pcj-blast - highly parallel similarity search implementation

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Blast

- Sequence alignment is essential for NGS
- There is a number of software packages for sequence alignment based on various a similarity search methods
- BLAST Basic Local Alignment Search Tool (1991)
  - The heruistic 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 runing on cloud or grid
  - Parallel versions of blast running on HPC systems

Fasta input (2 reads out of 1 milion)

>C1093377_2.0

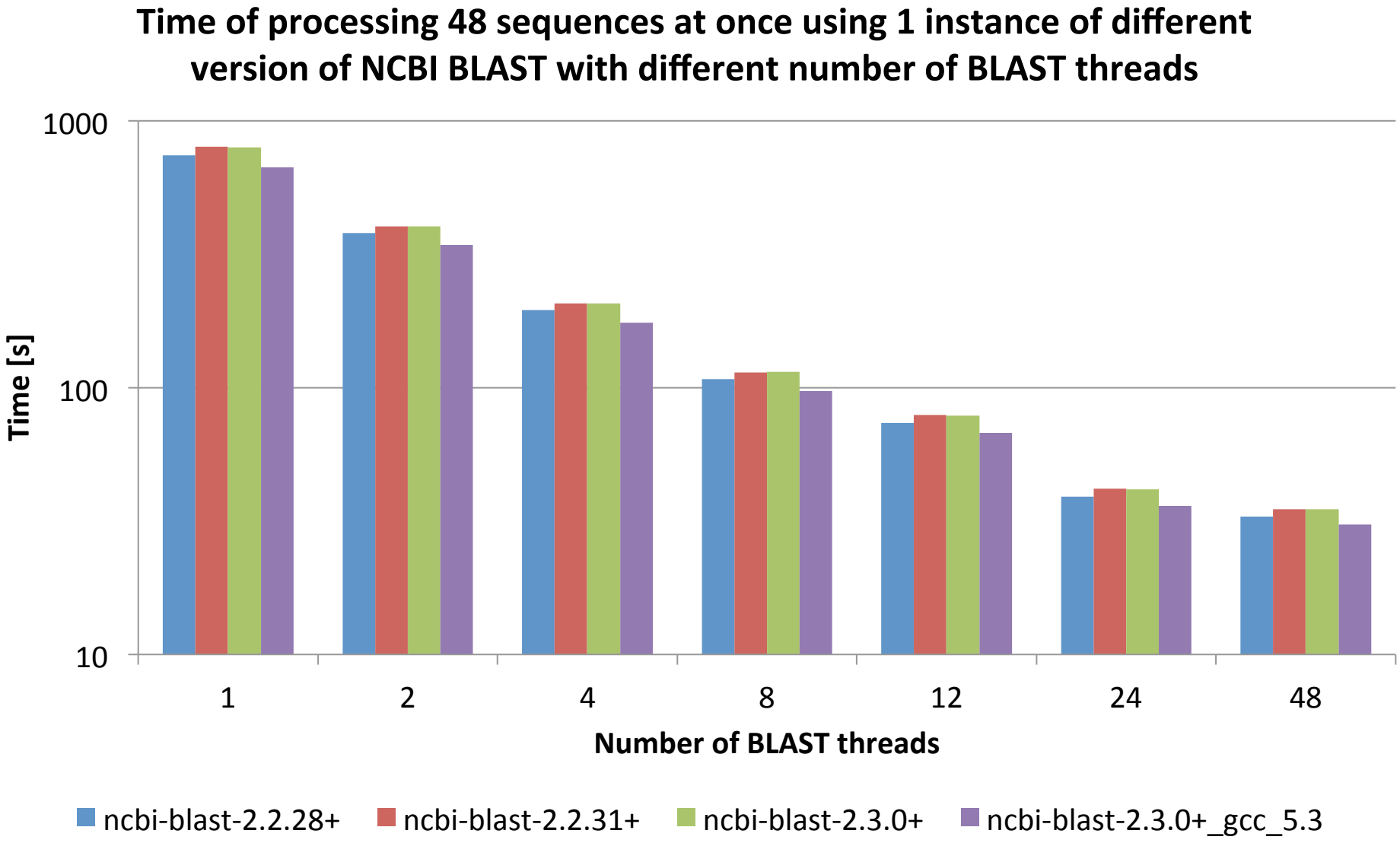
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
AAAAACACTTTGGGAGGCCAAGATGGGAAGATCTTTTGAGG
CCAGGCGTTCAAGACCAGTCTGGGCAATATGGAGAGACCT
GTCTCTACAAAAAAAATTAGCCAGACCTAGTGGCTGGCTGA
GGCAGGAGGATCATCTGAGCTCAGGAGATTGAGAT

>C1093379_2.0

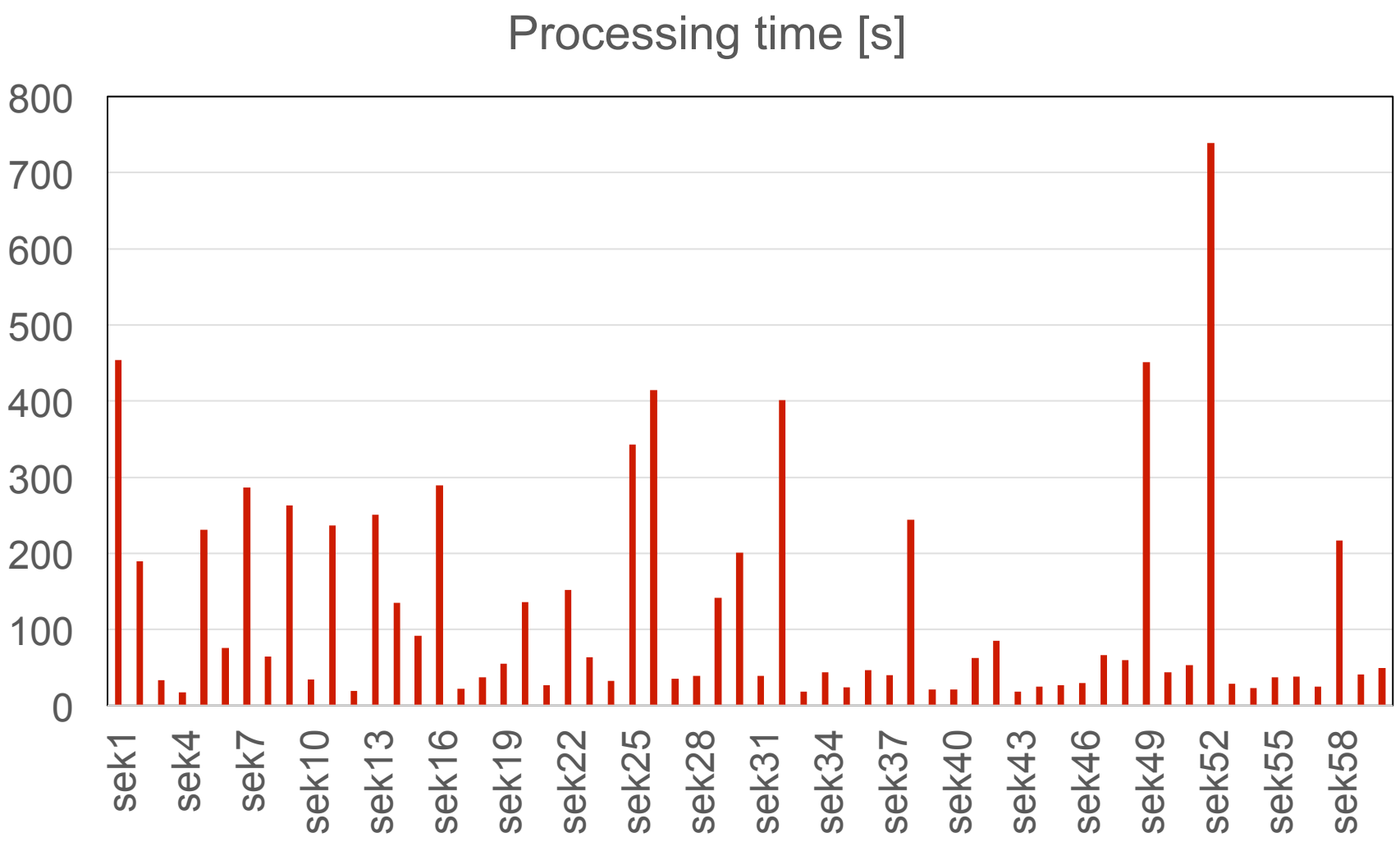
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
AAAATTTTAAGTTTTTCCTTATAAGGGAAATAAGCTTATTTCT
TTTAGAAGCAGAAACTGCAAATGGGGGTGTATGGAATTCTTT
TTTTTTTTTTTTTTTTTTTGCGACAAGGTCTCACTGTGTTGCCCA
GACTGGAGTGCAGTGGTGCAATCATAGCT

…

NCBI blast performance (XC40 single node)



Blast – processing time of reads changes



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
- …

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

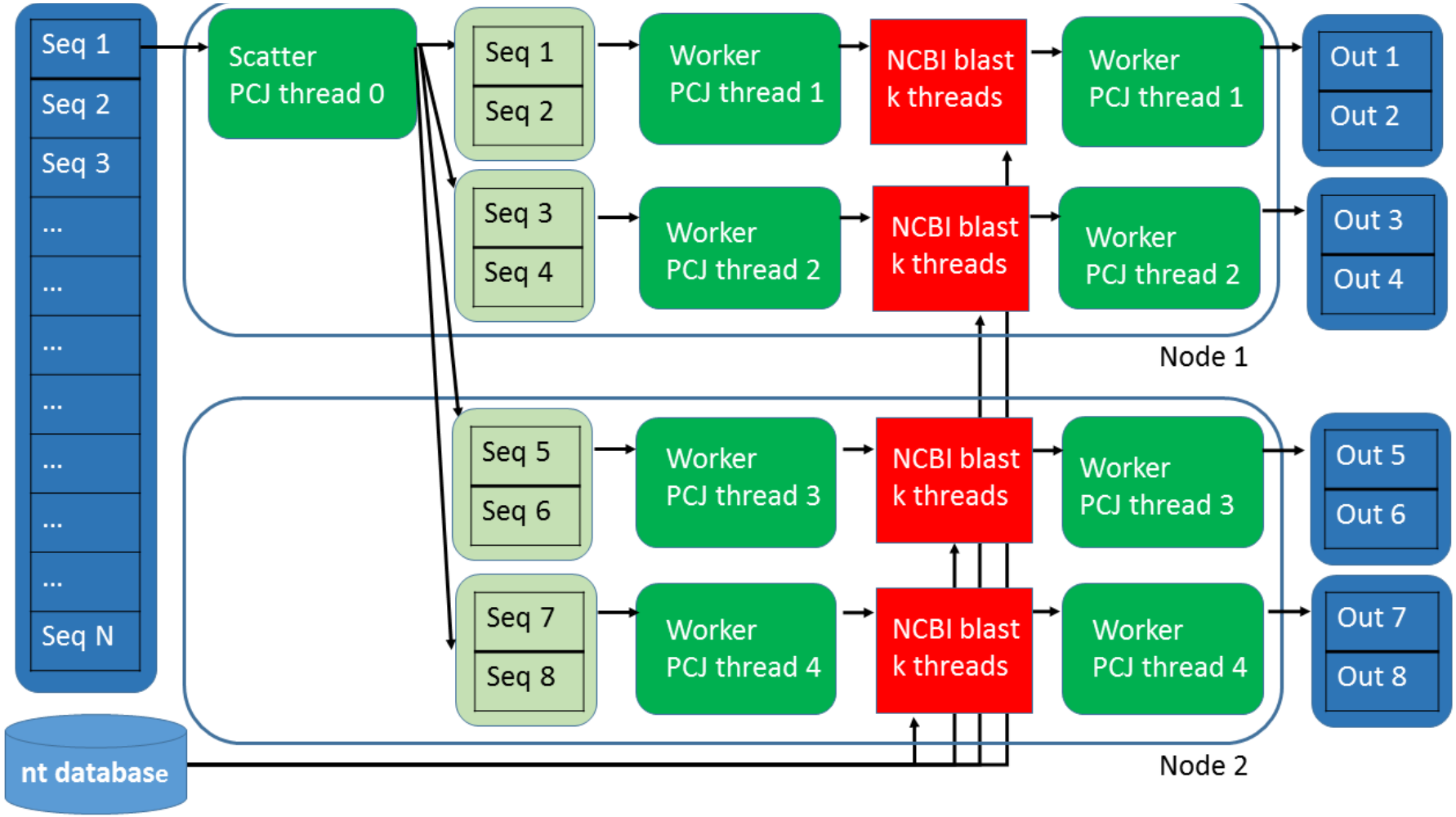
- The solution can be executed on any multinode system with Java 8 installed
- The I/O performance is important
  - thousands of blast instances reads blast database (52GB) concurrently
  - lustra filesystem performs worse than nfs

Pcj-blast

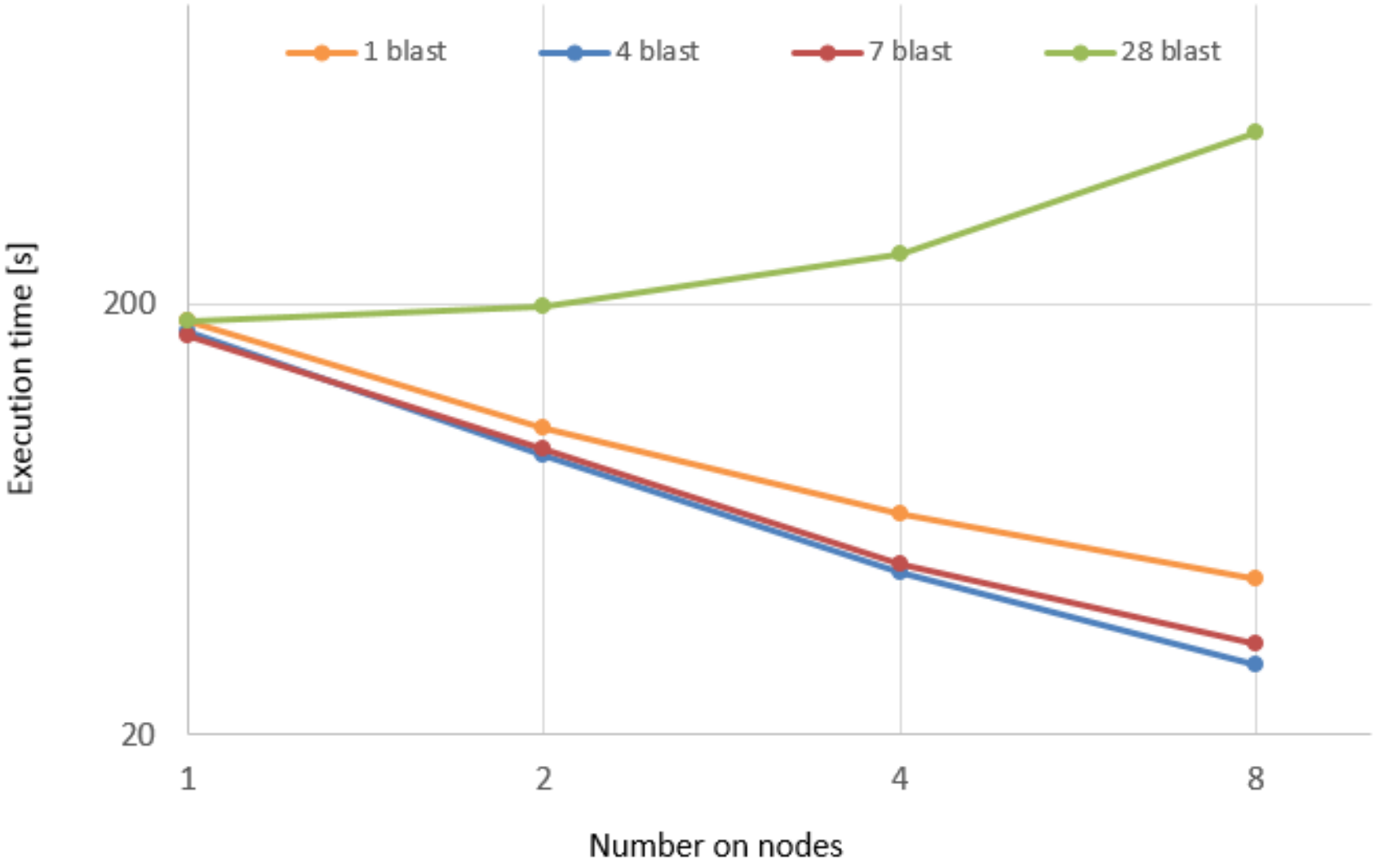
- Reads input sequence (fasta) line by line
- Blocks of lines (reads) are used as input for blast query
- Pcj-blast can start hundreds of blast instances
- NCBI blast is used
  pcj-blast not bounded to particular version
- One or more NCBI blast instances are run on the hardware node
- Output from each 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

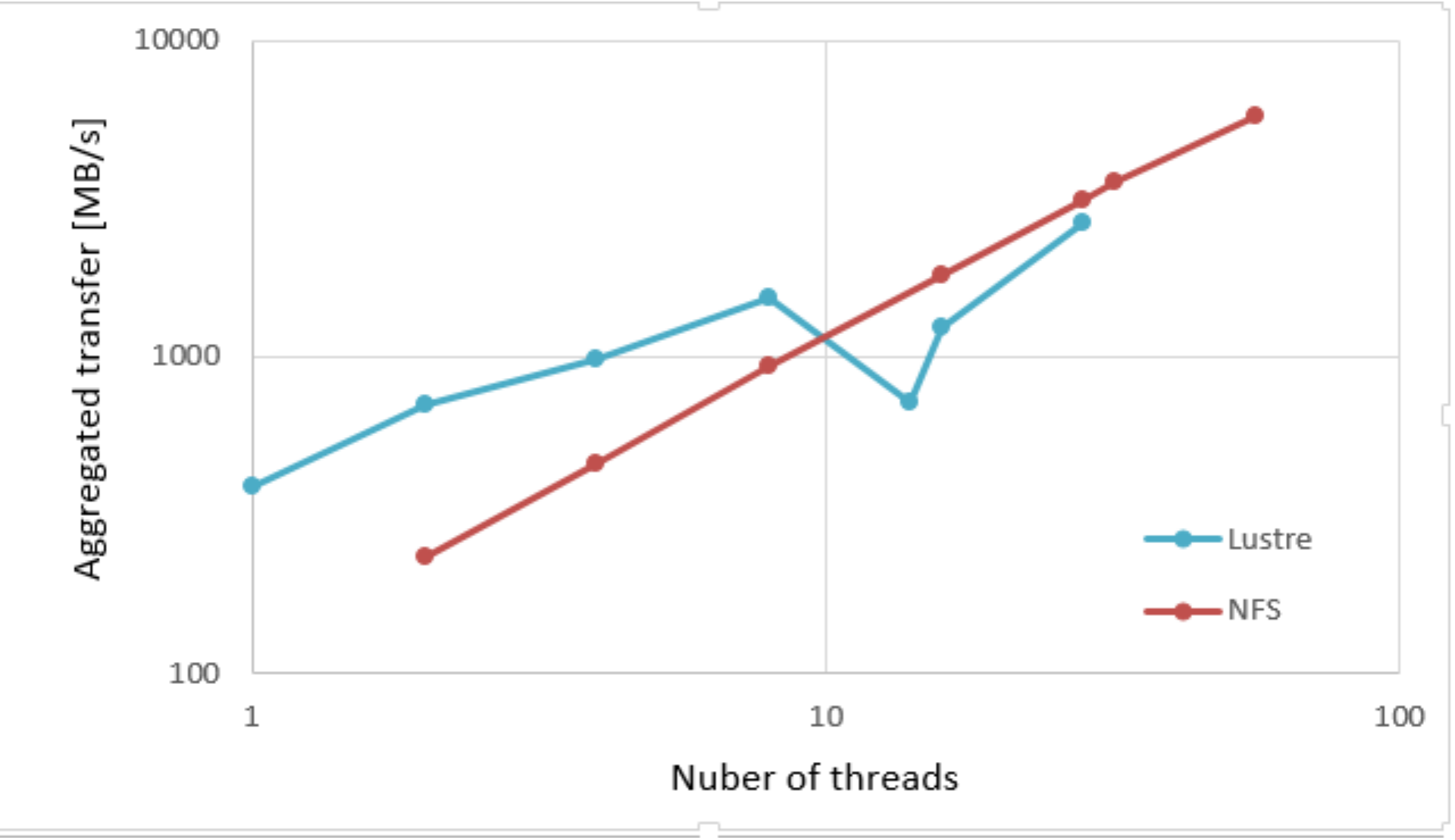
Pcj-blast


Seq 1
Seq 2
Seq 3
...
...
...
...
...
...
...
Seq N
Scatter
PCJ thread 0
Seq 1
Seq 2
Seq 3
Seq 4
Seq 5
Seq 6
Seq 7
Seq 8
Worker
PCJ thread 1
Worker
PCJ thread 2
Worker
PCJ thread 3
Worker
PCJ thread 4
NCBI blast
k threads
NCBI blast
k threads
NCBI blast
k threads
NCBI blast
k threads
Worker
PCJ thread 1
Worker
PCJ thread 2
Worker
PCJ thread 3
Worker
PCJ thread 4
Out 1
Out 2
Out 3
Out 4
Out 5
Out 6
Out 7
Out 8
Node 1
Node 2
nt database

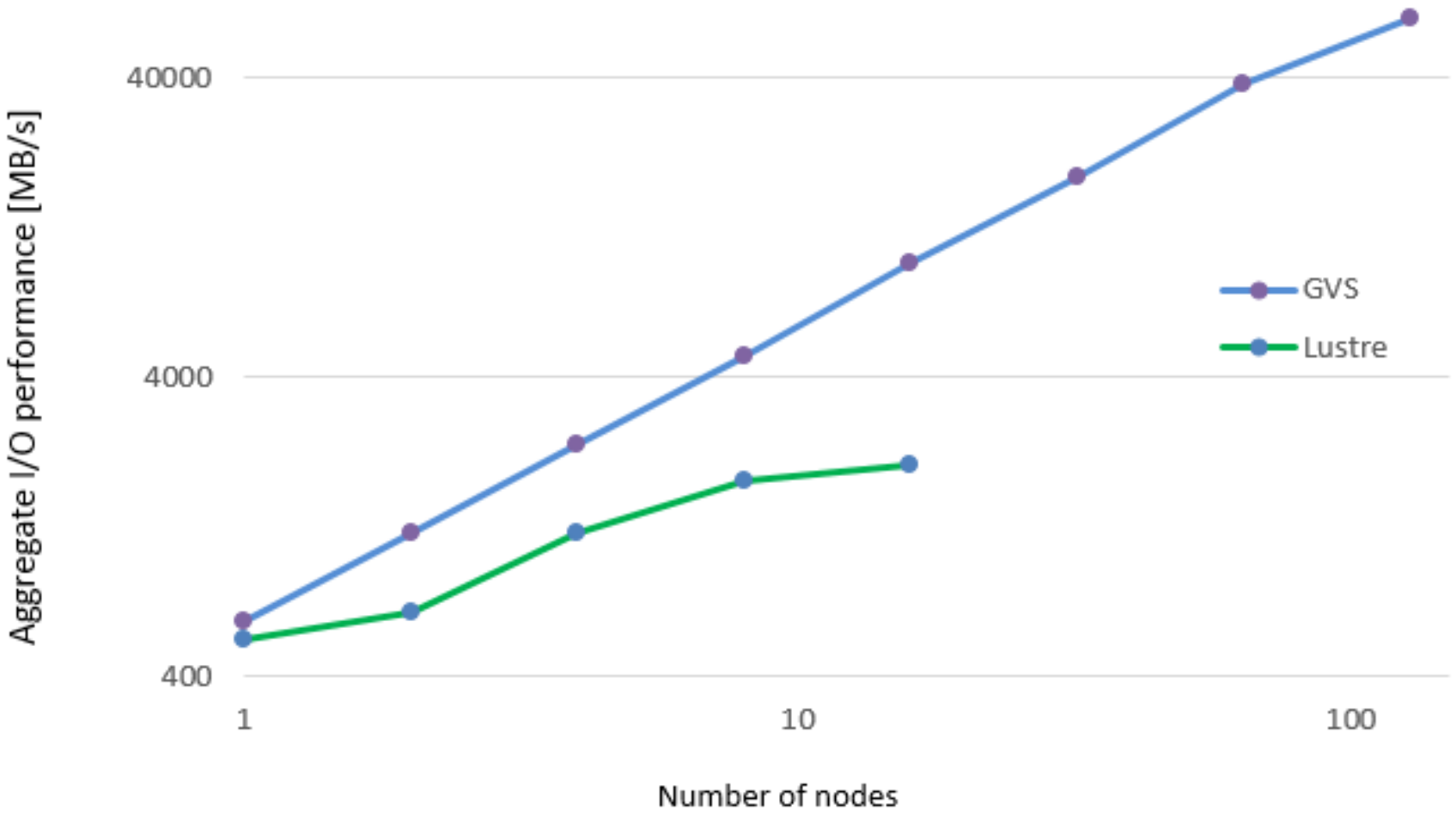
Multiple NCBI blast running on single node (X86 cluster)



I/O performance (x86 single file read)

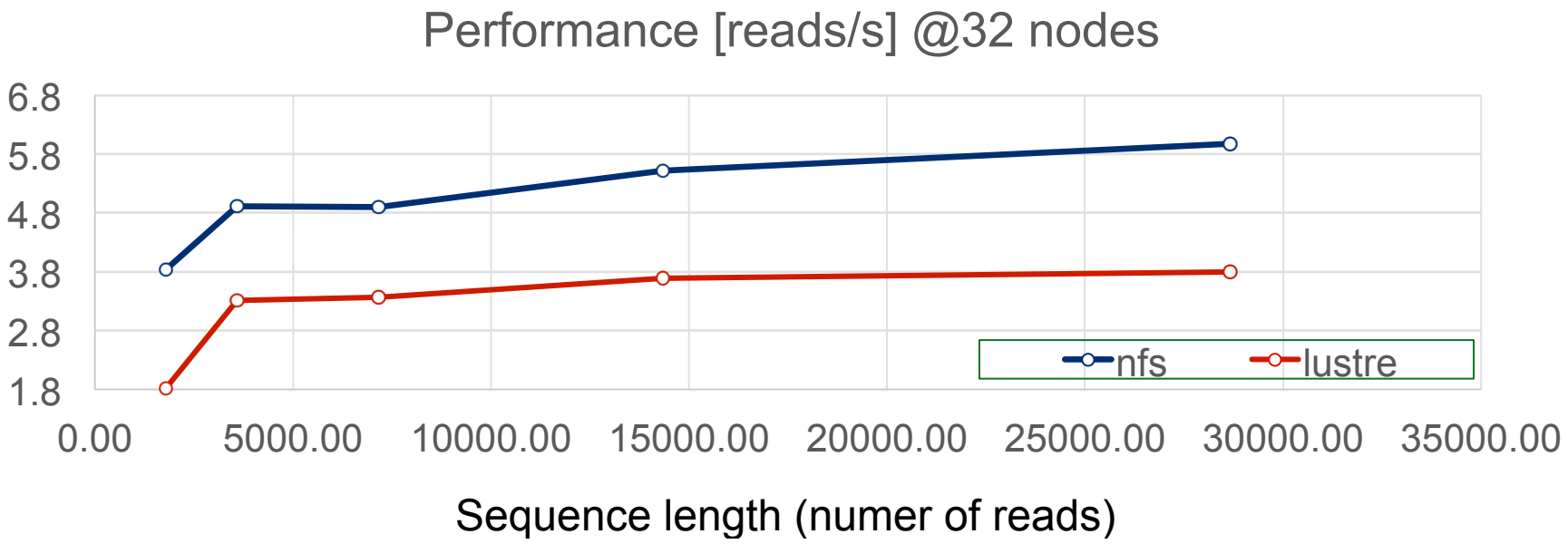


I/O performance (XC40 single file read)

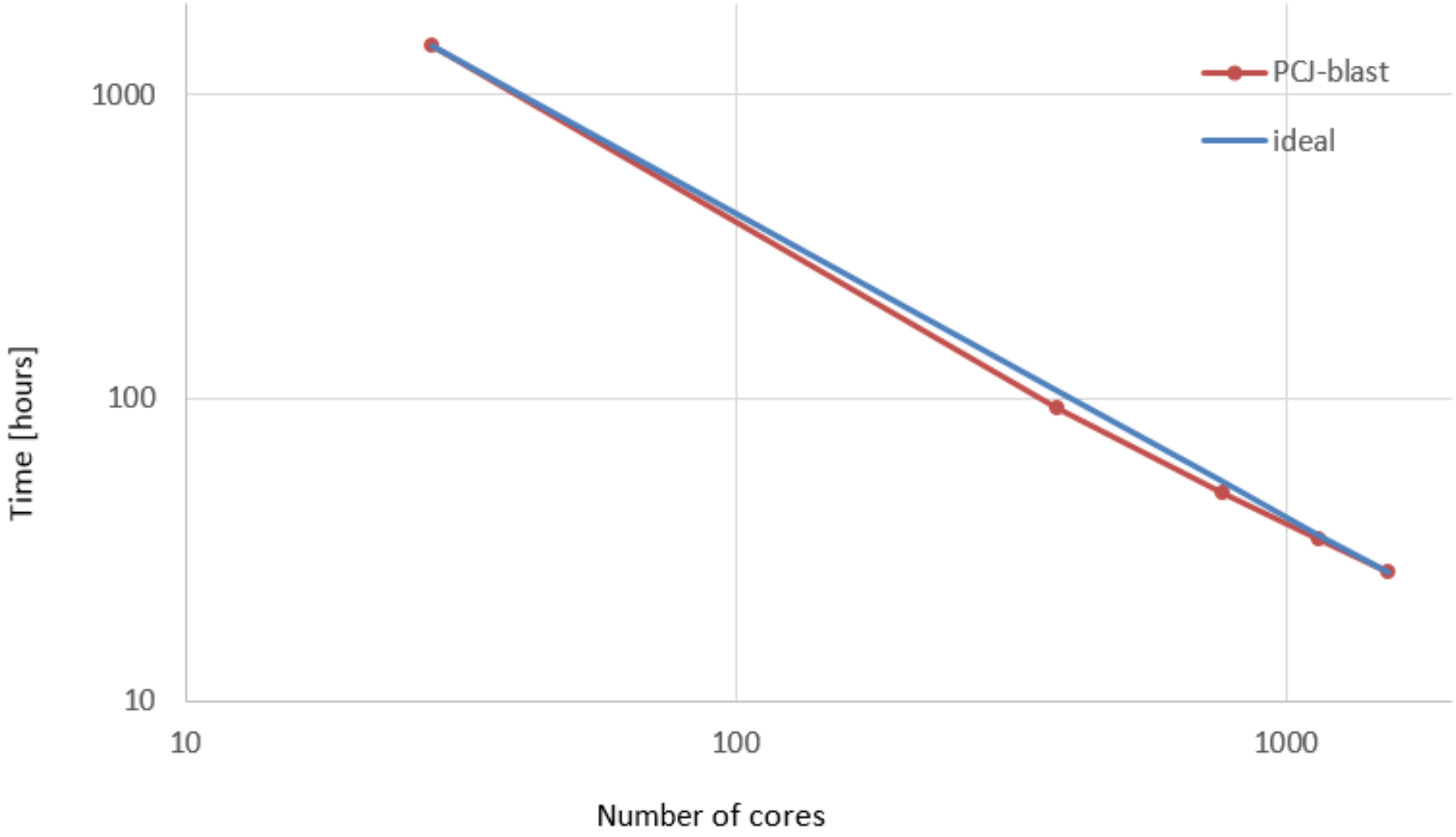


Blast (with PCJ) performance (x86 cluster)

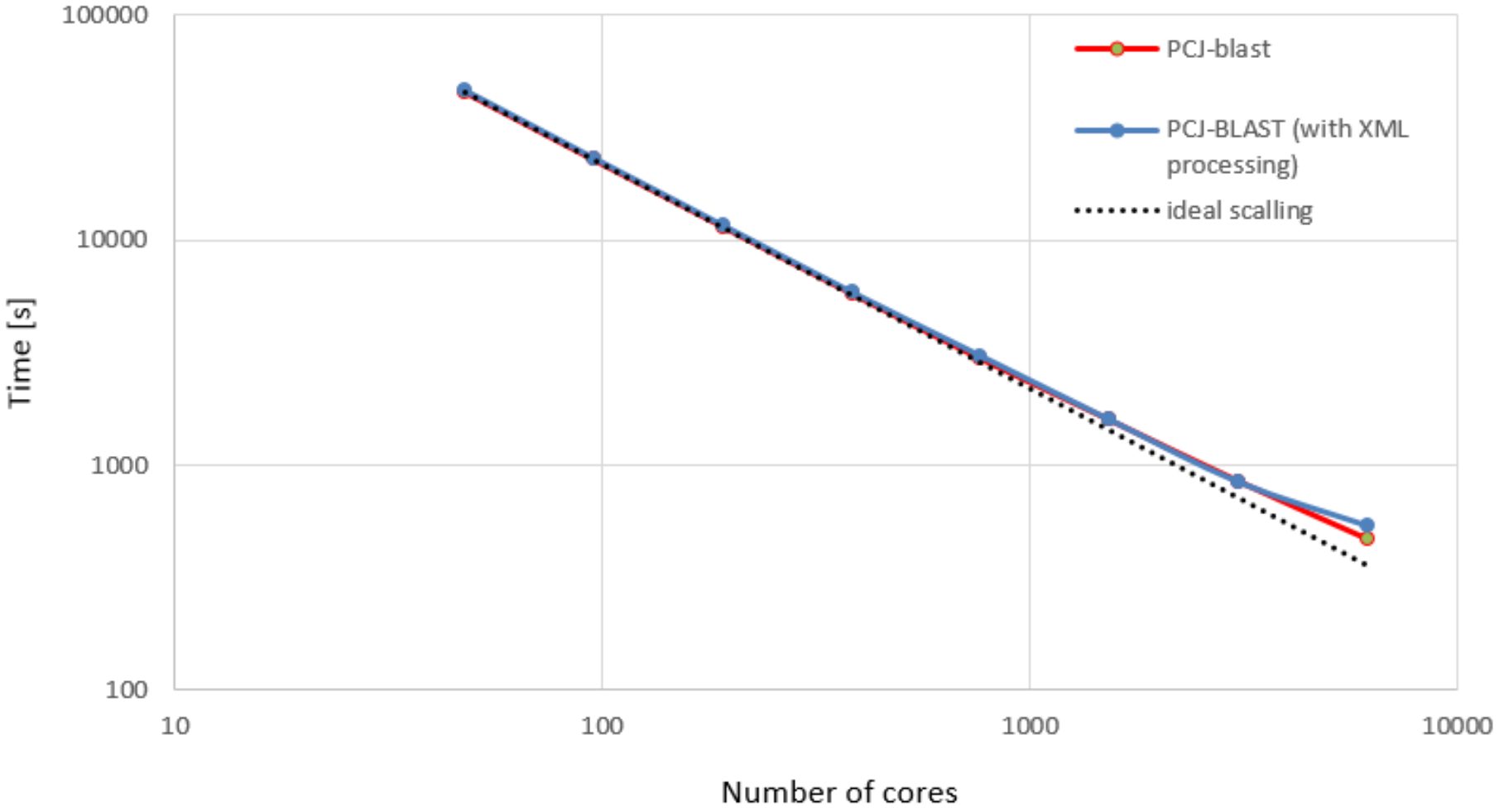
nodes	cores	Time [hours]	Time [days]	**1 mln reads**
1	28	1600.0	67.0	estimated
32	768	49.9	2.0	
48	1152	34.1	1.4	
64	1536	26.5	1.1	



Pcj-blast scalability (x86 cluster)



pcj-blast – scalability (Cray XC40)



parallel_blast.py
parallel_blast.py

Workflow development

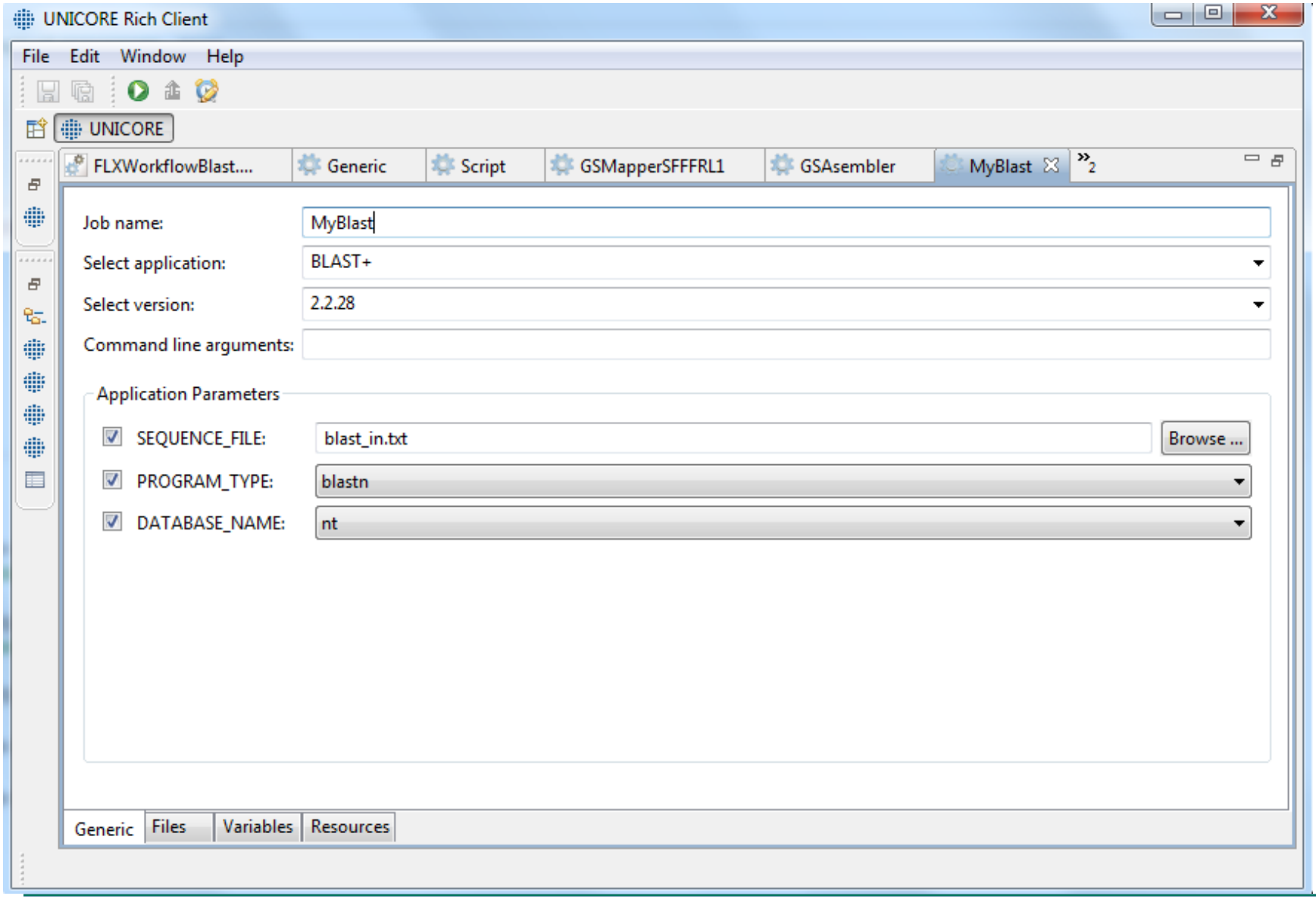
- Complicated workflow has been developed by Davit
- The bottleneck is sequence alignment with blast
  - typical data to process consists of ca. 1 mln reads
  - Input size ca. 300MB, output size (XML file) ca. 1TB
  - Blast outputs is than pro**c**essed by python scripts and R

New services for genetics

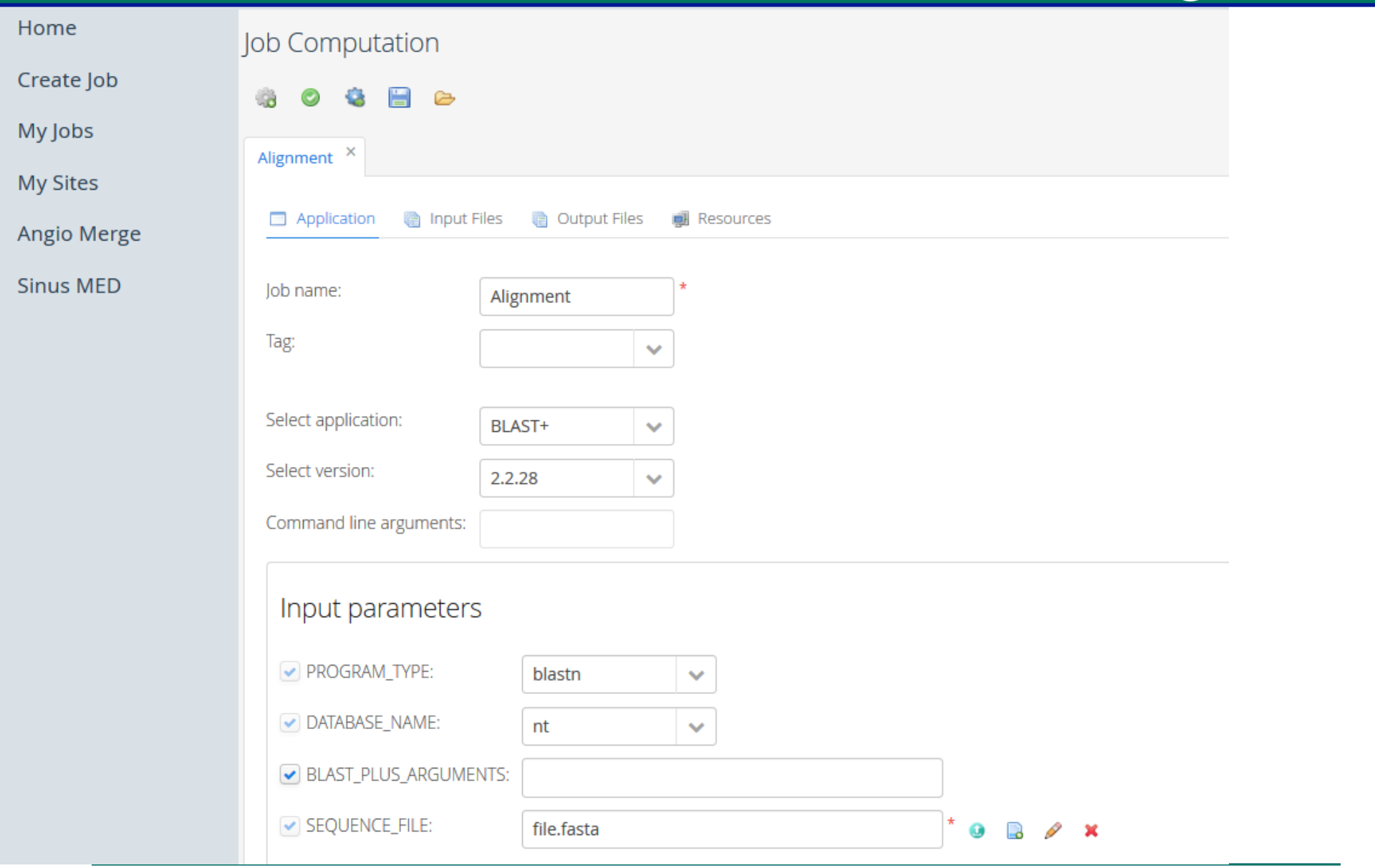
- Applications

Application	ACK	ICM	PCSS	TASK	WCSS
AutoDock	X	X		X	X
AutoDock Vina	X	X			
Blast	X	X			
Blast+	X	X			
BWA	X	X			
ClustalW2		X			X
Custal Omega	X	X		X	X
GATK		X			
MrBayes		X			
PicardTools	X	X			
R	X	X	X	X	X
GS Data Analysis Software		X			
Rosetta	X	X			X

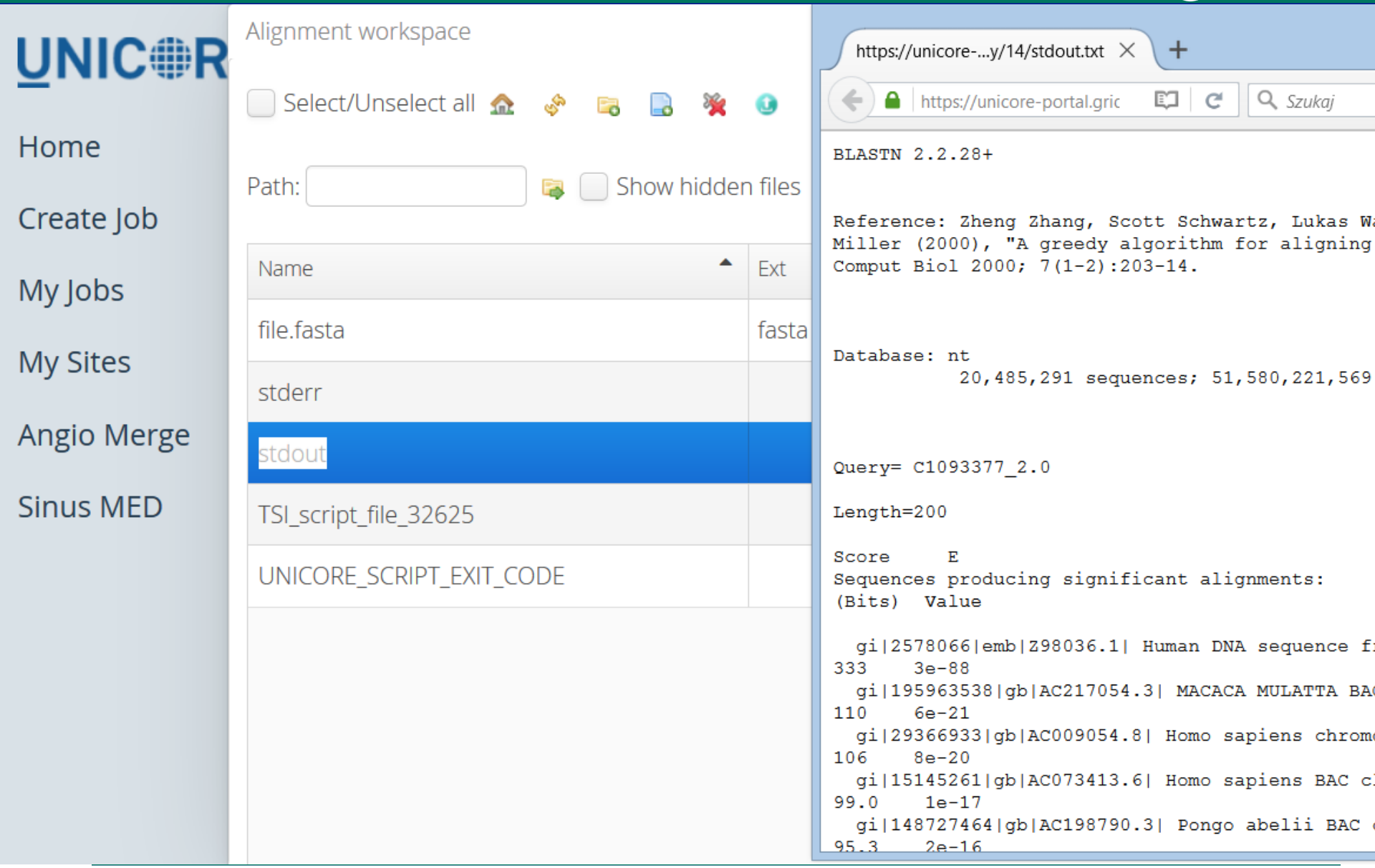
UNICORE RCP - Blast



UNICORE portal



UNICORE portal



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