HPC – Algorithms and Applications

Dwarf #6 – Unstructured Grids

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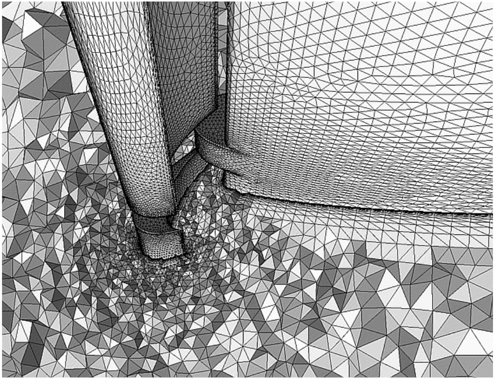
Dwarf #6 – Unstructured Grids

1. dense linear algebra
2. sparse linear algebra
3. spectral methods
4. N-body methods
5. structured grids
6. **unstructured grids**
7. Monte Carlo

Unstructured Grids – Characterisation

- (almost) no restrictions on grid generation, maximum flexibilty
- explicit storage of basic geometric and topological information $\rightarrow$ usually complicated data structures



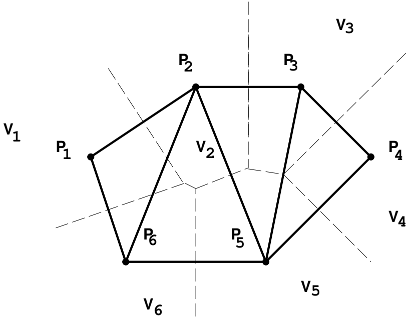
Example: Delaunay Triangulation

- assume: grid points are already given
- to do: generate triangular grid cells
- satisfy Delaunay property: circumcircle of any grid triangle does not contain other grid vertices
- leads to triangles with favourable properties: avoid acute/obtuse angles
- related to **Voronoi** diagrams (next slide)
- widespread (computer graphics, meshes for Finite Element methods, etc.)

Delaunay Triangulation and Voronoi Diagrams

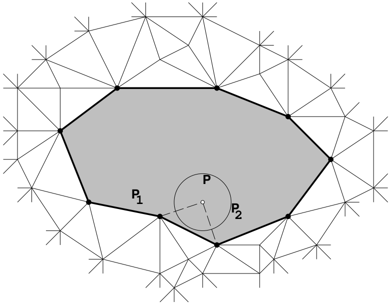
Algorithm

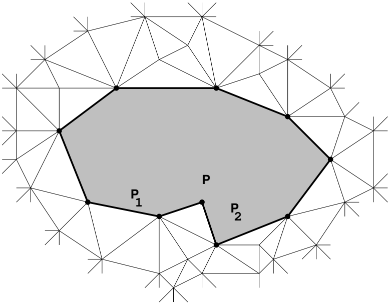
1. Voronoi region around each given grid point:
   $V_i = \{P : \|P - P_i\| < \|P - P_j\| \ \forall j \neq i\}$
2. connect points from adjacent Voronoi regions
3. leads to set of disjoint triangles (tetrahedra in 3D)



Example: Advancing Front Methods

- approach to generate both grid points and grid cells
- advance a *front* step-by-step towards interior
- starting from the boundary (*starting front*)





Advancing Front Methods (2)

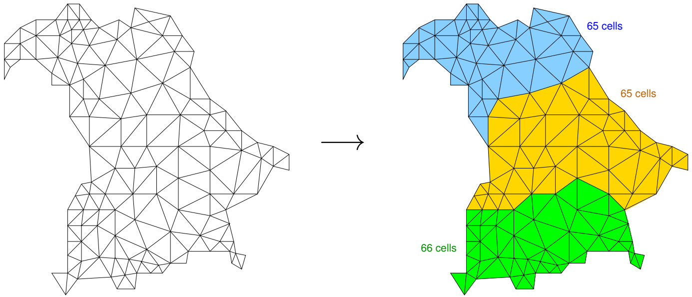
Algorithm:

1. choose an edge on the current front, say PQ
2. create a new point R at equal distance *d* from P and Q
3. determine all grid points lying within a circle around R, radius *r*
4. order these points w.r.t. distance from R
5. for all points, form triangles with P and Q;
   select one of these triangles
6. add triangle to grid (unless: intersections, . . .)
7. update triangulation and front line: add new cell, update edges

Partitioning Unstructured Grids

Partitioning problem:

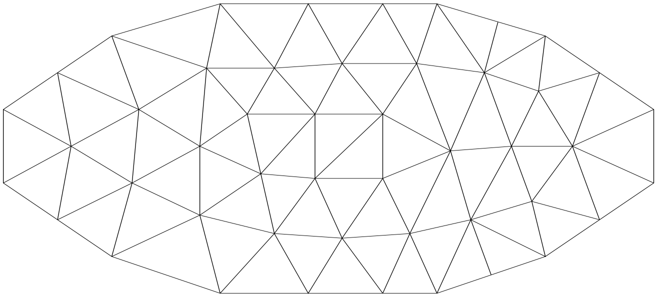
- divide grid into K partitions
- with uniform computational load
  $\rightarrow$ usually: partitions of equal size
- with minimal communication effort
  $\rightarrow$ minimise number of grid cells at partition boundaries



Graph-Based Partitioning

Graph-Representation of Grids:

- “standard” graph (V, E) for a grid:
  $V =$ grid vertices, $E =$ set of all grid cell edges
- vs. “dual” graph (V', E'):
  $V' =$ grid cells, $E' =$ tuples of adjacent grid cells



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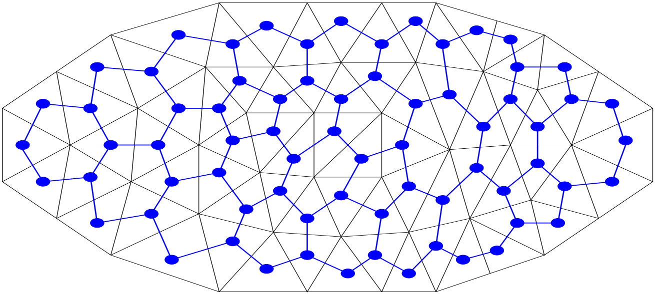
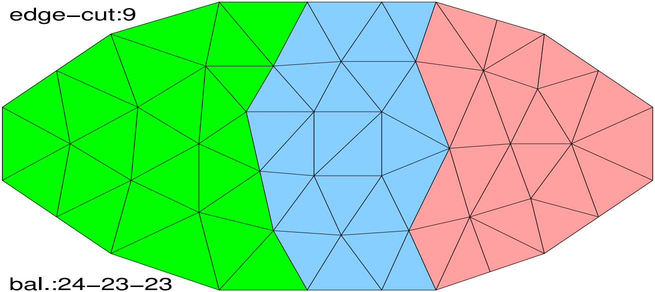


K-way Graph Partitioning

- divide V (or V') into K equal-sized partitions V_k:
$\bigcup_k V_k = V$, $|V_k| = |V|/K$, $V_k \cap V_j = \emptyset$ (if $k \neq j$)
- minimise **edge cut**: $\{(e,f) \in E : e \in V_k, f \notin V_k\}$
- NP-complete problem $\Rightarrow$ use heuristics-based algorithms



Multilevel k-Way Partitioning

Algorithm by Karypis and Kumar (1998):

1. **coarsening phase:**
   - successively collapse sets of vertices to reduce problem size
   - conserve vertex/edge weights
2. **partitioning phase:**
   - perform K-way partitioning on a coarse graph
3. **uncoarsening phase:**
   - successively expand collapsed vertices to obtain respective partitioning of the original graph
   - postprocessing after each uncoarsening step to improve load balance

Coarsening Phase

Coarsening by **Matching:**

- “matching”: set of edges, where no two edges share a common vertex
- “maximal” matching: a matching, where no further edges can be added
  (but some vertices might still be without a match)
- in contrast: “perfect” matching (matching covers all vertices)

Matching-based Coarsening:

- two vertices connected by an edge of the matching will be collapsed
- stop coarsening, if graph is small enough or matching does no longer lead to sufficient coarsening

Algorithms for Matching

Random Matching:

- vertices are visited in random order
- an unmatched vertex u randomly selects an unmatched connected vertex v
  $\rightarrow (u, v)$ is added to the matching
- vertices stay unmatched, if they no longer have an unmatched neighbour

$\Rightarrow$ simple, greedy approach; however, does not consider minimisation of edge-cut

Algorithms for Matching (2)

Heavy Edge Matching:

- use weighted edges: $W(e)$ and $W(A) := \sum_{e \in A} W(e)$
- E_{i+1} and E_i the edges of coarse/fine graph due to a matching M_i, then: $W(E_{i+1}) = W(E_i) - W(M_i)$
- heuristics: use heavy edges for matching
- again: visit vertices in random order;
  pick edge (to unmatched vertex) with the largest edge weight

$\Rightarrow$ greedy approach, heuristics to keep edge-cut low, but does not guarantee minimisation of edge-cut

Algorithms for Matching (3)

Modified Heavy Edge Matching:

- experience: coarse graphs with low average degree (number of outgoing edges) of edges lead to partitions with lower edge-cut
- chose random vertex $v \rightarrow H(v)$ the set of adjacent edges with maximum weight
- for each $u \in H(v)$, define $W(v,u) = \sum W(e)$ for all edges e that
  - are adjacent to v, i.e. $e = (v, u')$
  - u' is connected to u
- determine maximum $W(v,u)$ and pick resp. (v,u) for matching

Collapse Graph after Matching

Determine Coarse Vertices:

- matching M_i computed for (V_i, E_i)
- each $m \in M_i$ becomes a vertex of V_{i+1}
- each non-matched $v \in V_i$ becomes a vertex of V_{i+1}
- weight vertices to preserve load balance info: weights are added for matched edges

Determine Coarse Edges:

- an edge between two vertices of V_{i+1} is generated, if an edge in E_i connects any of the former members
- the edge weights are added over all such connections $\rightarrow$ preserve edge-cut

Partitioning of the Coarse Graph

Options:

- coarsen until only k graph vertices are left?
  $\rightarrow$ bad partitions (vertices no longer equally weighted);
  $\rightarrow$ matching does not reduce graph size well for small partitions
- switch to multilevel recursive bisection
  $\rightarrow$ turns out as successful choice
- Fiedler vector for partitioning (spectral methods)
  $\rightarrow$ solve eigenvalue problem on the adjacency matrix
- geometric methods (coordinates required)
- combinatorial methods

Uncoarsening of the Graph Partitions

Backprojection:

- partitioning P_{i+1} given on coarse graph
- put vertex v of P_i to partition $p \in P_i$, if match-vertex of v belongs to p in P_{i+1}

Local Refinement:

- even, if P_i might be (locally) optimal, P_{i+1} can be improved, as more degrees of freedom are available
- approach: swap vertices between partitions to reduce edge cut (until a local minimum is reached)

Local Refinement Algorithm

- define *neighbourhood* $N(v)$ for each vertex v: set of adjacent partitions
- for each vertex, compute gains for moving v into each of the partitions in $N(v)$
- move vertex from partition a to $b \in N(v)$, if
  1. gain $g(v, b)$ is large (largest among $N(v)$ and
  2. balancing is maintained:

$$W_i[b] + W(v) \leq W_{\max} \quad \text{and} \quad W_i[a] - W(v) \geq W_{\min}$$

- *greedy refinement*: visit vertices at partition boundaries in random order; move to the partition with largest gain
- in addition: move vertex, if edge cut stays equal but balance is improved

Local Refinement Algorithm (2)

Determine gain of vertex:

- sum up weights of edges to neighbour partition

$$\rightarrow \text{external degree:} \quad \mathrm{ED}[v,b] := \sum_{u \in P_b} W(v,u)$$

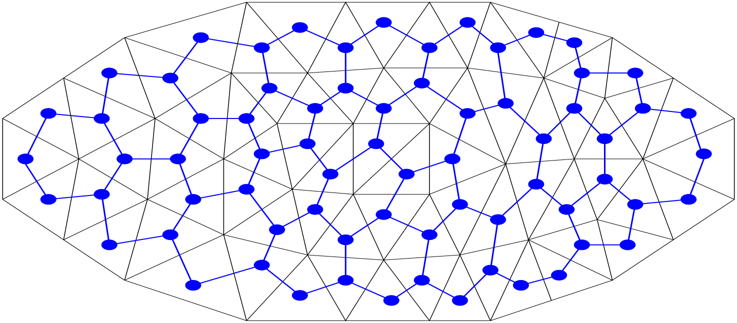
- sum up weights of edges in the same partition

$$\rightarrow \text{internal degree:} \quad \mathrm{ID}[v] := \sum_{u \in P[v]} W(v,u)$$

- gain of moving v to b: $g[v,b] = \mathrm{ED}[v,b] - \mathrm{ID}[v]$

MLkP-Example – Coarsening Phase

Start with dual graph:



MLkP-Example – Coarsening Phase

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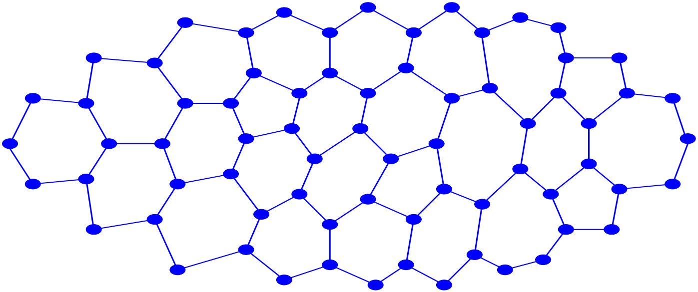
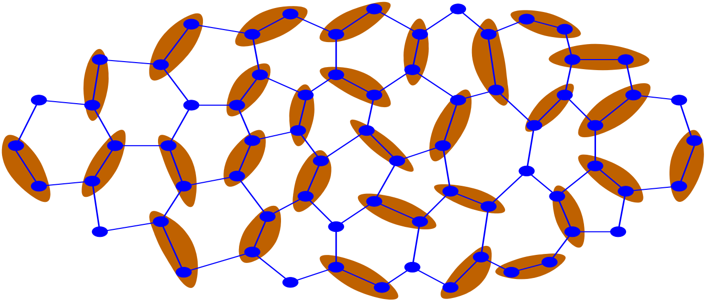


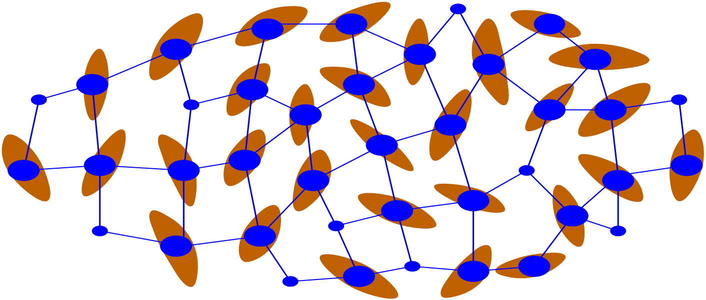
MLkP-Example – Coarsening Phase

Random matching:



MLkP-Example – Coarsening Phase

Collapse vertices and re-build adjacency graph:



(bigger discs indicated heavier vertices, i.e. multiple grid cells)

MLkP-Example – Coarsening Phase

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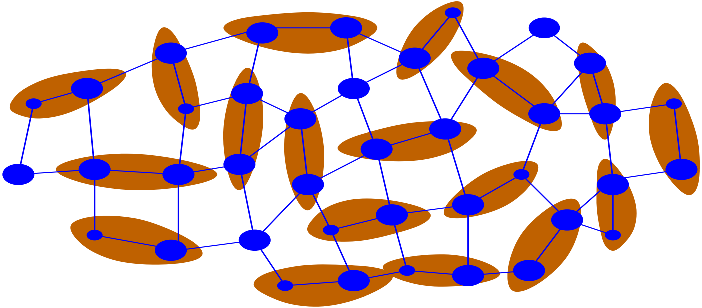

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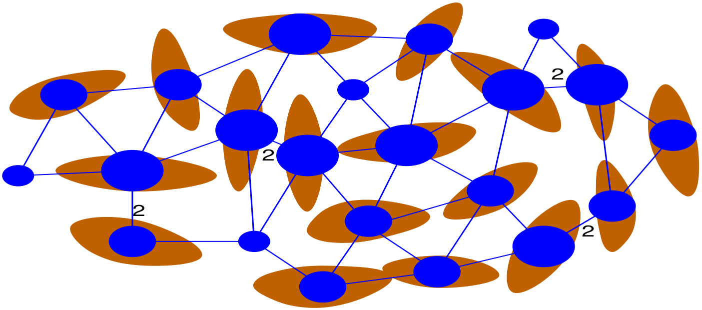
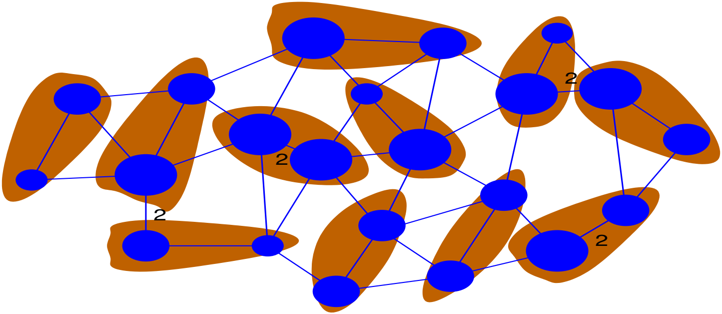


(multiple edges between matchings lead to edge weights > 1)

MLkP-Example – Coarsening Phase

Random matching:



MLkP-Example – Coarsening Phase

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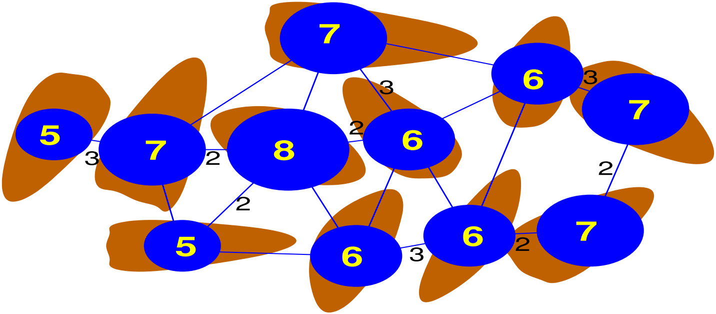
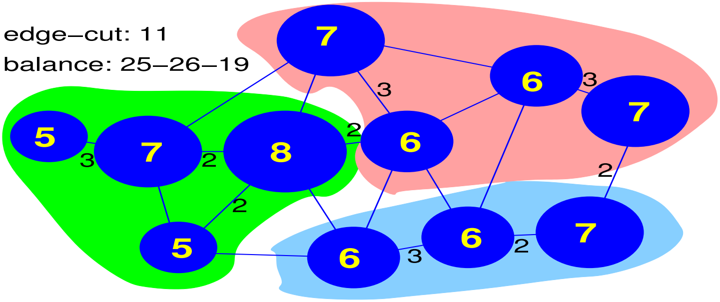


(yellow numbers indicated vertex weights)

MLkP-Example – Partitioning

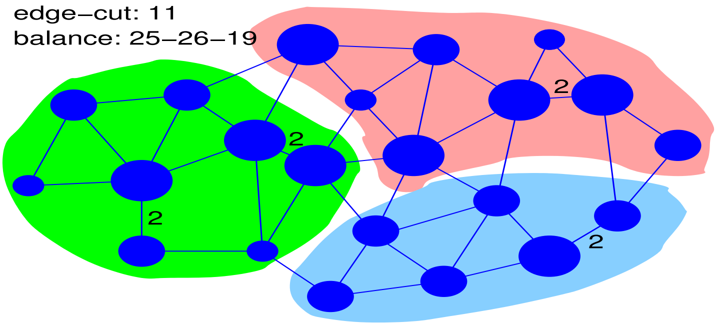
Determine initial partitioning on coarsened graph:



(minimize edge-cut: do not cut 2-/3-weighted edges)

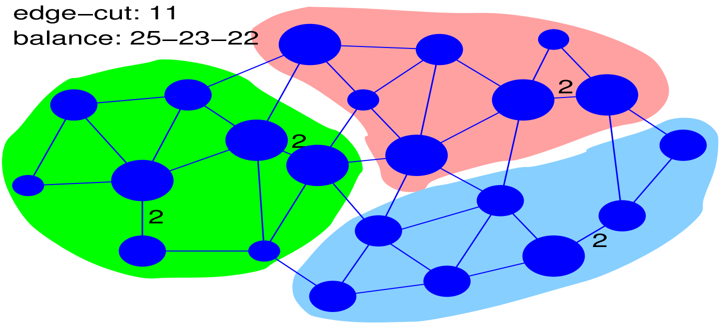
MLkP-Example – Uncoarsening Phase

Inflate collapsed vertices:



MLkP-Example – Uncoarsening Phase

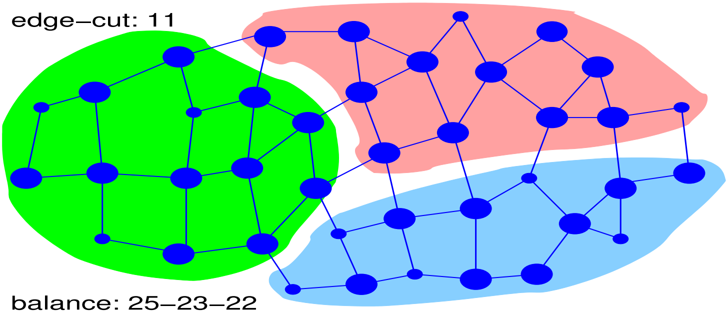
Local improvement:



(right-most vertex moves from pink to blue partition)

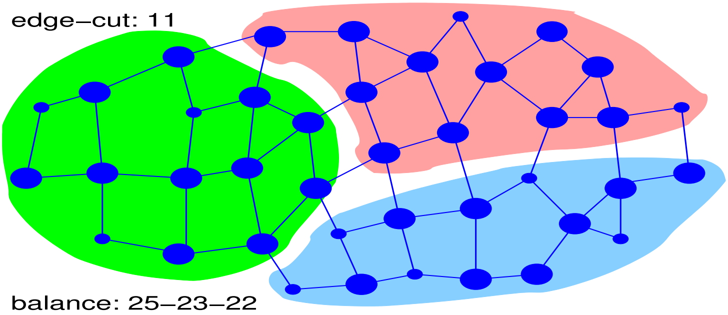
MLkP-Example – Uncoarsening Phase

Inflate collapsed vertices:



MLkP-Example – Uncoarsening Phase

Local improvement:



(here: no vertex moves that improve edge-cut or balance)

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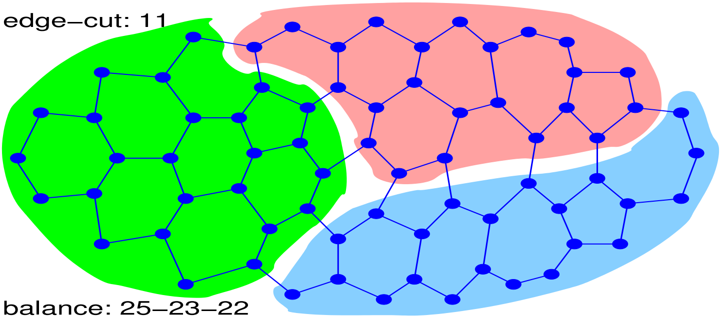
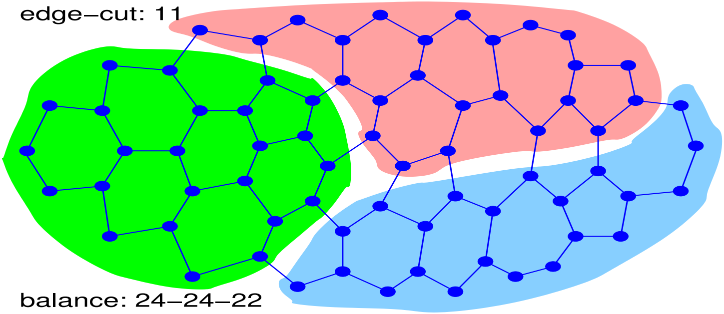


MLkP-Example – Uncoarsening Phase

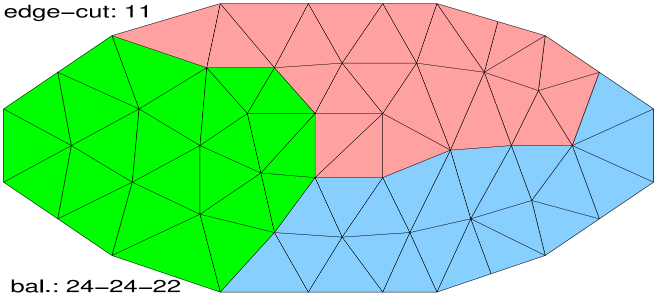
Local improvement:



(top-left vertex moves from green to pink partition)

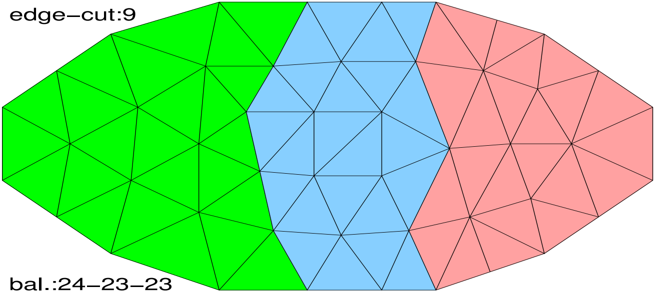
MLkP-Example – Computed Partition

Partitioning obtained via (our) MLkP algorithm:



MLkP-Example – Computed Partition

Compare with optimal(?) partitioning:



Analyse: what choices lead to different partitioning?