Distributed hybrid Gröbner bases computation

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Overview

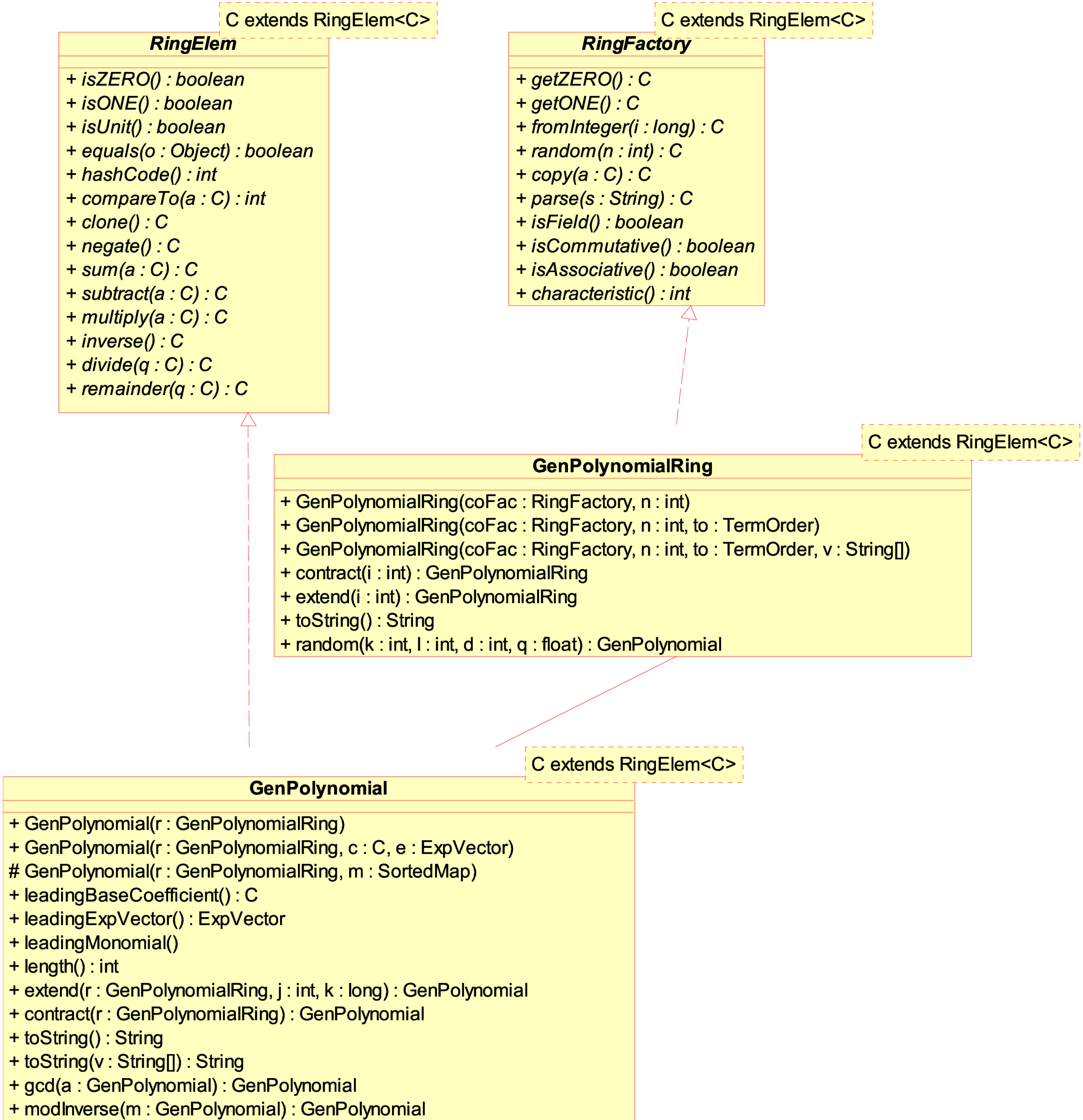
- Introduction to JAS
- Gröbner bases
  - sequential and parallel algorithm
  - problems with parallel computation
- Distributed and distributed hybrid algorithm
  - execution middle-ware
  - data structure middle-ware
- Evaluation
  - termination, selection strategies, hardware
- Conclusions and future 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

- 250+ classes and interfaces
- plus ~120 JUnit test classes,3800+ assertion tests
- uses JDK 1.6 with generic types
  - Javadoc API documentation
  - logging with Apache Log4j
  - build tool is Apache Ant
  - revision control with Subversion
  - public git repository
- 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

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

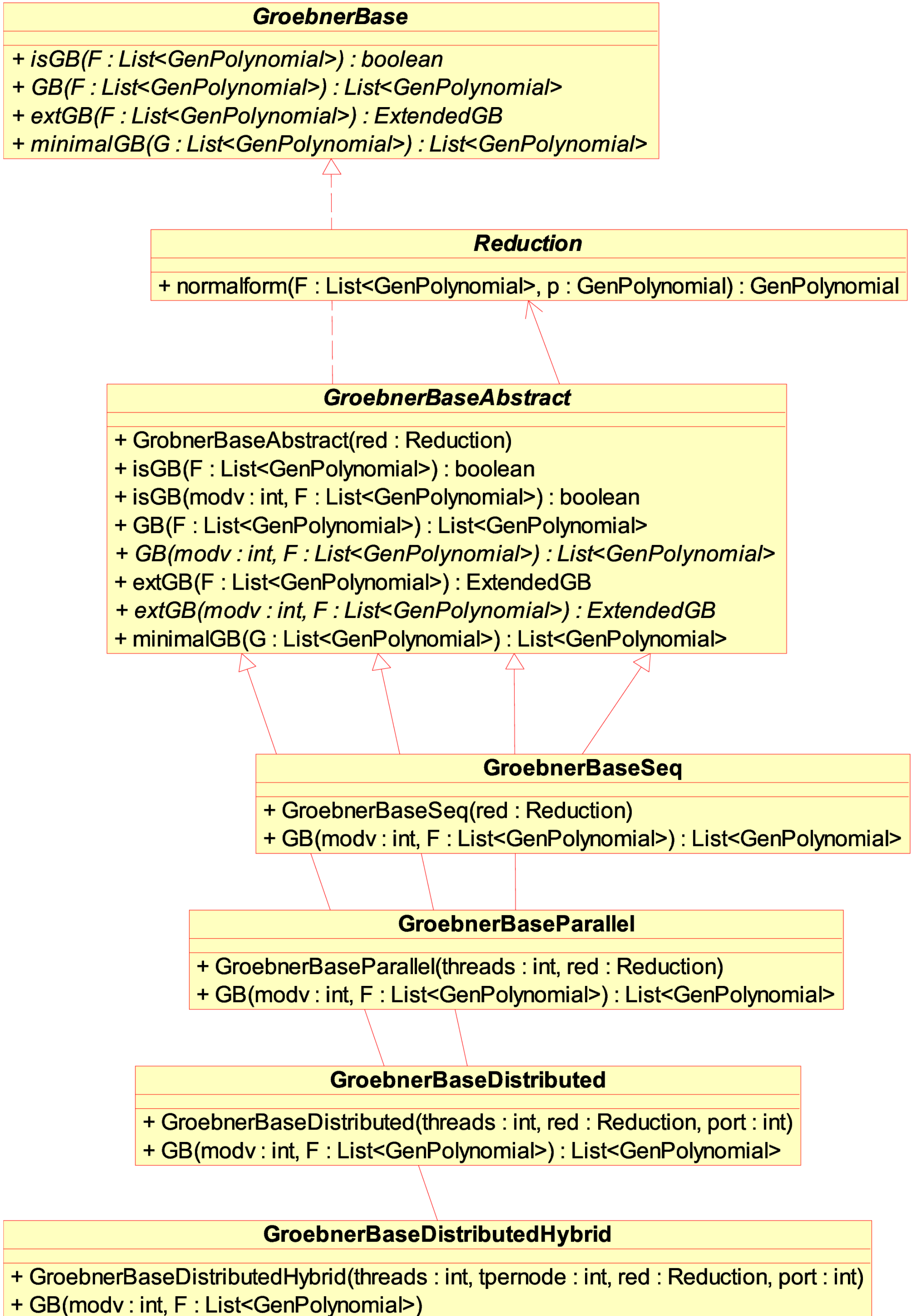
Buchberger algorithm

```
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
```

Problems with the GB algorithm

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



GroebnerBase

+ isGB(F : List<GenPolynomial>) : boolean
+ GB(F : List<GenPolynomial>) : List<GenPolynomial>
+ extGB(F : List<GenPolynomial>) : 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>

GroebnerBaseSeq

+ GroebnerBaseSeq(red : Reduction)
+ GB(modv : int, F : 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>

GroebnerBaseDistributedHybrid

+ GroebnerBaseDistributedHybrid(threads : int, tpernode : int, red : Reduction, port : int)
+ GB(modv : int, F : List<GenPolynomial>)

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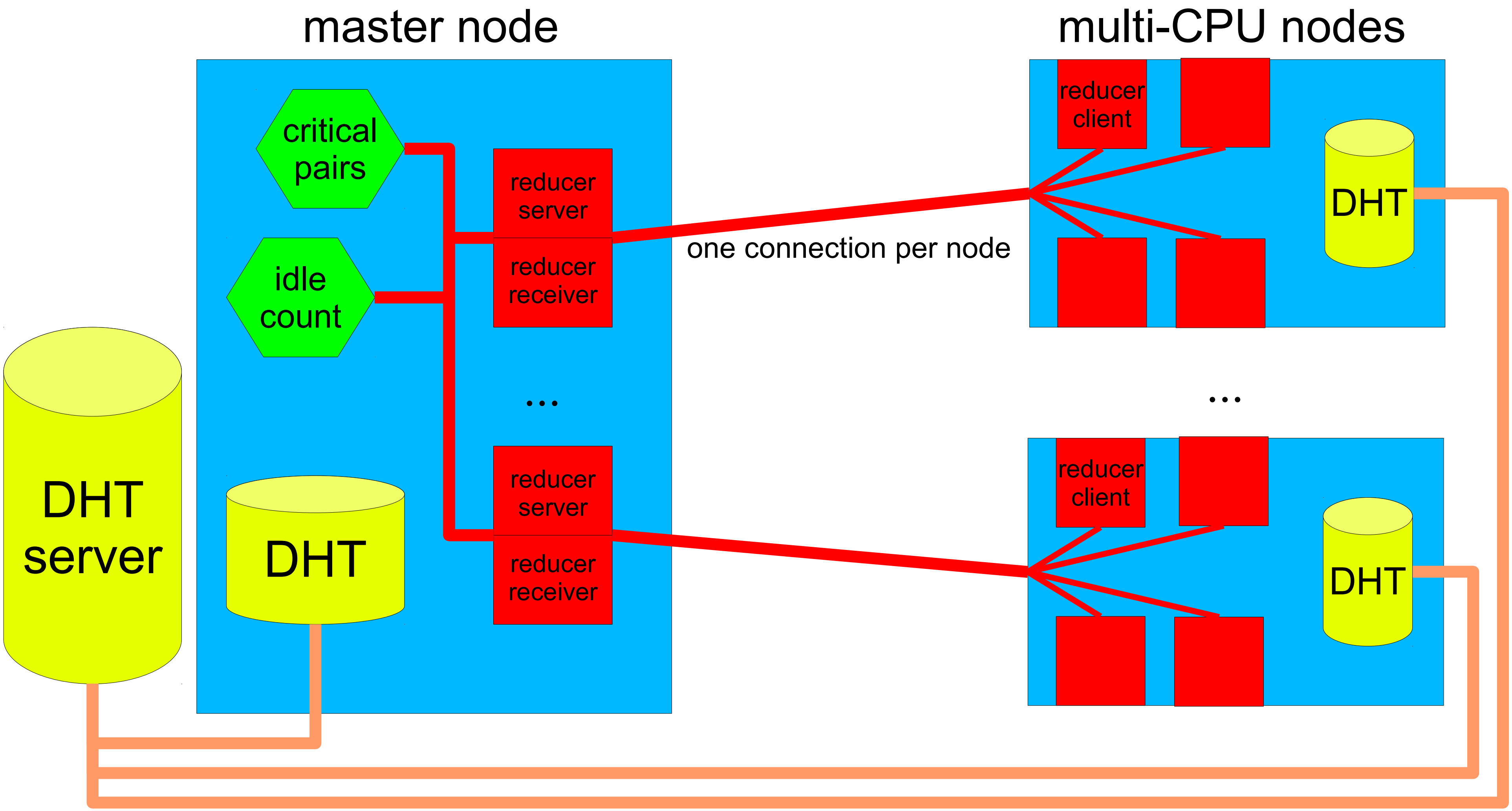
bwGRiD cluster architecture

- 8-core CPU nodes @ 2.83 GHz, 16GB, 140 nodes
- shared Lustre home directories
- 10Gbit InfiniBand and 1Gbit 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 over InfiniBand
- no Java high performance interface to InfiniBand
- alternative Java via MPI not studied
- other middle-ware ProActive or GridGain not studied

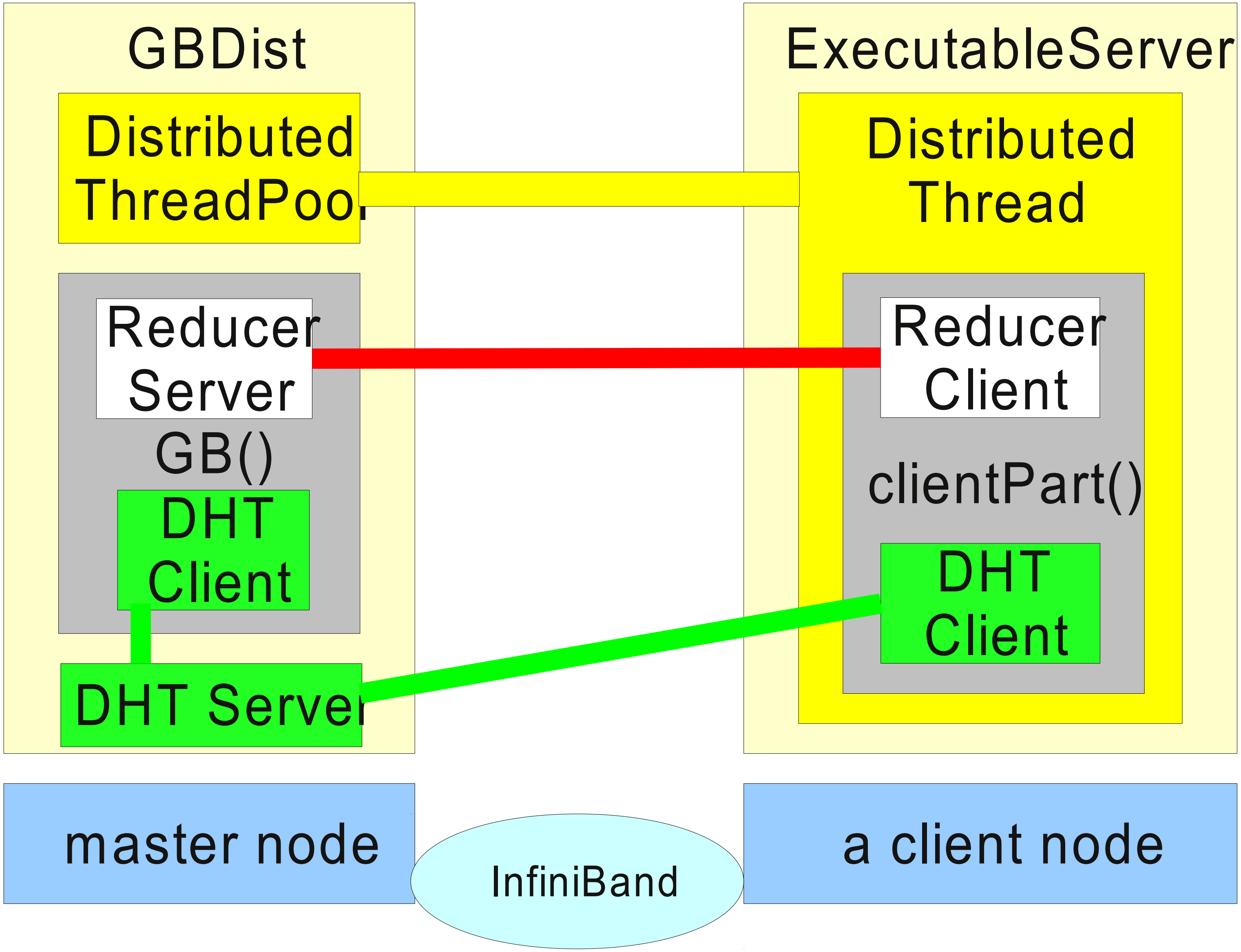
Distributed hybrid GB algorithm

- main method `GB()`
- distribute list G via distributed hash table (DHT)
- start `HybridReducerServer` threads for each node
  - together with a `HybridReducerReceiver` thread
- `clientPart()` starts multiple `HybridReducerClients` threads
- establish one control network connection per node
- select pair and send to distributed client
  - send index of polynomial in G
- clients perform S-polynomial and normalform computation send result back to master
- master eventually inserts new pairs to B and adds polynomial to G in DHT

Thread to node mapping



Middleware overview



Execution middle-ware (nodes)

same as for distributed algorithm

- 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)

same as for distributed algorithm

- 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)

Execution middle-ware usage

mostly same as for distributed algorithm

- Gröbner base master `GBDistHybrid`
- initialize `DistThreadPool` with PBS node list
- initialize `GroebnerBaseDistributedHybrid`
- `execute()` method of `GBDistHybrid`
  - add remote computation classes as jobs
  - execute `clientPart()` method in jobs
    - is `HybridReducerClient` above
  - calls main `GB()` method
    - start `HybridReducerServer` above
    - which then starts `HybridReducerReceiver`

Communication middle-ware

- one (TCP/IP) connection per compute node
- request and result messages can overlap
- solved with tagged message channel
  - message is tagged with a label, so receive() can select messages with specific tags
- implemented in class `TaggedSocketChannel`
- methods with tag parameter
  - `send(tag,object)` and `receive(tag)`
- implemented with blocking queues for each tag and a separate receiving thread
- alternative: `java.nio.channels.Selector`

Data structure middle-ware

improved version

- 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 `GroebnerBaseDistributedHybrid` constructor and `clientPart()` method
- then only indexes of polynomials need to be communicated

Distributed polynomial list

improved version

- distributed list implemented as distributed hash table (DHT)
- key is list index
- implemented with generic types
- class `DistHashTable` extends `java.util.AbstractMap`
- 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

DHT implementation (1)

improved version

- 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`
- in future implement DHT with decentralized control

DHT implementation (2)

improved version

- in master process de-serialization of polynomials is now avoided
- broadcast to clients in master now use serialized polynomials in marshaled objects
- 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

Marshalled objects

- reduce serialization overhead in DHT for polynomials
- use class `MarshalledObject` from `java.rmi`
- polynomials on DHT master are no more de-serialized and re-serialized
- serialization and de-serialization takes place only upon entry and exit in client side DHT
- timing samples from distributed and hybrid GB
  - sum of encoding and decoding
  - plus sum of marshalled object encoding and decoding

example	1	2	3	4
plain	2461	2364	1289	1100
marshall	487	765	394	594

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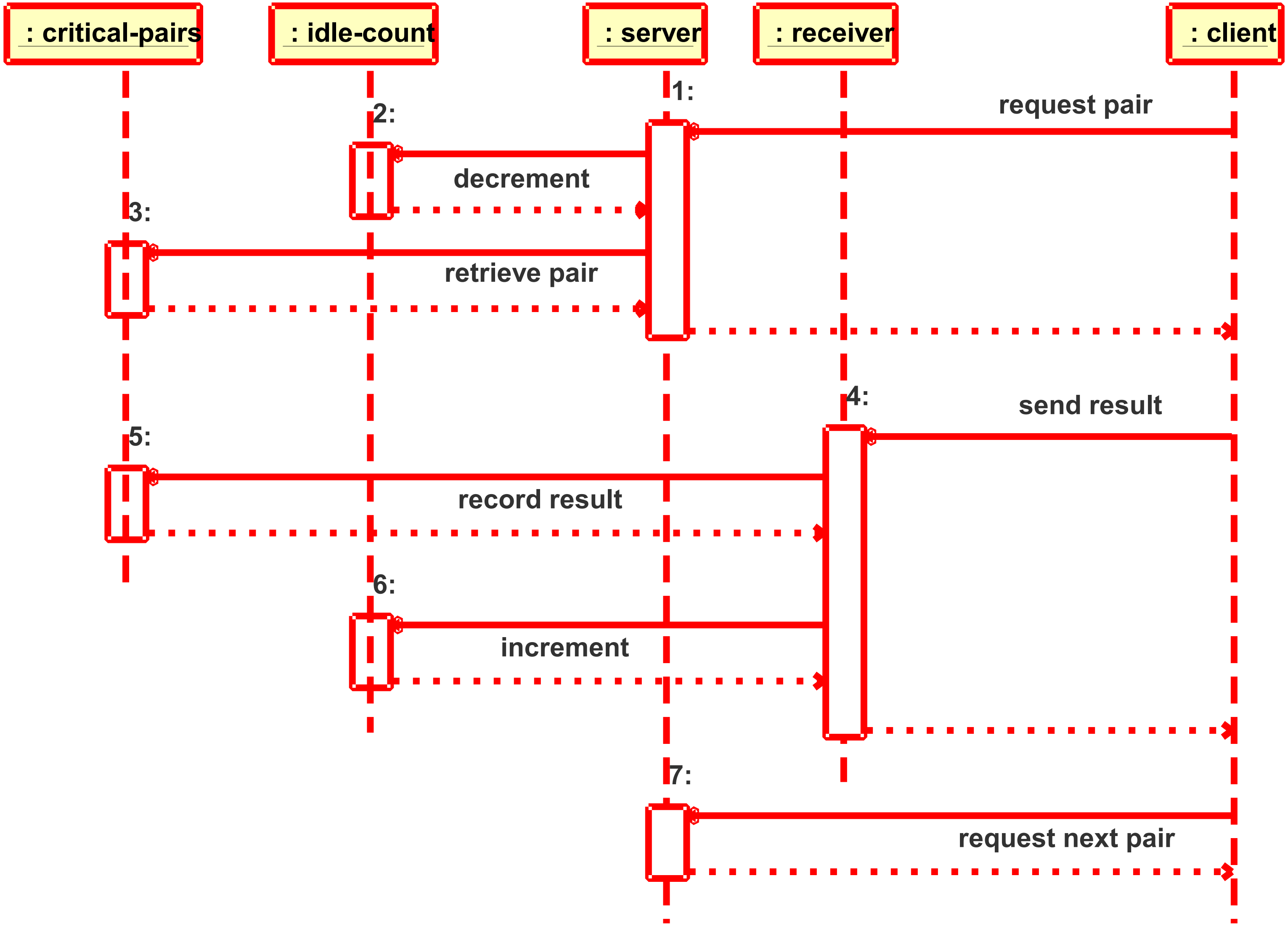
Termination (1)

- single thread can check if B is empty
- tests in case of multiple threads
  - B is empty
  - and all threads are idle
- distributed hybrid termination
  - idle client requests critical pair
  - thread on master waits for such requests, then
    - if B is empty and all threads are idle then terminate
    - if B is not empty then take pair and send to reducer client
    - if B is empty and threads are working, then sleep and recheck on wake-up
  - thread on master responsible for multiple node threads

Termination (2)



Termination (3)

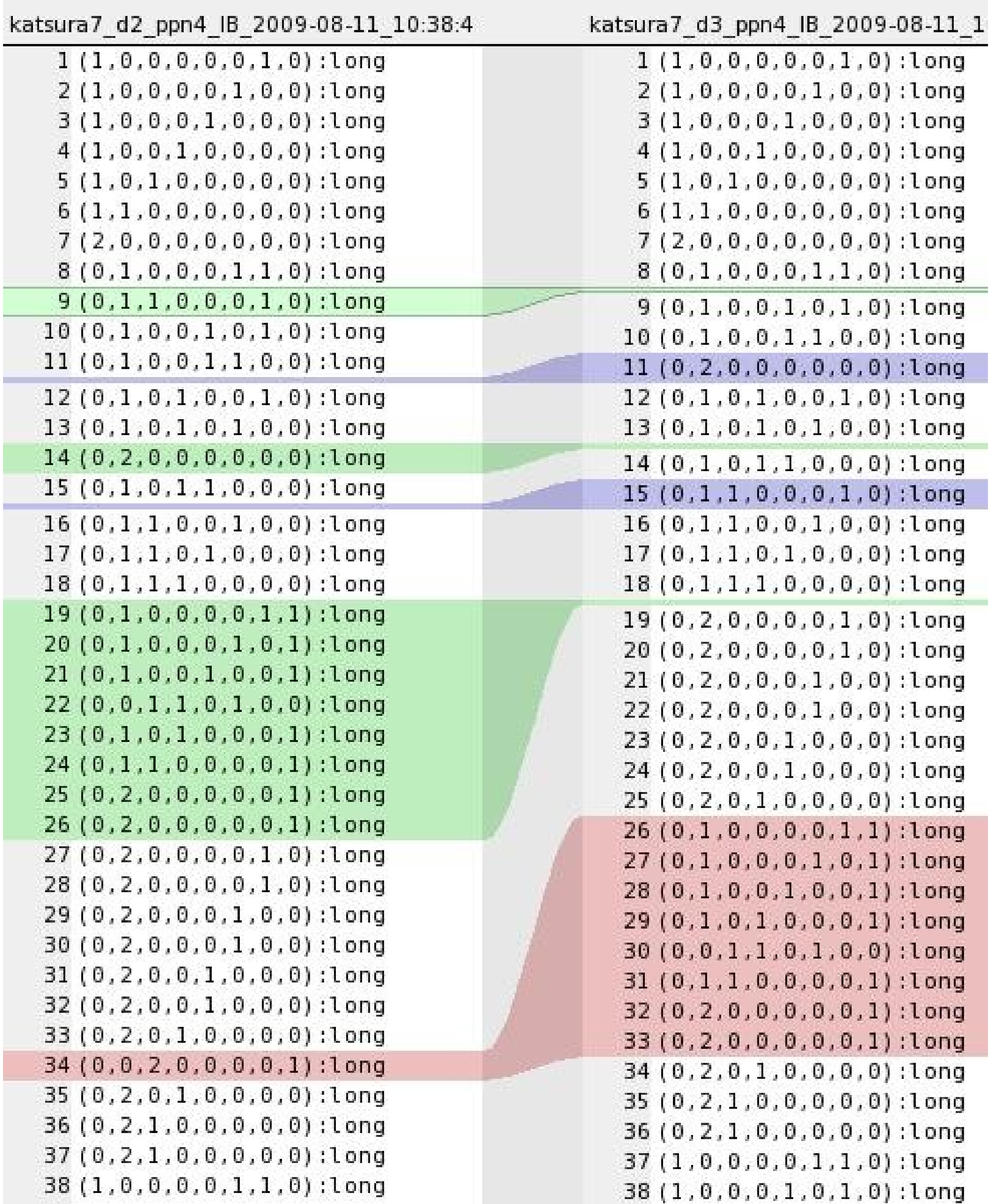
- multiple requests over the same connection
- uses `TaggedSocketChannel`
- send critical pair: receiving thread may not be the same as requesting thread
- pair handling thread may be blocked for requests
- so helper thread `HybridReducerReceiver` for result polynomials is required
  - record the result in the pair-list data structure
  - update idle threads count
  - send back acknowledgment
  - need to identify exact receiving thread: message tag

Termination (4)

- processing sequence in a master thread
  - receive reduction request
  - update idle threads count
  - retrieve a critical pair and update the pair-list
  - send pair-index to client
- acknowledgment ensures that the reduction request does not overlap with the other steps
- acknowledgment reduces parallelism, but required for book-keeping

Termination (5)

- processing sequence of client reducer thread
  - send pair request to master
  - receive pair index
  - process pair
    - retrieve polynomials from DTH via index
    - compute S-polynomial and a normal form
  - send result polynomial to master receiver
  - wait for acknowledgment from master



```
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 1 (1,0,0,0,0,0,1,0):long                      1 (1,0,0,0,0,0,1,0):long
 2 (1,0,0,0,0,1,0,0):long                      2 (1,0,0,0,0,1,0,0):long
 3 (1,0,0,0,1,0,0,0):long                      3 (1,0,0,0,1,0,0,0):long
 4 (1,0,0,1,0,0,0,0):long                      4 (1,0,0,1,0,0,0,0):long
 5 (1,0,1,0,0,0,0,0):long                      5 (1,0,1,0,0,0,0,0):long
 6 (1,1,0,0,0,0,0,0):long                      6 (1,1,0,0,0,0,0,0):long
 7 (2,0,0,0,0,0,0,0):long                      7 (2,0,0,0,0,0,0,0):long
 8 (0,1,0,0,0,1,1,0):long                      8 (0,1,0,0,0,1,1,0):long
 9 (0,1,1,0,0,0,1,0):long
10 (0,1,0,0,1,0,1,0):long                      9 (0,1,0,0,1,0,1,0):long
11 (0,1,0,0,1,1,0,0):long                     10 (0,1,0,0,1,1,0,0):long
                                              11 (0,2,0,0,0,0,0,0):long
12 (0,1,0,1,0,0,1,0):long                     12 (0,1,0,1,0,0,1,0):long
13 (0,1,0,1,0,1,0,0):long                     13 (0,1,0,1,0,1,0,0):long
14 (0,2,0,0,0,0,0,0):long
15 (0,1,0,1,1,0,0,0):long                     14 (0,1,0,1,1,0,0,0):long
                                              15 (0,1,1,0,0,0,1,0):long
16 (0,1,1,0,0,1,0,0):long                     16 (0,1,1,0,0,1,0,0):long
17 (0,1,1,0,1,0,0,0):long                     17 (0,1,1,0,1,0,0,0):long
18 (0,1,1,1,0,0,0,0):long                     18 (0,1,1,1,0,0,0,0):long
19 (0,1,0,0,0,0,1,1):long
20 (0,1,0,0,0,1,0,1):long
21 (0,1,0,0,1,0,0,1):long
22 (0,0,1,1,0,1,0,0):long
23 (0,1,0,1,0,0,0,1):long
24 (0,1,1,0,0,0,0,1):long
25 (0,2,0,0,0,0,0,1):long
26 (0,2,0,0,0,0,0,1):long
27 (0,2,0,0,0,0,1,0):long                     19 (0,2,0,0,0,0,1,0):long
28 (0,2,0,0,0,0,1,0):long                     20 (0,2,0,0,0,0,1,0):long
29 (0,2,0,0,0,1,0,0):long                     21 (0,2,0,0,0,1,0,0):long
30 (0,2,0,0,0,1,0,0):long                     22 (0,2,0,0,0,1,0,0):long
31 (0,2,0,0,1,0,0,0):long                     23 (0,2,0,0,1,0,0,0):long
32 (0,2,0,0,1,0,0,0):long                     24 (0,2,0,0,1,0,0,0):long
33 (0,2,0,1,0,0,0,0):long                     25 (0,2,0,1,0,0,0,0):long
                                              26 (0,1,0,0,0,0,1,1):long
                                              27 (0,1,0,0,0,1,0,1):long
                                              28 (0,1,0,0,1,0,0,1):long
                                              29 (0,1,0,1,0,0,0,1):long
                                              30 (0,0,1,1,0,1,0,0):long
                                              31 (0,1,1,0,0,0,0,1):long
                                              32 (0,2,0,0,0,0,0,1):long
                                              33 (0,2,0,0,0,0,0,1):long
34 (0,0,2,0,0,0,0,1):long
35 (0,2,0,1,0,0,0,0):long                     34 (0,2,0,1,0,0,0,0):long
36 (0,2,1,0,0,0,0,0):long                     35 (0,2,1,0,0,0,0,0):long
37 (0,2,1,0,0,0,0,0):long                     36 (0,2,1,0,0,0,0,0):long
38 (1,0,0,0,0,1,1,0):long                     37 (1,0,0,0,0,1,1,0):long
                                              38 (1,0,0,0,1,0,1,0):long
```

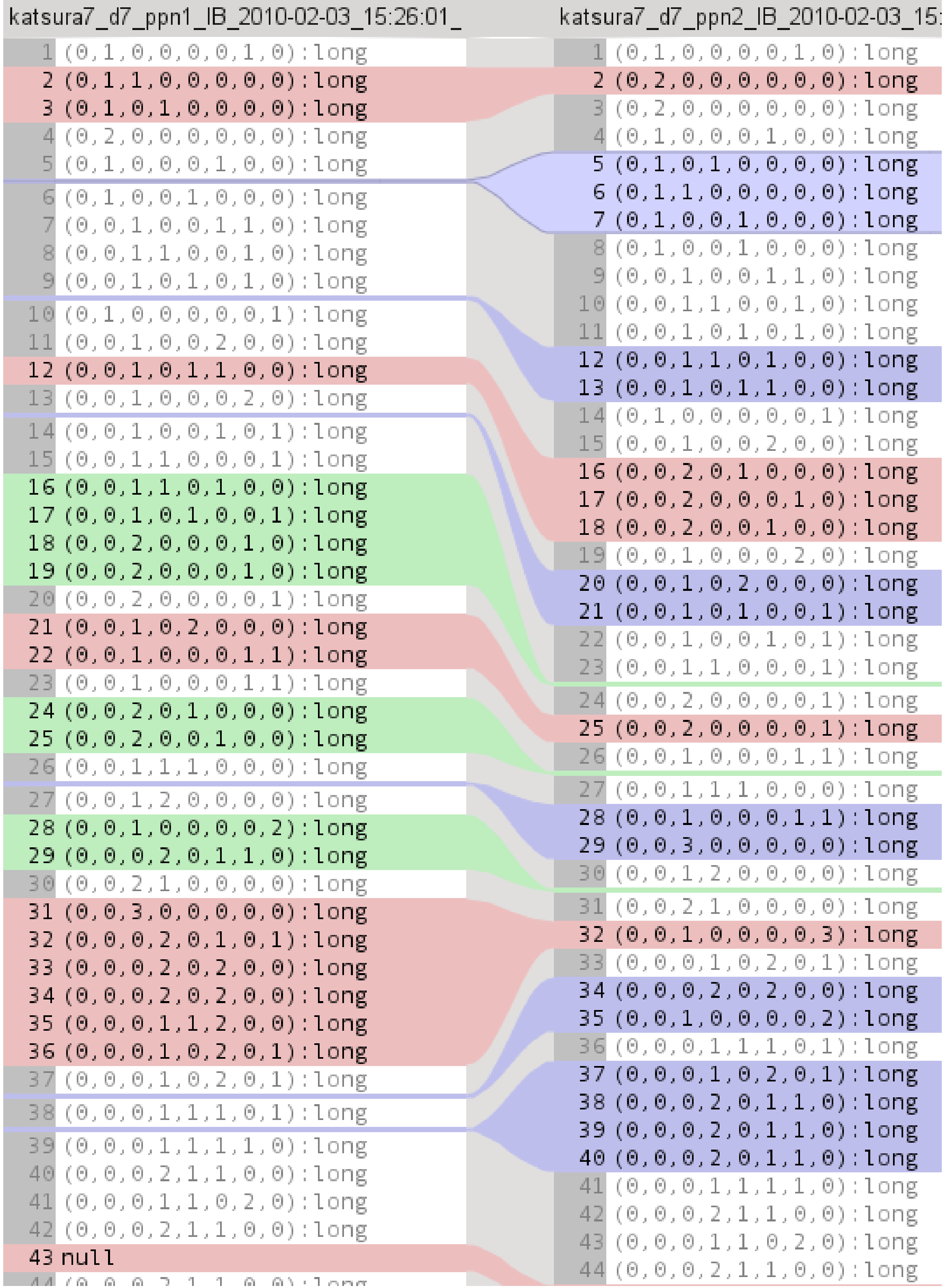

```
katsura7_d7_ppn1_IB_2010-02-03_15:26:01_
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 2 (0,1,1,0,0,0,0,0):long
 3 (0,1,0,1,0,0,0,0):long
 4 (0,2,0,0,0,0,0,0):long
 5 (0,1,0,0,0,1,0,0):long
 6 (0,1,0,0,1,0,0,0):long
 7 (0,0,1,0,0,1,1,0):long
 8 (0,0,1,1,0,0,1,0):long
 9 (0,0,1,0,1,0,1,0):long
10 (0,1,0,0,0,0,0,1):long
11 (0,0,1,0,0,2,0,0):long
12 (0,0,1,0,1,1,0,0):long
13 (0,0,1,0,0,0,2,0):long
14 (0,0,1,0,0,1,0,1):long
15 (0,0,1,1,0,0,0,1):long
16 (0,0,1,1,0,1,0,0):long
17 (0,0,1,0,1,0,0,1):long
18 (0,0,2,0,0,0,1,0):long
19 (0,0,2,0,0,0,1,0):long
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21 (0,0,1,0,2,0,0,0):long
22 (0,0,1,0,0,0,1,1):long
23 (0,0,1,0,0,0,1,1):long
24 (0,0,2,0,1,0,0,0):long
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41 (0,0,0,1,1,0,2,0):long
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43 null
44 (0,0,0,2,1,1,0,0):long
```

```
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21 (0,0,1,0,1,0,0,1):long
22 (0,0,1,0,0,1,0,1):long
23 (0,0,1,1,0,0,0,1):long
24 (0,0,2,0,0,0,0,1):long
25 (0,0,2,0,0,0,0,1):long
26 (0,0,1,0,0,0,1,1):long
27 (0,0,1,1,1,0,0,0):long
28 (0,0,1,0,0,0,1,1):long
29 (0,0,3,0,0,0,0,0):long
30 (0,0,1,2,0,0,0,0):long
31 (0,0,2,1,0,0,0,0):long
32 (0,0,1,0,0,0,0,3):long
33 (0,0,0,1,0,2,0,1):long
34 (0,0,0,2,0,2,0,0):long
35 (0,0,1,0,0,0,0,2):long
36 (0,0,0,1,1,1,0,1):long
37 (0,0,0,1,0,2,0,1):long
38 (0,0,0,2,0,1,1,0):long
39 (0,0,0,2,0,1,1,0):long
40 (0,0,0,2,0,1,1,0):long
41 (0,0,0,1,1,1,1,0):long
42 (0,0,0,2,1,1,0,0):long
43 (0,0,0,1,1,0,2,0):long
44 (0,0,0,2,1,1,0,0):long
```

Selection strategies (1)

- best to use the same order of polynomials and pairs as in sequential algorithm
- selection algorithm is sequential
  - so optimizations reduce parallelism
- Attardi & Traverso: 'strategy-accurate' algorithm
  - rest reduction sequential
  - only top-reduction in parallel

Selection strategies (2)

- 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

Hardware

- InfiniBand 10Gbit node to node
- 1 Gbit Ethernet shared between 14 nodes
- use TCP/IP stack on InfiniBand
- bypass TCP/IP stack eventually in JDK 1.7
    - JAS doesn't compile on JDK 1.7 due to compiler bug

Conclusions

- first version of a distributed hybrid 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, speed-up of ~4
- runtime of distributed hybrid is comparable to distributed version, speed-up of ~4
- reduced communication between nodes, shared channels
- serialization overhead reduced with marshaled objects
- less memory required on nodes comp. dist. version
- new package is now type-safe with generic types

Future work

- profile and study run-time behavior in detail
- investigate other grid middle-ware
- improve integration into the grid environment
- study other result selection strategies
- compute sequential Gröbner bases with respect to different term orders in parallel
- test with JDK 1.7
- test other examples

Thank you

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