Advanced Systems Lab

Spring 2024

Lecture: Memory bound computation, sparse linear algebra, OSKI

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Overview

Memory bound computations

Sparse linear algebra, OSKI

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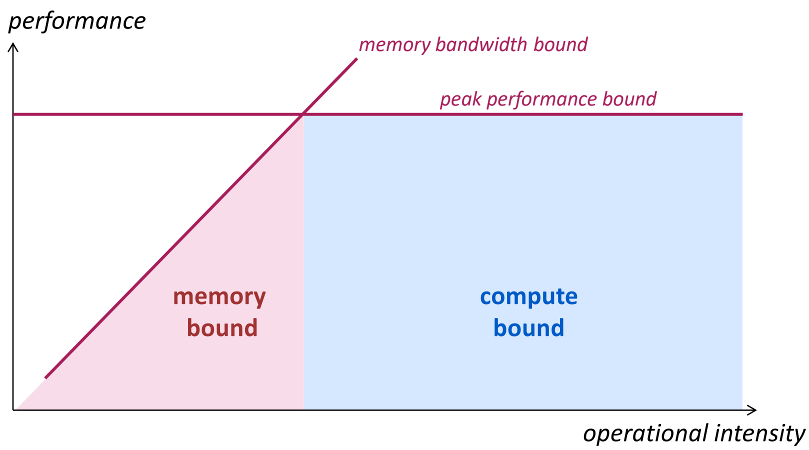
Memory Bound Computation

Data movement, not computation, is the bottleneck

Typically: Computations with operational intensity *I(n) = O(1)*



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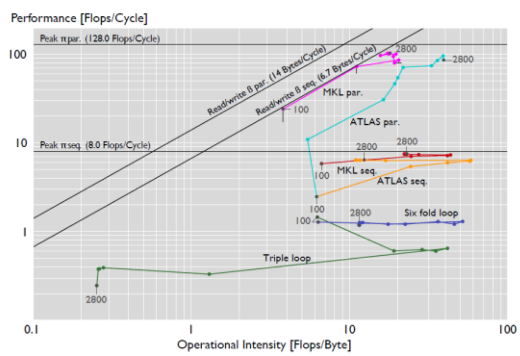
Memory Bound Or Not? Depends On …

The computer
- *Memory bandwidth*
- *Cache size*
- *Peak performance*

The algorithm
- *Dependencies*

How it is implemented
- *Good/bad locality*
- *SIMD or not*

How the measurement is done
- *Cold or warm cache*
- *In which cache data resides*
- *See next slide*



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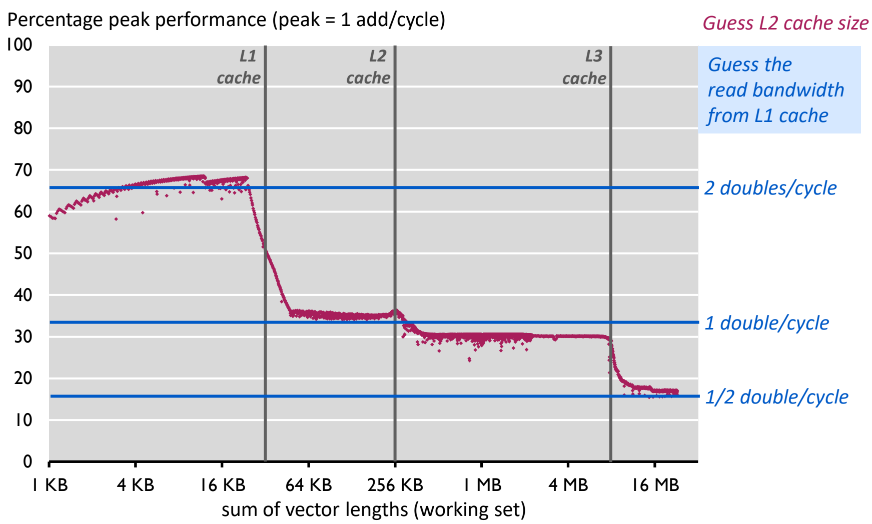
Example: BLAS 1, Warm Data & Code

z = x + y on Core i7 (Nehalem, one core, no SSE), icc 12.0 /O2 /fp:fast /Qipo



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Sparse Linear Algebra

Sparse matrix-vector multiplication (MVM)

Sparsity/Bebop/OSKI

References:

- *Eun-Jin Im, Katherine A. Yelick, Richard Vuduc. SPARSITY: An Optimization Framework for Sparse Matrix Kernels, Int'l Journal of High Performance Comp. App., 18(1), pp. 135-158, 2004*
- *Vuduc, R.; Demmel, J.W.; Yelick, K.A.; Kamil, S.; Nishtala, R.; Lee, B.; Performance Optimizations and Bounds for Sparse Matrix-Vector Multiply, pp. 26, Supercomputing, 2002*
- *Sparsity/Bebop website*

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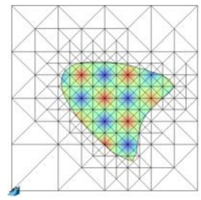
Sparse Linear Algebra

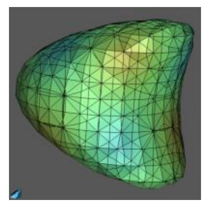
Very different characteristics from dense linear algebra (LAPACK etc.)

Applications:

- *finite element methods*
- *PDE solving*
- *physical/chemical simulation (e.g., fluid dynamics)*
- *linear programming*
- *scheduling*
- *signal processing (e.g., filters)*
- *…*

Core building block: Sparse MVM

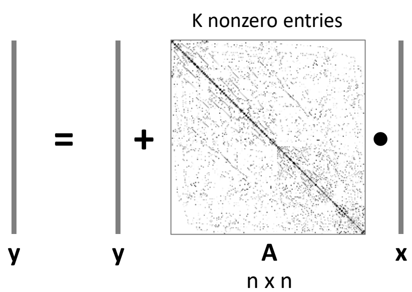




Graphics: http://aam.mathematik.uni-freiburg.de/IAM/homepages/claus/projects/unfitted-meshes_en.html

Sparse MVM (SMVM)

y = y + Ax, A sparse but known (below A is square)



Typically executed many times for fixed A

What is reused (possible temporal locality)?

Upper bound on operational intensity? $I(n) \leq \frac{2K}{8(K+3n)} \leq \frac{1}{4}$

Storage of Sparse Matrices

Standard storage is obviously inefficient: Many zeros are stored

- *Unnecessary operations*
- *Unnecessary data movement*
- *Bad operational intensity*

Several sparse storage formats are available

Popular for performance: Compressed sparse row (CSR) format

CSR

Assumptions:

- *A is m x n*
- *K nonzero entries*

A as matrix

b	c		c
	a		
		b	b
		c	

A in CSR:

`values`	b	c	c	a	b	b	c	*length K*
`col_idx`	0	1	3	1	2	3	2	*length K*

`row_start`	0	3	4	6	7	*length m+1*

Storage:

- *K doubles + (K+m+1) ints = Θ(max(K, m))*
- *Typically: Θ(K)*

Sparse MVM Using CSR

y = y + Ax

```
void smvm(int m, const double* values, const int* col_idx,
          const int* row_start, double* x, double* y)
{
  int i, j;
  double d;

  /* loop over m rows */
  for (i = 0; i < m; i++) {
    d = y[i]; /* scalar replacement since reused */

    /* loop over non-zero elements in row i */
    for (j = row_start[i]; j < row_start[i+1]; j++)
      d += values[j] * x[col_idx[j]];
    y[i] = d;
  }
}
```

CSR + sparse MVM: Advantages?

CSR

Advantages:

- *Only nonzero values are stored*
- *All three arrays for A (`values`, `col_idx`, `row_start`) accessed consecutively in MVM (good spatial locality)*
- *Good temporal locality with respect to y*

Disadvantages:

- *Insertion into A is costly*
- *Poor temporal locality with respect to x*

Impact of Matrix Sparsity on Performance

Adressing overhead (dense MVM vs. dense MVM in CSR):

- *~ 2x slower (example only)*

Fundamental difference between MVM and sparse MVM (SMVM):

- *Sparse MVM is input **dependent** (sparsity pattern of A)*
- *Changing the order of computation (e.g., when blocking) requires changing the data structure (CSR)*

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Bebop/Sparsity: SMVM Optimizations

Idea: Blocking for registers

Reason: Reuse x to reduce memory traffic

Execution: Block SMVM y = y + Ax into micro MVMs

- *Block size r x c becomes a parameter*
- *Consequence: Change A from CSR to r x c block-CSR (BCSR)*

BCSR: Next slide

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BCSR (Blocks of Size r x c)

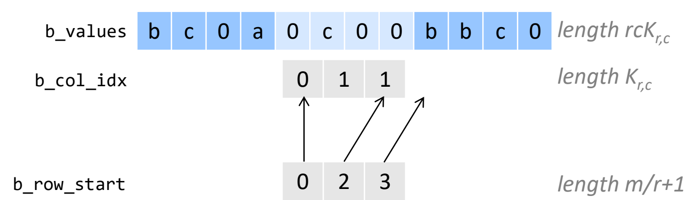
Assumptions:

- *A is m x n*
- *Block size r x c*
- $K_{r,c}$ *nonzero blocks*

A as matrix (r = c = 2)

b	c		c
	a		
		b	b
		c	

A in BCSR (r = c = 2):



Storage:

- $rcK_{r,c}$ *doubles +* $(K_{r,c}+m/r+1)$ *ints =* $\Theta(rcK_{r,c})$ *(in typical case* $K \geq m$*)*
- $rcK_{r,c} \geq K$

Sparse MVM Using 2 x 2 BCSR

```
void smvm_2x2(int bm, const int *b_row_start, const int *b_col_idx,
              const double *b_values, double *x, double *y)
{
  int i, j;
  double d0, d1, c0, c1;

  /* loop over bm block rows */
  for (i = 0; i < bm; i++) {
    d0 = y[2*i];   /* scalar replacement since reused */
    d1 = y[2*i+1];

    /* dense micro MVM */
    for (j = b_row_start[i]; j < b_row_start[i+1]; j++, b_values += 2*2) {
      c0 = x[2*b_col_idx[j]+0]; /* scalar replacement since reused */
      c1 = x[2*b_col_idx[j]+1];
      d0 += b_values[0] * c0;
      d1 += b_values[2] * c0;
      d0 += b_values[1] * c1;
      d1 += b_values[3] * c1;
    }
    y[2*i]   = d0;
    y[2*i+1] = d1;
  }
}
```

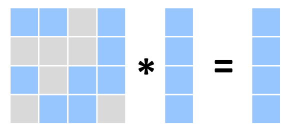
BCSR

Advantages:

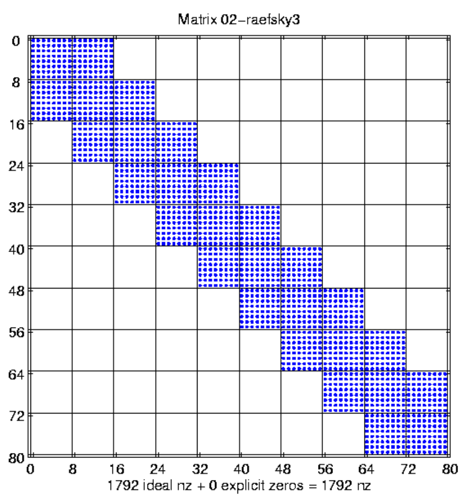
- *Temporal locality with respect to x and y*
- *Reduced storage for indexes*

Disadvantages:

- *Storage for values of A increased (zeros added)*
- *Computational overhead (also due to zeros)*



Which Block Size (r x c) is Optimal?

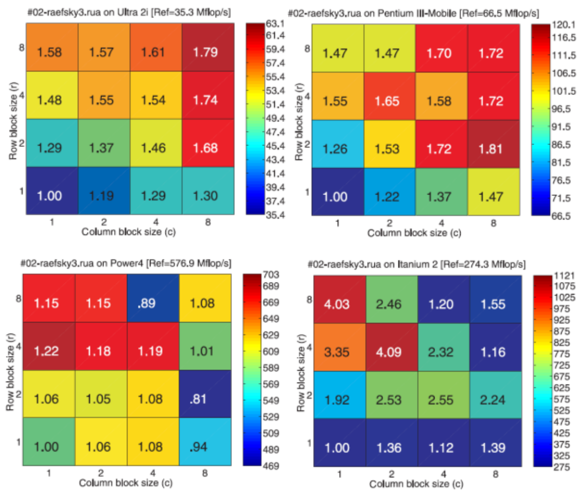


Example:

- 20,000 x 20,000 matrix (only part shown)
- Perfect 8 x 8 block structure
- No overhead when blocked r x c, with r, c divides 8

source: R. Vuduc, Georgia Tech

Speed-up Through r x c Blocking



- *machine dependent*
- *hard to predict*

Source: *Eun-Jin Im, Katherine A. Yelick, Richard Vuduc. SPARSITY: An Optimization Framework for Sparse Matrix Kernels, Int'l Journal of High Performance Comp. App., 18(1), pp. 135-158, 2004*

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How to Find the Best Blocking for given A?

Best block size is hard to predict (see previous slide)

Solution 1: Searching over all r x c within a range, e.g., 1 ≤ r,c ≤ 12

- *Conversion of A in CSR to BCSR roughly as expensive as 10 SMVMs*
- *So total cost = 1440 SMVMs*
- *Too expensive*

Solution 2: Model

- *Estimate the gain through blocking*
- *Estimate the loss through blocking*
- *Pick best ratio*

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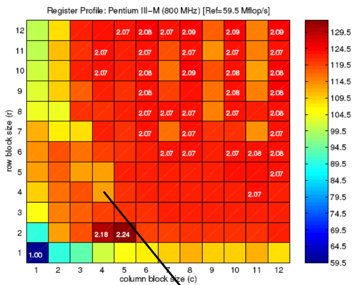
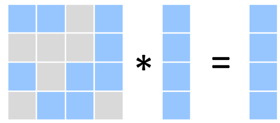
Model: Example

Gain by blocking (dense MVM)



Overhead (average) by blocking



16/9 = 1.77

1.4

1.4/1.77 = 0.79 (no gain)

Model: Doing that for all r and c and picking best

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Model

Goal: find best r x c for y = y + Ax

Gain through r x c blocking (estimation):

$$G_{r,c} = \frac{\textit{dense MVM performance in r x c BCSR}}{\textit{dense MVM performance in CSR}}$$

dependent on machine, independent of sparse matrix

Overhead through r x c blocking (estimation)
scan part of matrix A

$$O_{r,c} = \frac{\textit{number of matrix values in r x c BCSR}}{\textit{number of matrix values in CSR}}$$

independent of machine, dependent on sparse matrix

Expected gain: $G_{r,c}/O_{r,c}$

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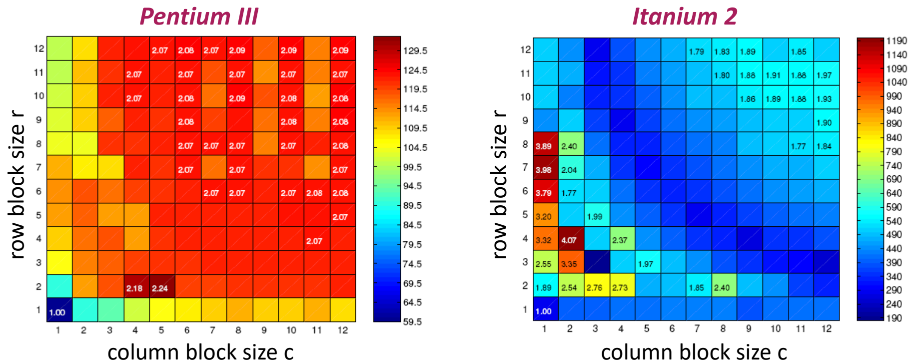
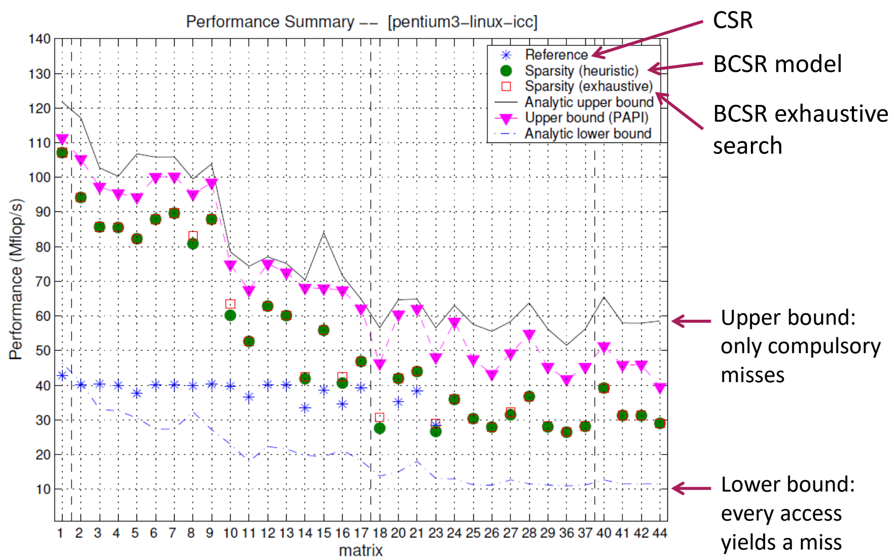
Gain from Blocking (Dense Matrix in BCSR)



- *machine dependent*
- *hard to predict*

Source: Eun-Jin Im, Katherine A. Yelick, Richard Vuduc. *SPARSITY: An Optimization Framework for Sparse Matrix Kernels*, *Int'l Journal of High Performance Comp. App.*, 18(1), pp. 135-158, 2004

Typical Result (assumes cold cache)



Source: Eun-Jin Im, Katherine A. Yelick, Richard Vuduc. *SPARSITY: An Optimization Framework for Sparse Matrix Kernels*, *Int'l Journal of High Performance Comp. App.*, 18(1), pp. 135-158, 2004

Principles in Bebop/Sparsity Optimization

Optimization for memory hierarchy = increasing locality

- *Blocking for registers (micro-MVMs)*
- *Requires change of data structure for A*
- *Optimizations are input dependent (on sparse structure of A)*

Fast basic blocks for small sizes (micro-MVM):

- *Unrolling + scalar replacement*

Search for the fastest over a relevant set of algorithm/implementation alternatives (parameters r, c)

- *Use of performance model (versus measuring runtime) to evaluate expected gain*

Different from ATLAS

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SMVM: Other Ideas

Value compression

Index compression

Pattern-based compression

Multiple inputs

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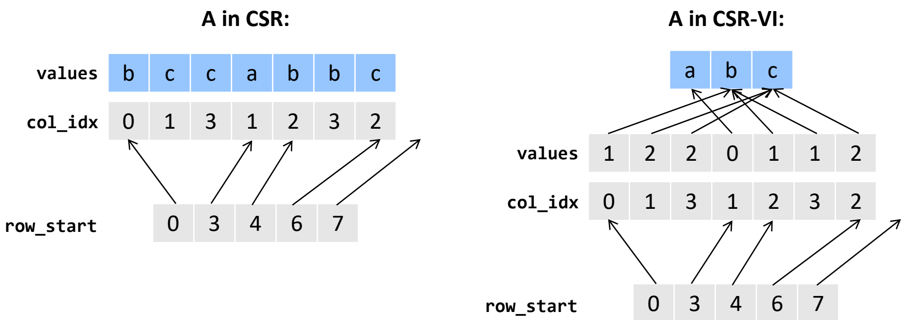
Value Compression

b	c		c
	a		
		b	b
		c	

Situation: Matrix A contains many duplicate values

Idea: Store only unique ones plus index information



Kourtis, Goumas, and Koziris, Improving the Performance of Multithreaded Sparse Matrix-Vector Multiplication using Index and Value Compression, pp. 511-519, ICPP 2008

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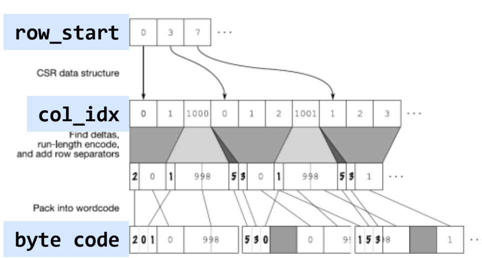
Index Compression

Situation: Matrix A contains sequences of nonzero entries

Idea: Use special byte code to jointly compress `col_idx` and `row_start`

Coding



Decoding

0: acc = acc * 256 + arg;
1: col = col + acc * 256 + arg; acc = 0;
   emit_element(row, col); col = col + 1;
2: col = col + acc * 256 + arg; acc = 0;
   emit_element(row, col);
   emit_element(row, col + 1); col = col + 2;
3: col = col + acc * 256 + arg; acc = 0;
   emit_element(row, col);
   emit_element(row, col + 1);
   emit_element(row, col + 2); col = col + 3;
4: col = col + acc * 256 + arg; acc = 0;
   emit_element(row, col);
   emit_element(row, col + 1);
   emit_element(row, col + 2);
   emit_element(row, col + 3); col = col + 4;
5: row = row + 1; col = 0;

Source: *Willcock and Lumsdaine, Accelerating Sparse Matrix Computations via Data Compression, pp. 307-316, ICS 2006*

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Pattern-Based Compression

Situation: After blocking A, many blocks have the same nonzero pattern

Idea: Use special BCSR format to avoid storing zeros;
needs specialized micro-MVM kernel for each pattern

A as matrix

b	c		c
	a		
		b	b
		c	

Values in 2 x 2 BCSR

b	c	0	a	0	c	0	0	b	b	c	0

Values in 2 x 2 PBR

b	c	a	c	b	b	c

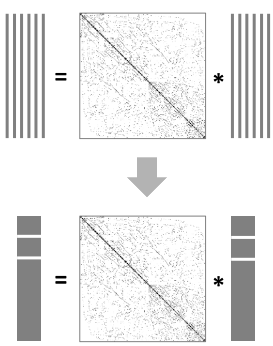
+ bit string: 1101 0100 1110

Source: *Belgin, Back, and Ribbens, Pattern-based Sparse Matrix Representation for Memory-Efficient SMVM Kernels, pp. 100-109, ICS 2009*

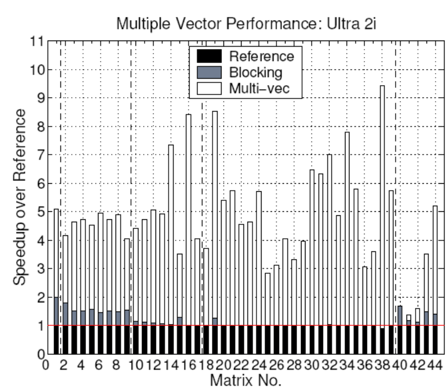
Multiple Inputs

Situation: Compute SMVM y = y + Ax for several independent x

Experiments: up to 9x speedup for 9 vectors



enables blocking across
MVMs like MMM



Source: Eun-Jin Im, Katherine A. Yelick, Richard Vuduc. *SPARSITY: An Optimization Framework for Sparse Matrix Kernels*, *Int'l Journal of High Performance Comp. App.*, 18(1), pp. 135-158, 2004