How to Write Fast Numerical Code

Spring 2017

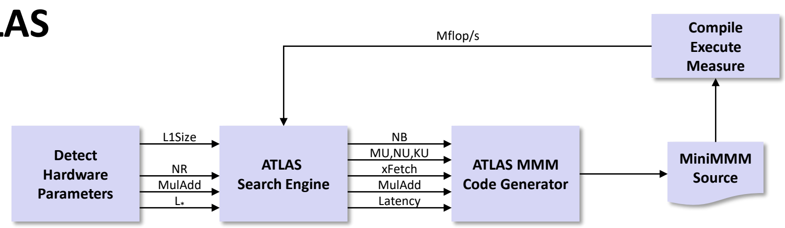
Lecture: Memory bound computation, sparse linear algebra, OSKI

Instructor: Markus Püschel

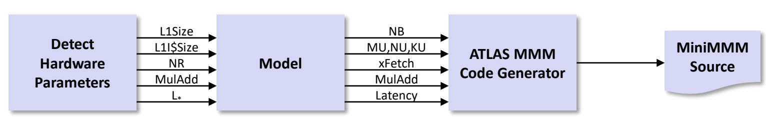
TA: Alen Stojanov, Georg Ofenbeck, Gagandeep Singh

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

ATLAS



Model-Based ATLAS



source: Pingali, Yotov, Cornell U.

Principles

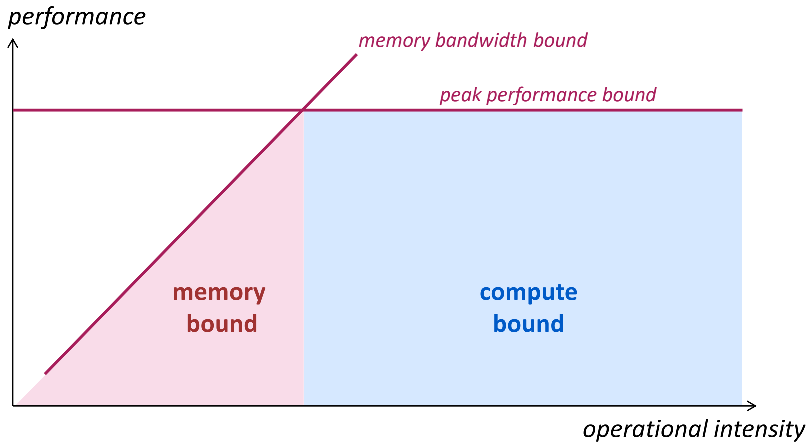
- **Optimization for memory hierarchy**
  - Blocking for cache
  - Blocking for registers
- **Basic block optimizations**
  - Loop order for ILP
  - Unrolling + scalar replacement
  - Scheduling & software pipelining
- **Optimizations for virtual memory**
  - Buffering (copying spread-out data into contiguous memory)
- **Autotuning**
  - Search over parameters (ATLAS)
  - Model to estimate parameters (Model-based ATLAS)
- ***All high performance MMM libraries do some of these (but possibly in a different way)***

Today

- **Memory bound computations**
- **Sparse linear algebra, OSKI**

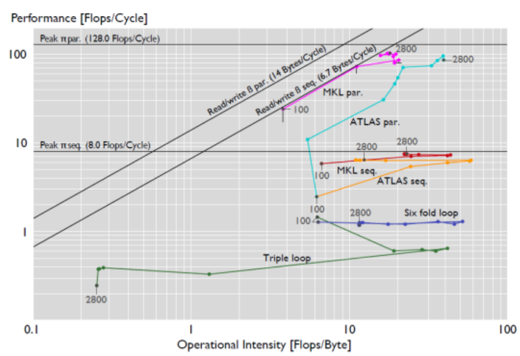
Memory Bound Computation

- **Data movement, not computation, is the bottleneck**
- **Typically: Computations with operational intensity *I(n) = O(1)***



Memory Bound Or Not? Depends On …

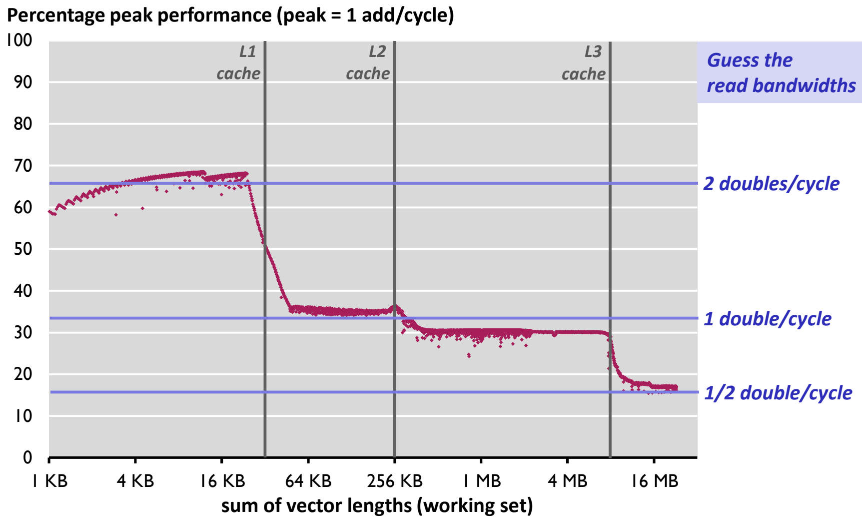
- **The computer**
  - Memory bandwidth
  - Peak performance
- **How it is implemented**
  - Good/bad locality
  - SIMD or not



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

Example: BLAS 1, Warm Data & Code

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



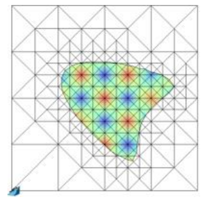
Sparse Linear Algebra

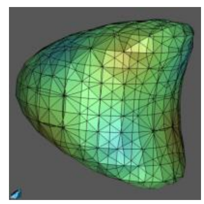
- **Sparse matrix-vector multiplication (MVM)**
- **Sparsity/Bebop/OSKI**

- **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

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***

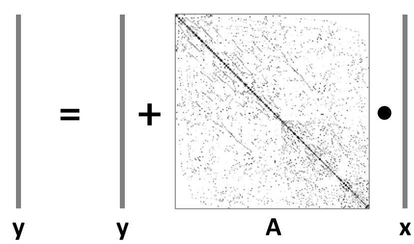




Graphics: http://aam.mathematik.uni-freiburg.de/IAM/homepages/claus/projects/unfitted-meshes_en.html

Sparse MVM (SMVM)

- **y = y + Ax, A sparse but known**



- **Typically executed many times for fixed A**
- **What is reused (temporal locality)?**
- **Upper bound on operational intensity?**

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**
- **Most popular: Compressed sparse row (CSR) format**
  - blackboard

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 (blocking) requires changing the data structure (CSR)

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: Blackboard**

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):

`b_values`	b c 0 a 0 c 0 0 b b c 0	*length* $rcK_{r,c}$
`b_col_idx`	0 1 1	*length* $K_{r,c}$
`b_row_start`	0 2 3	*length m/r+1*

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

Sparse MVM Using 2 x 2 BCSR

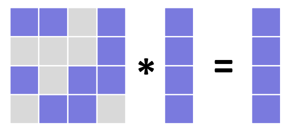
```
void smvm_2x2(int bm, const int *b_row_start, const int *b_col_idx,
              const double *b_values, double *x, double *y)
{
  int i, j;
  double d0, d1, c0, c1;

  /* 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;
  }
}
```

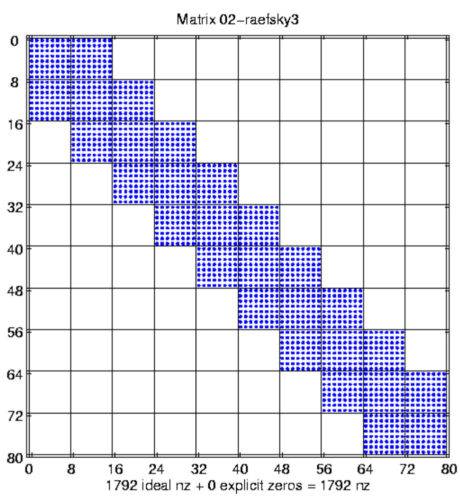
BCSR

- **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)



- **Main factors (since memory bound):**
  - ***Plus:*** increased temporal locality on x + reduced index storage = reduced memory traffic
  - ***Minus:*** more zeros = increased memory traffic

Which Block Size (r x c) is Optimal?

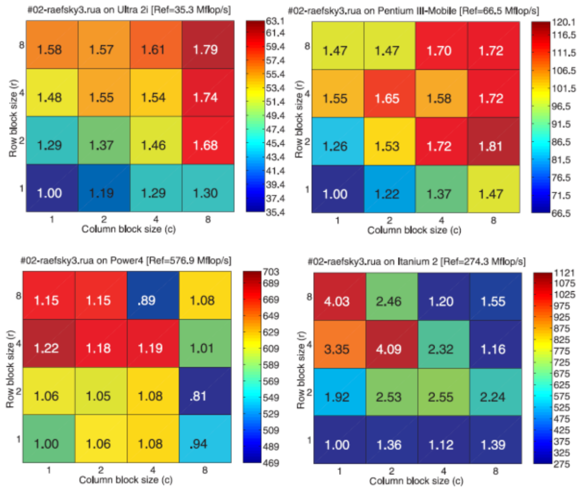


Example:

- **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, LLNL

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
  - 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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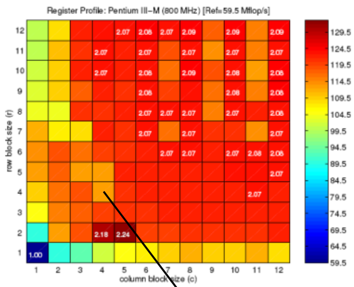
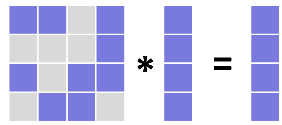
Model: Example

Gain by blocking (dense MVM)



1.4

Overhead (average) by blocking



16/9 = 1.77

1.4/1.77 = 0.79 (no gain)

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

Model

- ***Goal:*** **find best r x c for y = y + Ax**
- ***Gain*** **through r x c blocking (estimation):**

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

dependent on machine, independent of sparse matrix

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

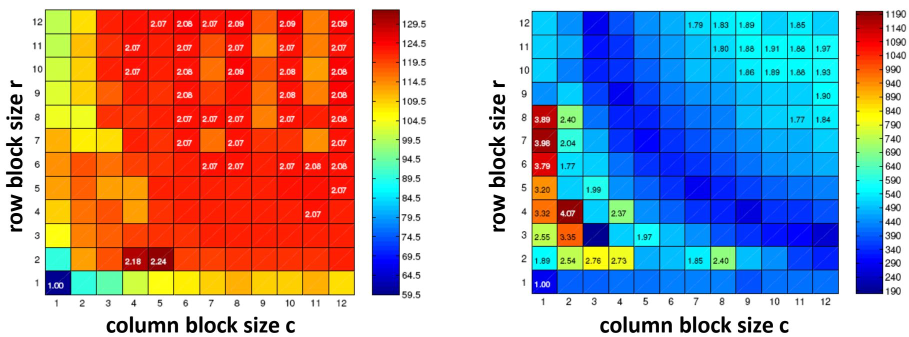
$$O_{r,c} = \frac{\text{number of matrix values in } r \times c \text{ BCSR}}{\text{number of matrix values in CSR}}$$

independent of machine, dependent on sparse matrix

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

Gain from Blocking (Dense Matrix in BCSR)

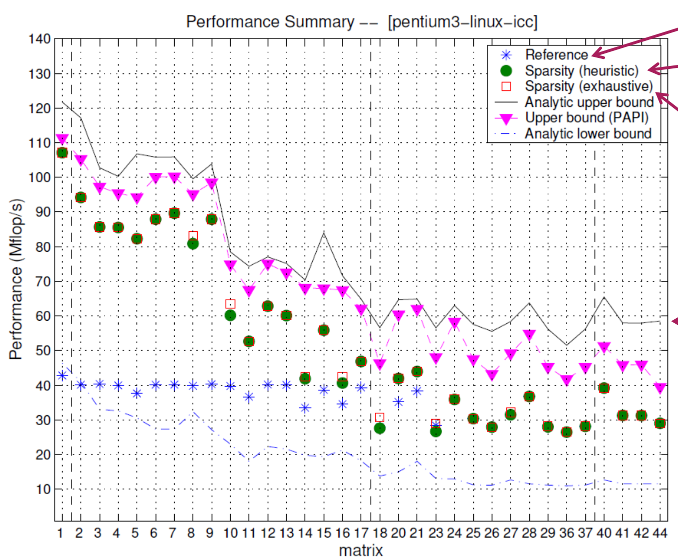
Pentium III *Itanium 2*



- *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



CSR

BCSR model

BCSR exhaustive search

Analytical upper bound
how obtained?
(blackboard)

Figure: 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

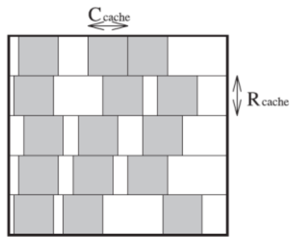
Different from ATLAS

SMVM: Other Ideas

- **Cache blocking**
- **Value compression**
- **Index compression**
- **Pattern-based compression**
- **Special scenario: Multiple inputs**

Cache Blocking

- **Idea: divide sparse matrix into blocks of sparse matrices**



- **Experiments:**
  - Requires very large matrices (x and y do not fit into cache)
  - Speed-up up to 2.2x, only for few matrices, with 1 x 1 BCSR

Figure: *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*

Value Compression

- ***Situation:*** **Matrix A contains many duplicate values**
- ***Idea:*** **Store only unique ones plus index information**

b	c		c
	a		
		b	b
		c	

A in CSR:

`values`	b	c	c	a	b	b	c
`col_idx`	0	1	3	1	2	3	2
`row_start`	0	3	4	6	7		

A in CSR-VI:

a	b	c

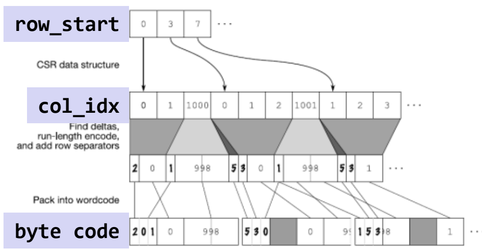
`values`	1	2	2	0	1	1	2
`col_idx`	0	1	3	1	2	3	2
`row_start`	0	3	4	6	7		

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

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;

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

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

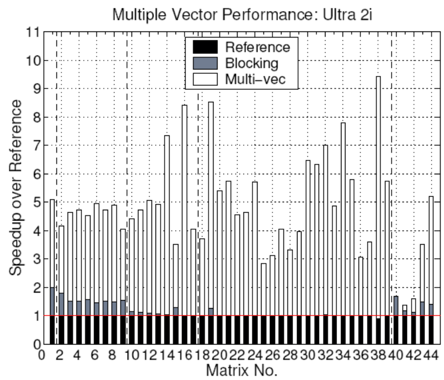
b	c	a	c	b	b	c

+ bit string: 1101 0100 1110

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

Special scenario: Multiple inputs

- **Situation: Compute SMVM y = y + Ax for several independent x**
- **Blackboard**
- **Experiments:**
  up to 9x speedup for 9 vectors



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