Parallel Generation of Transversal Hypergraphs

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joint work with
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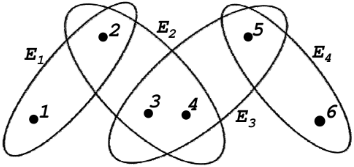
Hypergraphs

- For a finite set V of vertices, $\mathcal{H} = (V, \mathcal{E})$ is a hypergraph if $\mathcal{E}$ (called hyperedges) is a collection of subsets of V.

  Example: $\mathcal{H} = (123456,\ \{12,\ 234,\ 345,\ 56\})$.



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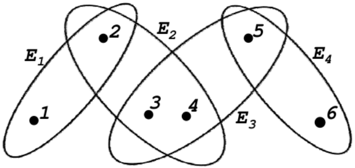

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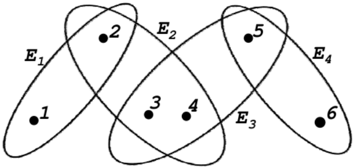

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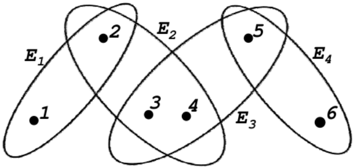

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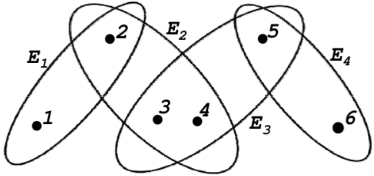
  Example: $\{25\}$ is a minimal transversal of $\mathcal{H}$; $\{235\}$ is a transversal but not minimal.

Transversal Hypergraph Generation (THG)

- The transversal hypergraph $\mathrm{Tr}(\mathcal{H})$ is the family of all minimal transversals of $\mathcal{H}$.

  Example: $\mathcal{H} = (123456, \{12, 234, 345, 56\})$,
  $\mathrm{Tr}(\mathcal{H}) = (123456, \{135, 136, 145, 146, 236, 246, 25\})$.



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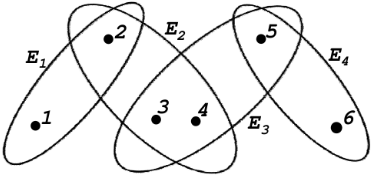

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  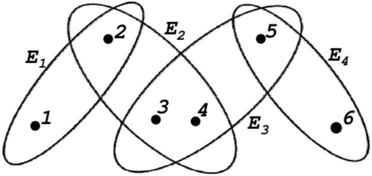

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- **Numerous applications**: data mining, computational biology, artificial intelligence and logic, cryptography, semantic web, mobile communication systems, e-commerce, etc.

THG Application I: Mining Emerging Patterns (1/2)

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- **Example** [Bailey, 2003]: given two classes of transactions
  $A = \{\{a, f, h, j\}, \{c, f, h, j\}, \{b, d, g, j\}, \{c, e, g, j\}\}$,
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  Question: what are the minimal contrasts between them?
  Answer: $\{af, ah, fj, hj\}, \{cj, fj, hj\}, \{b\}, \{ce, cg, cj\}$.

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- **How to find the minimal contrasts**
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- Relationship to hypergraphs: for each transaction t in A, we construct a hypergraph $\mathcal{H} = (V, \mathcal{E})$, where V consists of the elements of t, and $E_i = t \setminus t_i$ for each $t_i \in B$. Then, $\mathrm{Tr}(\mathcal{H})$ corresponds precisely the contrast patterns for t.

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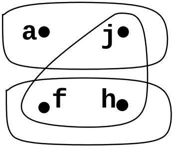
- For instance, for the first transaction in A, we have

  $t = \{a, f, h, j\}$,
  $\mathcal{H} = (afhj, \{fh, fhj, aj, fh\})$,
  $\mathrm{Tr}(\mathcal{H}) = (afhj, \{af, ah, fj, hj\})$



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- Let $Q = \{q_1, \ldots, q_n\}$ be the reactions and $S = \{s_1, \ldots, s_m\}$ the species. A metabolic network can be described by a $m \times n$ matrix N where N_{ij} is the *rate* of s_i in the reaction q_j.

  Example: a metet with 5 reactions and 4 species, and N as

	PYR	NADH	H	LAC	NAD
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H	4	1	1	6	0
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- A *steady state* (or equilibrium) is any vector $\vec{x} \in \mathbb{R}^n$ such that $\vec{x} \neq \vec{O}$ and $N\vec{x} = \vec{O}$.

  Example: $\vec{x} = {}^t\begin{pmatrix} -1 & -1 & -1 & 1 & 1 \end{pmatrix}$.

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- Elementary modes are the fundamental states of a metabolic network. They can be efficiently computed from the matrix N using optimization techniques (Gagneur and Klamt, 2004).

THG Application II: Knock-out Strategies in MetNet

- Let $T \subset Q$ be a set of *target reactions* to be avoided.

  A *cut set* is a subset $C \subset Q$ such that for a steady state $\vec{x}$:

  $$\mathrm{supp}(\vec{x}) \subseteq Q \setminus C \quad \Rightarrow \quad \mathrm{supp}(\vec{x}) \subseteq Q \setminus T$$

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- **Proposition.** Let $\mathcal{E}$ denote the elementary modes X such that $X \cap T \neq \emptyset$. Then, we have:

  $$C \in \mathcal{K} \quad \Longleftrightarrow \quad (\forall X \in \mathcal{E})\ X \cap C \neq \emptyset.$$

  That is, in hypergraph terms, $\mathcal{K} = \mathrm{Tr}(\mathcal{E})$.

THG: State-of-the-Art (1/3)

- Berge (1987): for two hypergraphs $\mathcal{H}' = (V, \mathcal{E}')$ and $\mathcal{H}'' = (V, \mathcal{E}'')$ we have

$$\mathrm{Tr}(\mathcal{H}' \cup \mathcal{H}'') = \mathrm{Min}(\mathrm{Tr}(\mathcal{H}') \vee \mathrm{Tr}(\mathcal{H}'')),$$

where

$$\mathcal{H}' \vee \mathcal{H}'' = (V, \{E' \cup E'' \mid (E', E'') \in \mathcal{E}' \times \mathcal{E}''\}),$$

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This algorithm suggests an **incremental approach**. More precisely, let $\mathcal{E} = \{E_1, \ldots, E_m\}$ and $\mathcal{H}_i = (V, \{E_1, \ldots, E_i\})$ for $i = 1 \cdots m$. Then,

$$\mathrm{Tr}(\mathcal{H}_{i+1}) = \mathrm{Min}(\mathrm{Tr}(\mathcal{H}_i) \vee (V, \{\{v\} \mid v \in E_{i+1}\})).$$

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- **Fredman and Khachiyan**'s algorithm (1996), implemented by **Boros, Elbassioni, Gurvich and Khachiyan** (BEGK03):
  – test the duality of a pair of monotone boolean functions;
  – incremental quasi-polynomial time algorithm.

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- **Kavvadias and Stavropoulos** (KS05):
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- **Lower Bounds**:
  Takata (2007): Berge's algorithm is not output-polynomial;
  Hagen (2008): None of BMR03, DL05 and KS05 is.

Our Parallel Transversal Algorithm: ParTran

- Apply Berge's formula in a divide-n-conquer manner where $\mathcal{H}'$ and $\mathcal{H}''$ are of similar order.

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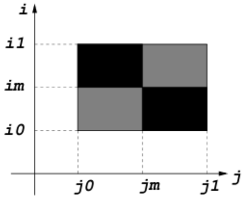

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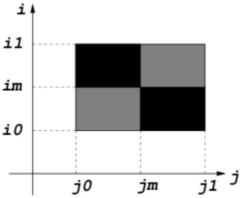

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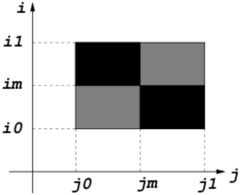


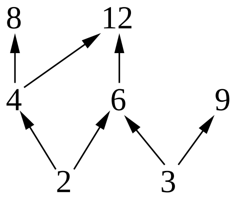
- Compute Min, again in a divide-n-conquer manner.
- Parallelism is created by the divide-n-conquer recursive calls.

The Core Operation: Min

- We describe a procedure ParMinPoset, in the following, for parallel computation of the minimal elements of a partially ordered set.
- Our computations for $\mathrm{Tr}(\mathcal{H})$ and $\mathcal{H}' \vee \mathcal{H}''$ follow the same scheme.

Partially Ordered Set (POSET)

- $(A, \preceq)$ is a poset if $\preceq$ is a binary relation on A which is reflexive, antisymmetric, and transitive.
- $x \in A$ is **minimal** for $\preceq$ if for all $y \in A$ we have: $y \preceq x \;\Rightarrow y = x$.
- $\mathrm{Min}(A, \preceq)$, or simply $\mathrm{Min}(A)$ designates the set of the minimal elements of A.
- A poset example for the integer divisibility relation:



A Simple Procedure but ...

Algorithm 1: SerMinPoset

Input : a poset $A = \{a_0, \cdots, a_{n-1}\}$
Output : Min(A)

for *i from* 0 *to* $n-2$ **do**
    if a_i *is not* `marked` **then**
        for *j from* $i+1$ *to* $n-1$ **do**
            if a_j *is not* `marked` **then**
                if $a_j \preceq a_i$ **then**
                    mark a_i; break inner loop
                if $a_i \preceq a_j$ **then**
                    mark a_j

$A \leftarrow$ {unmarked elements in A}
return A

- Poor locality: A is scanned for n times, $Q(n) = \Theta(n^2/L)$.
- Parallelizing these loops require **locks**.

Challenges and Solutions

- Improve data locality, say cache complexity $Q(n) \in O(\frac{n^2}{ZL})$ instead of $\Theta(n^2/L)$; Z and L are the cache size and line size.
- Load balancing.
- Obtain good scalability on multi-cores.
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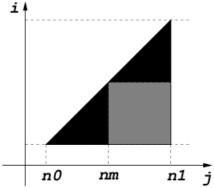
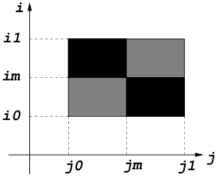




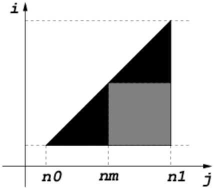
- Traverse the iteration space in a divide-n-conquer manner (Matteo Frigo's techniques for cache oblivious stencil computations and N-body problems (2005)).
- Generate A and compute $\mathrm{Min}(A)$ concurrently.

Parallel Min Algorithm

Algorithm 2: ParMinPoset(A)

if $|A| \leq MIN\_BASE$ **then**
  return SerMinPoset(A)
$(A^-, A^+) \leftarrow$ Split(A)
$A^- \leftarrow$ **spawn** ParMinPoset(A^-)
$A^+ \leftarrow$ **spawn** ParMinPoset(A^+)
sync
$(A^-, A^+) \leftarrow$ ParMinMerge(A^-, A^+)
return Union(A^-, A^+)

*MIN_BASE must be large enough to **reduce parallelization overheads** and small enough to **increase data locality**.



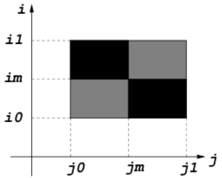
Parallel Merge of Min(B) and Min(C) (1/2)

Algorithm 3: ParMinMerge(B, C) for Min(B) $= B$ and Min(C) $= C$

if $|B| \leq$ MIN_MERGE_BASE *and* $|C| \leq$ MIN_MERGE_BASE **then**
  return SerMinMerge(B, C)

else if $|B| >$ MIN_MERGE_BASE *and* $|C| >$ MIN_MERGE_BASE **then**
  $(B^-, B^+) \leftarrow$ Split(B); $(C^-, C^+) \leftarrow$ Split(C)
  $(B^-, C^-) \leftarrow$ **spawn** ParMinMerge(B^-, C^-)
  $(B^+, C^+) \leftarrow$ **spawn** ParMinMerge(B^+, C^+)
  sync
  $(B^-, C^+) \leftarrow$ **spawn** ParMinMerge(B^-, C^+)
  $(B^+, C^-) \leftarrow$ **spawn** ParMinMerge(B^+, C^-)
  sync
  return (Union(B^-, B^+), Union(C^-, C^+))

. . . .



Parallel Merge of Min(B) and Min(C) (2/2)

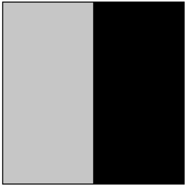
Algorithm 4: ParMinMerge(B, C) for Min(B) $= B$ and Min(C) $= C$

if $|B| \leq$ MIN_MERGE_BASE *and* $|C| \leq$ MIN_MERGE_BASE **then**
  . . . .

else if $|B| >$ MIN_MERGE_BASE *and* $|C| >$ MIN_MERGE_BASE **then**
  . . . .

else if $|B| >$ MIN_MERGE_BASE *and* $|C| \leq$ MIN_MERGE_BASE **then**
  $(B^-, B^+) \leftarrow$ Split(B)
  $(B^-, C) \leftarrow$ ParMinMerge(B^-, C)
  $(B^+, C) \leftarrow$ ParMinMerge(B^+, C)
  return (Union(B^-, B^+), C)

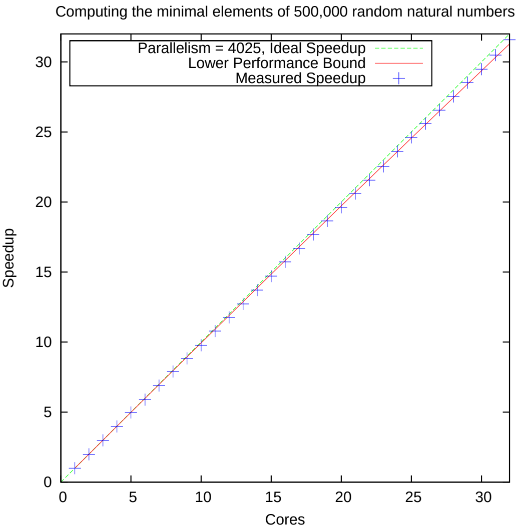
. . . .



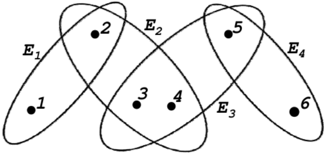
Complexity Results

- Our results are for the fork-join multi-threading parallelism (M. Frigo, C. E. Leiserson, and K. H. Randall, 1998) and the ideal cache model (M. Frigo, C. E. Leiserson, H. Prokop, & S. Ramachandran, 1999)
- The worst case occurs when $A = \mathrm{Min}(A)$ holds.
- In this case, setting all thresholds to one, we have:
  - the cache complexity $Q(n) \in \Theta(\frac{n^2}{ZL} + \frac{n}{L})$
  - the work $T_1(n) \in \Theta(n^2)$
  - the critical path (or span) $T_\infty(n) \in \Theta(n)$
  - and thus the parallelism is $\Theta(n)$

Scalability Analysis by Cilkview



ParTran: Example



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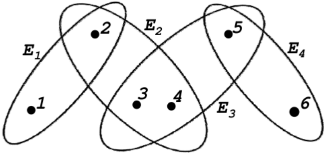

- $\mathrm{Tr}(\mathcal{H}) = \mathrm{Min}(\mathrm{Tr}(E_1 \cup E_2) \vee \mathrm{Tr}(E_3 \cup E_4))$

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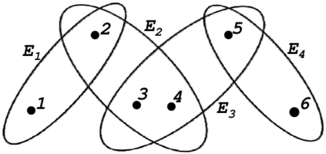

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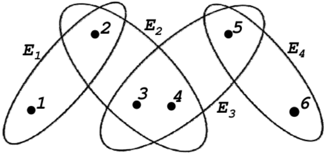

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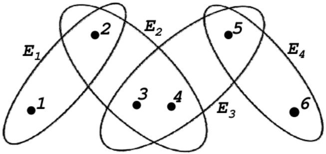

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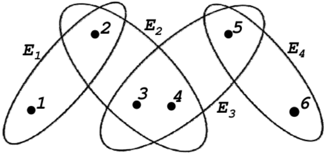
  $= \mathrm{MinMerge}(\{12, 13, 24\}, \{14, 2\}) = \{\mathbf{13}, \mathbf{14}, \mathbf{2}\}$

  $\mathrm{Min}(\{3, 4, 5\} \vee \{5, 6\})$
  $= \mathrm{MinMerge}(\cdots) = \cdots = \{\mathbf{36}, \mathbf{46}, \mathbf{5}\}$

ParTran: Example



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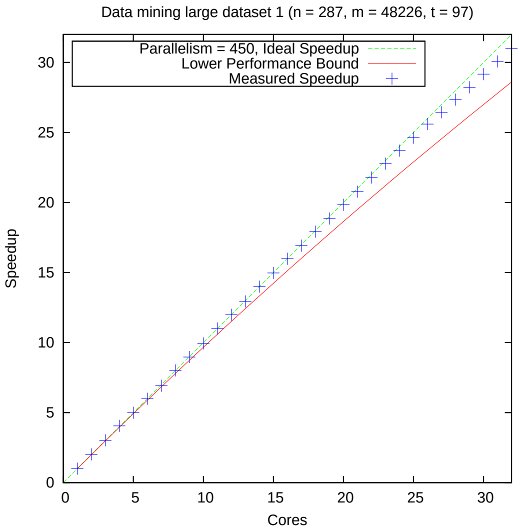
  $= \mathrm{Min}(\{13, 14, 2\} \vee \{36, 46, 5\}) = \mathrm{MinMerge}(\cdots)$
  $= \{\mathbf{135}, \mathbf{136}, \mathbf{145}, \mathbf{146}, \mathbf{236}, \mathbf{246}, \mathbf{25}\}$

Solving some Well-known Problems

Parameters			BEGK	BMR	*KS	ParTran		ParTran's Gain	
n	m	t	(s)	(s)	(s)	1P(s)	32P(s)	KS/1P	KS/32P
Threshold hypergraphs									
140	4900	71	22	194	11	0.01	-	1000	-
160	6400	81	40	460	23	0.01	-	2000	-
180	8100	91	75	1000	44	0.01	-	4000	-
200	10000	101	289	1968	82	0.02	-	4000	-
Dual Matching hypergraphs									
34	131072	17	911	2360	57	9	0.6	6	100
36	262144	18	2188	12463	197	23	1.8	9	110
38	524288	19	8756	36600	655	56	3.5	12	186
40	1048576	20	35171	201142	2167	131	7.1	17	304
Data Mining hypergraphs									
287	48226	97	1332	1241	1648	92	3	18	549
287	92699	99	4388	4280	6672	651	21	10	318
287	108721	99	5898	7238	9331	1146	36	8	259

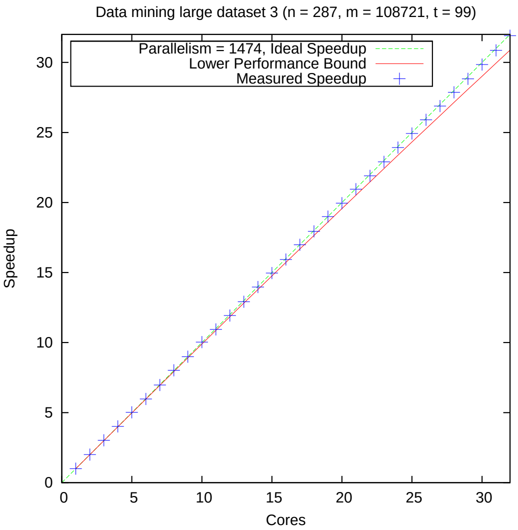
*KS: Kavvadias and Stavropoulos, http://lca.ceid.upatras.gr/estavrop/transversal/.
(Journal of Graph Algorithms and Applications, 9(2):239-264, 2005).

Scalability Analysis by Cilkview



ParTran for data mining problem #1

Scalability Analysis by Cilkview



ParTran for data mining problem #3

Solving some Classical Hypergraphs

Kuratowski Hypergraphs (K_n^r)

Parameters				KS	ParTran				
n	r	m	t	(s)	1P	16P		32P	
					(s)	(s)	Speedup	(s)	Speedup
30	5	142506	27405	6500	88	6	14.7	3.5	25.0
40	5	658008	91390	>15 hr	915	58	15.8	30	30.5
30	7	2035800	593775	>15 hr	72465	4648	15.6	2320	31.2

Lovasz Hypergraphs

Parameters				KS	ParTran				
n	r	m	t	(s)	1P	16P		32P	
					(s)	(s)	Speedup	(s)	Speedup
36	8	69281	69281	8000	119	13	8.9	10	11.5
45	9	623530	623530	>15 hr	8765	609	14.2	347	25.3
55	10	6235301	6235301	>15 hr	-	60509	-	30596	-

Conclusion and Work in Progress

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Conclusion and Work in Progress

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- Our program performs well on a number of large problems.
- We have identified the *computation of the minimal elements of a poset* as a core routine in many applications. Up to our knowledge, we provide the first parallel and cache-efficient algorithm for this task.
- Work in progress:
  - apply the techniques of Kavvadias and Stavropoulos (and others) to improve the performance of our program for some small size hypergraphs.
  - attack other graph-theoretic algorithms and their applications.

Acknowledgements

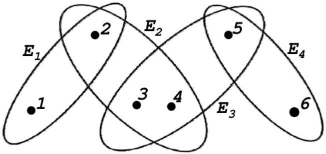
Sincere thanks to our colleagues Dimitris J. Kavvadias and Elias C. Stavropoulos for providing us with their program (implementing the KS algorithm) and their test suits in a timely manner.

We are grateful to Matteo Frigo for fruitful discussions on cache-oblivious algorithms and Cilk++.

Our benchmarks were made possible by the dedicated resource program of SHARCNET.

Thank you!

Incremental Approach: Example



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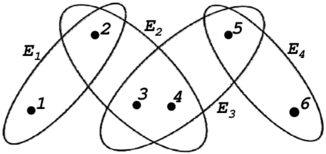

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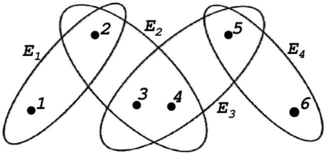

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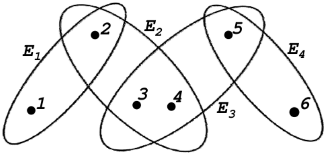

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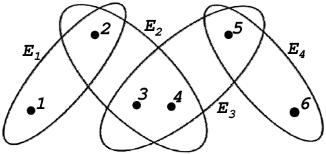
Incremental Approach: Example



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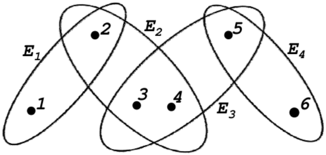

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Note: the growth of the intermediate expression!

Parallel $\mathrm{Tr}(\mathcal{H})$ Top Algorithm

Algorithm 5: ParTran

if $|\mathcal{H}| \leq$ TR_BASE **then**
  return SerTran($\mathcal{H}$);
$(\mathcal{H}^-, \mathcal{H}^+) \leftarrow$ Split($\mathcal{H}$)
$\mathcal{H}^- \leftarrow$ **spawn** ParTran($\mathcal{H}^-$)
$\mathcal{H}^+ \leftarrow$ **spawn** ParTran($\mathcal{H}^+$)
sync
return ParHypMerge($\mathcal{H}^-, \mathcal{H}^+$)