Sparse Matrix Algorithms

combinatorics + numerical methods + applications = SuiteSparse

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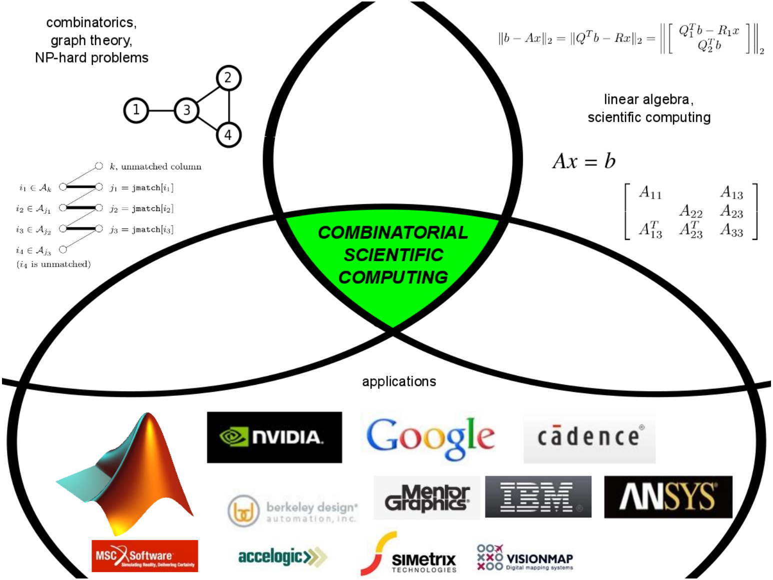
Outline

- **Computer Science + Applied Math =**
  $$\left[\begin{array}{c} \text{high-performance combinatorial scientific computing} \\ +\text{many applications enabled by my contributions} \end{array}\right]$$
- **Sparse matrix algorithms**
- **Contributions to the field**
  - from theory, to algorithms, to reliable software, to applications
  - sparse LU for circuit simulation (KLU)
  - sparse Cholesky update/downdate (CHOLMOD)
  - approximate minimum degree (AMD)
  - unsymmetric multifrontal LU (UMFPACK)
  - multifrontal QR (SuiteSparseQR)
- **Current work**
  - GPU-accelerated sparse LU, Cholesky, and QR
  - NVIDIA Academic Partner / Texas A&M CUDA Research Center
  - GPU-based methods, partnership with NVIDIA
  - graph partitioning
  - sparse SVD
- **Future vision**

Computer Science + Applied Math = combinatorial scientific computing + applications



Sparse Direct Methods: Algorithms + Code

Impact: new algorithms and useful code

- solve $Ax = b$ when A is sparse (LU, Chol, QR, ...)
- sparse least-squares problems
- rank estimates, sparse null space bases
- sparse SVD
- solve $Ax = b$, then let A undergo a low-rank change
- fill-reducing orderings, graph partitioning
- all in highly reliable, high performance code
- 3x more reliable than NASA's most extreme effort
- enabling a vast domain of commercial, academic, and government lab applications
- ...

Solve $Lx = b$ with L unit lower triangular; L, x, b are sparse

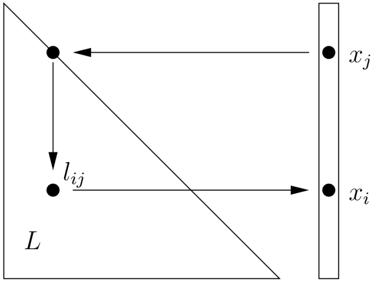
$x = b$
for $j = 0$ to $n - 1$ **do**
  if $x_j \neq 0$
    for each $i > j$ for which $l_{ij} \neq 0$ **do**
      $x_i = x_i - l_{ij} x_j$

- non-optimal time $O(n + |b| + f)$, where $f =$ flop count
- problem: outer loop and the test for $x_j \neq 0$
- solution: suppose we knew $\mathcal{X}$, the nonzero pattern of x
- optimal time $O(|b| + f)$, but how do we find $\mathcal{X}$? (Gilbert/Peierls)

Solve $Lx = b$ with L unit lower triangular; L, x, b are sparse

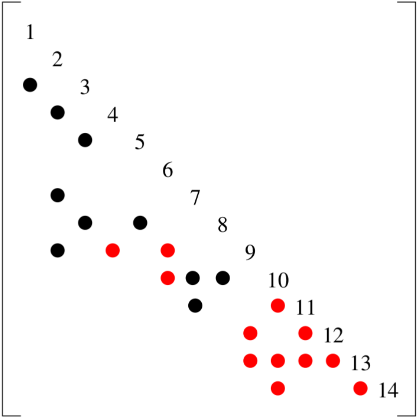
$x = b$
for $j = 0$ to $n - 1$ **do**
  if $x_j \neq 0$
    for each $i > j$ for which $l_{ij} \neq 0$ **do**
      $x_i = x_i - l_{ij} x_j$

- if $b_i \neq 0$ then $x_i \neq 0$
- if $x_j \neq 0$ and $\exists i (l_{ij} \neq 0)$
  then $x_i \neq 0$
- start with pattern $\mathcal{B}$ of b
- graph $\mathcal{L}$: edge (j, i) if $l_{ij} \neq 0$
- $\mathcal{X} = \text{Reach}_{\mathcal{L}}(\mathcal{B})$
  (Gilbert/Peierls)

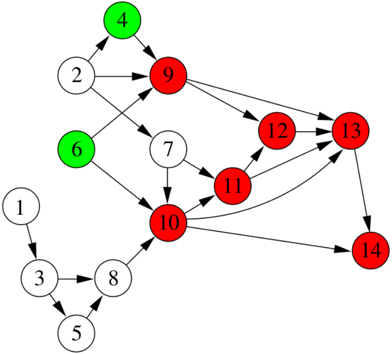


Sparse matrix algorithms

Lower triangular matrix L



Graph G_L



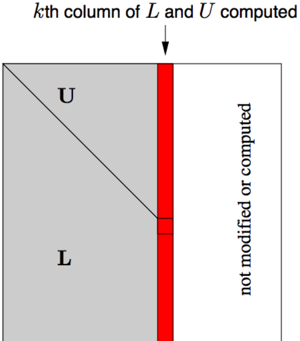
If $\mathcal{B} = \{4, 6\}$ then $\mathcal{X} = \{6, 10, 11, 4, 9, 12, 13, 14\}$

KLU: left looking LU

Each column of L and U computed via sparse Lx=b

```
L = speye(n) ; U = speye(n) ;
for k = 1:n
    x = L \ A(:,k)
    U(1:k,k) = x(1:k)
    L(k:n,k) = x(k:n) / U(k,k)
```

- $LU = PAQ$
- Q: fill-reducing preordering
- P: partial pivoting
- also exploits permutation to block triangular form
- appears in commercial and government lab circuit simulators

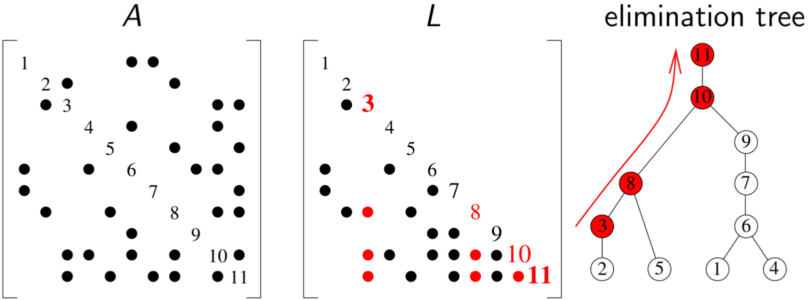


Sparse Cholesky update/downdate

The update/downdate problem:

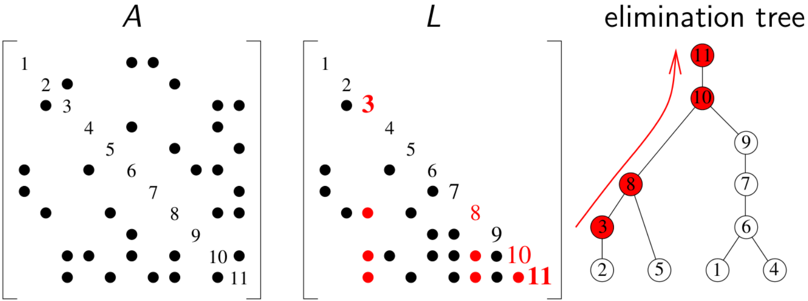
- Given $A = LL^T$
- A undergoes a low-rank change
- compute $\overline{L}\,\overline{L}^T = A \pm ww^T$
- arises in optimization, crack propagation, robotics, new data in least-squares, short-ciruit power analysis, ...

Sparse Cholesky update/downdate



Key results

- if $\mathcal{L}$ doesn't change: columns in L that change = path from $\min \mathcal{W}$ to root of the etree
- if $\mathcal{L}$ does change, follow the path in etree of $\overline{L}$
- Update/downdate in time proportional to the number of entries in L that change



Solving for just one component

- Suppose b is all zero except b_3, and all you want is x_3
- Forward solve: just up the path
- Back solve: just down the path
- Time is O(entries in L along the path), not O(nnz in L)

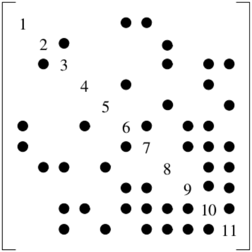
Sparse Cholesky update/downdate

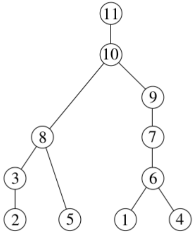
CHOLMOD update/downdate: key results / impact

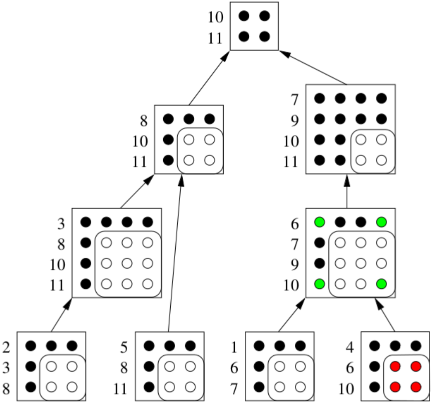
- update/downdate faster than a $Lx = b$ solve for dense b
- example application: LPDASA (Hager and Davis)
  - maintains Cholesky factorization of $A_F A_F^T$ for basis set F
  - update/downdate as basis set changes
- example: g2o (Kümmerle et al), iSAM
  - robotics, simultaneous localization and mapping
  - builds a map of its surroundings
  - update/downdate as new images arrive
- example: crack propagation (Pais, Kim, Davis et al)
  - structural engineering problem: crack in aircraft fuselage
  - update/downdate as crack progresses through airframe
- example: short-circuit power analysis
  - hypersparse solve, cut numerics by 10x to 100x

Multifrontal method

- Classic symmetric multifrontal method (Duff, Reid, others)
- Cliques + elimination tree = sequence of frontal matrices
- Dense factorization within a front; assemble data into parent

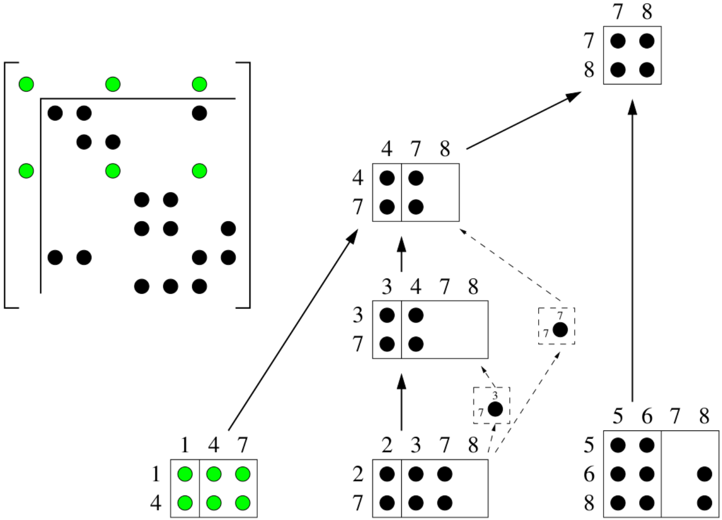






UMFPACK: unsymmetric multifrontal method

- Frontal matrices become rectangular
- Assemble data into ancestors, not just parents



UMFPACK: unsymmetric multifrontal method

Key results / impact

- sparse `lu` in MATLAB, `x = A \ b`
- used in many commercial CAD tools, Mathematics, Octave, ...

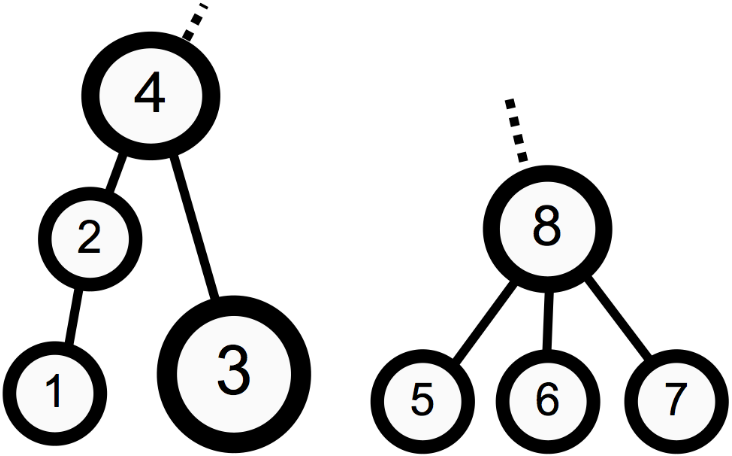
SuiteSparseQR: multifrontal sparse QR factorization

Key results / impact

- rectangular fronts like UMFPACK, but simpler frontal matrix assembly
- multicore parallelism
- amenable to GPU implementation (in progress)
- sparse `qr` in MATLAB, and `x=A\b`
- on the GPU:
  - novel "Bucket QR" scheduler and custom GPU kernels
  - up to 150 GFlops on the Kepler K20c
  - up to 20x speedup vs CPU algorithm (5x to 10x typical)
  - prototype multi-GPU: another $\sim$ 2x on 2 GPUs

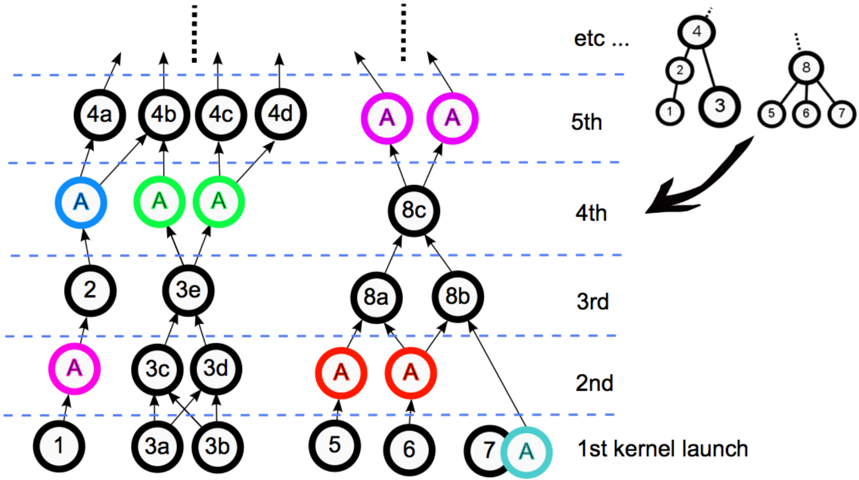
Highly-concurrent heterogeneous parallel computing

Consider a subtree of frontal matrices on the GPU

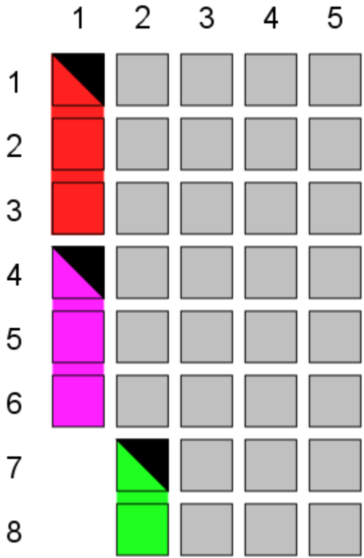


Highly-concurrent heterogeneous parallel computing

Expanded to show GPU kernel launches



GPU-based heterogeneous parallel computing



With no pipelining...

Householder bundles:

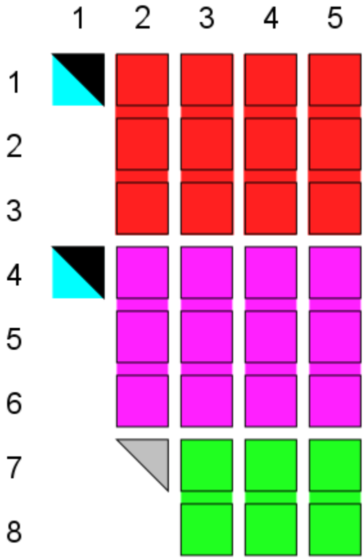
(1,2,3) new

(4,5,6) new

(7,8) new

first kernel launch same
as pipelined method

GPU-based heterogeneous parallel computing



With no pipelining...

Householder bundles:

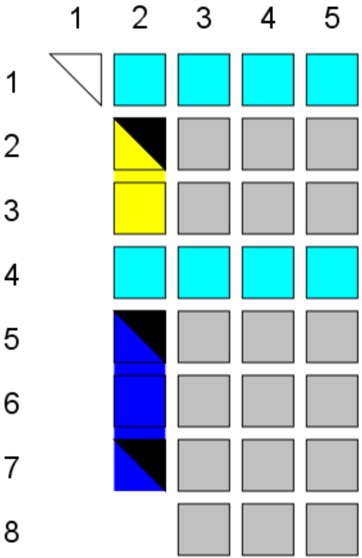
(1,2,3) applied

(4,5,6) applied

(7,8) applied

(1,4) new

GPU-based heterogeneous parallel computing



With no pipelining...

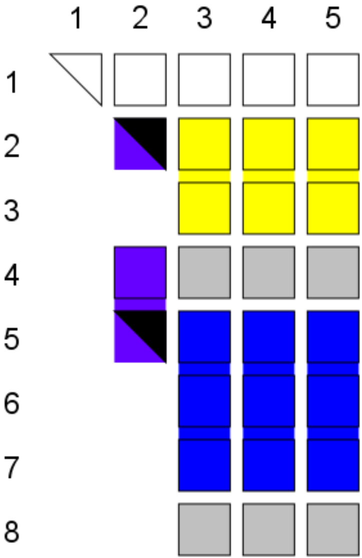
Householder bundles:

(2,3) new

(5,6,7) new

(1,4) applied

GPU-based heterogeneous parallel computing



With no pipelining...

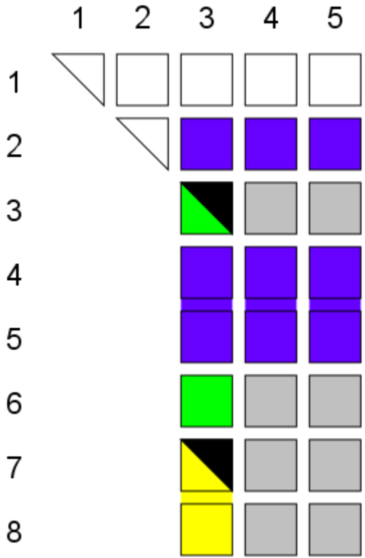
Householder bundles:

(2,3) applied

(5,6,7) applied

(2,4,5) new

GPU-based heterogeneous parallel computing



With no pipelining...

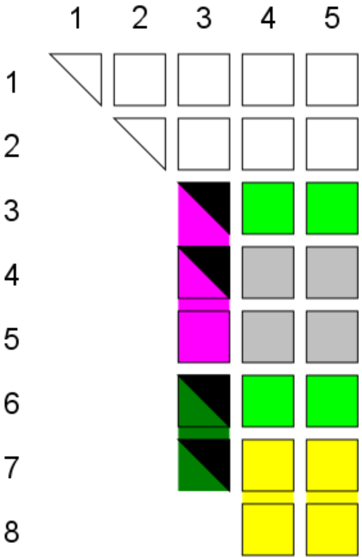
Householder bundles:

(3,6) new

(7,8) new

(2,4,5) applied

GPU-based heterogeneous parallel computing



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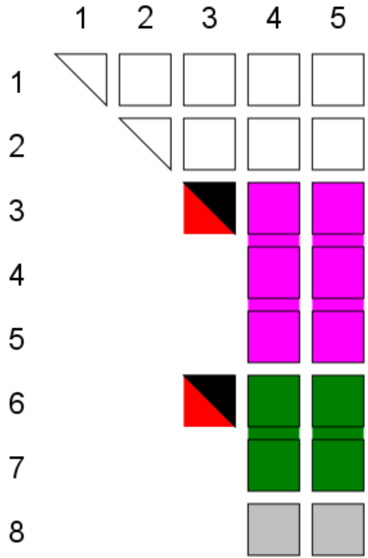

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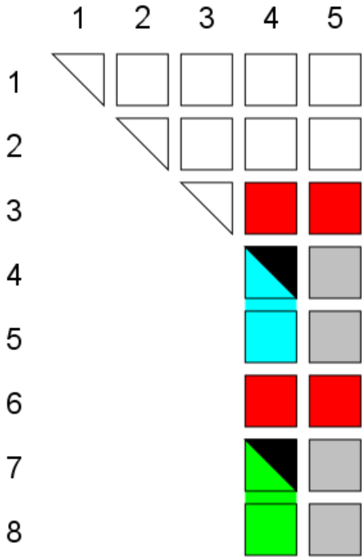

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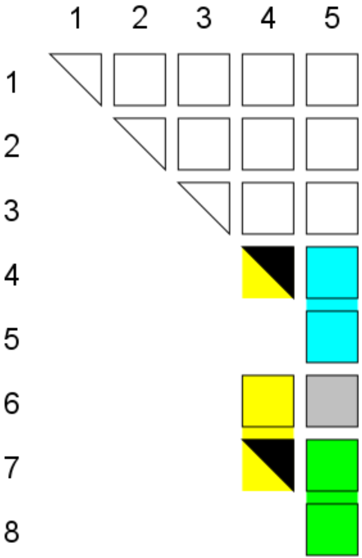

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(7,8) applied

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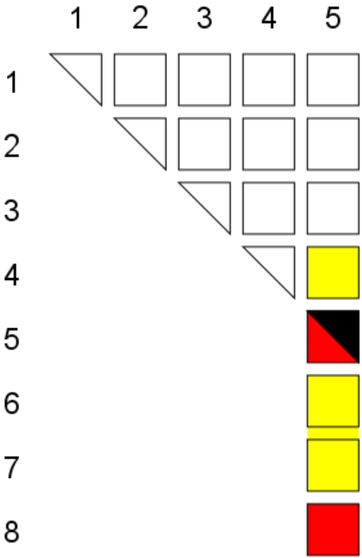

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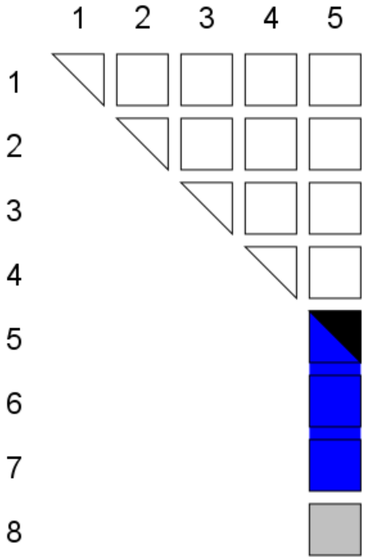

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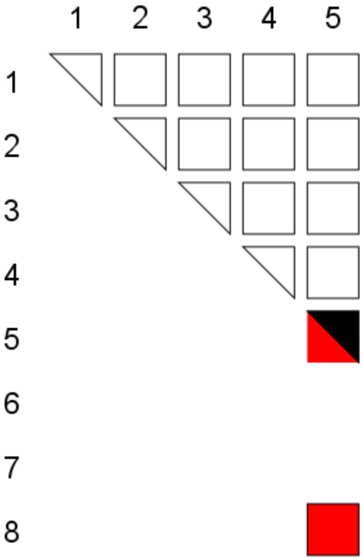
GPU-based heterogeneous parallel computing



With no pipelining...

Householder bundles:

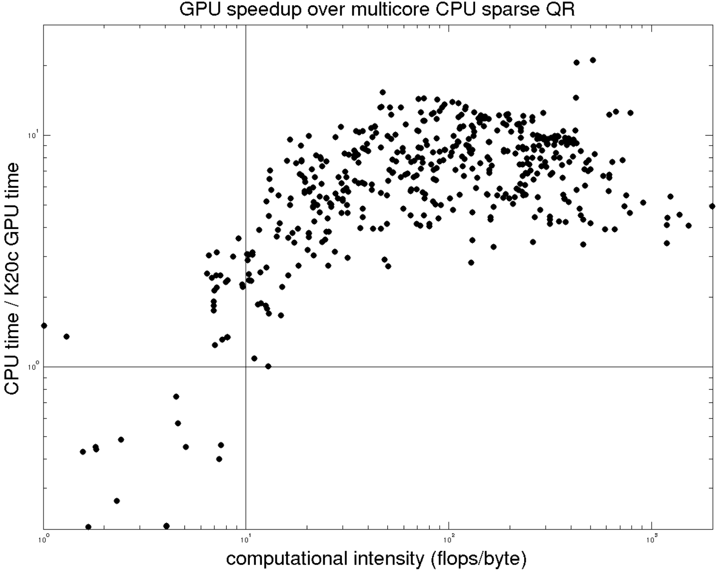
(5,8) new

Highly-concurrent heterogeneous parallel computing

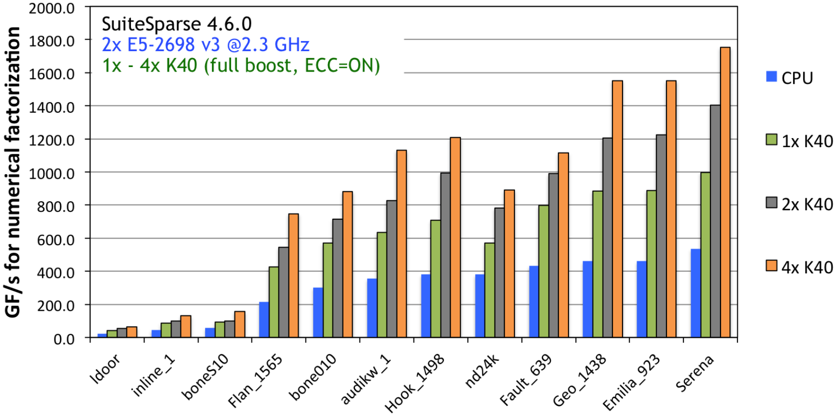
- **Putting it all together ...**

	C2070	K20	K40
GPU kernels:			
apply block Householder	183 Gflops	260 Gflops	$\sim$500
factorize 3 tiles	27 Gflops	20 Gflops	$\sim$50
dense QR for large front	107 Gflops	120 Gflops	
sparse QR on GPU	80 Gflops	150 Gflops	
peak speedup over CPU	11x	20x	
typical speedup over CPU	5x	10x	

Performance on many matrices



Supernodal Sparse Cholesky on the GPU



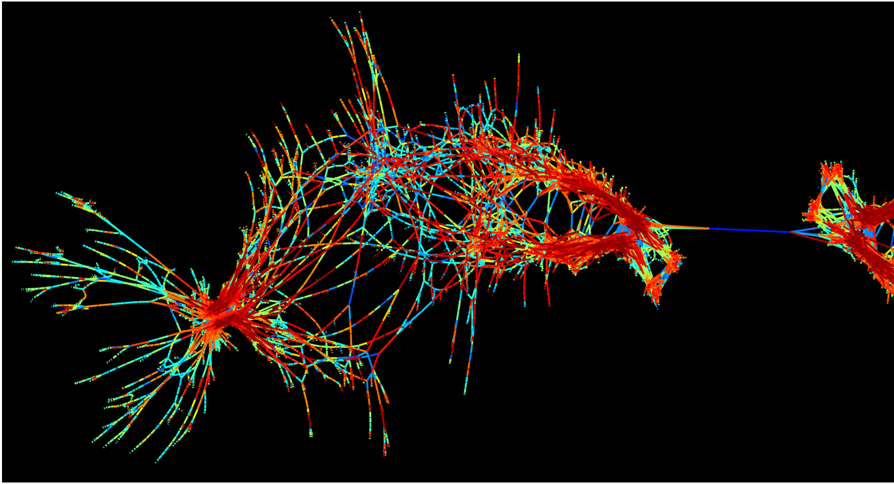
SuiteSparse: features in the packages

- orderings: AMD, COLAMD, CAMD, CCOLAMD, BTF
- CHOLMOD: Supernodal Cholesky, with update/downdate, +GPU
- SPQR: multifrontal QR, +GPU
- UMFPACK: multifrontal LU
- KLU: light-weight sparse LU, well-suited to circuits, power
- SPQR_RANK: sparse null set basis, rank estimation, pseudo-inverse
- FACTORIZE: object oriented wrapper for MATLAB. `F=factorize(A) ; x=F\b ; x=inverse(A)*b` (no inverse).
- UFget: MATLAB interface to SuiteSparse Matrix Collection
- CSparse: sparse LU, Cholesky, QR, matrix ops, update/downdate, ...
- Sparseinv: sparse inverse subset
- many matrix operators (sparse matrix multiply, transpose, ...)
- to appear: sparse SVD, edge and vertex graph partitioning
- 9 Collected Algorithms of the ACM, more on the way
- all packages have MATLAB interfaces (or just use `x=A\b`!)

Future vision

- **Computer Science + Applied Math**
  (combinatorics + linear algebra + graph algorithms) =
  $$\left[\begin{array}{c}\text{high-performance combinatorial scientific computing}\\ +\text{many applications enabled by my contributions}\end{array}\right]$$
- computational mathematics: the future is heterogeneous; driven by power constraints, need for parallelism
- high impact – getting it out the door
  - novel algorithms: delivered in widely used robust software
  - Collected Algorithms of the ACM
  - enabling academic projects: Julia, R, Octave, FEnICS, ROS.org, ...
  - current collaborations: UTK, UF, NVIDIA, Lawrence Livermore, Harvard, ...
  - growing industrial impact: MathWorks, Google, NVIDIA, Mentor Graphics, Cadence, MSC Software, Berkeley Design Automation, ...
  - applications: optimization, robotics, circuit simulation, computer graphics, computer vision, finite-element methods, geophysics, stellar evolution, financial simulation, ...

Computer Science + Math + Music = Art



- algorithmic translation of music into visual art
- theme artwork, London Electronic Music Festival