Introduction to Parallel Computing (CMSC416 / CMSC818X)

Course Overview

Abhinav Bhatele, Department of Computer Science
About the instructor

• Ph.D. from the University of Illinois

• Spent eight years at Lawrence Livermore National Laboratory

• Started at the University of Maryland in 2019
Masking guideline

Epidemiology studies say that masks are a significant defense against the spread of COVID-19 and other respiratory viruses. Therefore, I recommend wearing a KN95 mask while indoors for added protection.

Choose kindness!
Introductions

• Name

• Junior/Senior/MS/PhD

• Something interesting/ unique about yourself

• Why this course? (optional)
This course is

• An introduction to parallel computing

• 416: Upper Level CS Coursework / General Track / Area 1: Systems

• 818X: Qualifying course for MS/PhD: Computer Systems

• Work expected:
  • Four to five programming assignments
  • Four quizzes
  • Midterm exam: in class on October 27
  • Final exam: on December 14 (8:00-10:00 am)
Course topics

- Introduction to parallel computing (1 week)
- Distributed memory parallel programming (3 weeks)
- Shared memory parallel programming (2 weeks)
- Parallel algorithms (2 weeks)
- Performance analysis (1 week)
- Performance issues (2 weeks)
- Parallel simulation codes (2 weeks)
Tools we will use for the class

• Syllabus, lecture slides, assignment descriptions on course website:
  • http://www.cs.umd.edu/class/fall2022/cmsc416

• Assignment submissions and quizzes on ELMS

• Discussions: Piazza
  • piazza.com/umd/fall2021/cmsc416cmsc818x

• If you want to send an email, cc both TAs and me
  • Put [CMSC416] or [CMSC818X] in the subject line
Zaratan accounts

- The TAs will provide instructions for logging on to zaratan

- Helpful resources:
  - https://www.glue.umd.edu/hpcc/help/usage.html
  - https://missing.csail.mit.edu
  - https://gitlab.cs.umd.edu/mmarsh/quick-refs
Excused absence

Any student who needs to be excused for an absence from a single lecture, due to a medically necessitated absence shall make a reasonable attempt to inform the instructor of his/her illness prior to the class. Upon returning to the class, present the instructor with a self-signed note attesting to the date of their illness. Each note must contain an acknowledgment by the student that the information provided is true and correct. Providing false information to University officials is prohibited under Part 9(i) of the Code of Student Conduct (V-1.00(B) University of Maryland Code of Student Conduct) and may result in disciplinary action.

Self-documentation may not be used for Major Scheduled Grading Events (midterm and final exams) and it may only be used for one class meeting during the semester. Any student who needs to be excused for a prolonged absence (two or more consecutive class meetings), or for a Major Scheduled Grading Event, must provide written documentation of the illness from the Health Center or from an outside health care provider. This documentation must verify dates of treatment and indicate the timeframe that the student was unable to meet academic responsibilities. In addition, it must contain the name and phone number of the medical service provider to be used if verification is needed. No diagnostic information will ever be requested.
What is parallel computing?

- Serial or sequential computing: doing a task in sequence on a single processor
- Parallel computing: breaking up a task into sub-tasks and doing them in parallel (concurrently) on a set of processors (often connected by a network)
- Some tasks do not need any communication: embarrassingly parallel
What is parallel computing?

• Does it include:
  • Grid computing
  • Distributed computing
  • Cloud computing

• Does it include:
  • Superscalar processors
  • Vector processors
  • Accelerators (GPUs, FPGAs)
The need for parallel computing or HPC

HPC stands for High Performance Computing

Drug discovery

https://www.nature.com/articles/nature21414
The need for parallel computing or HPC

HPC stands for High Performance Computing

Drug discovery

Weather forecasting

https://www.nature.com/articles/nature21414

https://www.ncl.ucar.edu/Applications/wrf.shtml
The need for parallel computing or HPC

HPC stands for High Performance Computing

Drug discovery

Weather forecasting

Study of the universe

HPC stands for High Performance Computing.
Why do we need parallelism?

• Make some science simulations feasible in the lifetime of humans
  • Either due to speed or memory requirements
• Provide answers in realtime or near realtime
Large supercomputers

- Top500 list: https://www.top500.org/lists/top500/2020/06/

<table>
<thead>
<tr>
<th>Rank</th>
<th>System</th>
<th>Cores</th>
<th>Rmax (TFlop/s)</th>
<th>Rpeak (TFlop/s)</th>
<th>Power (kW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.20GHz, Tsubame interconnect D, Fujitsu RIKEN Center for Computational Science Japan</td>
<td>7,299,072</td>
<td>415,530.8</td>
<td>513,854.7</td>
<td>28,305</td>
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<td>2</td>
<td>Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States</td>
<td>2,414,592</td>
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<td>209,794.9</td>
<td>10,096</td>
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<tr>
<td>3</td>
<td>Sierra - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States</td>
<td>1,572,480</td>
<td>96,640.0</td>
<td>125,712.0</td>
<td>7,438</td>
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<tr>
<td>4</td>
<td>Sunway TaihuLight - Sunway MPP, Sunway SW24010 260C 1.8GHz, Sunway, NRPC National Supercomputing Center in Wuxi China</td>
<td>10,649,600</td>
<td>93,014.6</td>
<td>125,435.9</td>
<td>15,371</td>
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<td>5</td>
<td>Tianhe-2A - TH-YB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.20GHz, TH Express-2, Matrix 2000, NUDT National Super Computer Center in Guangzhou China</td>
<td>4,981,760</td>
<td>61,444.5</td>
<td>100,678.7</td>
<td>18,482</td>
</tr>
</tbody>
</table>
Parallel architecture

- A set of nodes or processing elements connected by a network.

https://computing.llnl.gov/tutorials/parallel_comp
Interconnection networks

- Different topologies for connecting nodes together
- Used in the past: torus, hypercube
- More popular currently: fat-tree, dragonfly

Torus

Fat-tree

Dragonfly

A group with 96 Aries routers

Column all-to-all (black) links

Row all-to-all (green) links

Two-level dragonfly with multiple groups

Inter-group (blue) links (not all links are shown)
I/O sub-system / Parallel file system

- Home directories and scratch space typically on a parallel file system
- Mounted on all login and compute nodes

http://wiki.lustre.org/Introduction_to_Lustre
System software: models and runtimes

- Parallel programming model
  - Parallelism is achieved by making calls to a library and the execution model depends on the library used.

- Parallel runtime [system]:
  - Implements the parallel execution model

- Shared memory/address-space
  - Pthreads, OpenMP

- Distributed memory
  - MPI, Charm

User code
Parallel runtime
Communication library
Operating system
Cores, sockets, nodes

- **Core**: a single execution unit that has a private L1 cache and can execute instructions independently.

- **Processor**: several cores on a single Integrated Circuit (IC) or chip are called a multi-core processor.

- **Socket**: physical connector into which an IC/chip or processor is inserted.

- **Node**: a packaging of sockets - motherboard or printed circuit board (PCB) that has multiple sockets.

https://hpc-wiki.info/hpc/HPC-Dictionary
Rackmount servers
Rackmount servers
Rackmount server motherboard

https://www.anandtech.com/show/15924/chenbro-announces-rb13804-dual-socket-1u-xeon-4-bay-hpc-barebones-server

https://www.anandtech.com/show/7003/the-haswell-review-intel-core-i74770k-i54560k-tested
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Job scheduling
Job scheduling

- HPC systems use job or batch scheduling
- Each user submits their parallel programs for execution to a “job” scheduler

<table>
<thead>
<tr>
<th>Job Queue</th>
</tr>
</thead>
<tbody>
<tr>
<td>#Nodes Requested</td>
</tr>
<tr>
<td>------------</td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>6</td>
</tr>
</tbody>
</table>
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- The scheduler decides:
  - what job to schedule next (based on an algorithm: FCFS, priority-based, ….)
  - what resources (compute nodes) to allocate to the ready job

<table>
<thead>
<tr>
<th></th>
<th>#Nodes</th>
<th>Time Requested</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>128</td>
<td>30 mins</td>
</tr>
<tr>
<td>2</td>
<td>64</td>
<td>24 hours</td>
</tr>
<tr>
<td>3</td>
<td>56</td>
<td>6 hours</td>
</tr>
<tr>
<td>4</td>
<td>192</td>
<td>12 hours</td>
</tr>
<tr>
<td>5</td>
<td>…</td>
<td>…</td>
</tr>
<tr>
<td>6</td>
<td>…</td>
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- Compute nodes: dedicated to each job
- Network, filesystem: shared by all jobs
Compute nodes vs. login nodes

- **Compute nodes**: dedicated nodes for running jobs
  - Can only be accessed when they have been allocated to a user by the job scheduler
- **Login nodes**: nodes shared by all users to compile their programs, submit jobs etc.
Supercomputers vs. commodity clusters

- Supercomputer refers to a large expensive installation, typically using custom hardware
  - High-speed interconnect
  - IBM Blue Gene, Cray XT, Cray XC
- Cluster refers to a cluster of nodes, typically put together using commodity (off-the-shelf) hardware
Serial vs. parallel code

- Thread: a thread or path of execution managed by the OS
  - Threads share the same memory address space
- Process: heavy-weight, processes do not share resources such as memory, file descriptors etc.
- Serial or sequential code: can only run on a single thread or process
- Parallel code: can be run on one or more threads or processes
Scaling and scalable

- Scaling: running a parallel program on 1 to \( n \) processes
  - 1, 2, 3, \ldots , n
  - 1, 2, 4, 8, \ldots , n
- Scalable: A program is scalable if its performance improves when using more resources
Scaling and scalable

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- **Scalable**: A program is scalable if its performance improves when using more resources
Weak versus strong scaling

- **Strong scaling:** *Fixed total* problem size as we run on more processes
  - Sorting n numbers on 1 process, 2 processes, 4 processes, …

- **Weak scaling:** Fixed problem size per process but *increasing total* problem size as we run on more processes
  - Sorting n numbers on 1 process
  - 2n numbers on 2 processes
  - 4n numbers on 4 processes
Speedup and efficiency

- **Speedup**: Ratio of execution time on one process to that on $p$ processes

  \[
  \text{Speedup} = \frac{t_1}{t_p}
  \]

- **Efficiency**: Speedup per process

  \[
  \text{Efficiency} = \frac{t_1}{t_p \times p}
  \]
Amdahl’s law

• Speedup is limited by the serial portion of the code
  • Often referred to as the serial “bottleneck”

• Lets say only a fraction $f$ of the code can be parallelized on $p$ processes

\[
\text{Speedup} = \frac{1}{(1 - f) + f/p}
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Amdahl’s law

\[ \text{Speedup} = \frac{1}{(1 - f) + f/p} \]

Total time on 1 process = 100s
Serial portion = 40s
Portion that can be parallelized = 60s

\[ f = \frac{60}{100} = 0.6 \]

\[ \text{Speedup} = \frac{1}{(1 - 0.6) + 0.6/p} \]
Communication and synchronization

- Each process may execute serial code independently for a while
- When data is needed from other (remote) processes, messaging occurs
  - Referred to as communication or synchronization or MPI messages
- Intra-node vs. inter-node communication
- Bulk synchronous programs: All processes compute simultaneously, then synchronize together
Different models of parallel computation

- SIMD: Single Instruction Multiple Data
- MIMD: Multiple Instruction Multiple Data
- SPMD: Single Program Multiple Data
  - Typical in HPC