HPC-BLAST: Distributed BLAST for Xeon Phi Clusters

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Introduction

Advancing sequencing technology is creating an exponential growth in the size of genomic databases. The Basic Local Alignment Search Tool (BLAST) is cornerstone of many bioinformatics workflows, and it is crucial that its performance keeps pace with the growth. HPC-BLAST is designed to address the performance gap between NCBI BLAST and this explosion of data, delivering a solution that is scalable, forward thinking, and ready for emerging architectures.

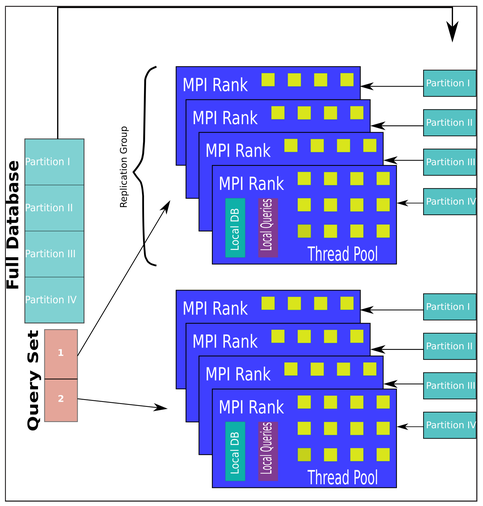
Objectives

Deliver a highly parallel version of BLAST targeting the Intel Xeon Phi architecture, as follows:

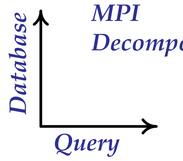
1. Port NCBI-BLAST to the Intel Xeon Phi.
2. Expose and exploit additional parallelism using a dual-layer approach.
3. Add managed I/O, dynamic load balancing, and checkpoint/restart capability.
4. Coordinate with NCBI and Intel.
5. Explore improved vectorization.

Approach

MPI-Level

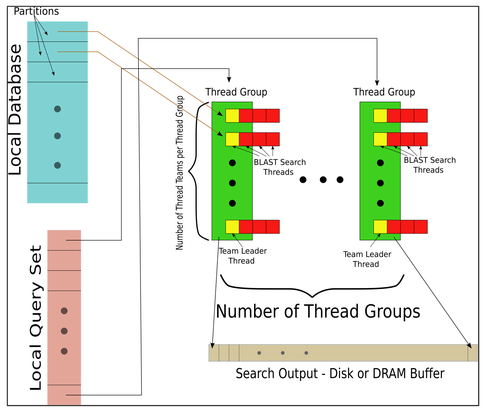


MPI Decomposition

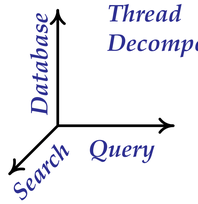


- A **REPLICATION GROUP** consists of one or more MPI ranks that collectively contain a **COMPLETE COPY** of the subject database.
- **MULTIPLE REPLICATION GROUPS** allow for distribution of the **QUERY SEQUENCES.**
- **MULTIPLE MPI RANKS** within a replication group allow for distribution of the **SEARCH DATABASE.**

Thread-level

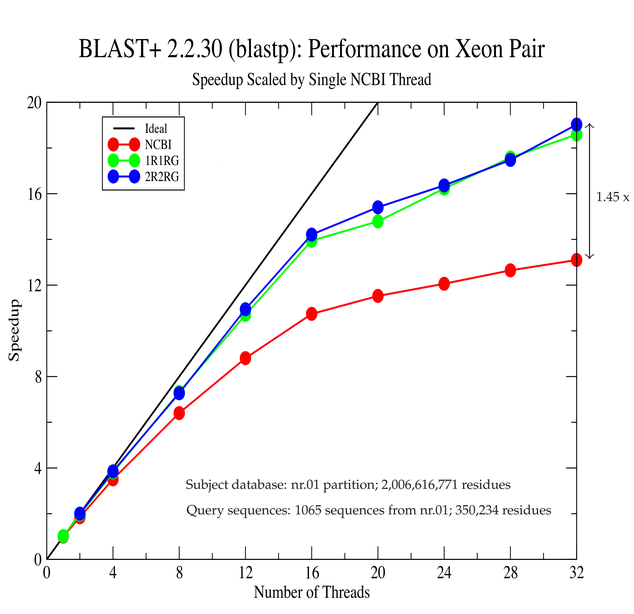


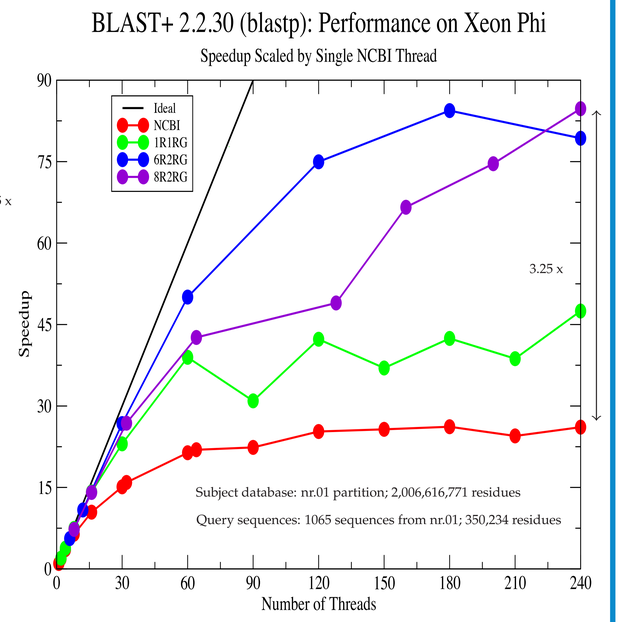
Thread Decomposition

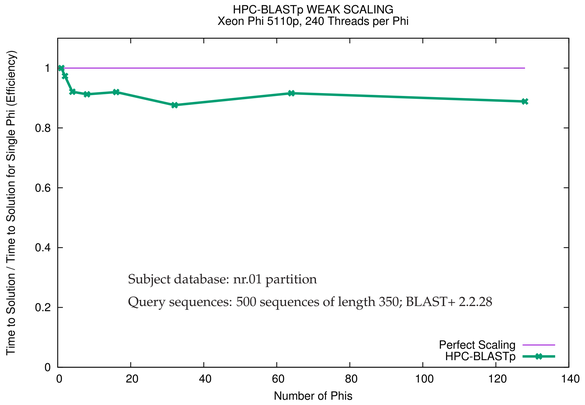


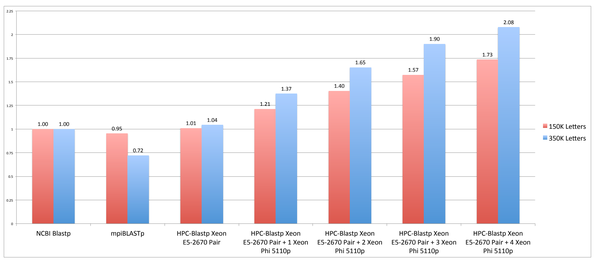
- A **THREAD GROUP** consists of one or more **THREAD LEADERS** that collectively contain a **COMPLETE COPY** of the subject database.
- **MULTIPLE THREAD GROUPS** allow for distribution of the **QUERY SEQUENCES.**
- **MULTIPLE LEADER THREADS** within a thread group allow for distribution of the **SEARCH DATABASE.**
- **MULTIPLE SEARCH THREADS** provide threads to the **CORE BLAST SEARCH ALGORITHM.**

Results & Conclusions









Subject database: nr (entire database); Query sequences: sampled from subjects: 444 (red) and 1065 (blue); BLAST+ 2.2.28; mpiBLAST 1.6.0.

Best results to date indicate that HPC-BLAST runs approximately 40% faster for blastn and 45% faster for blastp than NCBI BLAST+ on Intel Xeon processors and around 773% faster for blastn and 225% for blastp than NCBI BLAST+ on Intel Xeon Phi coprocessors. HPC-BLAST also demonstrates near constant 90% parallel efficiency with weak scaling across 128 Intel Xeon Phi coprocessors. Combined, these results indicate that HPC-BLAST offers substantial performance improvements over NCBI BLAST+ on highly parallel computing platforms.

Future Research

Current efforts include implementing a parallel, contention-aware I/O scheme and incorporating a hierarchical management layer to facilitate efficient dynamic load balancing and fault tolerance.

Future research targets developing scalable solutions for exascale through improved load balancing, dynamic job reconfiguration and database rebalancing, and improved vectorization.

Acknowledgments

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