PCJ-BLAST – massively parallel sequence alignment using NCBI Blast and PCJ Java library

Piotr Bała  
bala@icm.edu.pl  
ICM University of Warsaw

Marek Nowicki  
faramir@mat.umk.pl  
ICM University of Warsaw
N. Copernicus University

Davit Bzhalava  
davit.bzhalava@ki.se  
Karolinska Instituut
Blast

- Sequence alignment is essential for NGS
- There is a number of software packages for sequence alignment based on various similarity search methods
- BLAST Basic Local Alignment Search Tool (1991)
  - The heuristic algorithm it uses is much faster than other approaches
  - The search time can be long (days or weeks) for large datasets
- NCBI blast is the most widely used implementation

- There is strong interest in using large computer systems to run blast
  - Blast running on cloud or grid
  - Parallel versions of blast running on HPC systems
>C1093377_2.0
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
AAAAAACACTTTTGGGAGGGCCAAGGATGGGAAGATCTTTTGAGGGCAGGGCGTTCAAGACCAGCTCTGAGCAATATGGAGAGACCTGTCTCTACAAAAAAAATTAGCCAGACCTAGTGGCTGGCTGAAGGAGGATCATCTGAGCTCAGGAGATTGAGAT

>C1093379_2.0
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               
NCBI blast performance (XC40 single node)

Time of processing 48 sequences at once using 1 instance of different version of NCBI BLAST with different number of BLAST threads

- ncbi-blast-2.2.28+
- ncbi-blast-2.2.31+
- ncbi-blast-2.3.0+
- ncbi-blast-2.3.0+_gcc_5.3
Blast – processing time of reads changes

Processing time [s]
Parallel blast implementations

- mpiBLAST – uses old version (2012) of blast
- parallel_blast.py – limited to single node, regular split of input
- Paracel BLAST (based on NCBI blast 2.2.26) – costly!
- The BlueGene implementation – limited to IBM BGQ systems
- pioBLAST parallel version which uses MPIIO – memory problems while reference database is large

- SparkBLAST – Apache Spark implementation running on AWS cloud (PhD thesis 2016)
Pcj-blast

- Parallel version developed using PCJ (Parallel Computing in Java library developed at ICM)
- Java code is responsible for reading fasta input and execute NCBI-blast on set of sequences (reads)
- The NCBI blast (currently 2.2.28) is executed with the `–num_threads` option
  - For 28 core nodes: 4 PCJ threads with `–num_threads=7`

- The solution can be executed on any multinode system with Java 8 installed
- The I/O performance is important
  - thousands of blast instances reads blast database (52GB) concurrently
  - lustra filesystem performs worse than nfs
Pcj-blast

- Reads input sequence (fasta) line by line
- Blocks of lines (reads) are used as input for blast query
- Pcj-blast can start hundreds of blast instances
- NCBI blast is used
  - pcj-blast not bounded to particular version
- One or more NCBI blast instances are run on the hardware node
- Output from each node (text or XML) is gathered
- Output is postprocessed and is stored in a single file
  - Postprocessing is parallelized

- Pcj-blast can be run on HPC systems, clusters
  - Requires Java 8 and NCBI blast installed
Multiple NCBI blast running on single node (X86 cluster)
I/O performance (x86 single file read)
I/O performance (XC40 single file read)

- Aggregate I/O performance [MB/s]
- Number of nodes
- GVS
- Lustre

Graph showing the comparison between GVS and Lustre in terms of aggregate I/O performance over different numbers of nodes.
pcj-blast scalability (x86 cluster)
pcj-blast scalability (Cray XC40)
PGAS languages

- http://www.pgas.org
- Independent threads
- Local and shared (global) variables
- Global variables visible to all threads
- One-sided communication
  - Communication details hidden to programmer
- Main operations:
  - Synchronization (barrier)
  - get
  - put
Java library

- pcj.icm.edu.pl

- Designed based on PGAS (Partitioned Global Address Space) paradigm
- Simple and easy to use
- Does not introduce extensions to the Java language
  - no new compilers nor pre-processor
- Does not require additional libraries
- Works with Java 1.8, 1.9
  - Version for Java 1.7 available
- Good performance
- Good scalability (already beyond 50k+ cores)
PCJ – memory layout

![Diagram showing the memory layout of PCJ threads on physical nodes. The diagram includes visual representations of threads, CPUs, shared variables, and local variables.]
PCJ – memory layout and communication

Physical node

1. PCJ thread 0
2. PCJ thread 1
3. PCJ thread 2
4. PCJ thread 3

Physical node

5. PCJ thread 4
6. PCJ thread 5
7. PCJ thread 6
8. PCJ thread 7

CPU

CPU

CPU

CPU

CPU

CPU

CPU

Shared variables

Local variables

16/05/2017
Main functionality:
- Synchronization
- Get data from other thread (get)
- Send data to other thread (put)

Additional functionality:
- Broadcast
- Monitoring of the variable change (useful with put())
- Parallel I/O
- Groups of threads
import org.pcj.*

public class PcjHelloWorld implements StartPoint {

    @Override
    public void main() {
        System.out.println("Hello!"erior
    }

    public static void main(String[] args) {
        PCJ.deploy(PcjHelloWorld.class,
                    new NodesDescription("nodes.txt"));
    }
}

PCJ – main methods

```
@Shared(ExampleGetPut.class)    // Define storage
enum Shared { a, array }

if (PCJ.myId() == 0) c = (double) PCJ.get(3, Shared.a);

if (PCJ.myId() == 0) PCJ.put(5.0, 3, Shared.a);
if (PCJ.myId() == 0) PCJ.put(5.0, 3, Shared.array, p);

if (PCJ.myId() == 0) PCJ.broadcast(5.0, Shared.a);

public static void PCJ.barrier();
public static int PCJ.threadCount();
public static int PCJ.myId();
```
@Shared(ExampleRead.class)  // Define storage
enum Shared { a }

double a;

double al;

if (PCJ.myId() == 0) {
    Scanner s = new Scanner(System.in);
    al = s.nextDouble();
    PCJ.broadcast(al, Shared.a);
} else {
    PCJ.waitFor(Shared.a);
}

PCJ.barrier()
@Shared (PcjGather.class)
enum Shared { a }
double a
PcjFuture aL[] = new PcjFuture[PCJ.threadCount()];
double sum = 0.0;
if (PCJ.myId() == 0) {
    for (int p = 0; p < PCJ.threadCount(); p++) {
        aL[p] = PCJ.asyncGet(p, Shared.a);
    }
    for (int p = 0; p < PCJ.threadCount(); p++) {
        sum = sum + (double) aL[p].get();
    }
}
Graph500 – kernel 2 (BFS) Cray XC40

Scale 27

- TEPS in millions
- Number of tasks

- PCJ 64pn interlagos
- PCJ 4pn istanbul
- PCJ 16pn okeanos
- MPI 64pn interlagos
- MPI 4pn istanbul
Neural network optimization using GA (connectom of C. Elagans)
Pi Estimate (blue), BFS (orange), WordCount (red)
PCJ-BLAST – massively parallel sequence alignment using NCBI Blast and PCJ Java library

PCJ: pcj.icm.edu.pl

Piotr Bała  
bala@icm.edu.pl  
ICM University of Warsaw

Marek Nowicki  
faramir@mat.umk.pl  
ICM University of Warsaw  
N. Copernicus University

Davit Bzhalava  
davit.bzhalava@ki.se  
Karolinska Institutet