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Distributed Gröbner bases computation with MPJ

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EOOPS at AINA 2013, Barcelona

Overview

- Introduction to JAS
- Communication middle-ware: sockets and MPJ
  - execution middle-ware
  - data structure middle-ware
  - comparison
- Gröbner bases: sockets and MPJ
  - sequential and parallel algorithm
  - distributed algorithm
  - hybrid multi-threaded distributed algorithm
- 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) and jruby (Java Ruby) interactive scripting front ends

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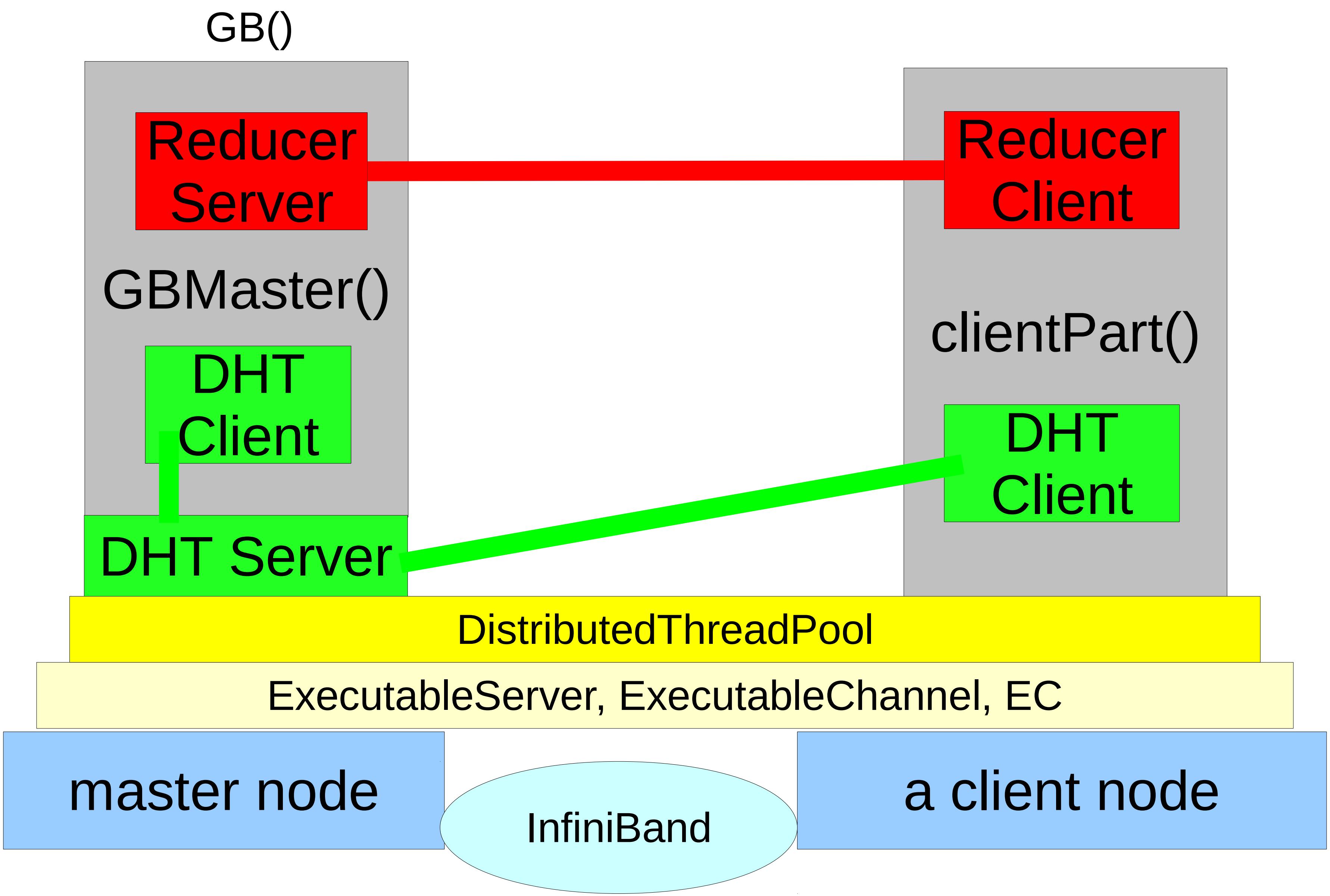
Socket middle-ware overview



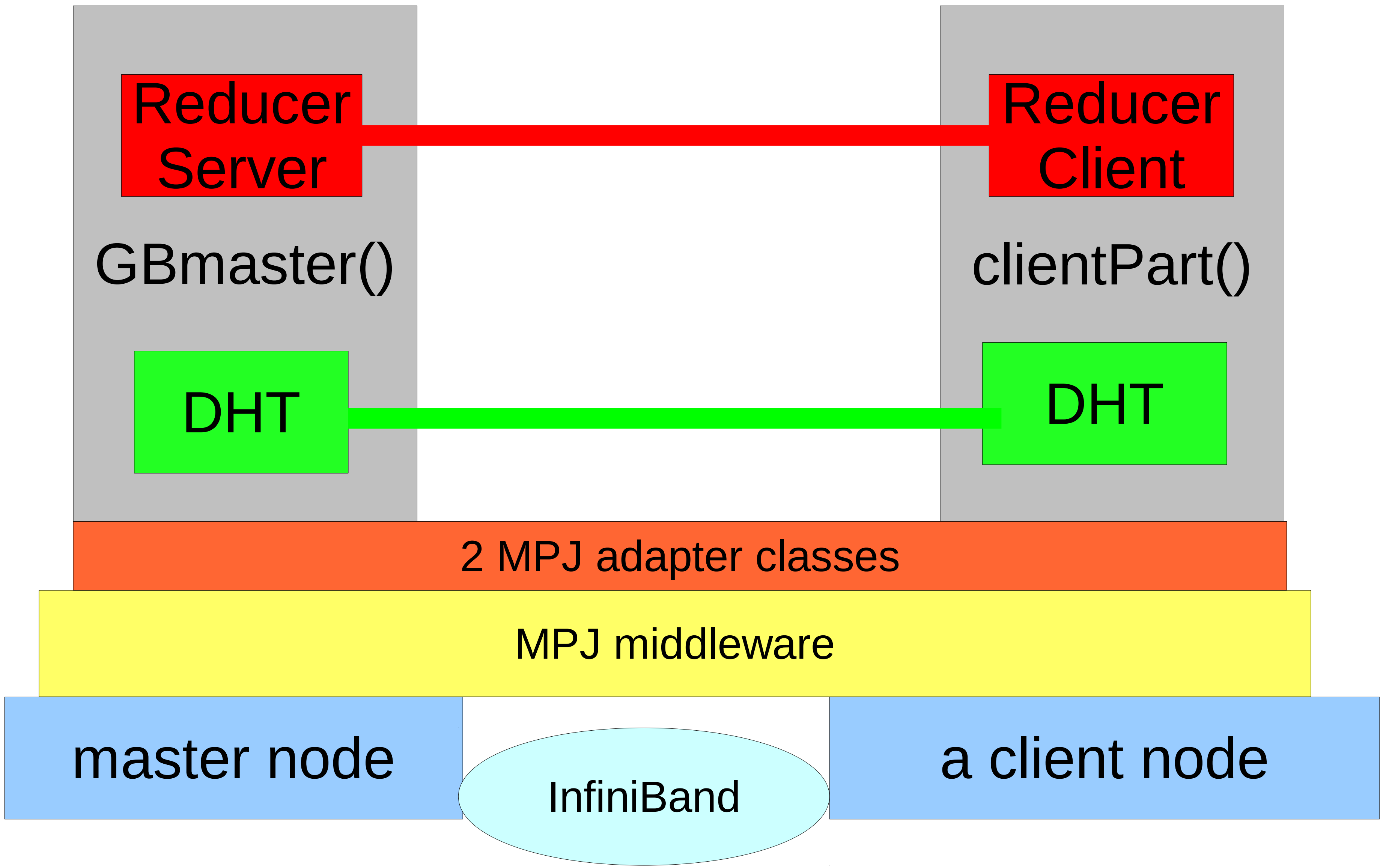
EC execution middle-ware (1)

- on compute nodes do basic bootstrapping
  - daemon class `ExecutableServer`
  - runs thread with `Executor` for each connection
  - receives objects and execute the `run()` method
  - multiple processes as threads in one JVM
- on master start `DistThreadPool`
  - start threads for each compute node
  - starts connections to all nodes with `ExecutableChannel`, gives the name EC
  - can start multiple tasks on nodes: multiple cores

EC execution middle-ware (2)

- client-server programming model
- list of compute nodes taken from PBS
- method `addJob()` on master
- send a job to a remote node and wait until termination
- method GB() executed on master
  - schedules clientPart() method/class as distributed threads to nodes
  - runs GBMaster()
    - starts DHT client
    - initialize communication channels
    - start further threads

MPJ middle-ware overview



MPJ execution middle-ware

- single-program multiple-data (SPMD) programming model
- execution within MPJ runtime environment
- `GB()` method executed on all nodes
  - rank 0: execute `GBmaster()`
  - rank > 0: execute `clientPart()`
- adapters between JAS and MPJ
  - `MPJEngine`
  - `MPJChannel`
- ibvdev not thread-safe in FastMPJ V1.0b

JAS to MPJ adapters

- MPJEngine
  - `getCommunicator()` delegates to `mpi.MPI.Init()`
  - `terminate()` delegates to `mpi.MPI.Finalize()`
  - `waitRequest()` within a global lock
  - `get*Lock(.)` to obtain global locks
- MPJChannel
  - `send()` delegates to `mpi.Comm.Send()`
  - `receive()` delegates to `mpi.Comm.Recv()`
  - also be used for `Isend`, `Irecv` together with `Request.Wait()`

Data structure middle-ware

- sending of polynomials to nodes involves
  - serialization and de-serialization time
  - and communication time
- minimize communication by replicating list on each node in a distributed data structure
- avoid explicit sending in GB to simplify protocol
- distributed list implemented as distributed hash table (DHT)
- key is list index
- implemented with generic types

DHT overview

- class `DistHashTable` extends `java.util.AbstractMap`
  - same for EC and MPJ versions
- 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 is received back
- no guaranty that value is received on all nodes

DHT-EC implementation

- client part on node use shared memory `TreeMap`
- implemented as central control DHT
  - `put()` sends key-value pair to a master
  - master broadcasts key-value pair to all nodes
  - `get()` method takes value from local `TreeMap`
  - clients to master use marshaled objects
  - no de-serialization in master
  - increases the CPU load on the master
  - doubles memory requirements on master

DHT-MPJ implementation

- class `DistHashTableMPJ`
- no central control, using MPI broadcast infra-structure
  - `put()` uses `mpi.Comm.Send()` to broadcast
  - separate threads use `mpi.Comm.Recv()` to retrieve message and store key-value pair
  - `get()` takes value from internal `TreeMap`
- MPJ must be thread-safe or a global lock must be maintained

Middle-ware comparison (1)

- MPJ simpler to use in PBS environment
  - set of well organized scripts from MPI run-time
- EC more flexible in dynamic task management
  - use of Threads and `java.util.concurrent`
- TCP/IP Sockets versus `mpi.Comm`
  - point-to-point with EC, explicit Channel management required, using object streams
  - n-to-n with MPI, all communication connections available via send/recv to MPI rank

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Middle-ware comparison (2)

- distributed HT data structure in EC and MPJ
- DHT semantics are different
  - DHT-EC maintains consistent key-value mappings after settling
  - DHT-MPJ can have inconsistent key-value mappings depending on timings
    - can be handled in distributed GB by master
- DHT uses threads and shared memory HT
  - problem with thread safety in MPJ with ibvdev

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  - sequential and parallel algorithm
  - distributed algorithm
  - hybrid multi-threaded distributed algorithm
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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 polynomial greatest common divisors
- 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

Buchberger algorithm

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

G = F; // needed on all compute nodes
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

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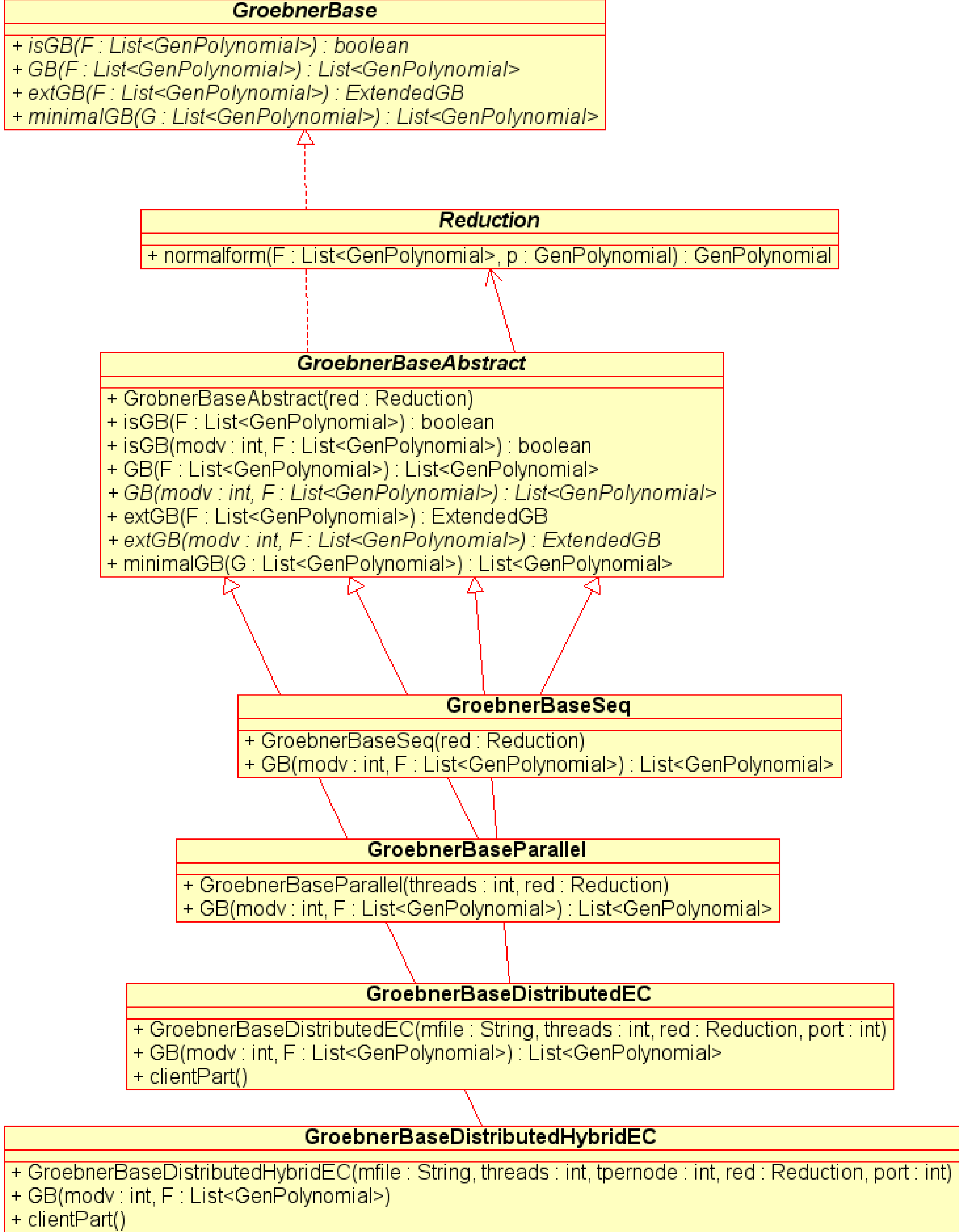

GroebnerBase
+ isGB(F : List<GenPolynomial>) : boolean
+ GB(F : List<GenPolynomial>) : List<GenPolynomial>
+ extGB(F : List<GenPolynomial>) : ExtendedGB
+ minimalGB(G : List<GenPolynomial>) : List<GenPolynomial>
Reduction
+ normalform(F : List<GenPolynomial>, p : GenPolynomial) : GenPolynomial
GroebnerBaseAbstract
+ 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>
GroebnerBaseDistributedEC
+ GroebnerBaseDistributedEC(mfile : String, threads : int, red : Reduction, port : int)
+ GB(modv : int, F : List<GenPolynomial>) : List<GenPolynomial>
+ clientPart()
GroebnerBaseDistributedHybridEC
+ GroebnerBaseDistributedHybridEC(mfile : String, threads : int, tpernode : int, red : Reduction, port : int)
+ GB(modv : int, F : List<GenPolynomial>)
+ clientPart()

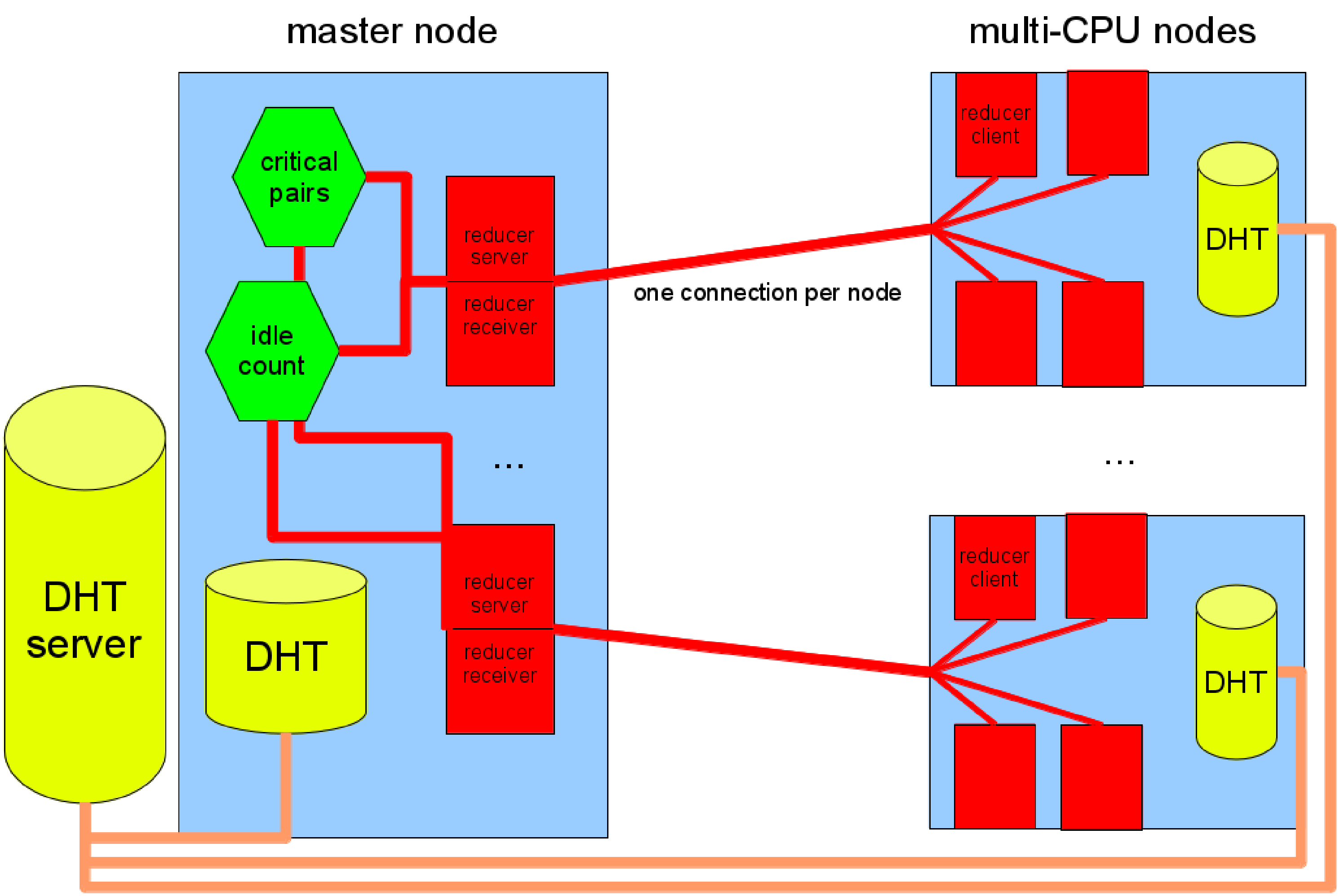
Sequential and parallel GB

- critical pair list `B` implemented as thread-safe working queues
- implementations for different selection strategies
  - `OrderedPairlist`, optimized Buchberger
  - `CriticalPairlist`, stay similar to sequential
  - `OrderedSyzPairlist`, Gebauer-Möller version
- selection and removal with `getNext()`
- addition with `put()`
- polynomial list is in shared memory on master

Distributed GB

- master maintains critical pair list and communicates with the distributed workers
- simple version with one JVM process per node
  - can also have multiple JVM processes on a node
- hybrid version with multiple threads per node
  - one channel from master to nodes
  - one DHT per node shared by all threads
- top level GB algorithms same for sockets EC and MPJ
  - only use different middle-wares

Thread to node mapping (EC)



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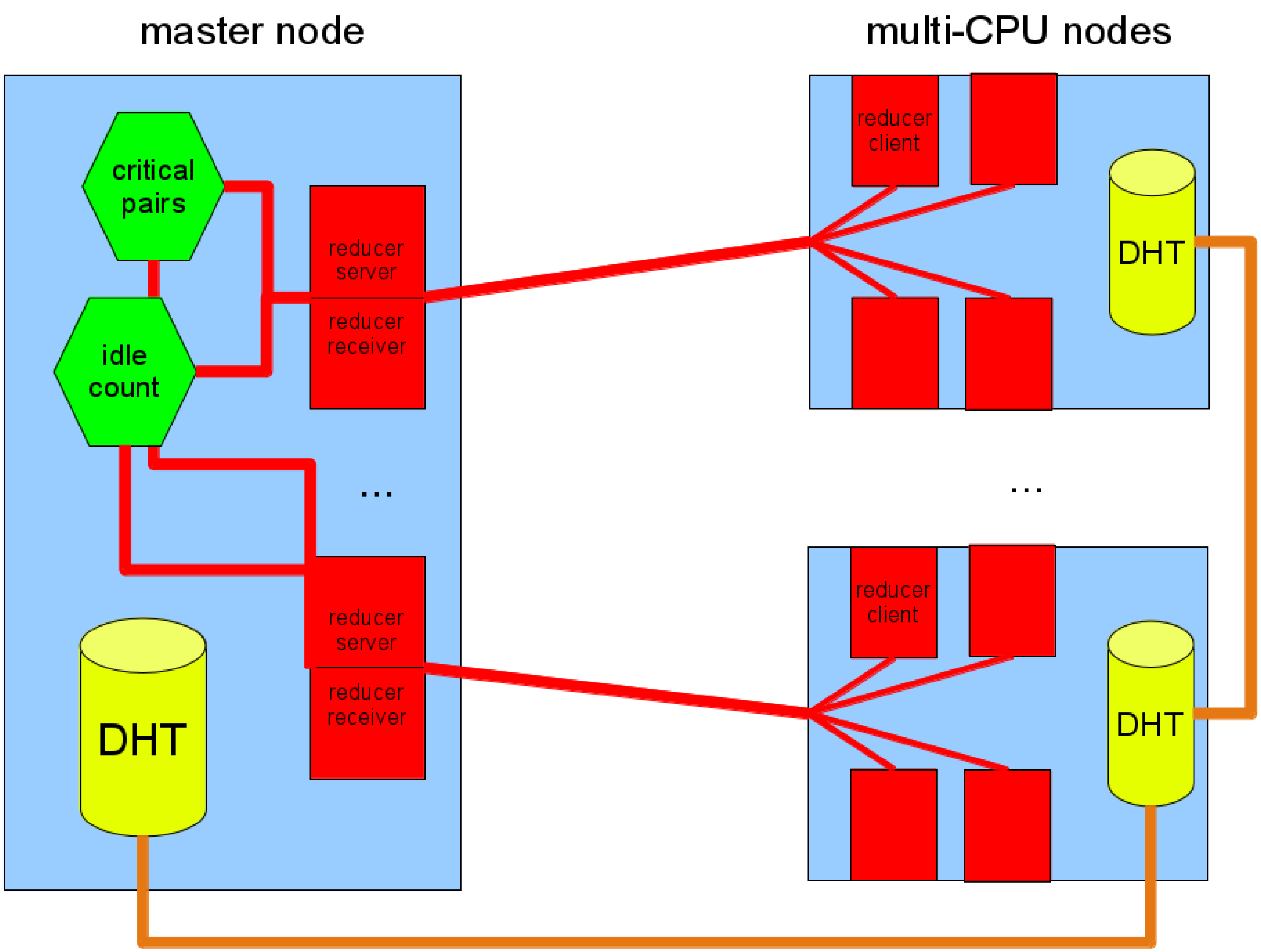
Thread to node mapping (MPJ)



GB comparison

- middle-ware design allows the easy replacement of underlying communication system
- get maximal overlap between communication and computation with DHT data structure
- MPJ less flexible than EC but more easy to use
- FastMPJ uses `java.nio` and own low-level code
  - niodev is thread-safe, works well with IP over IB
  - ibvdev is not thread safe at the moment
- EC uses Socket from `java.io, java.net`
  - use IP over IB, plain Ethernet too slow

Performance

- all tests on same hardware, network IP over IB
- same Java version 1.6, different JVM releases
- same example “Katsura 8 modulo 2^127-1”
- improvements over the last two years in JVMs and JAS
  - sequential GB: 20%
  - parallel GB: 40 – 60%
  - distributed hybrid GB: 50%
- EC vs MPJ depends on threads per node
- GB speed-up achieved, EC: 8.9, MPJ: 12.8

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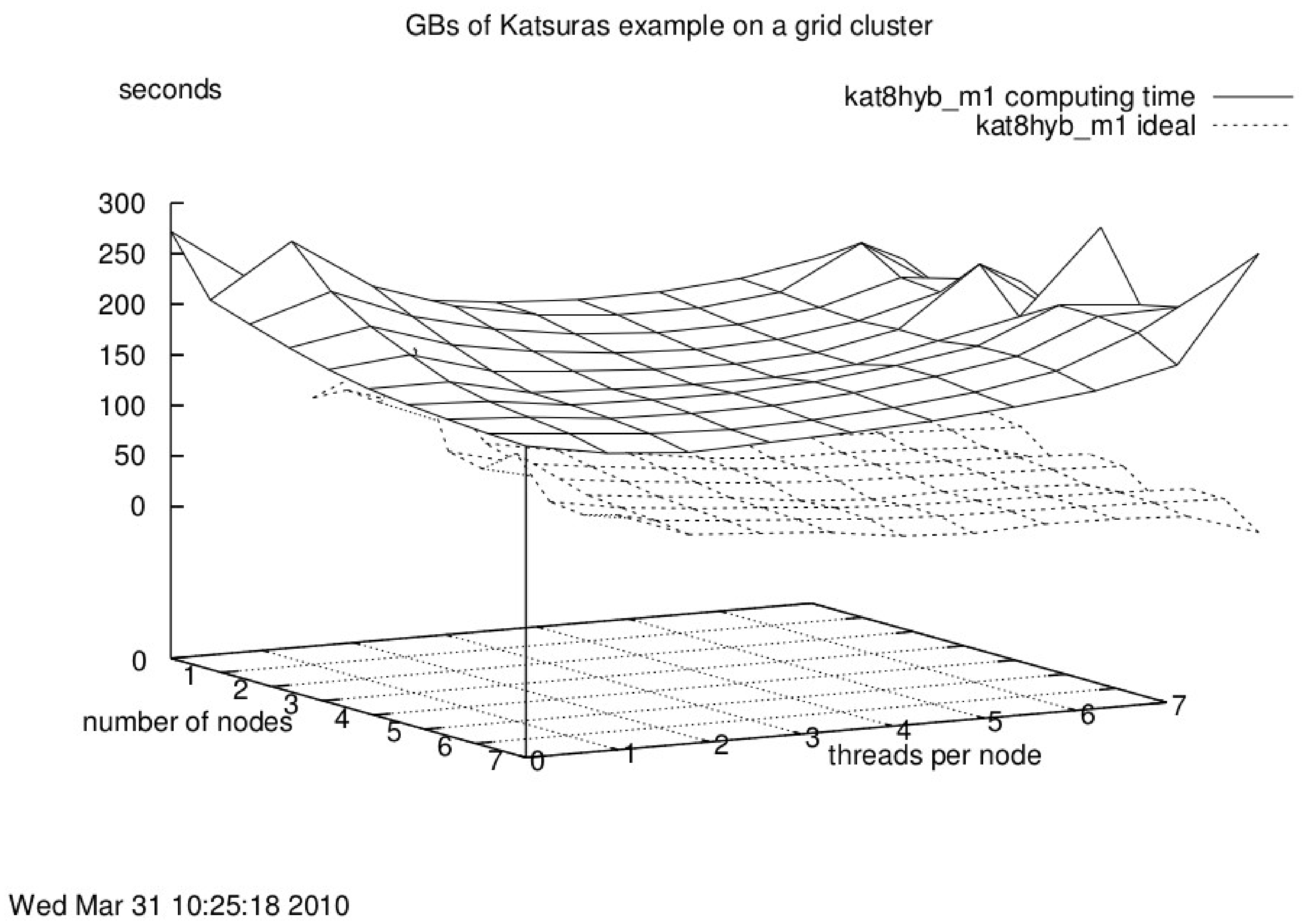
time EC GB run in 2010



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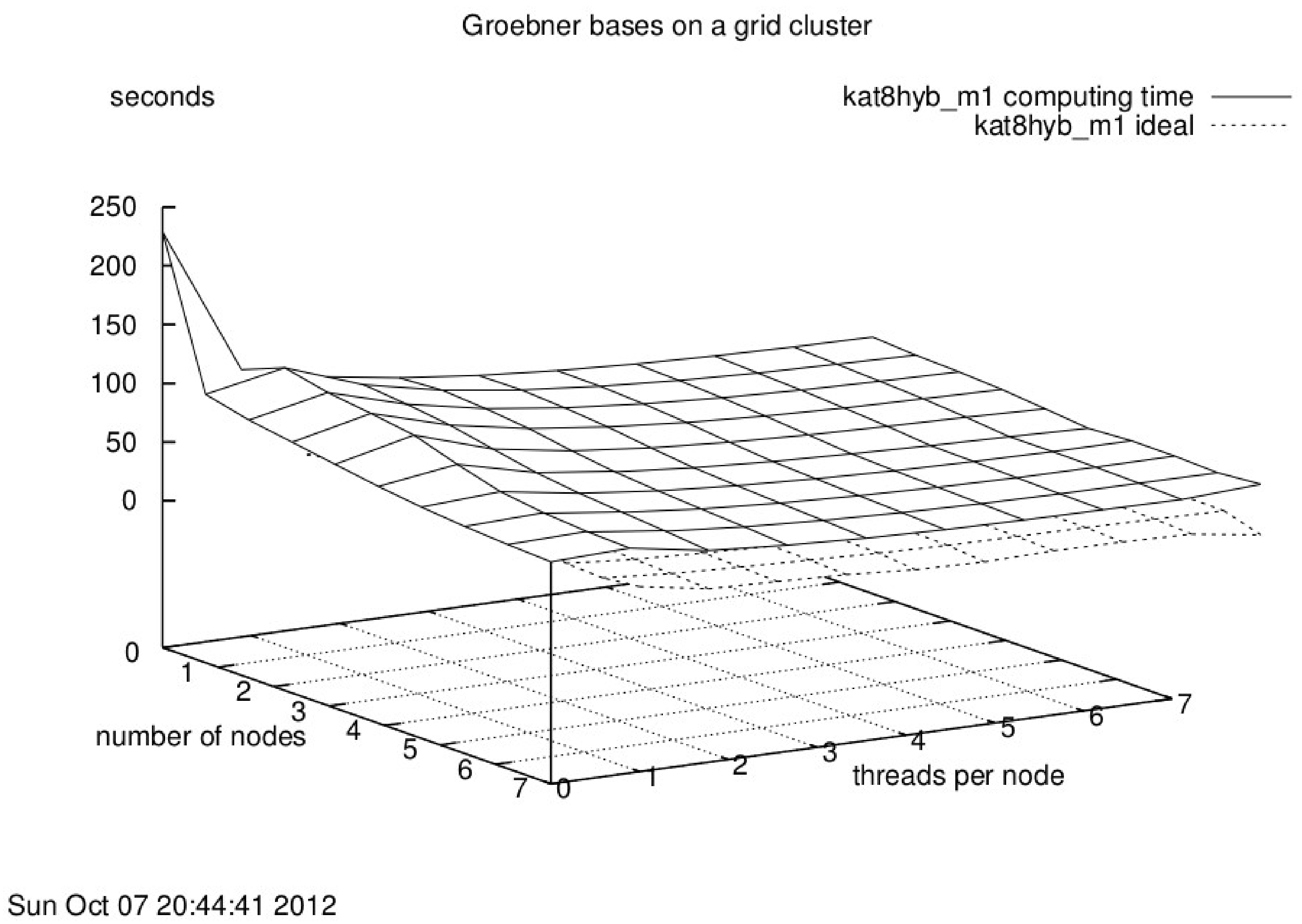
time same EC GB run in 2012



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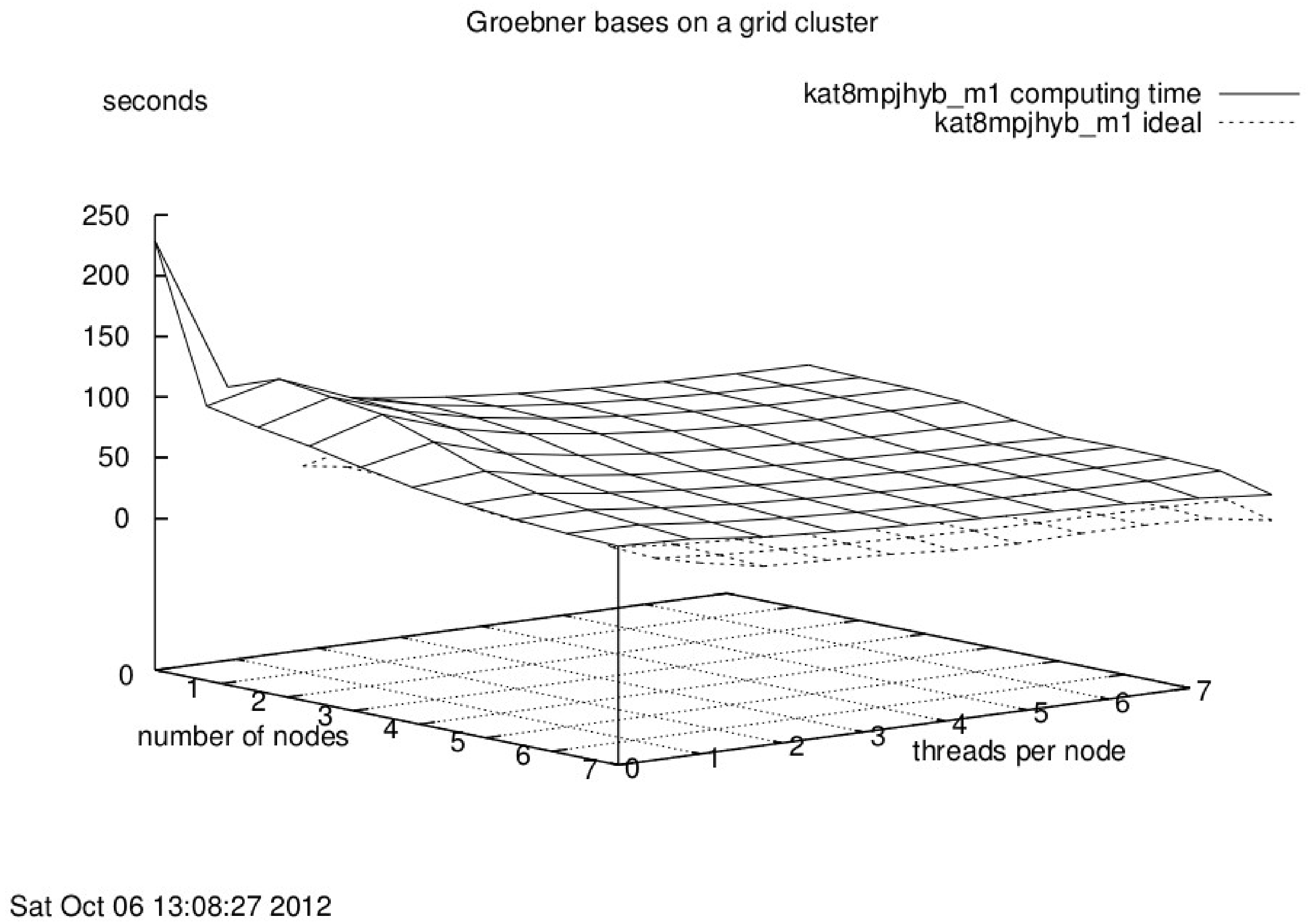
time MPJ GB run in 2012



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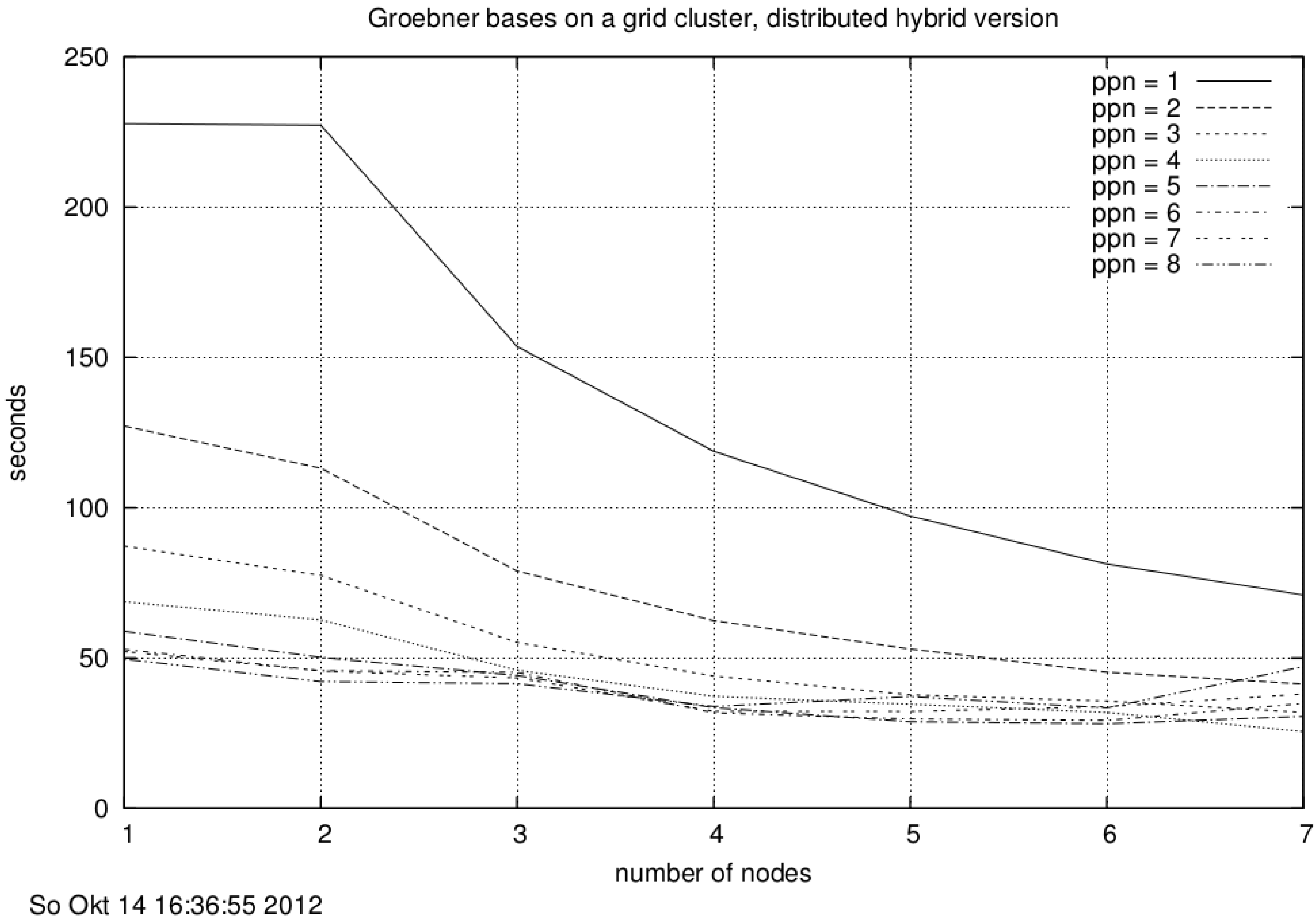
time EC GB run: different ppn



ppn = process / threads per node

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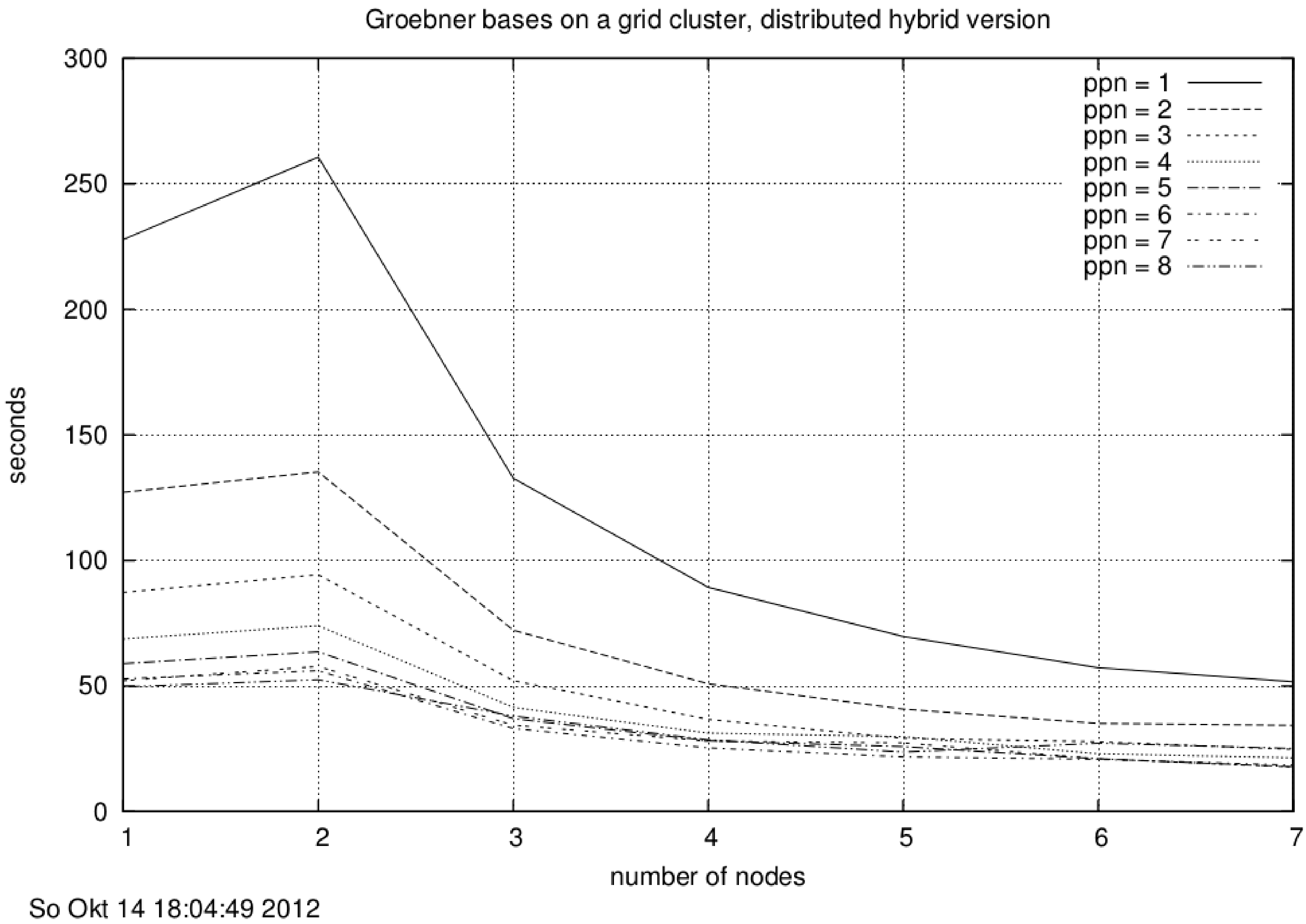
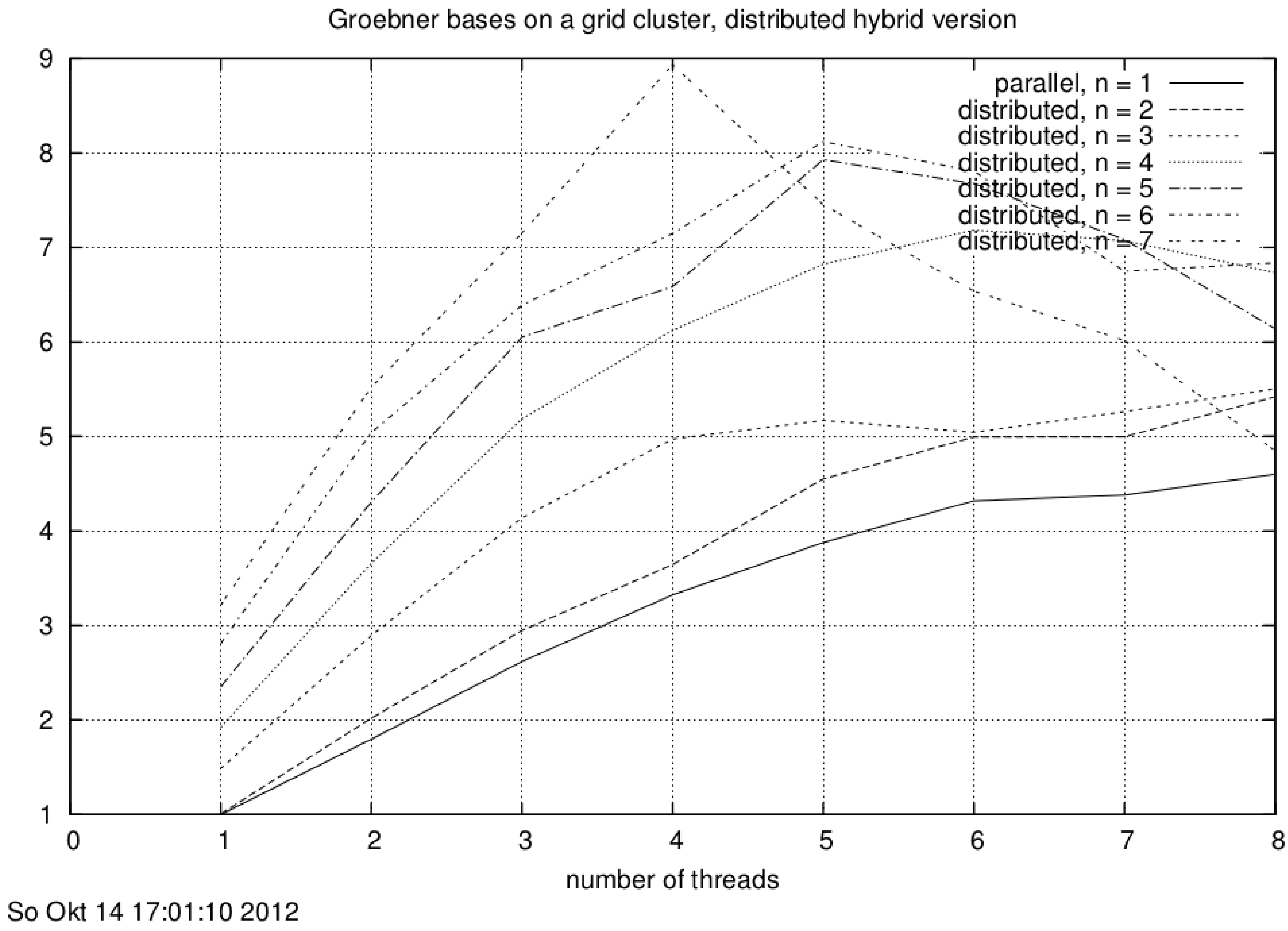
time MPJ GB run: different ppn



ppn = process / threads per node

speed-up EC GB: nodes



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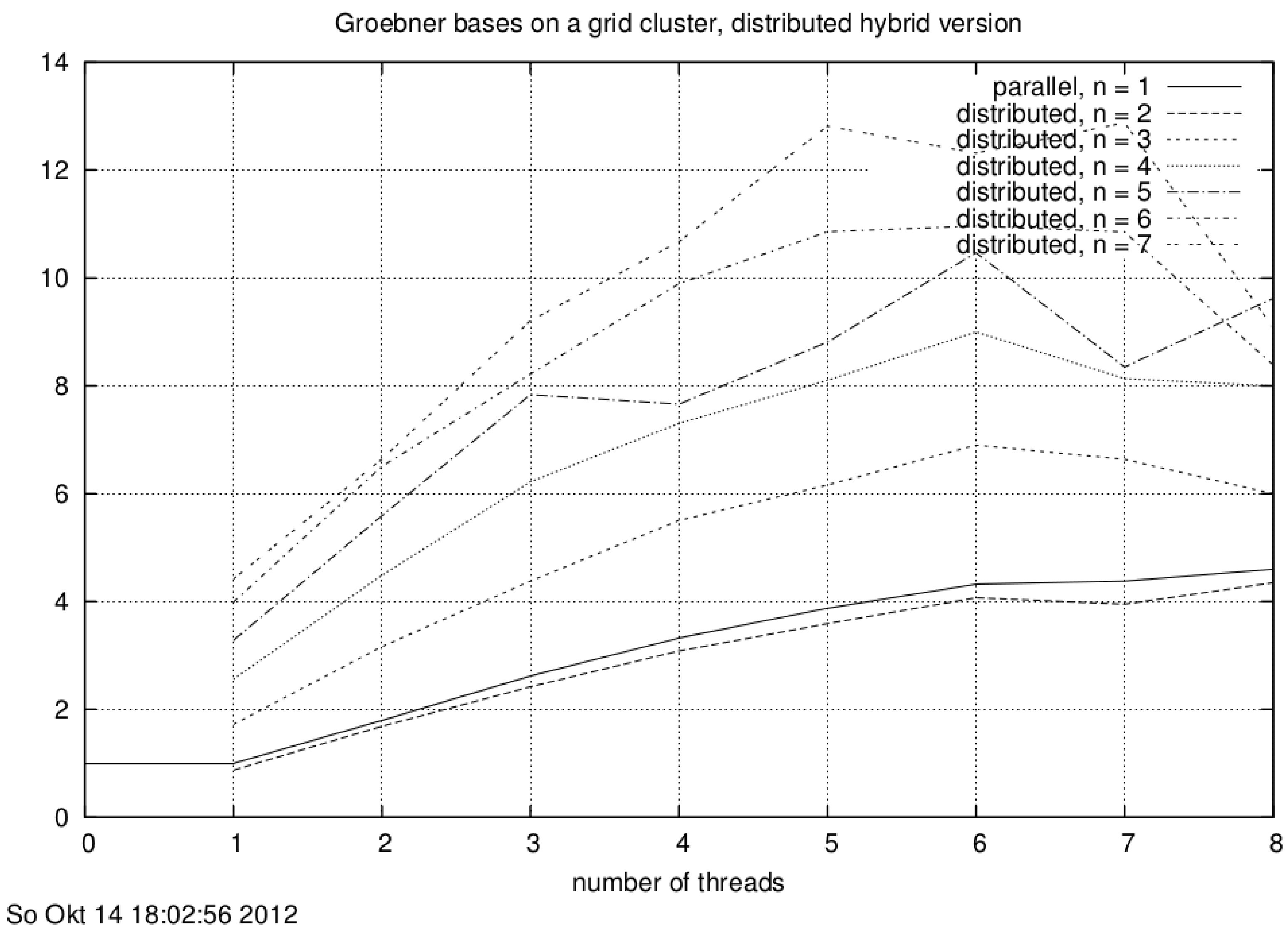
speed-up MPJ GB: nodes



Conclusions (1)

- distributed hybrid GB algorithm
  - communication based on EC sockets or MPJ
  - FastMPJ has support for direkt InfiniBand
- improvements within 2 years of 40-60%
  - JVM more optimized, JAS better optimized
- achieved speed-up with IP over IB on 8 nodes
  - 12.8 for FastMPJ and 5-7 threads per node
  - 8.9 for sockets EC and 4-6 threads per node
- EC for small number of threads per node faster
- FastMPJ is 50% faster for 5-7 threads per node

Conclusions (2)

- both run on a HPC cluster in PBS environment
- reduced communication overhead between nodes, main objects in shared memory
- less memory required on nodes compared to pure distributed version
- both packages are type-safe with generic types
- developed classes fit in Gröbner base class hierarchy

Future work

- fix or work around thread safety issues in FastMPJ
- investigate InfiniBand ibvdev device performance
- profile and study run-time behaviour in detail
- investigate further optimizations of the GB algorithms: F4, F5, GGV, ARRI, ...

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Thank you for your attention

Questions ?

Comments ?

http://krum.rz.uni-mannheim.de/jas/

Acknowledgements

- thanks to: Thomas Becker, Raphael Jolly, Werner K. Seiler, Axel Kramer, Dongming Wang, Thomas Sturm, Hans-Günther Kruse, Markus Aleksy
- thanks to the referees

more slides

bwGRiD cluster architecture

- 8-core CPU nodes @ 2.83 GHz, 16GB, 140 nodes
- shared Lustre home directories
- 20Gbit InfiniBand and 1Gbit Ethernet interconnect
- managed by PBS batch system, Moab scheduler
- running Java 64bit server VM 1.6 with 4+GB mem
- start Java VMs with daemons on allocated nodes
- communication via TCP/IP over InfiniBand
- other middle-ware ProActive or GridGain not studied

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JAS Implementation overview

- 340+ classes and interfaces
- plus ~150 JUnit test classes,5000+ assertions
- 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), jruby (Java Ruby) scripts
  - support for Sage compatible polynomial expressions
- Android version based on Ruboto using jruby

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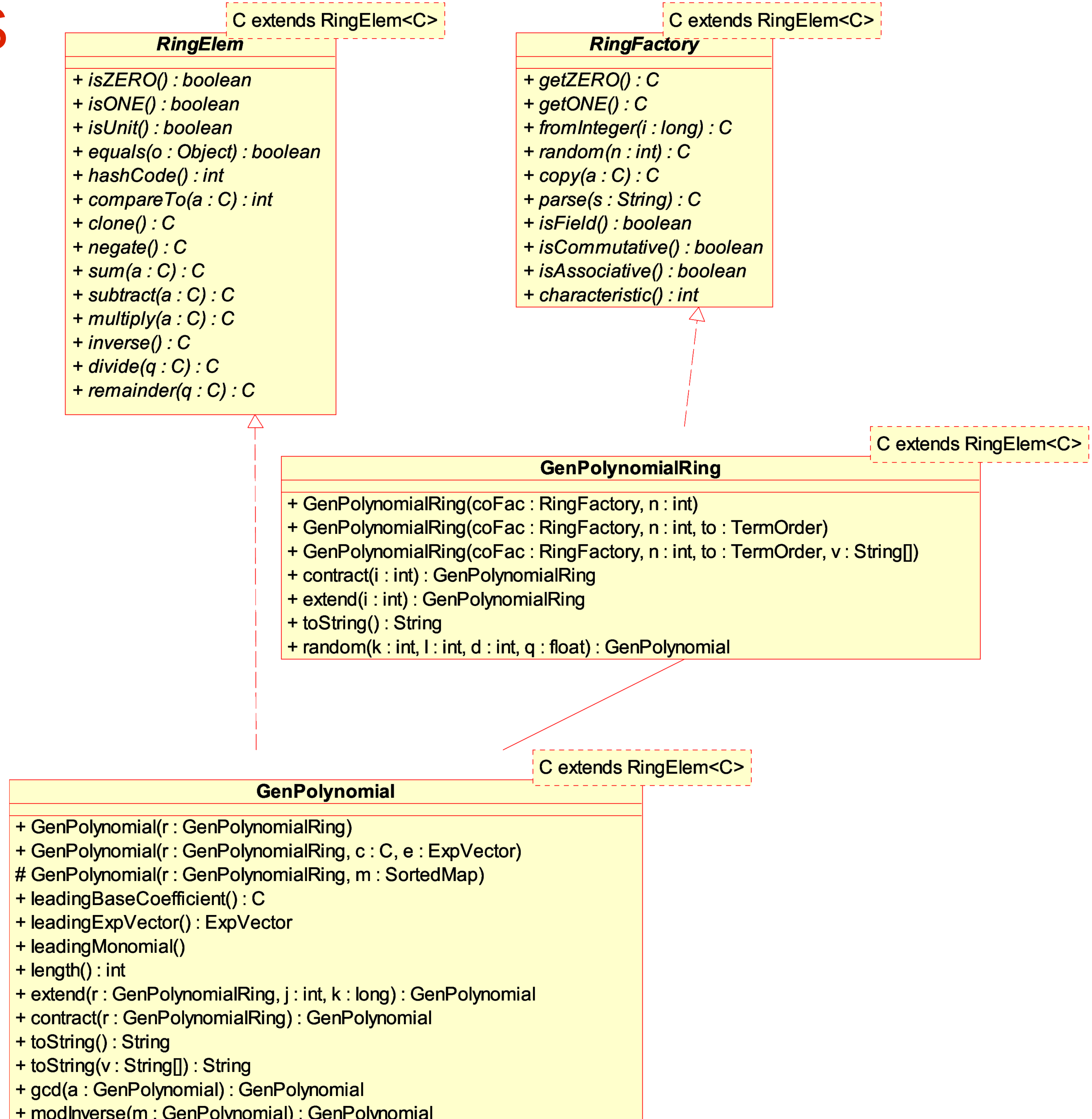
C extends RingElem<C>
RingElem
+ isZERO() : boolean
+ isONE() : boolean
+ isUnit() : boolean
+ equals(o : Object) : boolean
+ hashCode() : int
+ compareTo(a : C) : int
+ clone() : C
+ negate() : C
+ sum(a : C) : C
+ subtract(a : C) : C
+ multiply(a : C) : C
+ inverse() : C
+ divide(q : C) : C
+ remainder(q : 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; 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);
}
```