Algorithms of Scientific Computing

Hierarchical Methods and Sparse Grids

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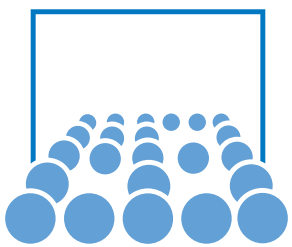


Part VII

Algorithms and Data Structures for Sparse Grids

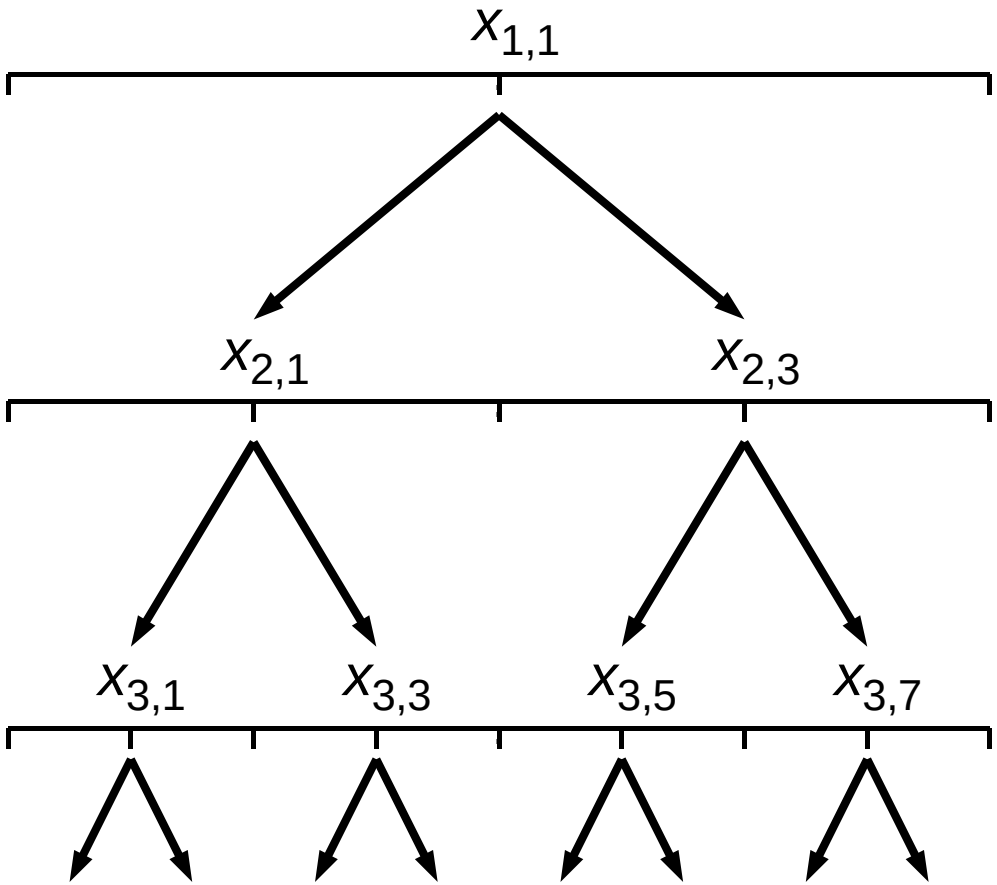
Algorithms and Data Structures

- We will now look at typical sparse grid algorithms
- Can, e.g., be used for solution of PDE in previous part
- Algorithms depend on data structure:
  - Efficient traversal of sparse grid necessary
  - Thus, we deal with data structures for sparse grids, too

Data Structures ($d = 1$)

- How to store function $u : [0, 1] \to \mathbb{R}$ in hierarchical representation (i.e. surplusses $v_{\vec{l},\vec{i}}$)?
- Order and store grid points and associated values in binary tree
  - Root is node $x_{1,1} = 1/2$
  - Children of node $x_{l,i}$ are – if existent – the grid points $x_{l+1,2i-1}$ and $x_{l+1,2i+1}$ of level $l + 1$
  - Alternative point of view if child does not exist: Complete subtree of binary tree starting from child with all surplusses set to 0

Data Structures ($d = 1$) (2)



Typical Algorithms ($d = 1$)

Hierarchization and Dehierarchization

- Prototype for typical algorithm (c.f. worksheet 4)
- Our data structure has to allow
  1. Iteration over all grid points, considering the hierarchical relations
     - E.g. for hierarchization: first handle all grid points in the support of $\phi_{l,i}$, then compute $v_{l,i}$
  2. Access to *hierarchical neighbors*: grid points at interval boundaries of support of $\phi_{l,i}$ (if possible – exception for points 0 and 1 as not in the tree), e.g. to compute

$$v_{l,i} = u_{l,i} - \frac{1}{2}(u_l + u_r).$$

Typical Algorithms ($d = 1$) (2)

- Hierarchical neighbors are easy to find geometrically

$$x_{l,i-1}, \qquad x_{l,i+1}$$

- But have even indices $\Rightarrow$ really are on another level ($< l$)
- In the binary tree structure:
  - Can be found on way from root to node
  - One is parent node
- For hierarchization/dehierarchization: pass hierarchical neighbors as additional parameters
- Developing algorithms:
  - Try to store all information to process one node at the node and its hierarchical neighbors
  - Access to other nodes typically expensive
  - Tree traversal with “supply of hierarchical neighbors” only linear in number of nodes

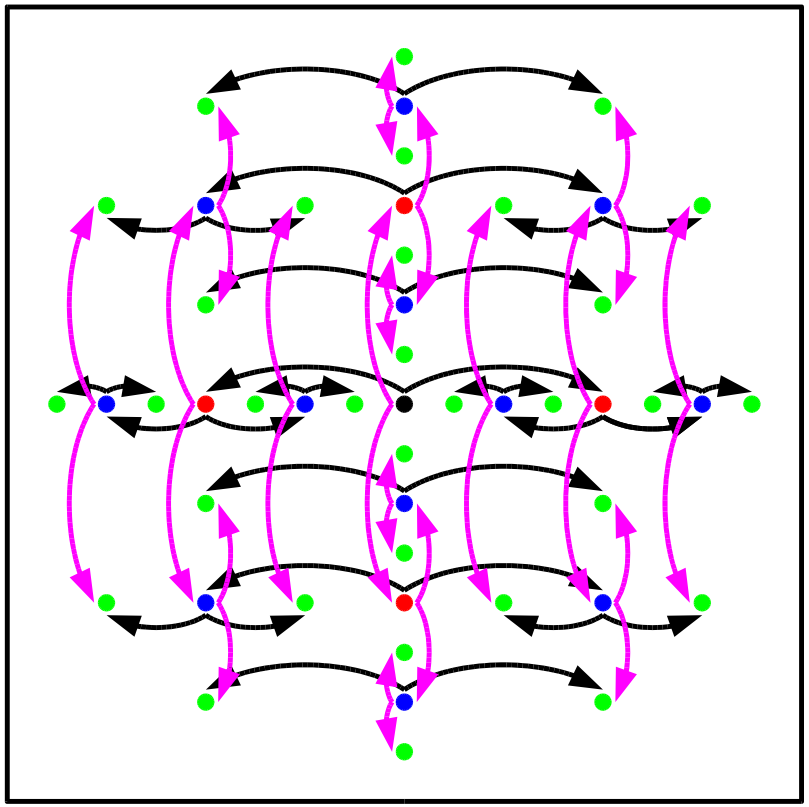
Data Structures and Typical Algorithms ($d > 1$)

- What data structure to use in more than one dimension?
- Algorithmically: use construction of basis functions as product of one-dimensional hats. Ideally:
  - Use a loop $1, \ldots, d$ over the dimension
  - Apply $1d$ algorithm on one-dimensional structures in each dimension (see also worksheet 7)

$\Rightarrow$ Need access to hierarchical neighbors in each spacial direction; implies to create binary tree structure in each dimension

- Disadvantages:
  - Storage requirements ($2d$ pointers)
  - High effort to keep structure consistent when inserting or deleting points

Data Structures and Typical Algorithms ($d > 1$) (2)



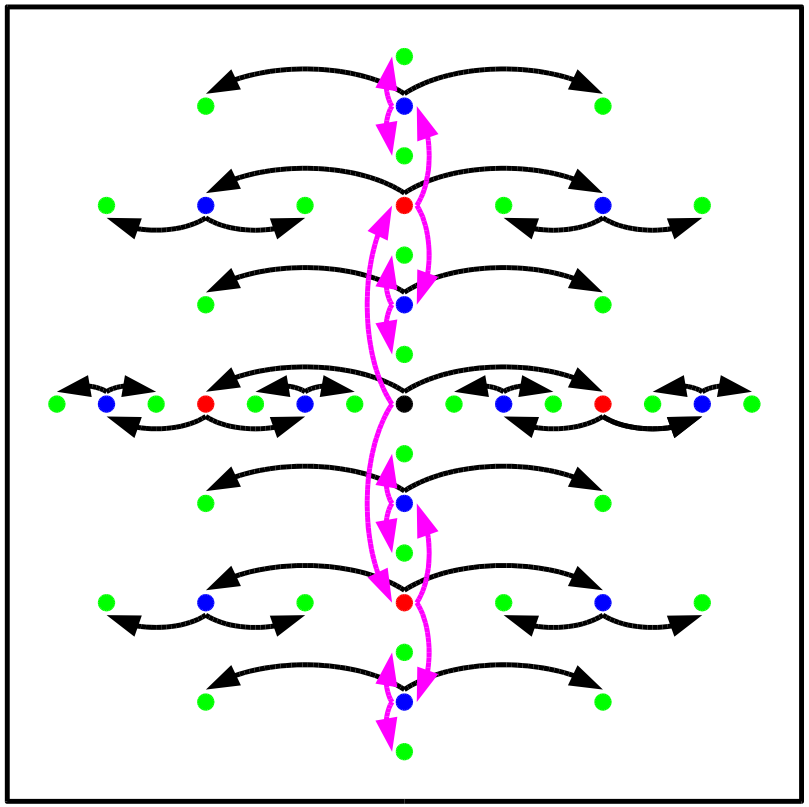
If you could recognize anything, it would be binary tree structures for rows (black) and columns (magenta)

Data Structures and Typical Algorithms ($d > 1$) (3)

Often better:

- Store in a node only two pointers for one direction (e.g. x_1)
- A binary tree of nodes is a row (a $1d$ structure parallel to the x_1 axis)
- For next spacial direction x_2, only a binary tree in x_2 direction required
- Stores one plane parallel to $x1 - -x2$ coordinate plane; nodes are the binary trees with $1d$ structures
- For each additional spatial direction x_d build binary tree with $(d-1)$-dimensional structures as nodes
- Disadvantage: Access to hierarchical neighbors not that easy any more (except for x_1-direction)
- But can be achieved without much more computational effort by suitable reordering of loops and tree traversals

Data Structures and Typical Algorithms ($d > 1$) (4)



Already more clear: One plane (two-dimensional structure) consists of one binary tree (magenta) of which the nodes are binary trees (black) for each row

Data Structures and Typical Algorithms ($d > 1$) (5)

Hash table

- Much more comfortable (and not half inefficient) alternative
- Store magnitudes as target values, with, e.g., $(\vec{l}, \vec{i})$ as keys
- No need to care about tree structures
- Only have to compute indices of designated node (hierarchical neighbor, . . .)

$\Rightarrow$ Best solution for your own sparse grid experiments

Further assumptions on data structures

- Algorithms will assume that all hierarchical neighbors exist for each grid point

$\Rightarrow$ If creating grid points adaptively, create them if necessary

- No further assumptions

Solving Differential Equations on Sparse Grids

Preliminary Considerations

- Finite elements: method to transform DE to system of linear equations

$$M\vec{v} = \vec{f}$$

  for hierarchical surplusses (threaded in vector $\vec{v}$)
- Linear system has to be solved

- Problem: matrix in hierarchical basis not sparse, but densely populated
- So many non-zero entries that explicit assembly can be too expensive
- Even worse: prohibits direct solution, e.g. via Cholesky decomposition

Preliminary Considerations (2)

Less problematic than it seems:

- Matrix can be applied to vector in linear time in length of vector (algorithmically tricky!)
- Use iterative solvers:
  - Only have to implement application of matrix to a given vector

    $$\vec{v} \mapsto M\vec{v}$$

    (algorithmically challenging and interesting)
  - Algorithmically less interesting part is done by someone else (conjugated gradients (CG), ...)
- We consider it at the example of matrix B (L_2 scalar product)
- Matrix A for energy scalar product less clear, but can be done similarly

Matrix-Vector multiplication

Computing $M\vec{v}$, with $M = B$, $b_{i,j} := \int_0^1 \phi_j(x)\phi_i(x)\,dx$

- Given: hierarchical coefficients $v_{\vec{l},\vec{i}}$
- Compute in each node $\vec{l},\vec{i}$ the corresponding component of $M\vec{v}$:

$$\int_\Omega \phi_{\vec{l},\vec{i}} \left(\sum_{\vec{l}',\vec{j}} v_{\vec{l}',\vec{j}} \phi_{\vec{l}',\vec{j}} \right) d\vec{x} = \sum_{\vec{l}',\vec{j}} \left(\int_\Omega \phi_{\vec{l},\vec{i}} \phi_{\vec{l}',\vec{j}}\, d\vec{x} \right) v_{\vec{l}',\vec{j}} = \sum_{\vec{l}',\vec{j}} \left(\phi_{\vec{l},\vec{i}}, \phi_{\vec{l}',\vec{j}} \right)_2 v_{\vec{l}',\vec{j}}$$

- Think of transport of contributions:
  - Transport surplus at $\vec{l}',\vec{j}$ with weight $(\phi_{\vec{l},\vec{i}}, \phi_{\vec{l}',\vec{j}})_2$ to position $\vec{l},\vec{i}$
  - Everything that arrives at a node is summed up
- It is possible with effort proportional to number of unknowns (squared would be too easy)!

Multiplication with B, $d = 1$

- Order $1d$ unknowns by level l (and within level by index i, e.g.) – important for mathematics, not for implementation
- Example for $n = 3$:

$$B\vec{v} = \left(\begin{array}{c|cc|ccccc} 1/3 & 1/8 & 1/8 & 1/32 & 3/32 & 3/32 & 1/32 \\ \hline 1/8 & 1/6 & 0 & 1/16 & 1/16 & 0 & 0 \\ 1/8 & 0 & 1/6 & 0 & 0 & 1/16 & 1/16 \\ \hline 1/32 & 1/16 & 0 & 1/12 & 0 & 0 & 0 \\ 3/32 & 1/16 & 0 & 0 & 1/12 & 0 & 0 \\ 3/32 & 0 & 1/16 & 0 & 0 & 1/12 & 0 \\ 1/32 & 0 & 1/16 & 0 & 0 & 0 & 1/12 \end{array}\right) \left(\begin{array}{c} v_{1,1} \\ \hline v_{2,1} \\ v_{2,3} \\ \hline v_{3,1} \\ v_{3,3} \\ v_{3,5} \\ v_{3,7} \end{array}\right)$$

- If follows from hierarchical structure:
  Surplusses have always to be propagated up or down the tree, never sidewards

Splitting of B

- We now split transports depending on direction in tree structure into
  - procedure *down*, which does transport towards leaves,
  - procedure *up*, which does transport towards root
- Note: splitting not necessary for $d = 1$, but helpful to derive operations and necessary for $d > 1$

- In matrix notation this corresponds to

$$B =: B^D + B^U$$

- B^D corresponds to down, contains entries of B below diagonal (strictly lower triangular matrix)
- B^U corresponds to up, contains entries on and above diagonal (upper triangular matrix)

Multiplication with B, $d = 1$: down

- Down computes in node $\vec{l}, \vec{i}$

$$\int_\Omega \phi_{l,i} \left(\sum_{l' < l, j} v_{l',j} \phi_{l',j} \right) dx,$$

- Value depends only on linear interpolant between hierarchical neighbors of $x_{\vec{l},\vec{i}}$!

$\Rightarrow$ Take procedure for dehierarchization

- Modify it to compute integral as

$$h_l \frac{u_l + u_r}{2}.$$

before computing function value $u_{\vec{l},\vec{i}}$

Multiplication with B, $d = 1$: up

Up is more difficult...

- Contribution of other basis functions not linear on support

To understand up operations, we consider the following:

- We can neglect the diagonal for the following considerations (unproblematic, as no communication of different nodes)
- B is symmetric, thus B^U and B^D are transposed
- Multiplication with B^D did consist mainly of operations

$$u_{l,i} := u_{l,i} + \frac{u_l + u_r}{2}$$

- They can be described by matrix $B^D_{\vec{l},\vec{i}}$ (how does it look like?)

Multiplication with B, $d = 1$: up (2)

- Multiplication with transposed of matrix $B^D_{\vec{l},\vec{i}}$ as follows:

$$u_r := u_r + \frac{u_{l,i}}{2}; \quad u_l := u_l + \frac{u_{l,i}}{2}$$

- Multiplication with h_l corresponds to diagonal matrix (slightly transposed)
- Now only apply those building blocks in reverse order (due to $(CD)^T = C^T D^T$) $\Rightarrow$ bottom-up tree traversal

$\Rightarrow$ Multiplication with B with constant cost per node (even though much more coefficients in B are non-zero): $\mathcal{O}(N)$

Multiplication with B, $d > 1$

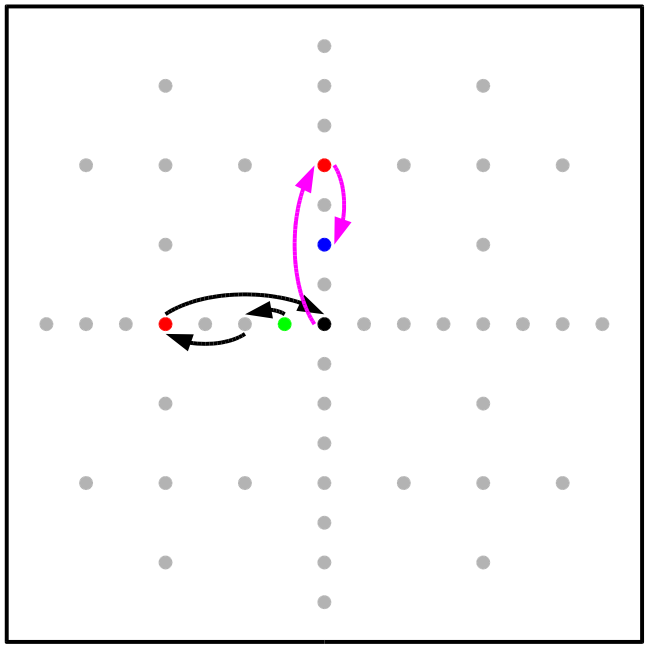
- In multi-dimensional case, we can write weights as products of $1d$ weights:

$$\left(\phi_{\vec{l},\vec{i}}, \phi_{\vec{l}',\vec{j}}\right)_2 = \prod_{k=1}^{d} \left(\phi_{l_k,i_k}, \phi_{l'_k,j_k}\right)_2$$

- This implies general strategy for d-dimensional problems:
  - Loop over the dimension
  - Loop over all $1d$ structures in corresponding direction
  - Apply $1d$ algorithm (up and down) there

Multiplication with B, $d > 1$ (2)

Example: transport of contributions

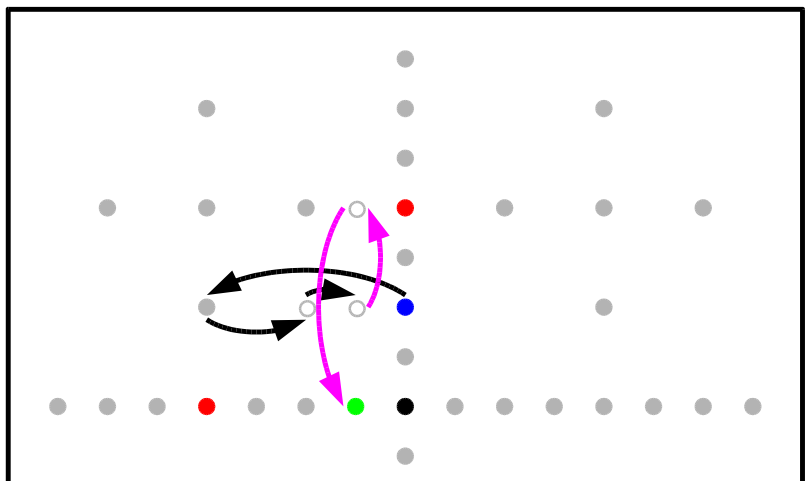


- Transport from grid point $\vec{l}', \vec{j} = (4,1),(7,1)$ to grid point $\vec{l}, \vec{i} = (1,3),(1,3)$
- Up along row (black arrows) computes weight $(\phi_{1,1}, \phi_{4,7})$, down along column (magenta) computes weight $(\phi_{3,3}, \phi_{1,1})$

Multiplication with B, $d > 1$ (2)

Troubles with that...

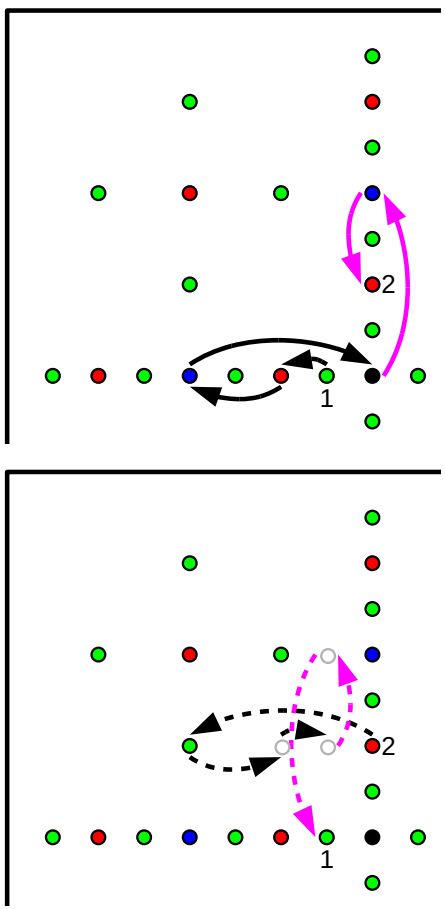
- Nice algorithm, but does not work on sparse grids
- Consider reverse direction – would be like this:

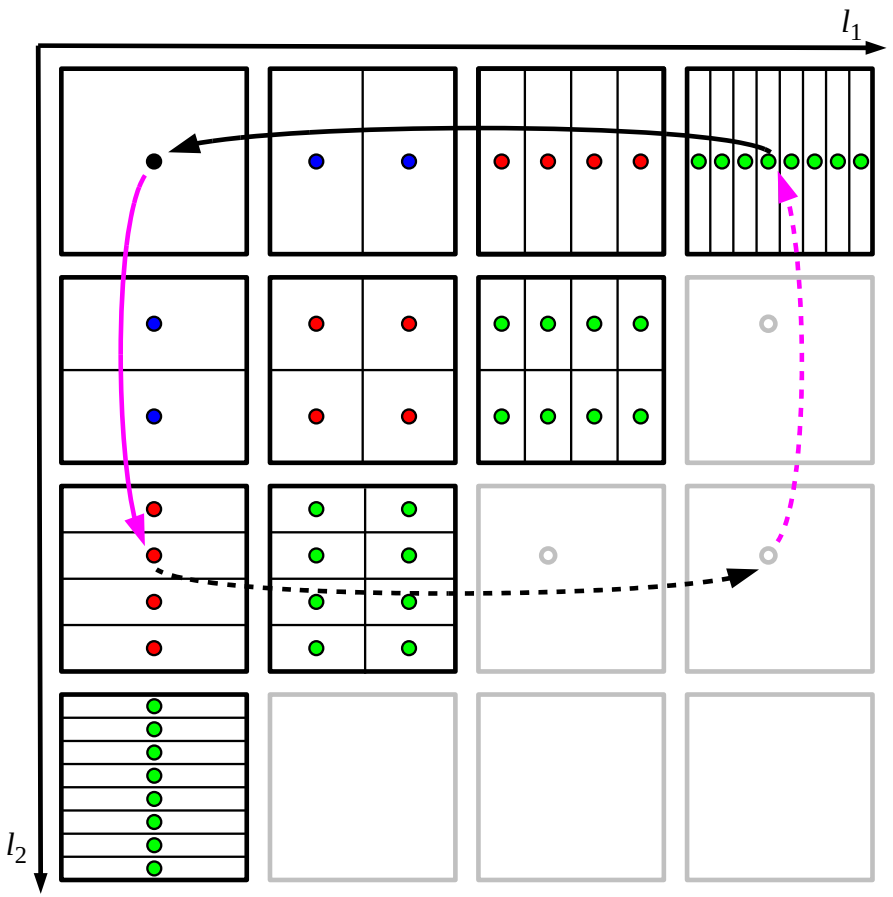


- Three grid points are missing!
- Creating all missing grid points on the fly $\Rightarrow$ full grid!

Multiplication with B, $d > 1$ (3)

Full scheme



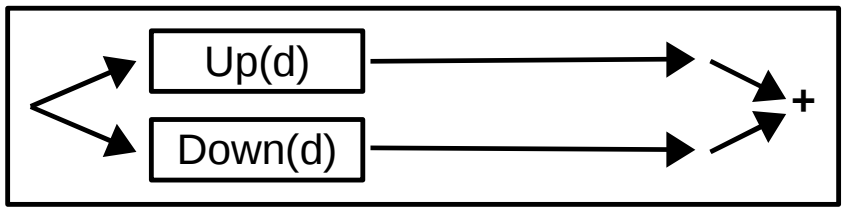


Multiplication with B, $d > 1$ (4)

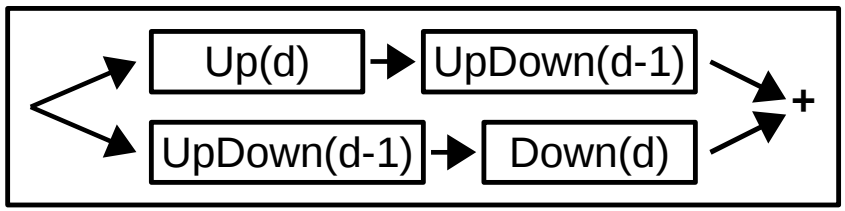
UpDown scheme

- It works, if we reorder up and down processes
  - Execute all ups before any down

UpDown(1):



UpDown(d):



All together...

- We have considered suitable data structures
  ...and efficient algorithms working on them
- We could now start
  - solving PDEs (iteratively)
  - integrate (and interpolate) multi-dimensional functions
  - and much more...