Graph Coarsening and Clustering on the GPU

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- Clustering $\simeq$ isolating 'related' groups of vertices in a graph.
- Relevant in: social networks, epidemiology, papers, metabolism, and ecosystems (Newman & Girvan, 2004).
- Our primary interests are speed and parallelisation.

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$$V = \bigcup_{C \in \mathcal{C}} C \qquad \text{as a disjoint union.}$$

- Quality of a clustering is measured by its modularity $\mathrm{mod}(\mathcal{C})$, introduced in 2004 by Newman and Girvan.

Modularity clustering

- Clustering modularity is defined as

$$\mathrm{mod}(\mathcal{C}) := \frac{\sum\limits_{C \in \mathcal{C}} \sum\limits_{\substack{\{u,v\} \in E \\ u,v \in C}} \omega(\{u, v\})}{\sum\limits_{e \in E} \omega(e)} - \frac{\sum\limits_{C \in \mathcal{C}} \left(\sum\limits_{v \in C} \zeta(v) \right)^2}{4 \left(\sum\limits_{e \in E} \omega(e) \right)^2}.$$

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- Here, vertex weights $\zeta : V \to \mathbb{R}_{\geq 0}$ are defined as

$$\zeta(v) := \sum_{\{u,v\} \in E} \omega(\{u,v\}).$$

Modularity clustering

- $\text{mod}(\mathcal{C})$ can be rewritten to

$$\frac{1}{4\,\Omega^2} \sum_{C \in \mathcal{C}} \left[\zeta(C)\,(2\,\Omega - \zeta(C)) - 2\,\Omega \left(\sum_{\substack{C' \in \mathcal{C} \\ C' \neq C}} \omega(\text{cut}(C, C')) \right) \right].$$

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- To calculate modularity, we only need to keep track of summed vertex weights of clusters and summed edge weights between clusters.

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- This suggests a greedy agglomerative strategy (e.g. Zhu et al., 2008).

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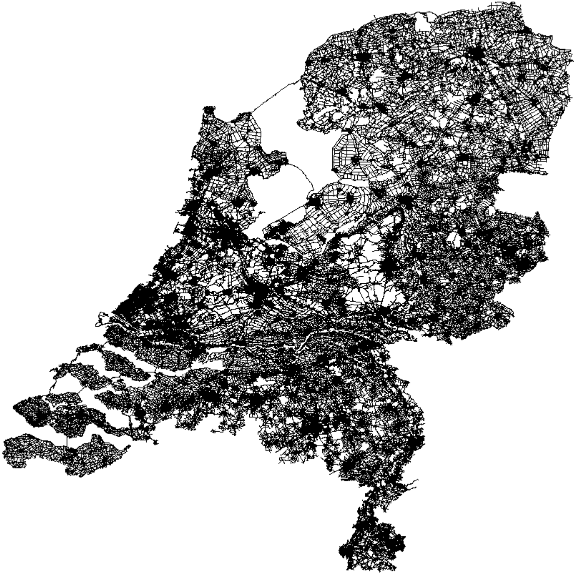
We make use of parallelism in steps 2 and 3.

Agglomerative clustering (`netherlands`)

0 iterations.



Agglomerative clustering (netherlands)

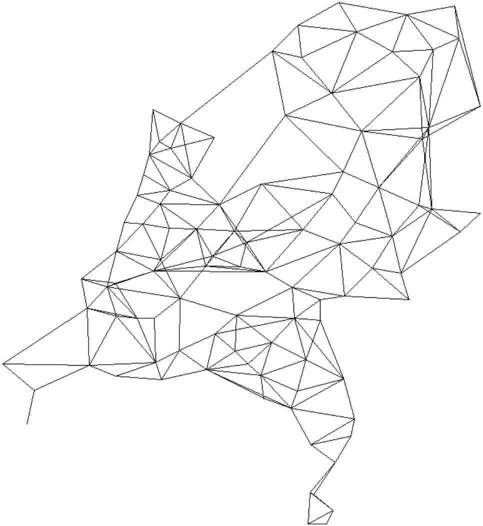
11 iterations.

Agglomerative clustering (netherlands)

21 iterations.

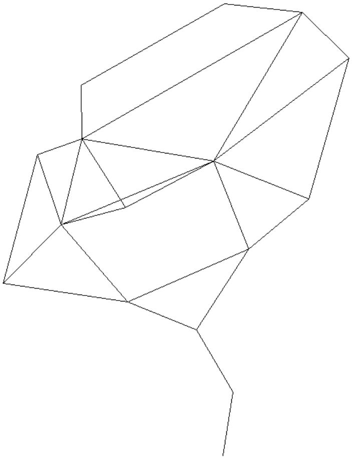
Agglomerative clustering (`netherlands`)

26 iterations.



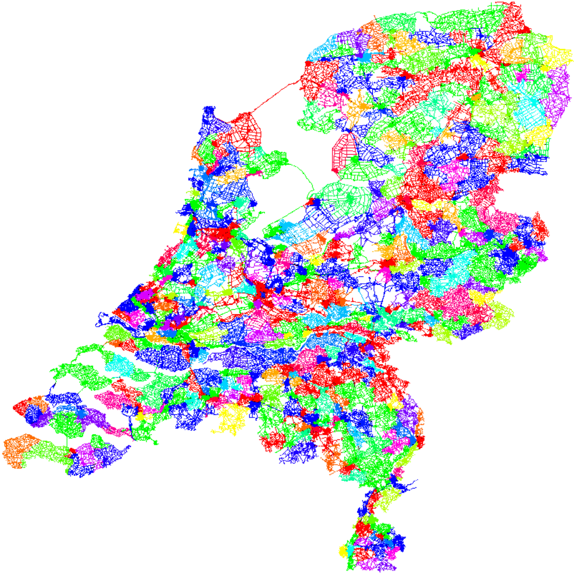
Agglomerative clustering (netherlands)

33 iterations.

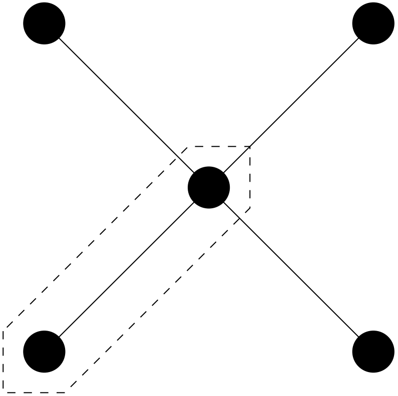


Agglomerative clustering (`netherlands`)

Final clustering.

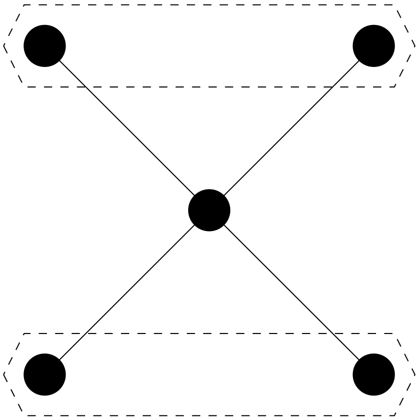


Star graphs



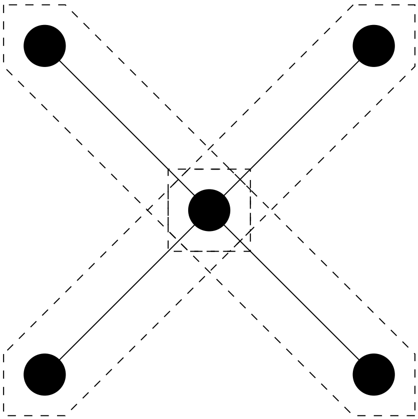
Agglomerative clustering slows down on star graphs.

Star graphs



Merging vertices with the same neighbours is bad for clustering.

Star graphs



So we merge multiple satellites to the same centre.

Centre potential

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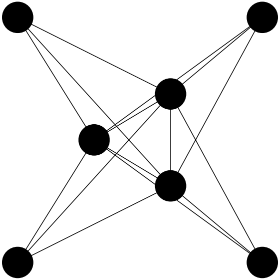
- We use $\mathrm{cp}(\cdot)$ to identify satellites and match these to centres.

Centre potential



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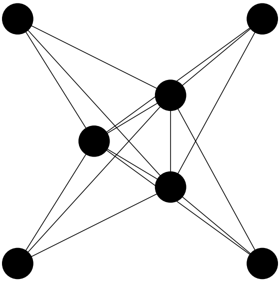

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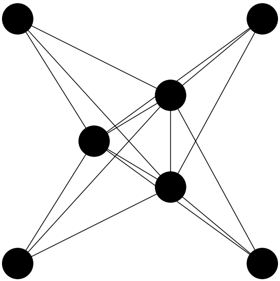

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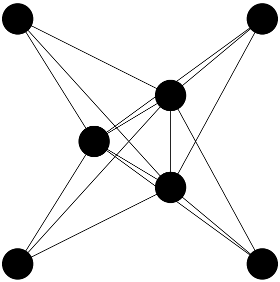

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$$\text{cp(satellite)} \leq \frac{1}{2} \qquad \text{and cp(satellite)} \to 0 \text{ as } k \to \infty,$$
$$\text{cp(centre)} \geq \frac{4}{3} \qquad \text{and cp(centre)} \to \infty \text{ as } k \to \infty.$$

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  - $$\zeta'(v') = \sum_{\pi(v)=v'} \zeta(v) \qquad \text{(sum vertex weights)},$$
  - $\pi(u) = \pi(v)$ if and only if $\mu(u) = \mu(v)$ (compress μ to π).

GPU coarsening (implementation)

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- Use μ, π, π^{-1}, and a bookkeeping array ρ in global GPU memory.

GPU coarsening (algorithm)

ρ	1	2	3	4	5	6	7	8	9	10	11	12
μ	9	2	3	22	9	9	22	2	3	3	2	4
π^{-1}												
π												

Initialise ρ sequentially and store μ.

GPU coarsening (algorithm)

ρ	1	2	3	4	5	6	7	8	9	10	11	12
μ	9	2	3	22	9	9	22	2	3	3	2	4
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Sort by increasing μ-value (`sort_by_key`).

GPU coarsening (algorithm)

ρ	2	8	11	3	9	10	12	1	5	6	4	7
μ	2	2	2	3	3	3	4	9	9	9	22	22
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Determine different matched groups (`adjacent_not_equal`).

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μ	1	0	0	1	0	0	1	1	0	0	1	0
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Extract boundaries for π^{-1} (`copy_index_if_nonzero`).

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Perform scan to find π indices (`inclusive_scan`).

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π	4	1	2	5	4	4	5	1	2	2	1	3

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- Gather weighted neighbours of $\rho(\pi^{-1}(i'))$ to $\rho(\pi^{-1}(i' + 1) - 1)$:

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- Sort the neighbour list by index.
- Compress the neighbour list by replacing subsequences $(j', \omega_1, j', \omega_2, \ldots, j', \omega_l)$ with $(j', \omega_1 + \omega_2 + \ldots + \omega_l)$.

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- This gives us a fine-grained shared-memory parallel clustering algorithm.
- We do not perform local improvement (Kernighan–Lin): changing cluster weights makes parallelising this very hard.

Results

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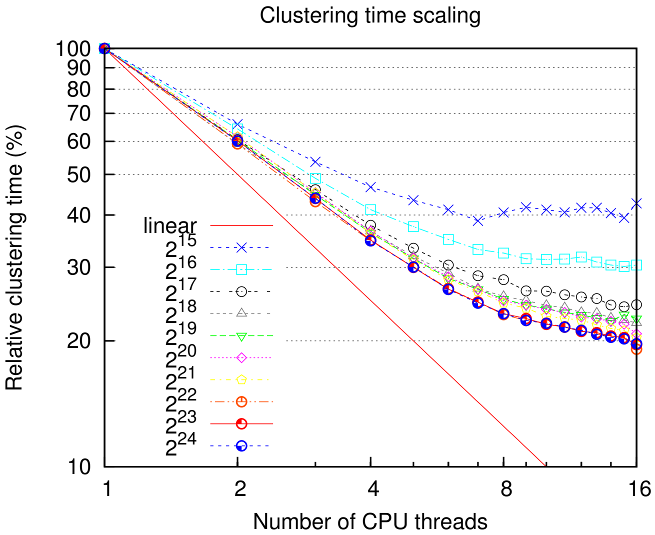
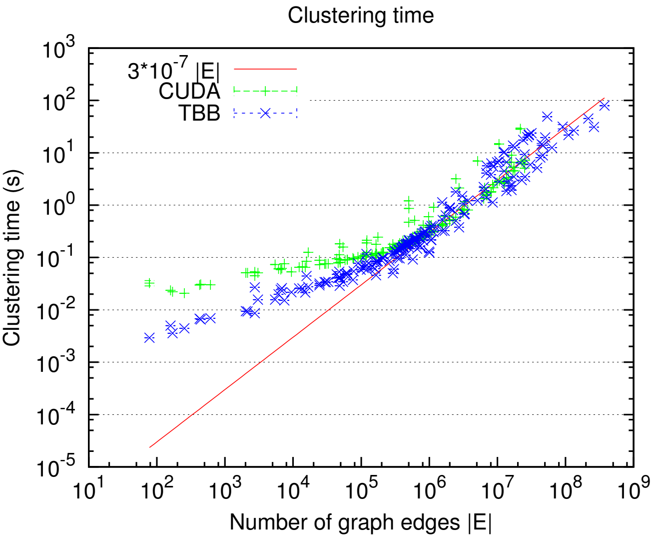
- Time: matching and CPU $\leftrightarrow$ GPU data transfer, not disk I/O.
- Test set: 10th DIMACS challenge.
- Test hardware: dual quad-core Xeon E5620 and an NVIDIA Tesla C2050 (thanks: the Little Green Machine project).

Results (scaling)



Results (time)



Results (quality)

	$\|V\|$	$\|E\|$	CUDA	TBB	Ovelgönne et al. (2010)
karate	34	78	0.363	0.383	0.412
jazz	198	2,742	0.314	0.369	0.444
email	1,133	5,451	0.440	0.473	0.572
PGP	10,680	24,316	0.809	0.841	0.880

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- Lower quality, because we do not use local refinement.

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- CUDA: road_central, $|V| = 14{,}081{,}816$, $|E| = 16{,}933{,}413$, modularity 0.996 clustering in 4.6 seconds.

Results (time)

- Our algorithm is very fast for large graphs.
- CUDA: road_central, $|V| = 14{,}081{,}816$, $|E| = 16{,}933{,}413$, modularity 0.996 clustering in 4.6 seconds.
- TBB: uk-2002, $|V| = 18{,}520{,}486$, $|E| = 261{,}787{,}258$, modularity 0.974 clustering in 31 seconds.

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- Comparison to state of the art: DIMACS challenge.

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- This algorithm is suitable for both multi-core CPUs and GPUs.
- We propose the centre potential to deal with star-like graphs.
- The algorithm is very fast, but quality could be improved by parallel local refinement.

Questions

$\exists$ any questions?

GPU matching problems

- Performing matching in parallel is problematic.

GPU matching problems

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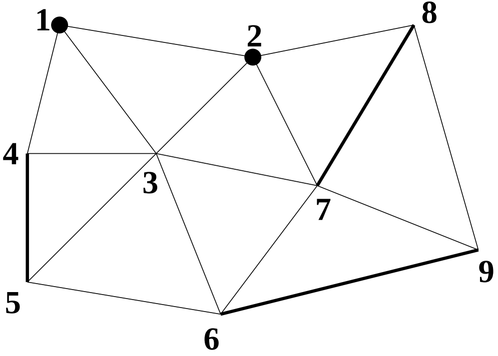
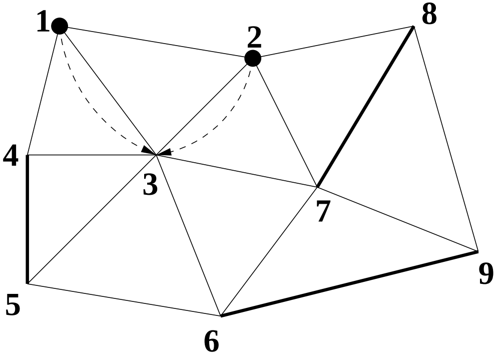
- Disjoint edges requirement leads to serialisation.

GPU matching problems



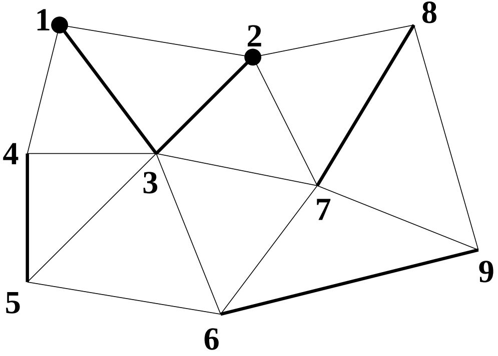
Suppose we match vertices simultaneously.

GPU matching problems



Vertices find an unmatched neighbour. . .

GPU matching problems



. . . but generate an invalid matching.

GPU matching

- To solve this we create two groups of vertices: **blue** and **red**.

GPU matching

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- **Blue** vertices propose.

GPU matching

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- **Red** vertices respond.

GPU matching

- To solve this we create two groups of vertices: **blue** and **red**.
- **Blue** vertices propose.
- **Red** vertices respond.
- Proposals that were responded to are matched.

GPU matching (implementation)

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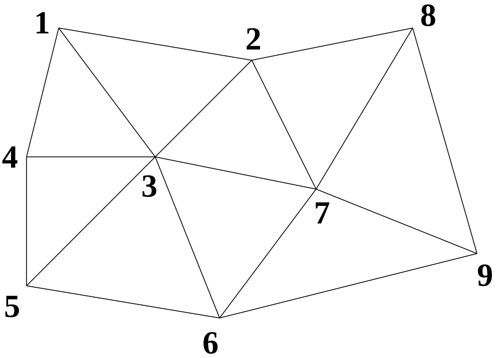
  - and its proposal/response value $\sigma(v)$.
- Both π and σ are stored in 1D arrays in global memory.

GPU matching (algorithm)

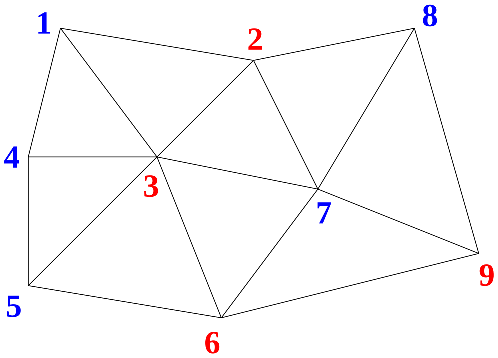
Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	-	-	-	-	-	-	-	-	-
σ	-	-	-	-	-	-	-	-	-

GPU matching (algorithm)

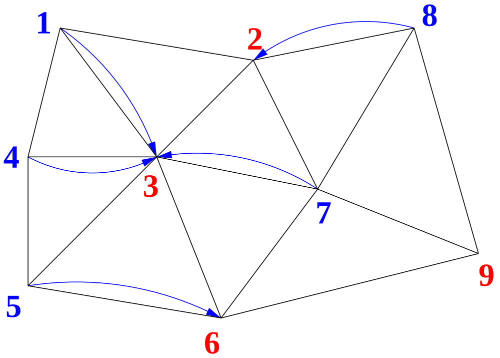
Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	**b**	**r**	**r**	**b**	**b**	**r**	**b**	**b**	**r**
σ	-	-	-	-	-	-	-	-	-

GPU matching (algorithm)

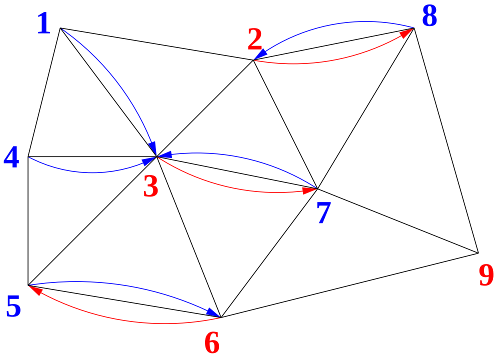
Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	**b**	**r**	**r**	**b**	**b**	**r**	**b**	**b**	**r**
σ	3	-	-	3	6	-	3	2	-

GPU matching (algorithm)

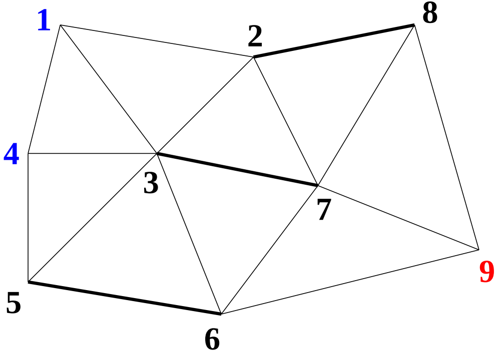
Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	**b**	**r**	**r**	**b**	**b**	**r**	**b**	**b**	**r**
σ	3	8	7	3	6	5	3	2	-

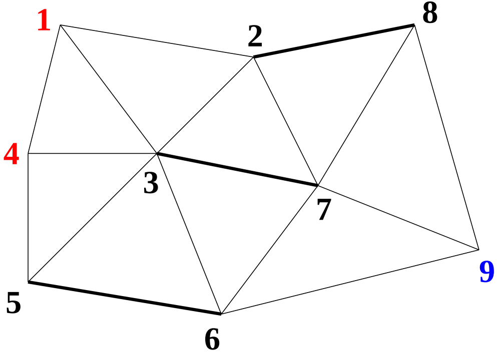
GPU matching (algorithm)

Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	**b**	2	3	**b**	5	5	3	2	**r**
σ	3	8	7	3	6	5	3	2	-

GPU matching (algorithm)

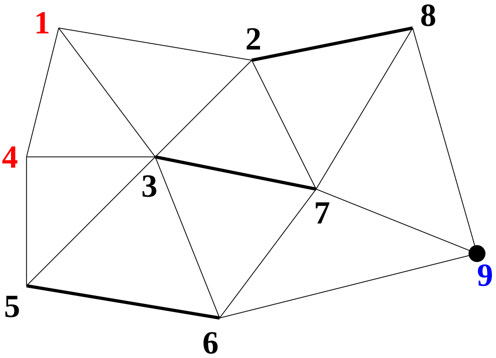


Colour
Propose
Respond
Match

	1	2	3	4	5	6	7	8	9
π	**r**	2	3	**r**	5	5	3	2	**b**
σ	3	8	7	3	6	5	3	2	-

GPU matching (algorithm)

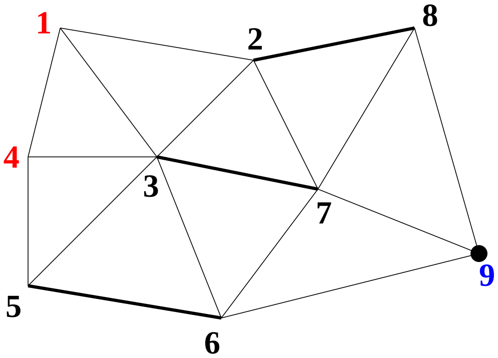
Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	**r**	2	3	**r**	5	5	3	2	**b**
σ	-	-	-	-	-	-	-	-	**d**

GPU matching (algorithm)

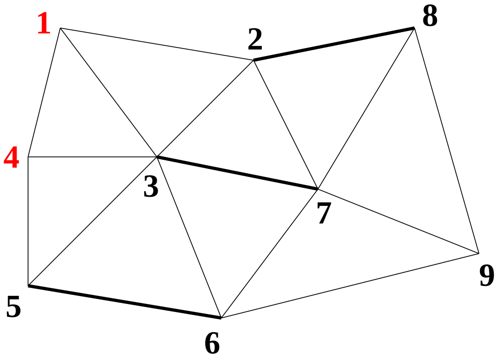
Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	r	2	3	r	5	5	3	2	b
σ	-	-	-	-	-	-	-	-	d

GPU matching (algorithm)

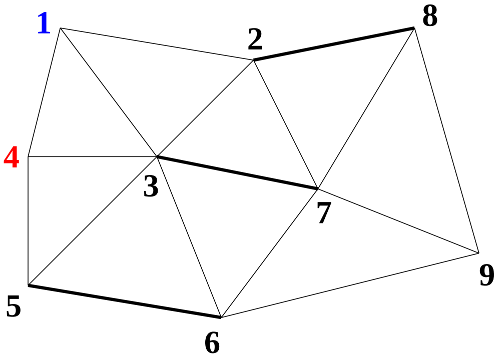
Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	**r**	2	3	**r**	5	5	3	2	**d**
σ	-	-	-	-	-	-	-	-	**d**

GPU matching (algorithm)

Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	**b**	2	3	**r**	5	5	3	2	**d**
σ	-	-	-	-	-	-	-	-	**d**

GPU matching (algorithm)

Colour
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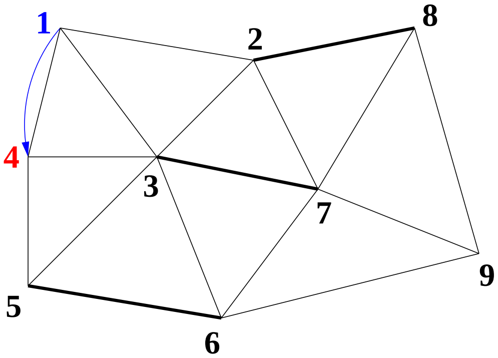
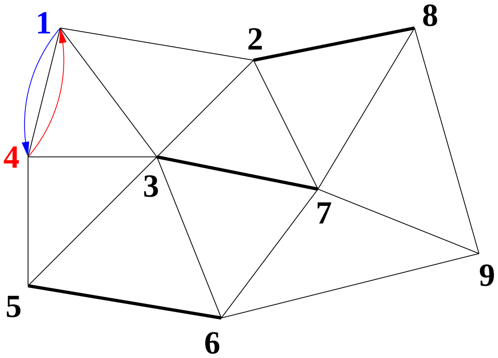


	1	2	3	4	5	6	7	8	9
π	**b**	2	3	**r**	5	5	3	2	**d**
σ	4	-	-	-	-	-	-	-	-

GPU matching (algorithm)

Colour
Propose
Respond
Match



	1	2	3	4	5	6	7	8	9
π	**b**	2	3	**r**	5	5	3	2	**d**
σ	4	-	-	1	-	-	-	-	-

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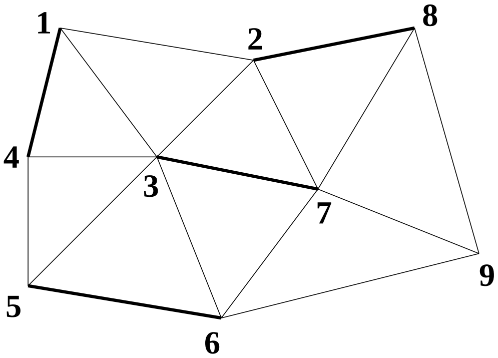
Respond
Match



	1	2	3	4	5	6	7	8	9
π	1	2	3	1	5	5	3	2	**d**
σ	4	-	-	1	-	-	-	-	-