Case study: A Jacobi smoother

The basics in two dimensions

Stencil schemes

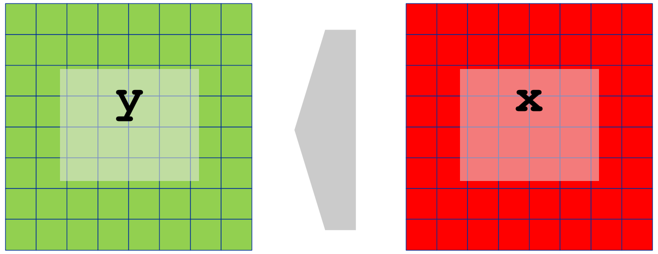
- Stencil schemes frequently occur in PDE solvers on regular lattice structures
- Basically a sparse matrix vector multiply (spMVM) embedded in an iterative scheme (outer loop)
- … but the regular access structure allows for matrix-free coding

```
do iter = 1, max_iterations

  Perform sweep over regular grid: y(:) ← x(:)

  Swap y ←→ x

enddo
```



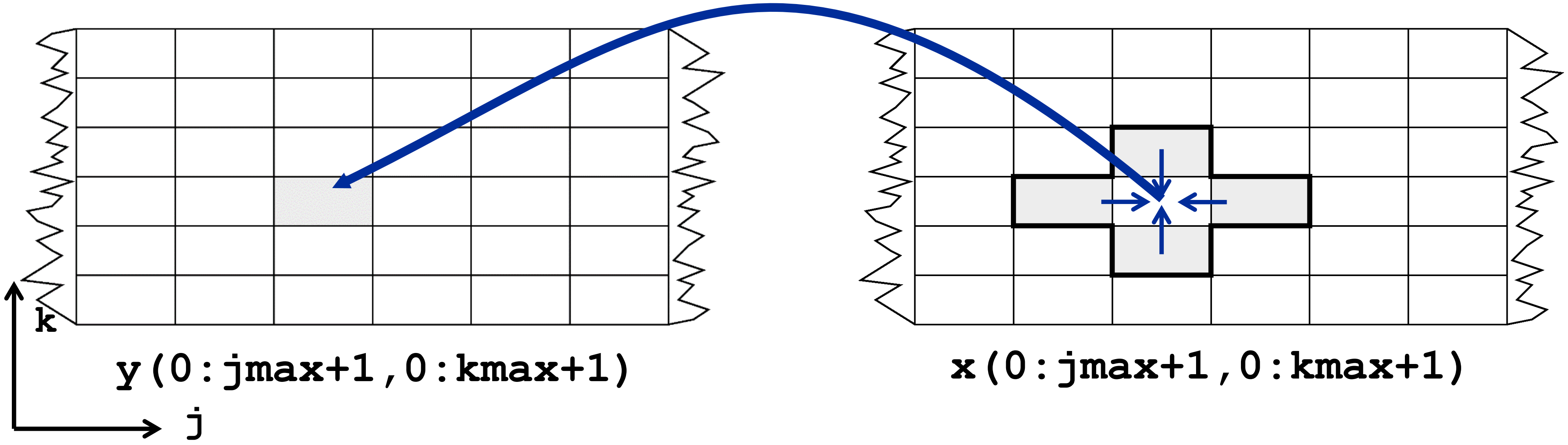
- Complexity of implementation and performance depends on
  - stencil operator, e.g. Jacobi-type, Gauss-Seidel-type, …
  - discretization, e.g. 7-pt or 27-pt in 3D,…

Jacobi-type 5-pt stencil in 2D

sweep

```
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
```

Lattice site update (LUP)



Appropriate performance metric: “Lattice site updates per second” [LUP/s]

(here: Multiply by 4 FLOP/LUP to get FLOP/s rate)

Jacobi 5-pt stencil 2D: data transfer analysis

RD+WR y(j,k)
(incl. write allocate)

Available in cache
(used 2 updates before)

RD x(j+1,k)

sweep

```
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
```

RD x(j,k-1)

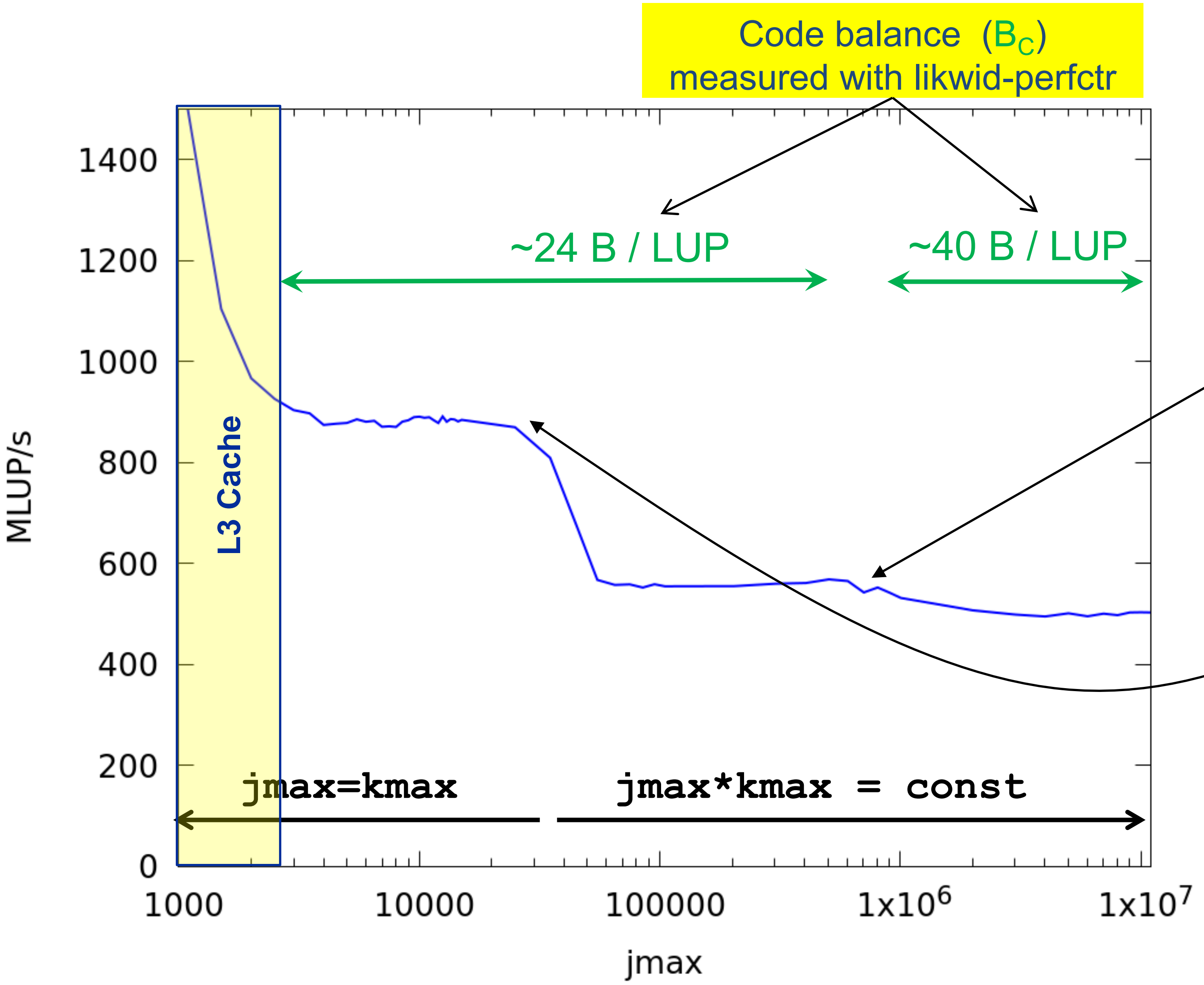
RD x(j,k+1)

Naive balance (incl. write allocate):

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

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

Jacobi 5-pt stencil 2D: Single core performance



Questions:

1. How to achieve 24 B/LUP also for large **`jmax`**?

2. How to sustain >800 MLUP/s for **`jmax`** > 10^4 ?

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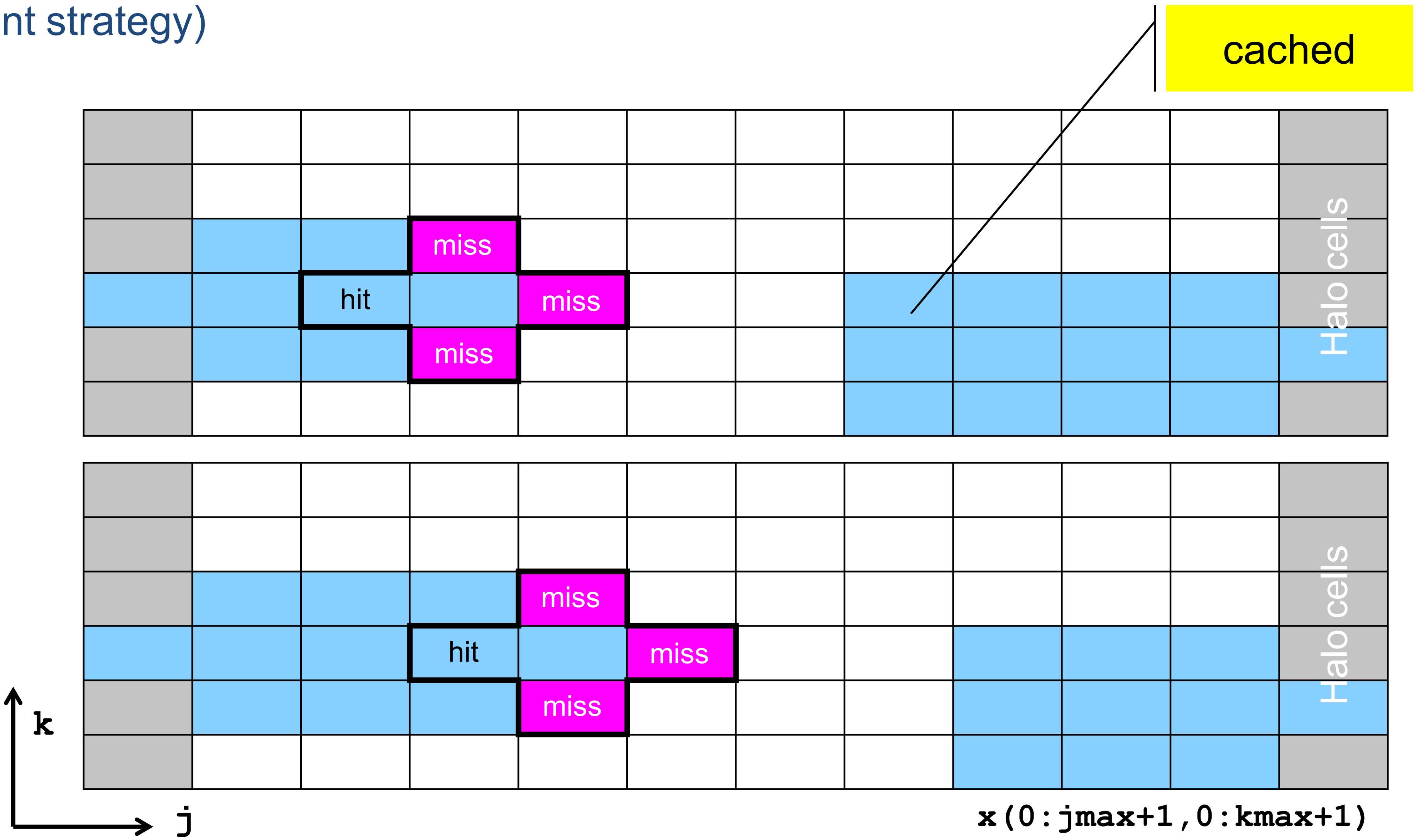
Case study: A Jacobi smoother

Layer conditions

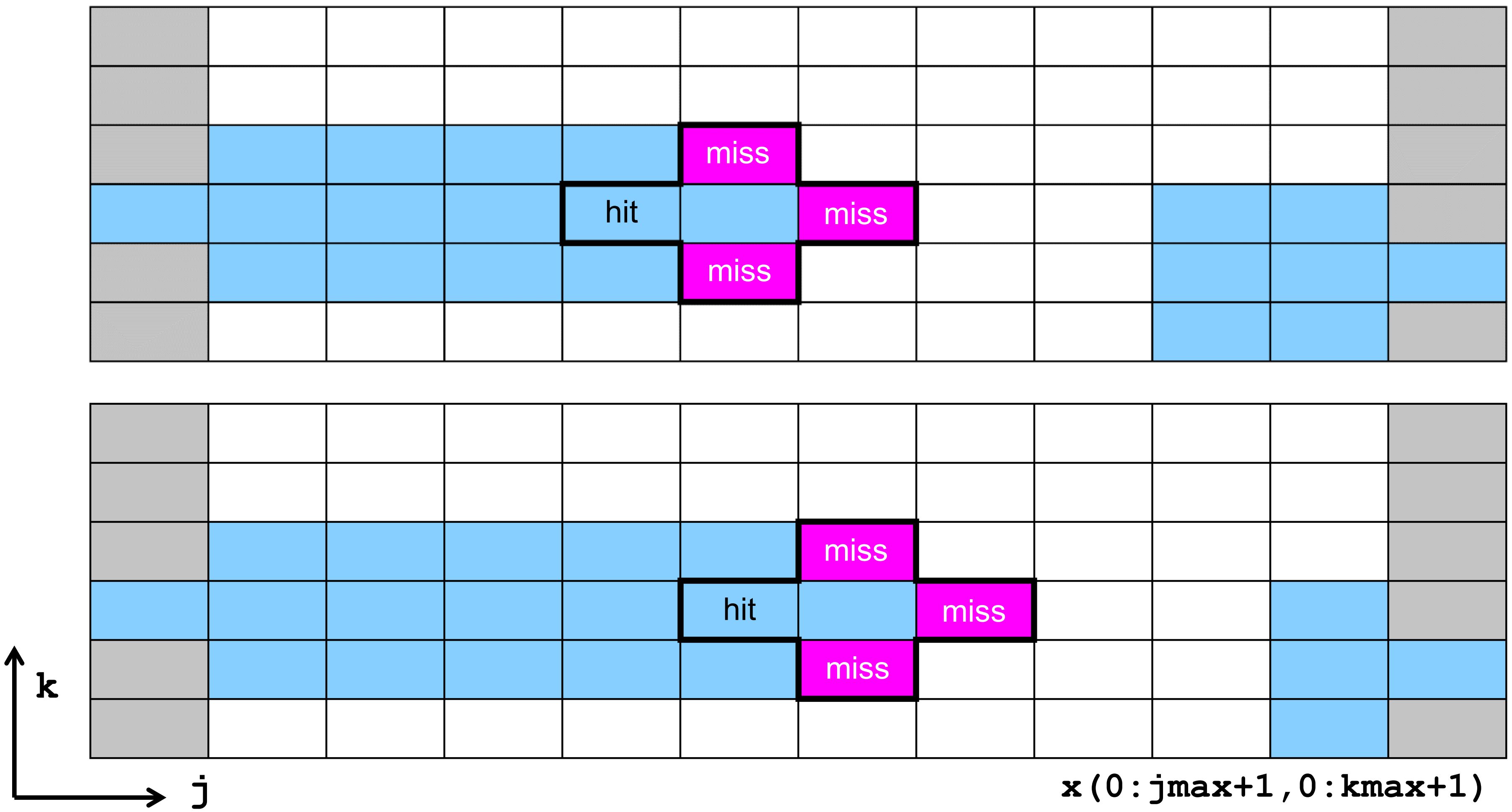
Analyzing the data flow

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



Analyzing the data flow

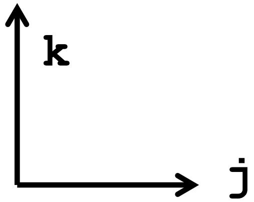
Worst case: Cache not large enough to hold 3 layers (rows) of grid (assume „Least Recently Used“ replacement strategy)

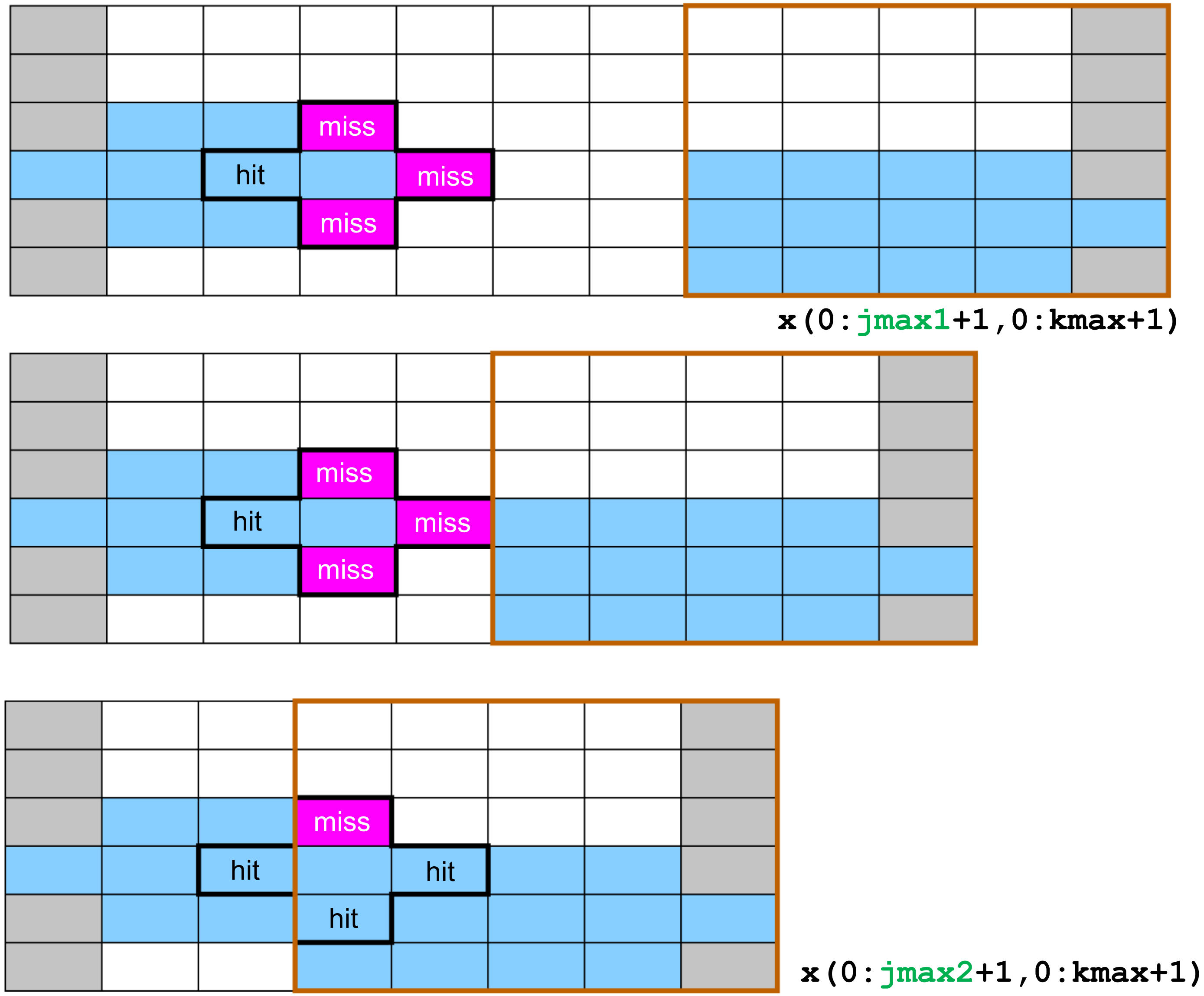


Analyzing the data flow

Reduce inner (j-) loop dimension successively

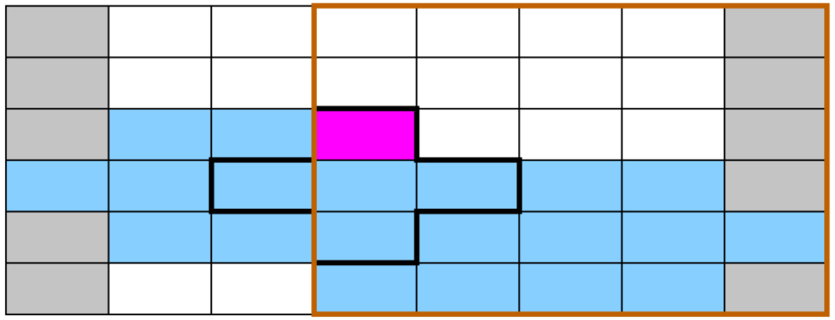
Best case: 3 “layers” of grid fit into the cache!





Analyzing the data flow: Layer condition

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



```
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
```

$$3 \times \mathtt{jmax} \times 8 \text{ byte} < \frac{C}{2}$$

"Layer condition"

3 rows of **jmax**

double precision

Safety margin (Rule of thumb)

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)

$$3 \times \mathbf{jmax} \times 8\ \text{byte} < \frac{C}{2}$$

Layer condition fulfilled?

YES

y: (1 RD + 1 WR) / LUP

x: 1 RD / LUP

```
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
```

B_C = 24 B / LUP

NO

y: (1 RD + 1 WR) / LUP

```
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
```

x: 3 RD / LUP

B_C = 40 B / LUP

Case study: A Jacobi smoother

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
```

New layer condition (blocking)

$$3 \times \mathbf{jblock} \times 8\ \text{byte} < \frac{C}{2}$$

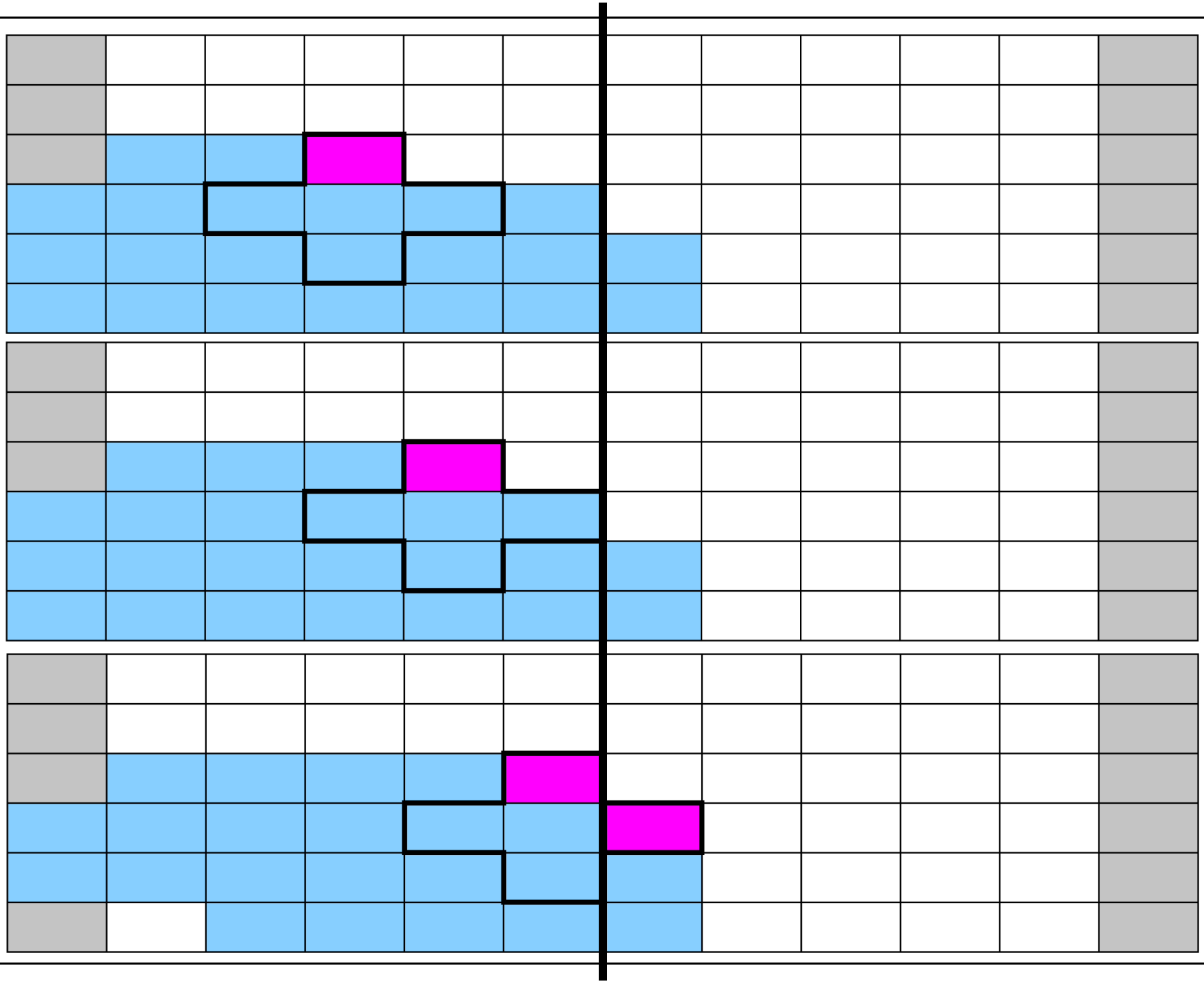
Determine for given C an appropriate **jblock** value:

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

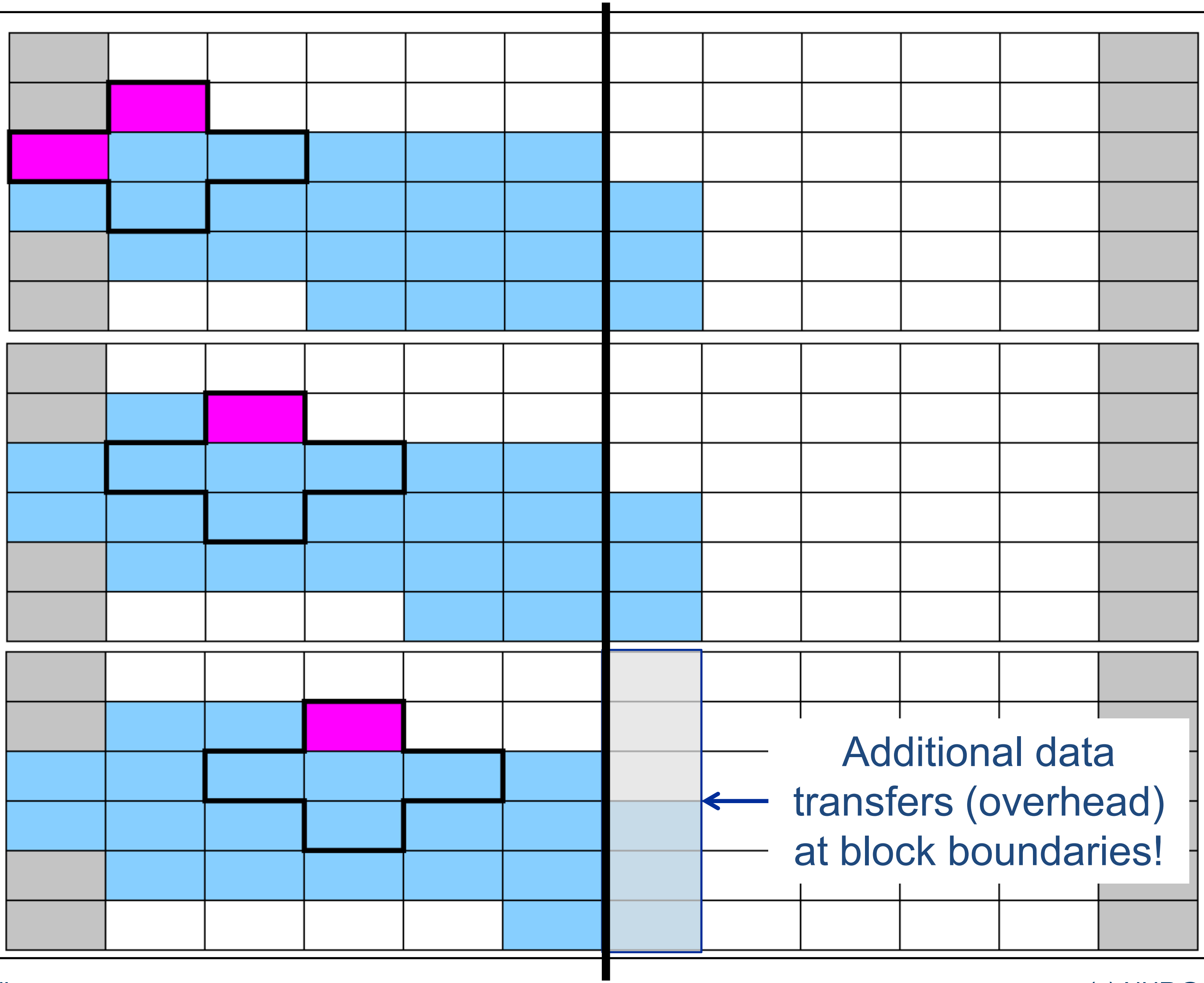
Establish the layer condition by blocking

Split domain into subblocks:

e.g. block size = 5



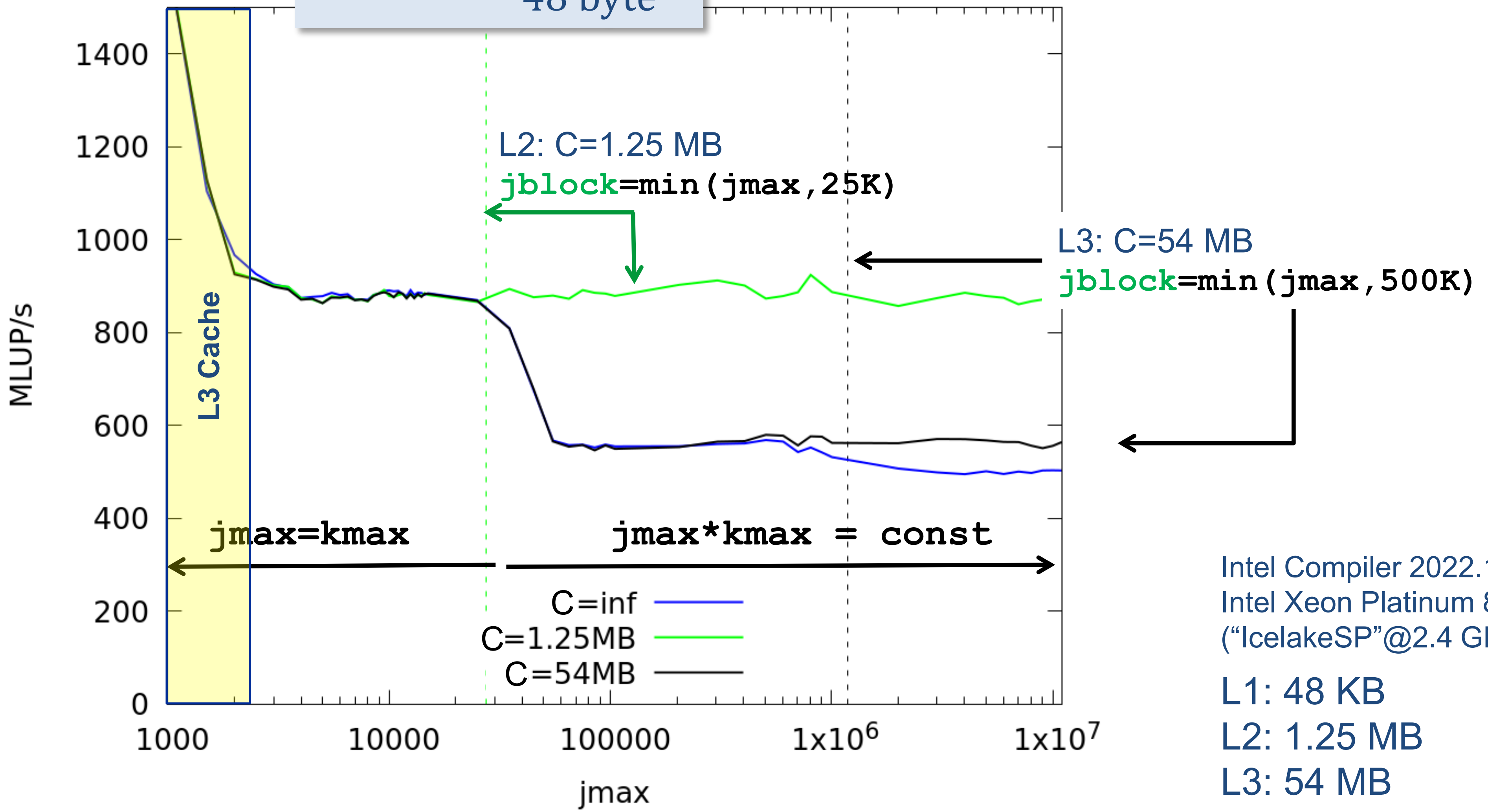
Establish the layer condition by blocking



Establish layer condition by spatial blocking

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

→ Which cache to block for?



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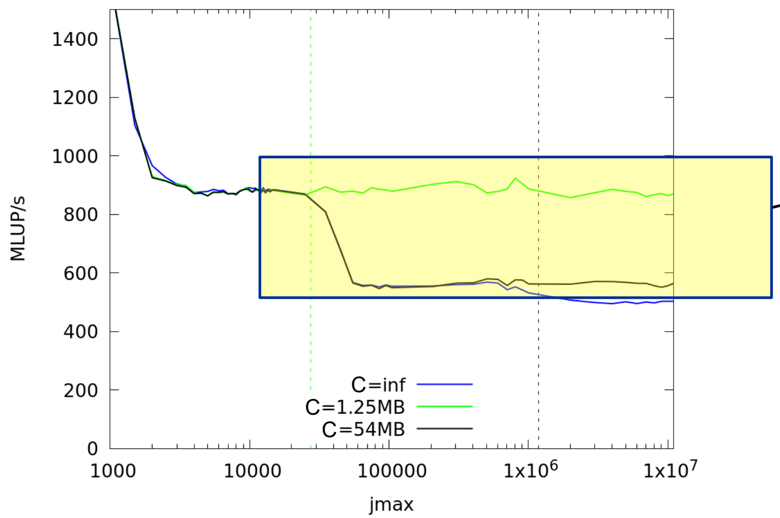
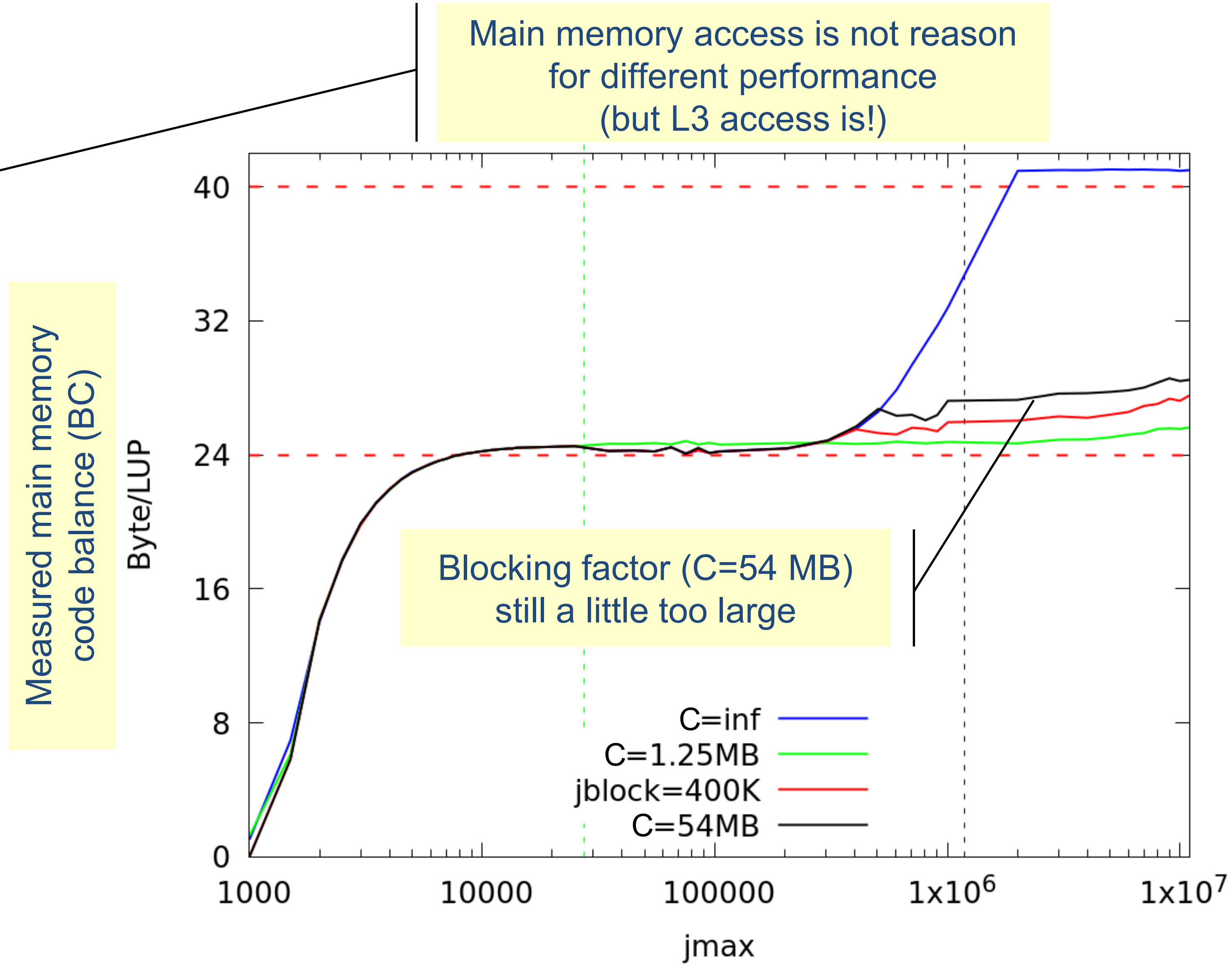
L1: 48 KB
L2: 1.25 MB
L3: 54 MB

Validating the model: Memory code balance





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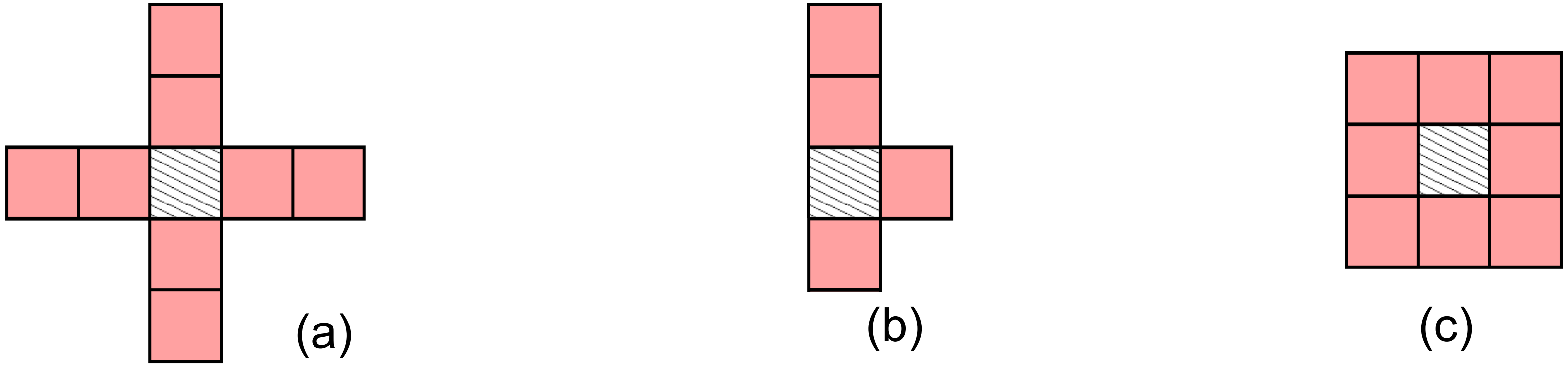
Stencil shapes and layer conditions in 2D



a) Long-range $r = 2$: 5 layers $(2r + 1)$

b) Asymmetric: 4 layers

c) 2D box: 3 layers

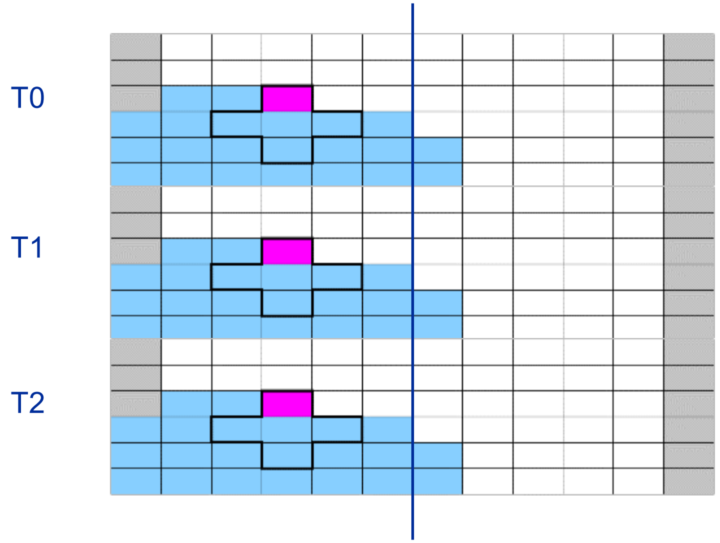
Case study: A Jacobi smoother

OpenMP parallelization

OpenMP parallelization of the blocked 2D stencil

Straightforward OpenMP work sharing:

```
do jb=1,jmax,jblock
!$OMP PARALLEL DO SCHEDULE(static)
  do k=1,kmax
    do j= jb, min(jb+jblock-1,jmax)
      y(j,k) = const * (x(j-1,k) + x(j+1,k) &
                     +  x(j,k-1) + x(j,k+1) )
    enddo
  enddo
!$OMP END PARALLEL DO
enddo
```



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

Layer condition:

$$3 \times \texttt{jblock} \times 8 \text{ byte} < \frac{C_t}{2}$$

Cache size available per thread

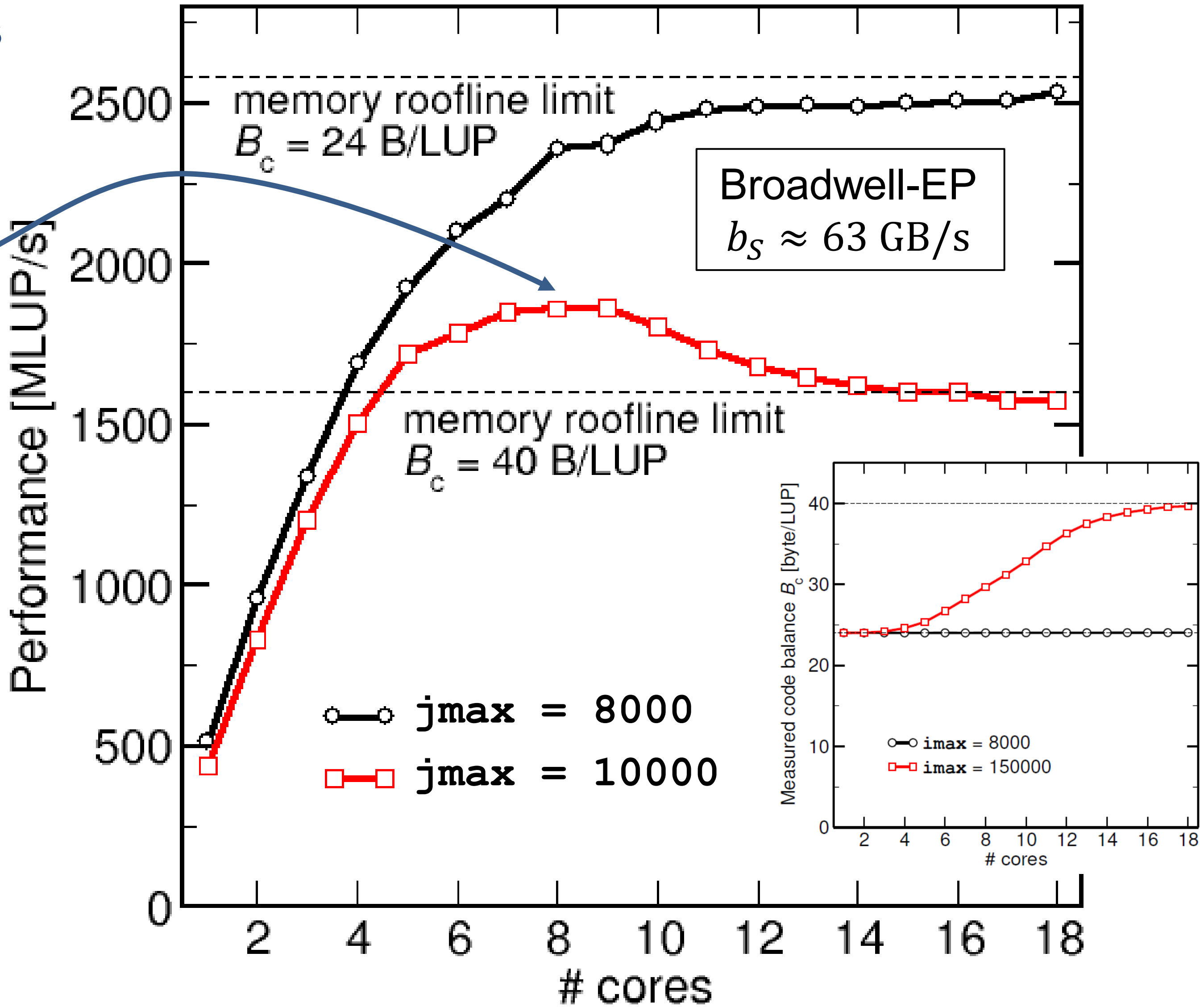
OpenMP parallelization and blocking for a shared cache

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 core-private caches *or*
     - Shared cache big enough to hold all layers for all threads
  2. Adaptive blocking for shared cache:

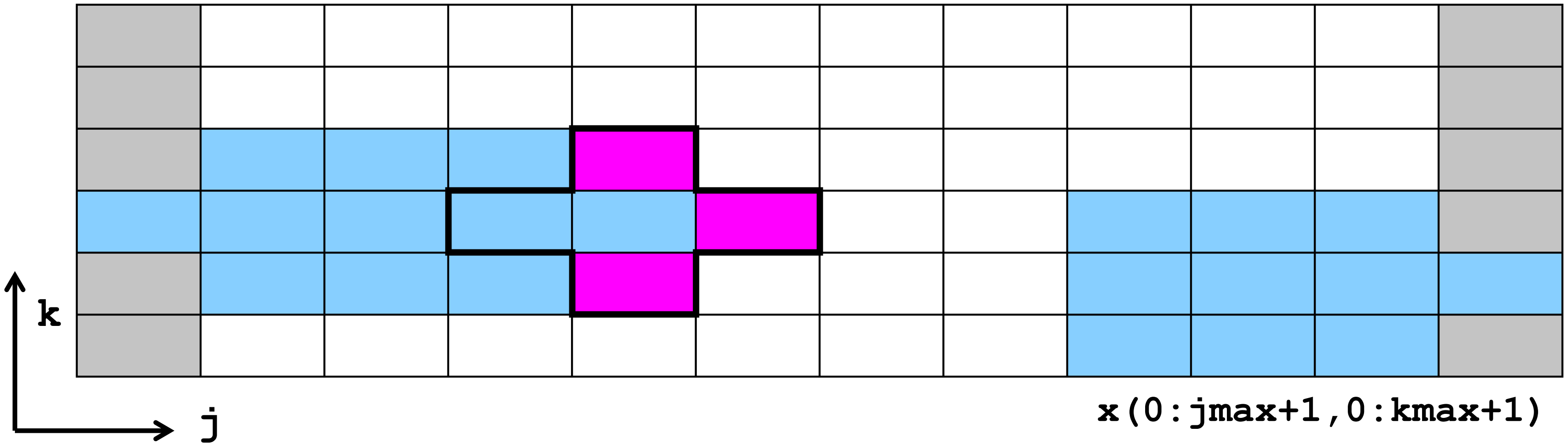
$$\mathbf{jblock} = \frac{C}{\#threads \times 48\ \text{byte}}$$



Case study: A Jacobi smoother

From 2D to 3D

2D:

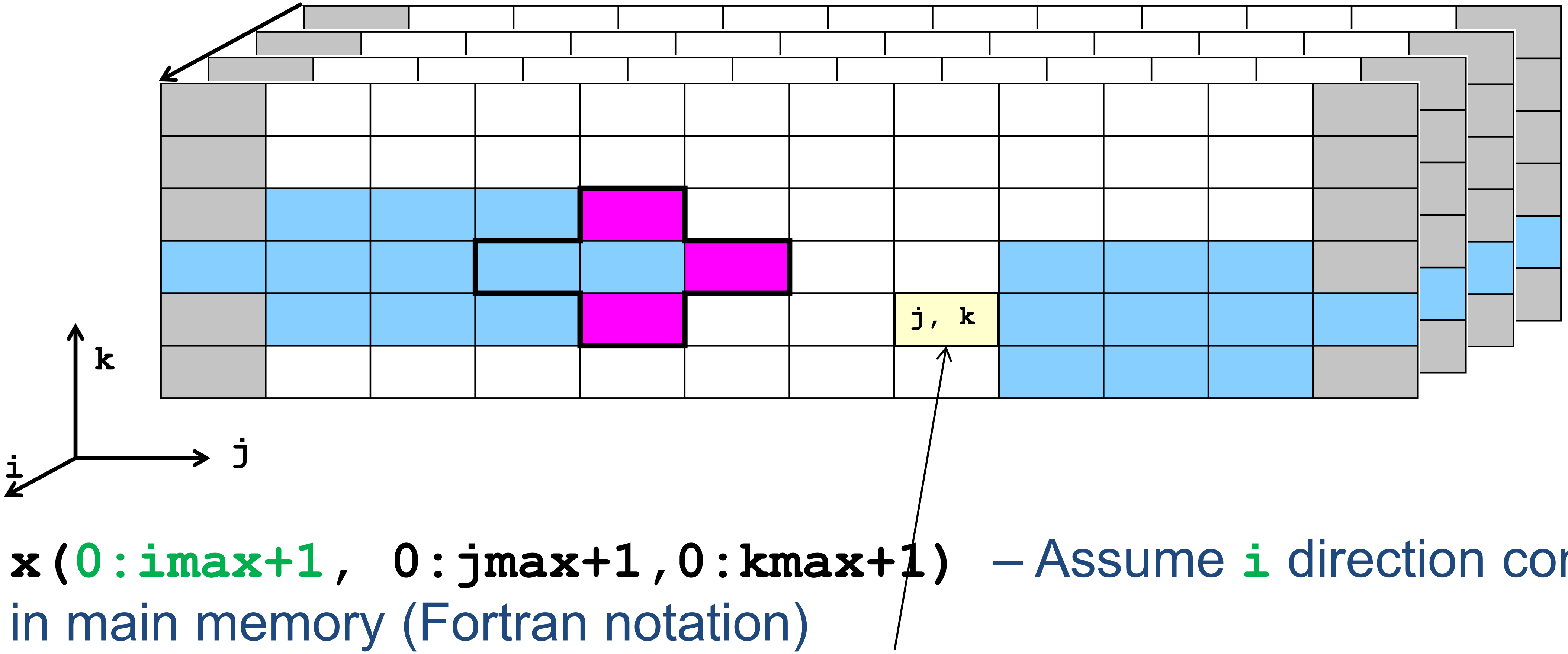


Towards 3D understanding

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

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

From 2D to 3D



- `x(0:imax+1, 0:jmax+1,0:kmax+1)` – Assume `i` direction contiguous in main memory (Fortran notation)
- 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)`

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

$$3 \times \mathtt{jmax} \times 8\,\text{byte} < \frac{C}{2}$$

Optimal B_C = 24 B / LUP

```
do k=1,kmax
  do j=1,jmax
    do i=1,imax
      y(i,j,k) = 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) )
    enddo
  enddo
enddo
```

3D

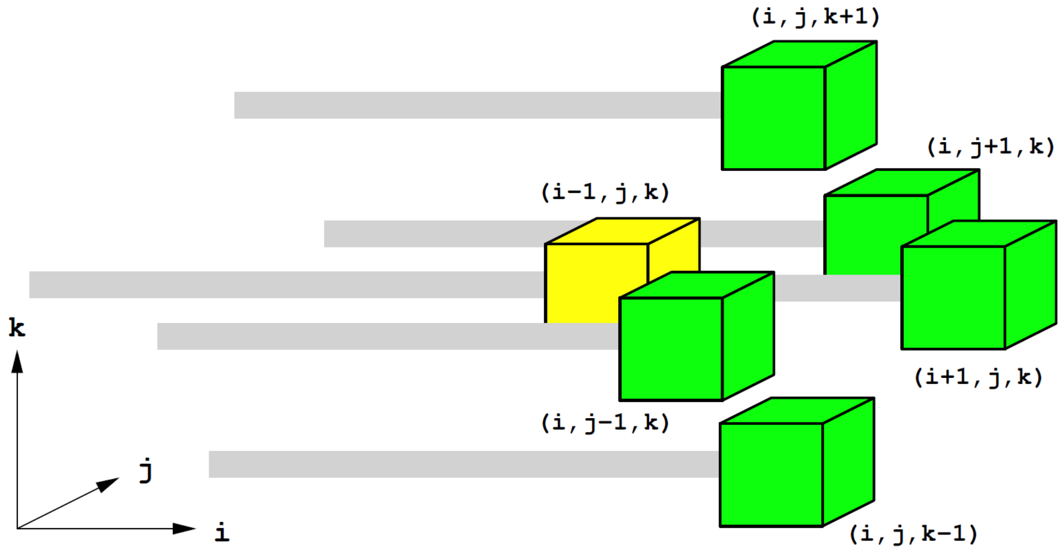
$$3 \times \mathtt{jmax} \times \mathtt{imax} \times 8\,\text{byte} < \frac{C}{2}$$

Optimal B_C = 24 B / LUP

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?

Stencil references

- J. Hammer, G. Hager, J. Eitzinger, and G. Wellein: Automatic Loop Kernel Analysis and Performance Modeling With Kerncraft. Proc. PMBS15, the 6th International Workshop on Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems, in conjunction with ACM/IEEE Supercomputing 2015 (SC15), November 16, 2015, Austin, TX. DOI: 10.1145/2832087.2832092, Preprint: arXiv:1509.03778
- H. Stengel, J. Treibig, G. Hager, and G. Wellein: Quantifying performance bottlenecks of stencil computations using the Execution-Cache-Memory model. Proc. ICS15, DOI: 10.1145/2751205.2751240, Preprint: arXiv:1410.5010
- 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). DOI:10.1002/cpe.3489 Preprint: arXiv:1304.7664
- 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).
- G. Wellein, G. Hager, T. Zeiser, M. Wittmann and H. Fehske: Efficient temporal blocking for stencil computations by multicore-aware wavefront parallelization. Proc. COMPSAC 2009. DOI: 10.1109/COMPSAC.2009.82