Disk-Based Parallel Computing: A New Paradigm

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Experience at Interactive, Parallel Computational Algebra

- I: What do we want and what can we expect from applying parallel techniques to pure mathematical research tools?
- 1. ParGAP: Parallel GAP, 1995 DIMACS Workshop
- 2. ParGCL: Parallel GCL (GNU Common Lisp/parallel Maxima), 1995 ISSAC-95: STAR/MPI
- 3. Marshalgen for C/C++; 2003-2004 (Nguyen, Ke, Wu and Cooperman); Like pickling for python, serialization for Java; but now, use **Boost.serialization** for C/C++: http://www.boost.org/libs/serialization/doc/index.html
- 4. DMTCP: Distributed Multi-Threaded Checkpointing, 2007 (alpha version: Ansel, Rieker and Cooperman); checkpoint-restart = saveWorkspace/loadWorkspace
- 1. SCIEnce Project: Symbolic Computation Infrastructure in Europe, 2006-2011 (consortium) http://symbolic-computing.org

Experience at Interactive, Parallel Computational Algebra (Others)

I: What do we want and what can we expect from applying parallel techniques to pure mathematical research tools?

- Symbolic Computing over Grid: SCIEnce, 2006- 2011 (U. St. Andrews, RISC-Linz, IeAT-Timisoara, Eindhoven, Tech. Uni. Berlin, Uni-Paderborn, Ecole Polytechnique, Heriot-Watt, MapleSof) http://symbolic-computing.org
 year 3.2M euro Framework VI Project (RII3-CT-2005-026133) Goal: produce a portable framework (SymGrid-Services) that will ... Maple, GAP, muPad, KANT
- 2. Meat-Axe



Meataxe: Origins

Efficient Computation with Dense matrices over finite fields:

- First versions of the meataxe (1970's): based around compact representations of vectors over small finite fields (multiple field entries per byte when appropriate) and efficient vector addition and scalar-vector multiply algorithms.
- Next innovation (1980s and early 1990s): grease precompute all (or sometimes just some) linear combinations of a block of rows. In A += B*C, grease blocks of C.
- Around 2000, Jon Thackray started reorganizing the greased multiply working with blocks of rows of B to improve locality of memory access when working from disk, and to improve cache hit ratios.



Meataxe: New Development in C/Assembly Libraries

Steve Linton, Beth Holmes and Richard Parker
{sal,bh}@mcs.st-and.ac.uk,rparker@amadeuscapital.com

Greasing large matrices; key is multiply-add:



Subdivide A and B vertically and C in both directions. Fill L2 cache with pre-computed linear combinations of rows from the purple block of C. Work sequentially through red and blue strips modifying red strip. Repeat for all pair of strips of A and B.

- Highly optimized representations for matrices and low-level vector arithmetic (field-specific).
- Gaussian elimination can be efficiently reduced to multiply-adds.
- Random 25000x25000 dense matrices over GF(2) multiply in 50 s on Pentium 4/2.4 GHz (about 7 times faster than previously).



Software Demonstrations

1. ParGAP: Parallel GAP, 1995

http://www.ccs.neu.edu/home/gene/pargap.html
http://www.gap-system.org/Packages/pargap.html

- 2. ParGCL: Parallel GCL (GNU Common Lisp, parallel Maxima), 1995 http://www.ccs.neu.edu/home/gene/pargcl.html Compatible with older GCLs and with upcoming GCL-2.7: http://www.gnu.org/software/gcl/
- 3. DMTCP: Distributed Multi-Threaded Checkpointing, 2007 (alpha version: Ansel, Rieker and Cooperman);
 checkpoint-restart = saveWorkspace/loadWorkspace
 GPL; write to request a beta test copy when available
- 4. TOP-C/C++: Task Oriented Parallel C/C++, 1996 Easy task farming in C/C++; http://www.ccs.neu.edu/home/gene/topc.html



ParGAP

```
SendMsg( "Print(3+4)"); # send to slave 1 by default
SendMsq( "3+4", 2); # send to slave 2
RecvMsq(2);
SendRecvMsg( "3+4", 2);
squares := ParList( [1..100], x->x^2 );
SendRecvMsg( "Exec(\"pwd\")" ); # Your pwd will differ :-)
SendRecvMsg( "x:=0; for i in [1..10] do x:=x+i; od; x");
SendRecvMsg( "fro i in [1..10]; x:=x+1; od"); #syntax error tolerated
SendRecvMsq( "a:=45", 1);
SendRecvMsg( "a", 2); # "a" undefined, error-tolerant
myfnc := function() return 42; end;;
BroadcastMsg( PrintToString( "myfnc := ", myfnc ));
SendRecvMsq( "myfnc()", 1 );
FlushAllMsgs();
SendMsg( "while true do od;"); # start infinite loop
ParReset();
```



ParGCL

Similar capability for GCL: GNU Common Lisp; NOTE: Maxima based on GCL

```
(send-message '(print (+ 3 4)))
(send-message "(+ 3 4)" 2)
(receive-message 2)
(flush-all-messages)
(par-reset)
(send-receive-message '(progn (setq a 45) (+ 3 4)) 1)
```



DMTCP: Distirbuted Multi-Threaded Checkpointing

Alpha version of DMTCP:

- # Assume on startHost and initially using startPort
- ./dmtcp_master # start DMTCP checkpoint controller
- # Separate window:
- ./dmtcp_checkpoint sh pargap.sh
- # Request checkpoint of dmtcp_master (or request periodic ckpt)
- # After a checkpoint, can quit, or allow software to crash

./dmtcp_master # start new DMTCP controller

./dmtcp_restart ckpt_gap_17436930_2326_1170308795.mtcp \

ckpt_gap_17436930_2333_1170308795.mtcp \ ckpt_gap_17436930_2334_1170308795.mtcp

ssh remoteHost

- # Continue calling dmtcp_restart
- # Computation resumes after last process restarted



TOP-C: Task Oriented Parallel C/C++

Simple task farming in C/C++, plus extensions for *non-trivial* parallelism



TOP-C from the Command Line

./topcc --mpi myapp.c
[OR: ./topcc --pthread myapp.c
OR: ./topcc --seq myapp.c]

./a.out --TOPC-help

G. Cooperman, "TOP-C: A Task-Oriented Parallel C Interface", 5th International Symposium on High Performance Distributed Computing (HPDC-5), 1996, IEEE Press, pp. 141–150



Running TOP-C

./topcc -c -g -O2 /tmp/topc-2.5.0/examples/parfactor.c

- ./topcc -g -O2 parfactor.o
- ./a.out 123456789

```
FACTORING 123456789
master \rightarrow 1: 2
master -> 2: 1002
master -> 3: 2002
master -> 4: 3002
master -> 5: 4002
1 -> master: TRUE
  UPDATE: TRUE
master -> 1: 5002
. . .
2 -> master: FALSE
3 -> master: FALSE
3 3 3607 3803
```



Getting Help with TOP-C

gene@auditor:/tmp/topc-2.5.0/bin\$./a.out --TOPC-help

TOP-C Version 2.5.0 (September, 2004); (distributed (mpi) memory model) Usage: ./a.out [[TOPC_OPTION | APPLICATION_OPTION] ...] --TOPC-stats[=<0/1>] display stats before and after [default: false] --TOPC-verbose[=<0/1>] set verbose mode [default: false] --TOPC-num-slaves=<int> number of slaves (sys-defined default) --TOPC-aggregated-tasks=<int> number of tasks to aggregate [default: 1] --TOPC-slave-wait=<int> secs before slave starts (use w/ gdb attach) --TOPC-slave-timeout=<int> dist mem: secs to die if no msgs, 0=never [default: 1800] --TOPC-trace=<int> trace (0: notrace, 1: trace, 2: user trace fncs.) --TOPC-procgroup=<string> procgroup file (--mpi) [default: "./procgroup"] --TOPC-safety=<int> [0..20]: higher turns off optimizations,

The environment variable TOPC_OPTS and the init file ~/.topcrc are also examined for options (format: --TOPC-xxx ...). You can change the defaults in the application source code.



First-Ever Computations Using TOP-C Model/Tools

DOSIV threads	eads MPI (Message Passing Interface)	
TOP-C (shared mem.)	TOP-C (dist. mem.)	
<i>Ly</i> coset enum. (8,835,156 cosets)	Parallelization of GNU Common Lisp (GCL) Parallelization of GAP (Groups, Algorithms and Programming) Parallelization of Geant4	J_4 condensation (from perm deg. 173,067,389 to matrix dim. 5,693) (over $GL(112,2)$) Ly perm. rep. (deg. 9,606,125) (over $GL(111,5)$)
	Baby Monster perm. rep. (deg. $\approx 1.3 \times 10^{10}$) (over $GL(4370,2)$) J ₄ perm. rep. (deg. 173,067,389) (over $GL(1333,11)$)	Th condensation (from perm deg. 976,841,775 to matrix dim. 1,403) (over $GL(248,2)$)



Paradox: Interactive, Parallel Computation

- Paradox 1:
 - 1. Parallel Computing is good for accelerating long-running jobs.
 - 2. Interactive Computing is good for computationally steering a sequence of short jobs.
- Paradox 2:
 - 1. Large parallel jobs require reservation of large resources by placing job in a batch queue.
 - 2. Interactive jobs require immediate access to resources.
- Paradox 3:
 - Long-running jobs in computer algebra often generate large intermediate swell; computations overflow from RAM to disk



Different cases

- 1. Large resources (1000+) CPUs is not currently an interactive job
- 2. Moderate resources on a medium-size cluster can be used interactively, but one wants to save the "parallel workspace", while thinking about the problem, and then return later. REQUIREMENT: checkpointing
- 3. Multi-core CPUs on a desktop one ideally wants thread parallelism, to save on use of RAM and cache; This will become especially important with 4-core and 8-core CPUs.



William Stein's Question:

Parallel Implementations of Common Algorithms are Not in Standard Use Today. WHY?

1. 2-core desktop/laptop:

Advantage: twice the speed; *Disadvantage:* must learn a parallel programming tool; *Interactive computation:* twice the speed = 1 second per step instead of 2 second per step — not enough reward to overcome the learning barrier.

2. medium-size cluster (32 CPUs?):

- (a) **Task farming:** low barrier to entry *if someone else sets up the software*.
- (b) **Parallel programming:** high barrier to entry, but potential high rewards requires a new generation more accustomed to the tools??
- (c) **Checkpointing = SaveWorkspace:** highly desirable for long interactive sessions
- 3. large cluster (1000+ CPUs): *interactive computing*?????



PART II: Disk-Based Parallel Computing



Disk as the New RAM

Bandwidth of RAM: 3.2 GB/s (PC-3200 RAM, single channel) Bandwidth of Disk: ~ 50 MB/s Bandwidth of Cluster of 64 nodes: 3.2 GB/s

Issues: Bandwidth of Network, ability of CPU to keep up



Disk: the New RAM (example)

Initial Testbed: large search and enumeration

- Key data structure: sorted array
- Key algorithm: sorting ⇒ merge, union, intersection
 (sorting on disk done as external sort: 4 passes in practice; fewer
 passes when there are opportunities to pipeline it with previous phase
 of computation)

Problem: Insertion of new elements

Solution: Defer insertions; sort elements to insert; and merge them into sorted array in large batch



Duplicate Elimination in Baby Monster

Optimization: eliminate duplicate insertions before merge; Use a new hash array in RAM to accumulate elements to insert. Need only store one bit per hash element: 1 =present; 0 =not present

Example: AI search: enumeration of states via open queue, as in breadth-first search

- 1. If element to insert hashes to 0, it is new; add to open queue on disk
- 2. If element to insert hashes to 1, it is either a hash collision or a duplicate: add to *collision queue* on disk
- 3. Continue to read from open queue and hash its neighbors: neighbors will also be stored either in open queue or collision queue
- 4. sort collision queue and eliminate duplicates
- 5. sort open queue
- 6. merge collision queue, open queue and original sorted array on disk
- 7. elements of collision queue that are determined to be new become the next open queue, and we repeat step 1.



Duplicate Elimination in Baby Monster (case 2)

- Hash array too large for RAM; must be stored on disk
 - 1. All new elements to insert are saved on disk in open queue
 - 2. As neighbors of elements in open queue are expanded, portions of the open queue are transferred into a closed set
 - 3. The closed set is then externally sorted according to hash index
 - 4. The closed set is then merged into the existing hash array

NOTE: Both RAM-based and disk-based hash arrays adapt easily to distributed computing. Each node is responsible for a contiguous sequence of hash indexes.



Times for Different Phases of Baby Monster Computation

(joint work, Eric Robinson and C.)

Manager	Disk Time	CPU/RAM Time	Network Time
Read/Write	0.5 days	0 days	
Computation	0 days	3 days	2 days
Check	0 days	0 days	
Hash	$\ll 1 \text{ day}$	$\ll 1 \text{ day}$	—
Formatting/Sorting	$\ll 1 \text{ day}$	$\ll 1 \text{ day}$	
Duplicate Elimination	$\ll 1 \text{ day}$	< 1 day	—
Rebuilding	$\ll 1 \text{ day}$	6 days	—
Approximate Total	2 days	10 days	2 days

NOTE: Uses approximately 7 terabytes of disk space

NOTE: Between CPU time and RAM bandwidth, the computation is primarily limited by RAM bandwidth.

Using faster CPUs has almost no benefit! (Only faster RAM helps.)



Application: Search and Enumeration Problems

Branch-and-Bound, A* search

Given a state, and a generator/operation, produce a new state This gives rise to a natural graph in which nodes correspond to states, and edges are labelled by generators or operations. A search/enumeration proceeds by breadth-first search, developing a spanning tree. Potential applications (some of it is future work):

- Enumeration of Orbit Elements
- Orderly Generation of Brendan McKay (symmetry and search)
- Gröbner bases, Knuth-Bendix, similar "completion algorithms"
- SAT (satisfiability) *Example use: VLSI circuit verification*
- Integer Programming Example use: Travelling Salesman Problem, Airline schedules



Disk-Based Computation

General Philosophy in case of Search:



	Two-Bit Trick	Î	Memory
Space	Landmarks (A) Landmarks (B)	Time	Disk
	Disk-Based Hash Imperfect Hash		Infeasible



Two-Bit Trick

- Assumes dense, perfect hash function w/ inverses (no hash collisions)
- Breadth-first search, storing level of node *modulo 3* of spanning tree in hash table (2 bits/node)
- Given a node, can now find minimal length path to origin:
 - 1. Look up level of current state in hash table
 - 2. Given state, use operators to find all neighbors of node
 - 3. Look up levels of all neighboring states in hash table
 - 4. Choose a state whose level is one less than the current level, modulo 3
 - 5. Repeat on the newly chosen state

Showed Rubik's $2 \times 2 \times 2$ cube (corners, only) always solvable in 11 moves. Used 1 MB on a SUN-3 workstation having only 4 MB of RAM. G. Cooperman, L. Finkelstein, and N. Sarawagi, Applications of Cayley Graphs, Algebra, Algebraic Algorithms and Error-Correcting Codes (AAECC-8), Springer-Verlag Lecture Notes in Computer Science **508**, pp. 367–378, 1990. (Also in G. Cooperman and L. Finkelstein. "New methods for using Cayley graphs in interconnection networks", *Discrete Applied Mathematics*, **37/38**, pp. 95–118, 1992.)



Disk-Based Computation

- 1. Data Structure: Distributed Database of Key-Value Pairs
- 2. Building Blocks: Algorithmic Subroutines
- 3. Integration into General Search Routines
- 4. Example Large Computations: Baby Monster; Rubik's Cube
- 5. Other Applications
- 6. Natural API (in progress)



Disk-Based Computation

- 1. Data Structure: Distributed Database of Key-Value Pairs
 - (a) Goals
 - i. Key-Values: Set(key, value); Get(key); Delete(key)
 - ii. Duplicate Elimination
 - (b) Data Structures for Database
 - i. Distributed Hash Array
 - ii. Distributed Sorted Array
 - iii. Double Hashed Array: (hybrid of above two data structures)
- 2. Building Blocks: Algorithmic Subroutines



Disk-Based Computation

- 1. Data Structure: Distributed Database of Key-Value Pairs
 - (a) Goals
 - (b) Data Structures for Database

2. Building Blocks: Algorithmic Subroutines

distributed hashing, sorting, duplicate elimination, binary search, batching of queries, pipelining of computations, striped access to distributed data structures, on-the-fly compression and expansion of data structures, Bloom filters, two-phase commit in support of persistent data, structures, ...



Disk-Based Computation

- 1. Data Structure: Distributed Database of Key-Value Pairs
 - (a) Goals
 - (b) Data Structures for Database
- 2. Building Blocks: Algorithmic Subroutines
 - (a) **EXAMPLE: Bloom filters:** Use hash array with only one bit per hash entry; We wish only to record if key is present or not present in hash table; Use *k* hash functions, and for a given key, set *k* bits of hash table (one bit for each hash function); To test presence of key, test all *k* bits; This greatly reduces hash collisions.



Disk-Based Computation

1. Data Structure: Distributed Database of Key-Value Pairs

ii. Data Structures for Database

- i. Distributed Hash Array: Good for key-value database Batching of queries important for efficiency
- ii. Distributed Sorted Array: Good for duplicate elimination Given source of new key-values, externally sort it, and compare with original sorted array; Merge on the fly
- iii. Doubly Hashed Array: Good for duplicate elimination
 Key-value pairs stored in buckets, based on high bits of hash index;
 High bits also determines node to hold bucket;
 Key-value pair stored unsorted in bucket; For duplicate elimination,
 sort elements of bucket in RAM
- 2. Building Blocks: Algorithmic Subroutines



Disk-Based Computation

- 4. Example Large Computations:
 - (a) Construction of Permutation Representation of Baby Monster GOAL: enumerate al 13,571,955,000 "points"
 Each point given asvector of dimenstion 4,370 over GF(2) (547 bytes per "point")
 STORAGE: about 7 terabytes (13, 571, 955, 000 × 547 bytes)
 TIME: About 750 hours BOTTLENECK: RAM: limited by speed of reading vectors/matrices from RAM for matrix-vector multiplication
 - (b) Rubik's Cube



Disk-Based Computation

- 4. Example Large Computations:
 - (a) Construction of Permutation Representation of Baby Monster
 - (b) Rubik's Cube

 4.3×10^{19} states

Square subgroup of about 6.6×10^5 elements

SUBGOAL: enumerate all 6.5×10^{13} cosets $(4.3 \times 10^{19}/(6.6 \times 10^5))$

Reduction: Only enumerate cosets up to symmetries of cube

About 1.5×10^{12} symmetrized cosets

STORAGE: 1 byte per symmetrized coset (1.5 terabytes) times a factor of at least two for frontier expansion in search



Disk-Based Computation

5. Other Applications:

- (a) Integer Programming Example use: Travelling Salesman Problem, Airline schedules
- (b) SAT (satisfiability) Example use: VLSI circuit verification
- (c) Applications to distributed linear algebra
- 1. Natural API (in progress)



Why are CPU vendors selling multi-core instead of faster CPUs?

- Speed of electrical signal: $\approx 10^9$ cm/s
- 1 GHz clock rate
- Distance travelled by electrical signal in one clock cycle: $\approx 1 \text{ cm}$
- Chip linear dimension: $\approx 1 \text{ cm}$



Moore's Law (every 18 months)

- Twice as many gates/mm²
- Twice the clock speed
- Half the distance travelled by electrical signal per clock cycle



2000: New millenium

Define a chip unit as a chip rectangle such that an electrical signal can cross the diagonal in one clock cycle.



 \longleftrightarrow : distance travelled by eletrical signal in one clock cycle



mid-2001: 1.5 years later



1) 4 times as many units

2) Twice as many total gates $\Rightarrow 1/2$ as many gates/unit



2009: 9 years later



1) 4,096 times as many units

2) 64 times as many total gates \Rightarrow 1/64 as many gates/unit



Common sense check

- 1985 1995: pipelining
- 1990 2000: superscalar CPU's, ILP (Instruction Level Parallelism)
- 2000: Intel/H-P Itanium, EPIC (Explicitly Parallel Instruction Computer)
- 2002: Simultaneous MultiThreading: Intel Xeon Pentium-4 (Hyper-Threading)
- 2002: Dual Core Chips: IBM Power4
- 2005: Mainstream Dual Core: AMD/Intel, IBM Power5 (dual core + simultaneous multithreading = 4 processors)
- 2006: Cell Architecture (Playstation 3): Sony/Toshiba/IBM (1 core + 8 vector processors on-chip pipelined parallelism support)
- 2010: IRAM (?), CRAM (?)



Memory Wall

CPU/RAM	New, Two-Pass	Traditional
	Algorithm	Algorithm
2.66 GHz Pentium 4		
DDR-266 RAM	0.042 s	0.159 s
0.6 GHz Pentium III		
PC-100 RAM	0.131 s	0.097 s

Two-Pass Permutation Multiplication versus Traditional Algorithm (joint work: X. Ma, V.H. Nguyen and C.)

```
Object Z[N], Y[N]; // Object is ``int'' in above experiments
int X[N];
for (i=0; i<N; i++)
        Z[i]=Y[X[i]];</pre>
```



Why is Two-Pass Permutation Now Faster?

Two Large Reasons:

1. The Pentium 4 has a longer cache line.

The Pentium 4 has a 128 byte cache line: four times longer than the 32 byte cache line of the Pentium III.

- 2. The bandwidth of DDR-266 (PC-2100) RAM is higher, but the latency is not faster.
 - DDR-266/PC-2100 has a bandwidth of 2.2 GHz, as compared to 1.1 GHz for older PC-100 RAM.
 - The latency of DDR-266 RAM and PC-100 RAM are both about 25 ns.



Future Trends:

1. Higher bandwidth memory

- Evidence: Today, we see dual-channel memory offering effective 800 MHz system busses (seven times faster than DDR-266)
- Evidence: Some scientific applications, such as matrix multiplication, FFT, etc., are now being programmed to use the high-bandwidth memory (and greater parallelism) of video boards. (Some applications are even using dual video boards to double this speed.)
- **Side Effect:** Possibly *even longer CPU cache lines*, in order to keep up with the high bandwidth)
- 2. Latency mostly unchanged
 - The time to precharge the external buffer of a DRAM chip is increasing slightly, as lower on-chip voltages must be raised to the higher voltage levels of the motherboard. *This is a long-term problem, for as long as DRAM and CPU are on different chips!*



Relative Speeds: CPU, RAM, Disk and Network

CPU bandwidth	2,400 MB/s	$(3 \text{ GHz} \times 8 \text{ byte words})$
Network bandwidth	100 MB/s	(1 Gb/s theoretical max
(point-to-point)		for Gigabit Ethernet)
Network bandwidth	1,000 MB/s	(varies by vendor)
(aggregate)		
RAM bandwidth (DDR-400)	3,300 MB/s	(maximum)
Disk bandwidth (per disk)	50 MB/s	(typical)

Aggregate bandwidth of 50 disks: $50 \times 50 = 2,500$ MB/s



Duplicate Elimination

Optimization: eliminate duplicate insertions before merge; Use a new hash array in RAM to accumulate elements to insert. Need only store one bit per hash element: 1 =present; 0 =not present

Example: AI search: enumeration of states via open queue, as in breadth-first search

- 1. If element to insert hashes to 0, it is new; add to *open queue* on disk
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NOTE: Both RAM-based and disk-based hash arrays adapt easily to distributed computing. Each node is responsible for a contiguous sequence of hash indexes.



Optimization: Bloom Filters

Recall in-RAM hash array with one bit per hash element: 1 = present; 0 = not present; **Idea of Bloom filters:**

- 1. Make hash array *k* times larger (retain same load factor for hash array)
- 2. Define *k* distinct hash functions
- 3. For each new element, apply *all* of the k hash functions, and set each corresponding entry of the hash array to 1
- 4. If any entry of the hash array was formerly 0, then this element is new: add to *open queue*
- 5. Else, add to *collision queue*

Example: Assume for simplicity that no duplicates are generated. if the original hash array had a load factor of 1/2, then the new hash array will be *k* times larger, but the the size of the collision queue will be reduced by a factor of $1/2^k$.



Planned Computation for Rubik's Cube

(joint work, Daniel Kunkle and C.)

Rubik's cube has approximately 4.3×10^{19} states

20-year conjecture: all states of Rubik's cube can be solved in at most 20 moves (known as "God's number")

How close can we get?

Standard strategy: partition 4.3×10^{19} states into *cosets* of equal size

Previously (Reid, 1993): Each coset has approximately 10^{10} states; approximately 5×10^8 such cosets to check; all states solved in 29 moves (recently shaved to 27 moves)

Planned: Each coset has approximately 10⁴ states; after symmetries, *only* 10¹⁴ cosets to check; (required data structure fills about 6 terabytes of aggregate disk); small cosets imply that each can be checked fully.



Questions?

QUESTIONS?