



MVA PICH

MPI, PGAS and Hybrid MPI+PGAS Library

Bridging Neuroscience and HPC with MPI-LiFE

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Neuroscience: Challenges and Opportunities

- Advancements in imaging technology
 - MRI, CAT Scan, etc.
- Higher resolution neuroimaging data
- How do we handle huge amounts of this data?
- Requirement for more efficient and faster algorithms
- *Can High Performance Computing help?*

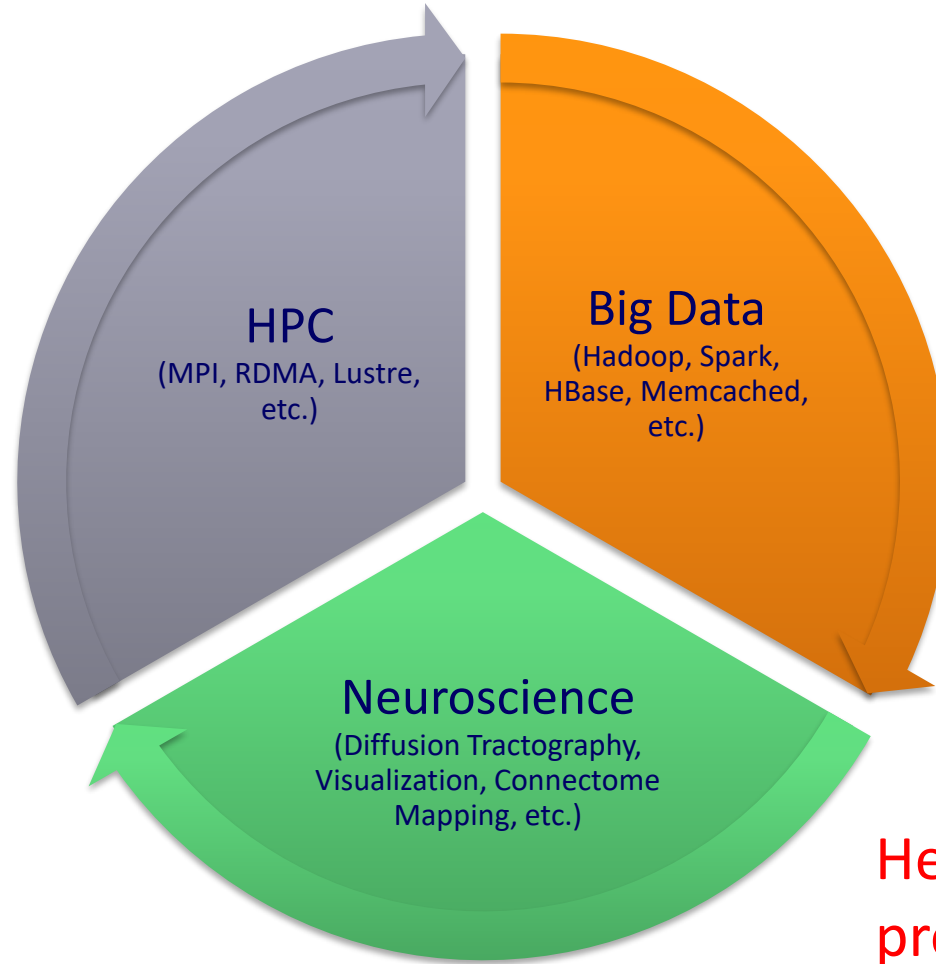
Advanced Computational Neuroscience Network (ACNN)

- Develop a new generation of sustainable interdisciplinary **Neuroscience Big Data** research
- Collaboration between University of Michigan, Indiana University, Northwestern University, **Ohio State University**, Case Western Reserve University, and Washington University
- Funded by **NSF**
- <http://www.neurosciencenetwork.org/>

Our Goal

- Accelerate Neuroscience Data
 - High-Performance Computing (HPC)
 - Different Programming Models (MPI, OpenMP and PGAS)
 - Big Data
 - Hadoop, Spark
 - Deep Learning
 - Caffe, Tensorflow

Bridging HPC and Neuroscience



Convergence of HPC, Big Data, and Neuroscience!

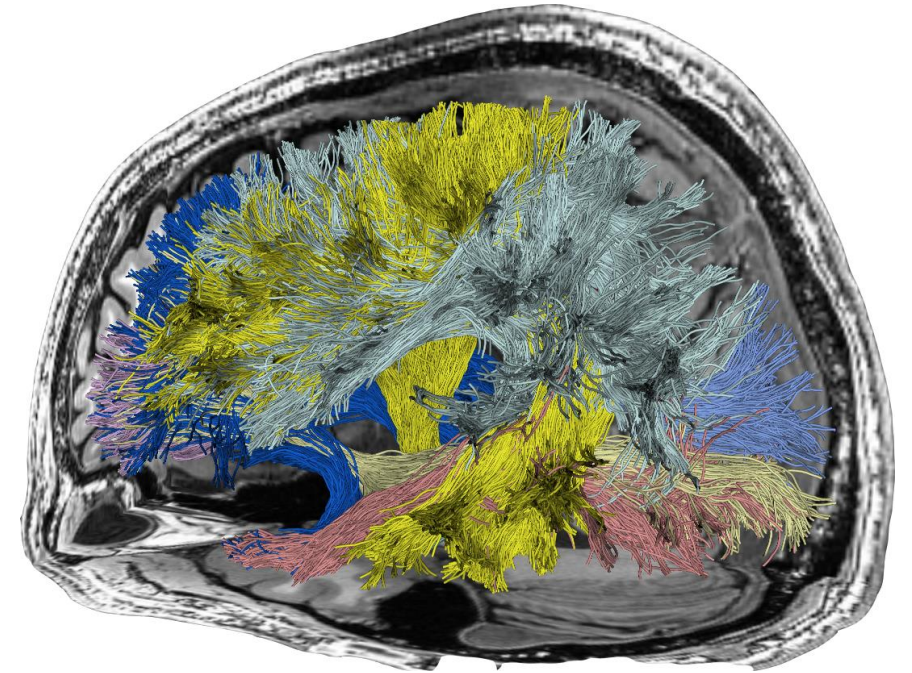
Heavy data analysis and processing requirements

Overview of the NeuroHPC project

- Aimed at bringing HPC to the field of Neuroscience
- **MPI-LiFE**
 - Scalable and distributed tool for statistical evaluation of brain connectomes
 - Based on LiFE method in the Encode Toolbox
 - MPI-based distributed sparse multiway matrix multiplication
 - Exploits efficient communication in MVAPICH2
 - Highly optimized for virtualized environments using Docker
 - Flexibility to run on any multi-core laptop, desktop, server, and cluster
- **MPI-LiFE 0.9 is now available for download!** (11/10/2017)
- For more information, visit <http://neurohpc.cse.ohio-state.edu/>

Brain-LiFE

- **Linear Fascicle Evaluation (LiFE¹)**
 - an approach to predict diffusion measurements in brain connectomes
 - evaluate evidence supporting white-matter connectomes generated using MRI and computational tractography
 - show evidence for white-matter tracts and connections between brain areas
 - heavily used by computational neuroscientists



Different colors show groups of white matter tracts connecting different portions of the brain

¹<https://github.com/francopestilli/life>

Brain-LiFE

- Originally written in MATLAB
 - Slow and inefficient
 - Convert to C to run outside MATLAB environment
 - Modularize and pipeline for distributed environment
- Based on Non-Negative Least Square (NNLS) constrained optimization
 - Uses large-scale sparse multiway matrix multiplication
 - Design, develop, and evaluate MPI-based algorithm
 - Dockerize solution

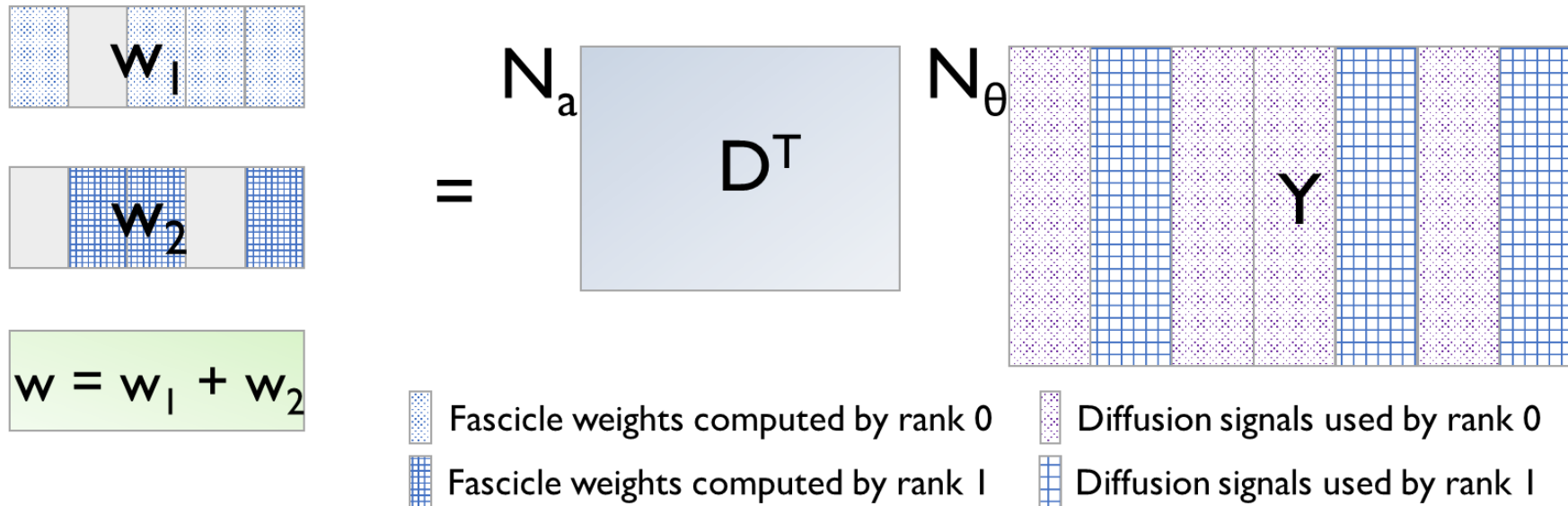
MPI-LiFE: Initial Design using MVAPICH2

- Computationally intensive tasks are the computations of sparse multiway matrix by vector products
 - $w = M^T y$ and $y = Mw$
 - Have been **parallelized** using **MPI** and **OpenMP** by dividing the task among multiple MPI processes
- Implementation uses **MVAPICH2**, from OSU team
 - Exploits efficient communication primitives to drastically improve performance
 - Uses high-performance networks to reduce communication latency

S. Gugnani, X. Lu, F. Pestilli, C.F. Caiafa, and D. K. Panda, MPI-LiFE: Designing High-Performance Linear Fascicle Evaluation of Brain Connectome with MPI, HiPC'17

MPI-based multiway matrix multiplication

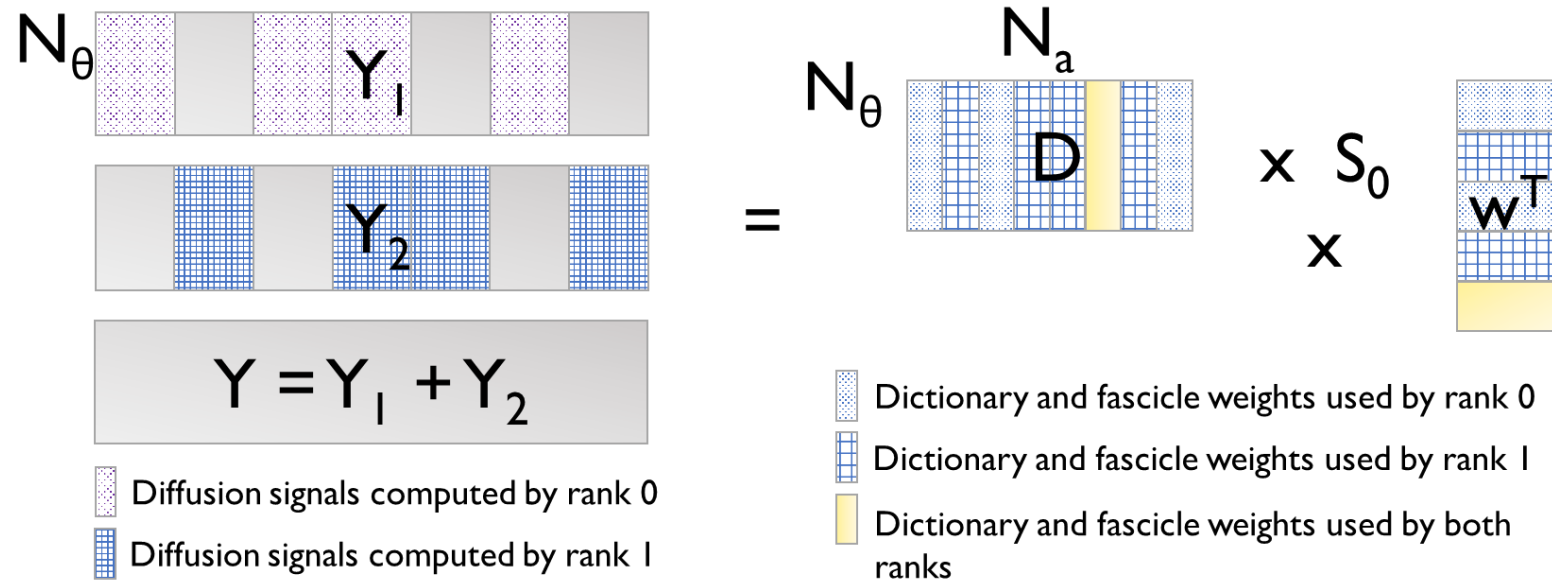
- $w = M^T y$
 - Distribution of data using MPI_Bcast, MPI_Scatter
 - Gathering of results using MPI_Gather
 - Use of OpenMP to parallelize computation within an MPI process



Computation of $w = M^T y$ using 2 MPI processes

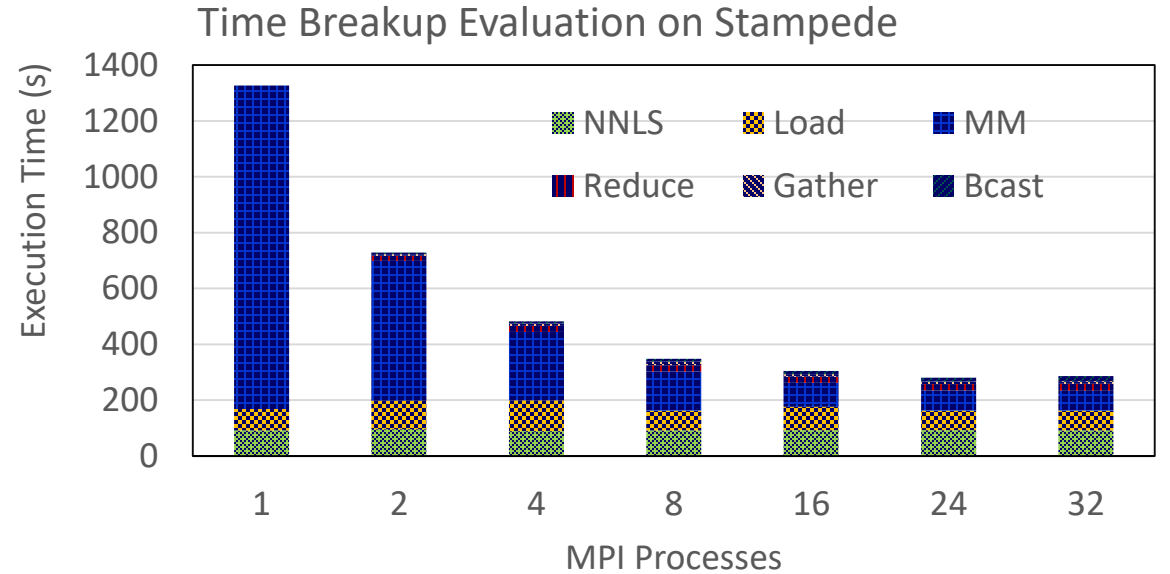
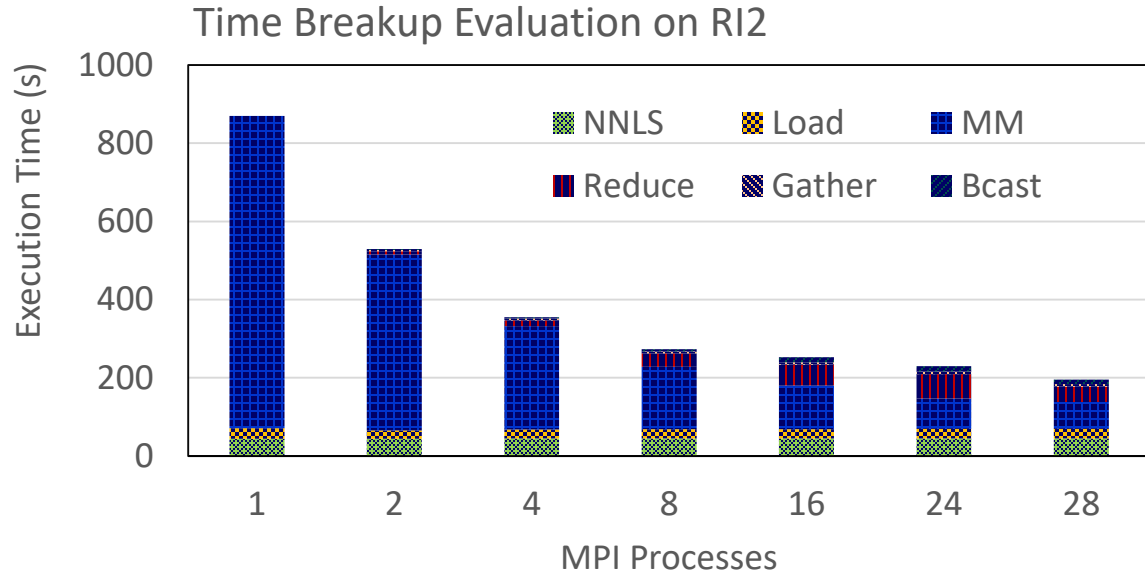
MPI-based multiway matrix multiplication

- $y = Mw$
 - Distribution of data using MPI_Bcast, MPI_Scatter
 - Gathering of results using MPI_Reduce
 - Use of OpenMP to parallelize computation within an MPI process



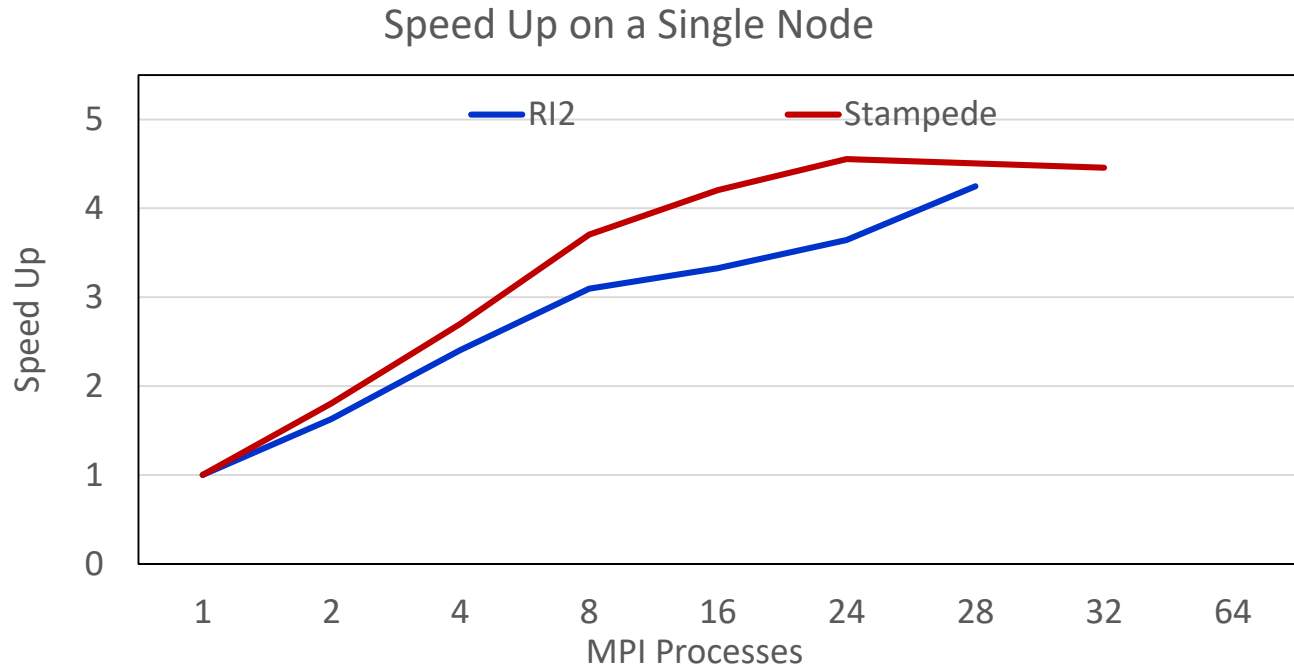
Computation of $y = Mw$ using 2 MPI processes

Evaluation with MVAPICH2: Single Xeon Node



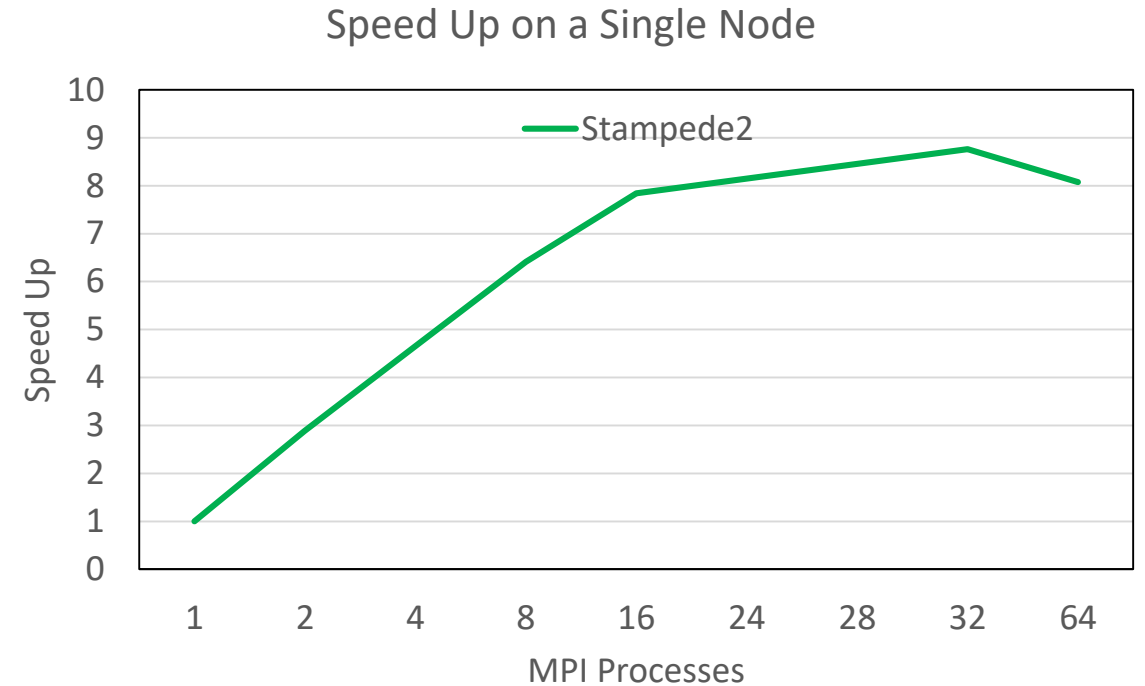
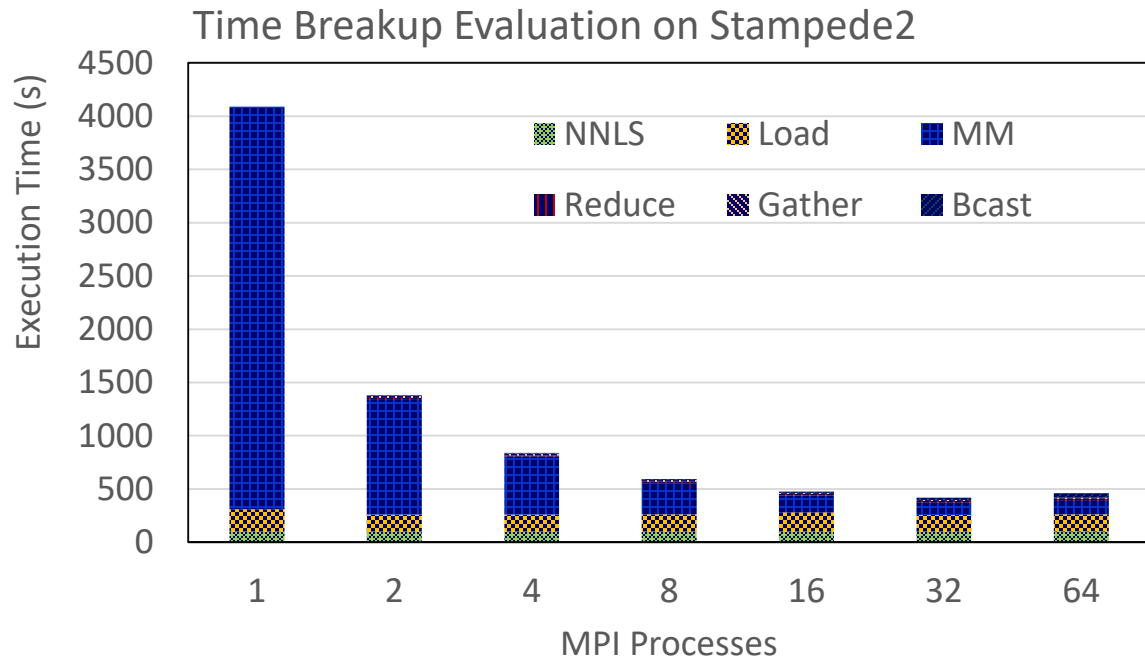
- Evaluation on
 - **OSU RI2** (Intel Broadwell CPUs, 28 cores, 128 GB memory per node)
 - **TACC Stampede** (Intel Sandy Bridge CPUs, 32 cores, 1 TB memory per node)
- Speed up of up to **4.2x** on RI2 and up to **4.5x** on Stampede

Evaluation with MVAPICH2: Single Xeon Node



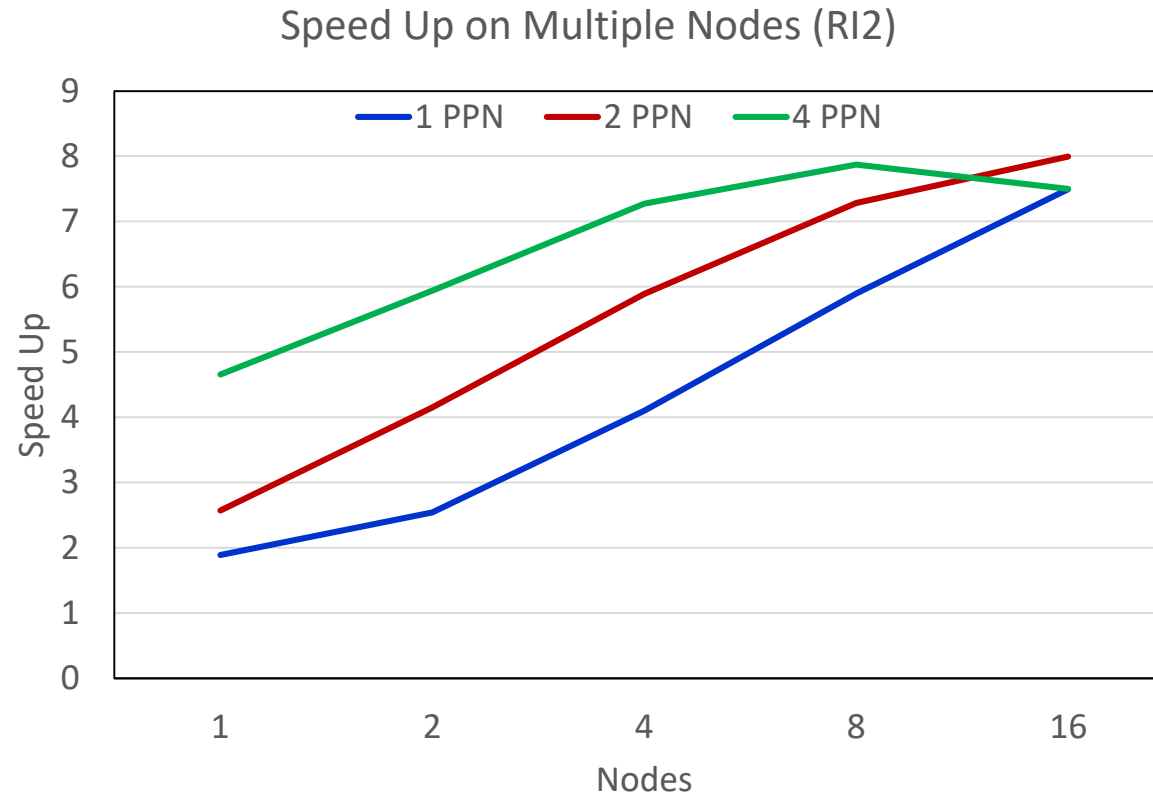
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Evaluation with MVAPICH2: Single KNL Node



- Evaluation on **TACC Stampede KNL** (Intel Xeon Phi KNL CPUs, 68 cores, 96 GB memory per node)
- Up to **8.7x** speed up

Evaluation with MVAPICH2: Multi-Node



- Evaluation on **OSU RI2** (Intel Broadwell CPUs, 28 cores, 128 GB memory per node)
- Up to **8.1x** speed up on RI2

MPI-LiFE: Continuing Work

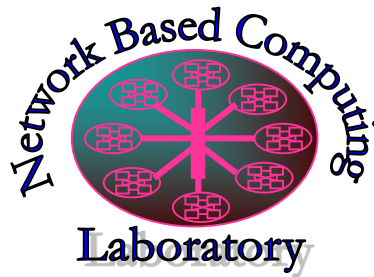
- Maximum parallelization is currently being achieved with MPI for the current LiFE algorithm
- Exploiting enhanced and optimized designs for scale-up and scale-out
 - MPI + OpenMP
 - PGAS Models (OpenSHMEM)
 - GPGPUs
- The sequential algorithm may need to be re-designed
 - May lead to better parallelization

Demo

- Demo on NSF Chameleon Cloud
 - 24 cores per node, Intel Haswell Processors
- Execution using dockerized version of MPI-LiFE
 - Available on docker hub: <https://hub.docker.com/r/neurohpc/neurohpc/>
- Analysis of tractography algorithm on a single dMRI scan
 - Demo run with 50 iterations

Thanks!

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Network-Based Computing Laboratory

<http://nowlab.cse.ohio-state.edu/>

The High Performance Neuroscience Project (NeuroHPC)

<http://neurohpc.cse.ohio-state.edu/>