Case study:
Sparse Matrix-Vector Multiplication

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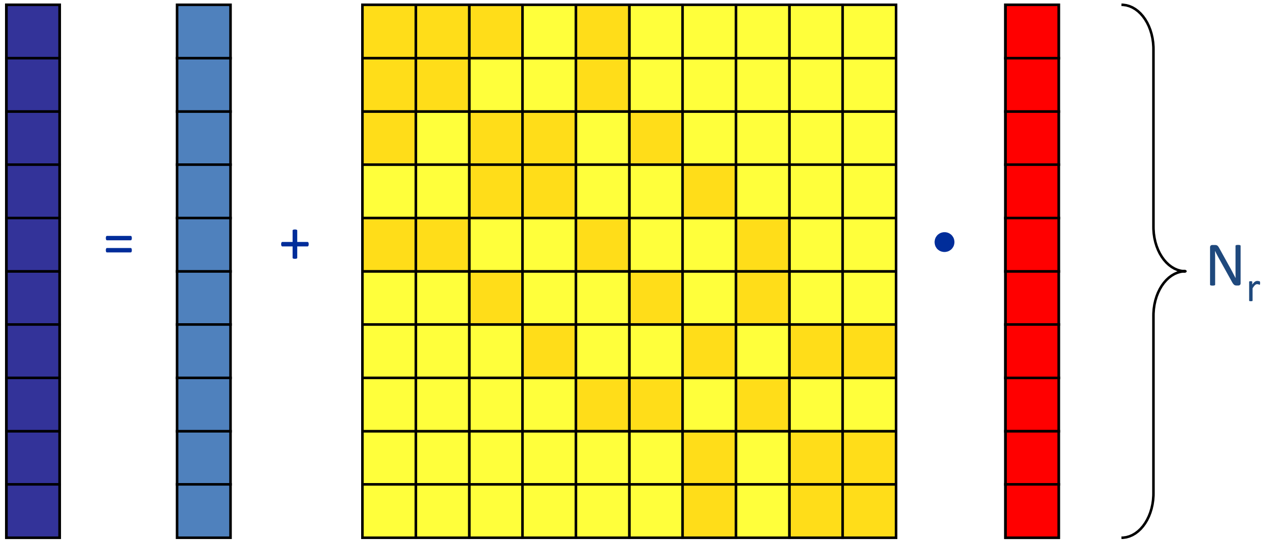
Sparse Matrix Vector Multiplication (SpMV)

- Key ingredient in some matrix diagonalization algorithms
  - Lanczos, Davidson, Jacobi-Davidson
- Store only N_{nz} nonzero elements of matrix and RHS, LHS vectors with N_r (number of matrix rows) entries
- "Sparse": $N_{nz} \sim N_r$
- Average number of nonzeros per row: $N_{nzr} = N_{nz}/N_r$

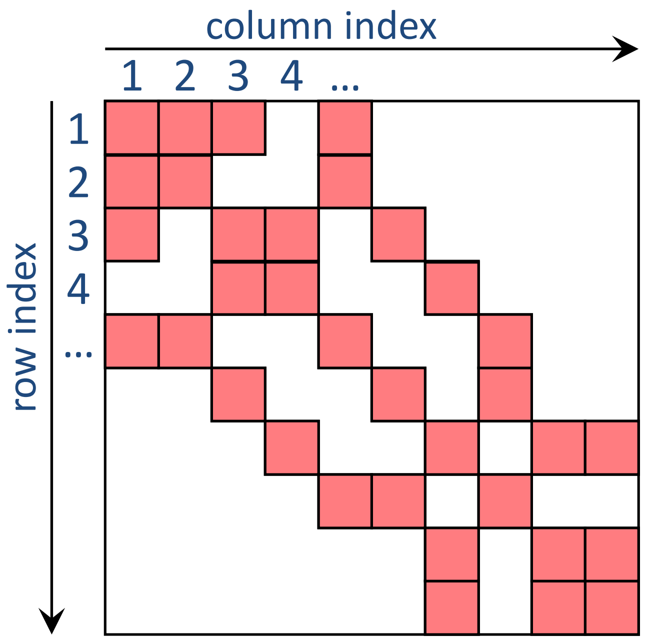


General case: some indirect addressing required!

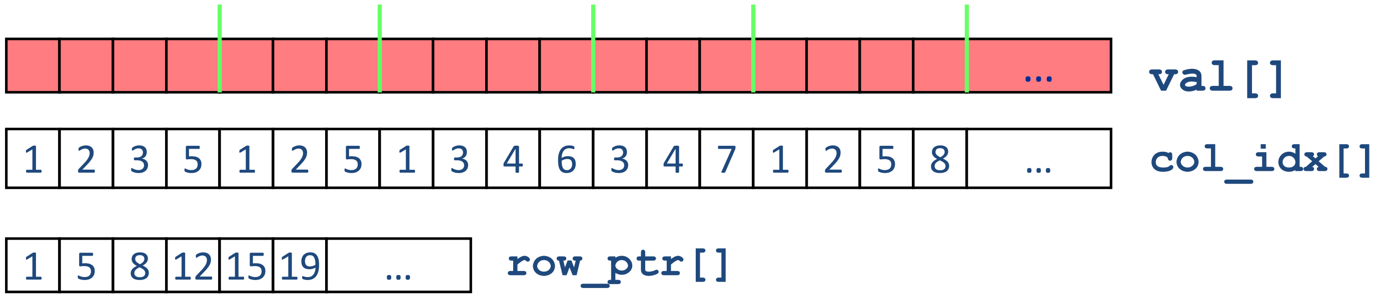
SpMVM characteristics

- For large problems, SpMV is inevitably memory-bound
  - Intra-socket saturation effect on modern multicores
- SpMV is easily parallelizable in shared and distributed memory
  - Load balancing
  - Communication overhead
- Data storage format is crucial for performance properties
  - Most useful general format on CPUs:
    Compressed Row Storage (CRS)
  - Depending on compute architecture

CRS matrix storage scheme



- **`val[]`** stores all the nonzeros (length N_{nz})
- **`col_idx[]`** stores the column index of each nonzero (length N_{nz})
- **`row_ptr[]`** stores the starting index of each new row in **`val[]`** (length: N_r)



Case study: Sparse matrix-vector multiply

- Strongly memory-bound for large data sets
  - Streaming, with partially indirect access:

```
!$OMP parallel do schedule(???)
do i = 1,Nr
 do j = row_ptr(i), row_ptr(i+1) - 1
  C(i) = C(i) + val(j) * B(col_idx(j))
 enddo
enddo
!$OMP end parallel do
```

  - Usually many spMVMs required to solve a problem

- Now let's look at some performance measurements…

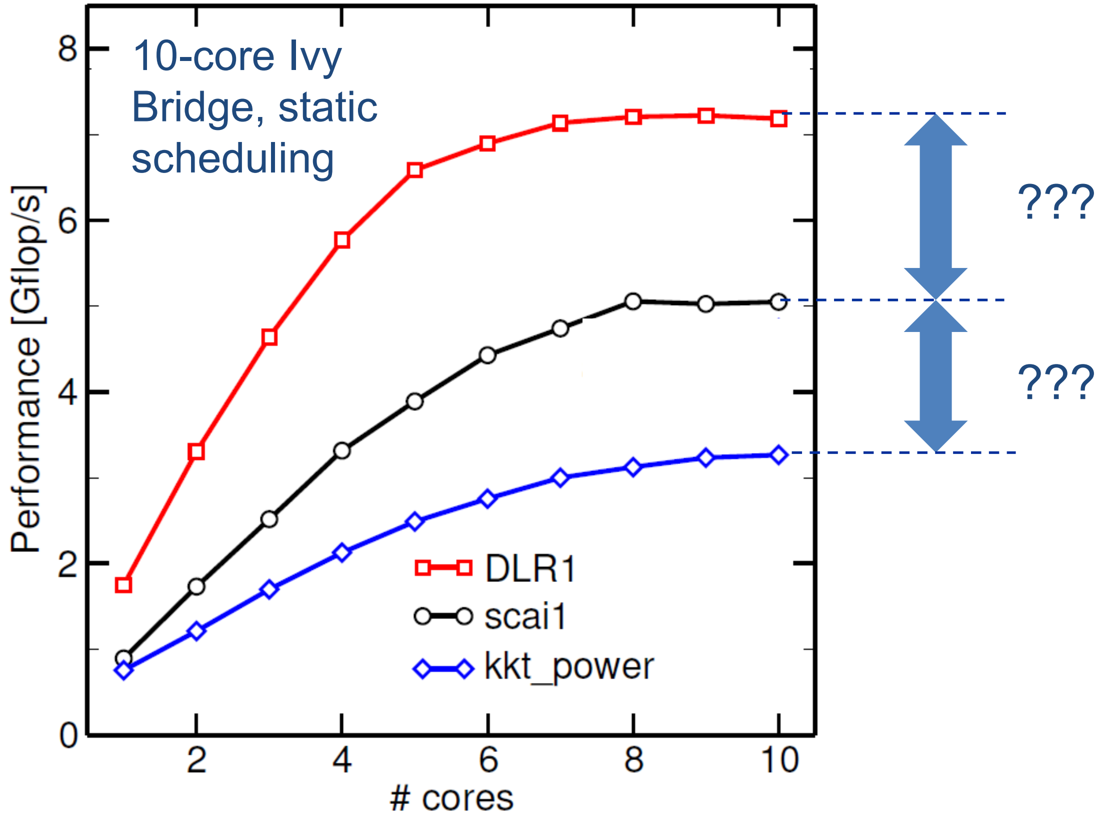
Performance characteristics

- Strongly memory-bound for large data sets → saturating performance across cores on the chip
- Performance seems to depend on the matrix

- Can we explain this?

- Is there a "light speed" for SpMV?

- Optimization?



SpMV node performance model – CRS (1)

```
do i = 1, Nr
 do j = row_ptr(i), row_ptr(i+1) - 1
  C(i) = C(i) + val(j) * B(col_idx(j))
 enddo
enddo
```

```
real*8      val(Nnz)
integer*4   col_idx(Nnz)
integer*4   row_ptr(Nr)
real*8      C(Nr)
real*8      B(Nc)
```

Min. load traffic [B]: $(8 + 4)\, N_{nz} + (4 + 8) N_r + 8\, N_c$

Min. store traffic [B]: $8\, N_r$

Total FLOP count [F]: $2\, N_{nz}$

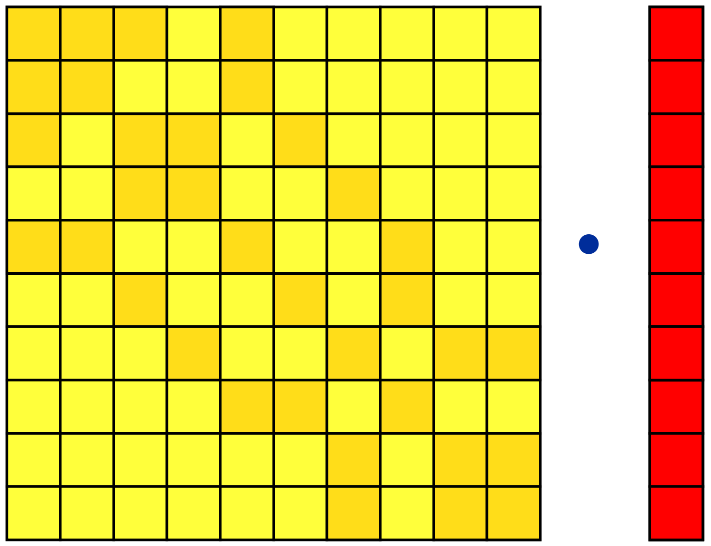
$$B_{C,min} = \frac{12\, N_{nz} + 20\, N_r + 8\, N_c}{2\, N_{nz}} \frac{B}{F} = \frac{12 + 20/N_{nzr} + 8/N_{nzc}}{2} \frac{B}{F}$$

Nonzeros per row ($N_{nzr} = {}^{N_{nz}}/_{N_r}$) or column ($N_{nzc} = {}^{N_{nz}}/_{N_c}$)

Lower bound for code balance: $B_{C,min} \geq 6\, \frac{\mathrm{B}}{\mathrm{F}}$ → $I_{\max} \leq \frac{1}{6} \frac{\mathrm{F}}{\mathrm{B}}$

SpMV node performance model – CRS (2)

```
do i = 1, Nr
 do j = row_ptr(i), row_ptr(i+1) - 1
  C(i) = C(i) + val(j) * B(col_idx(j))
 enddo
enddo
```



$$B_{C,min} = \frac{12 + 20/N_{nzr} + 8/N_{nzc}}{2} \frac{B}{F}$$

$$B_C\ (\alpha) = \frac{12 + 20/N_{nzr} + 8\,\alpha}{2} \frac{B}{F}$$

Parameter (α) quantifies additional traffic for **B(:)** (irregular access):

$$\alpha \geq {}^{1}/_{N_{nzc}}$$

$$\alpha N_{nzc} \geq 1$$

Consider square matrices: $N_{nzc} = N_{nzr}$ and $N_c = N_r$

Note: $B_C\left({}^{1}/_{N_{nzr}}\right) = B_{C,min}$

The “α effect”

DP CRS code balance

- α quantifies the traffic for loading the RHS
  - $\alpha = 0$ → RHS is in cache
  - $\alpha = 1/N_{nzr}$ → RHS loaded once
  - $\alpha = 1$ → no cache
  - $\alpha > 1$ → Houston, we have a problem!
- “Target” performance = b_S/B_c
- Caveat: Maximum memory BW may not be achieved with spMVM (see later)

$$B_C\,(\alpha) = \frac{12 + 20/N_{nzr} + 8\,\alpha}{2}\,\frac{B}{F}$$

$$= \left(6 + 4\,\alpha + \frac{10}{N_{nzr}}\right)\frac{B}{F}$$

Can we predict α?

- Not in general
- Simple cases (banded, block-structured): Similar to layer condition analysis

→ Determine α by measuring the actual memory traffic (→ measured code balance B_C^{meas})

Determine $\boldsymbol{\alpha}$ (RHS traffic quantification)

$$B_C\ (\alpha) = \left(6+4\alpha+\frac{10}{N_{nzr}}\right)\frac{\mathrm{B}}{\mathrm{F}} = \frac{V_{meas}}{N_{nz}\cdot 2\ \mathrm{F}} \quad (= B_C^{meas})$$

- V_{meas} is the measured overall memory data traffic (using, e.g., likwid-perfctr)
- Solve for α:

$$\alpha = \frac{1}{4}\left(\frac{V_{meas}}{N_{nz}\cdot 2\ \text{bytes}} - 6 - \frac{10}{N_{nzr}}\right)$$

Example: kkt_power matrix from the UoF collection on one Intel SNB socket

- $N_{nz} = 14.6\cdot 10^6, N_{nzr} = 7.1$
- $V_{meas} \approx 258\ \mathrm{MB}$

→ $\alpha = 0.36$, $\alpha N_{nzr} = 2.5$

→ RHS is loaded 2.5 times from memory

$$\frac{B_C\ (\alpha)}{B_{C,min}} = 1.11$$

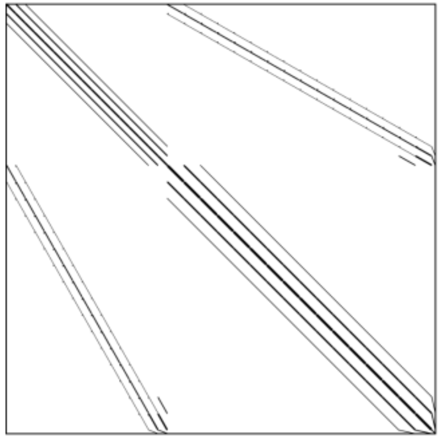
11% extra traffic → optimization potential!

Three different sparse matrices

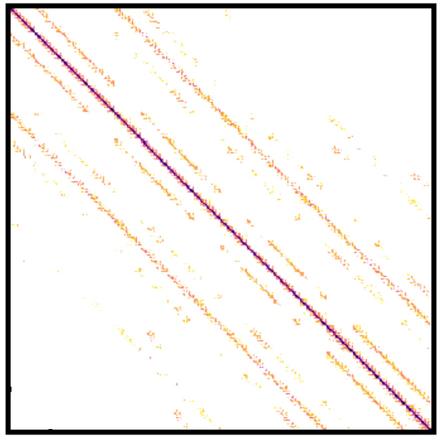
Benchmark system: Intel Xeon Ivy Bridge E5-2660v2, 2.2 GHz, $b_S = 46.6\,\mathrm{GB/s}$

→ Roofline: $P_{opt} = {}^{b_S}/_{B_{C,min}}$

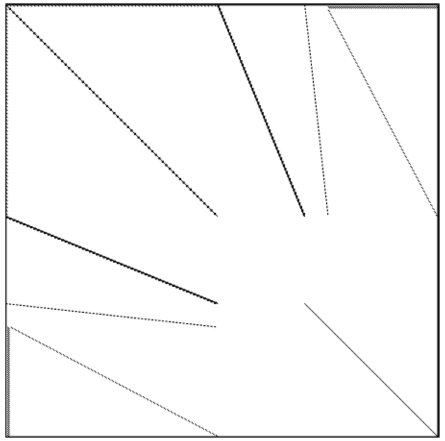
Matrix	N	N_{nzr}	$B_{C,min}$ [B/F]	P_{opt} [GF/s]
DLR1	278,502	143	6.1	7.64
scai1	3,405,035	7.0	8.0	5.83
kkt_power	2,063,494	7.08	8.0	5.83



DLR1

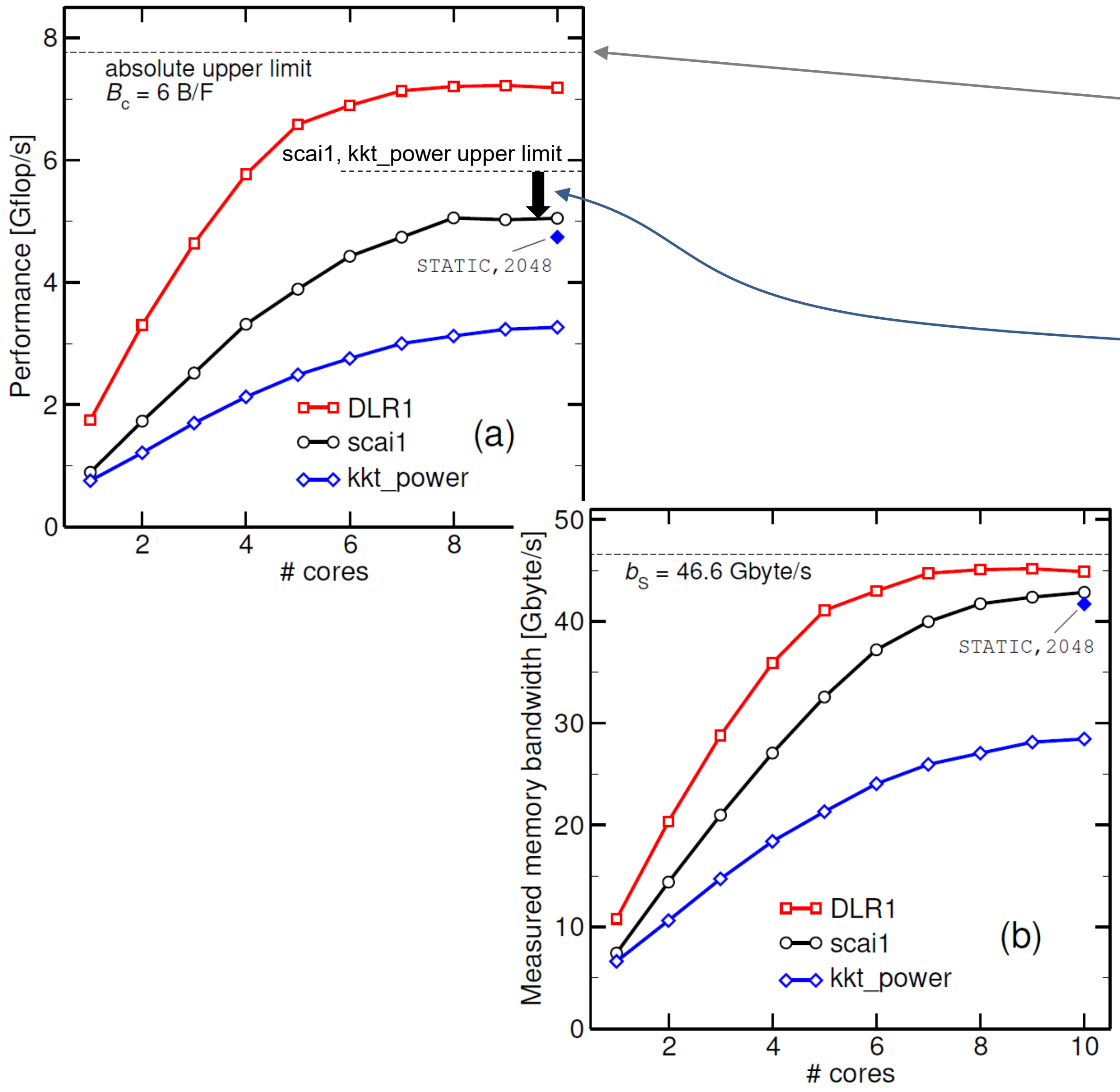


scai1



kkt_power

Now back to the start…



- $b_S = 46.6\,\mathrm{GB/s}\,, \quad B_c \;= 6\,\mathrm{B/F}$
- Maximum spMVM performance:

$$P_{max} = 7.8\,\mathrm{GF/s}$$

- **DLR1** causes (almost) minimum CRS code balance (as expected)

- **scai1** measured balance:

$B_c^{meas} \approx 8.5\,\mathrm{B/F} > B_{C,min}$ (6% higher than min)

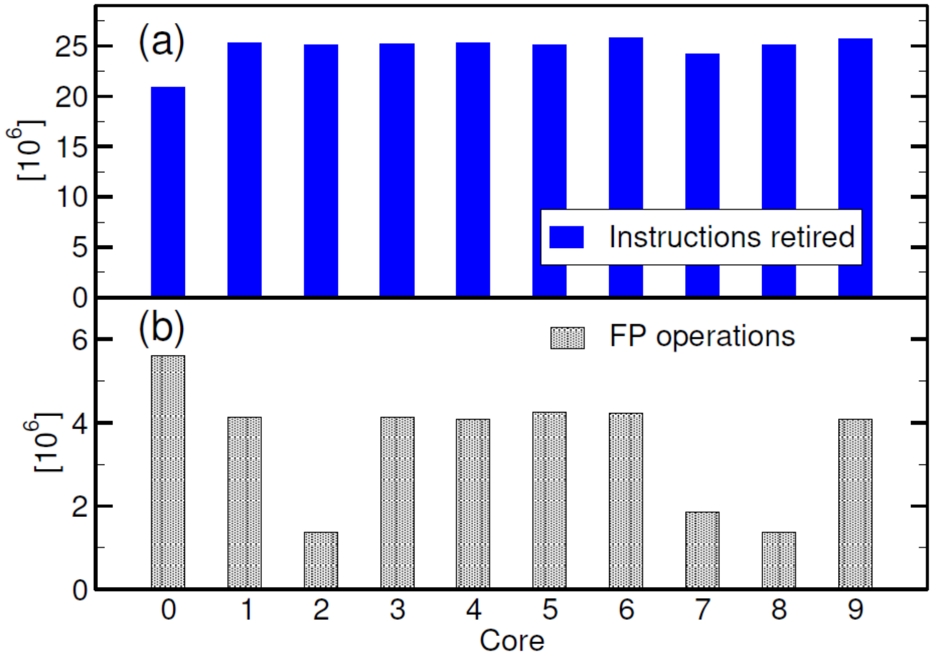
→ good BW utilization, slightly non-optimal α

- **kkt_power** measured balance:

$B_c^{meas} \approx 8.8\,\mathrm{B/F} > B_{C,min}$ (10% higher than min)

→ performance degraded by load imbalance, fix by block-cyclic schedule

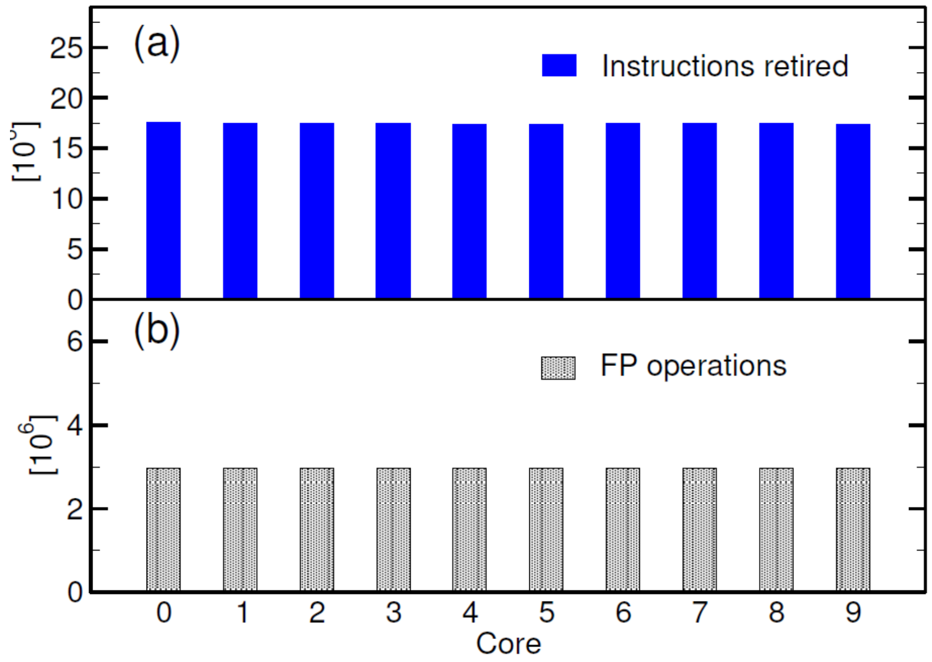
Investigating the load imbalance with kkt_power



Measurements with likwid-perfctr (MEM_DP group)

`static`

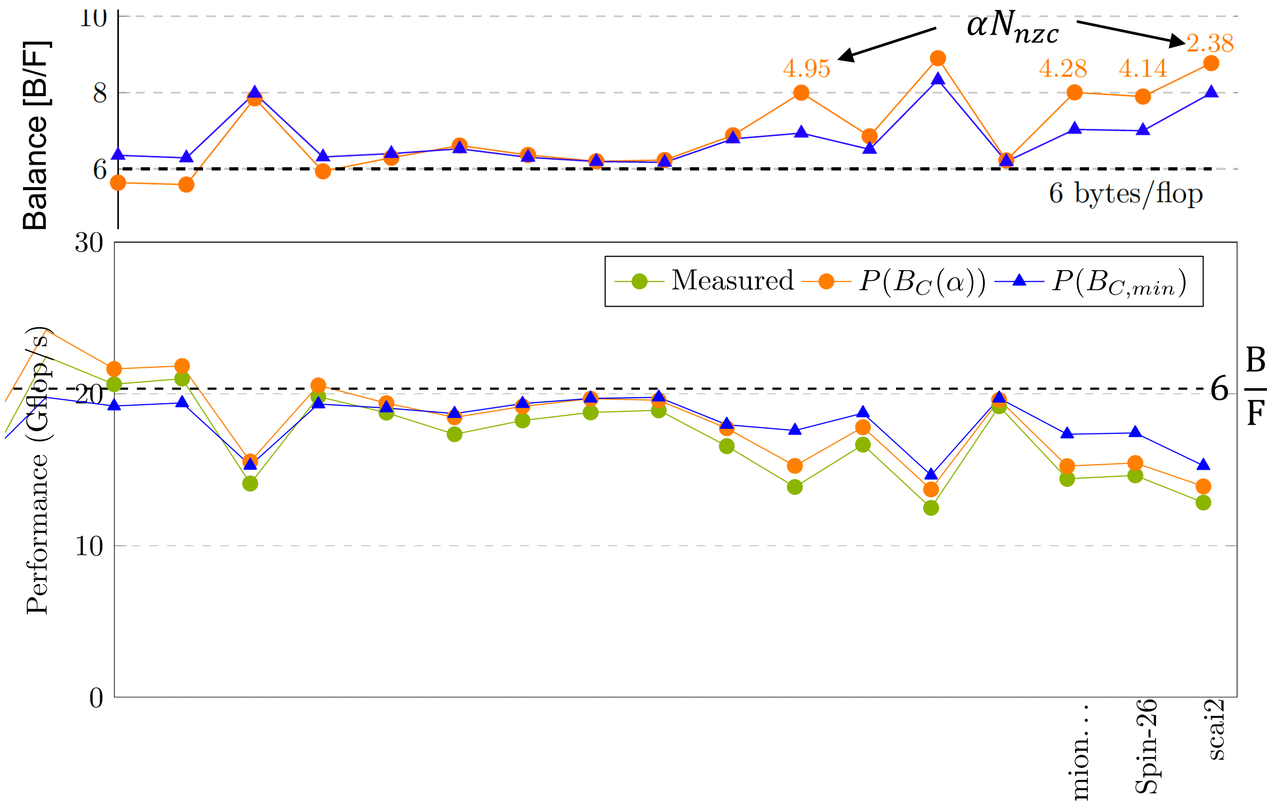
`static,2048`



→ Fewer overall instructions, (almost) BW saturation, 50% better performandce with load balancing

→ CPI value unchanged!

SpMV node performance model – CPU



Intel Xeon Platinum 9242
24c@2.8GHz (turbo)
$b_S = 122\ GB/s$

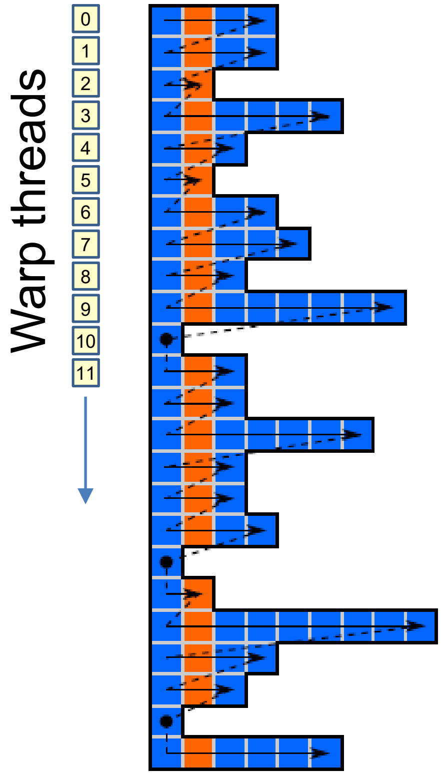
Matrices taken from: C. L. Alappat et al.: *ECM modeling and performance tuning of SpMV and Lattice QCD on A64FX.* In print. Preprint: arXiv:2103.0301

What about GPUs?

- GPUs need
  - Enough work per kernel launch in order to leverage their parallelism
  - Coalesced access to memory (consecutive threads in a warp should access consecutive memory addresses)

- Plain CRS for SpMV on GPUs is not a good idea
  1. Short inner loop
  2. Different amount of work per thread
  3. Non-coalesced memory access

- Remedy: Use SIMD/SIMT-friendly storage format
  - ELLPACK, SELL-C-σ, DIA, ESB,…



CRS SpMV in CUDA (y = Ax)

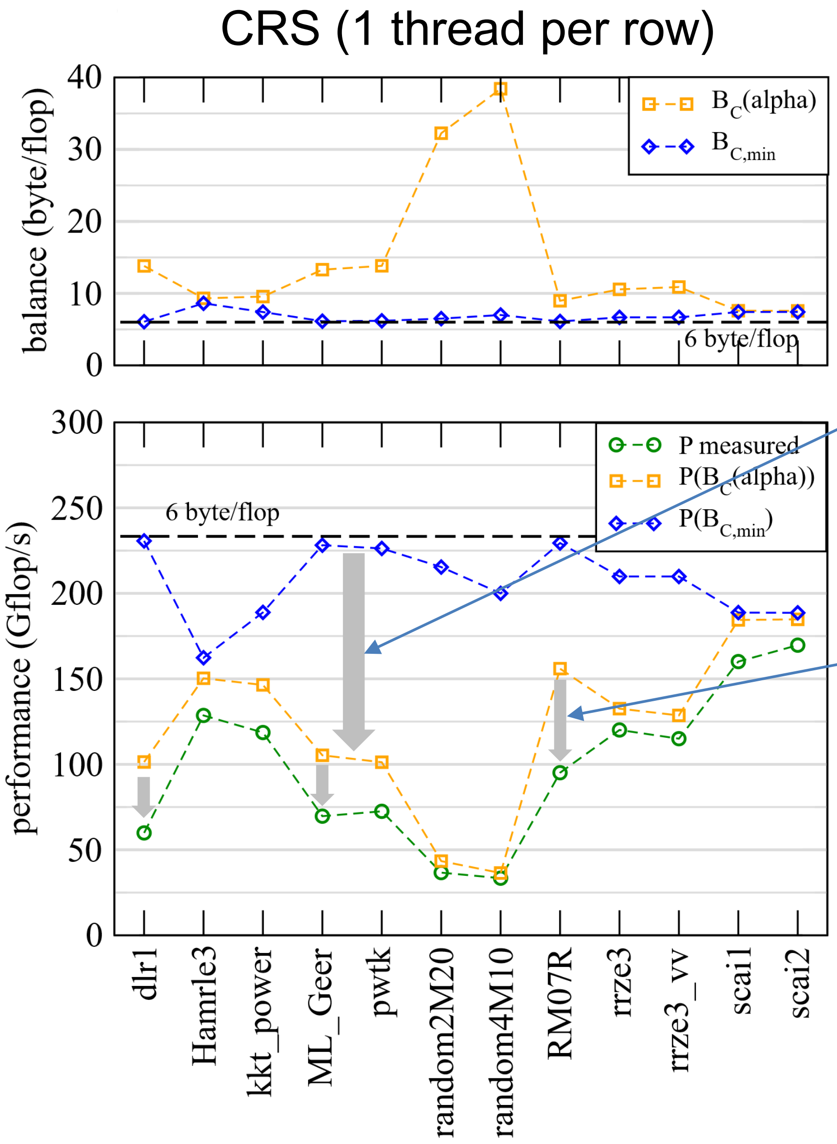
```
template <typename VT, typename IT>
__global__ static void
spmv_csr(const ST num_rows,
         const IT * RESTRICT row_ptrs, const IT * RESTRICT col_idxs,
         const VT * RESTRICT values,   const VT * RESTRICT x,
                                             VT * RESTRICT y)
{
    ST row = threadIdx.x + blockDim.x * blockIdx.x; // 1 thread per row

    if (row < num_rows) {
        VT sum{};
        for (IT j = row_ptrs[row]; j < row_ptrs[row + 1]; ++j) {
            sum += values[j] * x[col_idxs[j]];
        }
        y[row] = sum;
    }
}
```

$$B_c(\alpha) = \left(6 + 4\,\alpha + \frac{6}{N_{nzr}}\right)\frac{B}{F}$$

No write-allocate on GPUs for consecutive stores

SpMV CRS performance on a GPU



NVIDIA Ampere A100
Memory bandwidth $b_S = 1400\ \mathrm{GB/s}$

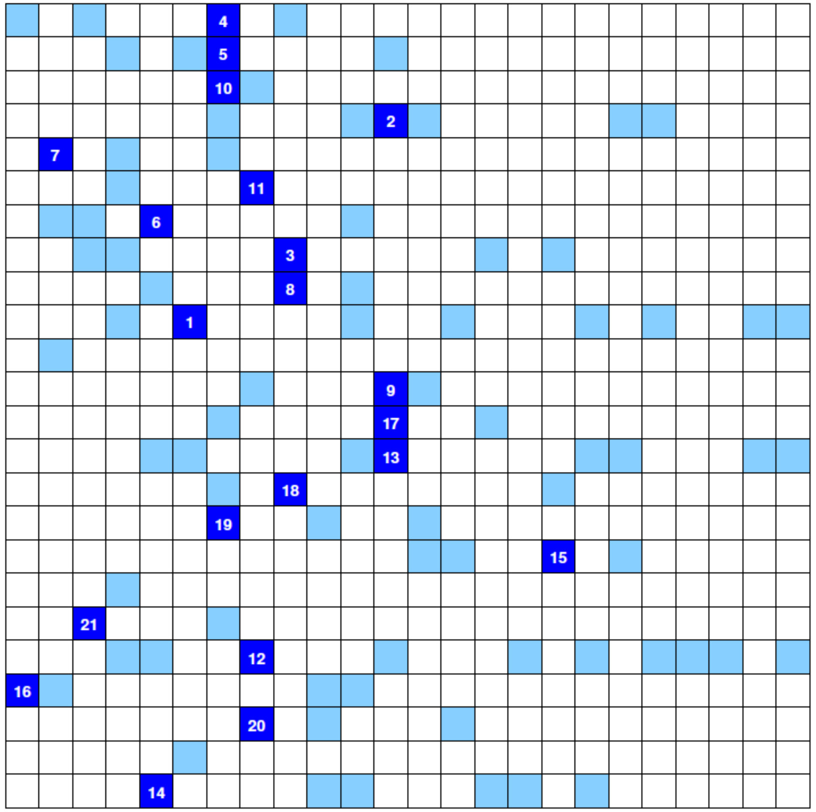
- Strong "α effect" – large deviation from optimal α for many matrices
  - Many cache lines touched b/c every thread handles one row → bad cache usage
- Mediocre memory bandwidth usage ($\ll 1400\ \mathrm{GB/s}$) in many cases
  - Non-coalesced memory access
  - Imbalance across rows/threads of warps

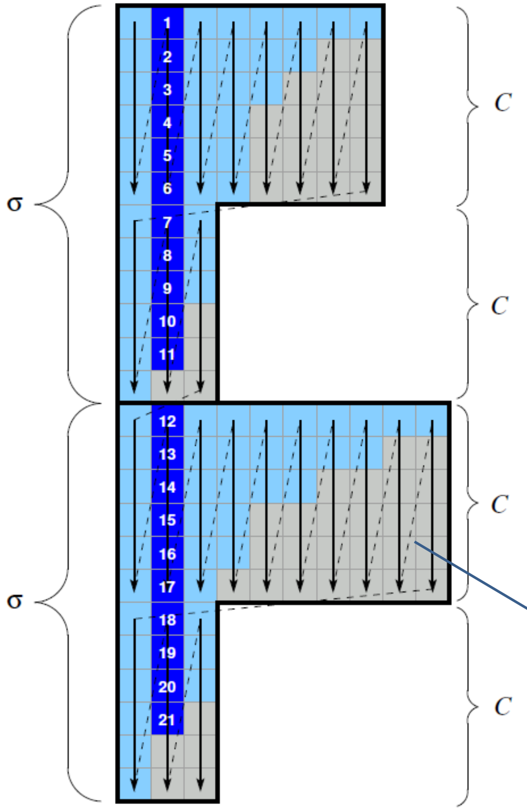
SELL-C-σ

M. Kreutzer et al.: *A Unified Sparse Matrix Data Format For Efficient General Sparse Matrix-vector Multiplication On Modern Processors With Wide SIMD Units*, SIAM SISC 2014, DOI: [10.1137/130930352](https://doi.org/10.1137/130930352)

Idea

- Sort rows according to length within sorting scope σ
- Store nonzeros column-major in zero-padded chunks of height C





"Chunk occupancy":

$$\beta = \frac{N_{nz}}{\sum_{i=0}^{N_c} C \cdot l_i}$$

l_i: width of chunk i

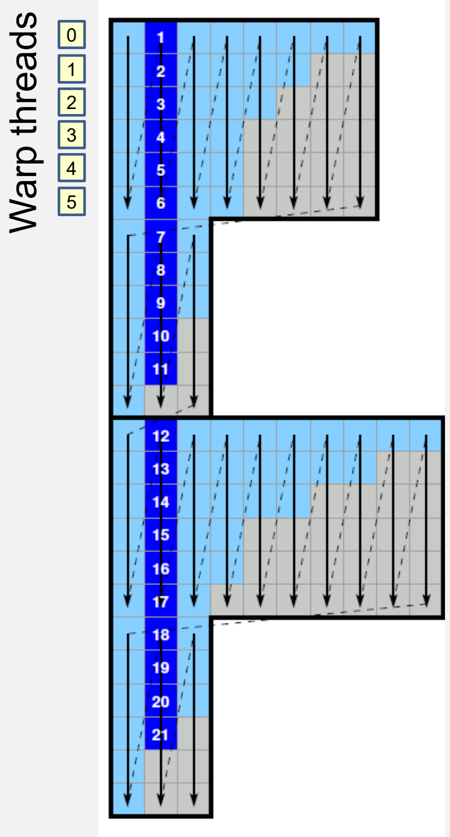
zero padding

SELL-C-σ SpMV in CUDA (y=Ax)

```
template <typename VT, typename IT> __global__ static void
spmv_scs(const ST C, const ST n_chunks,      const IT * RESTRICT chunk_ptrs,
         const IT * RESTRICT chunk_lengths, const IT * RESTRICT col_idxs,
         const VT * RESTRICT values, const VT * RESTRICT x, VT * RESTRICT y)
{
   ST row = threadIdx.x + blockDim.x * blockIdx.x;
   ST c   = row / C;  // the no. of the chunk
   ST idx = row % C;  // index inside the chunk

   if (row < n_chunks * C) {
       VT tmp{};
       IT cs = chunk_ptrs[c]; // points to start indices of chunks

       for (ST j = 0; j < chunk_lengths[c]; ++j) {
           tmp += values[cs + idx] * x[col_idxs[cs + idx]];
           cs += C;
       }
       y[row] = tmp;
   }
}
```



Code balance of SELL-C-σ (y=Ax)

Matrix data & column index

LHS update (write only)

chunk index

$$B_{SELL}(\alpha,\beta,N_{nzr}) = \left(\frac{1}{\beta}\left(\frac{\overbrace{8+4}}{2}\right) + \frac{8\alpha+\beta(8+4/C)/N_{nzr}}{2}\right)\frac{\text{bytes}}{\text{flop}}$$

$$= \left(\frac{6}{\beta} + 4\alpha + \frac{\beta(4+2/C)}{N_{nzr}}\right)\frac{\text{bytes}}{\text{flop}}$$

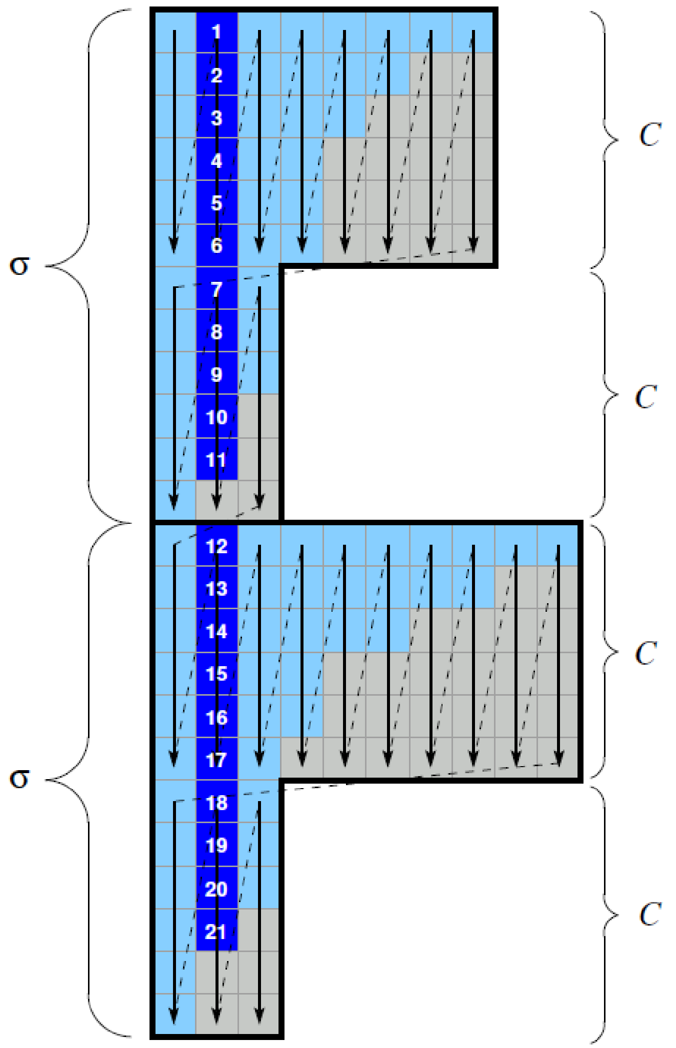
Optimal $\alpha = \frac{\beta}{N_{nzr}}$

When measuring B_C^{meas}, take care to use the "useful" number of flops (excluding zero padding) for work

How to choose the parameters C and σ on GPUs?

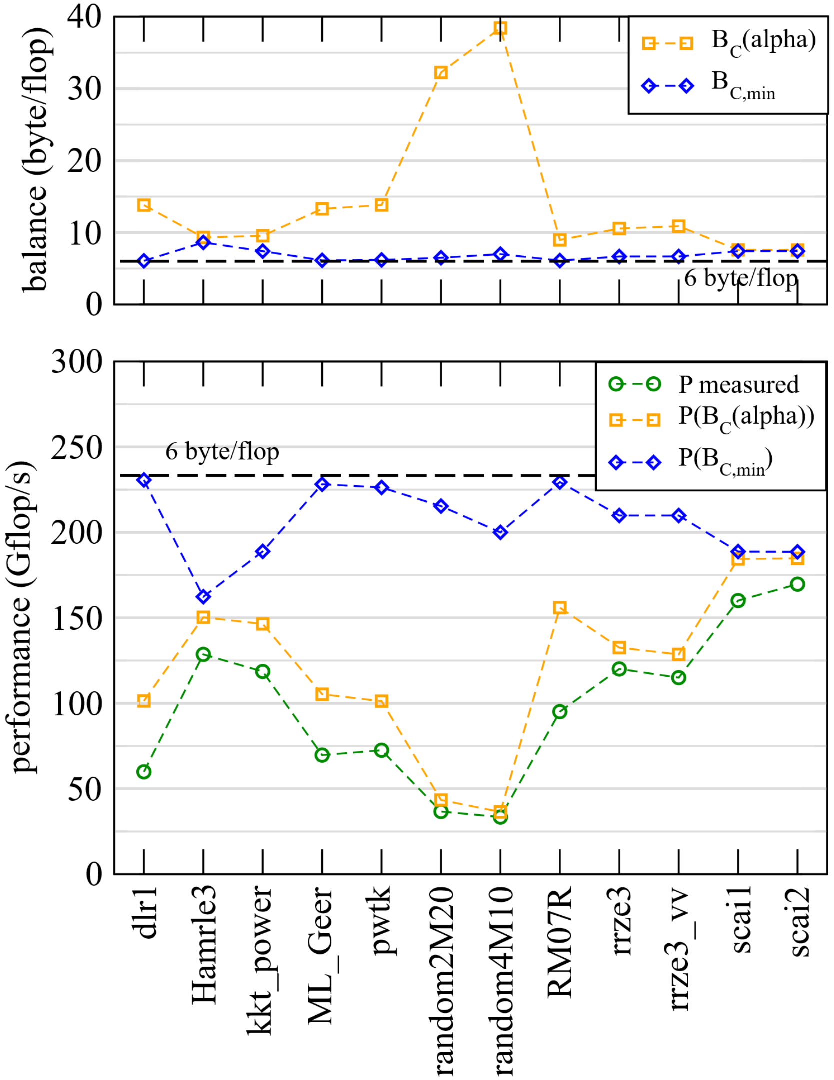
- C
  - $n \times$ warp size to allow good utilization of GPU threads and cache lines

- σ
  - As small as possible, as large as necessary
  - Large σ reduces zero padding (brings β closer to 1)
  - Sorting alters RHS access pattern → α depends on σ



SpMV node performance model – GPU

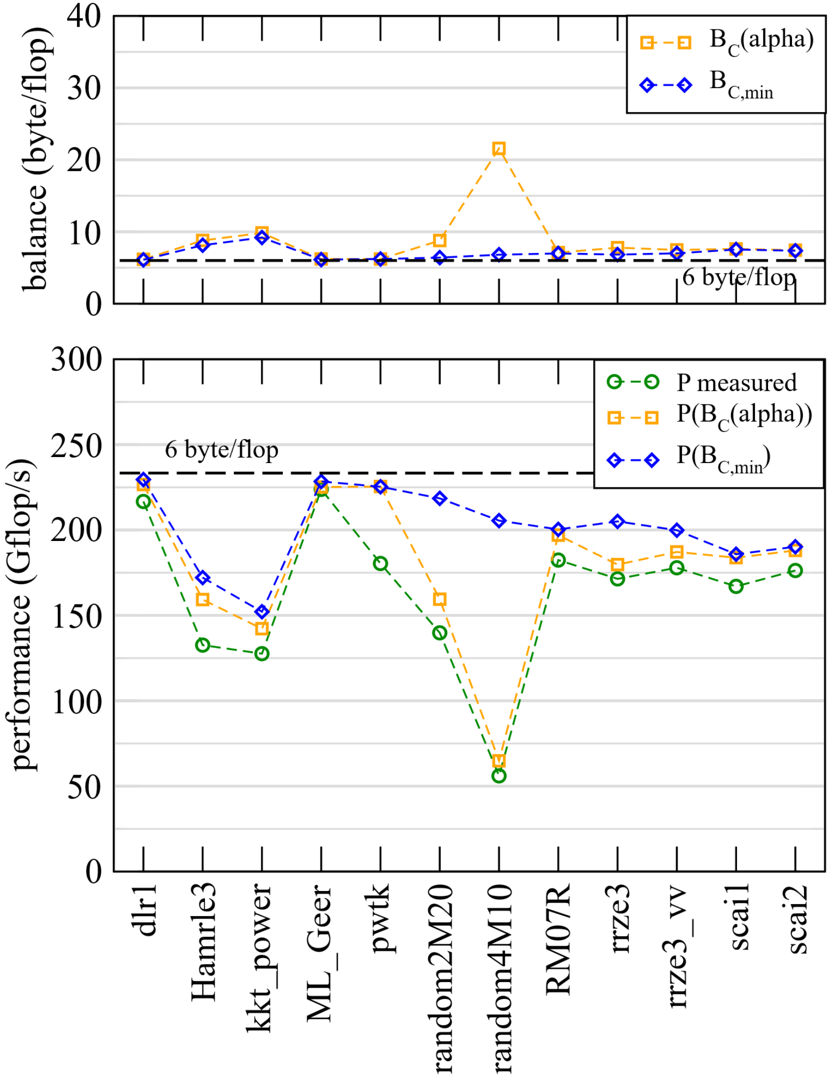
CRS (1 thread per row)



NVIDIA Ampere A100

$b_S = 1400\ \text{GB/s}$

SELL-32-128

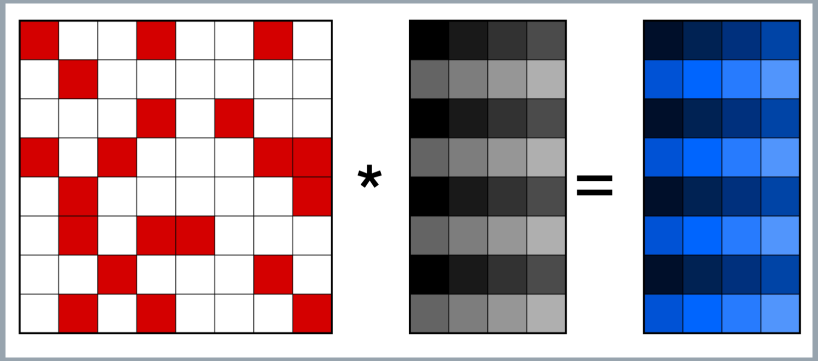


Roofline analysis for spMVM

- Conclusion from the Roofline analysis
  - The roofline model does not “work” for spMVM due to the RHS traffic uncertainties
  - We have “turned the model around” and measured the actual memory traffic to determine the RHS overhead
  - Result indicates:
    1. how much actual traffic the RHS generates
    2. how efficient the RHS access is (compare BW with max. BW)
    3. how much optimization potential we have with matrix reordering
- Do not forget about load balancing!
- Sparse matrix times multiple vectors bears the potential of huge savings in data volume
- Consequence: Modeling is not always 100% predictive. It‘s all about *learning more* about performance properties!

BACKUP

Applying sparse matrix to multiple vectors (Sparse Matrix Multiple Vectors: SpMMV)



Multiple RHS vectors (SpMMV)

Unchanged matrix applied to multiple RHS (`r`) vectors to yield multiple LHS (`r`) vectors

```
do s = 1,r
 do i = 1, Nr
  do j = row_ptr(i),row_ptr(i+1)-1
   C(i,s) = C(i,s) + val(j) *
            B(col_idx(j),s)
  enddo
 enddo
enddo
```

B_c unchanged, no reuse of matrix data

```
do i = 1, Nr
 do j = row_ptr(i),row_ptr(i+1)-1
  do s = 1,r
   C(i,s) = C(i,s) + val(j) *
            B(col_idx(j),s)
  enddo
 enddo
enddo
```

Higher B_c due to max reuse of matrix data

```
do i = 1, Nr
 do j = row_ptr(i),row_ptr(i+1)-1
  do s = 1,r
   C(s,i) = C(s,i) + val(j) *
            B(s,col_idx(j))
  enddo
 enddo
enddo
```

CL-friendly data structure (row major)

SpMMV code balance

One complete inner (`s`) loop traversal:

- $2r$ flops
- 12 bytes from matrix data (value + index)
- $\frac{16r}{N_{nzr}}$ bytes from the r LHS updates
- $\frac{4}{N_{nzr}}$ bytes from the row pointer
- $8r\alpha(r)$ bytes from the r RHS reads

```
do i = 1, Nr
 do j = row_ptr(i),row_ptr(i+1)-1
  do s = 1,r
   C(s,i) = C(s,i) + val(j) *
            B(s,col_idx(j))
  enddo
 enddo
enddo
```

$$B_c(r) = \frac{1}{2r}\left(12 + 8r\alpha(r) + \frac{16r+4}{N_{nzr}}\right)\frac{\mathrm{B}}{\mathrm{F}}$$

$$= \left(\frac{6}{r} + 4\alpha(r) + \frac{8+2/r}{N_{nzr}}\right)\frac{\mathrm{B}}{\mathrm{F}}$$

OK so what now???

SpMMV code balance

Let's check some limits to see if this makes sense!

$$B_c(r) = \left(\frac{6}{r} + 4\alpha(r) + \frac{8 + 2/r}{N_{nzr}}\right)\frac{\mathrm{B}}{\mathrm{F}}$$

$r = 1$ →

$$\left(6+4\alpha+\frac{10}{N_{nzr}}\right)\frac{\mathrm{B}}{\mathrm{F}}$$

reassuring ☺

$r \gg 1$ →

$$\left(4\alpha(r) + \frac{8}{N_{nzr}}\right)\frac{\mathrm{B}}{\mathrm{F}}$$

Can become very small for large N_{nzr} → decoupling from memory bandwidth is possible!

$N_{nzr} \gg 1$ →

$$\frac{6}{r}\,\frac{\mathrm{B}}{\mathrm{F}}$$

M. Kreutzer et al.: *Performance Engineering of the Kernel Polynomial Method on Large-Scale CPU-GPU Systems*. Proc. IPDPS15, DOI: 10.1109/IPDPS.2015.76

SELL-C-σ kernel on CPUs

Example $C = 4$ without further unrolling

```
for(i = 0; i < N/4; ++i)
{

  for(j = 0; j < cl[i]; ++j)
  {
    y[i*4+0] += val[cs[i]+j*4+0] *
                x[col[cs[i]+j*4+0]];
    y[i*4+1] += val[cs[i]+j*4+1] *
                x[col[cs[i]+j*4+1]];
    y[i*4+2] += val[cs[i]+j*4+2] *
                x[col[cs[i]+j*4+2]];
    y[i*4+3] += val[cs[i]+j*4+3] *
                x[col[cs[i]+j*4+3]];
  }
}
```

$C = 4$