Distributed parallel Gröbner bases computation

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ECDS at CISIS 2009, Fukuoka

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Overview

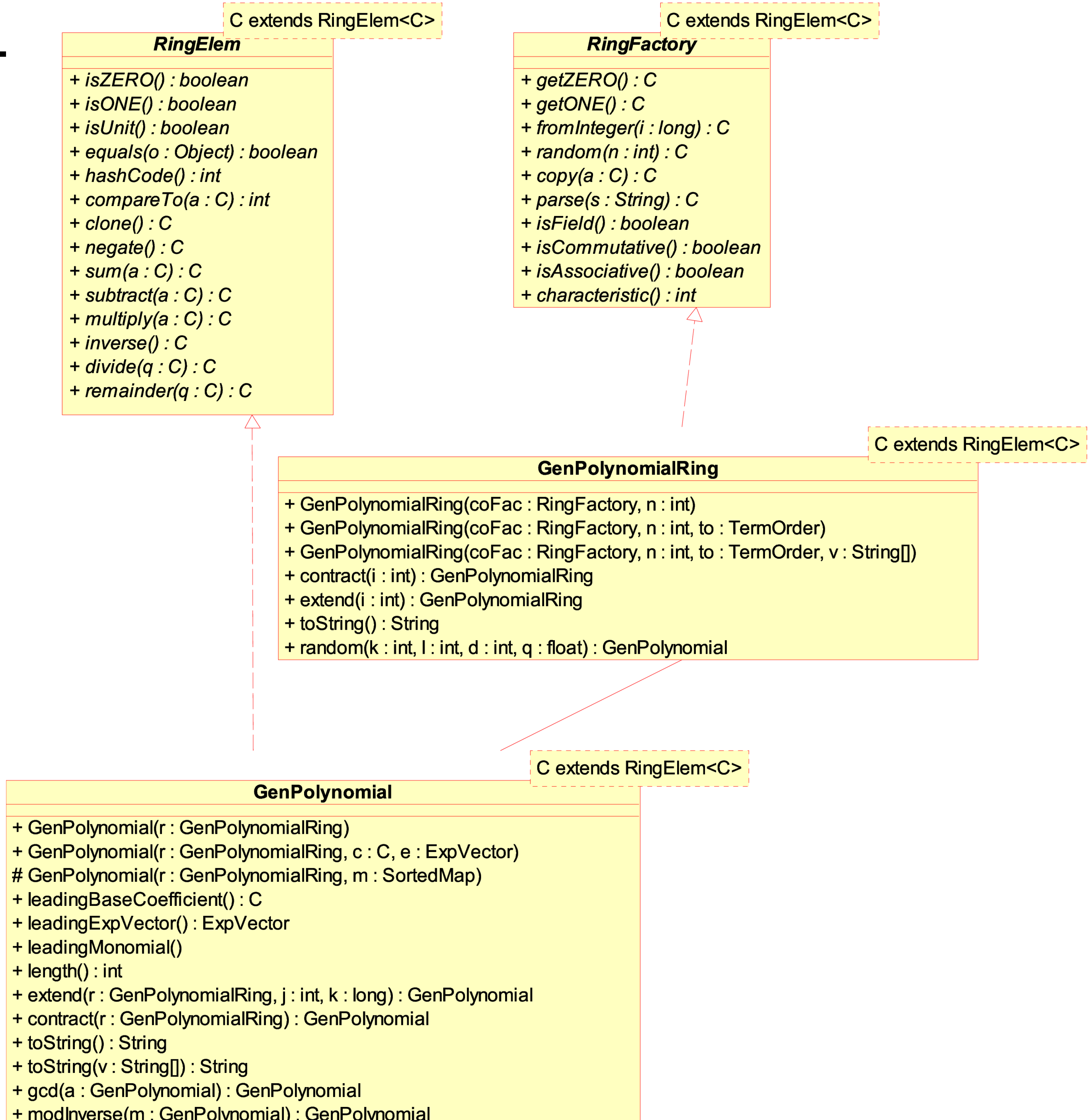
- Introduction to JAS
- Gröbner bases
  - problems with parallel computation
  - sequential and parallel algorithm
- Distributed algorithm
  - execution middle-ware
  - data structure middle-ware
  - workload paradox
- Conclusions and future work

Java Algebra System (JAS)

- object oriented design of a computer algebra system
  - = software collection for symbolic (non-numeric) computations
- type safe through Java generic types
- thread safe, ready for multi-core CPUs
- use dynamic memory system with GC
- 64-bit ready
- jython (Java Python) interactive scripting front end

Implementation overview

- 200+ classes and interfaces
- plus ~90 JUnit test cases
- uses JDK 1.6 with generic types
  - Javadoc API documentation
  - logging with Apache Log4j
  - build tool is Apache Ant
  - revision control with Subversion
- jython (Java Python) scripts
  - support for Sage like polynomial expressions
- open source, license is GPL or LGPL


C extends RingElem<C>
RingElem
+ isZERO() : boolean
+ isONE() : boolean
+ isUnit() : boolean
+ equals(o : Object) : boolean
+ hashCode() : int
+ compareTo(a : C) : int
+ clone() : C
+ negate() : C
+ sum(a : C) : C
+ subtract(a : C) : C
+ multiply(a : C) : C
+ inverse() : C
+ divide(q : C) : C
+ remainder(q : C) : C
C extends RingElem<C>
RingFactory
+ getZERO() : C
+ getONE() : C
+ fromInteger(i : long) : C
+ random(n : int) : C
+ copy(a : C) : C
+ parse(s : String) : C
+ isField() : boolean
+ isCommutative() : boolean
+ isAssociative() : boolean
+ characteristic() : int
C extends RingElem<C>
GenPolynomialRing
+ GenPolynomialRing(coFac : RingFactory, n : int)
+ GenPolynomialRing(coFac : RingFactory, n : int, to : TermOrder)
+ GenPolynomialRing(coFac : RingFactory, n : int, to : TermOrder, v : String[])
+ contract(i : int) : GenPolynomialRing
+ extend(i : int) : GenPolynomialRing
+ toString() : String
+ random(k : int, l : int, d : int, q : float) : GenPolynomial
C extends RingElem<C>
GenPolynomial
+ GenPolynomial(r : GenPolynomialRing)
+ GenPolynomial(r : GenPolynomialRing, c : C, e : ExpVector)
# GenPolynomial(r : GenPolynomialRing, m : SortedMap)
+ leadingBaseCoefficient() : C
+ leadingExpVector() : ExpVector
+ leadingMonomial()
+ length() : int
+ extend(r : GenPolynomialRing, j : int, k : long) : GenPolynomial
+ contract(r : GenPolynomialRing) : GenPolynomial
+ toString() : String
+ toString(v : String[]) : String
+ gcd(a : GenPolynomial) : GenPolynomial
+ modInverse(m : GenPolynomial) : GenPolynomial

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Example: Legendre polynomials

$P[0] = 1; \quad P[1] = x;$

$P[i] = 1/i \,((2i-1) * x * P[i-1] - (i-1) * P[i-2])$

```
BigRational fac = new BigRational();
String[] var = new String[]{ "x" };
GenPolynomialRing<BigRational> ring
 = new GenPolynomialRing<BigRational>(fac,1,var);
List<GenPolynomial<BigRational>> P
 = new ArrayList<GenPolynomial<BigRational>>(n);
GenPolynomial<BigRational> t, one, x, xc, xn; BigRational n21, nn;

one = ring.getONE(); x = ring.univariate(0);
P.add( one ); P.add( x );
for ( int i = 2; i < n; i++ ) {
        n21 = new BigRational( 2*i-1 );  xc = x.multiply( n21 );
        t = xc.multiply( P.get(i-1) );
        nn = new BigRational( i-1 ); xc = P.get(i-2).multiply( nn );
        t = t.subtract( xc );  nn = new BigRational(1,i);
        t = t.multiply( nn ); P.add( t );
}
      int i = 0;
      for ( GenPolynomial<BigRational> p : P ) {
          System.out.println("P["+(i++)+"] = " + P);
      }
```

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Gröbner bases

- canonical bases in polynomial rings $R = C[x_1, \ldots, x_n]$
- like Gauss elimination in linear algebra
- like Euclidean algorithm for univariate polynomials
- with a Gröbner base many problems can be solved
  - solution of non-linear systems of equations
  - existence of solutions
  - solution of parametric equations
- slower than multivariate Newton iteration in numerics
- but in computer algebra no round-off errors
- so guarantied correct results

Buchberger algorithm

```
algorithm: G = GB( F )
input: F a list of polynomials in R[x1,...,xn]
output: G a Gröbner Base of ideal(F)

G = F;
B = { (f,g) | f, g in G, f != g };
while ( B != {} ) {
  select and remove (f,g) from B;
  s = S-polynomial(f,g);
  h = normalform(G,s); // expensive operation
  if ( h != 0 ) {
     for ( f in G ) { add (f,h) to B }
     add h to G;
  }
} // termination ? Size of B changes
return G
```

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Problems with GB algorithm

- requires exponential space (in the number of variables)
- even for arbitrary many processors no polynomial time algorithm will exist

parallel computation hypothesis

- highly data depended
  - number of pairs unknown (size of B)
  - size of polynomials s and h unknown
    - size of coefficients
    - degrees, number of terms
- management of B is sequential
- strategy for the selection of pairs from B
  - depends moreover on speed of reducers

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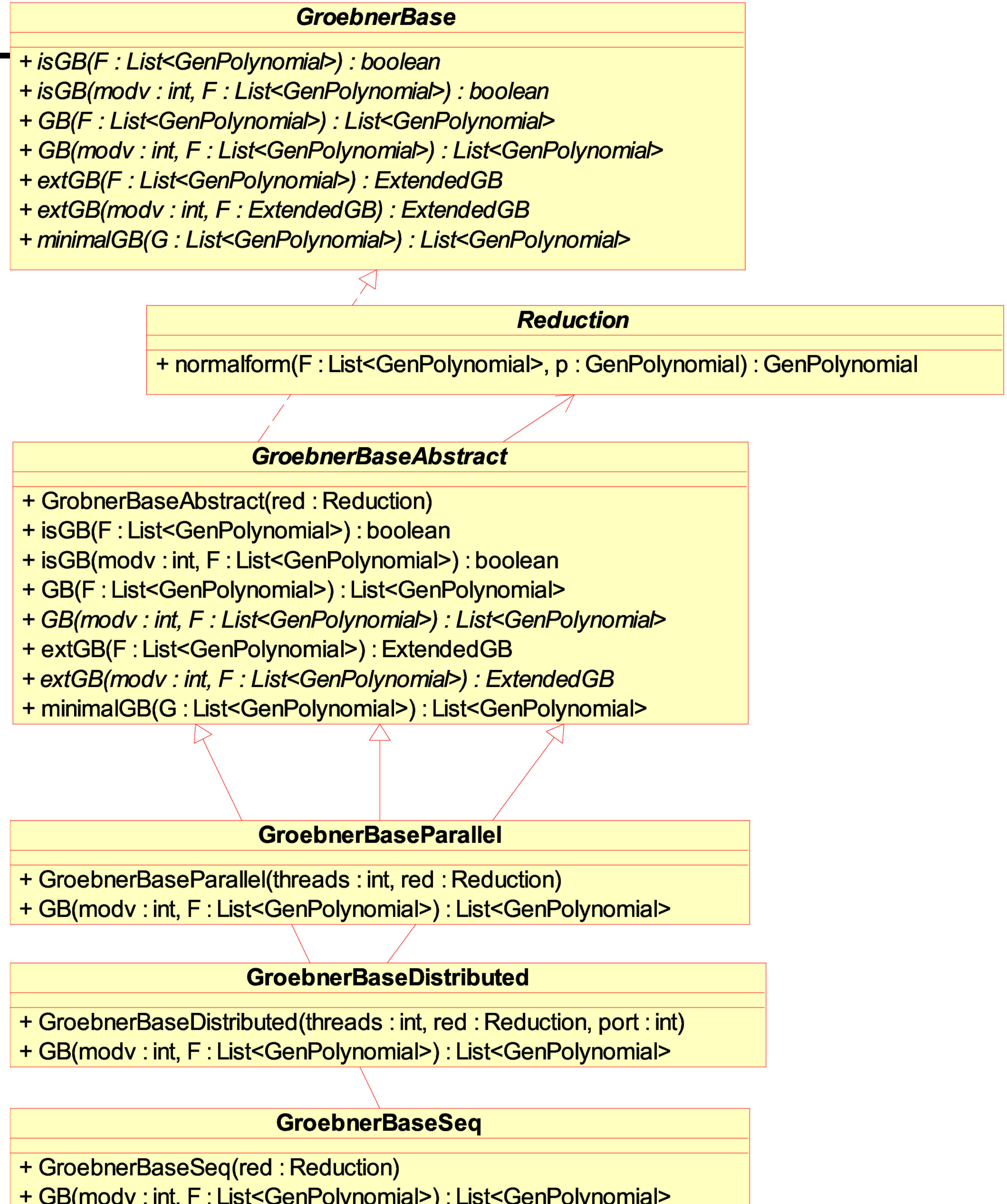
GroebnerBase
+ isGB(F : List<GenPolynomial>) : boolean
+ isGB(modv : int, F : List<GenPolynomial>) : boolean
+ GB(F : List<GenPolynomial>) : List<GenPolynomial>
+ GB(modv : int, F : List<GenPolynomial>) : List<GenPolynomial>
+ extGB(F : List<GenPolynomial>) : ExtendedGB
+ extGB(modv : int, F : ExtendedGB) : ExtendedGB
+ minimalGB(G : List<GenPolynomial>) : List<GenPolynomial>
Reduction
+ normalform(F : List<GenPolynomial>, p : GenPolynomial) : GenPolynomial
GroebnerBaseAbstract
+ GrobnerBaseAbstract(red : Reduction)
+ isGB(F : List<GenPolynomial>) : boolean
+ isGB(modv : int, F : List<GenPolynomial>) : boolean
+ GB(F : List<GenPolynomial>) : List<GenPolynomial>
+ GB(modv : int, F : List<GenPolynomial>) : List<GenPolynomial>
+ extGB(F : List<GenPolynomial>) : ExtendedGB
+ extGB(modv : int, F : List<GenPolynomial>) : ExtendedGB
+ minimalGB(G : List<GenPolynomial>) : List<GenPolynomial>
GroebnerBaseParallel
+ GroebnerBaseParallel(threads : int, red : Reduction)
+ GB(modv : int, F : List<GenPolynomial>) : List<GenPolynomial>
GroebnerBaseDistributed
+ GroebnerBaseDistributed(threads : int, red : Reduction, port : int)
+ GB(modv : int, F : List<GenPolynomial>) : List<GenPolynomial>
GroebnerBaseSeq
+ GroebnerBaseSeq(red : Reduction)
+ GB(modv : int, F : List<GenPolynomial>) : List<GenPolynomial>

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bwGRiD cluster architecture

- 8-core CPU nodes @ 2.83 GHz, 16GB, 140 nodes
- shared NFS/Lustre home directories
- InfiniBand and 1 G Ethernet interconnects
- managed by PBS batch system with Maui scheduler
- running Java 64bit server VM 1.6 with 4+GB memory
- start Java VMs with daemons on allocated nodes
- communication via TCP/IP interface to InfiniBand
- no Java high performance interface to InfiniBand
- alternative Java via MPI not studied
- other middle-ware ProActive or GridGain not studied

Distributed GB computation

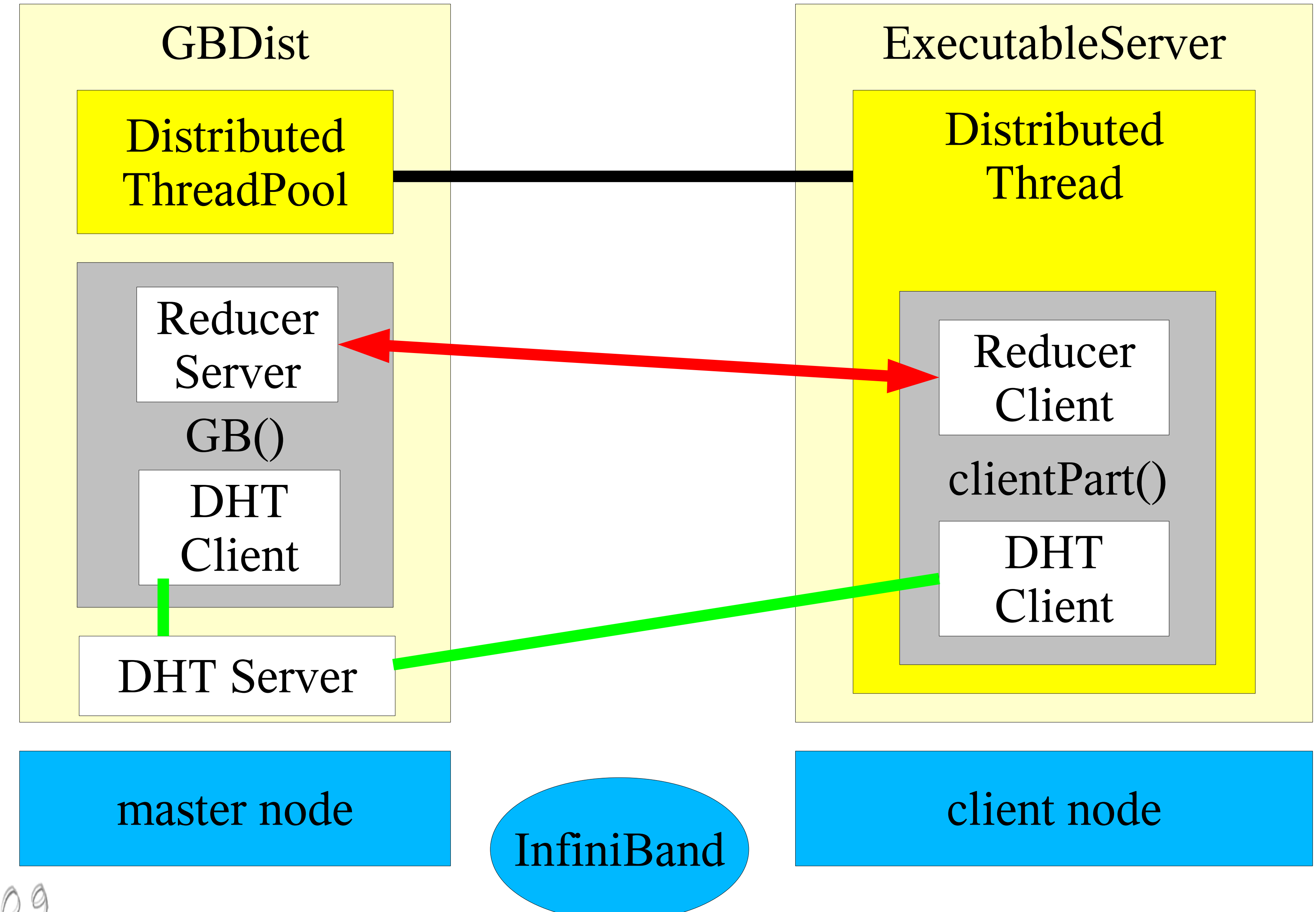
- main method GB()
- distribute list G via distributed hash table (DHT)
- start `ReducerServer` threads
- method `clientPart()` starts `ReducerClients`
- select pair and send to distributed client

    a) send polynomials them-selfs

    b) send index of polynomial in G
- client performs S-polynomial and normalform computation sends result back to master
- master eventually inserts new pairs to B and adds polynomial to G in DHT

```
mtype = { Get, Fin, Pair, Hpol };
proctype ReducerServer (chan pairs) {
 do
 :: idler++; pairs ? Get;
    if
    :: ( ! nextPair && idler == PROCNUM ) -> pairs ! Fin; break;
    :: ( ! nextPair ) -> skip; // sleep delay
    :: else skip;
    fi;
    idler--; getPair(); /* take pair from queue */
    pairs ! Pair; /* send to client */
 progress: skip;
    pairs ? Hpol; /* receive result */
    addPair(); /* add new pairs to queue */
 od;
}
    proctype ReducerClient (chan pairs) {
     do
     :: pairs ! Get;
        if
        :: pairs ? Fin  -> break;
        :: pairs ? Pair -> /*compute h-pol*/ pairs ! Hpol;
        fi
     od
    }
```

Middle-ware overview



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Execution middle-ware (nodes)

- on compute nodes do basic bootstrapping
  - start daemon class `ExecutableServer`
  - listens on connections (no security constrains)
  - start thread with `Executor` for each connection
  - receives (serialized) objects with `RemoteExecutable` interface
  - execute the `run()` method
  - communication and further logic is implemented in the `run()` method
  - multiple processes as threads in one JVM

Execution middle-ware (master)

- on master node
  - start `DistThreadPool` similar to `ThreadPool`
  - starts threads for each compute node
  - list of compute nodes taken from PBS
  - starts connections to all nodes with `ExecutableChannel`
  - can start multiple tasks on nodes to use multiple CPU cores via `open(n)` method
  - method `addJob()` on master
  - send a job to a remote node and wait until termination (RMI like)

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Execution middle-ware usage

- Gröbner base master `GBDist`
- initialize `DistThreadPool` with PBS node list
- initialize `GroebnerBaseDistributed`
- `execute()` method of `GBDist`
  - add remote computation classes as jobs
  - execute `clientPart()` method in jobs
    - is `ReducerClient` above
  - calls main `GB()` method
    - is `ReducerServer` above

Data structure middle-ware

- sending of polynomials involves
  - serialization and de-serialization time
  - and communication time
- avoid sending via a distributed data structure
- implemented as distributed list
- runs independently of main GB master
- setup in `GroebnerBaseDistributed` constructor and `clientPart()` method
- then only indexes of polynomials need to be communicated

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Distributed polynomial list

- distributed list implemented as distributed hash table (DHT)
- key is list index
- class `DistHashTable` similar to `java.util.HashMap`
- methods `clear(), get()` and `put()` as in `HashMap`
- method `getWait(key)` waits until a value for a key has arrived
- method `putWait(key,value)` waits until value has arrived at the master and is received back
- no guaranty that value is received on all nodes

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DHT implementation (1)

- implemented as central control DHT
- client part on node uses `TreeMap` as store
- client `DistributedHashTable` connects to master
- master class `DistributedHashTableServer`
- `put()` methods send key-value pair to a master
- master then broadcasts key-value pair to all nodes
- `get()` method takes value from local `TreeMap`

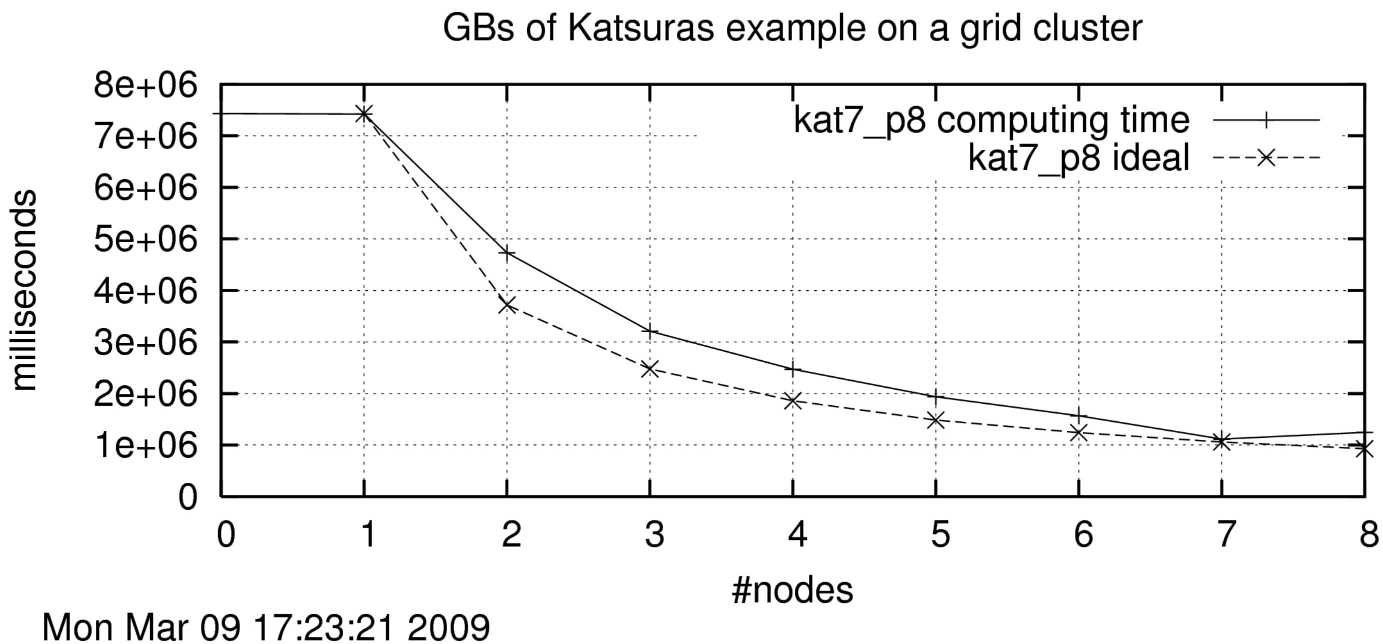
DHT implementation (2)

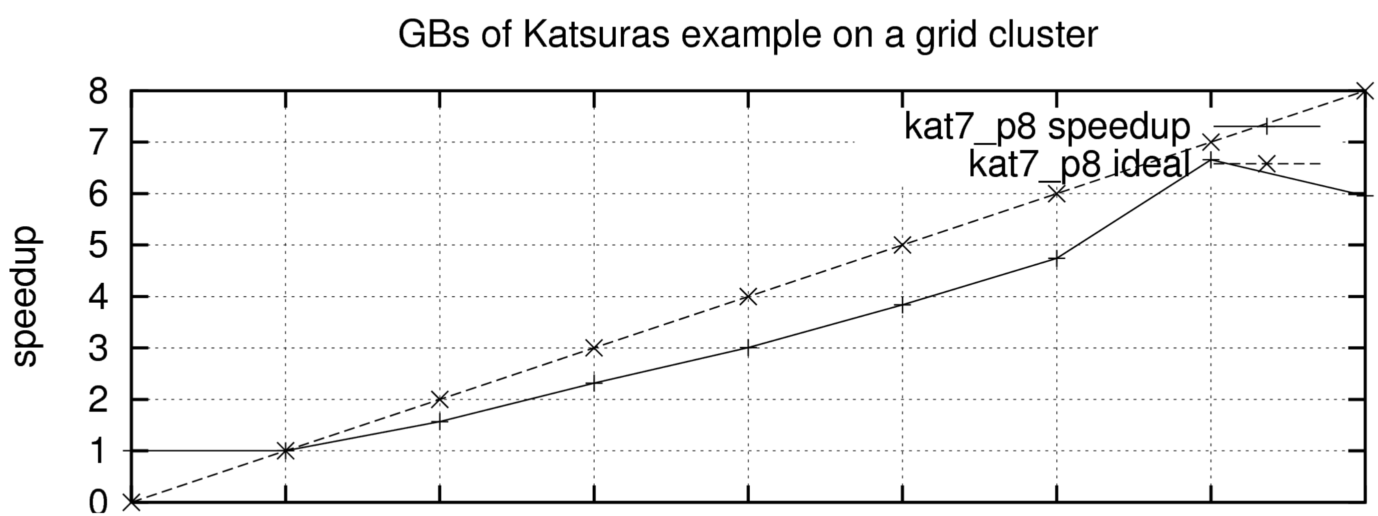
- in future implement DHT with decentralized control
- in future implement with generic types
- in master process de-serialization of polynomials should be avoided
- broadcast to clients in master serializes polynomials for every client again
- master is co-located to master of GB computation on same compute node
- this doubles memory requirements on master node
- this increases the CPU load on the master
  - limits scaling of master for more nodes

Performance

- multi-threaded computation
  - scales well to 8 CPU cores
  - 0.4 % overhead on one thread to sequential
- distributed computation
  - scales only to 4 compute nodes
  - absolute computing times comparable to multi-threaded case for up to 4 nodes
    - not too much communication overhead
    - can use multiple cores on nodes
  - InfiniBand is essential
- workload paradox, selection strategies

Multi-threaded Gröbner basis





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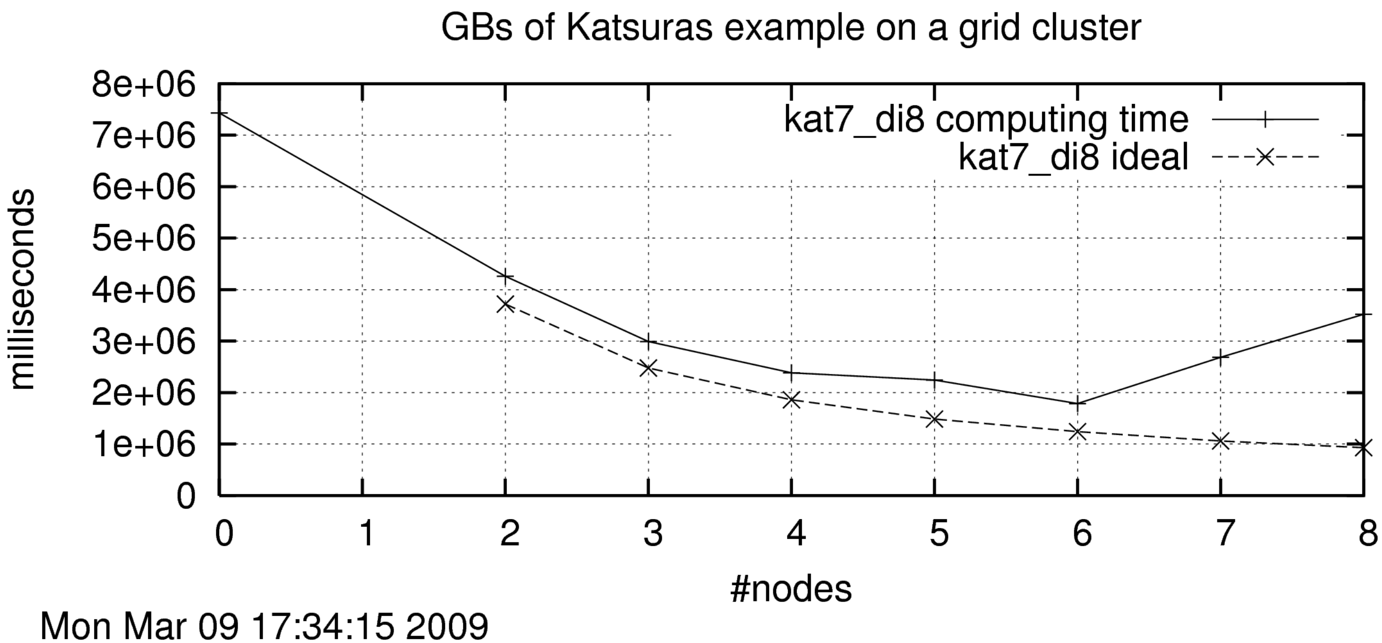
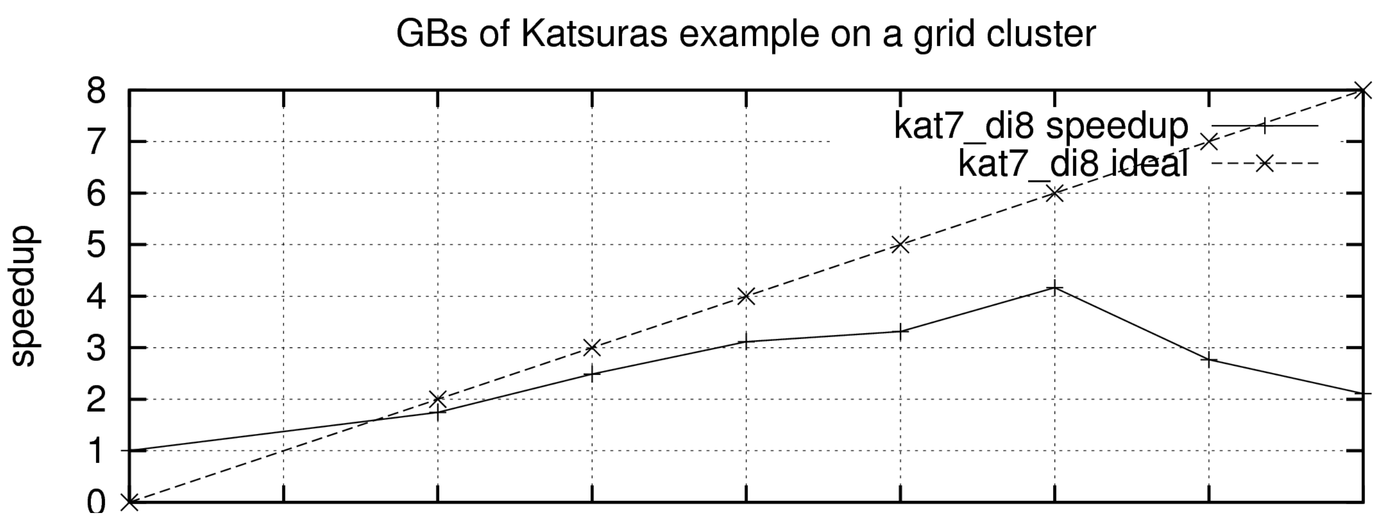
Distributed Gröbner basis





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Workload paradox

- parallel: 135 - 154 polynomials, 663 - 686 pairs
- distributed: 171 - 338 polynomials, 699 - 862 pairs
- possible pairs 9.045 – 56.953
  - rest avoided with 'criterions' and strategies
- different computation times in parallel reduction
  - pair polynomial size varies
  - size of polynomials in list varies
- different order of new pairs inserted in B
- different order of pairs removed from B

Table 1. Distributed timings, Katsura 6.

algo.	#threads	#VM	time	put	rem
seq	1	1	160.2	70	327
par	1	1	157.0	70	327
par	2	1	82.2	72	329
dist	1	1	177.2	77	334
dist	2	2	92.2	90	347
dist	4	2	56.2	112	369
dist	8	2	58.9	255	516
dist	4	4	51.2	117	374
dist	6	4	43.7	129	386
dist	8	4	62.9	259	519

Computing times in seconds on a 32 CPU Intel Xeon SMP computer running at 2.7 GHz and with 32 GB RAM. JVM 1.4.2 started with AggressiveHeap and UseParallelGC. Columns: #VMs = number of distinct Java virtual machines. put = number of polynomials put to pair list, rem = number of pairs removed from pair list.

Table 2. Multi-threaded timings, Katsura 7.

# threads	time	speedup	put	rem
seq	7435854	1.0	135	663
1	7424640	1.00	135	663
2	4733708	1.57	141	669
3	3212655	2.31	142	669
4	2470152	3.01	147	677
5	1937110	3.83	149	681
6	1568348	4.74	146	671
7	1116218	6.66	151	679
8	1247666	5.95	154	686

Columns: put = number of polynomials put to pair list, rem = number of pairs removed from pair list.

Table 3. Distributed timings, Katsura 7.

# nodes	time	speedup	put	rem
seq	7435854	1.0	135	663
2	4260202	1.74	171	699
3	2990191	2.48	195	726
4	2385904	3.11	216	745
5	2243687	3.31	233	764
6	1784650	4.16	255	786
7	2684213	2.77	287	814
8	3522735	2.11	338	862

Columns: put = number of polynomials put to pair list, rem = number of pairs removed from pair list.

Selection strategies

- best to use the same order of polynomials and pairs as in sequential algorithm
- selection algorithm is sequential
  - so optimizations reduce parallelism
- Amrhein & Gloor & Küchlin:
  - work parallel: n reductions in parallel
  - search parallel: select best from k results
- Kredel:
  - n reductions in parallel, select first finished
  - select result in same sequence as reduction is started, not the first finished

Conclusions

- first version of a distributed GB algorithm
- runs on a HPC cluster in PBS environment
- shared memory parallel version scales up to 8 CPUs
- runtime of distributed version is comparable to parallel version
- can the workload paradox be solved?
- developed classes fit in Gröbner base class hierarchy
- new package is type-safe with generic types (with the exception of the distributed hash table)

Future work

- profile and study run-time behavior in detail
- investigate other grid middle-ware
- improve integration into the grid environment
- improve serialization in distributed list
- study other result selection strategies
- develop hybrid GB algorithm
  - distributed and multi-threaded on nodes
- compute sequential Gröbner bases with respect to different term orders in parallel

Thank you

- Questions or Comments?
- http://krum.rz.uni-mannheim.de/jas
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  - the referees
  - and other colleagues