Programming Camp - Lecture 4

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Presentation outline

1. High Performance Computing
2. Parallel Computing

1 | High Performance Computing

Parallel Computing

Why do we need high performance

1. Quantitative, data-driven economic models are computationally complex
   - Finding equilibrium involves solving individual behavior and then iterating for many prices until markets clear;
   - Estimation requires solving model with many parameters guesses
   - Games with many players; industries with strategic behavior;
   - Auctions with many goods;
   - Migration with many cities;
2. Big data can easily overwhelm our laptops
   - Every housing transaction in the US (Corelogic, Green Library)
   - Product level databases (Neilsen, UC Chicago)

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→ A mix of hardware and software can push the boundary of what is feasible
   - Servers, with CPUs, GPUs, big RAM;
   - Parallel programming;
   - Distributed computing (many computers)

· Today: Show you the basics, and highlight what's out there

· Lots to learn from CS folk
   - Machine learning tools – e.g. Tensorflow & GPU – can be leveraged for scientific computing
   - Worth investing at this point in PhD

GPUs are changing machine learning and computer science

1 High Performance Computing

What type of computer cluster should you use?

- Paid services include Microsoft Azure, Amazon Web Services (AWS) and Google Cloud Platform.

	Paid Services	**University Cluster**
Monetary cost	[✗] Expensive, often paid by the hour	[✓] Free to students and faculty
Waiting times	[✓] Instantly available	[✗] Access often involves queues and waiting times
Ease of use	[✓] Low set up costs (e.g., turning on a computer + installing software)	[✗] Complicated to understand and use (high fixed costs)

1 High Performance Computing

1.1 University Clusters vs. Paid Services

1.2 Using Stanford Servers

Some Terminology

- **Computer cluster:**
  Collection of separate computer servers, called nodes, which are connected via a fast interconnect.
  Configuration allows many computers to work together.

- **Nodes:**
  Individual computers designed to accomplish specific tasks (e.g., login nodes, computing nodes).

- **Job Scheduler:** (SLURM)
  Software that organizes and assigns tasks to the computer cluster.
  Provides a framework to start, execute and monitor jobs within the cluster.

List of Stanford Servers

1. Farmshare: `rice` (login node), `wheat` (big memory node), and `oat` (gpu node).
   - Coursework, and non-sponsored research.
   - Can only connect to `rice`, and access other nodes from there.

2. Sherlock
   - Sponsored research. Need a faculty sponsor to get access to.
   - Humanities and Sciences partition available `hns`.
   - Connect to login nodes (low computing power) and schedule jobs in high performance nodes.

3. Other servers available tailored to other needs.
   - GSB server: `yen`.
   - Center for Population Health Sciences (PHS): HIPAA compliant; useful for PII data (e.g., Medicare).

Using the terminal

- Connect through SecureCRT (Windows) or the terminal (Mac).

- Connecting to Stanford servers:

  `ssh StanfordID@rice.stanford.edu`

  `ssh StanfordID@login.sherlock.stanford.edu`

- Some useful commands:

`pwd`	list current working directory
`cd`	change directory
`touch file.txt`	create a new file called file.txt
`vi file.txt`	open text editor in terminal
`module avail` or `ml avail`	show available modules
`module load X` or `ml X`	load module X into workspace
`module list`	list loaded modules

Transferring files to/from servers

- **Windows:**
  - Use SecureCRT + SecureFX (paid software, free for Stanford students). More information click here.

- **Mac:**
  - Use Cyberduck (free) or other paid software (e.g., Transmit).

- **Farmshare:**
  - Transfer through AFS: `http://afs.stanford.edu`
  - If working in batch jobs, store in `/farmshare/user_data/SUNetID`

- **Sherlock:**
  - Sherlock is pretty flexible. Once you need more information click here.

Write the following code using a text editor

test_matlab.m

```
clc; clear;
rng(29134)
a = random('normal',0,1,10,1)
mean(a)
disp("HELLO FROM MATLAB")
```

test_stata.do

```
set obs 10
set seed 1094
gen random = runiform()
summ random, d
disp "HELLO FROM STATA"
```

test_batch.sbatch

```
#!/bin/bash
#SBATCH -p normal
#SBATCH --job-name=test
#SBATCH --error=test_%j.err
#SBATCH --output=test_%j.out
#SBATCH --nodes=1
#SBATCH --mail-type=ALL
#SBATCH --mail-user=jimenezh@stanford.edu

echo "HELLO FROM BATCH"
cd /farmshare/user_data/jimenezh/test_server

module load matlab
matlab -nodesktop -nosplash -nodisplay < test_matlab.m > output_matlab.txt

module load stata-mp
stata-mp < test_stata.do > output_stata.txt
```

Steps:

Say that I have a `code.sbatch` ready to run.

1. Open Fetch / SecureFX to start your connection:
   Hostname: `rice.stanford.edu`
   Username: `<SUNet ID>`
   Password: `<SUNet Password>`
2. Go to `/farmshare/user_data/<SUNet ID>`.
3. Create a `test_data` folder and copy your code files there.
4. Start your ssh connection. Open the terminal and write:
   `ssh <SUNet ID>@rice.stanford.edu`
5. From the terminal, change to the Farmshare directory.
   `cd /farmshare/user_data/<SUNet ID>/test_data`
6. Run the code on the server.
   `sbatch test_batch.sbatch` or `srun test_batch.sbatch`.
7. Check your status with `squeue -u $USER`.

Other SLURM useful commands

- Submit jobs to specific partitions:
  `#SBATCH -p hns,normal`
  (other: `bigmem, gpu, long`).

- Request more / less time than default:
  `#SBATCH --time=01:00:00`
  (less time may make your code start faster).

- Request a specific amount of RAM:
  `#SBATCH --mem=128000`
  (note: not all memory - core combinations are available).

- Switch from `rice` node to a `wheat` node:
  `srun --qos=interactive --pty /bin/bash -l`

2 Parallel Computing

Why is some code faster than others?

- C is typically fastest language as it compiles code direct to machine readable code
  - Costs more in developer time though!
- Most languages convert your code to C which in turn converts to machine code
  - Matlab, Stata, Python (e.g. numpy, scipy)
- Built-in packages are highly optimized
  - $\beta = \mathbf{X'X}^{-1}\mathbf{X'Y}$ runs close to C
  - Parallelization and high performance algorithms under the hood

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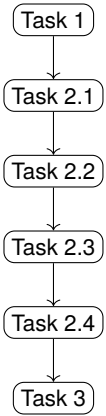
- Custom algorithms – like value functions w/loops — can be slow though
- Options to go faster
  1. Eliminate loops, use vectorized code
  2. Write inner loop in C
     - Matlab mex files
  3. Just-in-time compilers
     - Julia; Python-Numba, @njit
     - Run slower first time, then much faster
  4. Parallelization Today!
  5. Really parallel: GPU, multi-GPU nodes
     - Python: cupy, numba, dask, tensorflow; Julia...
     - Lots of digestible material from CS folks

Intuition for parallel computing

We are used to running code like this:



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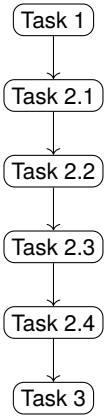
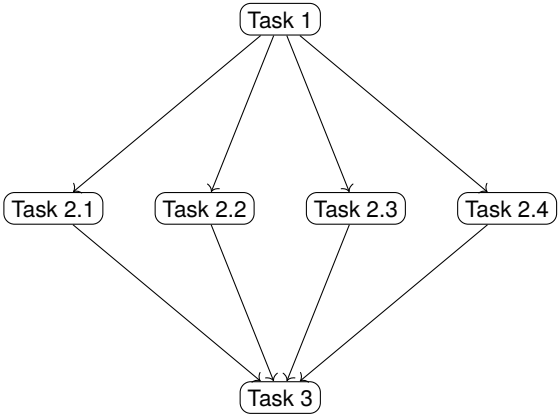


But we could do something else instead:



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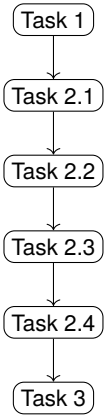

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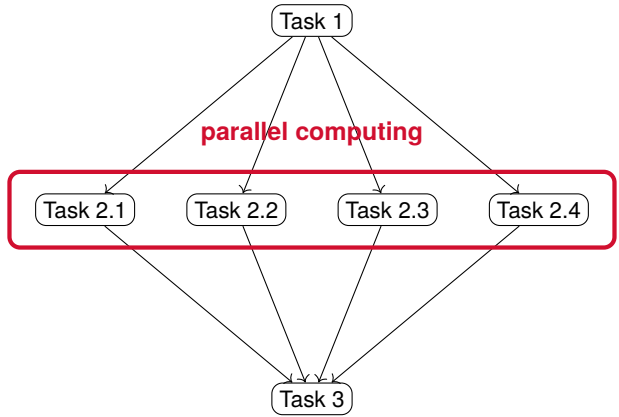

Explicit Parallelization

- Some software (e.g., Stata) has its own parallel implementation in the backend.
  We will discuss here explicit parallelization: asking software to run in parallel and implementing it ourselves.

- Parallel implementations allow code to run in as many CPUs as available in a computer.
  The number of CPUs is usually the same as the number of cores, but not always
  (CPUs = sockets $\times$ cores $\times$ threads per core).

- There are explicit parallel implementations in MATLAB (e.g., parfor), in R (e.g., BLAS), and Python (e.g., numba, joblib).

- When should you use parallel implementations in your code?
  - When little or no manipulation is needed to separate the problem into a number of parallel tasks.
  - No dependency or need for communication between these parallel tasks.
  - But be wary of overhead costs (tracking individual tasks, communicating results) — need “complicated enough” tasks!

- Common examples: bootstrap, Markov chain Monte Carlo, gradient computation in non-linear problems.

Parallelization on the GPU - kernal code

1. Vectorized code and *gpuArray()*
   1. Python: Cupy does many numpy operations using the GPU
   2. Python: Tensorflow Machine Learning libraries heavily vectorized

2. Cuda kernal
   - Traditiaonlly written in C CUDA (language for NVIDIA GPUS)
   - Now easy to write with Numba in Python (and Julia, matlab options)

   - CUDA Kernal: elementwise function to run on the “device” (aka the GPU)
   - The host (aka the CPU) sends blocks to be run in parallel on GPU

   - GPU memory is separate, need to initialize/end to GPU
   - Can scale to multiple GPUs

Parallelization on the GPU - kernal code

```
from __future__ import division
from numba import cuda
import numpy
import math
# CUDA kernel
@cuda.jit
def matmul(A, B, C):
    """ Perform matrix multiplication of C = A * B """
    row, col = cuda.grid(2)
    if row < C.shape[0] and col < C.shape[1]:
        tmp = 0.
        for k in range(A.shape[1]):
            tmp += A[row, k] * B[k, col]
        C[row, col] = tmp
```

Parallelization on the GPU - host code

```
A = numpy.full((24, 12), 3, numpy.float) # matrix containing all 3's
B = numpy.full((12, 22), 4, numpy.float) # matrix containing all 4's
# Copy the arrays to the device
A_global_mem = cuda.to_device(A)
B_global_mem = cuda.to_device(B)
# Allocate memory on the device for the result
C_global_mem = cuda.device_array((24, 22))
# Configure the blocks
threadsperblock = (16, 16)
blockspergrid_x = int(math.ceil(A.shape[0] / threadsperblock[0]))
blockspergrid_y = int(math.ceil(B.shape[1] / threadsperblock[1]))
blockspergrid = (blockspergrid_x, blockspergrid_y)

# Start the kernel
matmul[blockspergrid, threadsperblock](A_global_mem, B_global_mem, C_global_mem)
# Copy the result back to the host
C = C_global_mem.copy_to_host()
```

Example: Bootstrapping Clustered Standard Errors

- We imagine a setting where errors are correlated across individuals within groups. Denote by $g \in \{1, \ldots, G\}$ the given groups (e.g., states or classrooms) and by $n \in \{1, \ldots, N\}$ the individuals within each of these groups. We have $G \times N$ observations in our data.

- Imagine that the true model is $Y_{ng} = \beta \cdot X_{ng} + \eta_{ng}$ with $\eta_{ng} = \varepsilon_g + \varepsilon_{ng}$, $\varepsilon_g \sim$ i.i.d. $\mathcal{N}(0, 1)$ and $\varepsilon_{ng} \sim$ i.i.d. $\mathcal{N}(0, 1)$. Parametrization implies that errors are correlated across individuals within the same group.

- OLS still unbiased estimator for β. However, the formula for standard errors needs to account for correlation of unobservables within the same group. One idea to compute standard errors via bootstrap:
  1. Sample groups (with replacement) from the observed data.
  2. For each selected group, select all individuals in the group to construct a dataset of size $G \times I$, possibly w/ repeated obs.
  3. Estimate β via OLS within the bootstrapped data.
  4. Repeat 1-3 B times to compute the bootstrap estimator.

- We parametrize the model with $G = 50$, $N = 100$, $X_{ng} \sim$ i.i.d. $\mathcal{N}(0, 1)$ and $\beta = 2$.

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