Application Scaling Techniques on HPC Clusters

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Introduction

Modeling and Simulation Modeling and Simulation (M&S) are used extensively by FDA scientists[1]. M&S applications can overwhelm even HPC clusters. An FDA simulation project would require 28 years of computations per product on a single workstation. Applying our techniques reduces this run time to only seven days.

Bioinformatics FDA's Precision Medicine Initiative relies heavily on the next-generation sequencing technology which is associated with lengthy processing of exponentially growing sequence databases. A BLAST+ job consumes more than 22 days of computations. Applying the techniques reduces this run time to only few hours.

Deep Neural Networks Testing run time of 228 reduced to 3 weeks.

Big Data Analysis Interactome project, 1,800-year reduced to 6 months.

Materials & Methods

Scaling simulations:
➢ Partition simulation loops to delegate iterations to independent tasks.
➢ Adapt L'Ecuyer RngStream[2] technique to provide quality random numbers across all independent tasks.
➢ Use array job facility of the job schedulers to launch the tasks on all available cores and save all partial results.
➢ Merge all the partial results and summarize.

Scaling Bioinformatics:
➢ Partition queries and reference database into M and N subsets. Generate M x N unique combinations of the subsets.
➢ Use array job to launch M x N tasks, each task processing a unique combination of the subsets and save all partial results.
➢ Merge all the partial results and summarize.

Scaling Deep Neural Networks Testing:
➢ Create a look-up table, mapping contiguous intervals of sub-image IDs (total of L) to whole-slide image IDs.
➢ Use array job to launch L tasks, each task retrieving (using the look-up table) and processing a sub-image for testing and saving results.

Big Data Analysis:
➢ Split big data into P smaller subsets.
➢ Use array job to launch P tasks, each processing a subset and saving partial results.
➢ Merge all the partial results.

* Note: Number of array job tasks can exceed the max capacity.
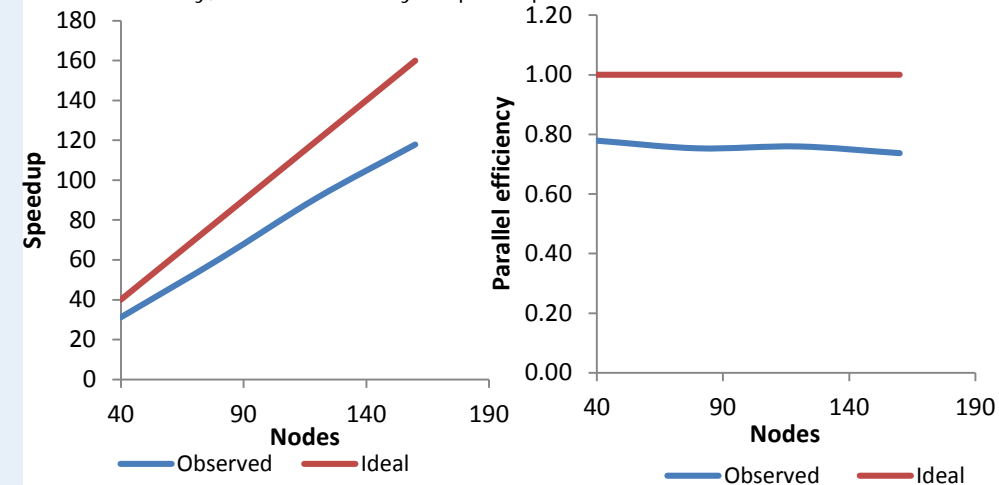
The challenge comes not from how big and fast the cluster can be, but how the HPC applications can be **scaled** to take advantage of all the resources in parallel and scalable manner.

Scan the QR code to access additional information online

Results

Speedup and parallel efficiency example using BlastX . Speedup increases sub-linearly; Parallel efficiency = speed up / number of nodes

Conclusions

• The scaling techniques presented here are already in use by FDA scientists.
• The techniques enable reduction of the data subset processed by each job task to a size that fits into the memory of the computing nodes where computations are performed. The resulting reduction in disk I/O produces excellent results, enabling substantial drops in run times.
• The described methods use only open source code, adds no hardware cost.

References

1. https://www.nuventra.com/resources/blog/simulation-transforms-regulatory-pathways/
2. http://simul.iro.umontreal.ca/