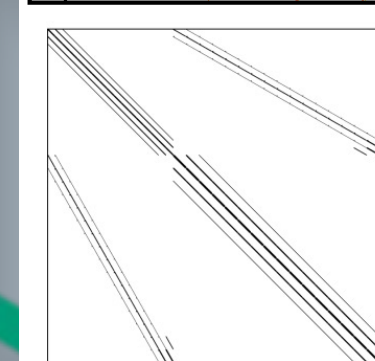
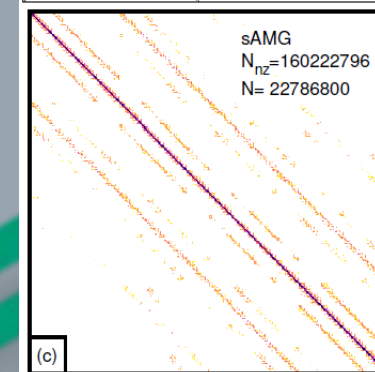
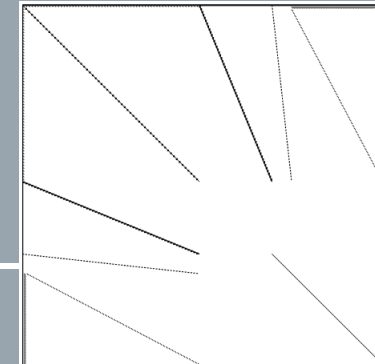


Sparse Matrix-Vector Multiplication

$$y = A x$$



Prof. Dr. G. Wellein^(a,b), Dr. G. Hager^(a)

^(a) Erlangen National High Performance Computing Center (NHR@FAU)

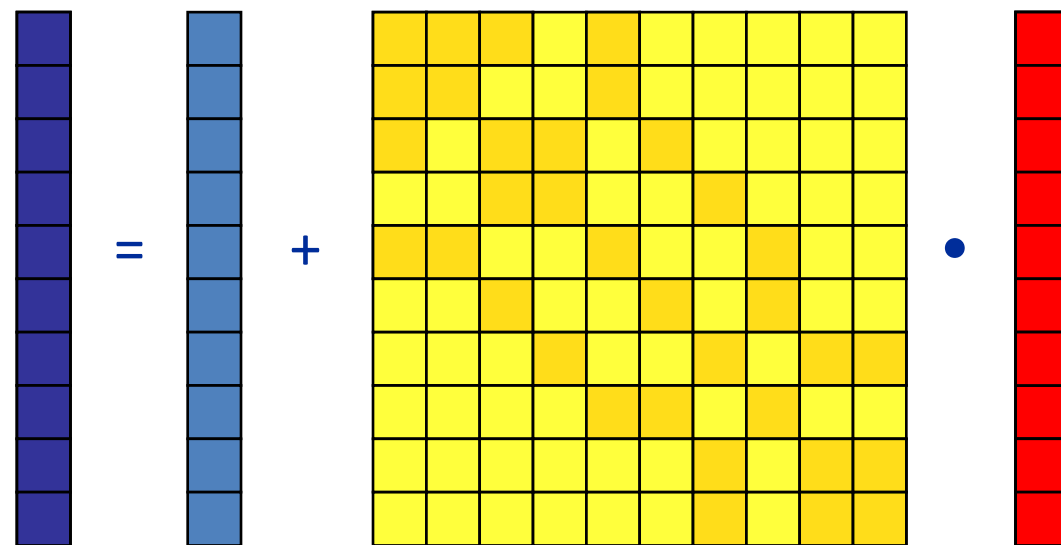
^(b) Department für Informatik

Friedrich-Alexander-Universität Erlangen-Nürnberg, Sommersemester 2024

Motivation

Algorithm 2. HPCG

```
1: while  $k \leq iter$  &  $r_{norm}/r_0 > tol$  do
2:    $z = MG(A,r)$ 
3:    $oldrtz = rtz$ 
4:    $rtz = \langle r,z \rangle$ 
5:    $\beta = rtz/oldrtz$ 
6:    $p = \beta * p + z$ 
7:    $Ap = A * p$ 
8:    $pAp = \langle p,Ap \rangle$ 
9:    $\alpha = rtz/pAp$ 
10:   $x = x + \alpha * p$ 
11:   $r = r - \alpha * Ap$ 
12:   $r_{norm} = \langle r,r \rangle$ 
13:   $r_{norm} = sqrt(r_{norm})$ 
14:   $k++$ 
```



Performance Modelling?
Optimal Performance?
Performance Optimizations?

Our SpMV plan

- Performance Engineering for SpMV – CPU
- Data layout considerations – GPUs

Boundary conditions:

- Node-level (OpenMP / CUDA)
- Application problems / matrices: Standard collection / own work

Roofline Model – Sparse Matrix Vector Multiplication

- SpMV: $y = A x$

Performance engineering of a single SpMV – general structure

- How to store and traverse SpMV
- Can we use RLM? What is the intensity of SpMV?
- Is there an maximum code intensity I for SpMV?
- Impact of matrix structure / OpenMP parallelization?
- CPU vs. GPU: Data layouts and more

Performance Engineering for Sparse Matrix-Vector Multiplication



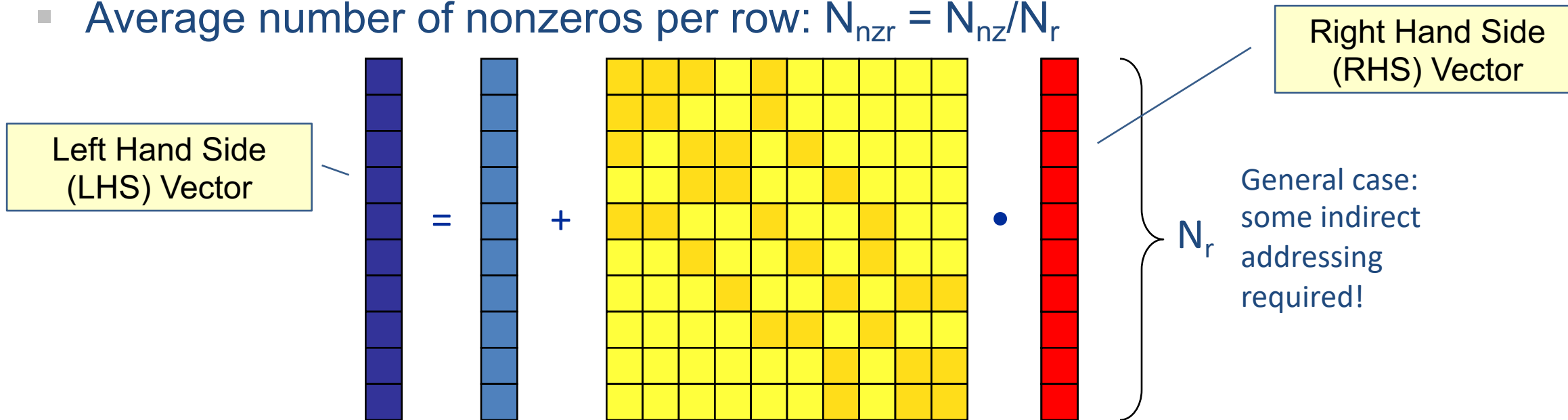
Sparse Matrix Vector Multiplication (SpMV)

Key ingredient in many sparse matrix solvers / matrix diagonalization algorithms

- Lanczos, Davidson, Jacobi-Davidson, CG, GMRES,.....

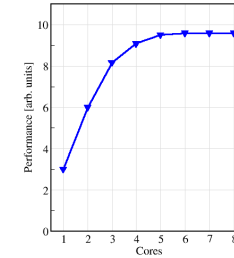
Minimize memory footprint:

- Store only N_{nz} nonzero elements of matrix with N_r (number of matrix rows) entries
- “Sparse”: $N_{nz} \sim N_r$ (assume square matrices $N_C=N_R$)
- Average number of nonzeros per row: $N_{nzc} = N_{nz}/N_r$

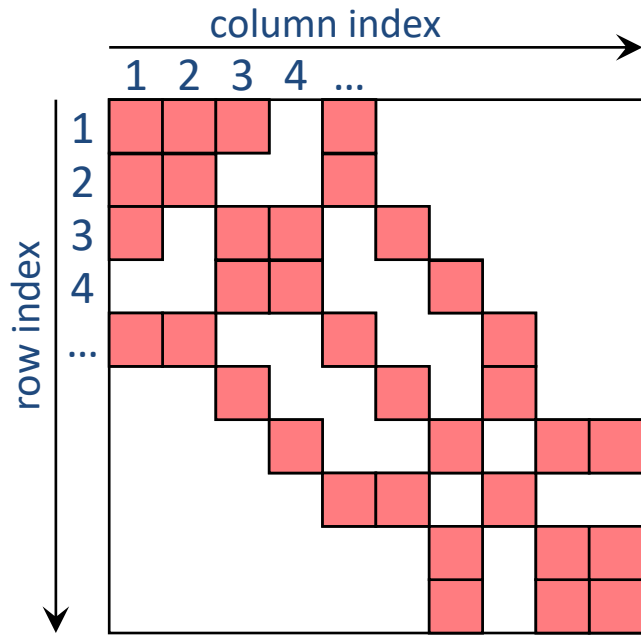


SpMVM characteristics

- 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**)
 - May depend on compute architecture and problem (sparsity pattern)

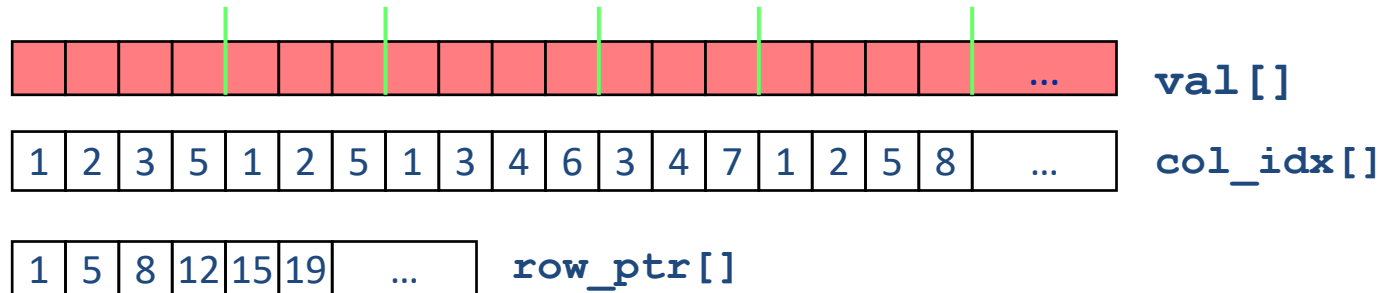


CRS matrix storage scheme



CRS data structure contains:

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



Case study: Sparse matrix-vector multiply

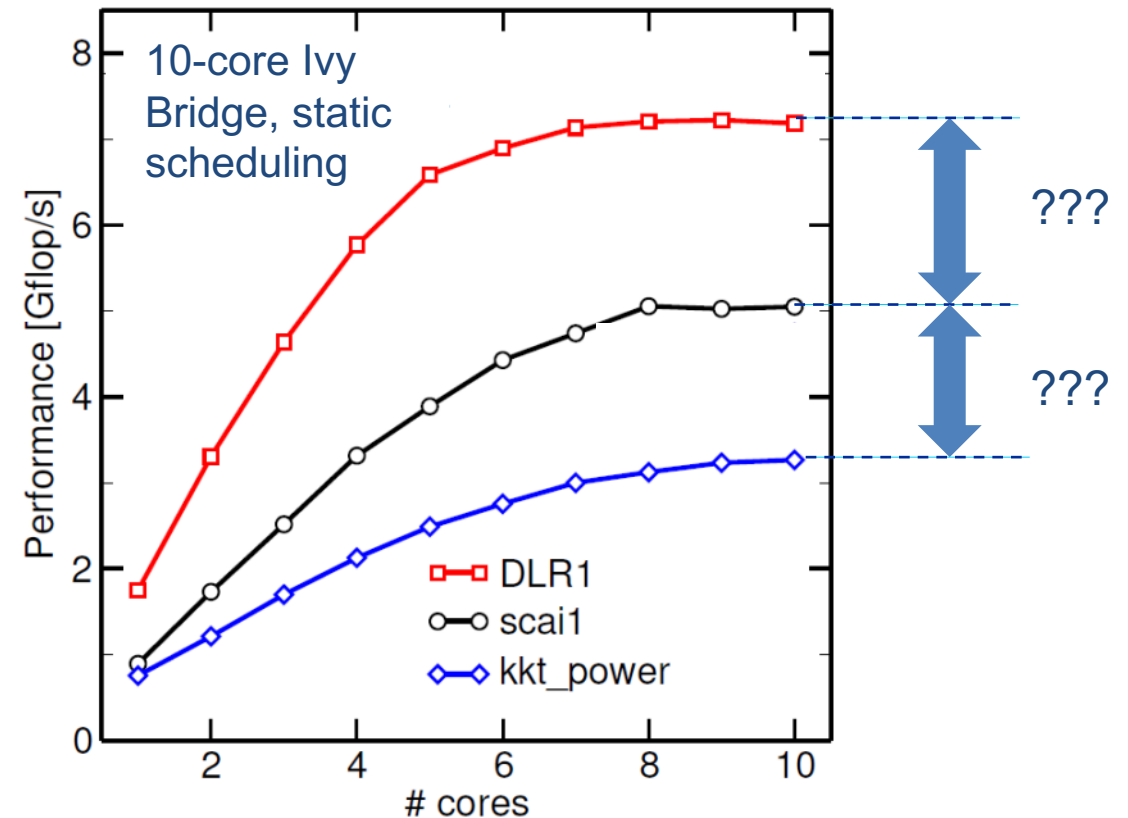
- Strongly memory-bound for large data sets
 - Mainly streaming data access (matrix data) mixed with partially indirect access (RHS data):

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

- Usually many spMV's required to solve a problem
- Typical dimensions: $N_R \approx 10^5, \dots, 10^9$ & $N_{NZR} \approx 10, \dots, 100$
- 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]: $2 N_{nz}$

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

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

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

SpMV node performance model – CRS (2)

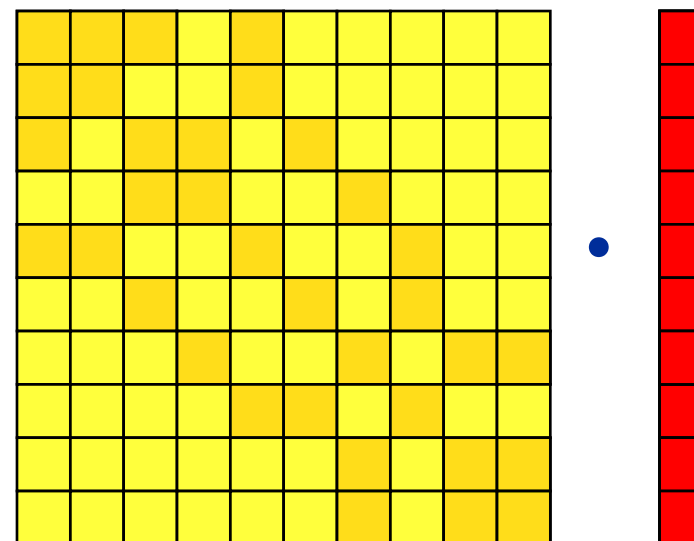
```
do i = 1, Nr
  do j = row_ptr(i), row_ptr(i+1) - 1
    C(i) = C(i) + val(j) * B(col_idx(j))
  enddo
enddo
```

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

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

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

Note: $B_C(1/N_{nzc}) = B_{C,min}$



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

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

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

The “ α effect”

CRS code balance

- α quantifies the traffic for loading the Right Hand Side (RHS) vector

- $\alpha = 0$ → RHS is in cache (RHS \ll cache size)
- $\alpha = 1/N_{nzs}$ → RHS loaded once
- $\alpha = 1$ → no cache
- $\alpha > 1$ → Houston, we have a problem!

$$B_C(\alpha) = \frac{12 + 20/N_{nzs} + 8\alpha}{2} \frac{B}{F}$$
$$= \left(6 + 4\alpha + \frac{10}{N_{nzs}}\right) \frac{B}{F}$$

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 α (RHS traffic quantification)

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

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

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

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

- $N_{nz} = 14.6 \cdot 10^6, N_{nzs} = 7.1$

- $V_{meas} \approx 258 \text{ MB}$

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

→ RHS is loaded 2.5 times from memory

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

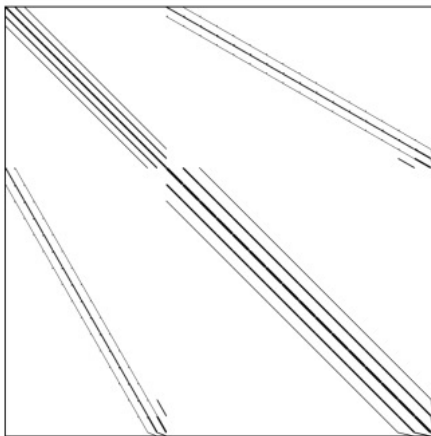
11% extra traffic → optimization potential!

Three different sparse matrices

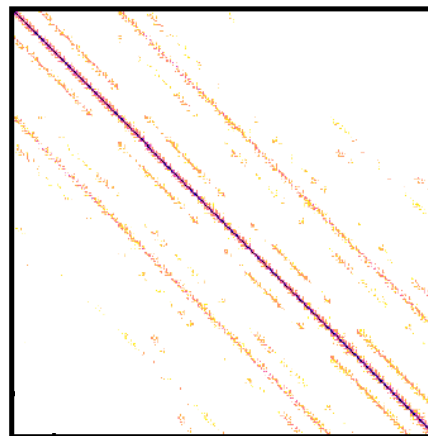
Roofline performance prediction : $P_{opt} = I * b_S = \frac{b_S}{B_{C,min}}$

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

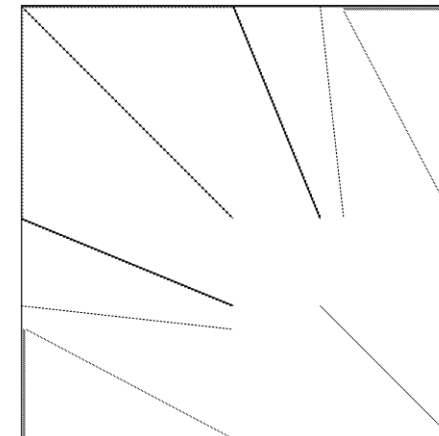
Matrix	N	N_{nzs}	$B_{C,min}$ [B/F]	P_{opt} [GF/s]
DLR1	278,502	143	6.1	7.64
scai1	3,405,035	7.0	8.0	5.83
kkt_power	2,063,494	7.08	8.0	5.83



DLR1

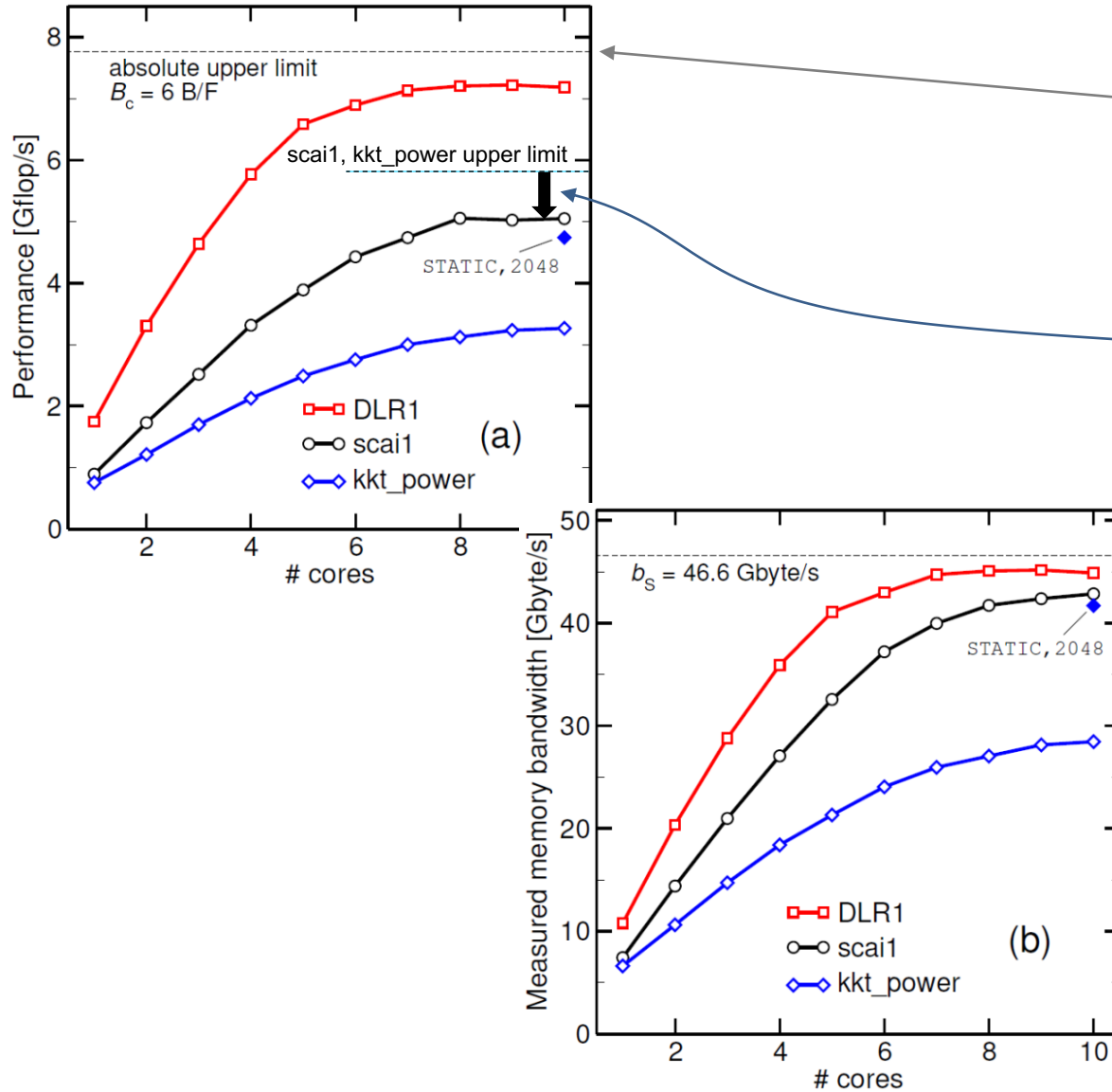


scai1



kkt_power

Now back to the start...



- $b_S = 46.6 \text{ GB/s}$, $B_C = 6 \text{ B/F}$
- Maximum spMVM performance:

$$P_{max} = 7.8 \text{ GF/s}$$

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

- **scai1** measured balance:

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

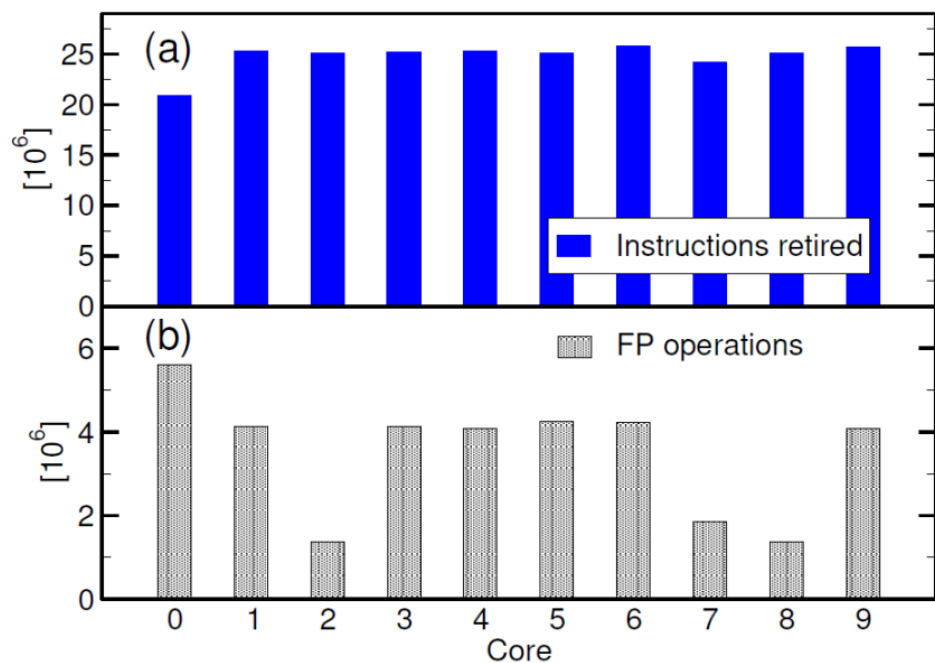
→ good BW utilization, slightly non-optimal α

- **kkt_power** measured balance:

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

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

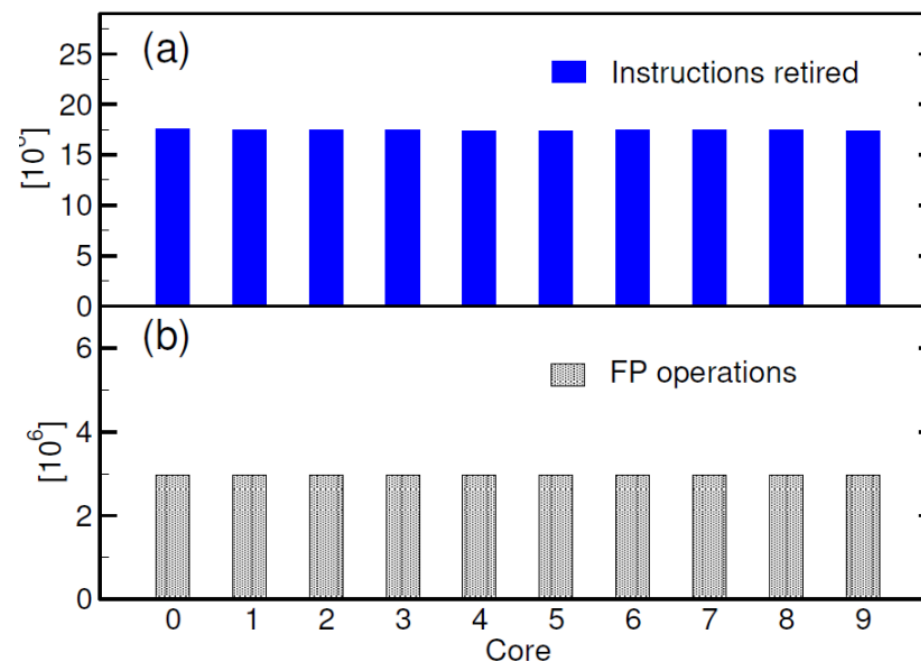
Investigating the load imbalance with kkt_power



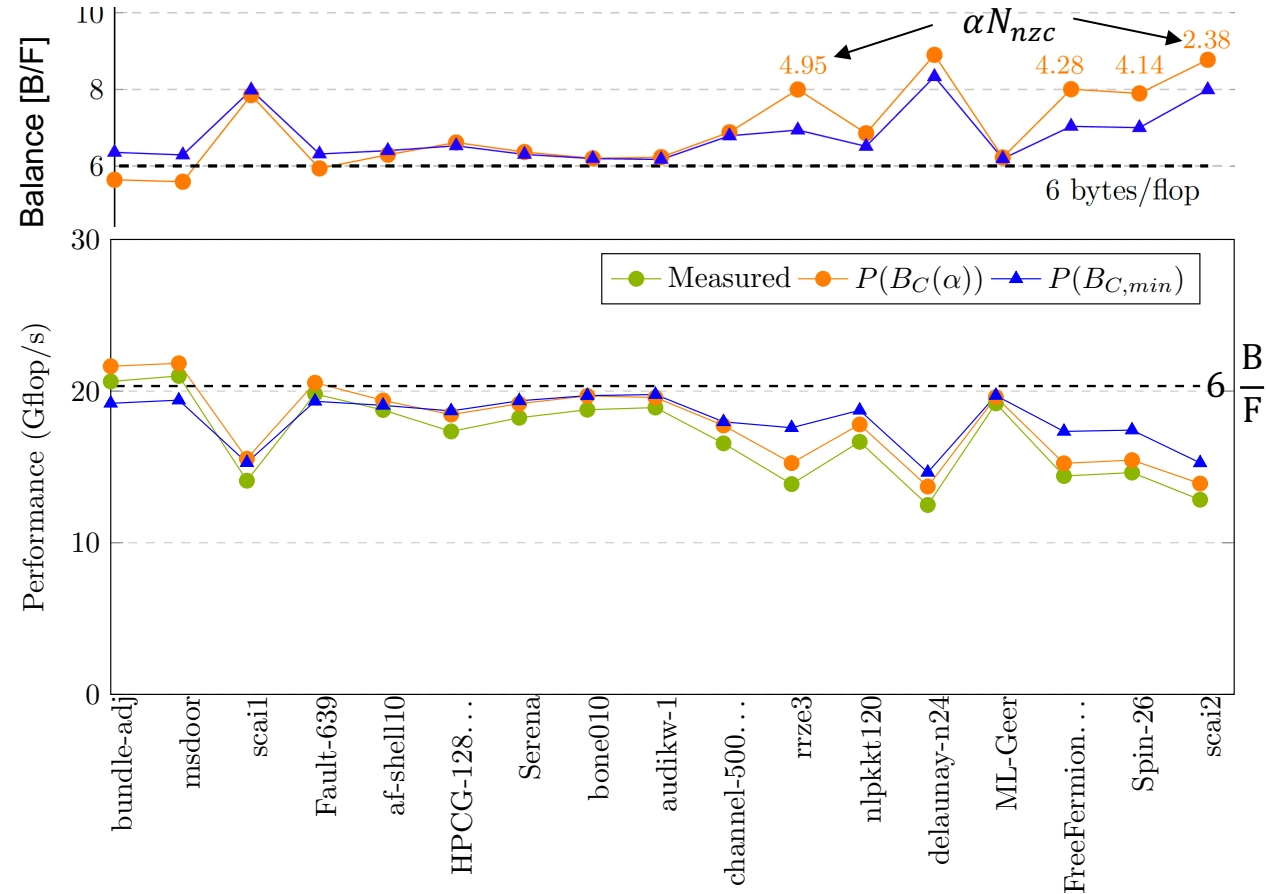
Measurements with likwid-perfctr (MEM_DP group)



- Fewer overall instructions, (almost) BW saturation, 50% better performance with load balancing
- CPI value unchanged!



SpMV node performance model – CPU



Intel Xeon Platinum 9242
 24c@2.8GHz (turbo)
 $b_s = 122 \text{ GB/s}$

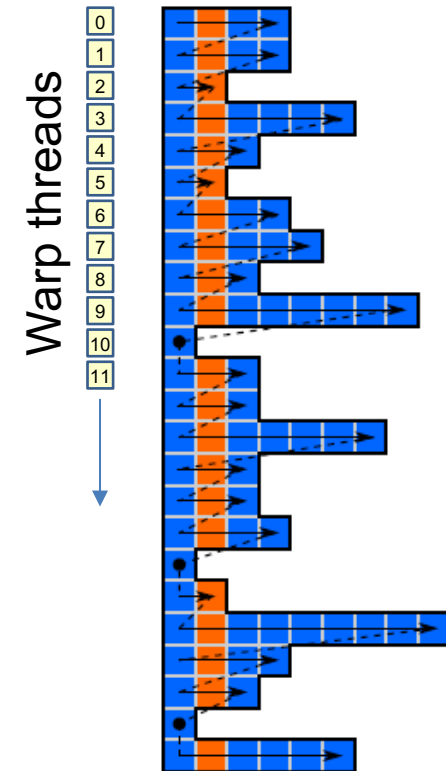
Matrices taken from: C. L. Alappat et al.: *ECM modeling and performance tuning of SpMV and Lattice QCD on A64FX*. In print. Preprint: [arXiv:2103.0301](https://arxiv.org/abs/2103.0301)

Data layout considerations – GPUs

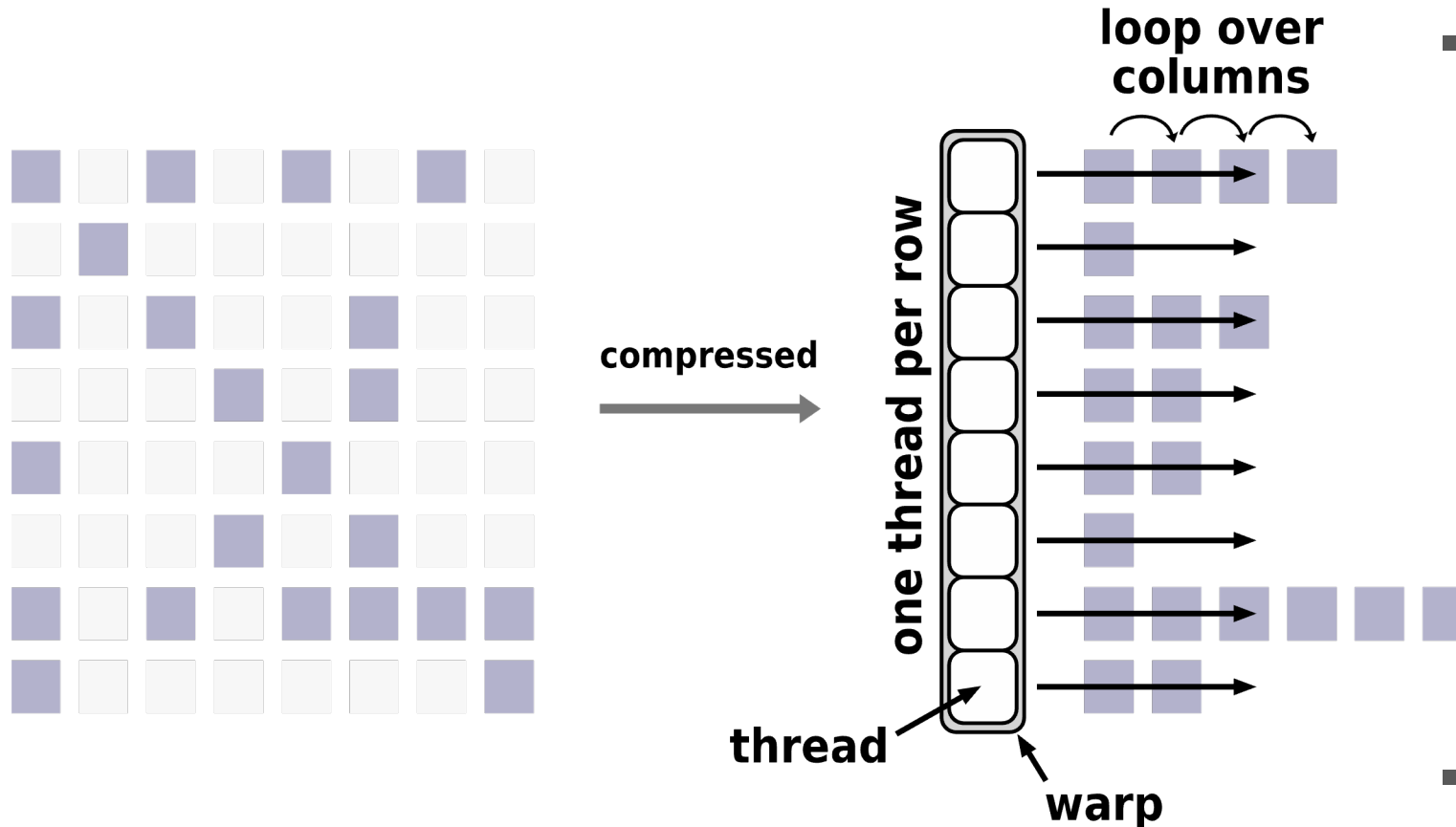


What about GPUs?

- GPUs need
 - Sufficient 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,...



What about GPUs?



- Each GPU thread computes one row, iterates over column indices
- This is the best mapping for CRS:
 - Enough parallelism to saturate the GPU (unless matrix is small)
 - Consecutive threads use similar data, spatial locality is used
 - No reduction among threads, each thread computes its own sum
- But plain CRS has problems on GPUs!

CRS SpMV in CUDA ($y = Ax$)

```
template <typename VT, typename IT>
__global__ static void
spmvr_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

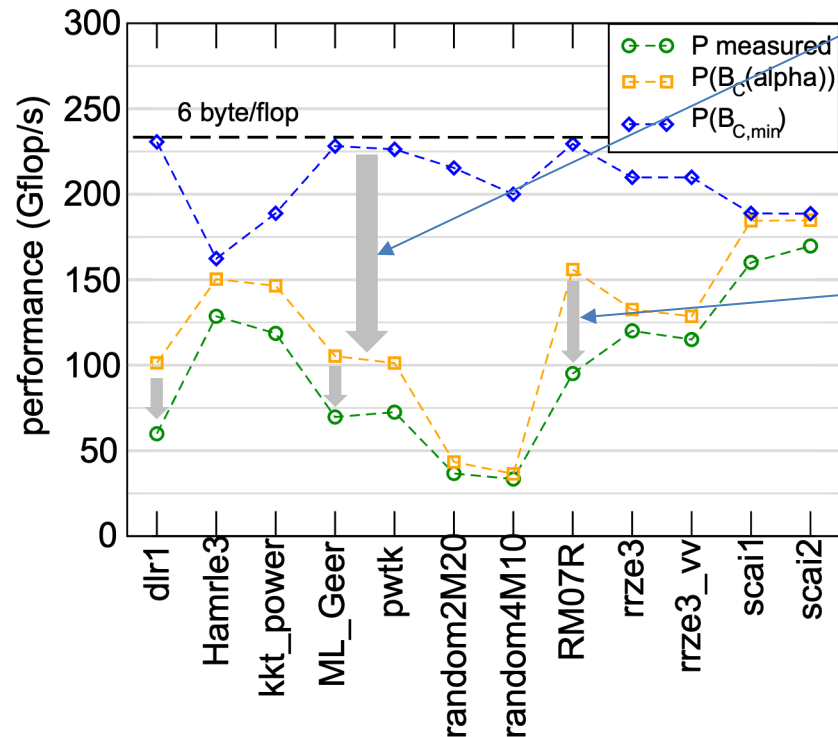
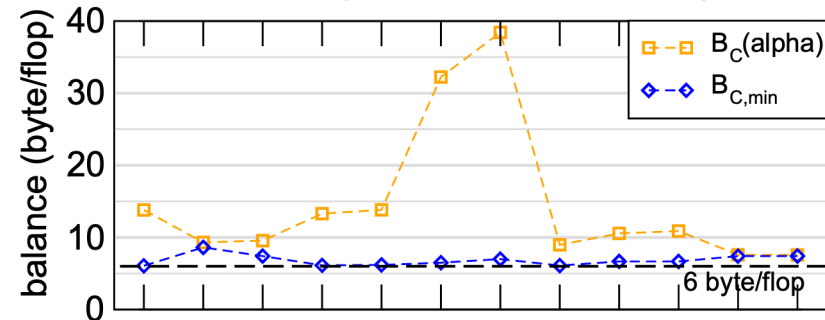
    if (row < num_rows) {
        VT sum{};
        for (IT j = row_ptrs[row]; j < row_ptrs[row + 1]; ++j) {
            sum += values[j] * x[col_idxs[j]];
        }
        y[row] = sum;
    }
}
```

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

No write-allocate on GPUs for consecutive stores

SpMV CRS performance on a GPU

CRS (1 thread per row)

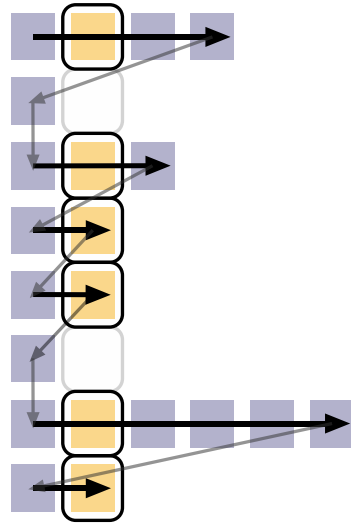


NVIDIA Ampere A100

Memory bandwidth $b_S = 1400$ GB/s

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

CRS SpMV on GPUs: scattered loads



in linear
memory

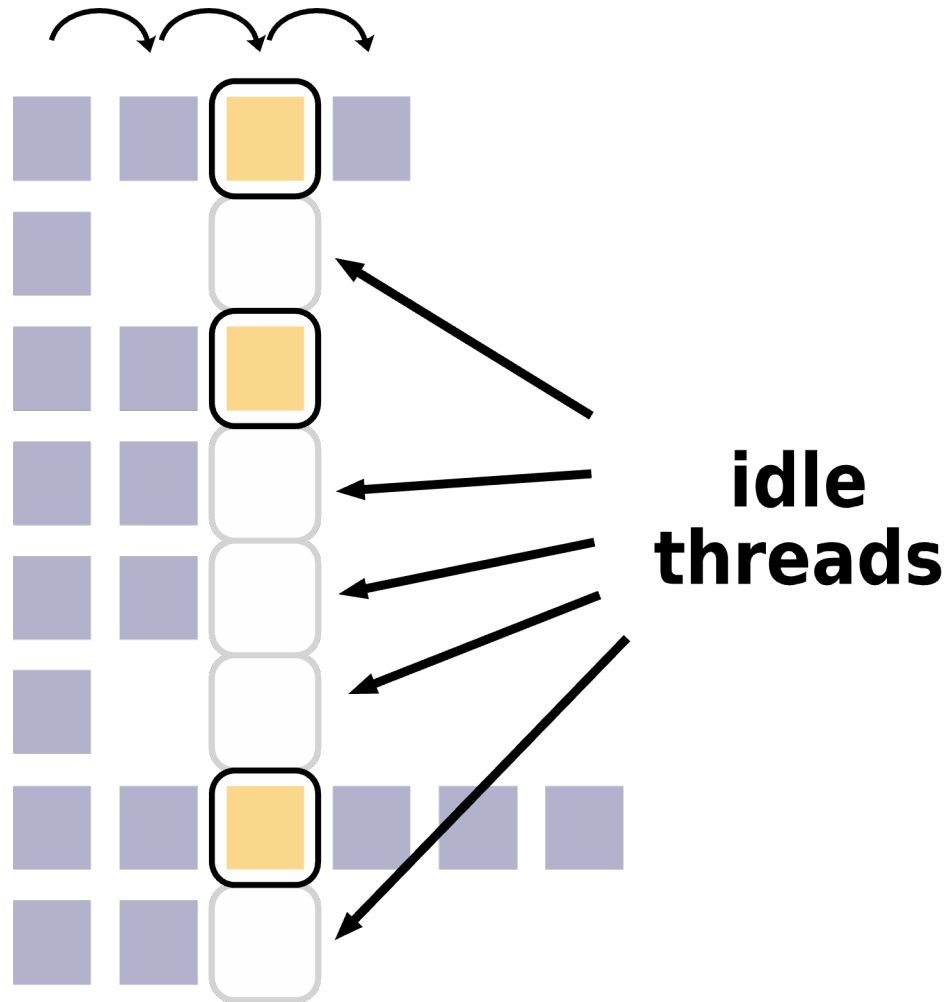


- Loads are executed in **lock step** on GPUs too
- GPUs prefer compact “**coalescable**” addresses for each load (i.e. consecutive access across threads)

CRS vs. GPU

- Row-wise storage format but access pattern orthogonal! → Scattered loads within warp
- Scattered loads need **more cycles**
- Scattered values occupy **more cache lines**
- **Higher latencies and redundant data transfers**

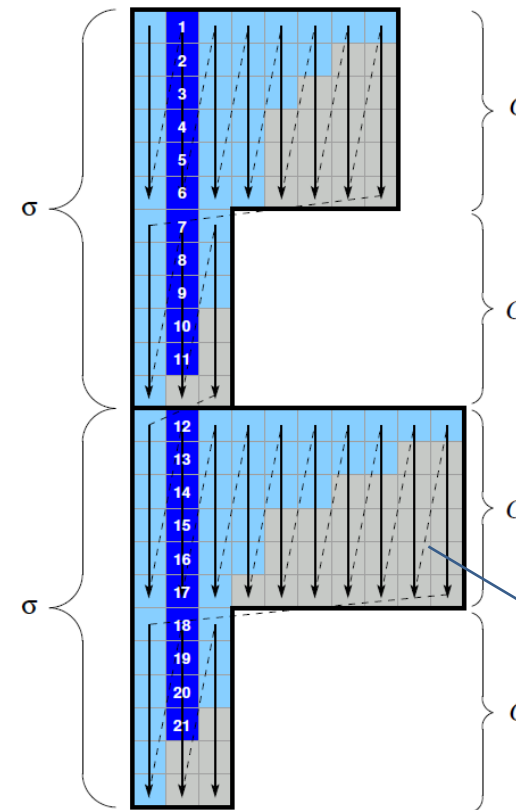
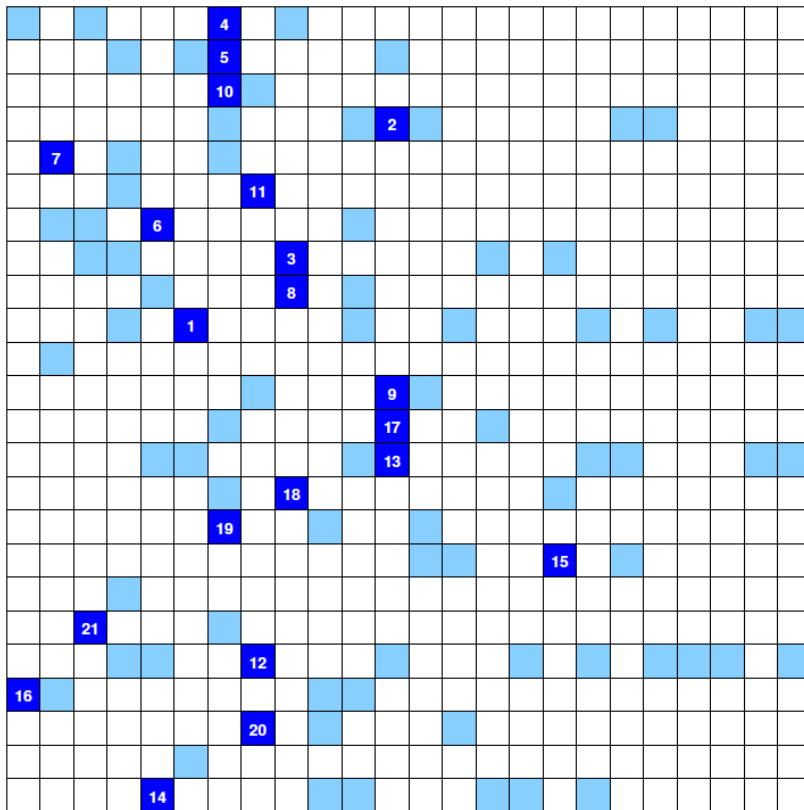
CRS SPMV on GPUs – Problems: Idle threads



- Threads are grouped in **warps**
- Threads in a warp execute in **lockstep**, similar to SIMD
- Problem: loop over column indices can have **different trip count** for each vector
- Threads in a warp that have completed the loop are **masked off**
- All threads in a warp have to **wait** for the thread with most non-zeros

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

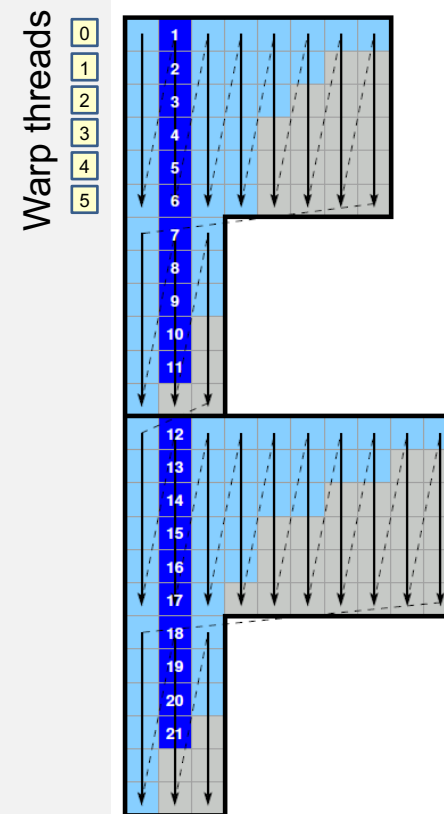
zero padding

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

$$B_{SELL}(\alpha, \beta, N_{nzs}) = \left(\frac{1}{\beta} \left(\frac{8+4}{2} \right) + \frac{8\alpha + \beta(8+4/C)/N_{nzs}}{2} \right) \frac{\text{bytes}}{\text{flop}}$$
$$= \left(\frac{6}{\beta} + 4\alpha + \frac{\beta(4+2/C)}{N_{nzs}} \right) \frac{\text{bytes}}{\text{flop}}$$

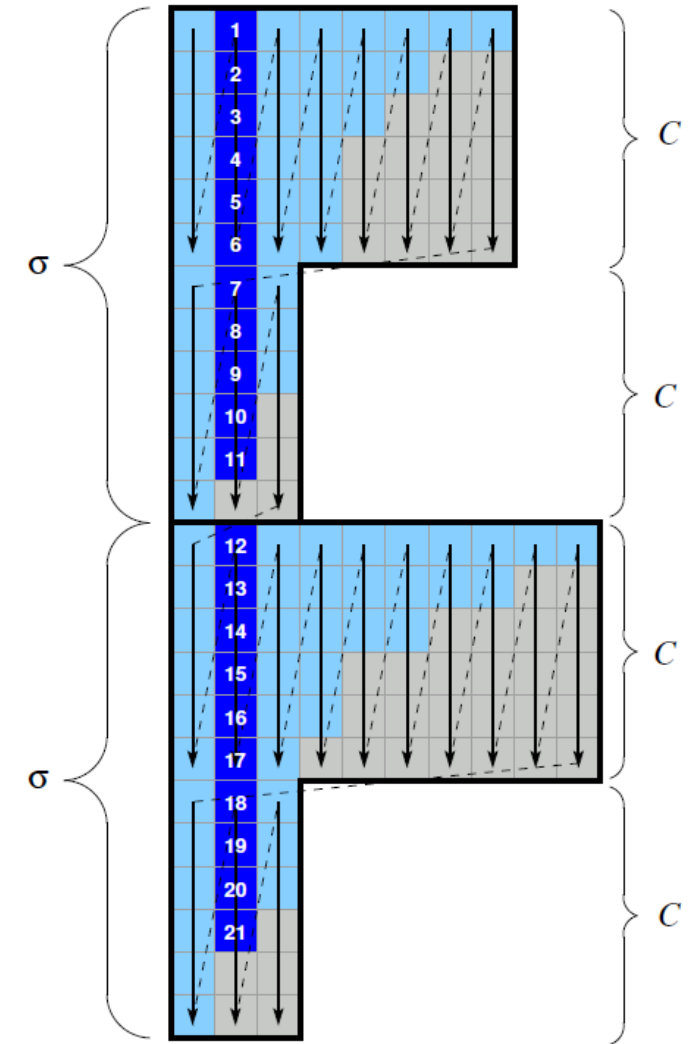
$$\text{Optimal } \alpha = \frac{\beta}{N_{nzs}}$$

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 \rightarrow α **depends on σ**

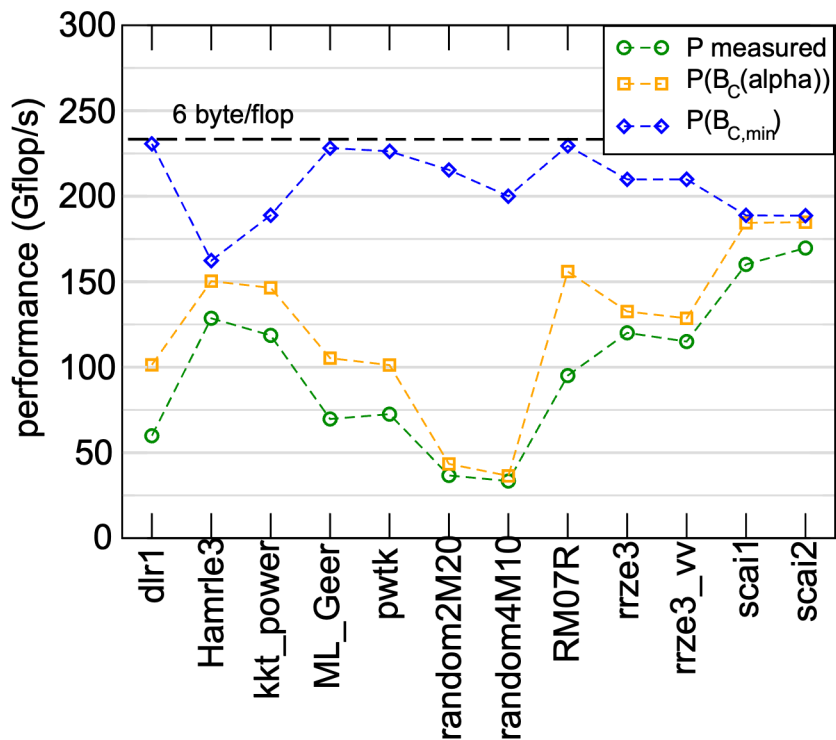
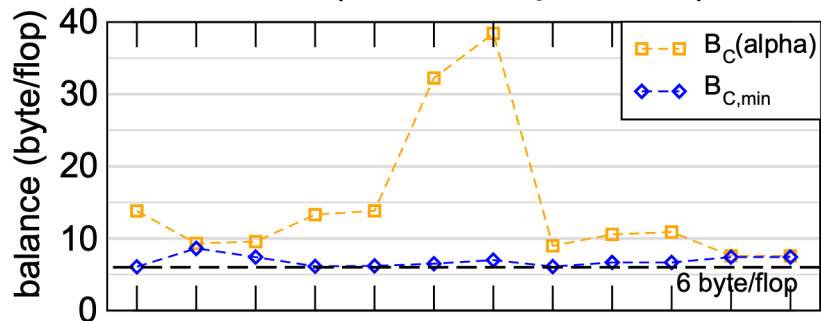


SpMV node performance model – GPU

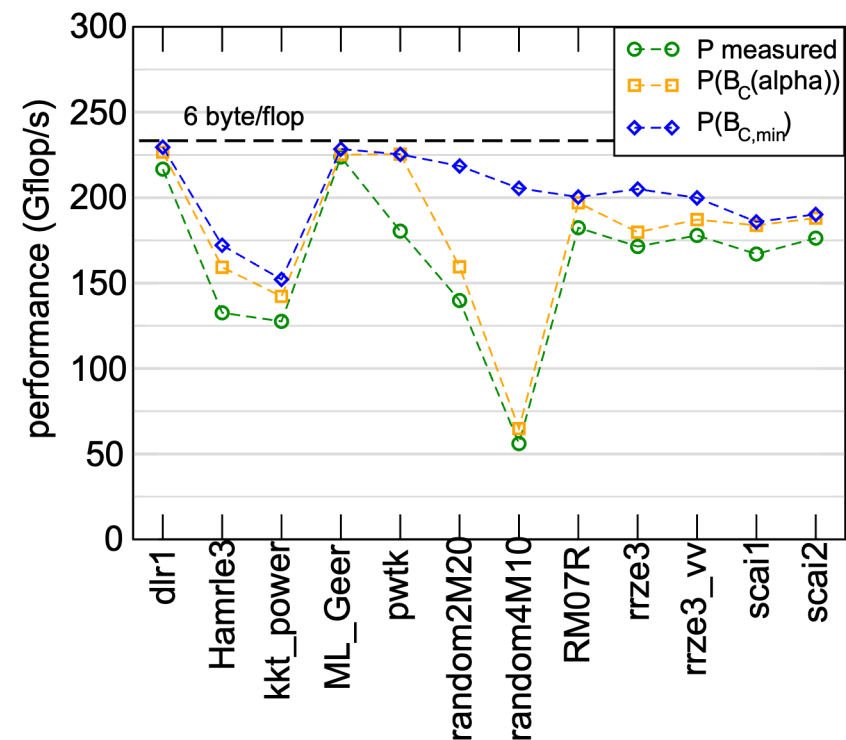
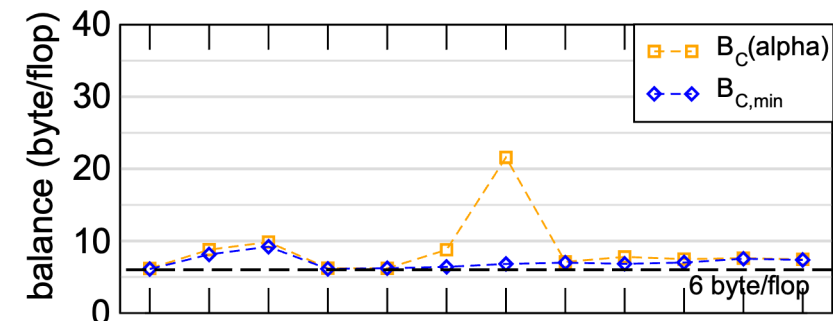
NVIDIA Ampere A100

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

CRS (1 thread per row)



SELL-32-128



SELL-C- σ kernel on CPUs

Example $C = 4$ without further unrolling

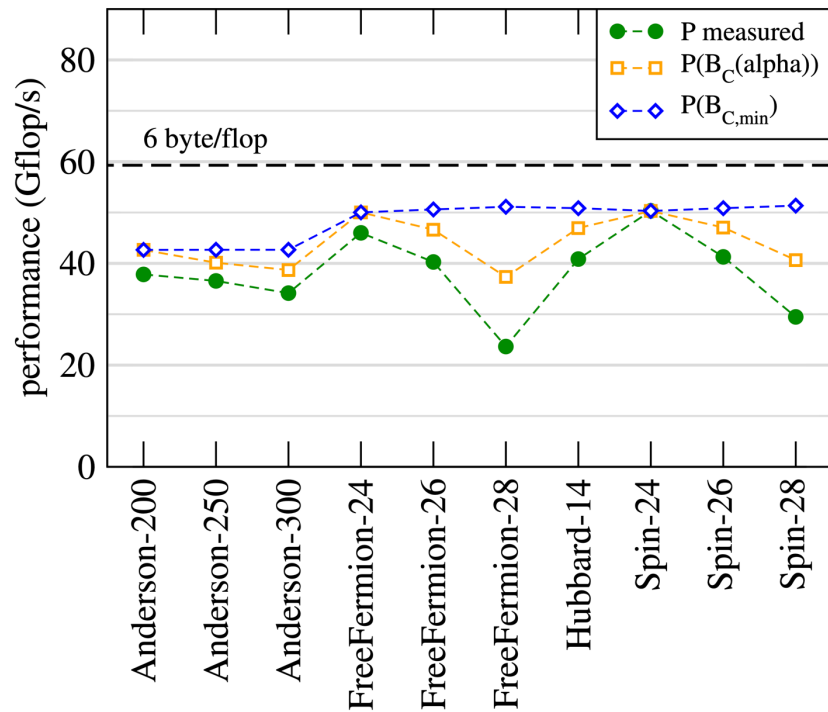
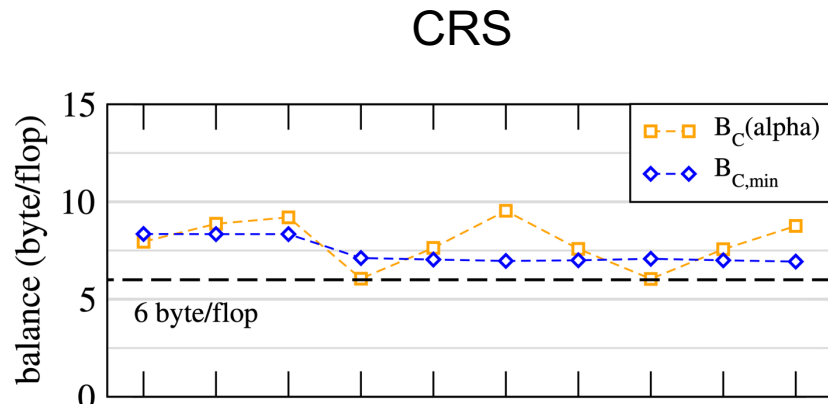
```
for (i = 0; i < N/4; ++i)
{
    for (j = 0; j < cl[i]; ++j)
    {
        y[i*4+0] += val[cs[i]+j*4+0] *
                    x[col[cs[i]+j*4+0]];
        y[i*4+1] += val[cs[i]+j*4+1] *
                    x[col[cs[i]+j*4+1]];
        y[i*4+2] += val[cs[i]+j*4+2] *
                    x[col[cs[i]+j*4+2]];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

Choice of C for CPUs:

- (Multiple of) SIMD length

$C = 4 \rightarrow$ AVX instructions

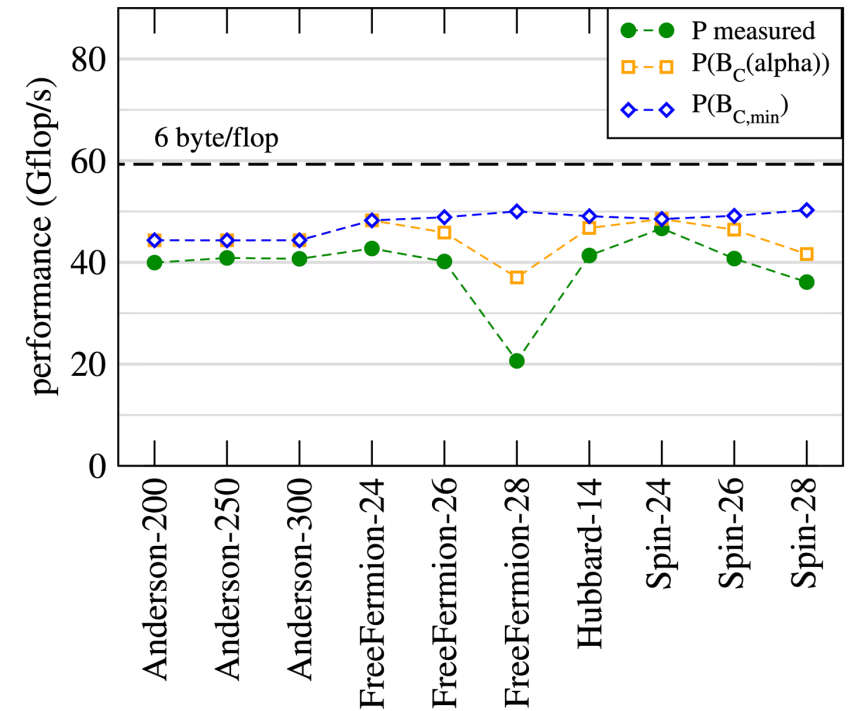
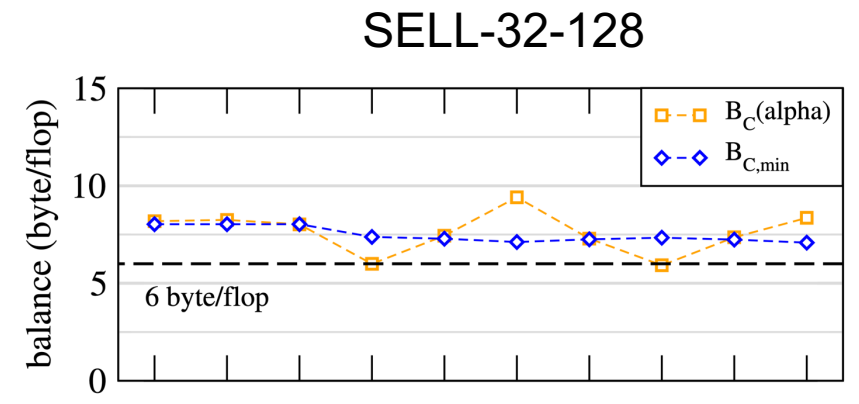
SpMV node performance model – CPU



Intel Ice Lake 8360 Y

$$b_S = 356 \text{ GB/s}$$

Different matrices!!!



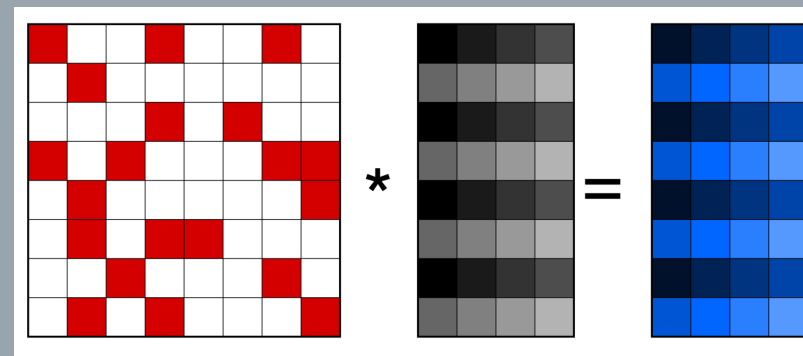
Roofline analysis for spMVM

- **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 (\mathbf{r}) vectors to yield multiple LHS (\mathbf{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)
- $\frac{16r}{N_{nzs}}$ bytes from the r LHS updates
- $\frac{4}{N_{nzs}}$ bytes from the row pointer
- $8r\alpha(r)$ bytes from the r RHS reads

$$B_c(r) = \frac{1}{2r} \left(12 + 8r\alpha(r) + \frac{16r + 4}{N_{nzs}} \right) \frac{B}{F}$$
$$= \left(\frac{6}{r} + 4\alpha(r) + \frac{8 + 2/r}{N_{nzs}} \right) \frac{B}{F}$$

```
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
```

OK so what now???

SpMMV code balance

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

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

$N_{nzs} \gg 1$

$r = 1$

$r \gg 1$

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

reassuring 😊

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

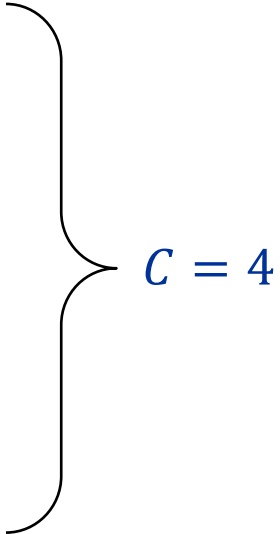
Can become very small for large N_{nzs} → decoupling from memory bandwidth is possible!

M. Kreuzer 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]];
    }
}
```



$C = 4$