High-Performance and Distributed Computing

Why?

- Code is too slow
- Can’t fit problem in memory

How?

- In approximate decreasing order of reward/effort:
  - Algorithms
  - Implementation
  - Parallel computing
    - Shared memory
    - Distributed memory

Algorithms

- Sorting ($n*\log(n)$ vs. n^2)
- Searching ($\log(n)$ vs. n)
- Shortest paths
- Don’t reinvent the wheel

Won’t discuss more today.

Implementation

- Make the code efficient before considering parallel computing
- 10x to 100x speedups not uncommon
- We’ll see some general guidelines

Why is code slow?

- Computing more than is necessary
- Accessing memory more than is necessary
- Compiled to inefficient low-level instructions

Example

```
x₁ = A\b₁ # solve Ax₁ = b₁
x₂ = A\b₂ # solve Ax₂ = b₂
```

How are linear systems solved?

- Idea: triangular systems are easy to solve
- Compute $A = LU$, where L is lower triangular and U is upper triangular (Gaussian elimination)
- Solve $x = U^{-1}L^{-1}b$

Example

```
x₁ = A\b₁ # solve Ax₁ = b₁
x₂ = A\b₂ # solve Ax₂ = b₂
# About twice as fast:
LU = lufact(A)
x₁ = LU\b₁
x₂ = LU\b₂
```

Example

- If matrix is symmetric positive definite, then Cholesky factorization is twice as fast as LU
  - `cholfact` in Julia
- **lufact.jl**

More

- Symmetric but not positive definite?
  - `bkfact` (Bunch-Kaufman)
- Sparsity
- **Large speedups possible by using better linear algebra** (4x speedup in our example)

In optimization

- When solving a sequence of LPs, can “hot-start” the simplex algorithm using previous optimal basic solution
  - Available in JuMP

Memory access

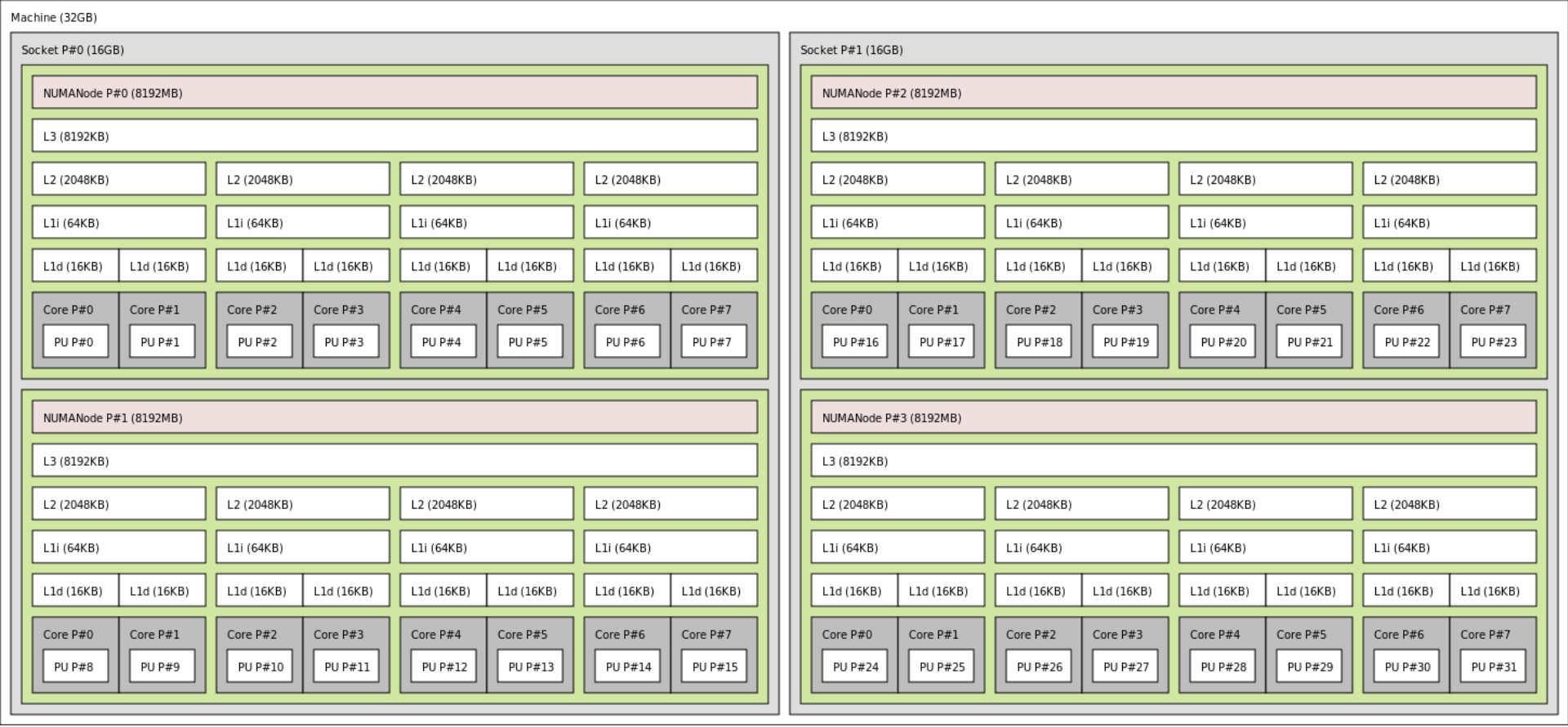
- RAM = Random-access memory
- Random memory access is about 100x slower than a floating-point operation

Memory access

- Random memory access is about 100x slower than a floating-point operation

Hardware solution

- Processor **predicts** which memory will be accessed soon and fetches it into a **cache** that’s faster to access
  - How?



Memory hierarchy of AMD Bulldozer (http://en.wikipedia.org/wiki/File:Hwloc.png)

Example

- Compute properties of a vector
  - L2, L1 norms and min/max element
- Single pass vs. built-in functions
- **locality.jl**

Example: reusing memory

```
function normalize!(x)
    n = norm(x)
    for i in 1:length(x)
        x[i] /= n
    end
end
```

Example: reusing memory

```
x = rand(100_000_000);  # 800Mb
@time x/norm(x);
```

“elapsed time: 0.65 seconds”

```
@time normalize!(x);       # includes compilation
```

“elapsed time: 0.49 seconds”

```
@time normalize!(x);
```

“elapsed time: 0.30 seconds”

Efficient low-level operations

- BLAS/LAPACK
  - http://www.netlib.org/lapack/
  - Efficient implementation of linear algebra operations
    - 20+ years of tuning
    - Commercial implementations
  - Used internally by MATLAB, Scipy, R, Julia
  - Good to use when possible!

Example: axpy

- BLAS function axpy: $y \leftarrow \alpha x + y$
- **axpy.jl**

Gradient descent example

- **gradient.jl**: Let's make this faster
- `x = x - (stepsize/2^k)*grad`
  - Creates a new vector at each iteration
  - Use AXPY instead
  - Also "...`fval - f(x - (stepsize/2^k)*grad)<...`"
- Solution: **gradient2.jl**

`f(x) = (1/2)*dot(x,Q*x); fgrad(x) = Q*x`

`Q*x` is computed twice. Restructure the code to use a single function that returns the value and gradient:

```
function genF(Q)
    function f_and_fgrad(x)
        grad = Q*x
        return ((1/2)*dot(x,grad), grad)
    end
end
```

- **gradient3.jl**

We’re still allocating a new vector for the gradient for each call to `f`. Instead use:

```
function genF(Q)
    function f_and_fgrad(x,grad_out)
        A_mul_B!(grad_out,Q,x)
        return (1/2)*dot(x,grad_out)
    end
end
```

- **gradient4.jl**

One more thing

Q is symmetric. Let's use a specialized function for symmetric matrix-vector products:

```
function f_and_fgrad(x,grad_out)
        # grad_out <- 1.0*Q*x + 0.0*grad_out
        BLAS.symv!('u',1.0,Q,x,0.0,grad_out)
        return (1/2)*dot(x,grad_out)
end
```

- **gradient5.jl**

Thoughts

- Reusing calculations, reusing memory, advanced linear algebra
- Applies to all languages
  - In Julia, don’t need to code critical parts in C

Thoughts

- “Premature optimization is the root of all evil” – Knuth
- Identify and fix bottlenecks **after** running
- Balance between readability and performance

Break

Parallel Computing

- Executing part of an algorithm using multiple simultaneous processors

Amdahl’s Law

- What can we expect?
- If 75% of an algorithm (by time) can be parallelized, what’s the best speedup we can obtain?

Amdahl's Law

More generally, if proportion x of algorithm can be parallelized, then with n parallel threads, the best execution time we can expect is:

$$(1-x) + x/n$$

What is easy to parallelize?

- Independent function evaluations
- Monte Carlo

Common, less trivial, uses:

- Linear algebra
- Physical simulations (chemistry, fluid dynamics, particles)

Shared memory

- All cores have access to the same RAM
- Example: your laptop
- Up to 100s of cores

Shared memory

What’s difficult?

- Multiple cores can write to the same block of memory at the same time
- Memory bandwidth is shared

Distributed memory

- “Network of computers”
- Communication? **Interconnect**
  - Bandwidth
  - Latency
- “distributed” vs. “parallel” computing

“Distributed” computing

- Slow interconnect, e.g. ethernet (ms latency), carrier pigeons
- Examples:
  - The cloud
  - Network of machines at a university
- Uses:
  - Mostly independent calculations with some synchronization

“Parallel” computing

- Fast interconnect, e.g. InfiniBand (µs latency)
- Examples:
  - “Supercomputers” (http://www.top500.org/lists/2013/11/)
  - High-performance clusters
- Uses:
  - Solving 100,000 x 100,000 dense linear system
  - Solving LPs with 10^9 variables
  - Numerical PDE simulations

Programming models

- Message passing (MPI)
  - Explicitly send and receive data
- Master-worker
  - Distribute tasks to workers
- MapReduce (saw this on Tuesday)

Parallel computing in Optimization

Math Meth Oper Res (2012) 76:67–93
DOI 10.1007/s00186-012-0390-9

ORIGINAL ARTICLE

Could we use a million cores to solve an integer program?

Thorsten Koch · Ted Ralphs · Yuji Shinano

School of Mathematics

How to solve QPs with 10^9 variables

Andreas Grothey, Jacek Gondzio

Parallel computing in Optimization

On a smaller scale (shared memory):

- Parallel barrier method
  - Using parallel sparse linear algebra
- No general parallel simplex method
- Parallel IP
  - Parallel branch & bound
- In JuMP: `Model(solver=GurobiSolver(Threads=10))`

Parallel linear algebra

- Via BLAS/LAPACK
- **threads.jl**

In Julia

- Distributed memory (except for BLAS)
  - Multiple processes on a single machine or across machines via ssh
- http://docs.julialang.org/en/release-0.2/manual/parallel-computing/
- **parfor.jl**
- **pmap.jl**

Case study

- Parallel computing for data-driven modeling optimization

Cutting-plane method

$$\min \sum f_n(x)$$

- f_n convex, non-smooth
- Can obtain subgradients:
  - $f_n(x') \geq f_n(x) + g^T(x'-x)$
- Idea:
  - Given a set of subgradients, we can form a piecewise linear model of each f_n

Cutting-plane method

$$\min \sum f_n(x)$$

- Idea:
  - Given a set of subgradients, we can form a piecewise linear model m_n of each f_n
- Algorithm:
  - Solve $\min \sum m_n(x)$
  - Evaluate each $f_n(x^*)$. If model $m_n(x^*)$ doesn't match $f_n(x^*)$, then update model with new subgradient and repeat.

Cutting-plane method

- Algorithm:
  - Solve $\min \sum m_n(x)$
  - **Evaluate each** $f_n(x^*)$. If model $m_n(x^*)$ doesn't match $f_n(x^*)$, then update model with new subgradient and repeat.
- Evaluation is trivially parallel.
- Classical parallel decomposition example in optimization

The problem

Decide the optimal capacity of each Hubway station using historical data

Our formulation

- x - vector of station capacities
- $f_n(x)$ - cost of reshuffling bikes between stations (once per hour) so that all demand is met
  - Assume demands (trips) for each day are **known in advance**, optimal reshuffling can be formulated as a network flow problem
- Objective: design station capacities to minimize reshuffling costs

The code

- Proof of concept, not polished
- Let’s run it on 50 cores…
- **master.jl** and **subproblem.jl**

Extensions

- Visualize solution
- Refine the model
- Time the master and subproblems, apply Amdahl’s law

Computing resources

- Amazon EC2
- University clusters

Thanks!