A Survey of Parallelism in Solving Numerical Optimization and Operations Research Problems

Jonathan Eckstein
Rutgers University, Piscataway, NJ, USA
(formerly of Thinking Machines Corporation)
(also consultant for Sandia National Laboratories)

RUTGERS

RUTGERS
Rutgers Business School
Newark and New Brunswick

Sandia National Laboratories

- I am not primarily a computer scientist

- I am not primarily a computer scientist

- I am “user” interested in implementing a particular (large) class of applications

- I am not primarily a computer scientist
- I am “user” interested in implementing a particular (large) class of applications

- I am not primarily a computer scientist
- I am “user” interested in implementing a particular (large) class of applications

- Well, a *relatively* sophisticated user…

Optimization

- Minimize some objective function of many variables
- Subject to constraints, for example
  - Equality constraints (linear or nonlinear)
  - Inequality constraints (linear or nonlinear)
  - General conic constraints (*e.g.* cone of positive semidefinite matrices)
  - Some or all variables integral of binary

- Applications
  - Engineering and system design
  - Transportation/logistics network planning and operation
  - Machine learning
  - Etc., etc...

Overgeneralization: Kinds of Optimization Algorithms

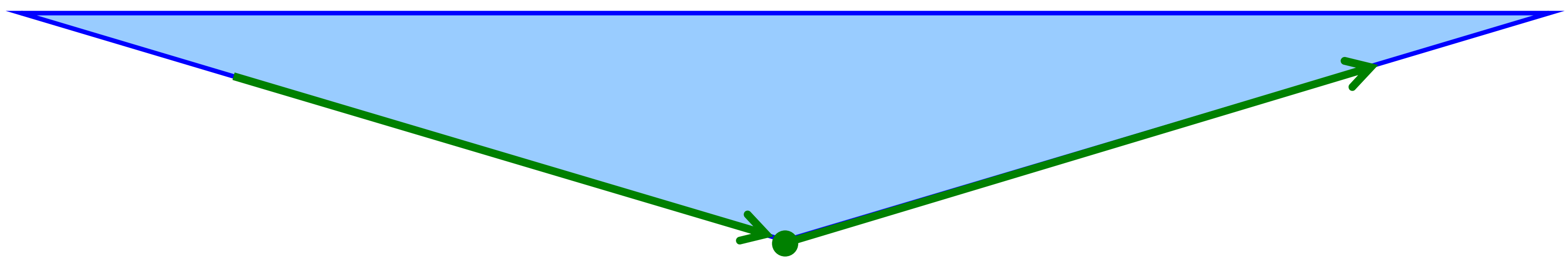
- For “easy” but perhaps very large problems
  - All variables typically continuous
  - Either looking only for local optima, or we know any local optimum is global (convex models)
  - Difficulty may arise extremely large scale

- For “hard” problems
  - Discrete variables, and not in a known “easy” special class like shortest path, assignment, max flow, etc., or…
  - Looking for a provably global optimum of a nonlinear continuous problem with local optima

Algorithms for "Easy" Problems

- Popular standard methods (not exhaustive!) that do not assume a particular block or subsystem structure
  - Active set (for example, simplex)
  - Newton barrier ("interior point")
  - Augmented Lagrangian
- *Decomposition* methods (many flavors) – exploit some kind of high-level structure

Non-Decomposition Methods: Active Set



- Canonical example: simplex
- Core operation: a *pivot*
  - o Have a usually sparse nonsingular matrix B factored into LU
  - o Replace one column of B with a different sparse vector
  - o Want to update the factors LU to match
- The general sparse case has resisted effective parallelization
- Dense case may be effectively parallelized (E *et al.* 1995 on CM-2, Elster *et al.* 2009 for GPU's)
- Some special cases like just "box" constraints are also fairly readily parallelizable

Non-Decomposition Methods: Newton Barrier

- Avoid combinatorics of constraint intersections
  - Use a barrier function to "smooth" the constraints (often in a "primal-dual" way)
  - Apply one iteration of Newton's method to the resulting nonlinear system of equations
  - Tighten the smoothing parameter and repeat
- Number of iterations grows weakly with problems size
- Main work: solve a linear system involving

$$M = \begin{bmatrix} H & -J^\top \\ J & D \end{bmatrix}$$

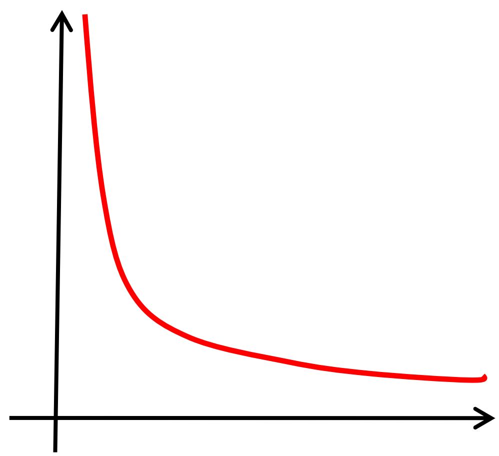
- System becomes increasingly ill-conditioned
- Must be solved to high accuracy

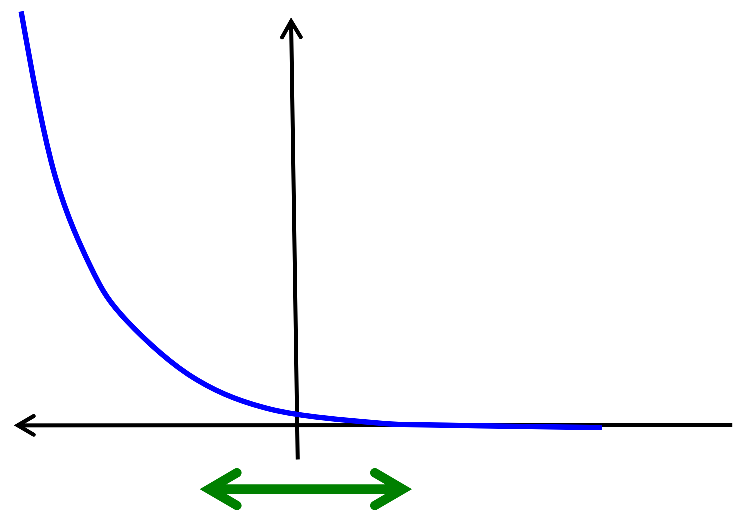
Non-Decomposition Methods: Newton Barrier

- Parallelization of this algorithm class is dominated by linear algebra issues
- Sparsity pattern and factoring of M is in general more complex than for the component matrices H, J, etc.
- Many applications generate sparsity patterns with low-diameter adjacency graphs
  - o PDE-oriented domain decomposition approaches may not apply
- Iterative linear methods can be tricky to apply due to the ill-conditioning and need for high accuracy
- A number of standard solvers offer SMP parallel options, but speedups tend to be very modest (i.e. 2 or 3)

Non-Decomposition Methods: Augmented Lagrangians

- Smooth constraints with a penalty instead of a barrier; use Lagrange multipliers to "shift" the penalty; do not have to increase penalty level indefinitely





- Creates a series of subproblems with no constraints, or much simpler constraints
- Subproblems are nonlinear optimizations (not linear systems)
- But may be solved to low accuracy
- Parallelization efforts focused on decomposition variants, but the standard, basic approach may be parallelizable

Decomposition Methods

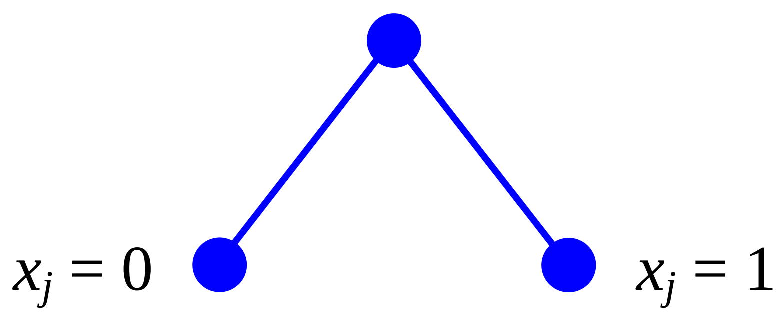
- Assume a problem structure of relatively weakly interacting subsystems
  - This situation is common in large-scale models
- There are many different ways to construct such methods, but there tends to be a common algorithmic pattern:
  - Solve a perturbed, independent optimization problem for each subsystem (potentially in parallel)
  - Perform a *coordination step* that adjusts the perturbations, and repeat
- Sometimes the coordination step is a non-trivial optimization problem of its own – a potential Amdahl’s law bottleneck
- Generally, “tail convergence” can be poor
- Some successful parallel applications, but highly domain-specific

Algorithms for “Hard” Problems: Branch and Bound

- *Branch and bound* is the most common algorithmic structure. Integer programming example:

$$\begin{aligned} \min \quad & c^\top x \\ \text{ST} \quad & Ax \le b \\ & x \in \{0,1\}^n \end{aligned}$$

  - Relax the $x \in \{0,1\}^n$ constraint to $\mathbf{0} \le x \le \mathbf{1}$ and solve as an LP
  - If all variables come out integer, we’re done
  - Otherwise, divide and conquer: choose j with $0 < x_j < 1$ and branch



Branch and Bound Example Continued

- Loop: pool of *subproblems* with subsets of fixed variables
  - Pick a subproblem out of the pool
  - Solve its LP
  - If the resulting objective is worse than some known solution, throw it away (prune)
  - Otherwise, divide the subproblem by fixing another variable and put the resulting children back in the pool

- The algorithm may be generalized/abstracted to many other settings
  - Including global optimization of continuous problems with local minima

Branch and Bound

- In the worst case, we will enumerate an exponentially large tree with all possible solutions at the leaves
- Thus, relatively small amounts of data can generate very difficult problems
- If the bound is "smart" and the branching is "smart", this class of algorithms can nevertheless be extremely useful and practical
  - For the example problem above, the LP bound may be greatly strengthened by using *polyhedral combinatorics* – adding additional linear constraints implied by combining $x \in \{0,1\}^n$ and $Ax \leq b$
  - Clever choices of branching variable or different ways of branching have enormous value

Parallelizing Branch and Bound

- Branch and bound is a “forgiving” algorithm to parallelize
  - o Idea: work on multiple parts of the tree at the same time
  - o But trees may be highly unbalanced and their shape is not predictable
  - o A variety of load-balancing approaches can work very well
- A number object-oriented parallel branch-and-bound frameworks/libraries exist, including
  - o PEBBL/PICO (E *et al.*)
  - o ALPS/BiCePS/BLIS (Ralphs *et al.*)
  - o BOB (Lecun *et al.*)
  - o OOBB (Gendron *et al.*)
- Most production integer programming solvers have an SMP parallel option: CPLEX, XPRESS-MP, GuRoBi, CBC

Effectiveness of Parallel Branch and Bound

- I have seen examples with near-linear speedup through hundreds of processors, and it should scale up further
- Sometimes there are even apparently superlinear speedup anomalies (for which there are reasonable explanations)
- I have also seen disappointing speedups. Why?
  - Non-scalable load balancing techniques
    - Central pool for SMPs or master-slave
  - Task granularity not matched to platform
    - Too fine $\Rightarrow$ excessive overhead
    - Too coarse $\Rightarrow$ too hard to balance load
  - Ramp-up/ramp-down issues
  - Synchronization penalties from requiring determinism

Big Picture: Where We Are (Both "Hard" and "Easy" Problems)

- Most numerical optimization is done by large, encapsulated solvers / callable libraries which encapsulate the expertise of numerical optimization experts
- Models are often passed to these libraries using specialized modeling languages
  - Leading example: AMPL
  - Digression – challenge to merge these optimization model description languages with a usable procedural language

Monolithic Solvers and Callable Libraries

- These libraries / solvers have some parameters (often poorly understood by our users), but are otherwise fairly monolithic
- Results
  - o Minimal or no speedups on LP and other continuous problems
  - o Moderate speedups on hard integer problems
  - o Usually available only on SMP platforms
- Why?
  - o "Hard" problems: we need to assemble the right teams
  - o "Easy" problems: we need a different approach

“Hard” Problems

- For branch-and-bound-related algorithms, the monolithic approach can take us much farther than we are today
- Today’s parallel implementations are somewhat weak, but the right combination of domain knowledge and implementation knowledge should yield monolithic solvers that could exploit parallelism far better

“Easy” (But Huge) Problems

- The monolithic approach will not get us much farther
- Fully analyzing the structure of a gigantic problem and picking the optimal problem partitioning & solution algorithm is a tall order
  - o To work effectively, a monolithic parallel solver must analyze the input model much more deeply than a serial one

New Approaches for Large "Easy" Problems

1. Better decomposition algorithms – but results will probably be application-specific

2. A "toolkit" approach for non-decomposition algorithms
   - Provide high-quality, rigorous fundamental optimization algorithms
     - Avoid user *ad hoc* approaches and "reinventing the wheel" for basic optimization algorithms
   - But give users control over data layout and function / gradient evaluation to best suit their application
   - Somewhat similar in spirit to CMSSL
   - Could still plug this framework to a monolithic solver that attempts to analyze problem structure and find good decomposition strategies

A Particular Approach I'm Working On

- "Outer loop": augmented Lagrangian with a relative error criterion (E + Silva 2010)
  - Generates a sequence of nonlinear box-constrained subproblems solved to gradually increasing accuracy
- "Inner loop": CG-DESCENT/ASA (Hager and Zhang 2005/2006), with minor modifications for parallelism
- User provides
  - "Primal layout": assignment of variables to processors (some may be replicated on multiple processors)
  - "Dual layout": assignment of constraints to processors (some may be replicated on multiple processors)
  - Function / gradient evaluators adapted to these layouts
- Asking for parallelization help from user, ...
  - but in a natural application domain (not matrix factoring)

Programming Environments

- What framework should we implement this in?
- What framework should we ask our users to employ for the function / gradient evaluator?
- What approach would make applications as portable as possible?

- C++ / MPI ? (what I do most of my current work in)
- CUDA ?
- OpenCL ?

- Yecch...

Programming Environments

- These environments are the assembly languages of parallelism

- Literally:
  - CUDA and OpenCL resemble C/PARIS, the assembly language of the CM-2

- Conceptually:
  - Low level of abstraction
  - Lots of clutter
  - Will only work (well) on certain families of platforms

Wish List

- We need a "C of parallelism"
  - o Something that allows reasonably low level control and is built for performance
  - o But also supports a proper level of abstraction
  - o ... and is not heavily platform dependent
- Is it possible? PGAS? Chapel? UPC? Fortress? ?
- Note:
  - o The #1 linear programming code of the 60's-80's (MPSX) was written in IBM/360 assembler
  - o Competitors were in FORTRAN
  - o In the 80's, they were swept aside by fast C codes
- If the right tools are there, they will get used

Wish List Continued

- Ideally, should be a superset of a recognizable standard language
  - We'll need users to code modules for us
  - Otherwise, it should interface easily to standard languages
- Aggregate operation support
  - Witness popularity of MATLAB, despite its many flaws
  - Also SciPy
- But also some kind of task / nested parallelism
  - More than just data parallelism and aggregate operations
- "Locality" support
  - Must express more than a flat global address space