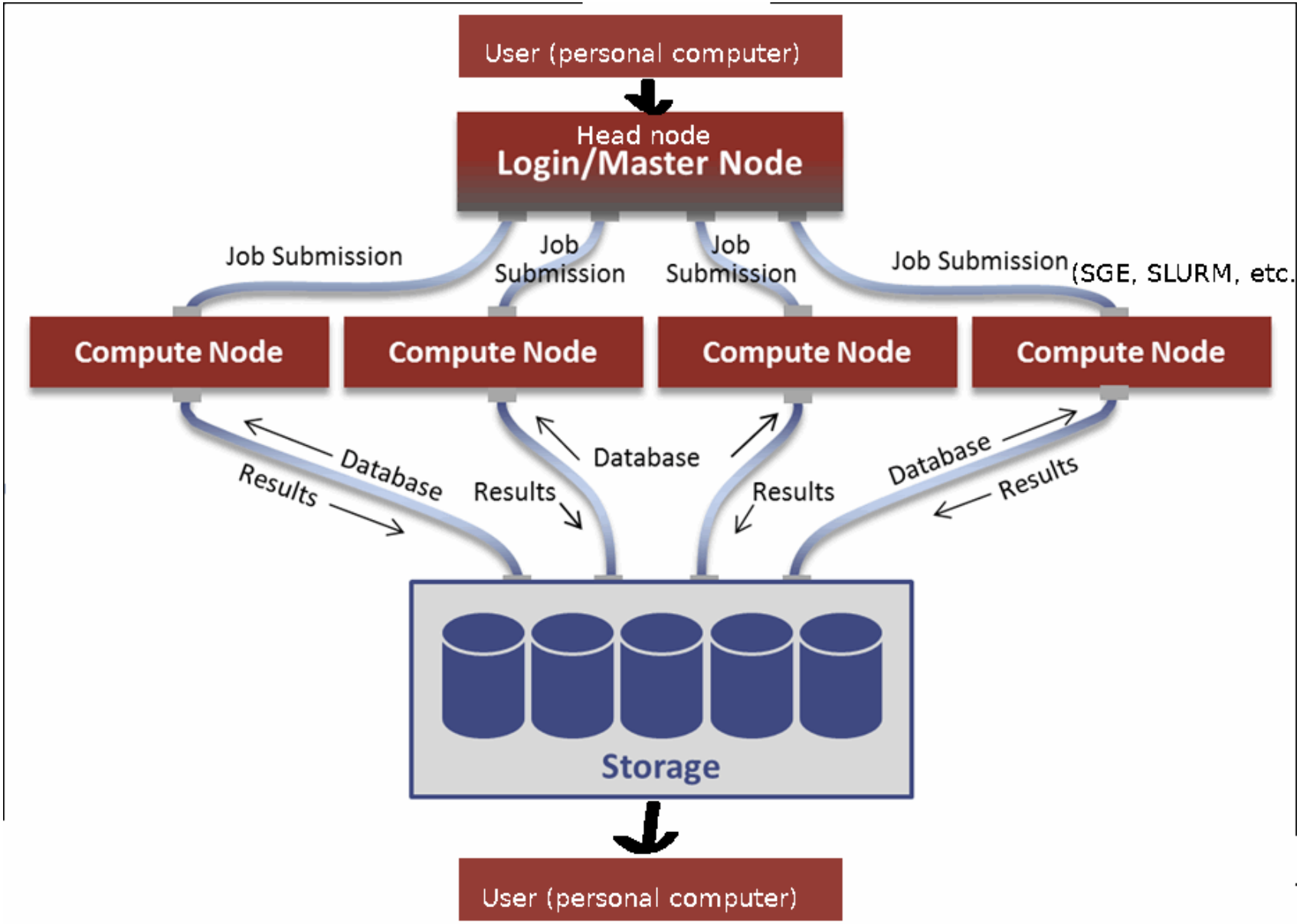

Using the cluster: submitting jobs

Workhorse command on SGE: qsub

Many options, including:

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-

Options are specified with a single -, as you saw in Lecture 8.

Using the cluster: checking jobs

Using the cluster: other helpful SGE commands

Appendix: other useful cluster things

Useful things: Windows file compatability