Parallel Graph Mining with GPUs

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BigMine14 #BigDataMining August 24, New York City

Frequent Subgraph Mining

- Discovering frequent subgraph patterns from a set of graphs (multi-graph) or a single graph.
- Practical applications in biology (PPI network), chemistry (similar compounds), or social networks (similar communities), etc
- The problem is computationally hard as it requires:
  - Enumeration of an exponential number of candidate subgraph patterns
  - Checking their presence in a set of graphs (subgraph isomorphism)
- We address multi-graph problem with Graphics Processing Units

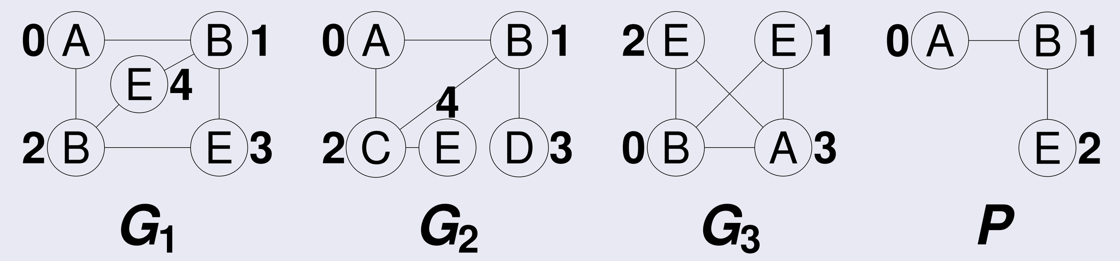


Figure : Graph database, $\mathcal{D} = \{G_1, G_2, G_3\}$ and pattern, P

Support: The number of graphs in $\mathcal{D} = \{G_i, \cdots G_n\}$ that contain P, i.e., $\sigma(P, \mathcal{D}) = |\{G : G \in \mathcal{D}$ and P subgraph isomorphic to $G\}|$.
Frequent Subgraph Mining: Given $\mathcal{D}$ and $minsup \in \mathbb{Z}$, find all frequent subgraph patterns, P, s.t. $\sigma(P, \mathcal{D}) \geq minsup$.

Graphics Processing Units (GPUs)

- GPUs have SIMT (single instruction multi-thread) architecture
- Energy efficient/less expensive choice for general purpose HPC
- Available programming platforms, such as NVIDIA CUDA[1]

Main challenges for graph mining:

- Serialized data for GPU kernels (no linked list or hashmap)
- Global memory coalescing as memory read in thread-groups
- Expensive GPU-CPU I/O transfer and dynamic allocation
- Algorithm steps are transformed into a set of parallel primitives (Prefix sum and Reduction etc.)

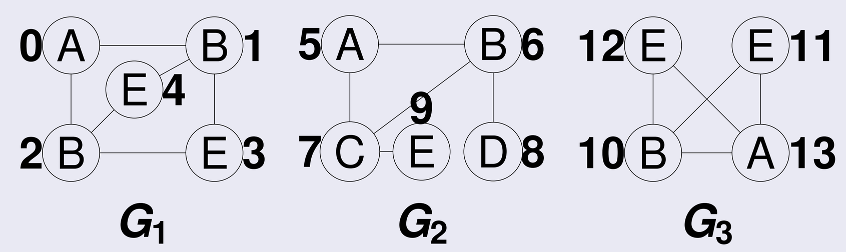
DFS code and Right-most Extension

- Graph mining algorithms [2,3] systematically generate all candidate subgraph patterns starting from a single edge
- gSpan algorithm [2] uses *minimal DFS code* [2] to uniquely represent patterns and avoid duplicates in candidate generation
- Perfoms right-most path extension from a minimal and frequent DFS code (subgraph pattern) by extending an edge
- Our variant keeps all occurences/embeddings [3] of the patterns (original gSpan does not) that grow with patterns

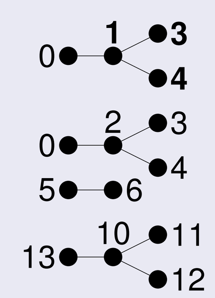
Graph Mining with GPUs

Algorithm: GraphMining($\mathcal{D}$, $minsup$, P, Embeddings $\Sigma_{\mathcal{D}}(P)$)
//Initial Call: $P = \emptyset, \Sigma_{\mathcal{D}}(P) = \emptyset$
(GPU step) Get all possible edges extensions (exts) $\mathcal{E}_{\mathcal{D}}(P)$ of P
(GPU step) Compute support for exts in $\mathcal{E}_{\mathcal{D}}(P)$ and remove infrequent exts
for each $e = (v_i, v_j, l_i, l_{ij}, l_j) \in \mathcal{E}_{\mathcal{D}}(P)$ **do**
  $P' \leftarrow P$ extended by e
  if $P' = minDFS(P')$ **then**
    output P'
    (GPU step) Create $\Sigma_{\mathcal{D}}(P')$
    GraphMining($\mathcal{D}$, $minsup$, P', $\Sigma_{\mathcal{D}}(P')$)
  end if
end for

Data Structures



(a) Graph database $\mathcal{D}$ with *global vertex ids*



Prefix tree rep.

Q_1 idx	Q_1 vid
-1	0
-1	0
-1	5
-1	13

Q_2 idx	Q_2 vid
0	1
1	2
2	6
3	10

Q_3 idx	Q_3 vid
0	3
0	4
1	3
1	4
3	11
3	12

In GPU memory

(b) Embeddings of $P = (0, 1, A, -, B)(1, 2, B, -, E)$

global id	0	1	2	3	4	5	6	7	8	9	10	11	12	13
N	1 2	0 3 4	0 3 4	1 2	1 2	6 7	5 7 8	5 6 9	6	7	11 12 13	10 13	10 11 12	10 11 12

index	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14
O	0	2	5	8	10	12	14	17	20	21	22	25	27	30	-1

(c) GPU representation (partial) of graph database

Figure : Graph database with *global vertex ids* and its storage in GPU memory.

Major GPU Steps

- **Pattern emumeration via embeddings:** Get all valid extensions on the right-most path of P in parallel
  - Look-up the neighborhood of each vertex, and set the entry in a large binary array for a valid forward/backward extension
  - Produce the ordered indexes by prefix sum and store extensions in EXT
  - Threads are allocated in column-major fashion for memory locality
  - EXT are segmented, EXT_k contains all exts from a pattern vertex
  - EXT_k contains blocks of elements corresponding to the same graph

Extensions

k	EXT_0							EXT_1				EXT_2			
v_i^g	0	0	0	0	5	13	13	1	1	6	10	3	4	11	12
v_j^g	2	2	1	1	7	11	12	3	4	8	12	2	2	13	13
l_j	B	B	B	B	C	E	E	E	E	D	E	B	B	A	A
B	0	0	0	1	1	0	0	0	1	1	0	0	1	1	0
scan **B**	0	0	0	0	1	2	2	0	0	1	2	0	0	1	1

Support Computation

	$(0,B)$			$(0,C)$			$(0,E)$			$(1,E)$			$(1,D)$		
F	1	0	0	0	1	0	0	0	1	1	0	1	0	1	0
scan of **F**	1			1			1			2			1		

Figure : The extensions of the pattern $P = (0, 1, A, -, B)(1, 2, B, -, E)$, and support computation of the extensions from vertices **0** and **1**.

Major GPU Steps

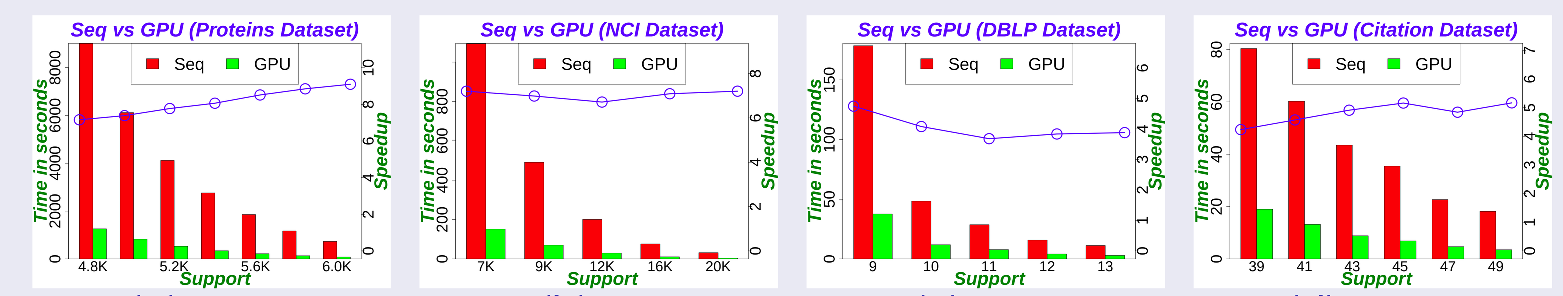
- **Support Computation:** Compute the support of P from the extensions
  - First, extract unique DFS code extensions from EXT
  - Support computation variants are based on the number of extentions processed in parallel : (a) single-ext, (b) single-seg, and (c) multi-seg
  - Number of threads is a bottleneck; single-seg which processes EXT_k demonstrates the best performance
- **Growing the Embeddings:**
  - Forward extensions from EXT_k introduces a new embeddings column
  - For the backward extensions the last embeddings column is filtered

Results

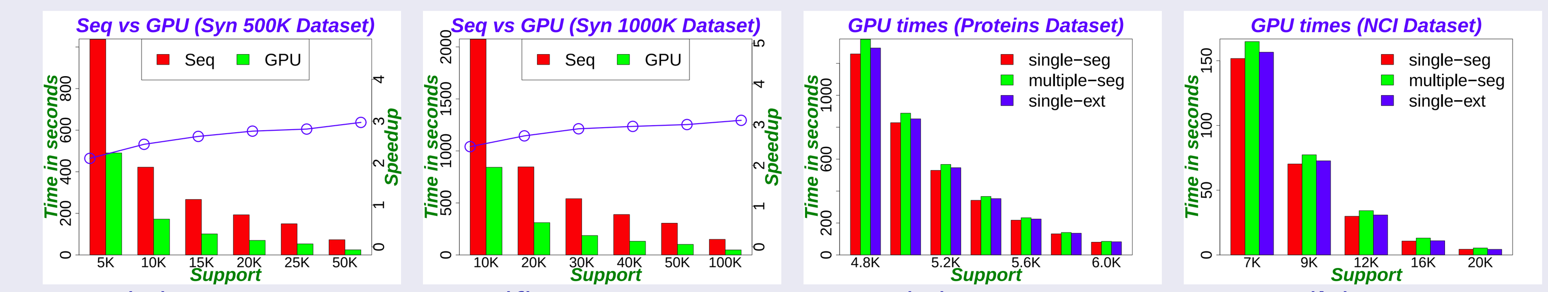
Setup: Sequential - Opteron 2.1GHz (256GB memory SMP 16 cores)
GPU - Tesla C2075 (448 cores and 6GB memory)

dataset	num of graphs	avg. $\lvert V\rvert$	avg. $\lvert E\rvert$	V labels	E labels	avg. deg	avg. clus. coeff.
Citation	81	469	541	15	1	2.042	0.008
Protein	6875	1113	4392	22	1	7.891	0.554
DBLP	21	205	300	26	26	2.796	0.594
NCI	24595	39	78	54	1	3.954	0.0014
Syn500K	500000	25	31	5	5	2.517	0.383
Syn1000K	1000000	25	31	5	5	2.517	0.383

Table : Properties of the datasets



(a) Protein (b) NCI (c) DBLP (d) Citation



(e) Syn 500K (f) Syn 1000K (g) Protein (h) NCI

Conclusions and Future Directions

- GPU memory is constrained for storing embeddings
- Investigate large graph mining in disributed setting
- Explore other accelerators, e.g. Intel Xeon Phi coprocessor

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Acknowledgements: This work was supported in part by NSF Awards CCF-1240646 and IIS-1302231.