



TABLE OF CONTENTS

01

INTRODUCTION

02

MapReduce

Large-Scale Frequent Subgraph
Mining in MapReduce

03

Pregel

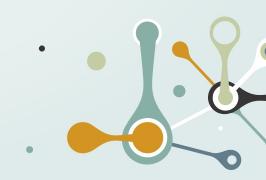
Frequent Subgraph Mining Based on Pregel

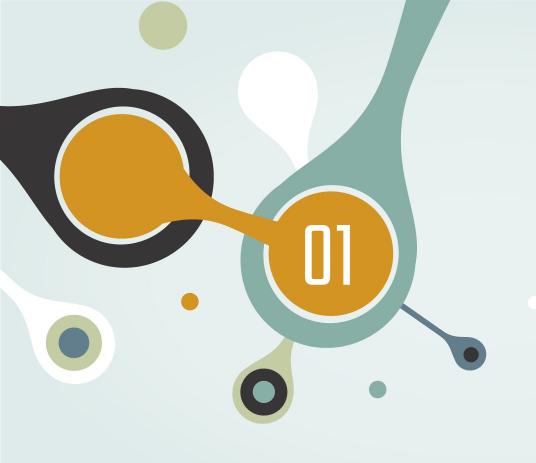
04

PARALLEL

Leveraging Multiple GPUs and CPUs for Graphlet Counting in Large Networks 05

CONCLUSION





INTRODUCTION



FREQUENT SUBGRAPH MINING



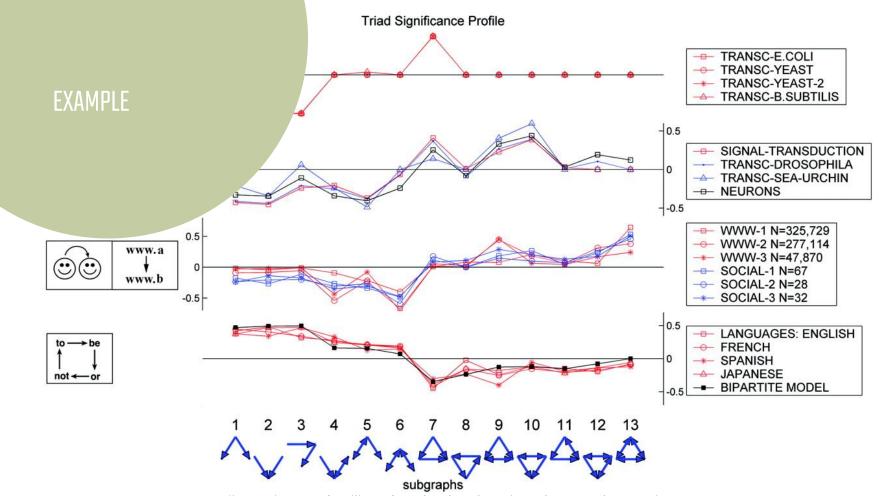
Goal of Frequent Subgraph Mining (FSM) is to extract frequent subgraphs from graphs.

- **Graph.** G = (V, E)
- Subgraph. G' = (V', E')

$$V' \subseteq V$$
 and $E' \subseteq E$

(Graph Isomorphism is in **NP**.) Subgraph Isomorphism is in **NP-Complete**.

Frequent Subgraphs are used in **chemistry**, **analysis of social networks**, etc.



Ron Milo et al. Superfamilies of Evolved and Designed Networks. In Science. 2004.

MapReduce

Large-Scale Frequent Subgraph Mining in MapReduce





INTRODUCTION

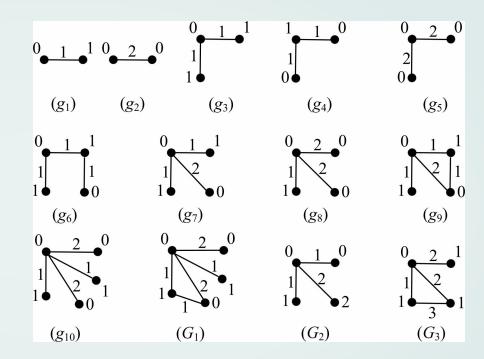


• **Transaction.** We usually mine 1 large graph, but in this case we will mine N small graphs.

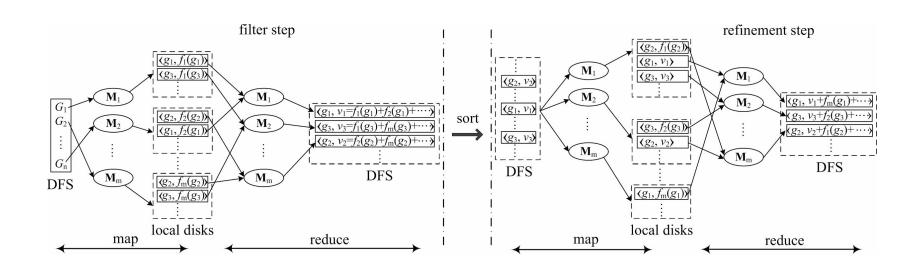
It is worth remembering that vertices and edges are labeled, in this case.

Like [4], MapReduce Frequent Subgraph Mining (MRFSM), which is based on MapReduce, is able to find subgraphs whose support is greater than θ , where θ is the threshold.

- $f(g_1) = |\{G_1, G_2, G_3\}| = 3$ $f(g_{10}) = |\{G_1\}| = 1$



MRFSM





FILTER



- **Map.** After dividing G into G_{ij} , G_{2j} , ..., G_{mj} we assign G_{ij} to M_{ij} , which signals g_{ij} if $f(g_{ij})/n_{ij} \ge \theta$, where $n_{ij} = |G_{ij}|$. **Reduce.** Write the union of the sets of the candidates to DFS.

Unfortunately, there is a risk of a large number of **false positives**, because it is possible for subgraphs to be frequent at the level of G_i but infrequent at the level of G.



FILTER



- Map. We distribute the graphs in G among the machines, randomly. M_j returns frequent subgraphs as well as infrequent subgraphs that are selected as detailed below.
- **Reduce.** If the upper bound of $f(g_i)$, i.e., f'(g), is greater than θ n, then we will promote g_i to candidate.

$$f^{\mathsf{T}}(g) = \sum f_{i}^{\mathsf{T}}(g)$$

If $f_i^{\mathsf{T}}(g)$ is unknown, then we will use $\lceil n_i \cdot \theta \rceil - 1$ as a proxy.



FILTER



It is possible for subgraphs to be infrequent at the level of G_i but frequent at the level of G.

 $G \setminus G_i$ is unknown. On M_i it is necessary to compute the **probability** of a subgraph that is infrequent at the level of G_i being globally frequent. In theory, frequency follows a **binomial distribution**.

If the upper bound of the probability is greater than ρ , then we will approve a locally infrequent subgraph.

BINOMIAL DISTRIBUTION

 $p = f(G') / n_i$

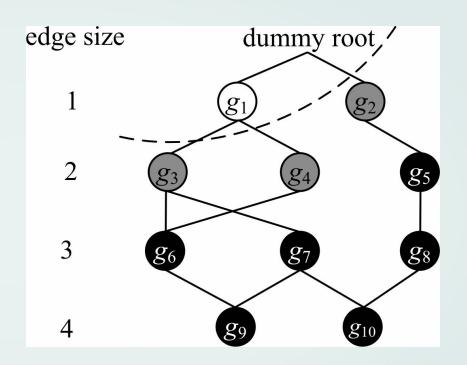
$$Pr \{\exists j \neq i, f_j(G') \geq \lceil \theta \cdot n_j \rceil \}$$

$$\leq \sum_{j \neq i} Pr \{ f_i(G') \geq \lceil \theta \cdot \rceil \}$$

$$= \sum_{j \neq i} \sum_{k = \lceil \theta \cdot n_j \rceil} {n_j \choose k} p^k (1 - p)^{n_j - k}$$

LATTICE

It is possible to construct a lattice by adding an edge at a time.





REFINEMENT



From **Sorting**, M, receives S — in other words, pairs of

- **keys**, which are subgraphs; and
- **values**, which are frequencies.

 $A^{i}(g)$ is the set of supergraphs of g, in case of M,

Map.

For example, g_7 and g_8 are subgraphs of g_{10} .

- Top-Down.
 - **First.** Pairs are in ascending order of size. $ub(g_{10}) = A^{i}(g_{7}) \cap A^{i}(g_{8})$
- Bottom-Up.
 - **First.** Pairs are in ascending order of size. $ub(g_{10}) = ub(g_7) \cap ub(g_8)$.
 - **Second.** Pairs are in descending order of size. In case of g_8 , it is necessary to mine $ub(g_8) \setminus lb(g_8)$, which is $ub(g_9) \setminus A'(g_{10})$.
- **Reduce.** Compute the frequencies of the frequent subgraphs, by summing.

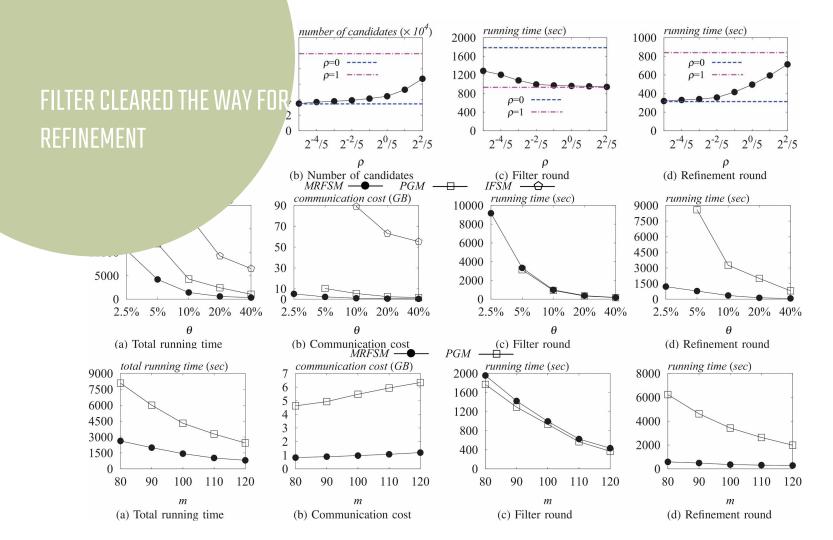


COMPRESSION



We need to reduce our overheads, via compression of canonical labeling.

Like [5], $G = (V, E, L_v, I_v, L_e)$, which is (de)compressed. Also, spanning trees, plus $E \setminus E'$, where E is the set of edges of I and E' is the set of edges of ST, are encoded. Indeed, there is some evidence that frequent subgraphs are commonly spanning trees.



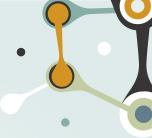
Pregel

Frequent Subgraph Mining Based on Pregel





Pregel



MapReduce is not specialized for graphs, but there is a variety of graph processing distributed systems such as **Pregel**.

With every superstep, we

- receive messages;
- do something; and
- **send** messages.

Bulk Synchronous Parallel (BPS) is used for Pregel. Indeed, there is a **barrier** between superstep and superstep.

Apache Giraph is the open-source equivalent of Pregel.



INTRODUCTION



Unfortunately, Pregel is not good with tasks that imply structure. See [6]. (:-) For this reason, we need a number of **aggregators**.

Zhao et al. propose Pregel-Based Frequent Subgraph Mining, a.k.a. **pegi**, which returns a set of frequent subgraphs, starting from a (labeled) graph.

N.B. If g is a subgraph of G, then we will call f(g) an **embedding** of g in G.

1 MACHINE

Algorithm 1: Baseline (G, τ) **Input** : G is a graph; τ is a support threshold. **Output**: *P* is a set of frequent subgraphs, initialized to \emptyset . 1 $P \leftarrow P^1 \leftarrow$ find frequent single edges in G; 2 foreach edge $e \in P^1$ do DFSMine (G, e); Function DFSMine(G, p)enumerate 1-edge extension of p and embeddings; foreach enumerated edge e for p do $p' \leftarrow p \cup \{e\};$ if e is a forward edge with target vertex v then if $\phi_{p'}(v) < \tau$ then continue; if $\phi(p') < \tau \lor p' \in P$ then continue; $P \leftarrow P \cup \{p'\}$; /* find an answer */ DFSMine (G, p'); 10

WMACHINES

Algorithm 2: master. compute()

```
1 switch phase do
        case VERTEX:
            V_f \leftarrow \text{GetAggregatedValue}(frq_v);
 3
            V_f \leftarrow get frequent vertices with images;
            V_t \leftarrow retrieve images of first vertex in V_f;
 5
            Aggregate(nxt_v, V_t);
 6
        case GROW:
 7
            e \leftarrow \mathsf{GrowPattern}(E_c, \Phi);
            Aggregate(nxt_e,e);
 9
       case UPDATE:
10
            V_t \leftarrow \text{GetAggregatedValue}(\text{nxt\_v});
11
            update global embedding tree by adding edges
12
            incident on V_t;
```

MASTER

WORKER

```
Algorithm 3: vertex. compute()
1 switch phase do
      case VERTEX: Aggregate(frq_v, this.l<sub>v</sub>);
      case EXTEND: ExploreEdge(V_t);
      case SUPPORT:
         foreach distinct message m do
             Aggregate(m.e, 1);
      case TARGET:
         if this is backtrack then update local
8
         embedding tree by removing last updated
         edges;
         e ← GetAggregatedValue(nxt_e);
         Aggregate(nxt_v, V_t(e));
10
```



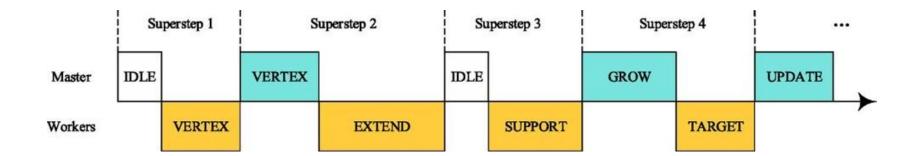
N MACHINES



pattern growth and embedding discovery

- Worker. Send labels of vertices.
- **Master.** Produce set of frequent vertices, that is, frequent subgraphs of size 1. Share target vertex.
- **Worker.** Starting from target vertex, send messages to neighbors.
- **Worker.** Upon receive, compute (local) support, which we share with aggregator.
- **Master.** Select edge to be added.
- Worker. Send embeddings.
- Master. Update embedding trees.
- etc.

FLOW



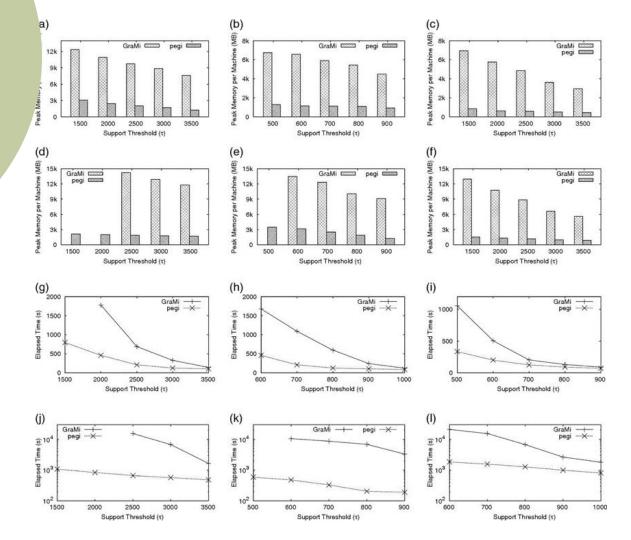


OPTIMIZATIONS

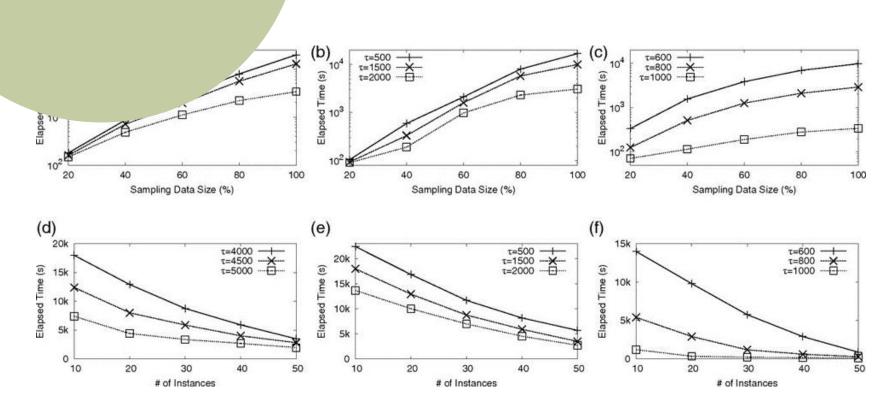


- **+Filter.** If the upper bound of the estimation of the support of *u* is less than the threshold, then we will skip *u*.
- **+Backward.** There is a large number of superstes and barriers. So, we do pattern grow until a new vertex is added.

GraphMi VERSUS pegi



SCALABILITY





GRAPHLETS



Graphlets are, by definition, **induced** subgraphs.

Graphlets enable the analysis of **higher-order** networks, which highlight connections that are in the background. For example, they are used to detect not only **communities** but also **roles**.

In case of graphlet counting, it is necessary

- to **enumerate**; and
- to count.

For example, k = 4. There are two to the power of sixteen (2^{2k}) subgraphs and only six graphlets in this case.

LEGO

It is possible to view a graph as the union of graphlets, instead of vertices and edges.





PARALLEL

Leveraging Multiple GPUs and CPUs for Graphlet Counting in Large Networks



INTRODUCTION



Rossi and Zhou propose an algorithm that is used to count the number of **connected** and **disconnected** graphlets of size $k = \{2, 3, 4\}$ at the graph level and at the edge level.

In comparison with CPUs, GPUs have the advantage of

- higher **performance** in terms of FLOPS, and
- higher **memory bandwidth** in terms of B/s.

Thus, Rossi and Zhou propose a hybrid algorithm, which is able to leverage multiple GPUs and CPUs. Authors present **load balancing** and **work stealing**, too.



VERTEX VERSUS EDGE



Unlike MapReduce and Pregel, which are vertexcentric, Rossi and Zhou propose an algorithm that counts the number of graphlets per edge.

 z_{ii} is the number of graphlets H_i per vertex v_i , x_{ii} is the number of graphlets H_i per edge e_i

$$Z_j = \sum Z_{ij}$$
 and $X_j = \sum X_{ij}$

Of course,

$$Z_j = X_j$$

 $Z_j = X_j$ Since the number of vertices is much less than the number of edges, *i.e.*,

$$N \ll M$$

, the average number of graphlets H_i per edge is less than the average number of graphlets H_i per vertex, i.e.,

$$X_i / M < Z_i / N$$

Overall, an edgecentric algorithm is better at **load balancing** than a vertexcentric algorithm.



GPUs AND CPUs



CPUs and GPUs have both their **pros and cons**.

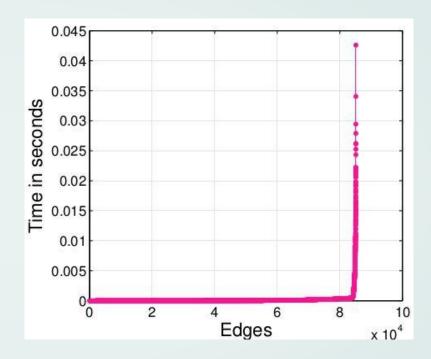
On the one hand, GPUs are, by definition, parallel, and as a result they are able to run a large number of tasks simultaneously. It is worth remembering that they are good at homogeneous tasks.

On the other hand, CPUs are able to run a wide range of tasks.

So, it makes sense to assign edges with a large number of neighbors to CPUs and thus to assign edges with a small number of neighbors to GPUs.

POWER LAW

Networks are known to show a **degree distribution** that is a power law.

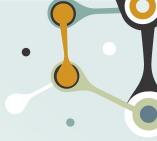


QUEUE

$$\Pi = \{\underbrace{e_1, \dots, e_k, e_{k+1}, \dots, e_{j-1}, e_j, e_{j+1}, \dots, e_M}_{\Pi_{\text{GPUs}}}\}$$



DETAILS



Edges are in descending order of **difficulty**, which is, by definition, proportional to number of neighbors.

$$\Gamma(e) = \Gamma(u, v) = \{\Gamma(u) \cup \Gamma(v) \setminus \{u, v\}\}\$$

The whole idea of graphlet counting is to make processes be independent. That it, we are able to mine neighborhood in parallel.

- **CPUs** are responsible for the first b_{CPUs} in the queue.
- **GPUs** are responsible for the last b_{GPUs}^{GPUs} in the queue. Tasks are assigned in a **round robin**.

$$b_{\text{CPUs}} < b_{\text{GPUs}}$$

Thanks to b_{CPUS} and b_{GPUS} it is possible to switch from single GPU, to multi-GPU, and to hybrid multi-core CPU-GPU.



TRIANGLES, CLIQUES, AND CYCLES



Rossi and Zhou propose a series of algorithms for CPUs and a series of algorithms for GPUs. The whole idea of the article is to make the most of their strength and weaknesses. For example, hash algorithms are used for CPUs and search algorithms are used for GPUs.

- T is the set of vertices that are in triangles with e,
- S_u is the set of vertices that are in **two-stars**, whose center is u, with e,

It is possible to compute the number of graphlets of size $k = \{2, 3, 4\}$ at the edge level and at the graph level, starting from the number of **triangles**, *i.e.*, $\mathbf{X}_{k,3'}$ the number of **cliques**, *i.e.*, $\mathbf{X}_{k,7'}$ and the number of **cycles**, *i.e.*, $\mathbf{X}_{k,10'}$ plus the number of vertices, i.e., N, and the number of edges, i.e., M.

$$\mathbf{X}_{k,3} = |7|$$

 $\mathbf{X}_{k,7}$ and $\mathbf{X}_{k,10'}$ are derived, starting with T and $S_{u'}$ too.

k=3

$$C_{3} = \sum_{e_{k}=(v,u)\in E} \mathbf{X}_{k,3} = \sum_{e_{k}=(v,u)\in E} |T|$$

$$C_{4} = \sum_{e_{k}=(v,u)\in E} |S_{v}| + |S_{u}|$$

$$e_k = \underbrace{|\mathcal{O}v| + |\mathcal{O}u|}_{|\mathcal{O}v| + |\mathcal{O}u|}$$

$$C_5 = \sum_{e_k = (v,u) \in E} N - (|S_v| + |S_u| + |T|) - 2$$

EDGE

It is worth remembering that T and S_u and S_u are known.

GRAPH

N and M are known.

$$X_{3} = \frac{1}{3} \cdot C_{3}$$

$$X_{4} = \frac{1}{2} \cdot C_{4}$$

$$X_{5} = C_{5}$$

$$X_{6} = \binom{N}{3} - (X_{3} + X_{4} + X_{5})$$

$$k=2$$

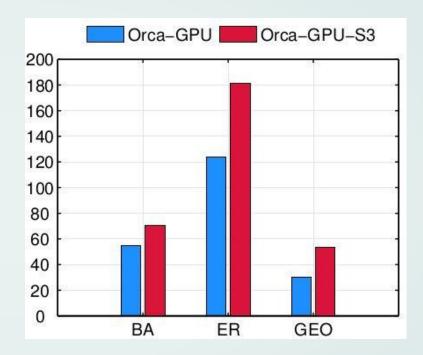
- the number of connected graphlets is equal to the number of edges
- the number of disconnected graphlets is equal to the complementary of the number of edges

$$X_1 = M$$

$$X_2 = \binom{N}{2} - M$$

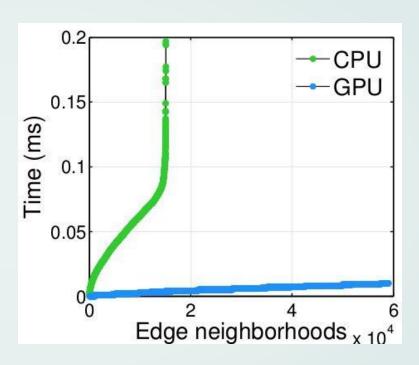
TIME

Compared to [7], which is designed in the single GPU setting, Rossi and Zhou have improved their times by 102%, on average.



DEGREE

In practice, degree provides an accurate estimation of the difficulty.





CONCLUSION





03

MapReduce

Based on MapReduce, it resolves issues that are caused by having a partial knowledge, via Probability.

Pregel

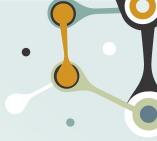
Unfortunately,
Pregel is not good
with
structure-related
tasks. Aggregators
are used for
coordination.

PARALLEL

Both GPUs and CPUs are used for graphlet counting. Also, it moves from vertexcentrism to edgecentrism.



References



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THANKS

Do you have any questions?

Susanna Pozzoli spozzoli@kth.se

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