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An Approach for Parallel Reading in Multiple Sequence Alignment

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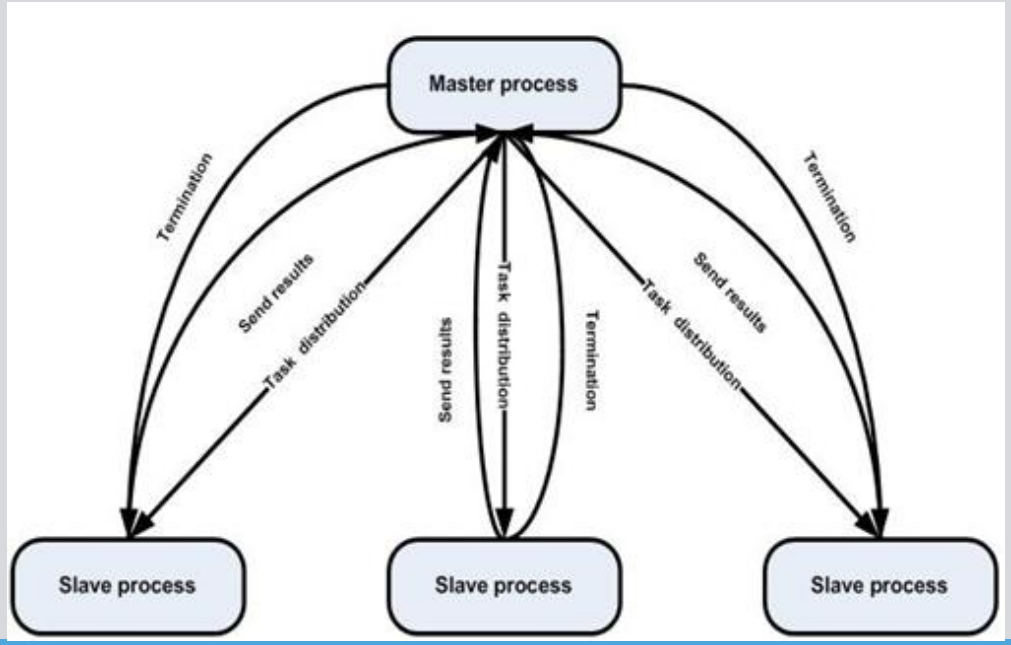
Introduction

- Multiple sequence alignment (MSA) is an important method for biological sequences analysis.
- This method is in search of evolutionary relationship among biological sequences.
- Amounts of genetic sequences of proteins, DNAs, RNAs are newly discovered every day, which require the adoption of advanced I/O techniques as well as efficient parallelism for sequence analyses.
- In this paper we propose a parallel I/O approach for multiple sequence alignment input reading.

ClustalW-MPI

- ClustalW-MPI is a parallel version of ClustalW software and applies the master-slave parallelism for multiple sequence alignment.
- ClustalW-MPI is capable of experimenting up to ~10K sequence sets.



Designing a Parallel I/O Interface for Multiple Sequence Alignment

- The structure of the parallel read routine is summarized as follows:
  - Predefine *group_size* and *read_chunk_size* parameters
  - Create an MPI Group '*processor_group*' whose entities are (i×*group_size*, i×*group_size*+1, …, (i+1)×*group_size*-1) for i^{th} group of processors
  - Create an MPI communicator '*group_comm*'
  - Create an MPI Group '*leader_group*' whose entities are (0, *group_size*, …, (N-1)×*group_size*)
  - Create an MPI communicator '*leader_comm*'
  - Create a string *read_buffer*[*file_size*]
  - *leader_comm* calls *MPI_file_open* sequence dataset
  - *leader_comm* iterates *MPI_read* calls to store the *read_chunk_size* chunk of input file to a *read_buffer*, until all sequence dataset are read
  - Broadcast operation of *read_buffer* between the *group_comm*
  - Reformulate *read_buffer* info to recognizable format of *seq*[*seq_id*][*each_seq_size*]
- Parameters of *group_size* and *read_chunk_size* are dependent of data file size, total number of processors, and the file system capacity. We determine these parameters heuristically after the synthetic benchmark of I/O performance.

Experimental Resource

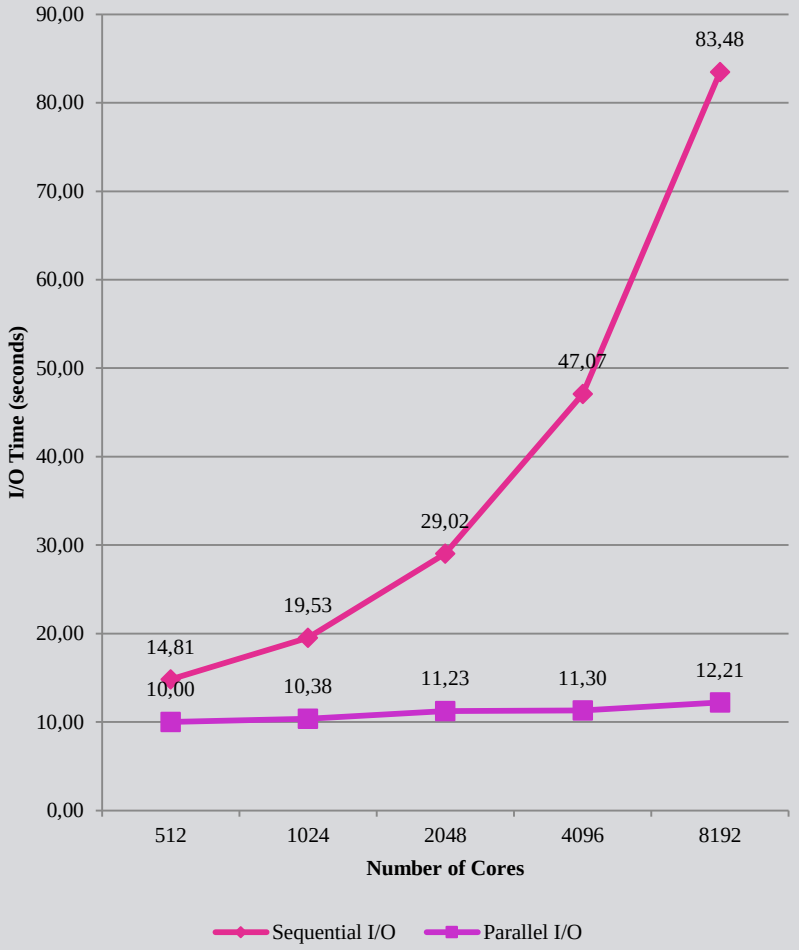
- JUQUEEN supercomputer.
- 458,752 cores in total.
- Each compute node contains 16 cores
- 4-way hyperthreading (use up to 64 cores-per-node)
- 16 GB RAM
- GPFS (General Parallel File System).

Sequence Dataset

- 4 different datasets ranging from tens of KiloBytes to a hundred MegaBytes.
- A subset of human influenza A virus type from NCBI.
- 8999 sequences approx. 16 MB.
- A dataset with 139 MB in size.

Parallel Reading Performance for Genetic Sequence Input

- Wall-time comparison between sequential and parallel file reading.
- Measured time is the total simulation time in seconds until all data inputs are broadcasted to all slaves.



Conclusion

- The use of MPI-I/O over a subset of MPI cores
- It is achieved by creating a number of subgroups under a global MPI communicator
- We verify the performance of our approach by comparing it with the traditional way of “sequential file reading and global broadcast”
- We apply it to the MPI version of multiple sequence alignment software ClustalW.
- In the production run over 8192 BlueGene/Q cores, the current approach provides 6.8 times speed-up than the original ClustalW-MPI implementation.

- Thank you for your attention!