Construction of general hierarchical matrices for multi-dimensional problems

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Winterschool on Hierarchical Matrices

General cluster tree

Goal: Cluster tree $\mathcal{T}_\mathcal{I}$ for general index set $\mathcal{I}$.

Definition: A labeled tree $\mathcal{T}_\mathcal{I}$ is a cluster tree for $\mathcal{I}$ if

- its root is labeled by $\mathcal{I}$,
- if $t \in \mathcal{T}_\mathcal{I}$ has sons, its label is the union of its sons' labels

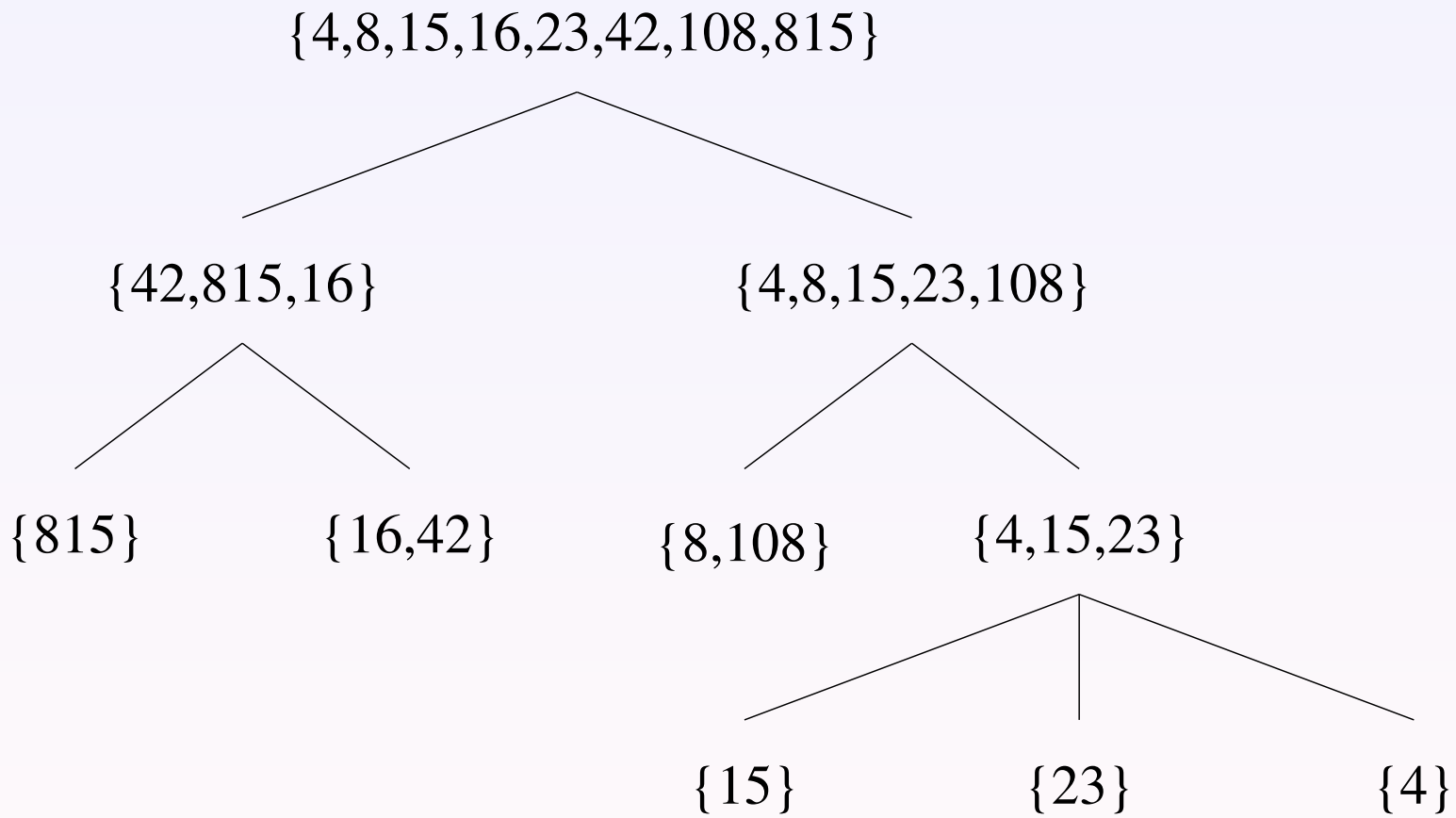
$$\hat{t} = \bigcup_{t' \in \operatorname{sons}(t)} \hat{t}',$$

- if $t \in \mathcal{T}_\mathcal{I}$ has sons, the labels of its sons are disjoint

$$t_1 \neq t_2 \Rightarrow \hat{t}_1 \cap \hat{t}_2 = \emptyset \qquad \text{for all } t_1, t_2 \in \operatorname{sons}(t).$$

Simple example

An acceptable cluster tree for the general index set $\mathcal{I} = \{4, 8, 15, 16, 23, 42, 108, 815\}$ could look as follows:



Properties

Levelwise disjoint: We have

$$t \neq s \Rightarrow \hat{t} \cap \hat{s} = \emptyset \qquad \text{for all } t, s \in \mathcal{T}_{\mathcal{I}} \text{ with } \operatorname{level}(t) = \operatorname{level}(s).$$

Inclusion: By a simple induction this implies

$$\hat{t} \cap \hat{s} \neq \emptyset \Rightarrow s \in \operatorname{sons}^*(t) \text{ or } t \in \operatorname{sons}^*(s) \qquad \text{for all } t, s \in \mathcal{T}_{\mathcal{I}}.$$

Partition: For all $i \in \mathcal{I}$, there is a $t \in \mathcal{T}_{\mathcal{I}}$ with $i \in \hat{t}$.

Leaf partition: Labels of the leaf clusters $\mathcal{L}_{\mathcal{I}}$ form disjoint partition of $\mathcal{I}$

$$\mathcal{I} = \dot{\bigcup_{t \in \mathcal{L}_{\mathcal{I}}}} \hat{t}.$$

How to construct?

In theory there are more than $n!$ possible cluster trees for an index set $\mathcal{I}$ with n elements.

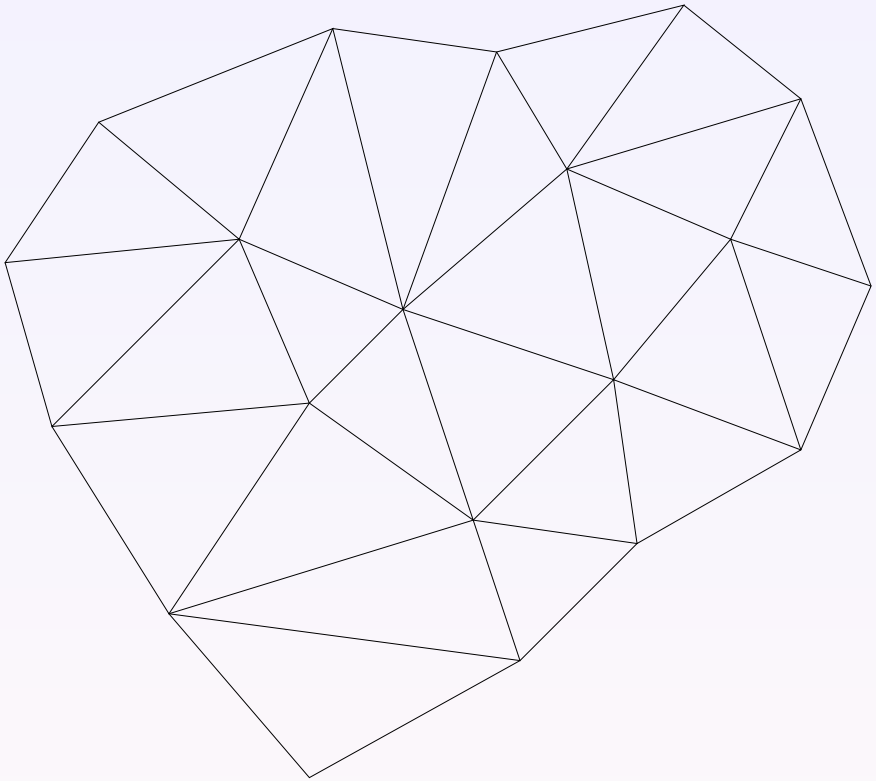
Goal: Construct cluster tree that is well-suited for low-rank approximations.

Approximation quality: Small diameters lead to good approximations.

Complexity: Small number of clusters and small number of levels lead to good efficiency.

General construction

Goal: Construct a good cluster tree for multi-dimensional meshes.



Consider an unstructured triangular mesh.

General construction

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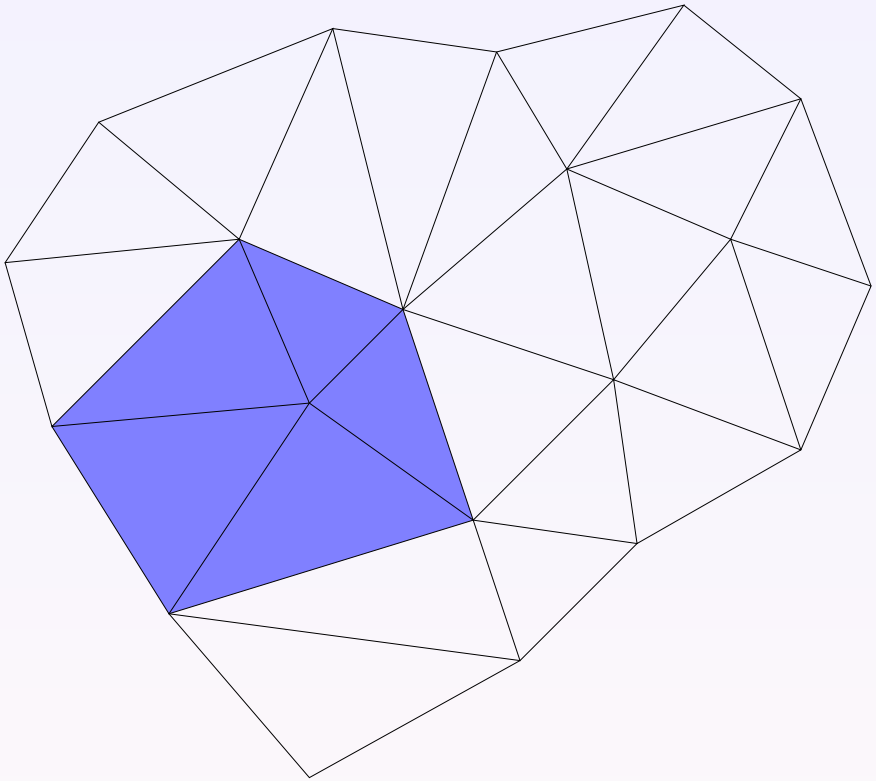

Nodal basis functions may have irregular polygonal supports.

Even overlapping supports are not uncommon.

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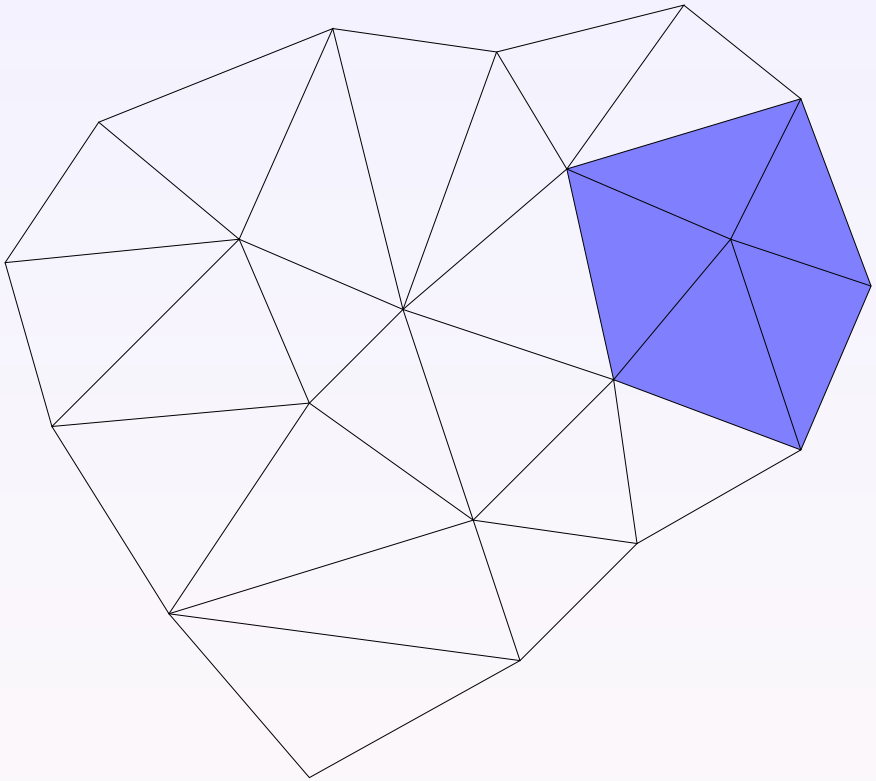

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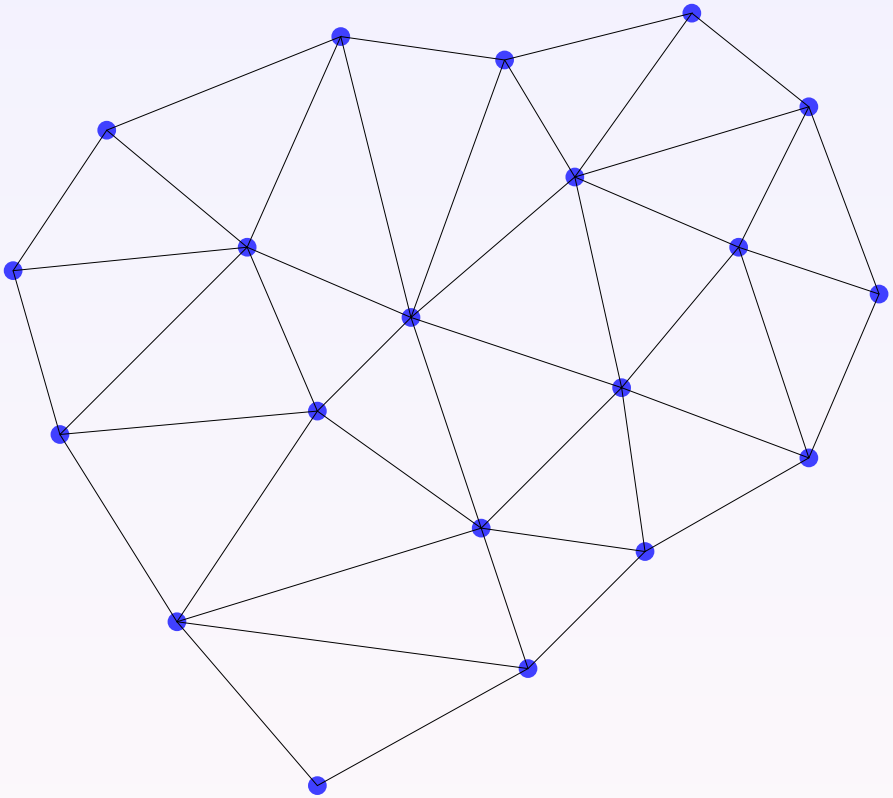

Idea: Replace each support by just one characteristic point.

No overlap, very simple geometric objects.

General construction

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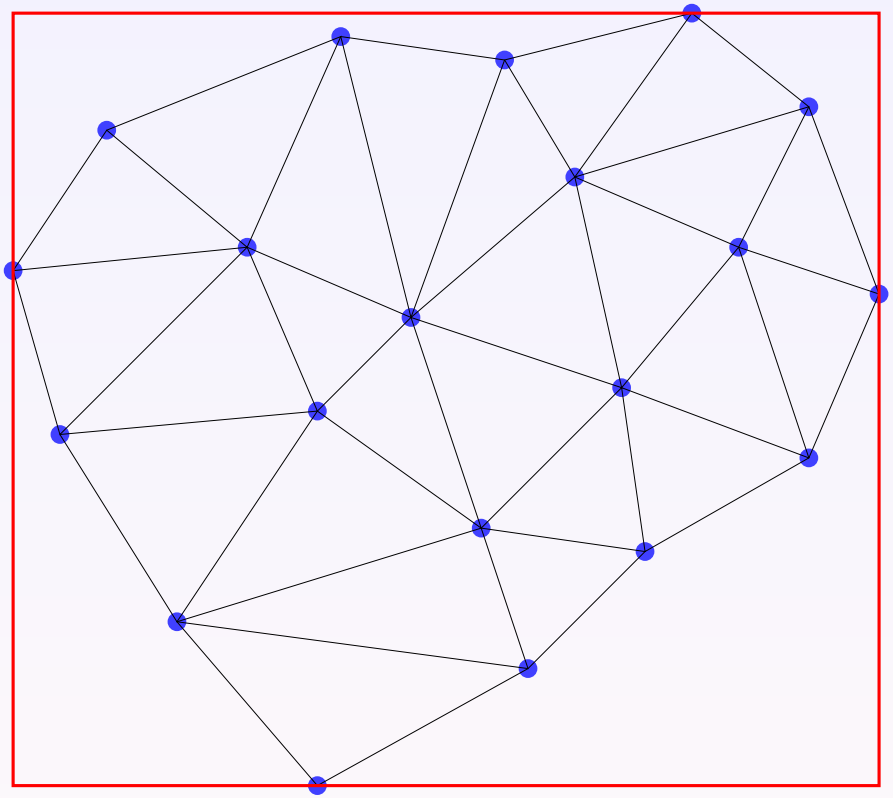

Find an axis-parallel box containing all points.

General construction

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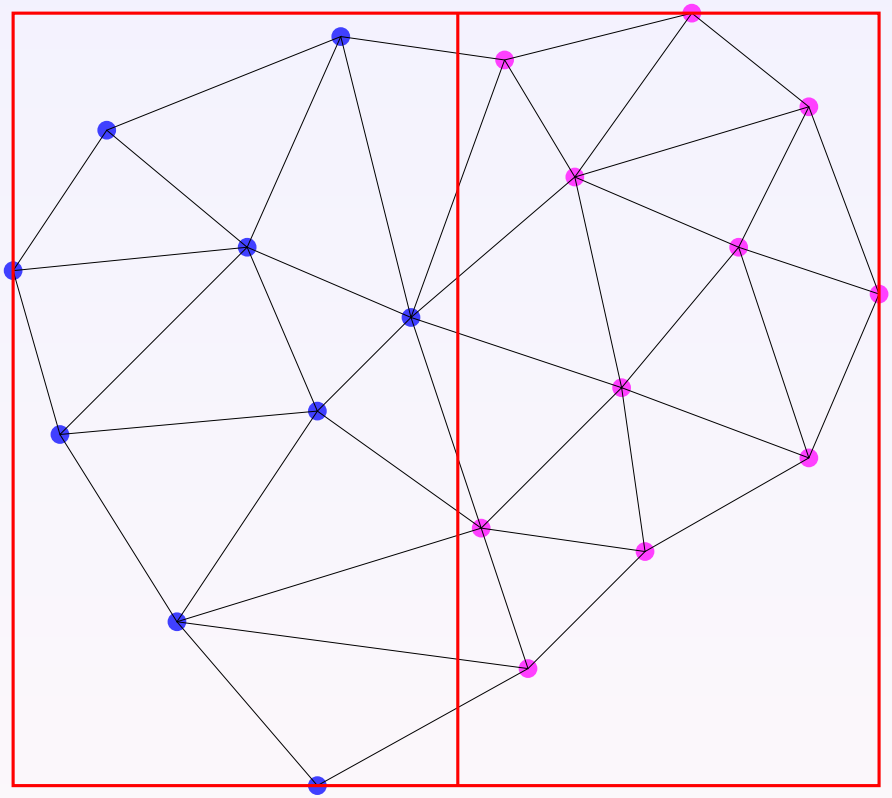
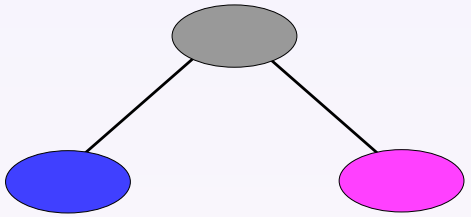


Splitting the box suggests a splitting of the point set.



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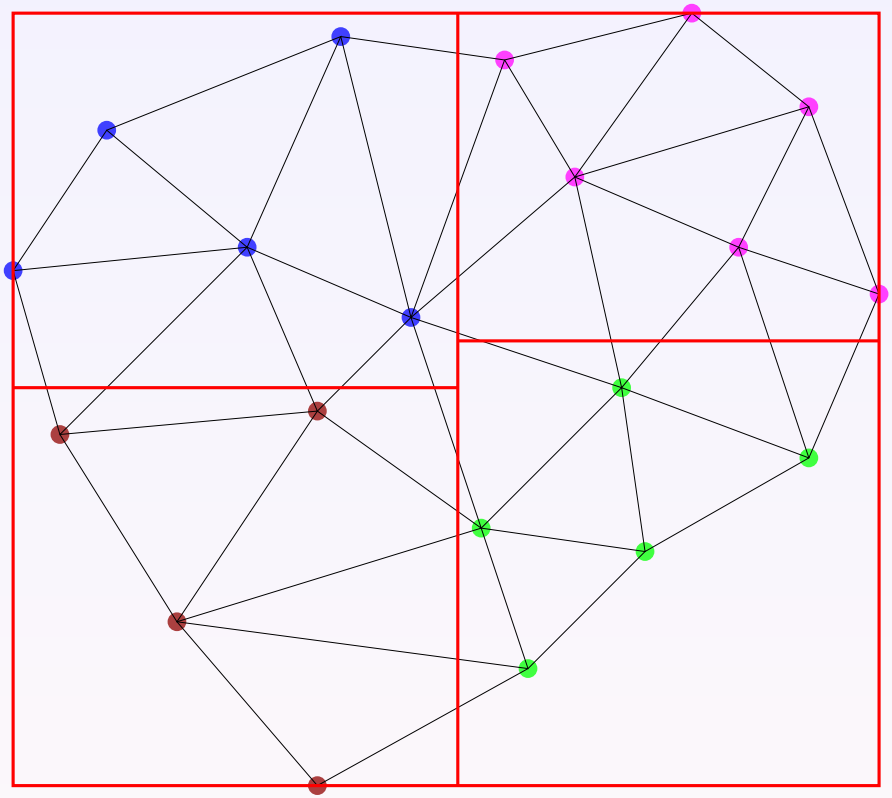
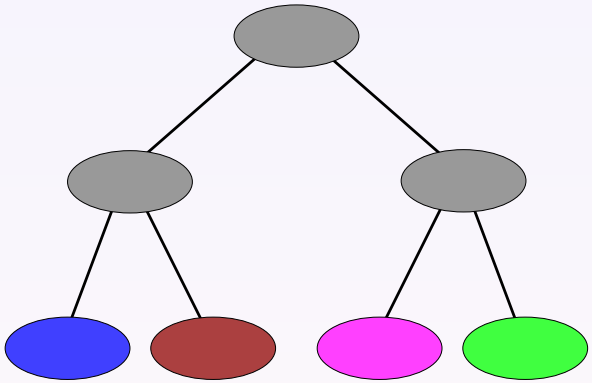


Repeatedly splitting yields a cluster tree.



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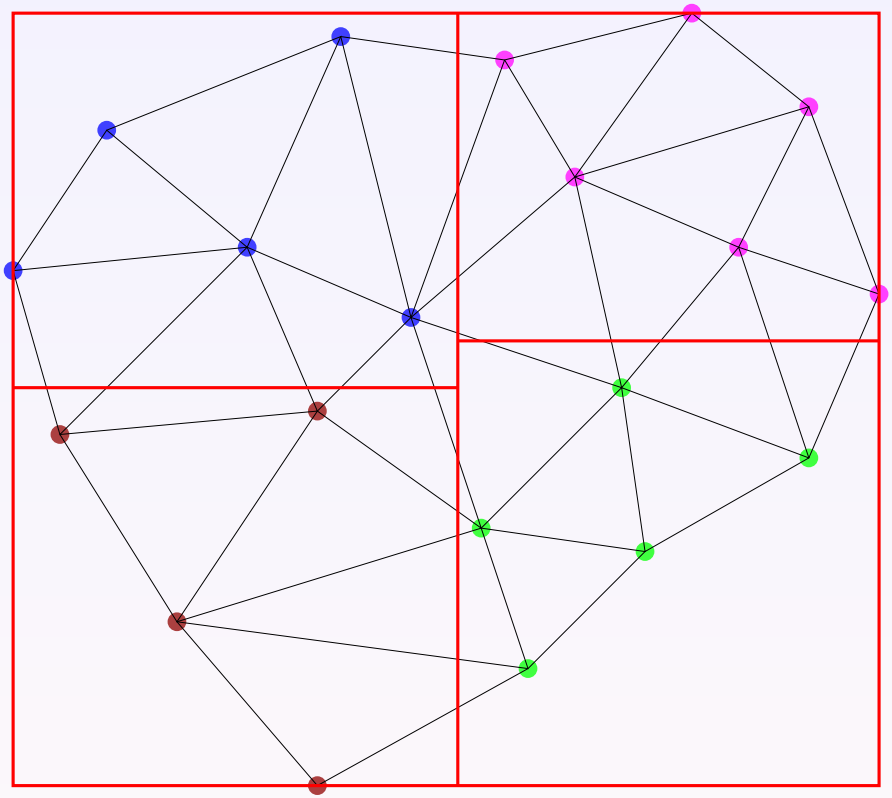

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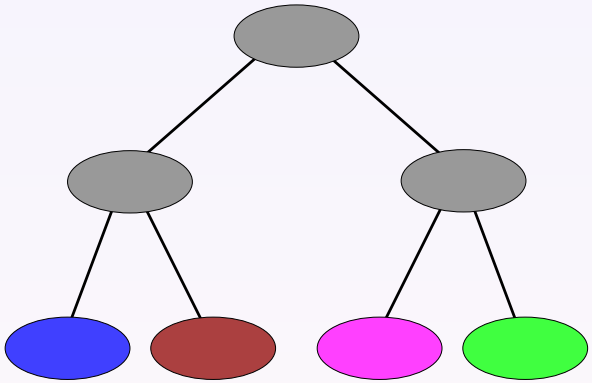
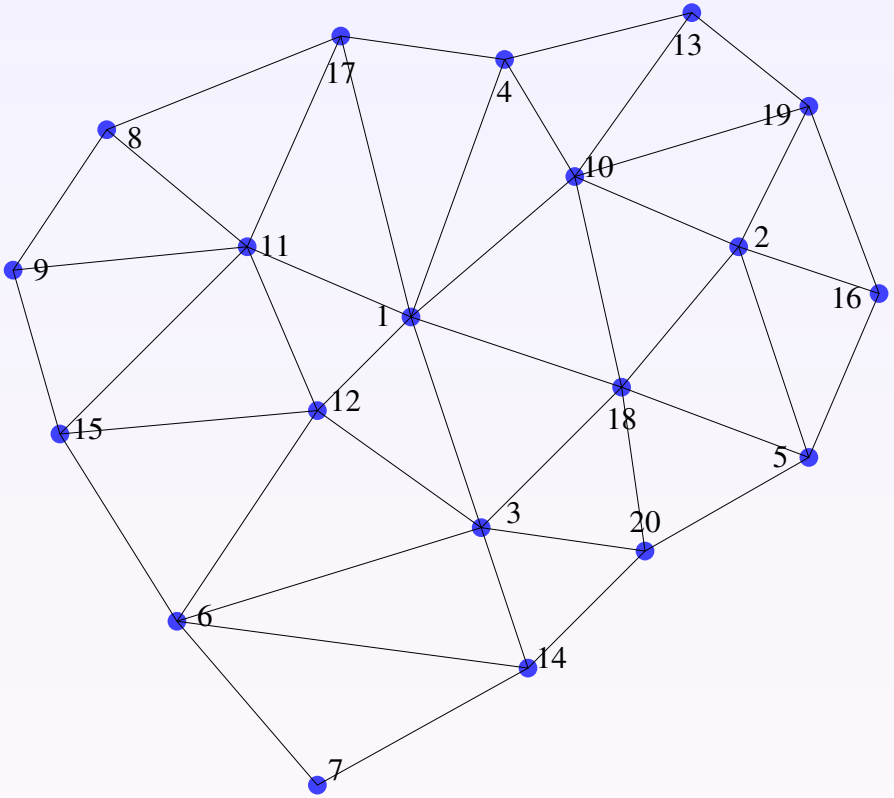


Result: Simple general algorithm for constructing cluster trees.

Splitting step

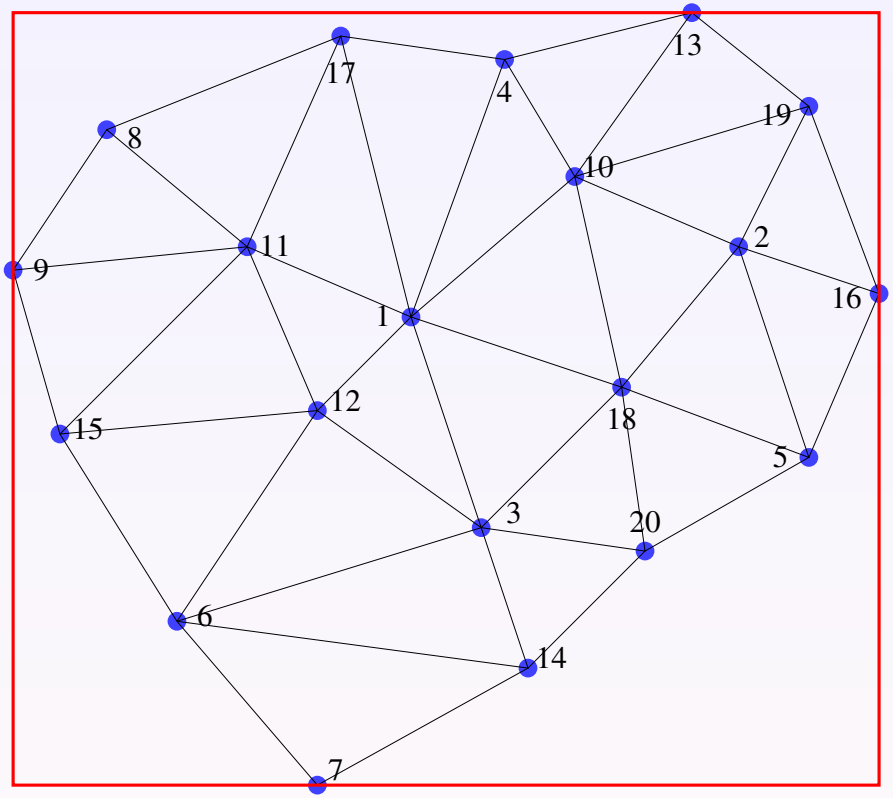
Basic operation: Split one cluster into two sons with consecutively numbered indices.



Consider characteristic points.

Splitting step

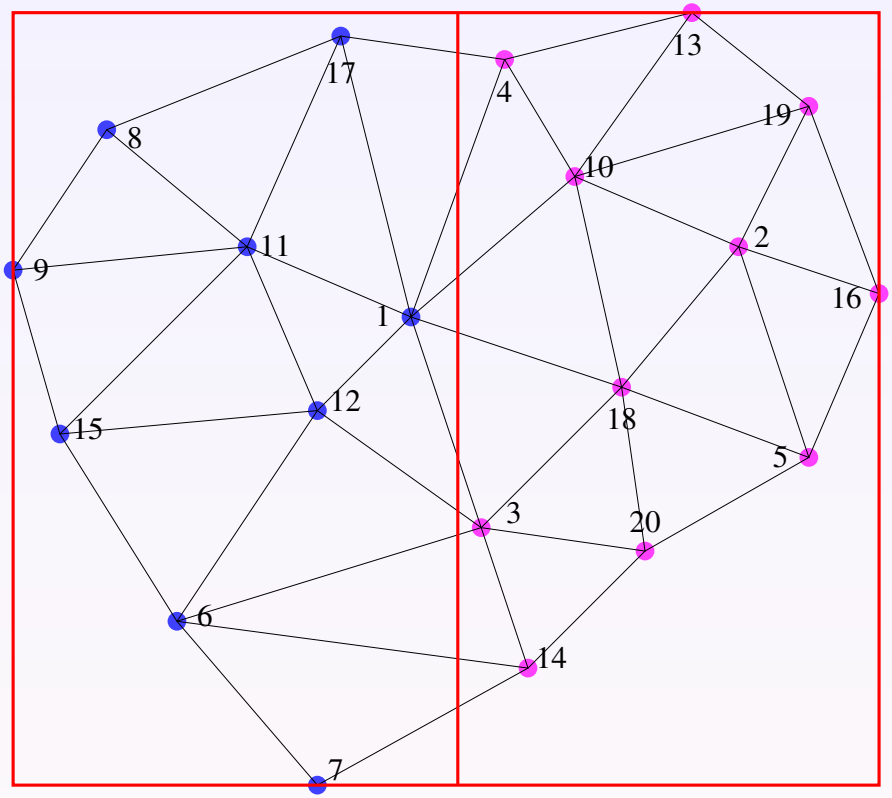
Basic operation: Split one cluster into two sons with consecutively numbered indices.



Find a bounding box.

Splitting step

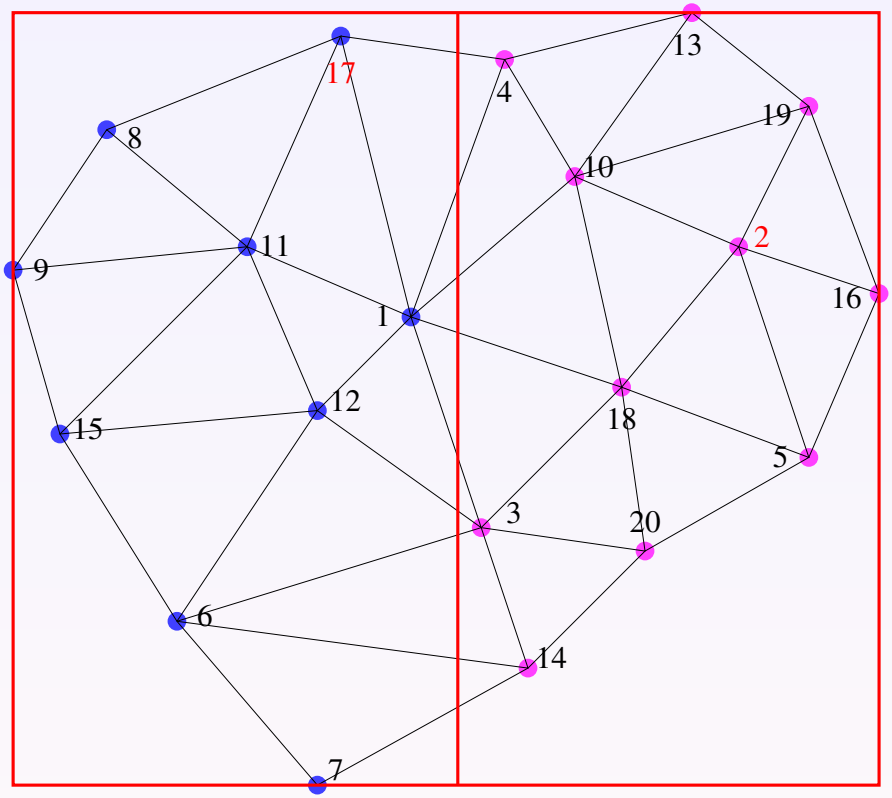
Basic operation: Split one cluster into two sons with consecutively numbered indices.



Split the bounding box.

Splitting step

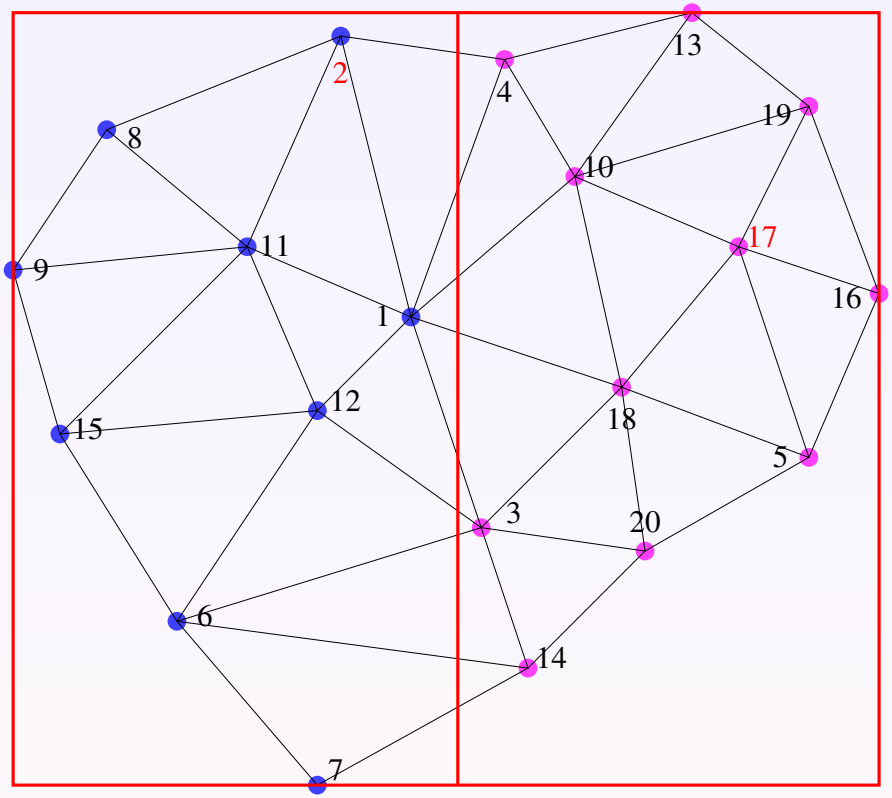
Basic operation: Split one cluster into two sons with consecutively numbered indices.



No consecutive ordering.

Splitting step

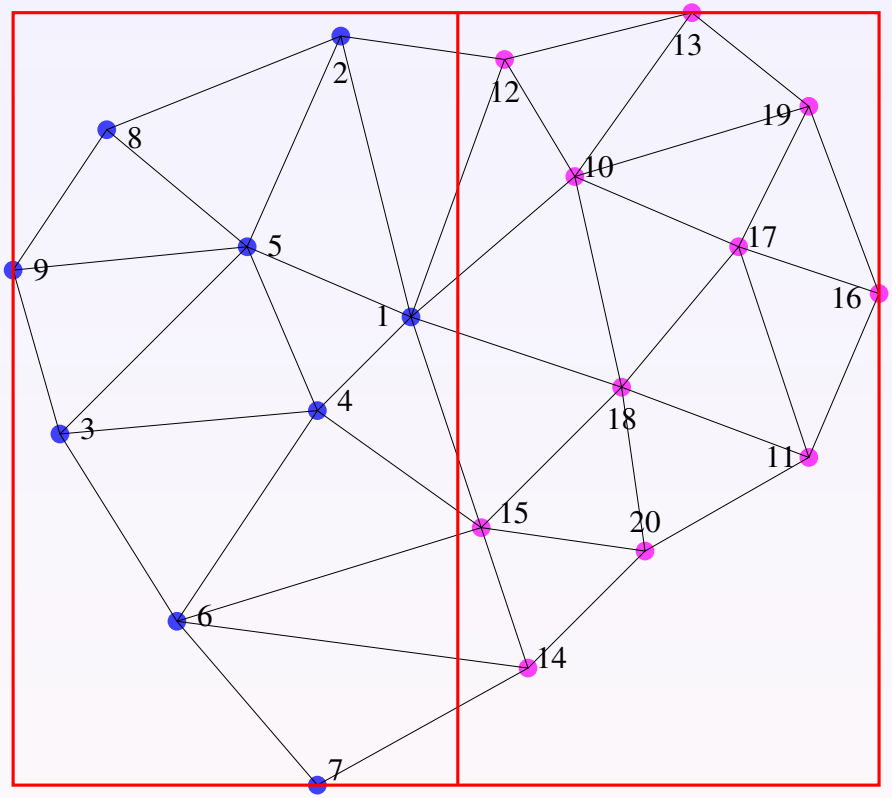
Basic operation: Split one cluster into two sons with consecutively numbered indices.



Fix ordering by exchanging numbers.

Splitting step

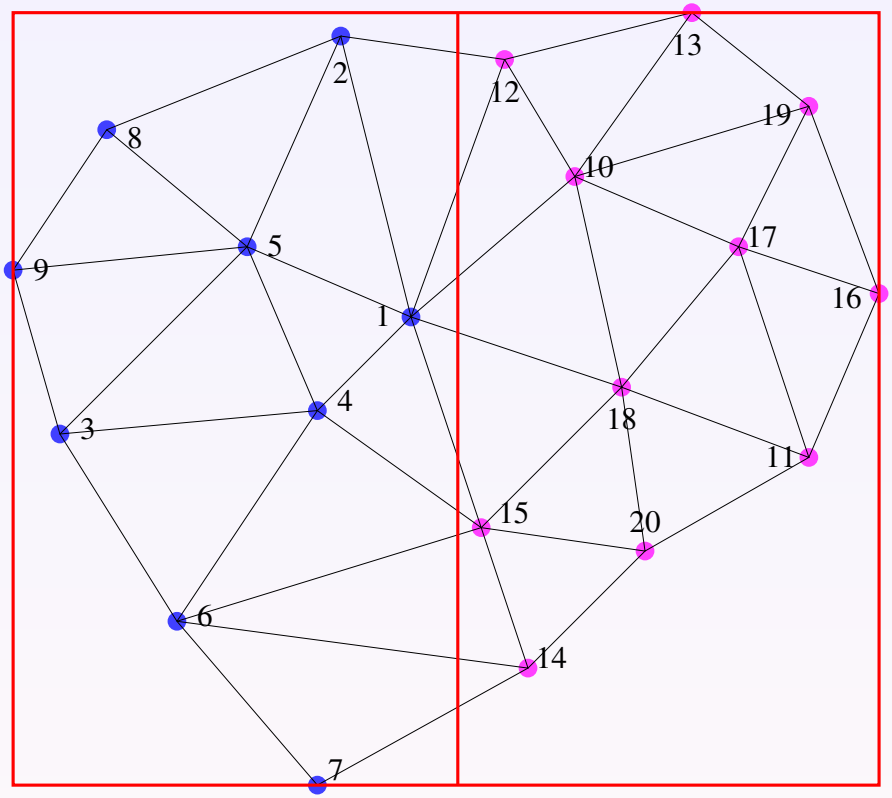
Basic operation: Split one cluster into two sons with consecutively numbered indices.



Keep exchanging until consecutive.

Splitting step

Basic operation: Split one cluster into two sons with consecutively numbered indices.



Keep exchanging until consecutive.

Result: Simple recursive algorithm for finding both a suitable cluster tree and a matching permutation of the indices.

Alternatives

Regular clustering:

- Cycle through coordinate directions instead of choosing direction of maximal extend.
- Do not shrink box adaptively.
- Guarantees geometrically similar boxes every d steps.

Cardinality-balanced clustering:

- Split into two sons of approximately equal cardinality.
- Guarantees balanced cluster tree.

Domain decomposition clustering:

- Split into two sons and their interface.
- Useful for handling sparse matrices, e.g., FEM.

General block cluster tree

Goal: Block cluster tree for general cluster trees $\mathcal{T}_\mathcal{I}$ and $\mathcal{T}_\mathcal{J}$.

Definition: A labeled tree $\mathcal{T}_{\mathcal{I}\times\mathcal{J}}$ is a block cluster tree for $\mathcal{T}_\mathcal{I}$ and $\mathcal{T}_\mathcal{J}$ if

- each node $b \in \mathcal{T}_{\mathcal{I}\times\mathcal{J}}$ is a pair $b = (t, s)$ of clusters $t \in \mathcal{T}_\mathcal{I}$, $s \in \mathcal{T}_\mathcal{J}$,
- the root of $\mathcal{T}_{\mathcal{I}\times\mathcal{J}}$ is the pair of the roots of $\mathcal{T}_\mathcal{I}$ and $\mathcal{T}_\mathcal{J}$,
- the label of $b = (t, s) \in \mathcal{T}_{\mathcal{I}\times\mathcal{J}}$ is the Cartesian product of the labels of t and s, i.e., $\hat{b} = \hat{t} \times \hat{s}$,
- if $b = (t, s) \in \mathcal{T}_{\mathcal{I}\times\mathcal{J}}$ has sons, we have

$$\operatorname{sons}(b) = \begin{cases} \{(t', s) \;:\; t' \in \operatorname{sons}(t)\} & \text{if } \operatorname{sons}(s) = \emptyset, \\ \{(t, s') \;:\; s' \in \operatorname{sons}(s)\} & \text{if } \operatorname{sons}(t) = \emptyset, \\ \{(t', s') \;:\; t' \in \operatorname{sons}(t), s' \in \operatorname{sons}(s)\} & \text{otherwise.} \end{cases}$$

Observation: A block cluster tree $\mathcal{T}_{\mathcal{I}\times\mathcal{J}}$ for $\mathcal{T}_\mathcal{I}$ and $\mathcal{T}_\mathcal{J}$ is a special cluster tree for the index set $\mathcal{I} \times \mathcal{J}$.

How to construct?

Observation: Since $\mathcal{T}_{\mathcal{I}\times\mathcal{J}}$ is a special cluster tree for $\mathcal{I}\times\mathcal{J}$, the labels of its leaves $\mathcal{L}_{\mathcal{I}\times\mathcal{J}}$ correspond to a disjoint partition of matrix entries

$$\{\hat{t}\times\hat{s} \;:\; b=(t,s)\in\mathcal{L}_{\mathcal{I}\times\mathcal{J}}\}.$$

This partition is used to define the hierarchical matrix.

Goals: Since we have to approximate each submatrix, we require

- that the number of leaves is small and
- that inadmissible leaves correspond to small index sets.

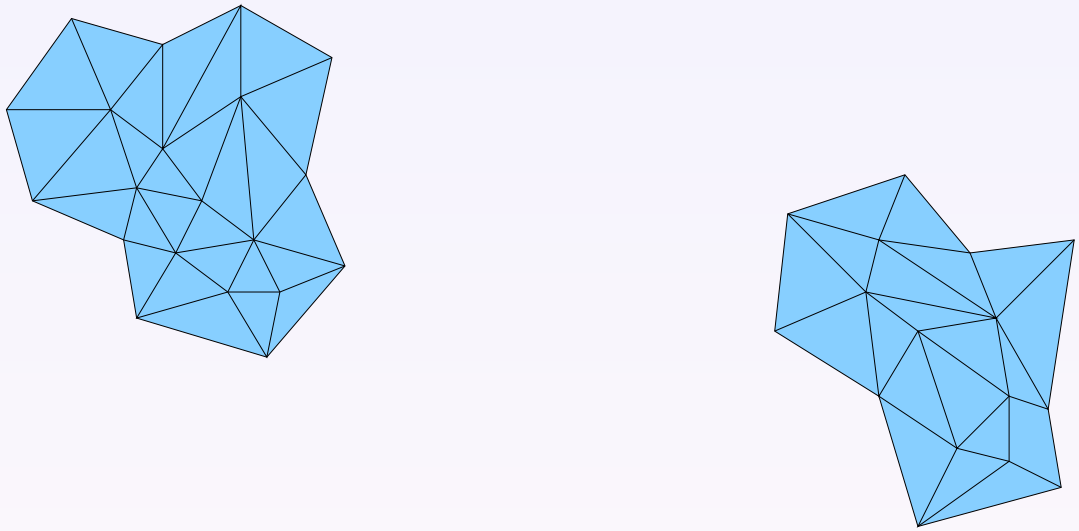
Algorithm: If $(t,s)\in\mathcal{T}_{\mathcal{I}\times\mathcal{J}}$ is admissible, make it a leaf.
Otherwise construct its sons and proceed by recursion.

Admissibility condition

Goal: Construct a good block partition for the admissibility condition

$$\operatorname{diam}(\tau) \leq 2 \operatorname{dist}(\tau, \sigma).$$

Problem: How to check the condition efficiently?



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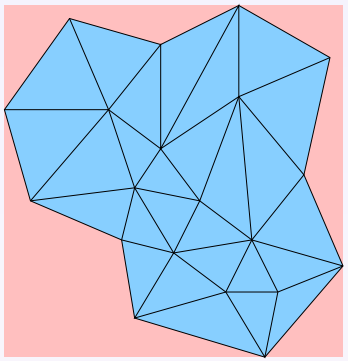

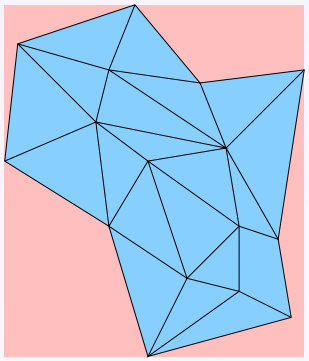

Idea: Replace subdomains τ, σ by larger domains B_t, B_s that can be handled efficiently, e.g., axis-parallel bounding boxes.

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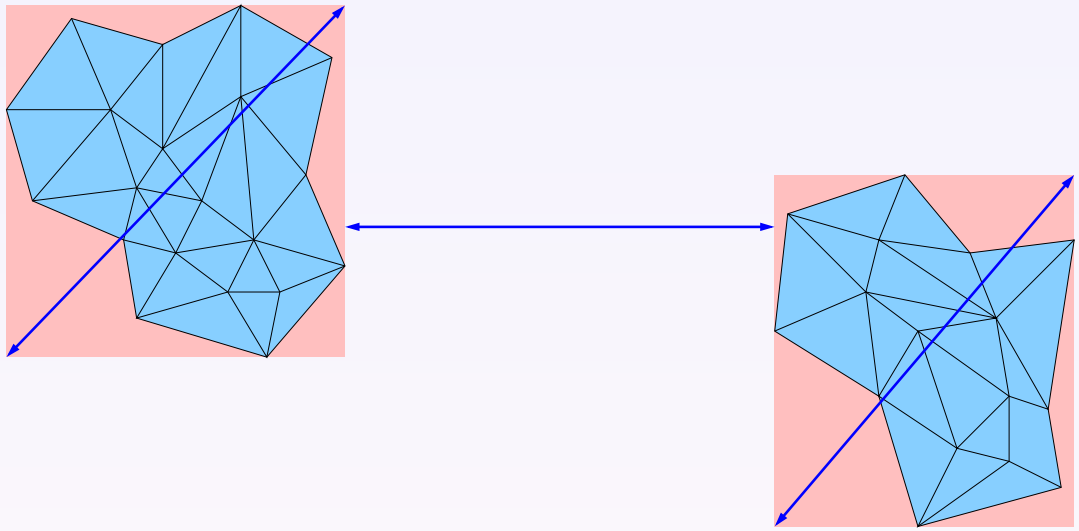

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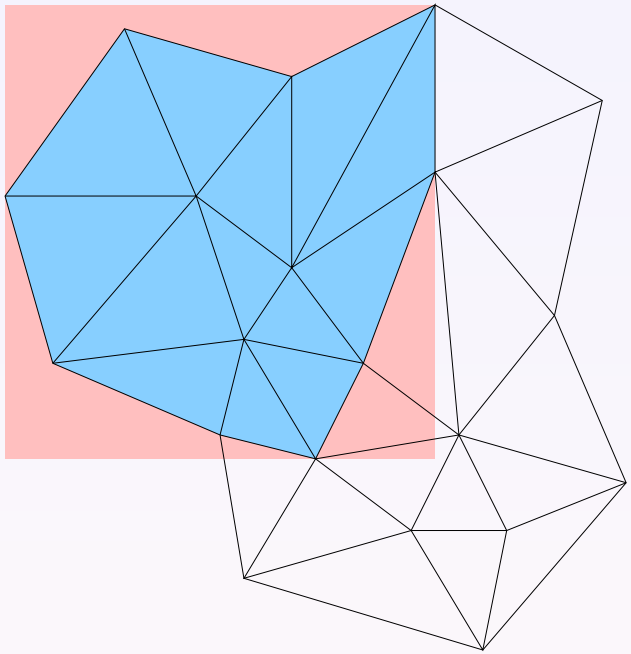
$$\operatorname{diam}(B_t) \leq 2 \operatorname{dist}(B_t, B_s) \qquad \Longrightarrow \qquad \operatorname{diam}(\tau) \leq 2 \operatorname{dist}(\tau, \sigma)$$

Construction of bounding boxes

Goal: Find minimal box B_t with $\tau \subseteq B_t$.

Recursion: Construct boxes for sons $t' \in \operatorname{sons}(t)$ of t and merge them.



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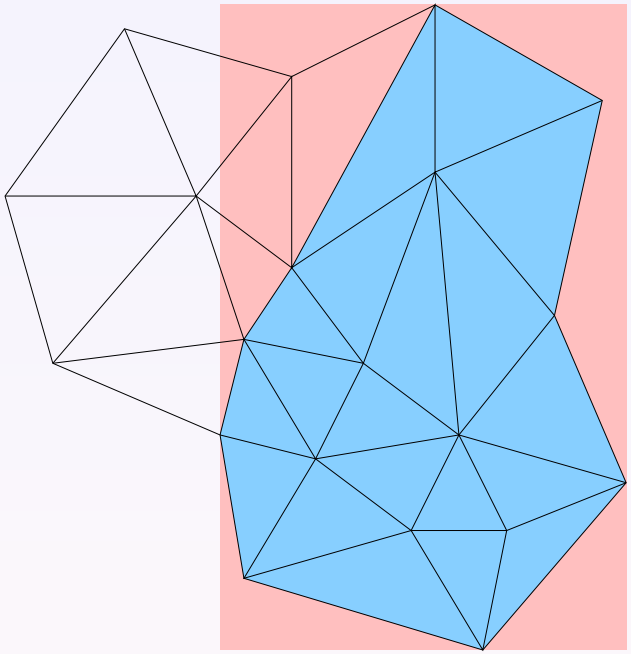

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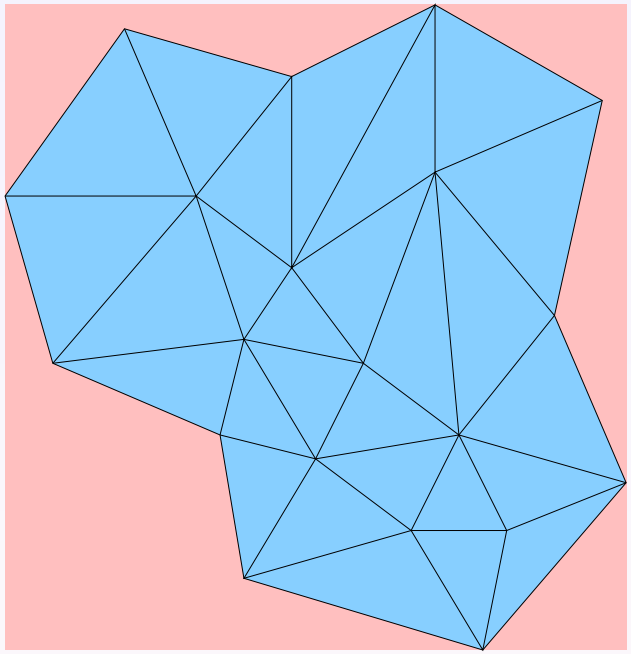

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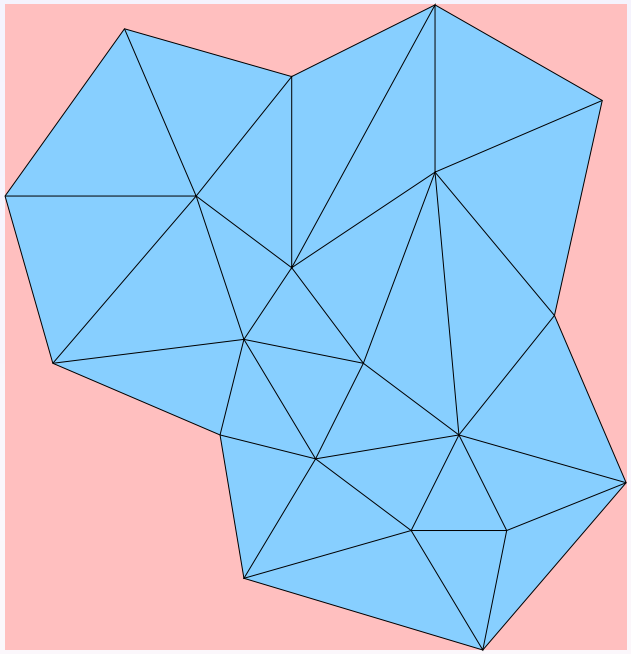
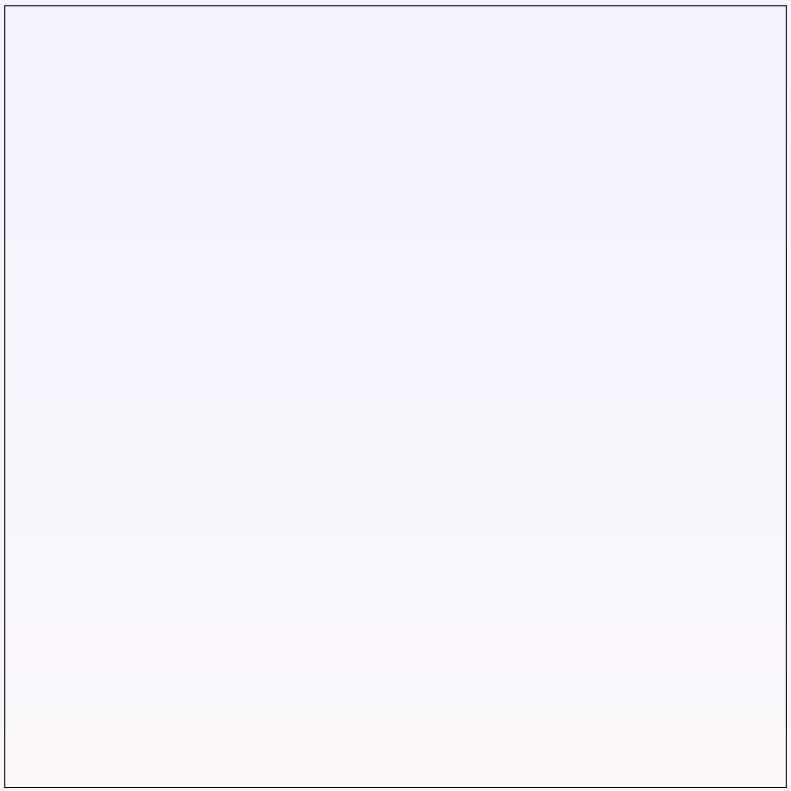


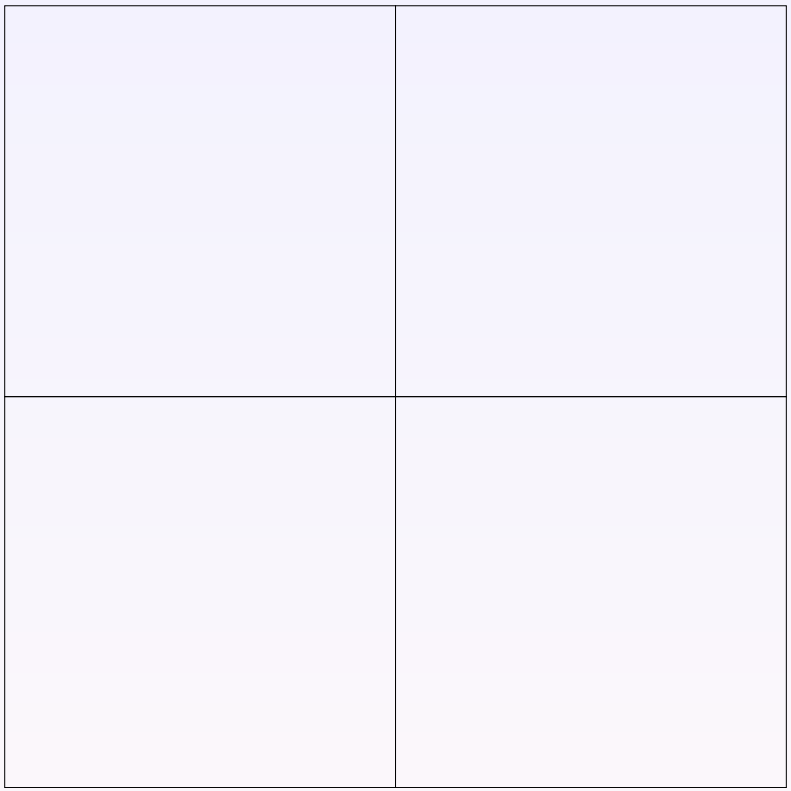
Result: Only $\mathcal{O}(n)$ operations for all bounding boxes.

Matrix structure



Start with the entire matrix.

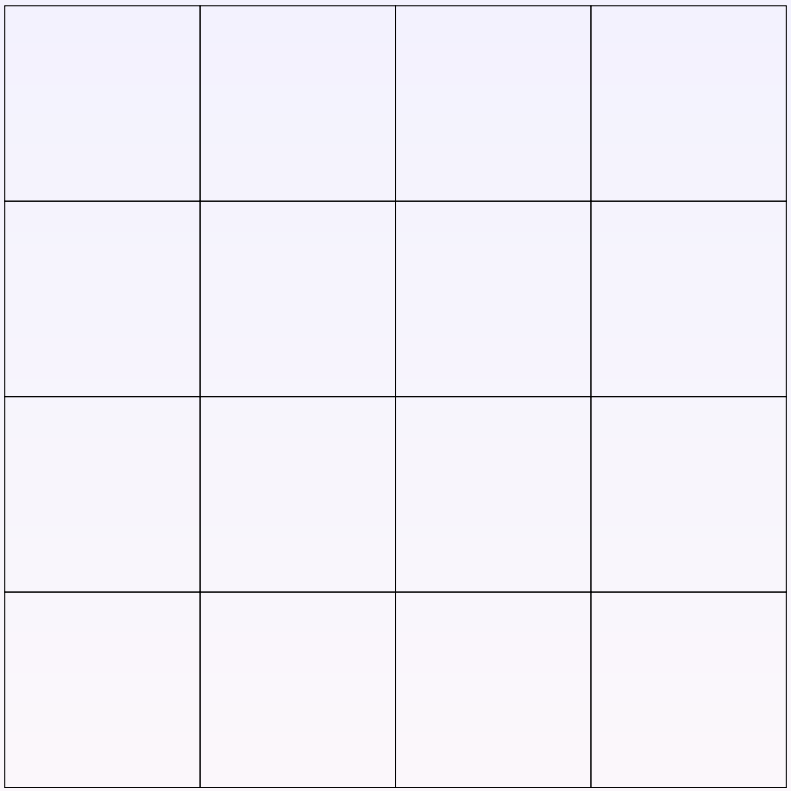
Matrix structure



Start with the entire matrix.

Subdivide according to the cluster tree.

Matrix structure



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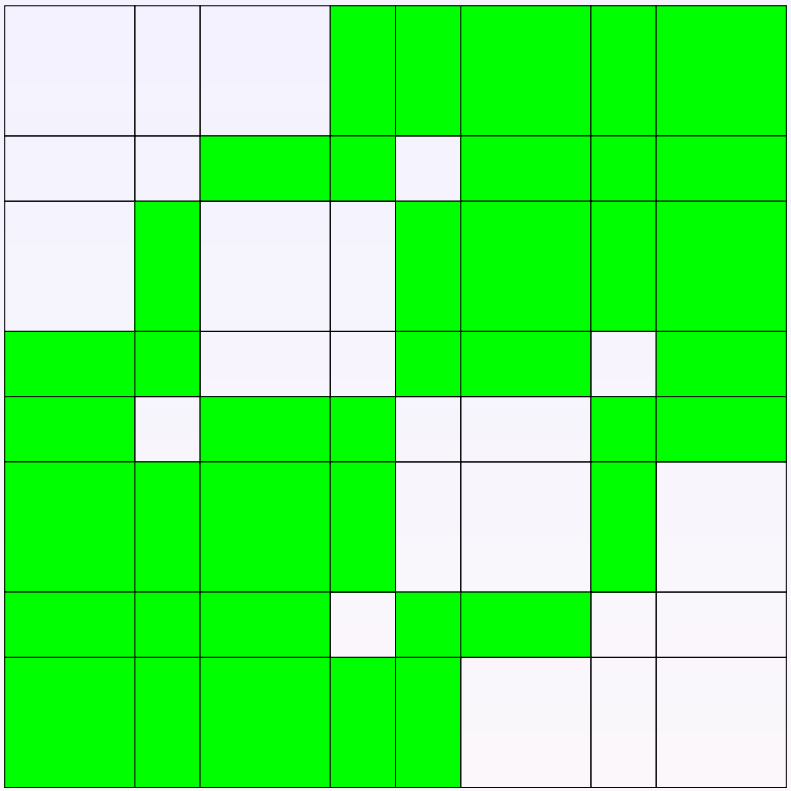
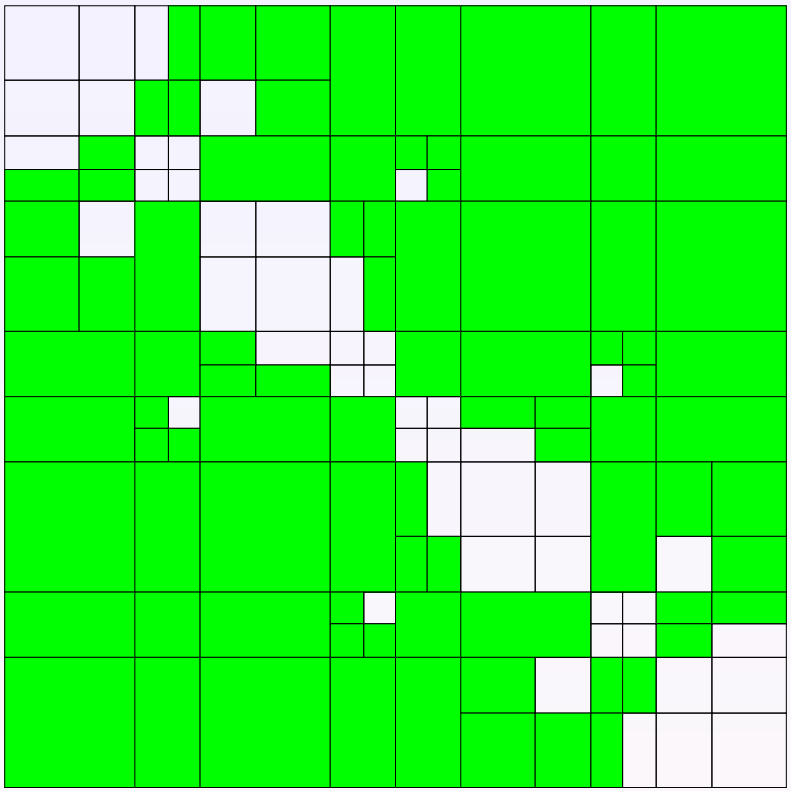


Start with the entire matrix.

Subdivide according to the cluster tree.

Mark admissible blocks and subdivide the others.

Matrix structure



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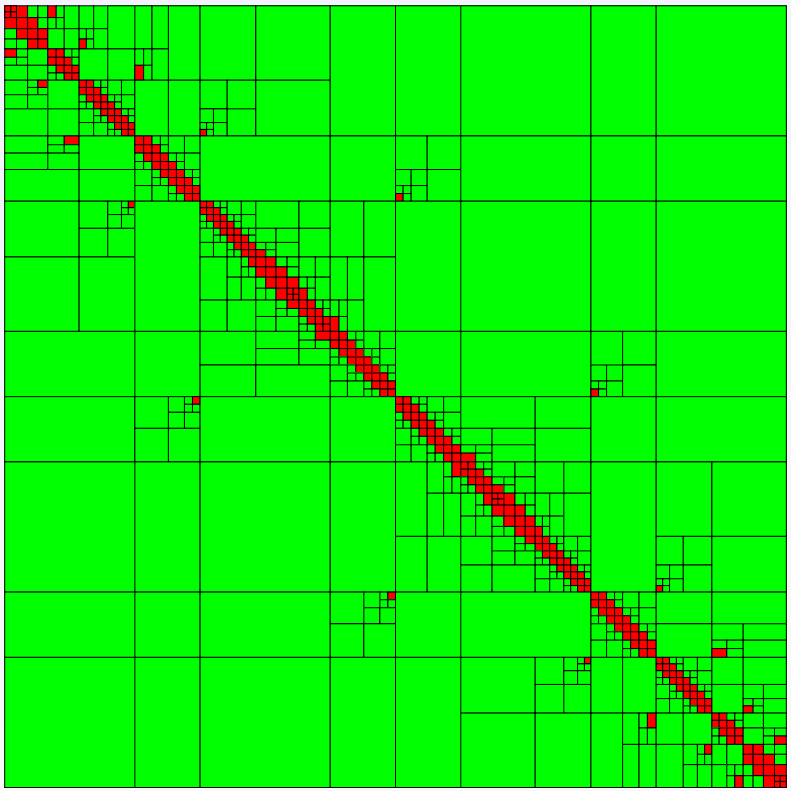


Start with the entire matrix.

Subdivide according to the cluster tree.

Mark admissible blocks and subdivide the others.

Result: $\mathcal{H}$-matrix structure.

Data structures for a cluster tree

Cluster: Consecutive sequence of indices, organized in a tree.

```
struct _cluster {
  int start;
  int size;
  double *bmin, *bmax;
  int sons;
  pcluster *son;
};
```

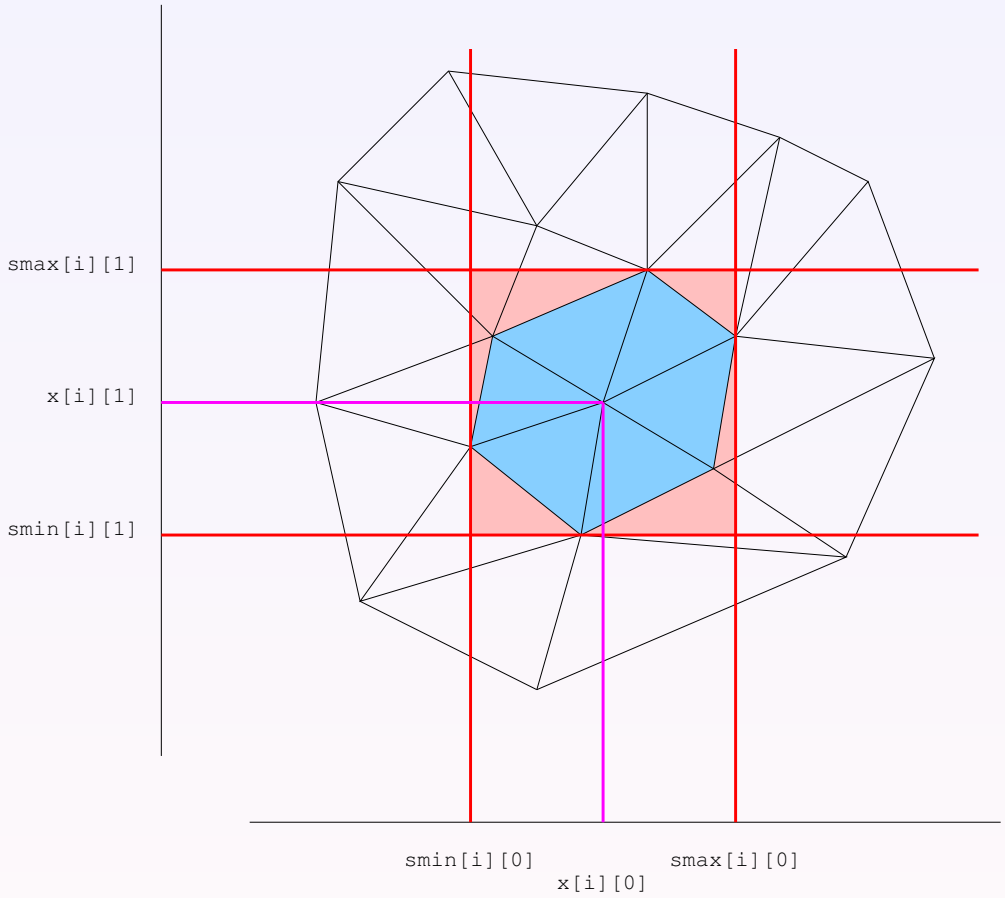
Cluster tree: Index permutation and pointer to root cluster.

```
struct _clustertree {
  int ndof;
  int nidx;
  int *dof2idx;
  int *idx2dof;
  pcluster root;
};
```

Data structure representing the geometry

Cluster factory: Contains coordinates of characteristic points and bounding boxes for supports of single basis functions.

```
struct _clusterfactory {
  double **x;
  double **smin;
  double **smax;
  int n;
  int d;
};
```



Splitting in HLib

```
static pcluster
split_geometrically(pclusterfactory factory, int *index,
                    int start, int sz, int leafsize)
{
  /* ... some initialization ... */
  if(sz <= leafsize)                        /* Stop if small enough */
    this = new_cluster(start, sz, 0);
  else {
    for(j=0; j<d; j++) {                    /* Determine bounding box */
      vmin[j] = vmax[j] = x[index[0]][j];
      for(i=1; i<sz; i++)
        if(x[index[i]][j] < vmin[j])       vmin[j] = x[index[i]][j];
        else if(vmax[j] < x[index[i]][j]) vmax[j] = x[index[i]][j];
    }
    jmax = 0; vdiff = vmax[0] - vmin[0]; /* Find maximal extent */
    for(j=1; j<d; j++)
      if(vmax[j] - vmin[j] > vdiff) { jmax = j; vdiff = vmax[j] - vmin[j]; }
    l = 0; r = sz-1;                        /* Rearrange array */
    vmid = 0.5 * (vmax[jmax] + vmin[jmax]);
    while(l < r) {
      while(l < sz && x[index[l]][jmax] <= vmid) l++;
      while(r >= 0 && x[index[r]][jmax] >  vmid) r--;
      if(l < r) { h = index[l]; index[l] = index[r]; index[r] = h; }
    }
    this = new_cluster(start, sz, 2);    /* Recursion */
    this->son[0] = split_geometrically(factory, index,   start,   l,    leafsize);
    this->son[1] = split_geometrically(factory, index+l, start+l, sz-l, leafsize);
  }

  return this;
}
```

Bounding boxes in HLib

```
static void
find_boundingbox(pcluster tau, pcclusterfactory factory)
{
  /* ... some initialization ... */

  if(sons > 0) {
    for(i=0; i<sons; i++)
     find_boundingbox(tau->son[i], factory);

    for(j=0; j<d; j++) {
      bmin[j] = son[0]->bmin; bmax[j] = son[0]->bmax;
    }
    for(i=1; i<sons; i++)
      for(j=0; j<d; j++) {
        bmin[j] = dmin(bmin[j], son[i]->bmin[j]);
        bmax[j] = dmax(bmax[j], son[i]->bmax[j]);
      }
  }
  else {
    for(j=0; j<d; j++) {
      bmin[j] = smin[index[0]]; bmax[j] = smax[index[0]];
    }
    for(i=1; i<size; i++)
      for(j=0; j<d; j++) {
        bmin[j] = dmin(bmin[j], smin[index[i]][j]);
        bmax[j] = dmax(bmax[j], smax[index[i]][j]);
      }
  }
}
```

Data structure for a block cluster tree

Block cluster: Contains row and column cluster, admissibility flags and pointers to sons.

```
typedef struct {
  unsigned weakadm : 1;
  unsigned minadm : 1;
  unsigned maxadm : 1;
} BlockType;

struct _blockcluster {
  pccluster row;
  pccluster col;
  BlockType type;
  pblockcluster *son;
  int block_rows;
  int block_cols;
};
```

Block tree in HLib

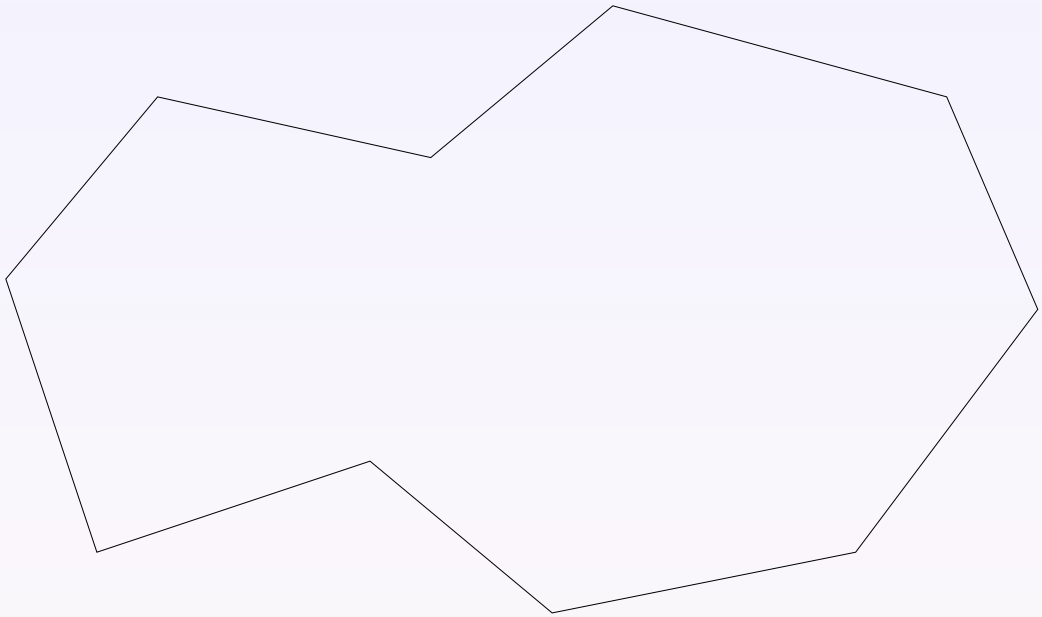
```
pblockcluster
build_blockcluster(pccluster row, pccluster col, double eta)
{
  dist = distance_cluster(row, col);
  diam_row = diameter_cluster(row);
  diam_col = diameter_cluster(col);
  type.maxadm = type.minadm = type.weakadm = 0;
  if(diam_row < eta*dist || diam_col < eta*dist) {
    type.minadm = type.weakadm = 1;
    bc = new_blockcluster(row, col, 0, 0, type);
  }
  else if(row->sons > 0 && col->sons > 0) {
    bc = new_blockcluster(row, col, row->sons, col->sons, type);
    for(j=0; j<col->sons; j++)
      for(i=0; i<row->sons; i++)
        bc->son[i+j*bc->block_rows] =
          build_blockcluster(row->son[i], col->son[j], eta);
  }
  else bc = new_blockcluster(row, col, 0, 0, type);
  return bc;
}
```

$\mathcal{H}$-matrix in HLib

```
psupermatrix
build_supermatrix_from_blockcluster(pcblockcluster bc, int k)
{
  if(bc->son) {
    s = new_supermatrix(block_rows, block_cols, rows, cols,
                        NULL, NULL, NULL);
    for(j=0; j<block_cols; j++) for(i=0; i<block_rows; i++)
      s->s[i+j*block_rows] =
        build_supermatrix_from_blockcluster(bc->son[i+j*block_rows], k, eps);
  }
  else if(bc->type.weakadm) {
    r = new_rkmatrix(k, rows, cols);
    s = new_supermatrix(1, 1, rows, cols, NULL, r, NULL);
  }
  else {
    f = new_fullmatrix(rows, cols);
    s = new_supermatrix(1, 1, rows, cols, NULL, NULL, f);
  }
  return s;
}
```

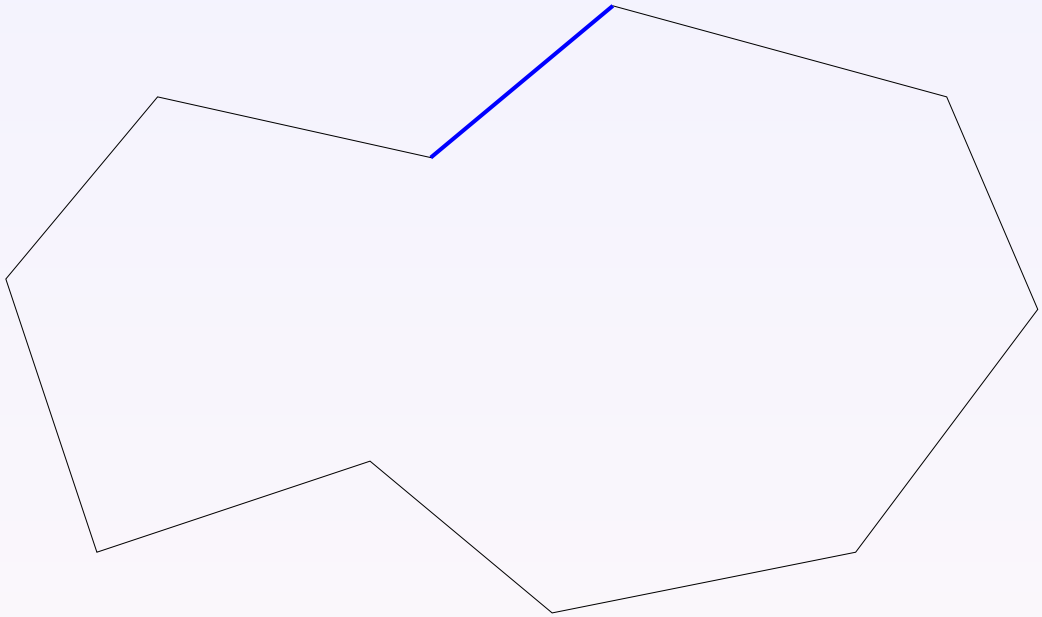
Example: Curve

Example: Polygonal curve in two-dimensional space with piecewise constant basis functions.



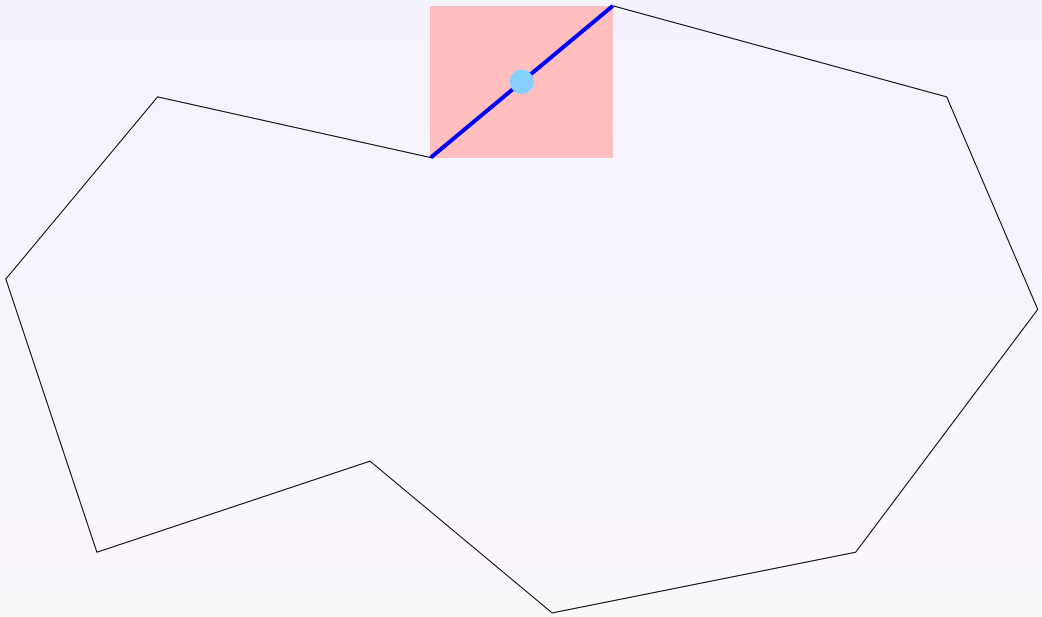
Example: Curve

Example: Polygonal curve in two-dimensional space with piecewise constant basis functions.



Example: Curve

Example: Polygonal curve in two-dimensional space with piecewise constant basis functions.



Observation: Midpoints are good characteristic points.
Optimal bounding boxes are easily found.

Setup of cluster factory

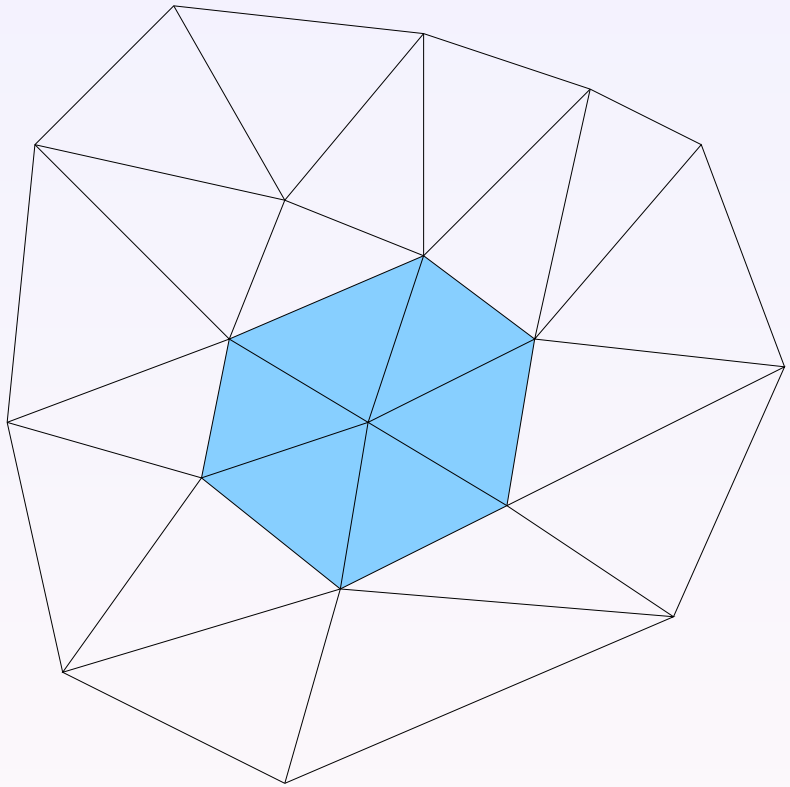
Approach: Represent curve by cyclic array of vertices, compute midpoints and bounding boxes, use general algorithm in HLib.

```
factory = new_clusterfactory(n, 2);

for(i=0; i<n; i++) {
  factory->x[i][0] = 0.5 * (vertex[i][0] + vertex[(i+1)%n][0]);
  factory->x[i][1] = 0.5 * (vertex[i][1] + vertex[(i+1)%n][1]);
  factory->smin[i][0] = dmin(vertex[i][0], vertex[(i+1)%n][0]);
  factory->smax[i][0] = dmax(vertex[i][0], vertex[(i+1)%n][0]);
  factory->smin[i][1] = dmin(vertex[i][1], vertex[(i+1)%n][1]);
  factory->smax[i][1] = dmax(vertex[i][1], vertex[(i+1)%n][1]);
}

cluster = create_clustertree(factory, HLIB_GEOMETRIC, 1, 0);
```

Result: Construction of a cluster tree requires only small amount of problem-specific code.

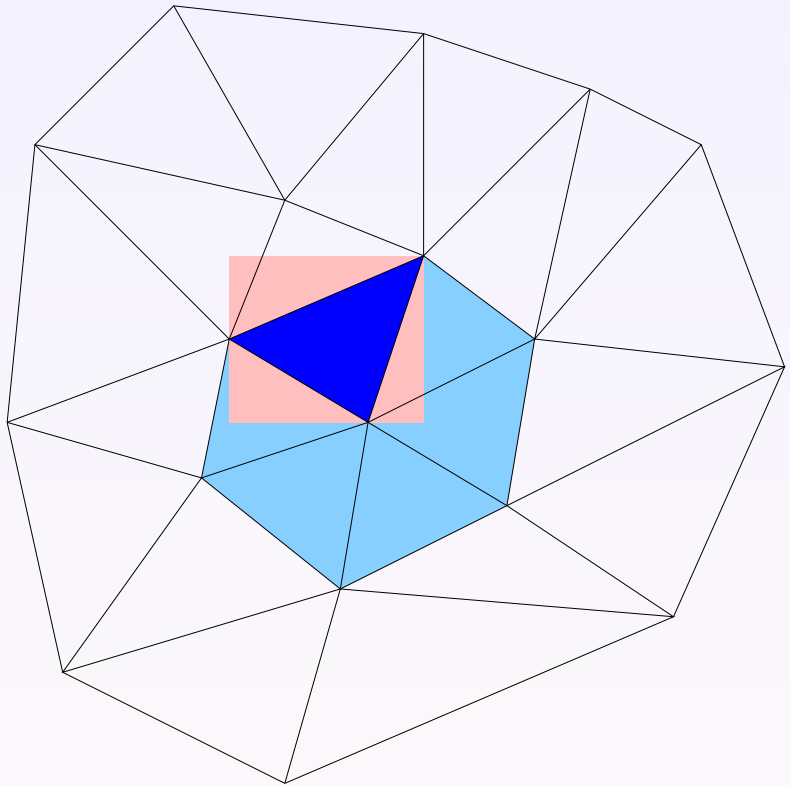
Example: FEM

Example: Polygonal mesh in two-dimensional space with piecewise linear nodal basis functions.



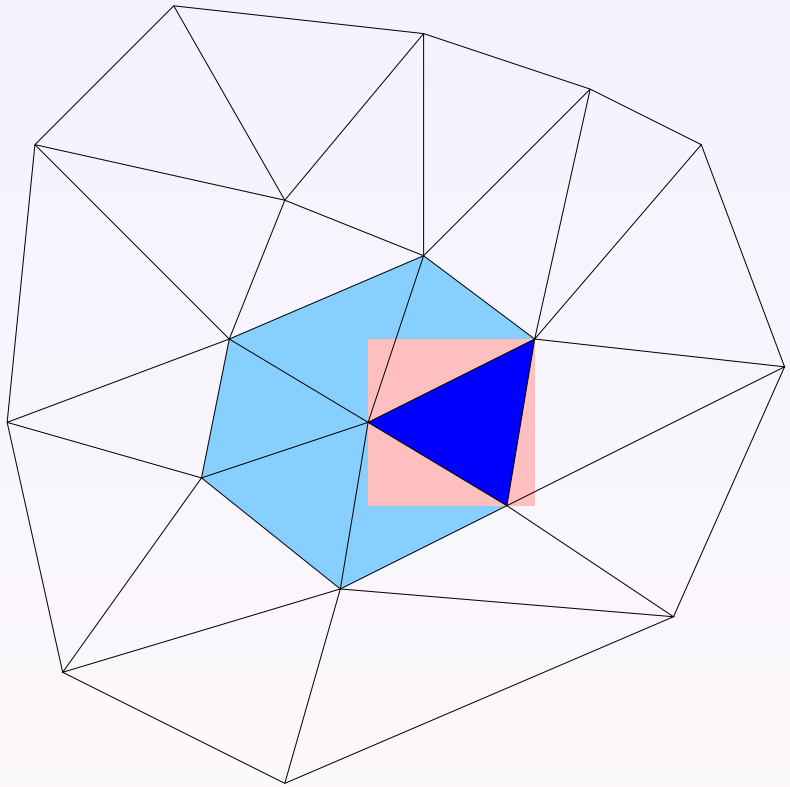
Example: FEM

Example: Polygonal mesh in two-dimensional space with piecewise linear nodal basis functions.



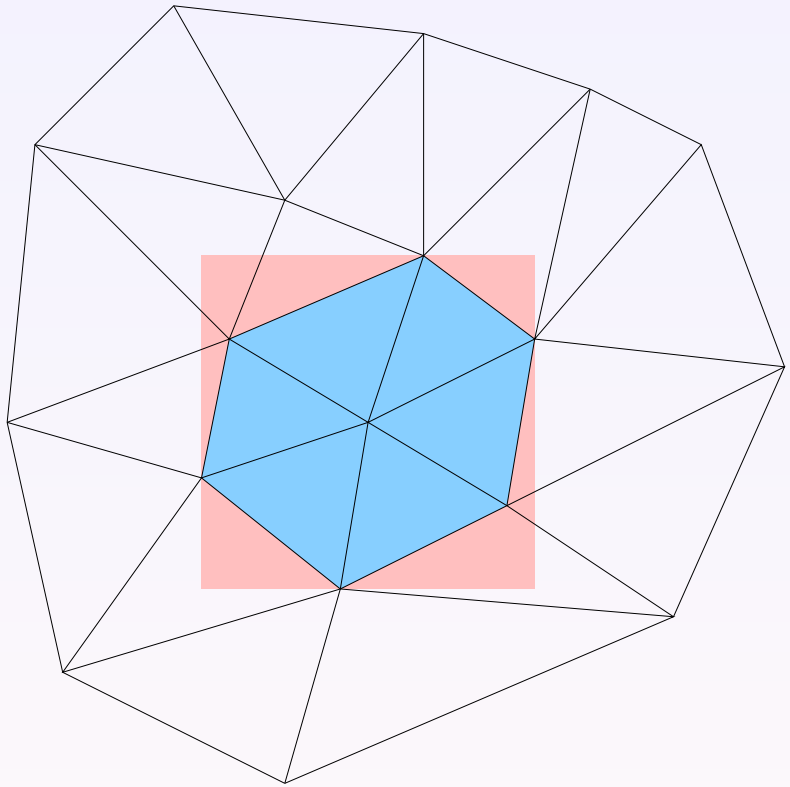
Example: FEM

Example: Polygonal mesh in two-dimensional space with piecewise linear nodal basis functions.



Example: FEM

Example: Polygonal mesh in two-dimensional space with piecewise linear nodal basis functions.



Observation: Nodal points are good characteristic points.
Optimal bounding boxes constructed from single triangles.

Setup of cluster factory

Approach: Represent polygon by array of vertices and array of triangles referencing the vertices, compute points and bounding boxes.

```
for(i=0; i<nv; i++) {
  factory->x[i][0] = vertex[i][0];
  factory->x[i][1] = vertex[i][1];
  factory->smin[i][0] = factory->smax[i][0] = vertex[i][0];
  factory->smin[i][1] = factory->smax[i][1] = vertex[i][1];
}

for(i=0; i<nt; i++) {
  tmin[0] = dmin(vertex[triangle[i][0]][0], dmin(vertex[triangle[i][1]][0],
                 vertex[triangle[i][2]][0]));
  tmax[0] = dmax(vertex[triangle[i][0]][0], dmax(vertex[triangle[i][1]][0],
                 vertex[triangle[i][2]][0]));
  tmin[1] = dmin(vertex[triangle[i][0]][1], dmin(vertex[triangle[i][1]][1],
                 vertex[triangle[i][2]][1]));
  tmax[1] = dmax(vertex[triangle[i][0]][1], dmax(vertex[triangle[i][1]][1],
                 vertex[triangle[i][2]][1]));

  for(j=0; j<3; j++) {
    k = triangle[i][j];
    factory->smin[k][0] = dmin(factory->smin[k][0], tmin[0]);
    factory->smax[k][0] = dmax(factory->smax[k][0], tmax[0]);
    factory->smin[k][1] = dmin(factory->smin[k][1], tmin[1]);
    factory->smax[k][1] = dmax(factory->smax[k][1], tmax[1]);
  }
}
```

Summary

Cluster tree: Constructed based on characteristic points by recursive bisection.

Block cluster tree: Recursive subdivision based on admissibility condition.

Admissibility condition: Evaluated using bounding boxes.

Implementation: `clusterfactory` structure contains simple geometric data, all trees and matrices can be constructed by standardized routines.