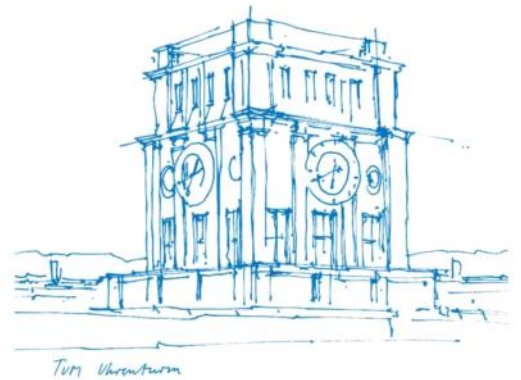


Algorithms for Scientific Computing

Organisation of the Course

Tobias Neckel
Technical University of Munich
Summer 2020



Content

Space-Filling Curves

- Hilbert Curve
- Peano Curve
- 2D vs. 3D
- Applications

 $1/4$ TN

Hierarchical Numerical Methods

- Hierarchical Basis (1D, ND)
- Sparse Grids
- Applications

 $1/2$

Discrete Fourier Transform & related Transforms

- Fast Fourier Transform
- Fast Discrete Cosine/Sine Transform
- Applications

 $1/4$

Persons

Lecture

- Tobias Neckel
- Felix Dietrich
- Christian Mendl

Tutorials

- Jean-Matthieu Gallard
- Santiago Narvaez

Corona Aspects

Lecture

- Asynchronous: Recorded videos
- Will be uploaded shortly before the corresponding lecture slot
- If desired: virtual office hours of lecturer once per week

Tutorials

- Asynchronous: WS + solutions published
- Synchronous: Interactive Q & A tutorial session
- For more details: See Moodle page

Exams

- State / TUM policy not yet clear
- Probably: usual format (written) in usual period (end of term) in unusual mode (other rooms, more distance)

Technical Aspects

- Moodle: Landing page, contains everything
- Interactive parts: either via zoom or BigBlueButton (will be announced via Moodle)

Lecture 1 - From Quadtrees to Space-Filling Orders

Donnerstag, 16. April 2020 16:21

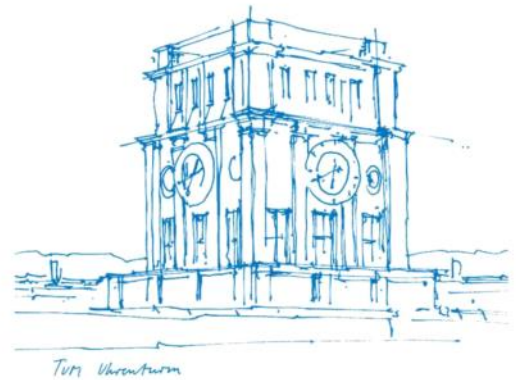
3 parts:

- I. Quadtrees
- II. Hilbert Orders
- III. Applications of Space-Filling Orders

Algorithms for Scientific Computing

From Quadtrees to Space-Filling Orders

Tobias Neckel
Technical University of Munich
Summer 2020



Part I

Quadtrees

Overview: Modelling of Geometric Objects

Surface-oriented models:

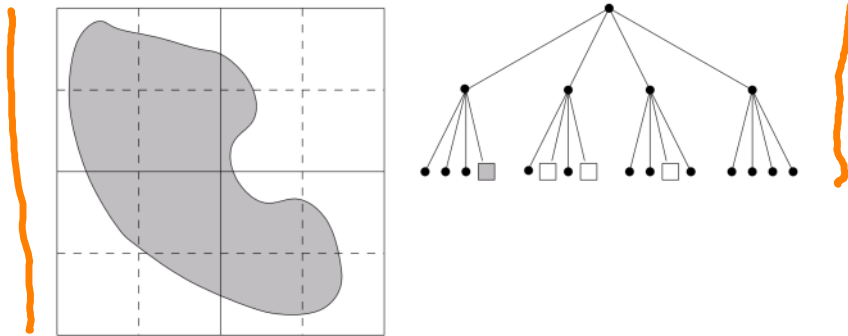
CAD

- wire-frame models
- augmented models using Bezier curves and planes
- typically described by graphs on nodes, edges, and faces

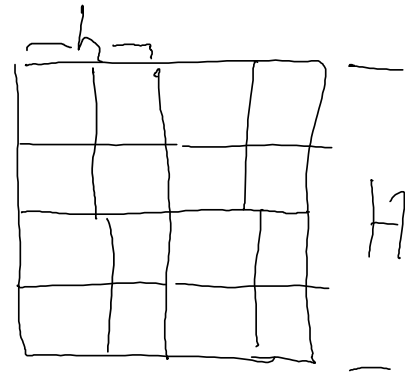
Volume-oriented models:

- Constructive Solid Geometry (boolean operations on primitives)
- voxel models: place object in a grid
- octrees: recursive refinement of voxel grids
- quadtrees: 2D analogon (voxel \rightsquigarrow pixel)

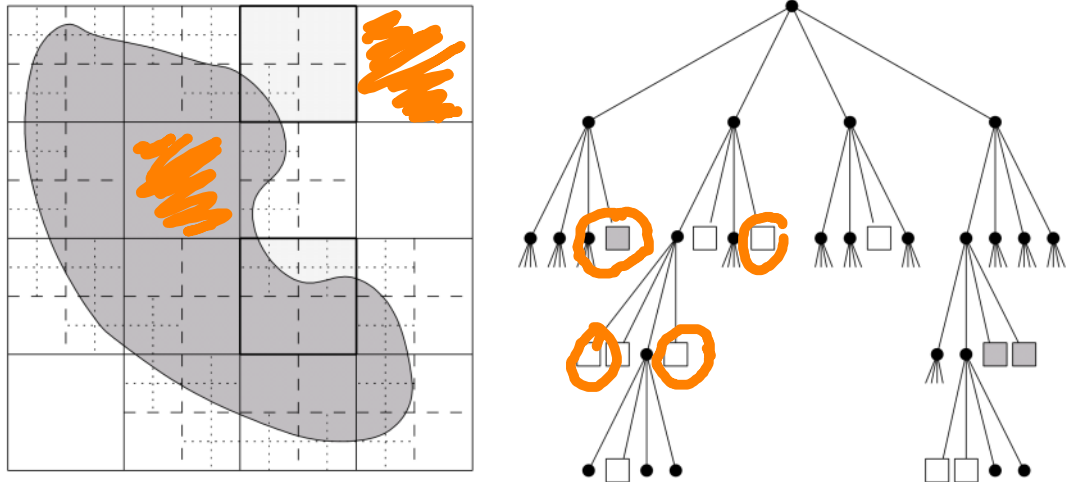
Quadrees to Describe Geometric Objects



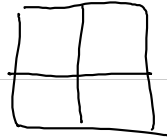
- start with an initial square (covering the entire domain)
- recursive substructuring in four subsquares



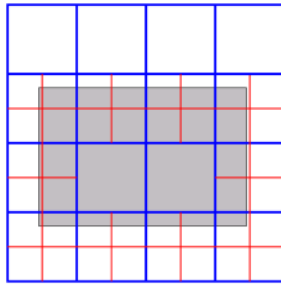
Quadrees to Describe Geometric Objects



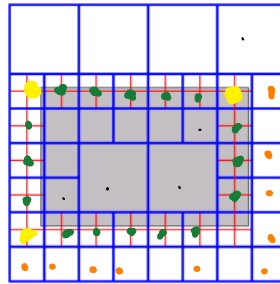
- start with an initial square (covering the entire domain)
- recursive substructuring in four subsquares
- adaptive refinement possible
- terminate, if squares entirely within or outside domain



Number of Quadtree Cells to Store a Rectangle



k=2



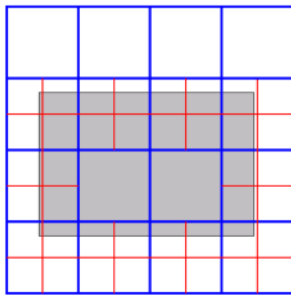
k=3

Terminal (t_k) and boundary (b_k) cells after k refinement steps (for $k > 2$):

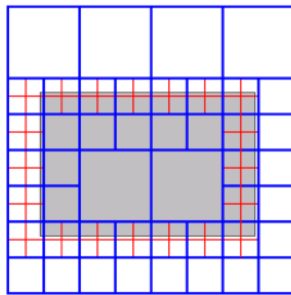
$$\begin{aligned} b_k &= 2 \cdot b_{k-1} \\ t_k &= t_{k-1} + 2 \cdot b_{k-1} \end{aligned} \Rightarrow \begin{aligned} b_k &= 2^{k-2} \cdot b_2 = \frac{5}{2} \cdot 2^k \\ t_k &= \dots = 5 \cdot 2^k - 14 \end{aligned}$$

$k \downarrow$	b	t
	$b_0 = 1$	$t_0 = 0$
	$b_1 = 4$	$t_1 = 0$
	$b_2 = 16$	$t_2 = 6$
	$b_3 = 4 + 16 = 20$	$t_3 = 6 + 7 + 13 = 26$
	$b_4 = 4 + 36 = 40$	$t_4 = 26 + 17 + 23 = 66$
	$b_k = 2b_{k-1} = 2 \cdot 2 \cdot \dots \cdot 2b_2$	
	$= 2^{k-2} \cdot \frac{5}{2} \cdot 2 \cdot 2 = \frac{5}{2} 2^k$	

Number of Quadtree Cells to Store a Rectangle



k=2

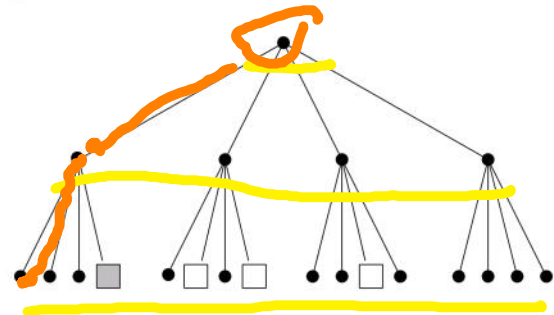
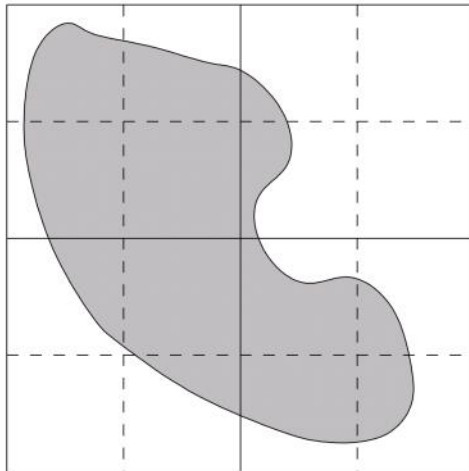


k=3

- uniformly ref. voxel-grid (level k): $(2^{d=2})^k = (2^k)^2 =: \mathcal{O}(N^2)$ cells
- quadtree-refined grid (level k): $\frac{15}{2} \cdot 2^k - 14 =: \mathcal{O}(N)$ cells
 \Rightarrow number of cells proportional to length of boundary ($N := 2^k$)

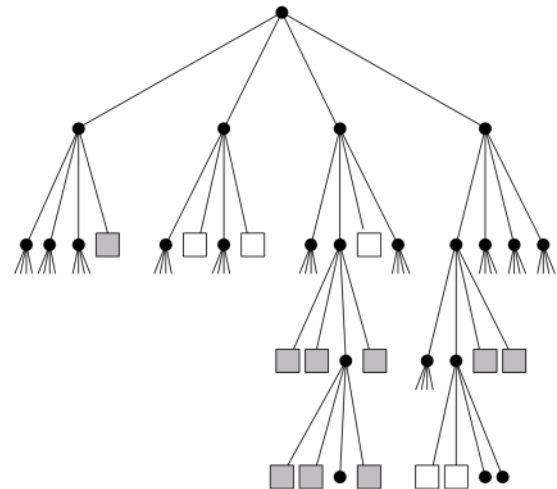
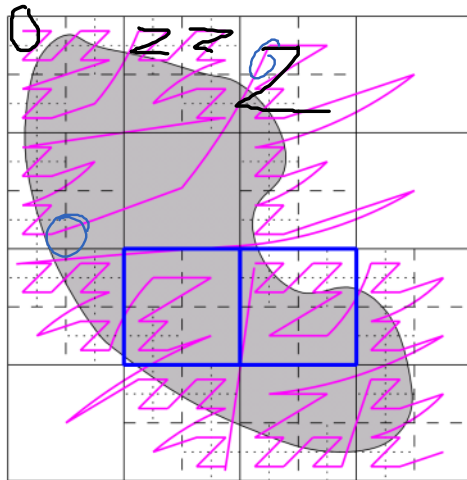
$$\begin{aligned}
 \ell_k &= \ell_{k-1} + 2b_{k-1} \\
 &= \ell_{k-2} + 2b_{k-2} + 2b_{k-1} \\
 &= \dots = \ell_2 + 2(b_{1,1} + \dots + b_2) \\
 &= \ell_2 + 2 \sum_{j=2}^{k-1} b_j \\
 &= \ell_2 + 2 \sum_{j=2}^{k-1} \left(\frac{5}{2} 2^j \right) \\
 &= \ell_2 + 5 \cdot \left(\sum_{j=2}^{k-1} 2^j \right) \\
 &= \ell_2 + 5 \left(\frac{2^k - 1}{2 - 1} - 2^0 - 2^1 \right) \\
 &= \ell_2 + 5 \cdot 2^k - 20 = 5 \cdot 2^k - 14
 \end{aligned}$$

Storing a Quadtree – Sequentialisation



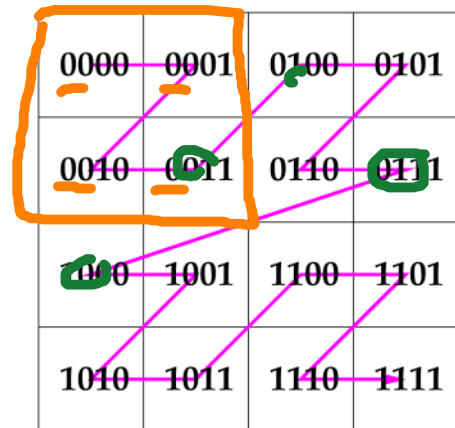
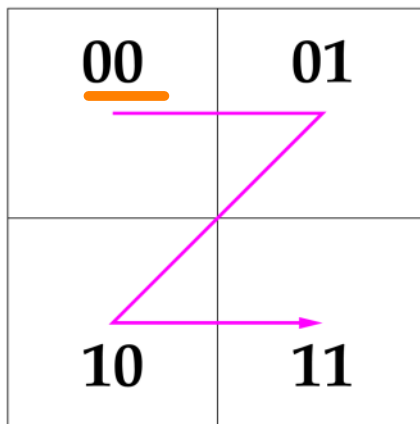
- sequentialise cell information according to **depth-first traversal**
- relative numbering of the child nodes determines sequential order

Storing a Quadtree – Sequentialisation



- sequentialise cell information according to **depth-first traversal**
- relative numbering of the child nodes determines sequential order
- here: leads to so-called **Morton order**

Morton Order ("Z curve")



Relation to bit arithmetics:

- odd digits: position in vertical direction
- even digits: position in horizontal direction

Morton Order and Cantor's Mapping

Georg Cantor (1877):

$$0.\underline{01}111001\dots \rightarrow \begin{pmatrix} 0.\underline{01}10\dots \\ 0.\underline{11}01\dots \end{pmatrix}$$

- **bijective** mapping $[0, 1] \rightarrow [0, 1]^2$
- proved identical cardinality of $[0, 1]$ and $[0, 1]^2$
- provoked the question: is there a **continuous** mapping? (i.e. a curve)

Similar: is there a contiguous order on the quadtree cells?

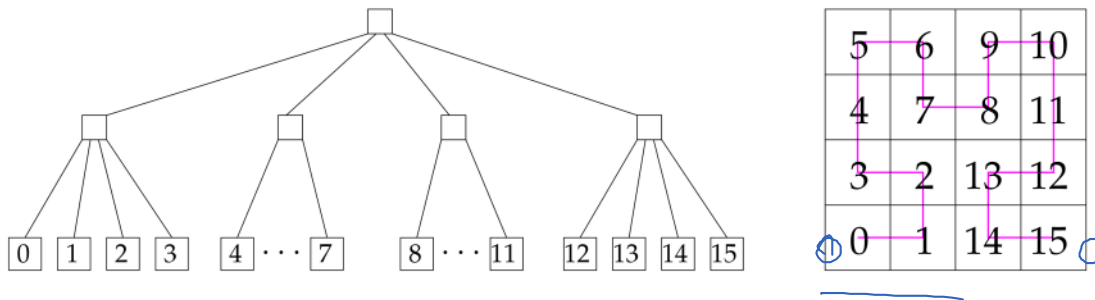
Preserving Neighbourship for a 2D Octree

Requirements:

- consider a simple 4×4 -grid
- uniformly refined
- subsequently numbered cells should be neighbours in 2D

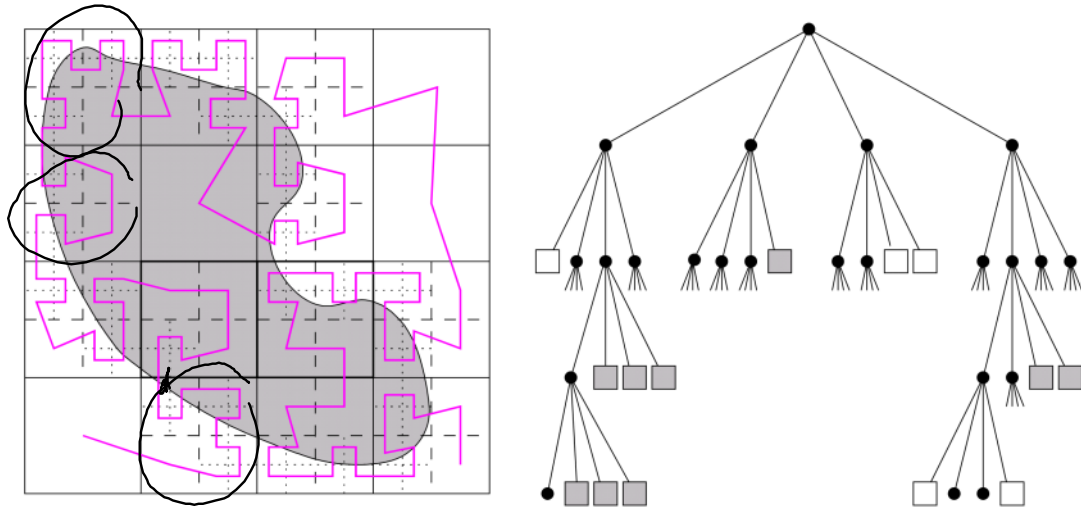
skaved edges

Leads to (more or less unique) numbering of children:



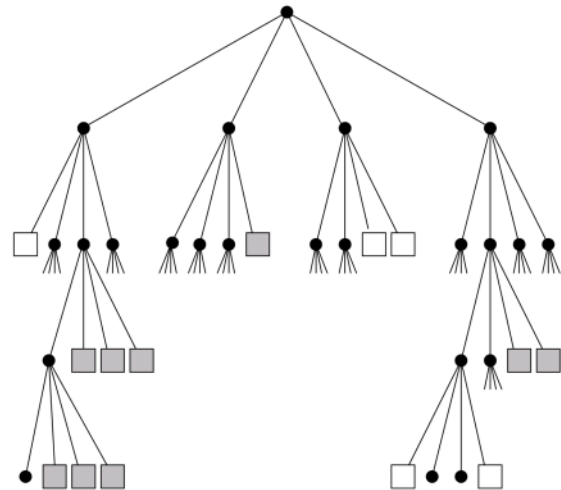
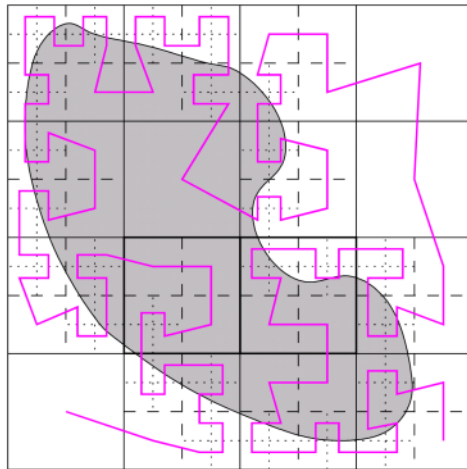
Hilbert

Preserving Neighbourship for a 2D Octree (2)



- adaptive refinement possible
- neighbours in sequential order remain neighbours in 2D

Preserving Neighbourship for a 2D Octree (2)



- adaptive refinement possible
- neighbours in sequential order remain neighbours in 2D
- here: similar to the concept of **Hilbert curves**

Open Questions

Algorithmics:

- How do we describe the sequential order algorithmically?
- What kind of operations are possible?
- Are there further “orderings” with the same or similar properties?

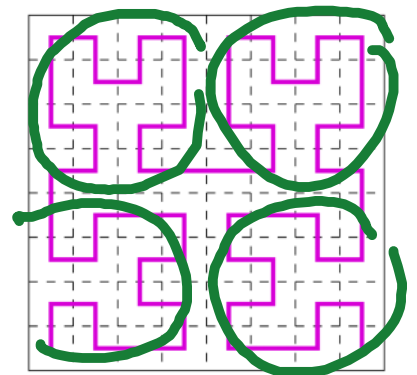
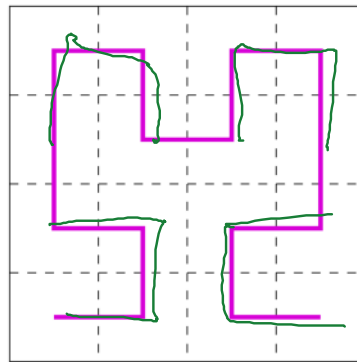
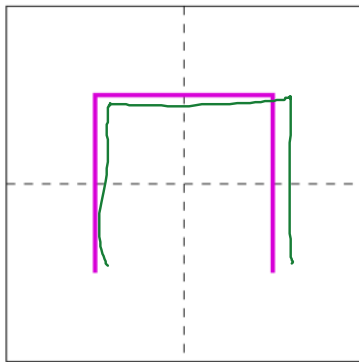
Applications:

- Can we quantify the “neighbour” property?
- In what applications can this property be useful?
- Which other properties and/or operations can be useful?

Part II

Hilbert Orders

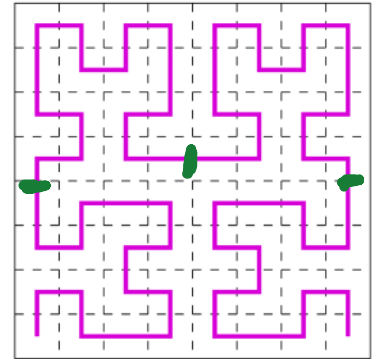
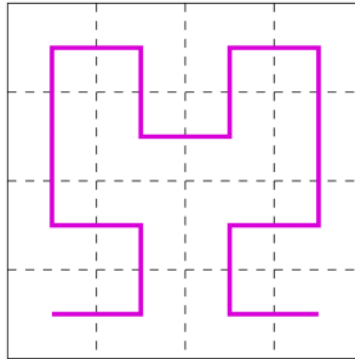
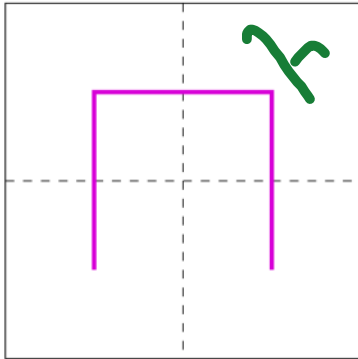
Construction of the Hilbert Order



Incremental construction of the Hilbert order:

- start with the basic pattern on 4 subsquares
- combine four numbering patterns to obtain a twice-as-large pattern
- proceed with further iterations

Construction of the Hilbert Order

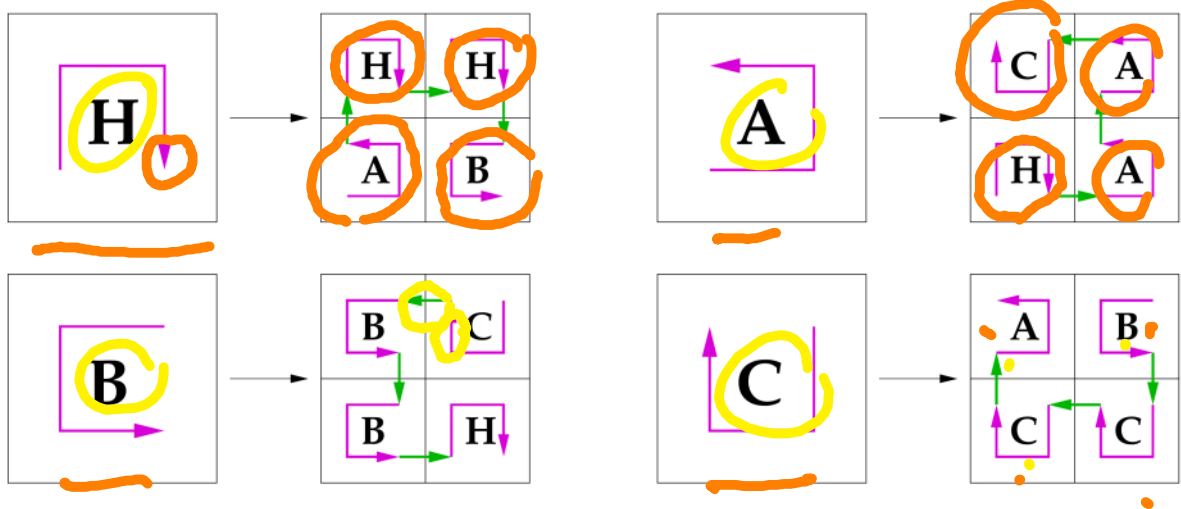


Recursive construction of the Hilbert order:

- start with the basic pattern on 4 subsquares
- for an existing grid and Hilbert order:
split each cell into 4 congruent subsquares
- order 4 subsquares following the rotated basic pattern,
such that a contiguous order is obtained

A Grammar for Describing the Hilbert Order

Examine pattern during the construction of the Hilbert order:



→ motivates a Grammar to generate the iterations

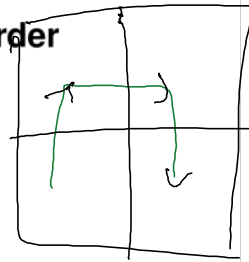
A Grammar for Describing the Hilbert Order

- Non-terminal symbols: $\{H, A, B, C\}$, start symbol H
- terminal characters: $\{\uparrow, \downarrow, \leftarrow, \rightarrow\}$
- productions:

$H \leftarrow A \uparrow H \rightarrow H \downarrow B$
 $A \leftarrow H \rightarrow A \uparrow A \leftarrow C$
 $B \leftarrow C \leftarrow B \downarrow B \rightarrow H$
 $C \leftarrow B \downarrow C \leftarrow C \uparrow A$

- replacement rule: in any word, all non-terminals have to be replaced at the same time
 → L-System (Lindenmayer)

⇒ the arrows describe the **iterations of the Hilbert curve** in "turtle graphics"



sub, pred, obj } sequence

Using the Grammar to Describe the Hilbert Curve

The grammar for the Hilbert order prepares the mathematical definition of the curve (and proof of continuity):

- there are only four basic patterns that occur (corresp. to the symbols $\{H, A, B, C\}$ of the grammar)
→ **closed recursive system!**
- two subsequent subsquares of the Hilbert-curve construction share a common edge(!)
→ follows from the fact that the move operators $\{\uparrow, \downarrow, \leftarrow, \rightarrow\}$ are sufficient to describe the operators
→ **contiguous order!** (leads to continuity of the curve)
- last but not least:
we have formalised the construction of the iterations (towards formal definition of a mapping)



Part III

Applications of Space-Filling Orders

Sequentialising Multi-dimensional Data

Examples of multi-dimensional data structures:

- Matrices
- Image data (images, tomographic data, movies, ...)
- discretisation meshes (to discretise mathematical models in physics/...; PDE, etc.)
- Coordinates (often used in connection with graphs)
- tables (also in data bases)
- in computational finance and financial mathematics: “baskets” of stocks/options/...

Sequentialising Multi-dimensional Data (2)

Typical algorithms and operations:

- traversal (update/processing of all data; simulation meshes, e.g.)
- matrix operations (linear algebra, etc.)
- sequentialisation (e.g. to store data on discs or in main memory)
- partitioning of data (for parallelisation or in divide-and-conquer algorithms)
- sorting of data (to simplify further operations)
- in general: nested loops

```
for i from 1 to n do  
    for j from 1 to m do        ...
```

Demands on Efficient Sequentialisation

Effective Sequentialisation:

- unique numbering \Rightarrow requires bijective mapping
- sequentialisation without “holes” (for data structures, e.g.)

Efficient Sequentialisation:

- preserve neighbourhood properties \Rightarrow data locality
- fast, simple index computation
- “smoothness”, stability vs. small changes
- dimensional symmetry (no fast or slow dimensions)
- “clustering” of data

Application Examples

- **range queries** in image and raster data bases
- **image browsing** and **image search** in image collections
- heuristical approaches for graph-based algorithms (nearest neighbour, traveling salesman)
- collision detection
- **parallelisation** of data
- efficient use of **cache memory** (in simulations, e.g.)

Also: everything that involves **Quadtrees/Octrees**:

- Searching (**collision detection**, **access to surface representations**, etc.)
- Fast access to level-of-detail infos (geodata, graphics, **games**, ...)
- Dynamically adaptive **meshes in scientific computing**
- many more ...