Parallel Computing in MARCC

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What is parallel computing?

Parallel computing is a problem-solving technique in which

- A problem is divided into parts.
- Each part's solution does not depend on the others'.
- Multiple parts are solved *simultaneously* by *different* processing units.

Example: baking 400 muffins in 1 vs. 2 vs. 4 ovens.

The gains are easy to understand:

- Get many processing units (n).
- Make them all work simultaneously.
- Speed up your solution by a factor of n.

... not so fast.

Caveats — What *can* you parallelize?

Idea from Economics:

$$V_t(m_t) = \max_{0 \leq c_t \leq m_t} u(c_t) + V_{t+1}(m_t - c_t), \qquad t = 1, ..., T.$$

Can we solve each t in a different processor *simultaneously*?

No! notice we can't find $V_t(\cdot)$ until we have found $V_{t+1}(\cdot)$.

Things we *could* do:

- If we have heterogeneous agents, solve each type in its own processor.
- If we are using a grid for m, given $V_{t+1}(\cdot)$
  - Solve $V_t(m)$ for different m's simultaneously in different processors.
  - Join the solutions to form $V_t(\cdot)$, move on to $V_{t-1}(\cdot)$.

Caveats — What *should* you parallelize?

Example: 400 muffins again. Should you simultaneously use 400 ovens?

At some point it becomes impractical.

- Coordinating parallel tasks has some costs. E.g.
  - Setting up the processing units.
  - Dividing the problem.
  - Transferring information to and from the units.
  - Combining the independent solutions.
- This is often called *overhead*.
- Overhead can easily make the parallel version of your solution slower than the sequential version!
- Therefore, test and optimize your parallelization strategy.

MARCC — MD Advanced Research Computing Center

- Computing facility.
- Funded by the State, managed by JHU and UMD-CP.
- Two purposes:
  - High performance computing. $> 23,000$ cores.
  - Reliable data storage.

Its resources are organized in *Partitions*

- You select which partition to send your jobs to.
- Each has its own characteristics:
  - Type of processor, number of available cores.
  - GPUs.
  - Time allowances.
  - Memory.
- Find detailed descriptions here.

MARCC — Resources

Example, each node in `parallel` partition

- 24 cores, 128GB RAM.
- Type of processor: Intel Haswell, 12-core, 2.5GHz, 30MB cache (2x).
- Can be used for up to 72 hours.

Software:

- Packaged in "modules" that you must load.
- See them with command: `module avail`.
- Matlab, Mathematica, Python, R, Julia, gcc (C++, Fortran), and many more.

Availability:

- Currently Econ. Dep. has 1,000 CPU-Hours/quarter. **Free**.
- Going mostly unused.

Getting Access to MARCC

- MARCC's usage is regulated through *allocations* of resources.
- "PIs" control who can access their allocations.
- Our allocation's PI (as of 2021) is Prof. Jonathan Wright.

Steps

1. Contact Professors Hwang, Moffitt, or Wright to request access.
2. Make sure Prof. Wright is aware that you will request an account.
3. Request an account here.
4. Wait for an approval email from MARCC.

Connecting to MARCC

MARCC uses the *Secure Shell (SSH)* protocol.

Options:

- **Command `ssh` in a terminal**:
  - Available by default in Unix and MacOS.
  - Available in Windows ≥ 10. Might need setup.
  - Find instructions here.
- **SSH client**:
  - A program dedicated to ssh connections. List of available ones.
  - For Windows: **PuTTy** is the most popular. I like **Bitvise**.

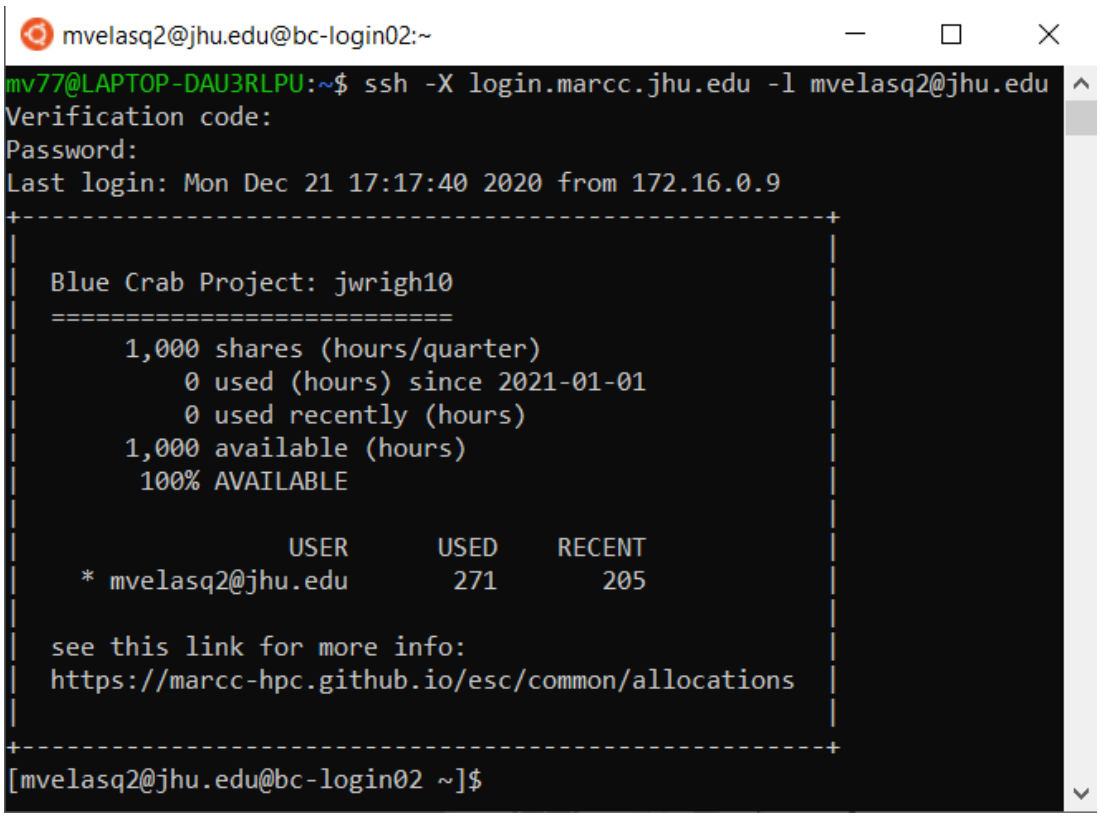
In both cases you will need Google Authenticator:

- Register the app with your MARCC account. Instructions.
- Use it to get your `Verification code`.

Example — Terminal

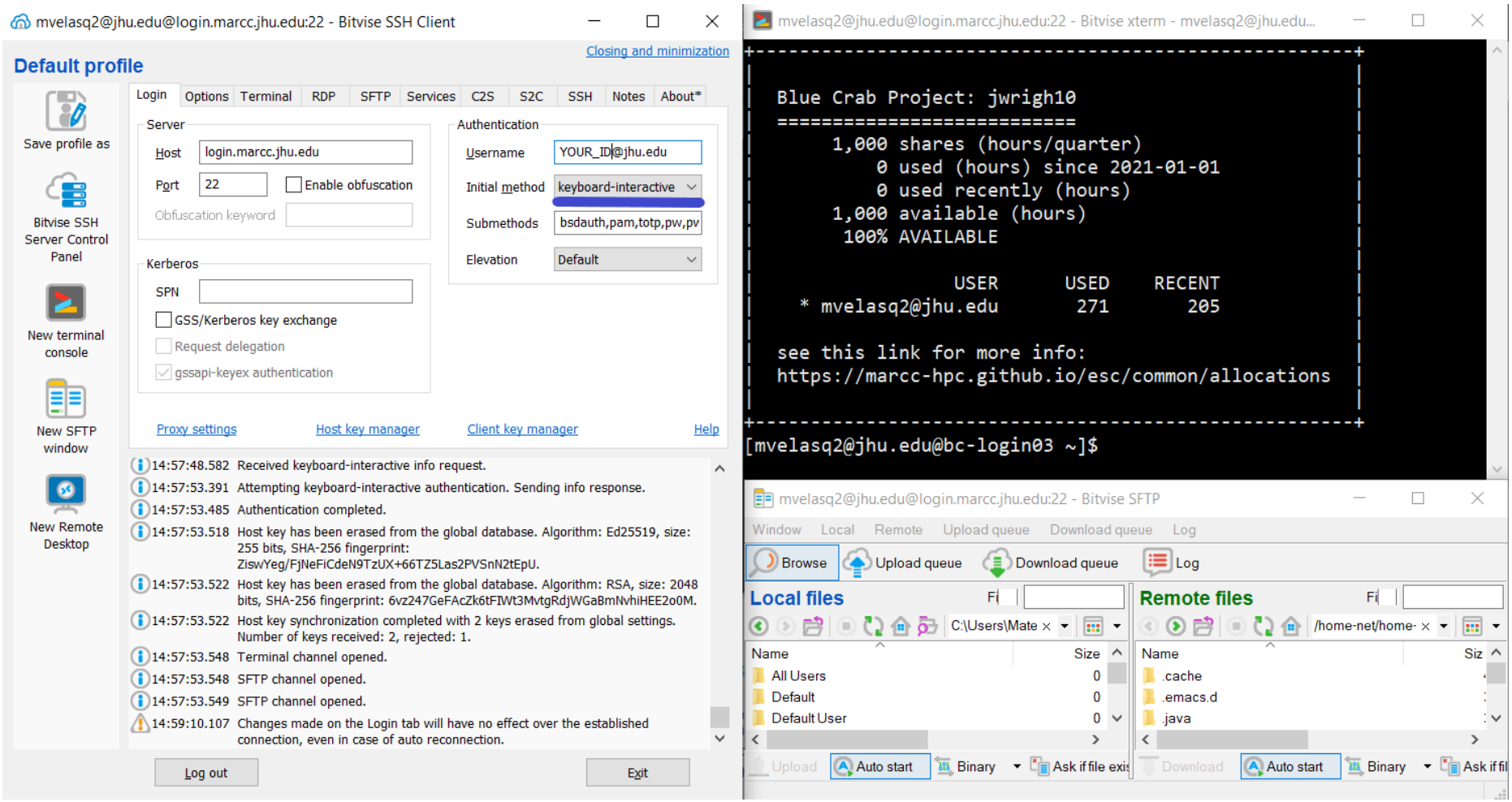
Command:

```
ssh -X login.marcc.jhu.edu -l user@jhu.edu
```



Example — Client (Bitvise)

Configure your client as in the left panel.



Transferring files — Globus

MARCC recommends a system called Globus. Instructions here.

Details:

- You need to set-up "endpoints".
- Your computer:
  - Endpoints → "Create a personal endpoint".
  - Download and install the client.
  - Will appear at `Endpoints/Administered By You`.
- MARCC:
  - Appears as `marcc#dtn`.
  - Select it and log in with your marcc credentials.
- Select both in `File Manager` and use the interface.
- You will get emails when transfers complete.

Examples — Matlab

- Different languages do parallel computing differently.
- Basic examples in R, Matlab and Python here.

... However, they share the same structure. Some subset of:

1. Create a `pool` or `cluster`.
2. Export the tools workers need. E.g., data, self-defined functions.
3. Execute the parallel operations.
4. "Paste" and format their results.
5. Shut down pool.

Lets go through the Matlab example.

SLURM — Workload Manager

Would be a mess to have everyone running jobs at the same time.

That is why SLURM exists.

- It is a resource administrator.
- You don't *just run* your jobs.
  - You write your instructions as a bash script.
  - Specify what resources you would like to use.
  - Send the request to SLURM.
  - It will assign your resources and run your script.
- Pros: order and predictability!
- Cons: there is a queue for resources.

SLURM Scripts

- You configure your request with lines starting with `#SBATCH`.
- Place them at the top of your bash script.

Some examples:

`#SBATCH --job-name` :

`#SBATCH --partition` : MARCC partition. Type of resources.

`#SBATCH --time` : maximum time allowed for your job.

`#SBATCH --cpus-per-task` : CPU cores to allocate to each task.

More here.

Confusing: `nodes` vs `cpus` vs `cores` vs `tasks`. Best guide I've found.

Let's see an example script for our Matlab job.

Hopefully we will do this part live!

For posterity:

- Get familiar with basic Linux commands: `cd`, `ls`, `cat`...
- Navigate to your script.
- Submit it with `> sbatch YOUR_SCRIPT.sh`

After that:

- You can see your jobs' status using command `sqme`.
- This will also give you your job's "id".
- `seff id` details your job's use of resources.
- `scancel id` cancels your job.

More here.

You can log off. Your job won't be stopped.

Additional resources and troubleshooting

- MARCC's help desk: `marcc-help@marcc.jhu.edu`.
- MARCC's website: `https://www.marcc.jhu.edu`.
- MARCC's own introductory session:
  - Go to this link.
  - Click on "This video".
  - Log-in with your JHU credentials.
- MARCC's guide for Matlab.
- Course from Princeton.
- My Github repository with Matlab, R, and Python examples.
- My own email: `mvelasq2@jhu.edu`.

Thank you and best of luck!