Graph Coloring in Parallel Processing and Scientific Computing

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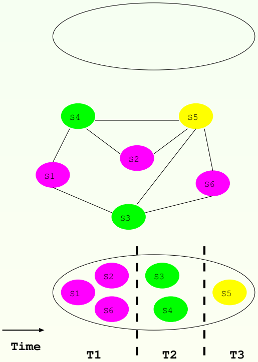
CSCAPES Workshop, June 2008, Santa Fe, NM

Coloring in parallel processing

- A distance-1 coloring of $G = (V, E)$ is
  - a mapping $\phi : V \rightarrow \{1, 2, \dots, q\}$ s.t. $\phi(u) \neq \phi(v)$ whenever $(u, v) \in E$
  - a partitioning of V into q independent sets

  The objective is to minimize q

- Distance-1 coloring is used to discover concurrency in parallel scientific computing. Examples:
  - iterative methods for sparse linear systems (Jones & Plassmann, 94)
  - adaptive mesh refinement
  - preconditioners (Saad, 96; Hysom & Pothen, 01)
  - eigenvalue computation (Manne, 98)
  - sparse tiling (Strout et al, 02)



Coloring in automatic differentiation: context

Procedure $\textsc{SparseCompute}(F : R^n \to R^m)$

S1. Determine the sparsity structure of the derivative (first or second) matrix $A \in R^{m \times n}$ of the function F

S2. Obtain a seed matrix $S \in \{0,1\}^{n \times q}$ with the smallest q

S3. Compute the numerical values of the entries of the compressed matrix $B = AS \in R^{m \times q}$

S4. Recover the numerical values of the entries of A from B

The seed matrix S partitions the columns of A:

$$s_{jk} = \begin{cases} 1 & \text{iff column } a_j \text{ belongs to group } k, \\ 0 & \text{otherwise.} \end{cases}$$

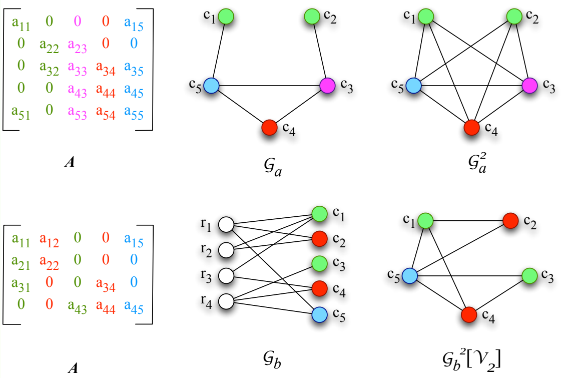
It is obtained using an appropriate coloring on the graph of A.

Coloring model variations in derivative computation via compression

Sources of problem variation:

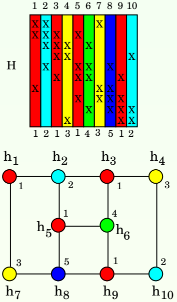
- Type of derivative matrix
  - Jacobian (nonsymmetric)
  - Hessian (symmetric)
- Recovery method
  - Direct
  - Substitution
- Dimension of partitioning (for the Jacobian case)
  - Unidirectional (only columns or rows)
  - Bidirectional (both columns and rows)

An archetypal model for direct methods



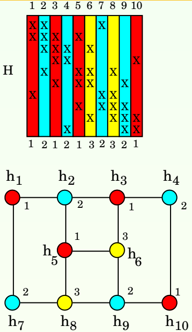
Structurally orthogonal partition of matrix A equivalent to:

- Distance-2 coloring of the adjacency graph $G_a(A) = (V, E)$ when A is symmetric (McCormick, 1983)
- Partial distance-2 coloring of the bipartite graph $G_b(A) = (V_1, V_2, E)$ when A is nonsymmetric (GMP, 2005)
- Distance-1 coloring of the appropriate square graph (Coleman and Moré, 1983)



$$\begin{pmatrix} h_{11} & h_{12} & h_{17} & 0 & 0 \\ h_{21}+h_{23}+h_{25} & h_{22} & 0 & 0 & 0 \\ h_{33} & h_{32} & h_{34} & h_{36} & 0 \\ h_{43} & h_{4,10} & h_{44} & 0 & 0 \\ h_{55} & h_{52} & 0 & h_{56} & h_{58} \\ h_{63}+h_{65}+h_{69} & 0 & 0 & h_{66} & 0 \\ h_{71} & 0 & h_{77} & 0 & h_{78} \\ h_{85}+h_{89} & 0 & 0 & 0 & h_{88} \\ h_{99} & h_{9,10} & 0 & h_{96} & h_{98} \\ h_{10,9} & h_{10,10} & h_{10,4} & 0 & 0 \end{pmatrix}$$

- Symmetrically orthogonal partition: whenever $h_{ij} \neq 0$
  - h_j only column in a group with nonzero at row i or
  - h_i only column in a group with nonzero at row j
- Star coloring: a vertex coloring ϕ of $G_a(H)$ s.t.
  - ϕ is a distance-1 coloring and
  - every path on 4 vertices (P_4) uses at least 3 colors
- SymOP equivalent to star coloring (Coleman and Moré, 84)



$$\begin{pmatrix} h_{11} & h_{12}+h_{17} & 0 \\ h_{21}+h_{23}+h_{25} & h_{22} & 0 \\ h_{33} & h_{32}+h_{34} & h_{36} \\ h_{43}+h_{4,10} & h_{44} & 0 \\ h_{55} & h_{52} & h_{56}+h_{58} \\ h_{63}+h_{65} & h_{69} & h_{66} \\ h_{71} & h_{77} & h_{78} \\ h_{85} & h_{87}+h_{89} & h_{88} \\ h_{9,10} & h_{99} & h_{96}+h_{98} \\ h_{10,10} & h_{10,4}+h_{10,9} & 0 \end{pmatrix}$$

- Substitutable partition: whenever $h_{ij} \neq 0$
  - h_j in a group where all nonzeros in row i are ordered before h_{ij} or
  - h_i in a group where all nonzeros in row j are ordered before h_{ij}
- Acyclic coloring: a vertex coloring ϕ of $G_a(H)$ s.t.
  - ϕ is a distance-1 coloring and
  - every cycle uses at least 3 colors
- Substitutable partition equivalent to acyclic coloring (Coleman and Cai, 86)

General sparsity pattern:

	unidirectional partition	bidirectional partition	
Jacobian	distance-2 coloring	star bicoloring	Direct
Hessian	star coloring (restricted star coloring)	NA	Direct
Jacobian	NA	acyclic bicoloring	Substitution
Hessian	acyclic coloring (triangular coloring)	NA	Substitution

Nonsym A $\quad G_b(A) = (V_1, V_2, E)$

Sym A $\quad G(A) = (V, E)$

Regular sparsity pattern (discretization of structured grids):

- Formula-based coloring (Goldfarb and Toint, 1984)
- Hierarchical coloring (Hovland, 2007)

Outline

1. Models
   - Parallel scientific computing
   - Derivative computation
2. Sequential algorithms
3. Case studies
4. Parallel algorithms
5. Summary

- Distance-k, star, and acyclic coloring are NP-hard (they are also hard to approximate)
- A greedy heuristic usually gives a good solution

  GREEDY($G = (V, E)$)

      Let $v_1, v_2, \ldots, v_n$ be an ordering of V

      for $i = 1$ to n **do**

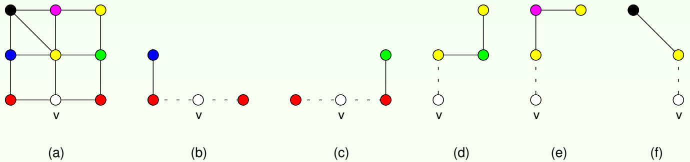
          determine forbidden colors to v_i

          assign v_i the smallest permissible color

      end-for
- For distance-k coloring, GREEDY can be implemented to run in $O(n\overline{d}_k)$ time, where $\overline{d}_k$ is the average degree-k
- We have developed $O(n\overline{d}_2)$-time heuristic algorithms for star and acyclic coloring

  Key idea: exploit the structure of two-colored induced subgraphs

A new star coloring heuristic algorithm

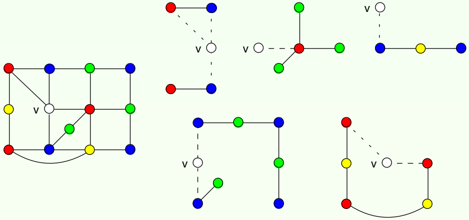


Algorithm (Input: $G = (V, E)$):
for each $v \in V$

1. Choose color for v
   - forbid colors used by neighbors $N(v)$ of v
   - forbid colors leading to two-colored P_4
     - $\forall \{w, x\} \subseteq N(v)$ where $\phi(w) = \phi(x)$, forbid colors used by $N(w)$ and $N(x)$
     - $\forall$ non-single-edge star S incident on v, forbid color of hub of S
2. Update collection of two-colored stars

Time: $O(|V|\bar{d}_2)$ Space: $O(|E|)$

A new acyclic coloring heuristic algorithm



Algorithm (Input: $G = (V, E)$):
for each $v \in V$

1. Choose color for v
   - forbid colors used by neighbors $N(v)$ of v
   - forbid colors leading to two-colored cycles
     - $\forall$ tree T incident on v, if v adj to ≥ 2 vertices of *same* color, forbid the other color in T
2. Update collection of two-colored trees (merge if necessary)

Time: $O(|V|\overline{d}_2 \cdot \alpha)$ Space: $O(|E|)$

Performance comparison:

new star and acyclic coloring algorithms vs previous algorithms

	$\lvert V \rvert$ in 1000	$\lvert E \rvert$ in 1000	MaxDeg	MinDeg	AvgDeg
range	10 – 150	50 – 17,000	8 – 860	0 – 230	3 – 600
sum	1,500	88,000	6,400	800	4,200

Table: Summary of size and density of test graphs (total: 29).

	D2	RS	NS	S	T-sl	A	D1
colors	9,240	8,749	7,636	7,558	5,065	4,110	1,757
time (min)	28.2	34.4	930	162	12.4	32.5	0.04

Table: Total number of colors and runtime, summed over all test cases.

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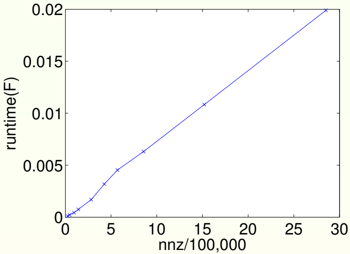
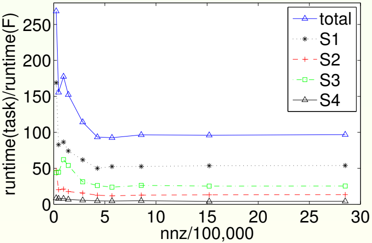
Experiments using ADOL-C

- Efficacy of the four-step scheme tested in two case studies
  1. Jacobian computation in a Simulated Moving Bed process (chromatographic separation in chemical engineering)
  2. Hessian computation in an optimal electric power flow problem
- Experiments showed
  - technique enabled cheap Jacobian/Hessian computation where dense computation is infeasible
  - observed results for each step matched analytical results





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Parallelizing greedy coloring

- Desired task: parallelize Greedy such that
  - speedup is $\Theta(p)$
  - number of colors used is roughly same as in serial
- A difficult task since Greedy is inherently sequential
- For D1 coloring, several approaches based on Luby's parallel algorithm for maximal independent set exist
- Some drawbacks:
  - no actual parallel implementation
  - many more colors than a serial implementation
  - poor parallel speedup on unstructured graphs

Generic parallelization techniques

- Basic standard techniques:
  balanced trees, pointer jumping,
  divide and conquer, strict partitioning
- Strict partitioning:
  - break up the given problem into p independent subproblems of almost equal sizes
  - solve the p subproblems concurrently using p processors

  Main work in SP lies in the decomposition step,
  often no easier than solving the original problem.
- Relaxed partitioning:
  - break up the given problem into p, not necessarily entirely independent, subproblems of almost equal sizes
  - solve the p subproblems concurrently
  - detect inconsistencies in the solutions concurrently
  - resolve any inconsistencies

  RP can be used successfully if the resolution in the fourth step
  involves only "local" adjustments.

RP applied to greedy coloring

Basic features of the algorithm:

- exploits features of data distribution
  - distinguishes between interior and boundary vertices
- proceeds in rounds, each having two phases:
  - tentative coloring
  - conflict detection
- tentative coloring phase organized in supersteps
  - each processor communicates only after coloring a subset of its assigned vertices using currently available information (infrequent, coarse-grain communication)
- randomization used in resolving conflicts

Framework($G = (V, E), s$)
Partition V into $V_1, V_2, \ldots, V_p$ using a graph partitioner
On each processor P_i, $i \in I = \{1, \ldots, p\}$
    for each boundary vtx $v \in V_i' = \{u : (u, v) \in E_i\}$
        assign v a random number $r(v)$
    $U_i \leftarrow V_i$
    while $\exists j \in I$, $U_j \neq \emptyset$ rounds
        Partition U_i into ℓ_i subsets $U_{i,1}, U_{i,2}, \ldots, U_{i,\ell_i}$, each of size s
        for $k = 1$ to ℓ_i **do**   supersteps for tentative coloring
            for each $v \in U_{i,k}$ **do**
                assign v a permissible color
            send colors of boundary vtxs in $U_{i,k}$ to relevant processors
            receive color information from relevant processors
        Wait until all incoming messages are received
        $R_i \leftarrow \emptyset$
        for each boundary vtx $v \in U_i$ **do**   conflict detection
            if $\exists (v, w) \in E_i$ s.t. $c(v) = c(w)$ and $r(v) < r(w)$ **then**
                $R_i \leftarrow R_i \cup \{v\}$
        $U_i \leftarrow R_i$ recolor in next round

Specializations of Framework

Framework can be specialized along several axes:

1. Color selection strategies:
   First Fit: search for smallest color starts at 1 on each processor
   Staggered FF: search for smallest color starts from different "bases"
2. Coloring order:
   interior vertices can be colored before, after, or interleaved with boundary vertices
3. Local vertex ordering:
   vertices on each processor can be ordered using various degree-based techniques
4. Supersteps:
   can be run synchronously or asynchronously
5. Inter-processor communication:
   can be customized or broadcast-based

How should the options in Framework be set?

An answer requires considering a complex set of factors, including

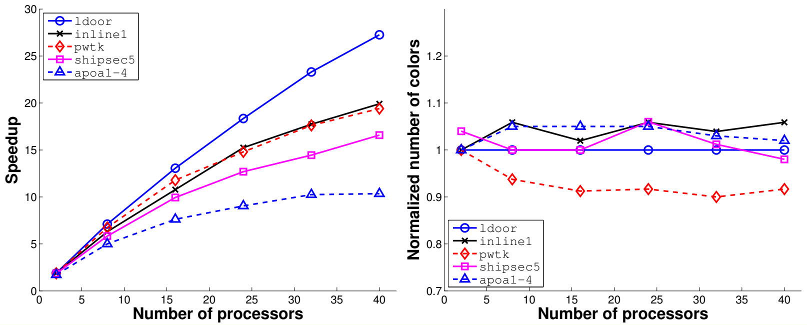
- size and density of input graph
- number of processors
- quality of initial partitioning
- characteristic of platform on which implementation is run

Determination bound to rely on experimentation

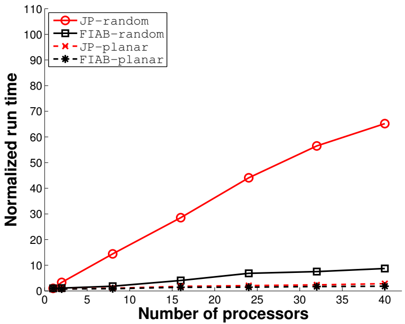
Lessons learned from experiments

Good parameter configuration for
large-size (millions of edges) graphs:

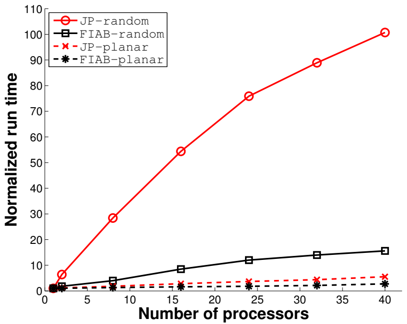
- moderately unstructured graphs
  (e.g. a typical application graph):
  1. a superstep size s in the order of 1000
  2. asynchronous supersteps
  3. a coloring order in which interior vertices appear either strictly before or strictly after boundary vertices
  4. First Fit color choice strategy
  5. customized inter-processor communication
- highly unstructured (e.g. random) graphs:
  - s in the order of 100
  - items 2 to 4 same as for moderately unstructured graphs
  - broadcast-based communication



Algorithm FBAC on Itanium 2 cluster.



Itanium 2



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Summary

- Current accomplishments:
  - Developed a unifying graph-theoretic framework for sparse derivative computation.
  - Designed and implemented new sequential algorithms for distance-k, star, acyclic, and other coloring problems.
  - C++ implementations assembled in a package called ColPack.
    - ColPack also includes various ordering routines for greedy coloring.
  - Integrated parts of ColPack with the AD tool ADOL-C.
  - Developed parallel algorithms for distance-1, distance-2, and restricted star coloring.
    - Algorithms scale well for a hundred processors.
    - Implementations made available via Zoltan.
- Planned activities:
  - Integrate coloring software with tools in OpenAD.
  - Develop algorithms for coloring problems in partial matrix computation.
  - Develop parallel star and acyclic coloring algorithms.
  - Develop parallel coloring algorithms for tera and petascale computation.
  - Collaborate with application and tool developers to "plug in" coloring technologies to enable CSE.

Further reading

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