



Performance Engineering Case Studies

Analytic performance modeling and its use

in scientific computing

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PE Case Study: A Jacobi Smoother

The basics in two dimensions

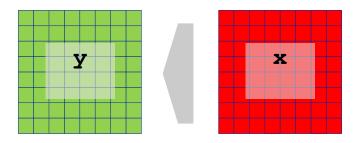


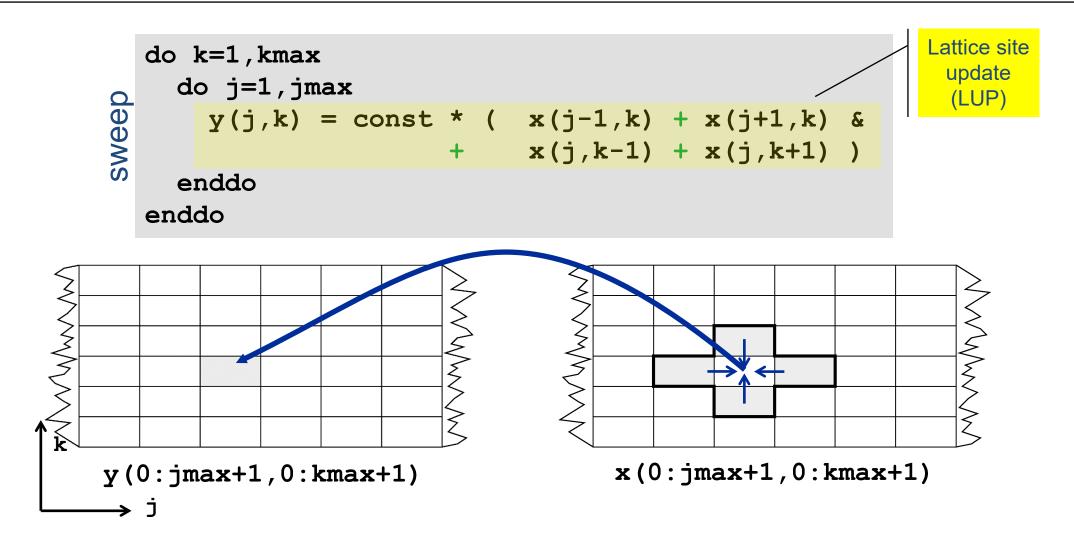
Stencil schemes

- Stencil schemes frequently occur in PDE solvers on regular lattice structures
- Basically a sparse matrix vector multiply (spMVM) embedded in an iterative scheme (outer loop)
- but the regular access structure allows for matrix-free coding



- stencil operator, e.g. Jacobi-type, Gauss-Seidel-type, ...
- discretization, e.g. 7-pt or 27-pt in 3D,...

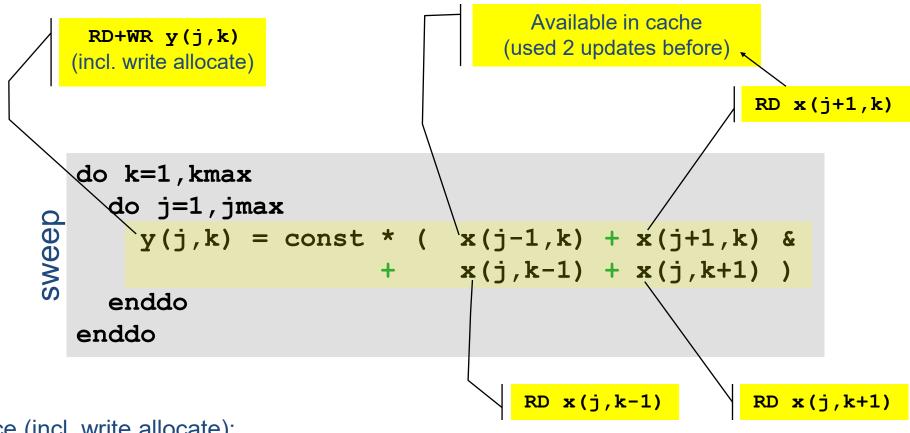




Appropriate performance metric: "Lattice site updates per second" [LUP/s] (here: Multiply by 4 FLOP/LUP to get FLOP/s rate)

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Jacobi 5-pt stencil 2D: data transfer analysis

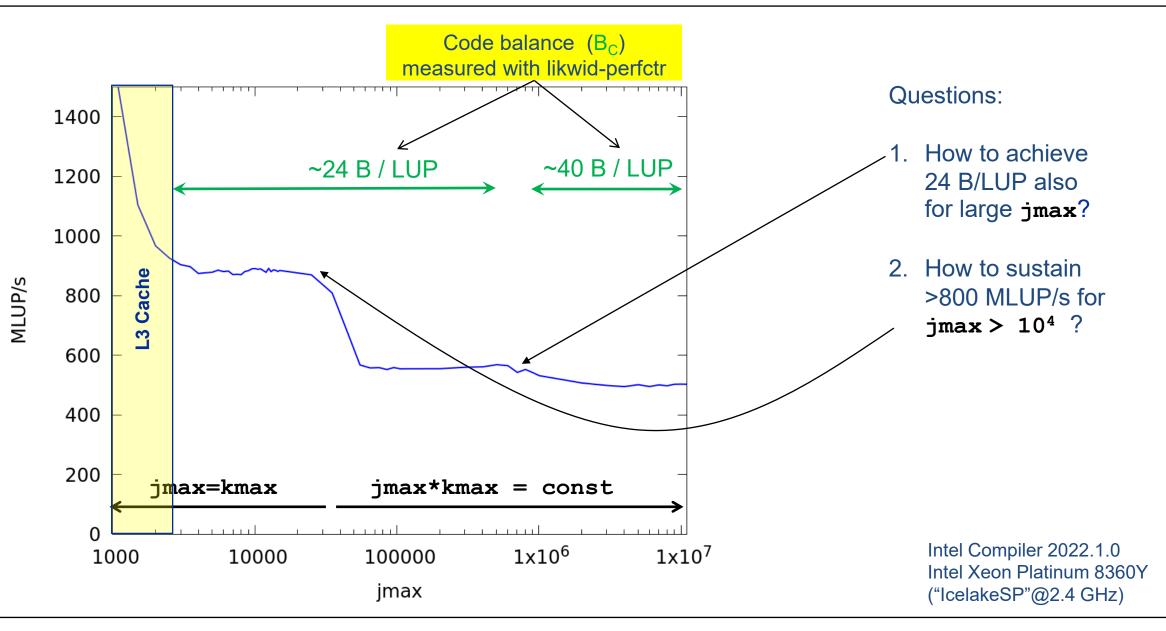


Naive balance (incl. write allocate):

```
x(:,:):3RD+
y(:,:):1WR+1RD
```

 \rightarrow B_C = 5 Words / LUP = 40 B / LUP (assuming double precision)

Jacobi 5-pt stencil 2D: Single core performance





Case study: A Jacobi smoother

Layer conditions



Analyzing the data flow

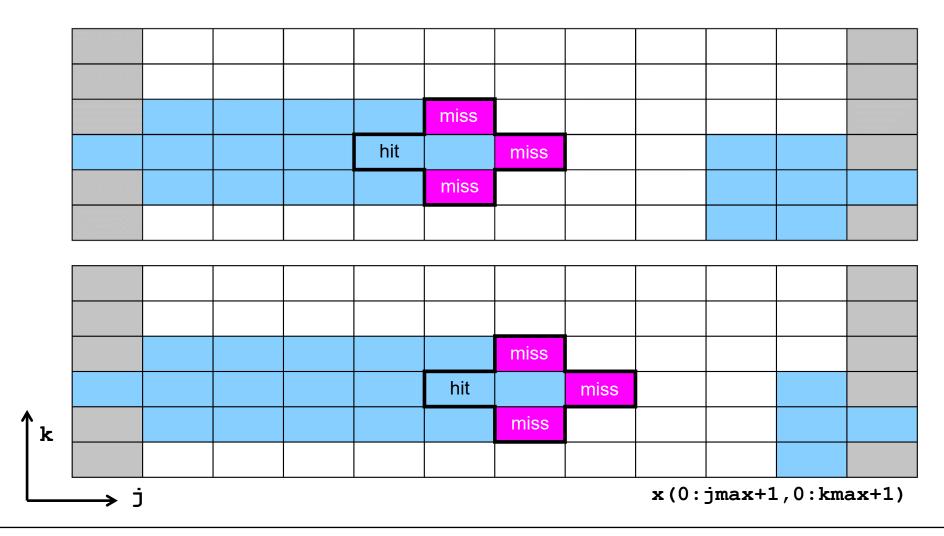
Worst case: Cache not large enough to hold 3 layers (rows) of grid (assume "Least Recently Used" replacement strategy) cached miss hit miss miss CG miss <u>a</u> hit miss miss k

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x(0:jmax+1,0:kmax+1)

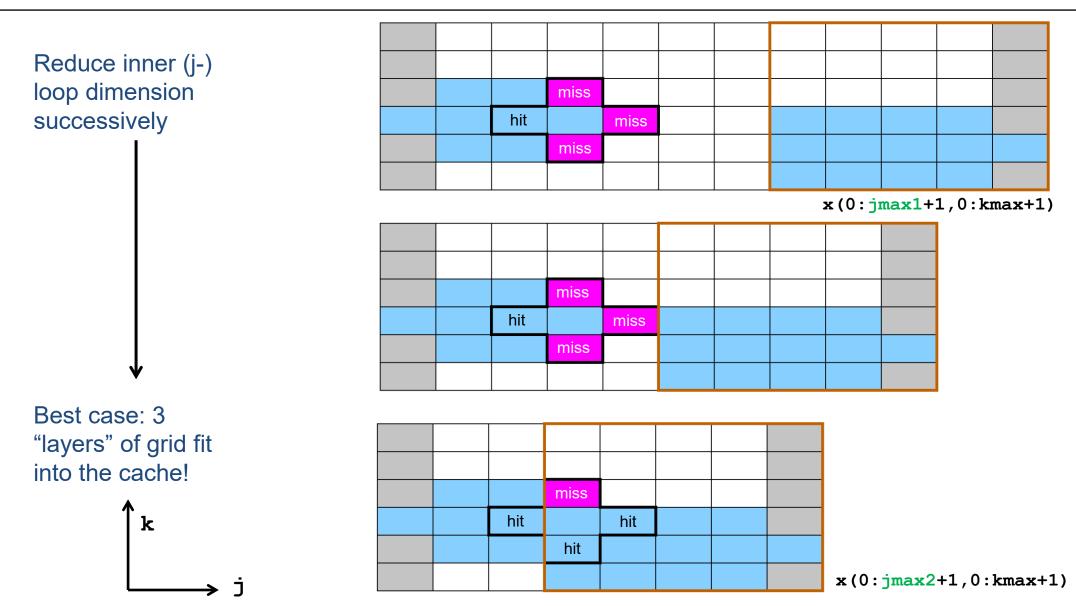
Analyzing the data flow

Worst case: Cache not large enough to hold 3 layers (rows) of grid (assume "Least Recently Used" replacement strategy)



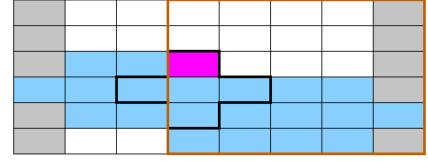
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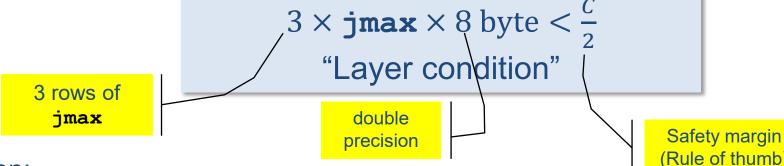
Analyzing the data flow



Analyzing the data flow: Layer condition

2D 5-pt Jacobi-type stencil, cache size *C*

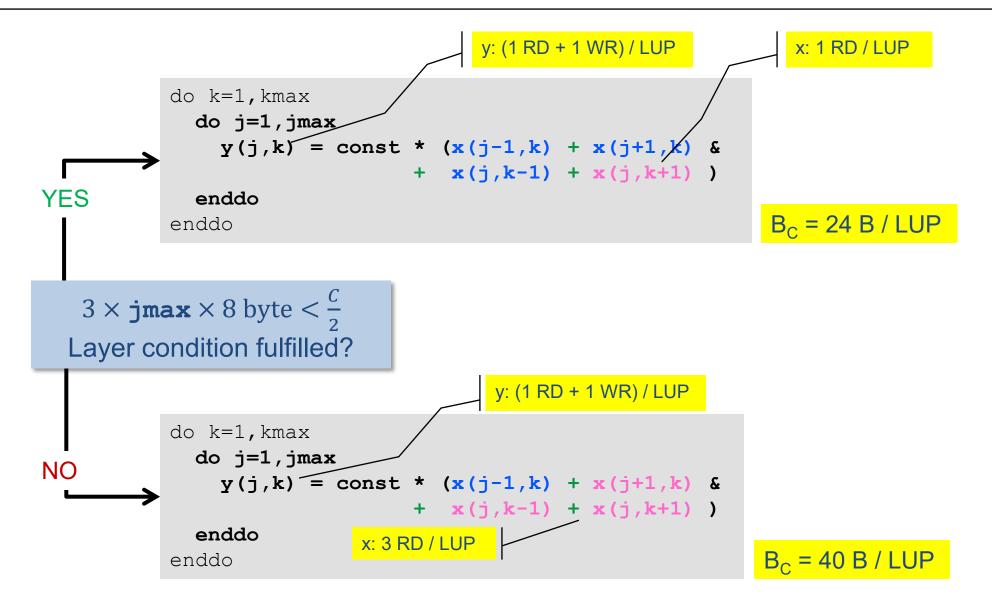




Layer condition:

- Does not depend on outer loop length (kmax)
- No strict guideline (cache associativity, data traffic for y not included)
- Needs to be adapted for other stencils (e.g., long-range stencils)

Analyzing the data flow: Layer condition (2D 5-pt Jacobi)



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Optimization by spatial blocking



Enforcing a layer condition (2D 5-pt Jacobi)

- How can we enforce a layer condition for all domain sizes?
- Idea: Spatial blocking
 - Reuse elements of x () as long as they stay in cache
 - Sweep can be executed in any order, e.g., compute blocks in j direction

"Spatial Blocking" of j loop:

```
do jb=1,jmax,jblock !

do k=1,kmax

do j=jb, min(jb+jblock-1,jmax) !inner loop length jblock

y(j,k) = const * (x(j-1,k) + x(j+1,k) & \\
 + x(j,k-1) + x(j,k+1) )

enddo

enddo

enddo

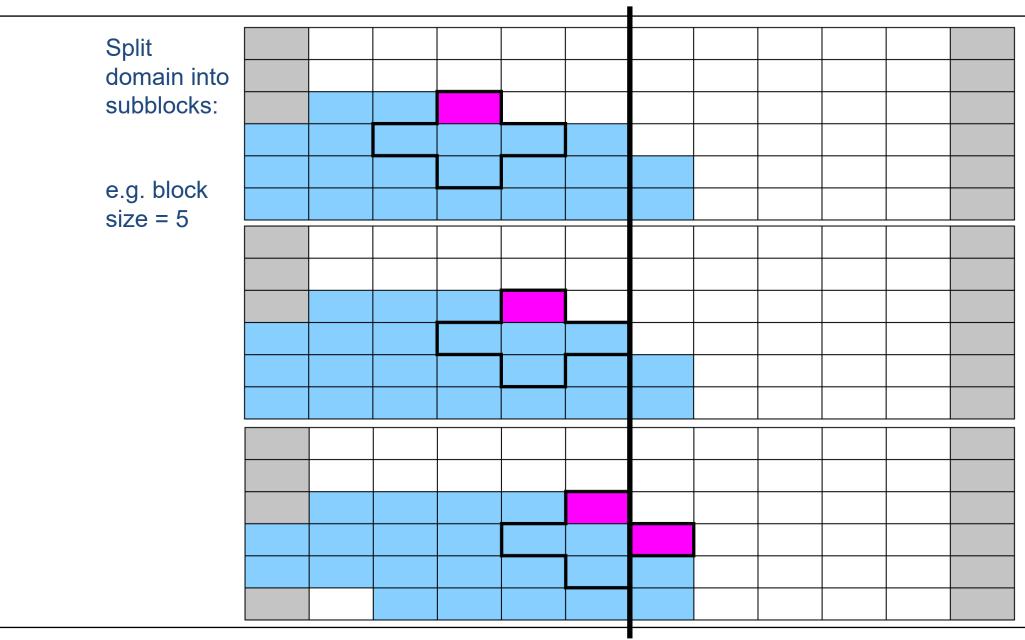
enddo
```

Determine for given *C* an appropriate jblock value:

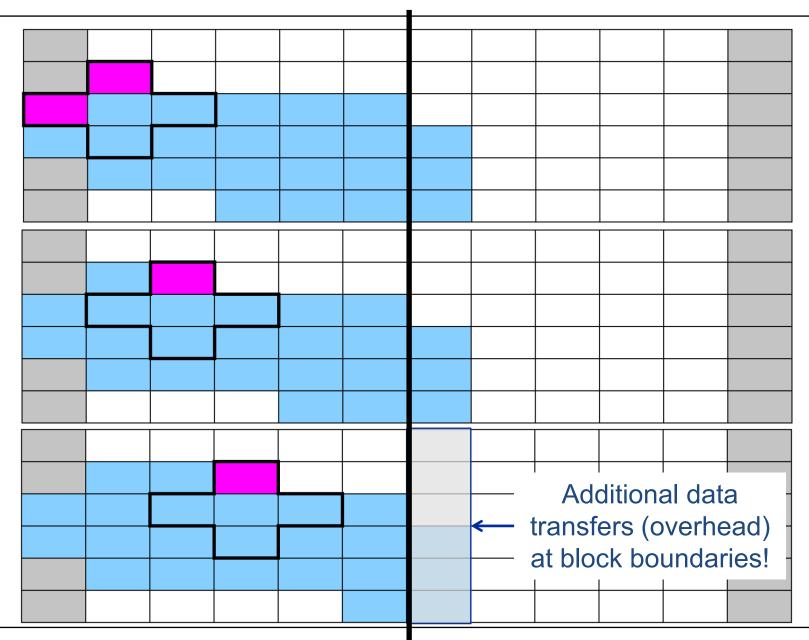
New layer condition (blocking) $3 \times \mathbf{jblock} \times 8 \text{ byte } < \frac{c}{2}$

$$jblock < \frac{C}{48 \text{ byte}}$$

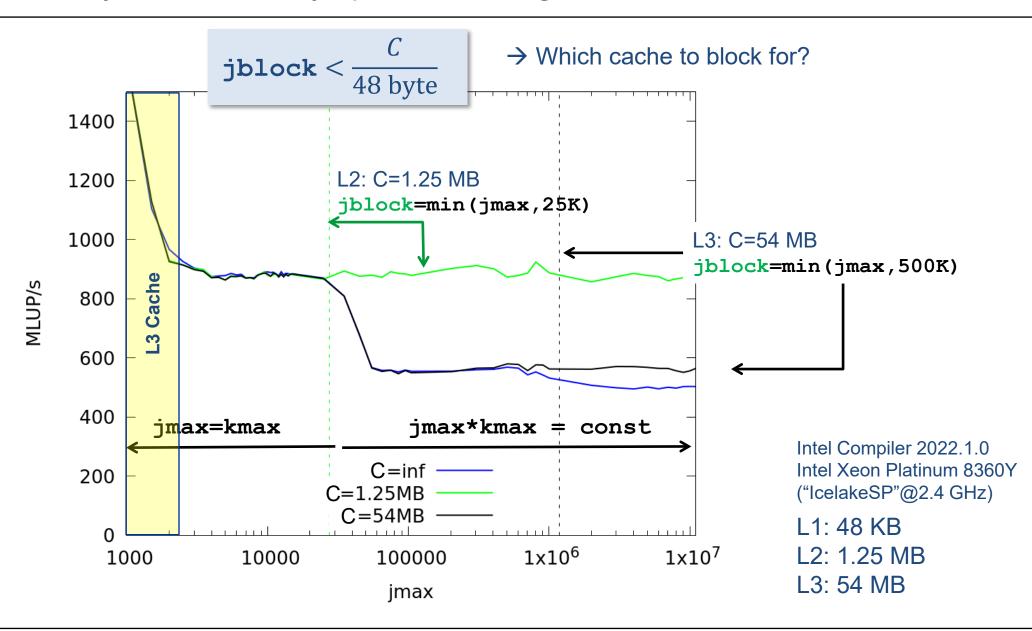
Establish the layer condition by blocking



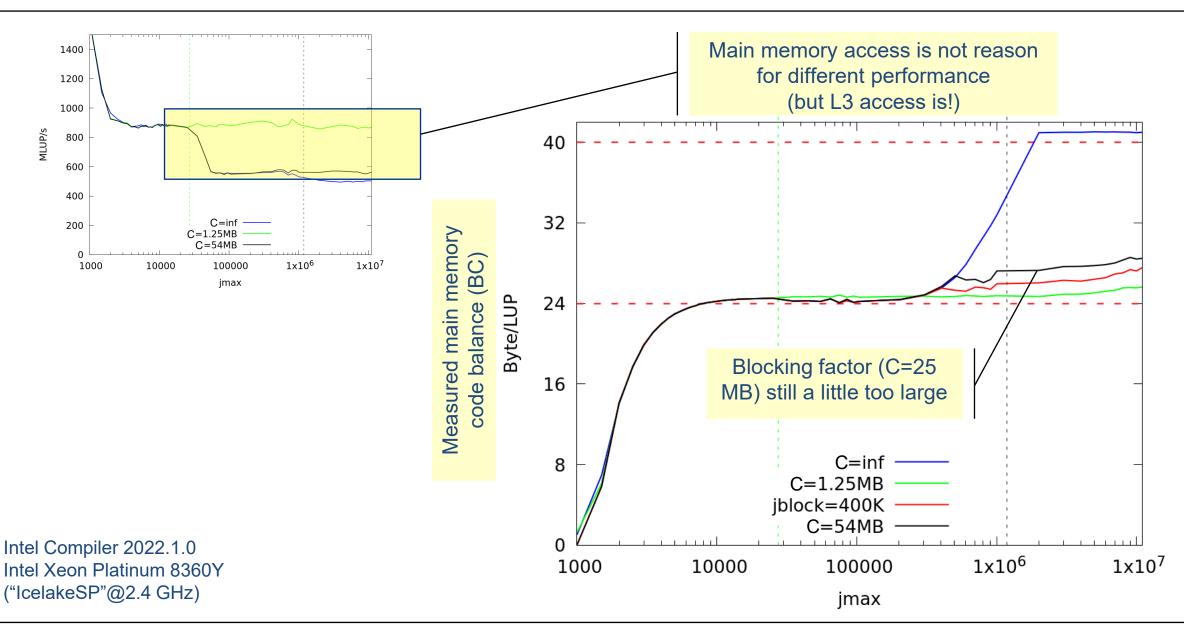
Establish the layer condition by blocking



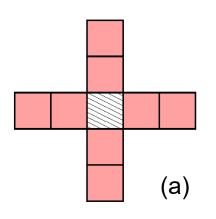
Establish layer condition by spatial blocking

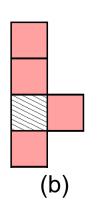


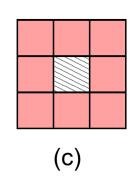
Validating the model: Memory code balance



Stencil shapes and layer conditions in 2D







- a) Long-range r = 2: 5 layers (2r + 1)
- b) Asymmetric: 4 layers
- c) 2D box: 3 layers



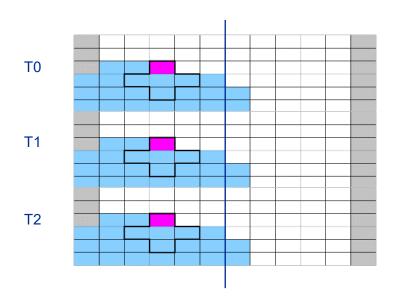
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OpenMP parallelization

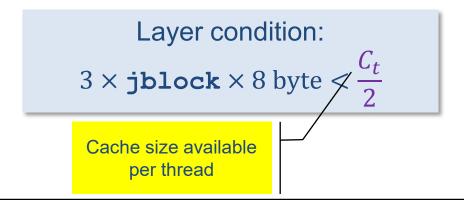


OpenMP parallelization of the blocked 2D stencil

Straightforward OpenMP work sharing:



Caveat: LC must be fulfilled per thread → shared cache causes smaller blocks!



enddo

OpenMP parallelization and blocking for a shared cache

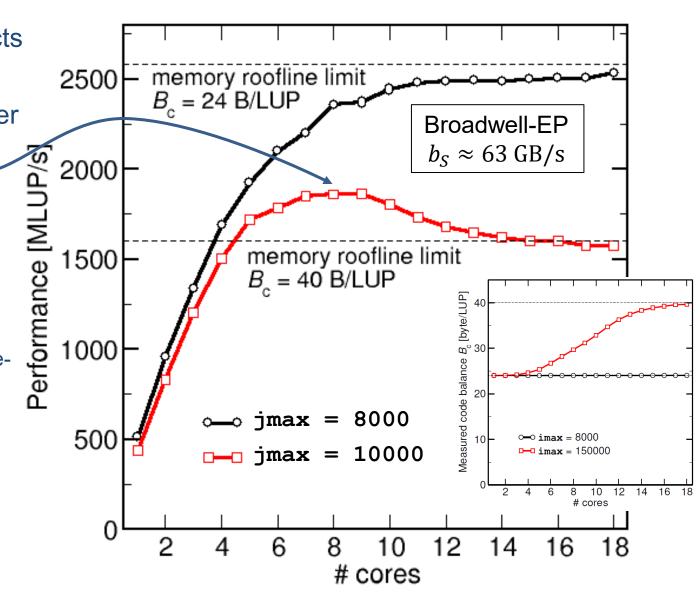
Layer conditions make for interesting effects

 Less and less shared cache available per thread as #threads goes up

LC may break "along the way"

- Solutions
 - 1. Choose small enough block or domain size
 - Layers either small enough to fit in coreprivate caches or
 - Shared cache big enough to hold all layers for all threads
 - 2. Adaptive blocking for shared cache:

$$jblock = \frac{C}{\#threads \times 48 \text{ byte}}$$



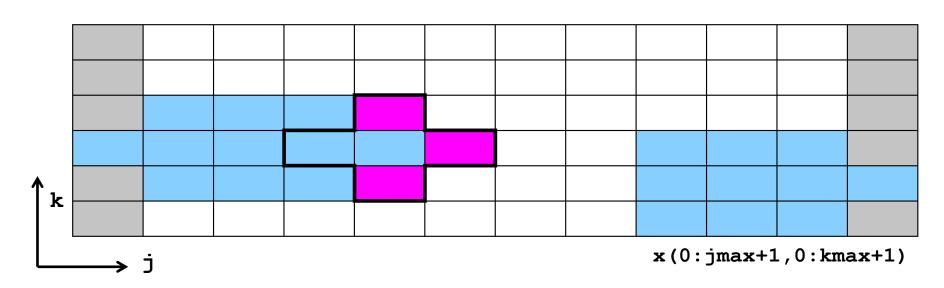


Case study: A Jacobi smoother

From 2D to 3D



2D:



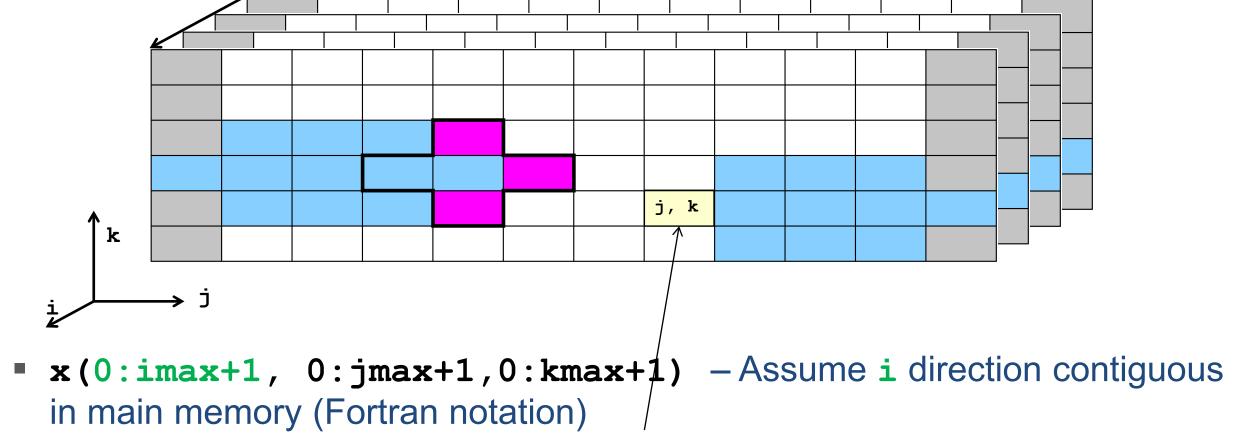
Towards 3D understanding

Picture can be considered as 2D cut of 3D domain for a (new) fixed i index:

```
x(0:jmax+1,0:kmax+1) \rightarrow x(i, 0:jmax+1,0:kmax+1)
```

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Stay at 2D picture and consider one cell of j-k plane as a contiguous slab of elements in i direction: x (0:imax, j,k)

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Layer condition: From 2D 5-pt to 3D 7-pt stencil

```
do k=1,kmax do j=1,jmax y(j,k) = const * (x(j-1,k) + x(j+1,k) & + x(j,k-1) + x(j,k+1)) enddo enddo 2D
```

```
3 \times \texttt{jmax} \times 8 \text{ byte} < \frac{c}{2}
```

Optimal $B_C = 24 B / LUP$

```
\begin{array}{l} \text{do } k=1,k\text{max} \\ \text{do } j=1,j\text{max} \\ \text{do } i=1,i\text{max} \\ \text{y(i,j,k)} = \text{const} * (x(i-1,j,k) + x(i+1,j,k) \\ & + x(i,j-1,k) + x(i,j+1,k) & \\ & + x(i,j,k-1) + x(i,j,k+1) ) \\ \text{enddo} \\ \text{enddo} \\ \text{enddo} \\ \text{enddo} \\ \end{array}
```

$$3 \times jmax \times imax \times 8 \text{ byte} < \frac{c}{2}$$

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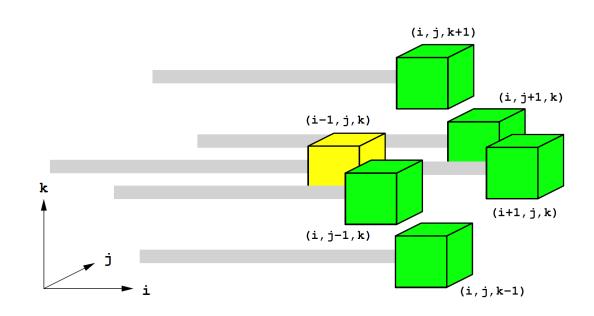
Optimal $B_C = 24 B / LUP$

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3D 7-pt stencil

There is actually more than one layer condition in 3D

- "Outer" LC:
 - 3 * imax * jmax
- "Inner" LC:
 - 3 * imax in the central layer



- → Code balance of
 - 24 B/LUP if outer LC fulfilled
 - 40 B/LUP if outer LC broken but inner LC fulfilled
 - 56 B/LUP if inner & outer LC broken

Online Layer Condition calculator: http://tiny.cc/LayerConditions

Conclusions from the stencil example

- We have made sense of the memory-bound performance vs. problem size
 - "Layer conditions" lead to predictions of code balance
 - "What part of the data comes from where" is a crucial question
 - The model works only if the bandwidth is "saturated"
 - In-cache modeling is more involved
- Avoiding slow data paths == re-establishing the most favorable layer condition
- Improved code showed the speedup predicted by the model
- Optimal blocking factor can be estimated
 - Be guided by the cache size the layer condition
 - No need for exhaustive scan of "optimization space"
- Food for thought
 - Multi-dimensional loop blocking would it make sense?
 - Can we choose a "better" OpenMP loop schedule?
 - What about temporal blocking?

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Stencil references

- T. M. Malas, G. Hager, H. Ltaief, and D. E. Keyes: Multi-dimensional intra-tile parallelization for memory-starved stencil computations. ACM Transactions on Parallel Computing 4(3), 12:1-12:32 (2017). DOI: 10.1145/3155290, Preprint: arXiv:1510.04995
- J. Hammer, G. Hager, J. Eitzinger, and G. Wellein: Automatic Loop Kernel Analysis and Performance Modeling With Kerncraft. Proc. <u>PMBS15</u>, the 6th International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems, in conjunction with ACM/IEEE Supercomputing 2015 (<u>SC15</u>), November 16, 2015, Austin, TX. <u>DOI: 10.1145/2832087.2832092</u>, Preprint: <u>arXiv:1509.03778</u>
- H. Stengel, J. Treibig, G. Hager, and G. Wellein: Quantifying performance bottlenecks of stencil computations using the Execution-Cache-Memory model. Proc. <u>ICS15</u>,
 DOI: 10.1145/2751205.2751240, Preprint: <u>arXiv:1410.5010</u>
- M. Wittmann, G. Hager, T. Zeiser, J. Treibig, and G. Wellein: Chip-level and multi-node analysis of energy-optimized lattice-Boltzmann CFD simulations. Concurrency and Computation: Practice and Experience (2015). <u>DOI:10.1002/cpe.3489</u>
 Preprint: <u>arXiv:1304.7664</u>
- J. Treibig, G. Wellein and G. Hager: Efficient multicore-aware parallelization strategies for iterative stencil computations.
 Journal of Computational Science 2 (2), 130-137 (2011). DOI 10.1016/j.jocs.2011.01.010
- M. Wittmann, G. Hager, J. Treibig and G. Wellein: Leveraging shared caches for parallel temporal blocking of stencil codes on multicore processors and clusters. Parallel Processing Letters 20 (4), 359-376 (2010).

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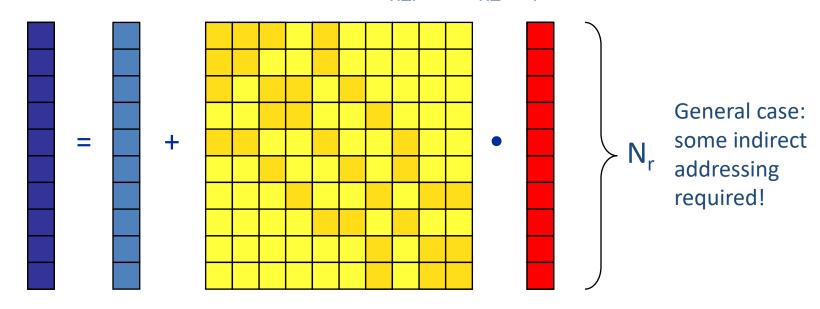


Case study: Sparse Matrix-Vector Multiplication



Sparse Matrix Vector Multiplication (SpMV)

- Key ingredient in numerous sparse linear algebra solvers
- Store only N_{nz} nonzero elements of matrix and RHS, LHS vectors with N_r (number of matrix rows) entries
- "Sparse": N_{nz} ~ N_r
- Average number of nonzeros per row: $N_{nzr} = N_{nz}/N_r$



Performance Modeling

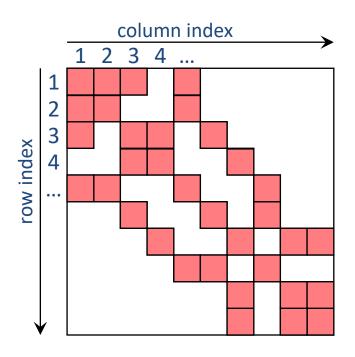
SpMVM characteristics

- 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

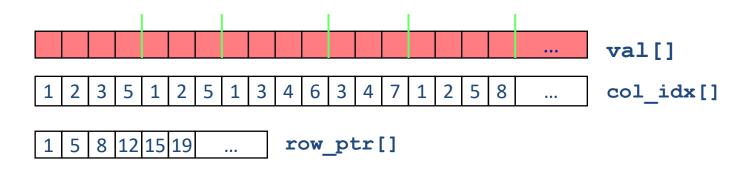
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CRS matrix storage scheme



- 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...

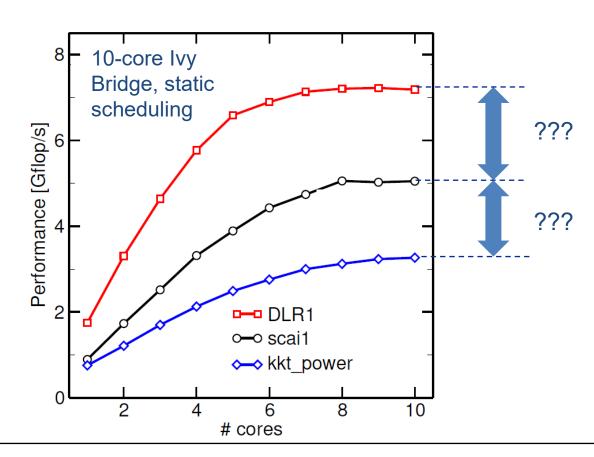
35

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, N_r
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(N<sub>nz</sub>)
integer*4 col_idx(N<sub>nz</sub>)
integer*4 row_ptr(N<sub>r</sub>)
real*8 C(N<sub>r</sub>)
real*8 B(N<sub>c</sub>)
```

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: $B_{C,min} \ge 6 \frac{B}{F} \longrightarrow I_{max} \le \frac{1}{6} \frac{F}{B}$

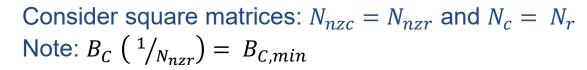
SpMV node performance model – CRS (2)

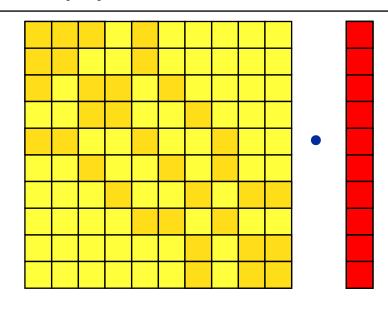
do i = 1,
$$N_r$$

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):

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

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

The " α effect"

DP CRS code balance

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

Can we predict α ?

- Not in general
- Simple cases (banded, block-structured): Similar to layer condition analysis
- \rightarrow Determine α by measuring the actual memory traffic (\rightarrow measured code balance B_C^{meas})

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

Determine α (RHS traffic quantification)

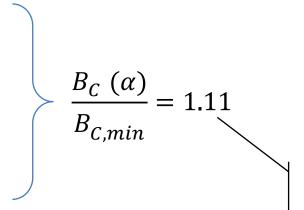
$$B_C(\alpha) = \left(6 + 4\alpha + \frac{10}{N_{nzr}}\right) \frac{B}{F} = \frac{V_{meas}}{N_{nz} \cdot 2 F} \quad (= B_C^{meas})$$

- 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

- $N_{nz} = 14.6 \cdot 10^6$, $N_{nzr} = 7.1$
- $V_{meas} \approx 258 \text{ MB}$
- $\rightarrow \alpha = 0.36$, $\alpha N_{nzr} = 2.5$
- → RHS is loaded 2.5 times from memory



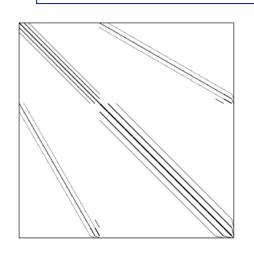
11% extra traffic → optimization potential!

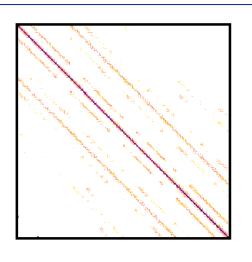
Three different sparse matrices

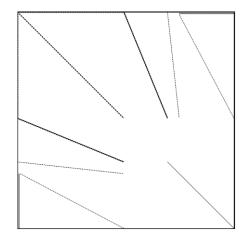
Benchmark system: Intel Xeon Ivy Bridge E5-2660v2, 2.2 GHz, $b_S = 46.6 \, \mathrm{GB/s}$

$$\rightarrow$$
 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





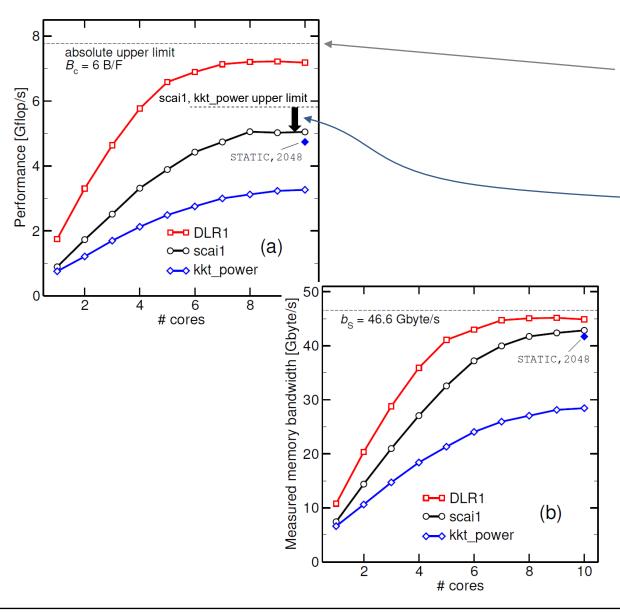


DLR1

scai1

kkt_power

Now back to the start...



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

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

- **DLR1** causes (almost) minimum CRS code balance (as expected)
- scai1 measured balance:

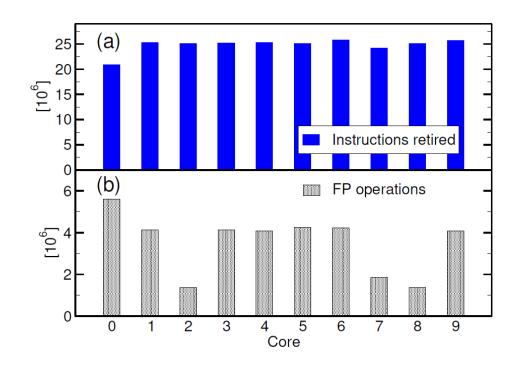
 $B_c^{meas} \approx 8.5 \text{ B/F} > B_{C,min}$ (6% higher than min)

- \rightarrow good BW utilization, slightly non-optimal α
- kkt_power measured balance:

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

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

Investigating the load imbalance with kkt_power

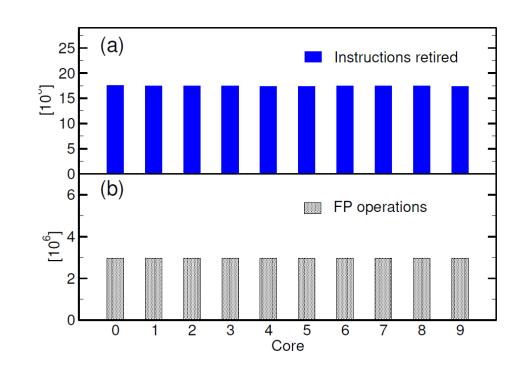


Measurements with likwid-perfctr (MEM_DP group)

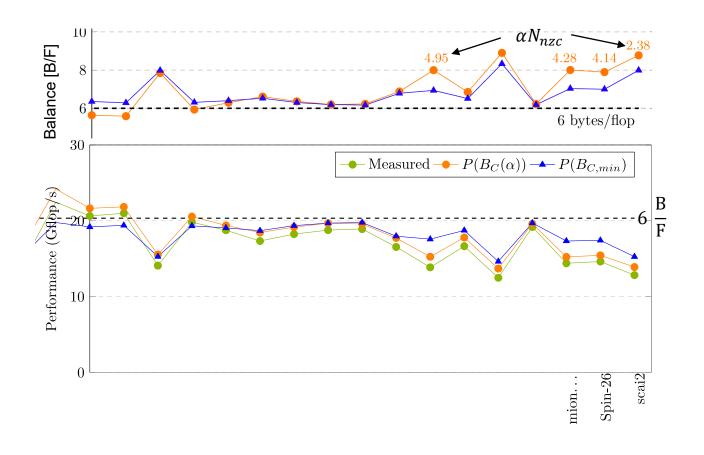
static

static,2048

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



SpMV node performance model – CPU



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

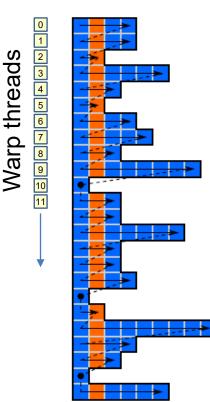
Matrices taken from: C. L. Alappat et al.: *ECM modeling and performance tuning of SpMV and Lattice QCD on A64FX.* DOI: 10.1002/cpe.6512

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)

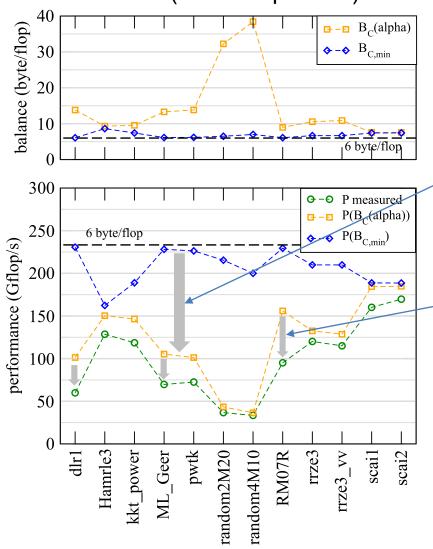
```
template <typename VT, typename IT>
global static void
spmv csr(const ST num rows,
         const IT * RESTRICT row_ptrs, const IT * RESTRICT col_idxs,
         const VT * RESTRICT values, const VT * RESTRICT x,
                                             VT * RESTRICT y)
   ST row = threadIdx.x + blockDim.x * blockIdx.x; // 1 thread per row
   if (row < num rows) {</pre>
       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





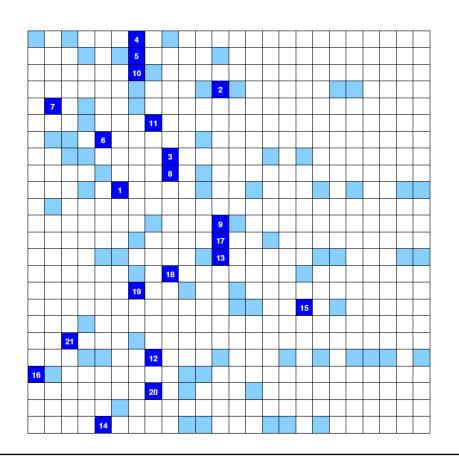
NVIDIA Ampere A100 Memory bandwidth $b_S = 1400 \text{ GB/s}$

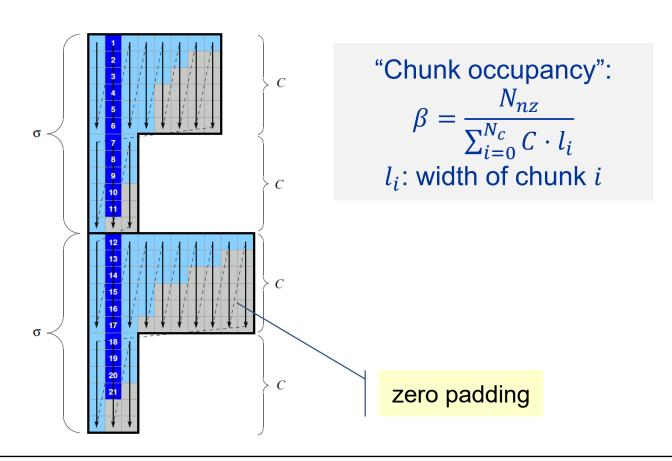
- Strong " α effect" large deviation from optimal α for many matrices
 - Many cache lines touched b/c every thread handles one row → bad cache usage
- Mediocre memory bandwidth usage
 (< 1400 GB/s) in many cases
 - Non-coalesced memory access
 - Imbalance across rows/threads of warps

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

Idea

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



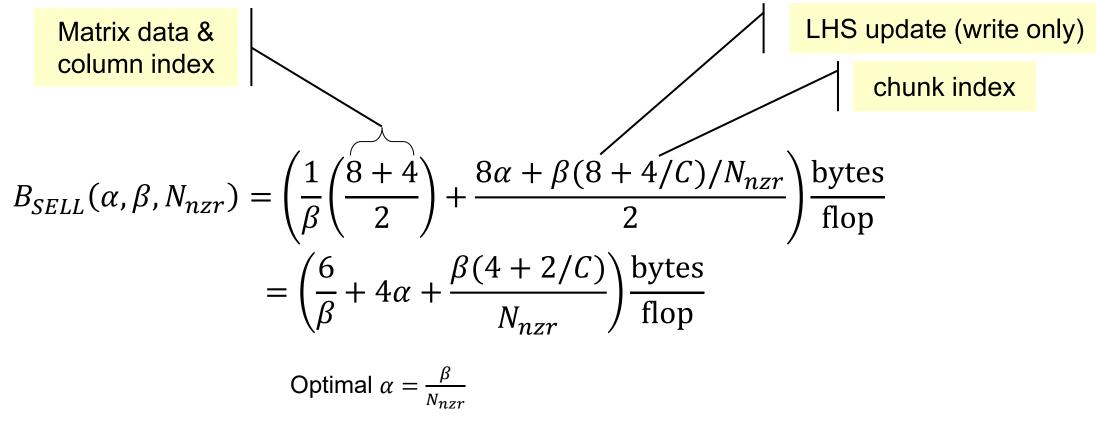


SELL-C- σ SpMV in CUDA (y=Ax)

```
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;
```

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Code balance of SELL-C- σ (y=Ax)



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

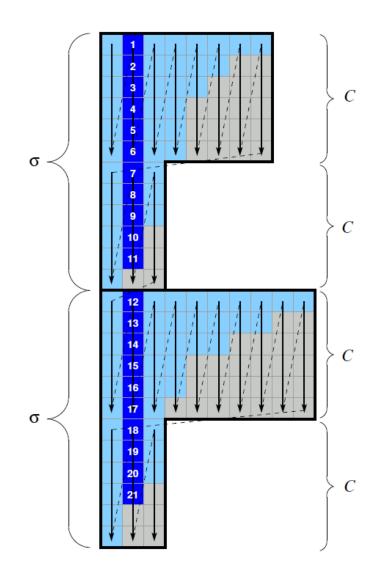


51

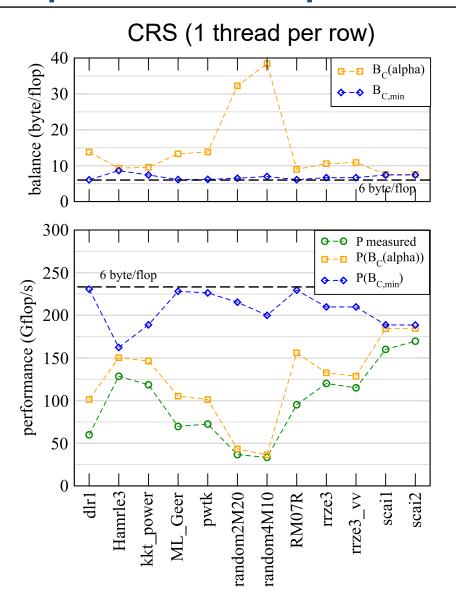
How to choose the parameters C and σ on GPUs?

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

- **O**
 - As small as possible, as large as necessary
 - Large σ reduces zero padding (brings β closer to 1)
 - Sorting alters RHS access pattern $\rightarrow \alpha$ depends on σ

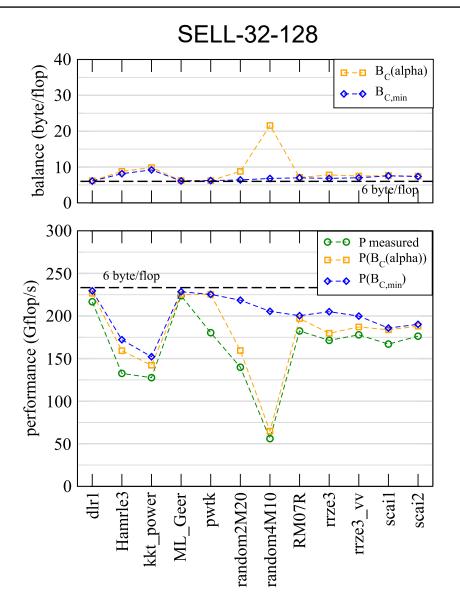


SpMV node performance model – GPU



NVIDIA Ampere A100

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



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!

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