CMSC 714
High Performance Computing
Lecture 2 - Introduction

https://www.cs.umd.edu/class/fall2023/cmsc714

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Notes

- Slides from 1st lecture posted
- Cluster accounts on zaratan handed out and first assignment probably late next week

Last time

- Why parallel computing?
  - speed, cost
- Parallel computing basics
  - Processing elements, memory, network, disks
  - SIMD, MIMD, SPMD, dataflow
  - networks
    - bus, ring, tree, mesh (2D or 3D), hypercube
  - memory
    - latency and throughput (bandwidth)
    - shared vs. distributed (physically and logically)
    - UMA vs. NUMA

Coordination

- Since parallelism in our view is processors working *together* to solve a problem
- Synchronization
    - protection of a single object (e.g., locks)
    - coordination of processors (e.g., barriers)
- Size of a unit of work by a processor
    - need to manage two issues
        - load balance - processors have equal work
        - coordination overhead - communication and synchronization
    - often called "grain" size - coarse grain vs. fine grain

Terminology: Serial vs. parallel code

- Thread: a unit of execution managed by the OS
  - Threads can share memory, multiple ones can run in the same address space
- Process: heavy-weight, processes do not share resources such as memory, file descriptors etc.
  - A process consists of an address space and one or more threads running in it
- Serial or sequential code: can only run in a single thread or process
- Parallel code: can be run on one or more threads or processes

Sources of Parallelism

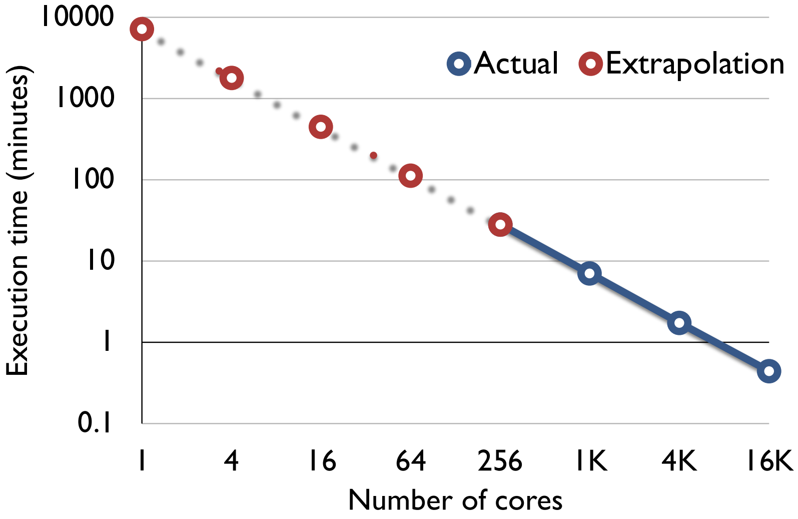
- Statements
  - called “control parallel”
  - can perform a series of steps in parallel
  - basis of dataflow computers
- Loops
  - called “data parallel”
  - most common source of parallelism for most programs
  - each processor/core gets one (or more) iterations to perform

Examples of Parallelism

- Easy (embarrassingly parallel)
  - multiple independent jobs (i.e., different simulations)
- Scientific
  - dense linear algebra (divide up matrix)
  - physical system simulations (divide physical space)
- Databases
  - biggest success of parallel computing (divide tuples)
    - exploits semantics of relational algebra
- AI
  - search problems (divide search space)
  - pattern recognition and image processing (divide image)

Metrics in Application Performance

- Speedup
  - ratio of time on one node to time on *n* nodes
  - hold problem size fixed (**strong** scaling)
  - should compare to best serial time
  - goal is linear speedup
  - super-linear speedup is possible due to:
    - adding more memory/cache
    - search problems
- Iso-Speedup (or scaled or **weak** speedup)
  - scale data size up with number of nodes
  - goal is a flat horizontal curve
- Amdahl's Law
  - max speedup is 1/(serial fraction of time), or 1 / (1 – f + f/s) as s →∞
- Computation to Communication Ratio
  - goal is to maximize this ratio



How to Write Parallel Programs

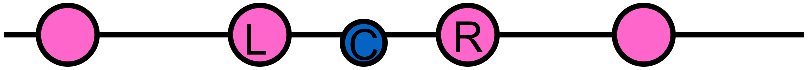
- Use old serial code
  - compiler converts it to parallel
  - called the dusty deck problem
- Serial Language plus Communication Library
  - no compiler changes required!
  - MPI uses this approach
- New language for parallel computing
  - requires all code to be re-written
  - hard to create a language that provides high performance on different platforms
- Hybrid Approach – old language(s), new constructs
  - PGAS – variants of C/Fortran/Java with combination of shared memory view of data, but awareness of data being distributed on the hardware
  - have parallel loops and synchronization operations

Application Example - Weather

- Typical of many scientific codes
  - computes results for three dimensional space
  - compute results at multiple time steps
  - uses equations to describe physics/chemistry of the problem
  - grids are used to discretize continuous space
    - granularity of grids is important to speed/accuracy
- Simplifications (for example, not in real code)
  - earth is flat (no mountains)
  - earth is round (poles are really flat, earth bulges at equator)
  - second order properties

Grid Points

- Divide Continuous space into discrete parts
  - for this code, grid size is fixed and uniform
    - possible to change grid size or use multiple grids
  - use three dimensional grid
    - two for latitude and longitude
    - one for elevation
    - Total of M * N * L points
- Design Choice: where is the grid point?
  - left, right, or center of the interval for a grid element



  - in multiple dimensions this multiplies:
    - for 3 dimensions have 27 possible positions

Variables

- One dimensional
  - m - geo-potential (gravitational effects)
- Two dimensional
  - pi - “shifted” surface pressure
  - sigmadot - vertical component of the wind velocity
- Three dimensional (primary variables)
  - <u,v> - wind velocity/direction vector
  - T - temperature
  - q - specific humidity
  - p - pressure
- Not included
  - clouds
  - precipitation
  - can be derived from others

Serial Computation

- Convert equations to discrete form
- Update from time t to $t + \delta_t$

```
foreach longitude, latitude, altitude
    ustar[i,j,k] = n * pi[i,j] * u[i,j,k]
    vstar[i,j,k] = m[j] * pi[i,j] * v[i,j,k]
    sdot[i,j,k] = pi[i,j] * sigmadot[i,j]
end
foreach longitude, latitude, altitude
    D = 4 * ((ustar[i,j,k] + ustar[i-1,j,k]) * (q[i,j,k] + q[i-1,j,k]) +
                terms in {i,j,k}{+,-}{1,2}
    piq[i,j,k] = piq[i,j,k] + D * delat
    similar terms for piu, piv, piT, and pi
end
foreach longitude, latitude, altitude
    q[i,j,k] = piq[i,j,k]/pi[i,j,k]
    u[i,j,k] = piu[i,j,k]/pi[i,j,k]
    v[i,j,k] = piv[i,j,k]/pi[i,j,k]
    T[i,j,k] = piT[i,j,k]/pi[i,j,k]
end
```

Shared Memory Version

- in each loop nest, iterations are independent
- use a parallel for-loop for each loop nest
- synchronize (barrier) after each loop nest
  - this is overly conservative, but works
  - could use a single sync variable per element, but would incur excessive overhead
- potential parallelism is M * N * L
- private variables: D, i, j, k
- Advantages of shared memory
  - easier to get something working (ignoring performance)
- Hard to debug
  - other processors can modify shared data

Distributed Memory Version

- decompose data to specific processors
  - assign a cube to each processor
    - maximize volume to surface ratio
    - which minimizes communication/computation ratio
  - called a <block,block,block> distribution
- need to communicate {i,j,k}{+,-}{1,2} terms at boundaries
  - use send/receive to move the data
  - no need for barriers, send/receive operations provide sync
    - do sends earlier in computation to hide communication time
- Advantages
  - easier to debug? maybe
  - consider data locality explicitly with data decomposition
    - better performance/scaling
- Problems
  - harder to get the code running

Database Applications

- Too much data to fit in memory (or sometimes disk)
  - data mining applications (K-Mart had a 4-5TB database many years ago)
  - imaging applications (NASA and others have sites with multiple petabytes to exabytes)
    - use a fork lift to load tapes by the pallet
- Sources of parallelism
  - within a large transaction
  - among multiple transactions
- Join operation
  - form a single table from two tables based on a common field
  - try to split join attribute into disjoint buckets
    - if know data distribution is uniform its easy
    - if not, try hashing

Parallel Search (TSP)

- may appear to be faster than 1/n
  - but this is not really the case either
- Algorithm
  - compute a path on a processor
    - if our path is shorter than the shortest one, send it to the others.
    - stop searching a path when it is longer than the shortest.
  - before computing next path, check for word of a new min path
  - stop when all paths have been explored.
- Why it appears to be faster than 1/n speedup
  - we found the path that was shorter sooner
  - however, the reason for this is a different search order!

Load balance and grain size

- Load balance: try to balance the amount of work (computation) assigned to different threads/ processes
  - Bring ratio of maximum to average load as close to 1 as possible
  - Secondary consideration: also load balance amount of communication
- Grain size: ratio of computation-to-communication
  - Coarse-grained (more computation) vs. fine-grained (more communication)

Ensuring a fair speedup

- T_{serial} = fastest of
  - best known serial algorithm
  - simulation of parallel computation
    - use parallel algorithm
    - run all processes on one processor
  - parallel algorithm run on one processor
- If speedup appears to be super-linear
  - check for memory hierarchy effects
    - increased cache or real memory may be reason
  - verify order of operations is the same in parallel and serial cases