# How to Write Fast Numerical Code

Spring 2019

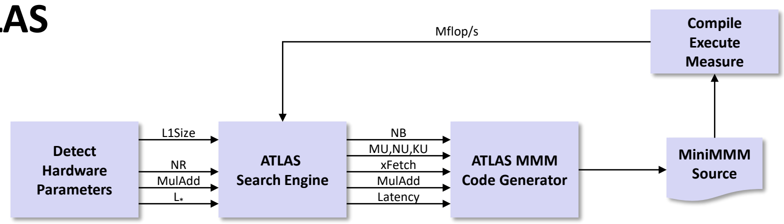
*Lecture:* Memory bound computation, sparse linear algebra, OSKI

**Instructor:** Markus Püschel

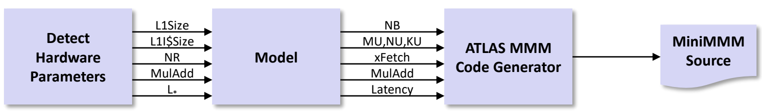
**TA:** Tyler Smith, Gagandeep Singh, Alen Stojanov

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

## ATLAS




## Model-Based ATLAS




*source: Pingali, Yotov, Cornell U.*

2

# 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 slightly different ways)***

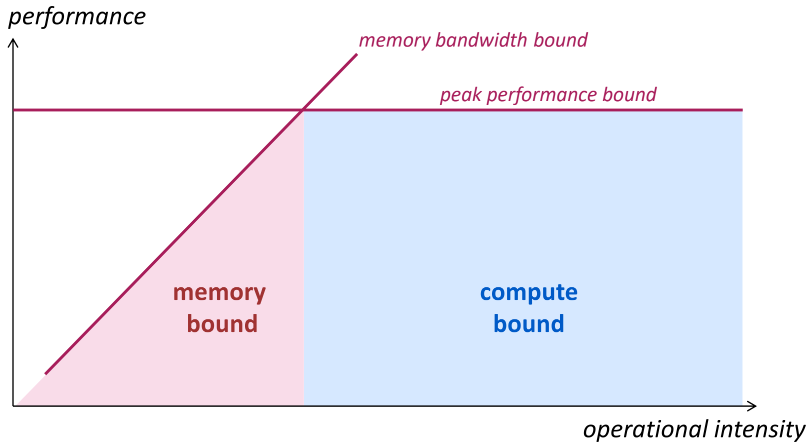


# Today

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

# Memory Bound Computation

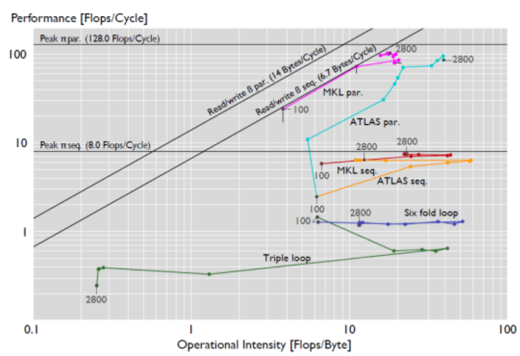
- Data movement, not computation, is the bottleneck
- Typically: Computations with operational intensity *I(n) = O(1)*






# Memory Bound Or Not? Depends On …

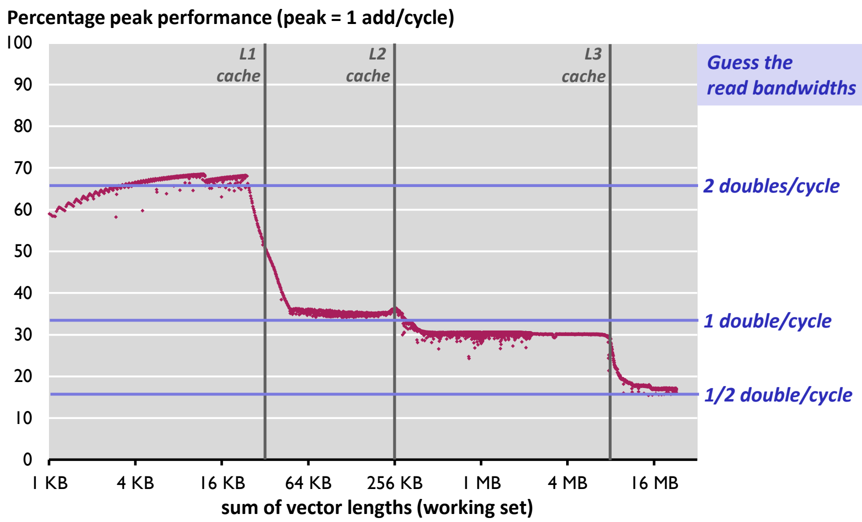
- **The computer**
  - Memory bandwidth
  - Peak performance
- **How it is implemented**
  - Good/bad locality
  - SIMD or not




- **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





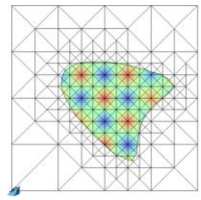

# Sparse Linear Algebra

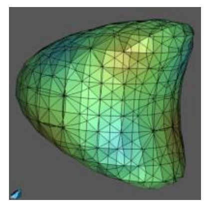
- **Sparse matrix-vector multiplication (MVM)**
- **Sparsity/Bebop/OSKI**

- **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***



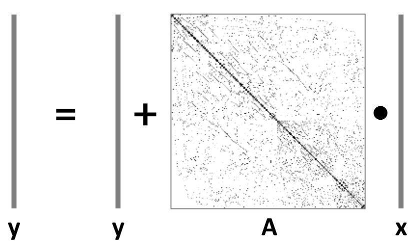


*Graphics: http://aam.mathematik.uni-freiburg.de/IAM/homepages/claus/projects/unfitted-meshes_en.html*



# Sparse MVM (SMVM)

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




- **Typically executed many times for fixed A**
- **What is reused (possible 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**
- **Popular for performance: 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

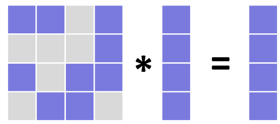
```
void smvm_2x2(int bm, const int *b_row_start, const int *b_col_idx,
              const double *b_values, double *x, double *y)
{
  int i, j;
  double d0, d1, c0, c1;

  /* 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

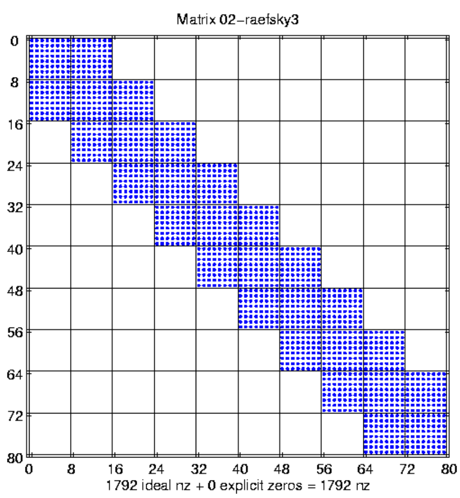
- **Advantages:**
  - Temporal locality with respect to x and y
  - Reduced storage for indexes
- **Disadvantages:**
  - Storage for values of A increased (zeros added)
  - Computational overhead (also due to zeros)




- **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?

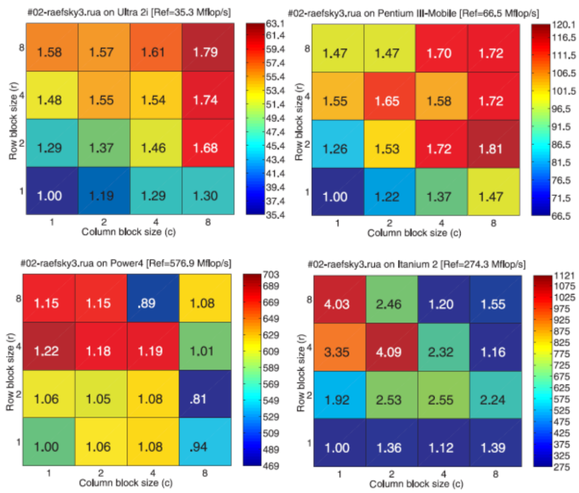



***Example:***

- **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*

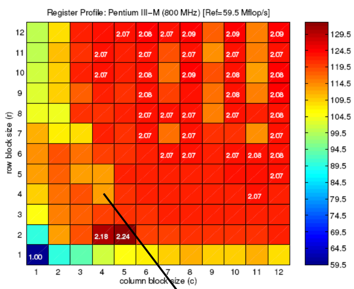


# How to Find the Best Blocking for given A?

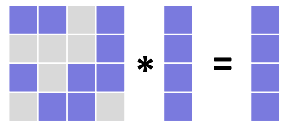
- **Best block size is hard to predict (see previous slide)**
- ***Solution 1:*** **Searching over all r x c within a range, e.g., 1 ≤ r,c ≤ 12**
  - Conversion of A in CSR to BCSR roughly as expensive as 10 SMVMs
  - Total cost: 1440 SMVMs
  - Too expensive
- ***Solution 2:*** **Model**
  - Estimate the gain through blocking
  - Estimate the loss through blocking
  - Pick best ratio

# 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**



# 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

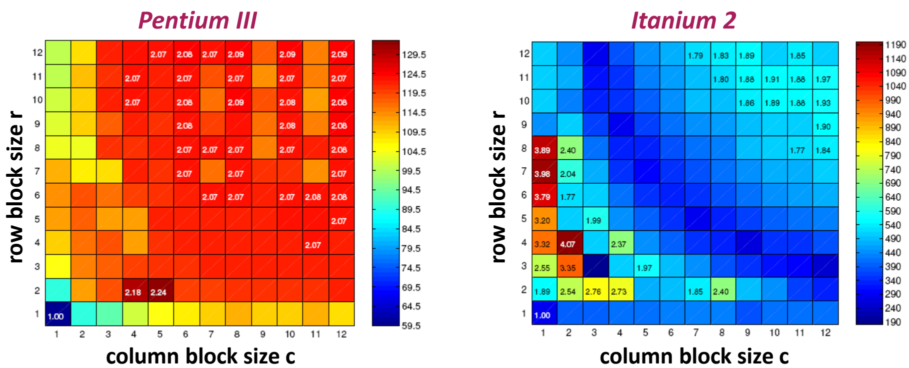
- ***Overhead*** **through r x c blocking (estimation)**
scan part of matrix A

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

independent of machine, dependent on sparse matrix

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

# Gain from Blocking (Dense Matrix in BCSR)

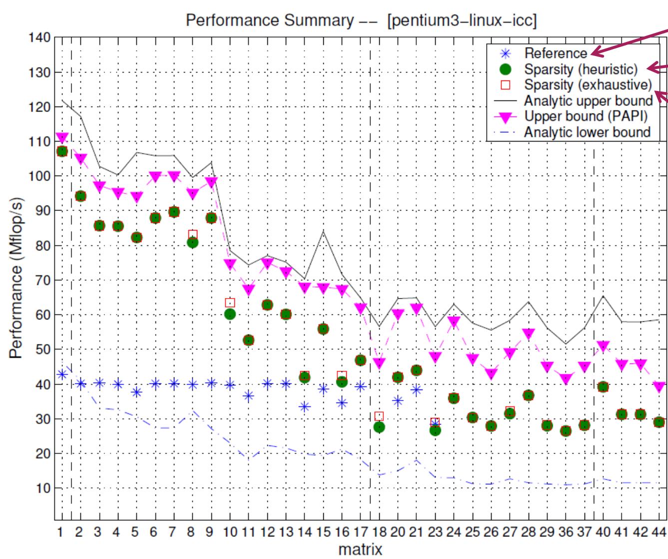



- *machine dependent*
- *hard to predict*

**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

25

# 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

26

# 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***

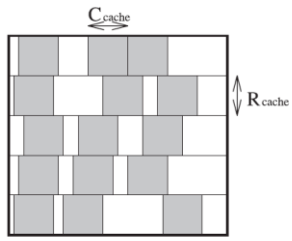


# SMVM: Other Ideas

- **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 | |

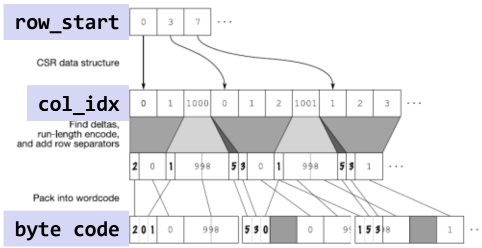
| | | | | | | | |
|---|---|---|---|---|---|---|---|
| `values` | 1 | 2 | 2 | 0 | 1 | 1 | 2 |
| `col_idx` | 0 | 1 | 3 | 1 | 2 | 3 | 2 |
| `row_start` | 0 | 3 | 4 | 6 | 7 | | |

*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**

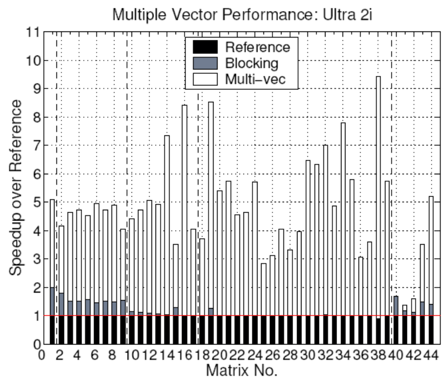
| | | | | | | |
|---|---|---|---|---|---|---|
| b | c | a | c | b | b | c |

**+ 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