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# Performance Analysis of MPI and Hybrid MrBayes Computational Biology Code on Multicore Systems

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Abstract—This research focuses on the performance analysis of the MPI-only and hybrid versions of the MrBayes computational biology program on multicore systems. We conducted experiments using two different multicore systems-one from the Virginia Polytechnic Institute and State University, Dori, and the other from the Texas A&M University Supercomputing Facility, Hydra. We used strong scaling and weak scaling to collect performance data for seven different datasets. We used three performance metrics to analyze performance: execution time, efficiency, and speedup. Also we collected energy consumption data for MrBayes for both versions. The results of this research show that the hybrid version has a higher execution than the MPI-only version. The results also show that the hybrid version experiences more speedup than the MPI version and that the hybrid version scales better than the MPI version. The energy consumption data collected shows that the hybrid version has higher energy consumption than the MPI version.

#### I. INTRODUCTION

The current trend in parallel computing has shifted towards hierarchically composed multicore systems. Programs that take a very long time to execute have been a driving force in parallel computing. These types of programs can be made parallel using a parallel programming paradigm such as MPI or OpenMP, and execution time will be reduced. Another method that suggests lower execution time is the combining of two different paradigms in one application. Combining two different techniques such as OpenMP and MPI in one program to make a hybrid application allows users to exploit multiple levels of parallelism on a multicore system.

OpenMP [2] is used for shared memory parallelism. It follows a fork and join model where initially there is one master thread. When the master thread reaches a parallel region, the thread will fork off many other threads to execute that particular area in parallel.

OpenMP is applied to a program using directives. It is very popular for fine-grained parallelism, particularly large for loops. These loops can be divided amongst other threads so that the problem can be worked on at the same time. With OpenMP and shared memory, we must watch out for data dependencies and the scope of variables to make sure that in the end, we obtain the correct results. MPI [1] is the interface used for message passing parallelism and distributed memory. MPI uses processes to execute parallel regions. Since MPI is dealing with distributed memory, each process originally only knows its own data. A process does not have access to another process's data. To communicate this data, processes must pass their data using messages. MPI is useful for coarse-grained parallelism.

Hybridization with OpenMP and MPI in one application allows for multiple levels of parallelism when using multicore clusters. OpenMP can be used per node for shared memory fine-grained parallelism amongst the cores on the node. MPI can be used for distributed memory coarse-grained parallelism between the nodes themselves.

This research focuses on the performance analysis of the MPI-only and hybrid versions of the MrBayes computational biology program on multicore systems. We conducted experiments using two different multicore systems. Two different methods of testing were conducted. Weak scaling was used on one system. Strong scaling was used on two systems. Execution time, speedup, and efficiency were used to compare the performance of both versions. Also we collected energy consumption data for MrBayes for both versions.

The remainder of this paper is organized as follows. Section II discusses the MrBayes application. Section III describes the experimental setup and the multicore systems used. Section IV shows the results obtained from the experiment. Section V is conclusions.

#### II. MRBAYES COMPUTATIONAL BIOLOGY PROGRAM

MrBayes [5] is a computational biology program used for Bayesian inference of phylogeny. The application takes as input a file containing a number of taxa and each taxon's data. The program then based on the taxa's data will construct a tree depicting the relationship of the organisms. There are many possible phylogenies to choose from. Bayesian inference is used to find the best tree to show this relationship.

$$Pr[Tree|Data] = \frac{Pr[Data|Tree] \times Pr[Tree]}{Pr[Data]}$$

*Pr[Data]* involves a summation over all possible trees and, for each tree, integration over all possible combinations of branch lengths and parameter values [4].

The posterior probability

# $\frac{Pr[Data|Tree] \times Pr[Tree]}{Pr[Data]}$

is impossible to calculate analytically. MrBayes uses Markov chain Monte Carlo simulation to approximate the posterior probability of trees [4]. MrBayes is a worthy target for parallel processing because the program does many computations and takes a very long time to execute. Evaluating real world data could potentially be very time consuming without parallelization thus rendering the application useless. Making the program parallel produces a lower execution time and produces results in an amount of time that is reasonable.

Both versions of MrBayes apply MPI to the Markov chains. The total number of chains is divided amongst the number of processes. The hybrid version is based on the MPI version. OpenMP is applied to parallelize large for loops in only one source file, mcmc, where the Monte Carlo chaining is handled, so OpenMP is not used as much as MPI in the application. The flow of the program is:

Read dataset and initialize

• The program reads in a dataset. The dataset specifies the number of taxa in the file. The dataset also contains the names of each taxon and their data

Set parameters

- set number of generations and number of chains
- Distribute number of chains amongst MPI processes
- Run analysis
  - run analysis for the set number of chains for the set number of generations

Seven datasets tested	Seven	datasets	tested
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Dataset	Number of Taxa	Table 1
Adh	54	
Avian	89	
Bglobin	17	
Cynmix	32	
Anolis	30	
Primates	12	
Replicase	9	

Table 1	shows	the 7	datas	ets and	l their
corresp	onding	num	ber of	taxa	

#### **III. EXPERIMENTAL SETUP**

The two multicore systems used were Dori, a machine from the Virginia Polytechnic Institute and State University, and Hydra [3] from the Texas A&M Supercomputing Facility. Dori uses an AMD Opteron processor chip. The hierarchical organization of Dori is 8 nodes with 2 dual core chips each so there are 32 cores. The makeup of Hydra is 52 nodes with 8 dual core Power5+ chips each for a total of 832 cores. The specifications and comparison of the two systems can be seen in Table 2.

	Dori	Hydra
Number of Nodes	8	52
CPUs per node	4	16
Cores per chip	2	2
Total Cores	32	832
CPU type	1.8 GHz AMD Opteron	1.9GHz IBM Power5+
Memory per node	6GB	32GB/49 nodes 64GB/3nodes

# **Table 2 Dori and Hydra Specifications**

Figure 1 illustrates the architecture of a dual core chip on Dori. Figure 2 shows the architecture of a dual core chip on the Hydra cluster.

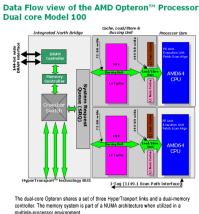


Figure 1 Dori AMD Opteron dual core chip

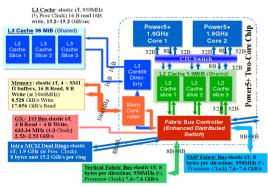


Figure 2 Power 5+ Dual Core Chip on Hydra

When executing hybrid MrBayes on Dori, shared memory parallelism is used on the 4 cores on each node, and MPI is used between the 8 nodes. With Hydra, shared memory parallelism is used on the 16 cores per node, and MPI is used between the nodes.

MrBayes was executed on both multicore systems using both versions. Each data set was run on a different number of cores for 10,000 generations using a different number of chains.

On Dori, we did strong scaling with MrBayes. For each dataset, 32 chains total were used. This number of chains was chosen because Dori has 32 cores and with this number of chains, each chain could be distributed to one core.

We did strong and weak scaling on Hydra. For the weak scaling, 16 chains per node were used. For strong scaling, 512 chains were used.

Dori was used to collect energy consumption data for MrBayes. Energy consumption on Dori is collected using the PowerPack software. The system has an external meter connected to the power supply and cables connected to each component to detect energy consumption and power data per node.

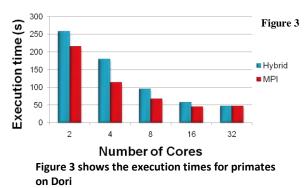
For the collection of energy data, we ran one dataset, primates, using both versions and collected energy consumption data.

# IV. PERFORMANCE ANALYSIS AND COMPARISON

To compare the performance of hybrid MrBayes to that of the MPI-only version, we use three performance metrics. Execution time is compared on each number of cores for each dataset. The speedup compares the speedup that both versions experienced with increasing cores. The efficiency is also used to compare the efficiency of both versions when running on multiple cores. Seven datasets were run on Dori. Only six were run on Hydra because of memory issues.

#### A. Results on Dori

The following charts show results after executing on the Dori multicore system using 2, 4, 8, 16, and 32 cores with 32 chains each.



Performance for primates-12 taxa

Speedup for primates-12 taxa

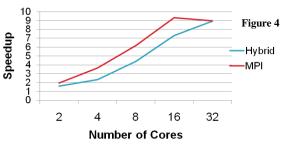


Figure 4 shows the speedup comparison for the primates dataset on Dori

Figure 3 and Figure 4 show performance data after executing one of the smaller datasets, primates, on Dori. Figure 5 shows the execution time on 5 different number of cores for the hybrid and MPI-only versions. The chart shows that the MPI-only version outperforms the hybrid version, but at 32 cores, the execution times are very close.

Figure 4 shows the speedup of both versions when executing the primates dataset. The results show that both versions experience speedup, however at 32 cores, the MPI-only version actually has a decrease in speedup while the hybrid version keeps experiencing increased speedup. The results show that 16 cores for the MPI version is the optimal number of cores to use when executing the primates dataset. The communication time when using 32 cores increases the execution time making it larger than that of 16 cores.

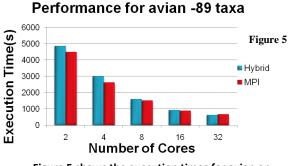


Figure 5 shows the execution times for avian on Dori

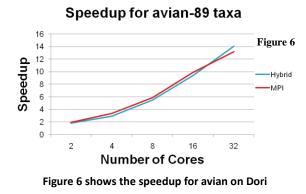
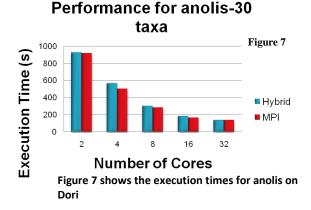
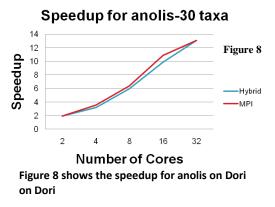


Figure 5 and Figure 6 show the performance data on Dori after running the largest dataset avian. These results show that MPI MrBayes has lower execution time than the hybrid version for up to 16 cores. At 32 cores, the hybrid version has a lower execution time. The speedup data shows that both versions experience increased speedup. At 32 cores, the speedup of the hybrid version is larger.





Figures 7 and 8 show the results after executing the anolis dataset. The hybrid version is slower than the MPI version. Figure 8 presenting the speedup shows that both versions experience increased speedup. At 32 cores, the two versions have close speedup values.

# B. Results on Hydra

On Hydra there were memory issues with all but two of the datasets. We could only run the two smallest datasets successfully. The amount of memory needed is proportional to the number of taxa in the dataset and also the number of chains needed. On Hydra, the number of chains was increased to 512 total, and this caused a problem with larger datasets.

To be able to execute on Hydra, we performed weak scaling. The work load, number of chains, increased as the number of cores increased. To keep the work load constant, we used sixteen chains per node. Sixteen was chosen because there are sixteen cores per node on Hydra.

The following data shows results on Hydra executing on up to 256 cores.

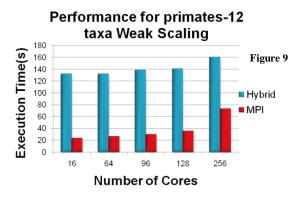


Figure 9 Execution time for primates on Hydra with weak scaling

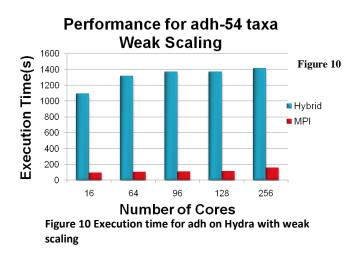
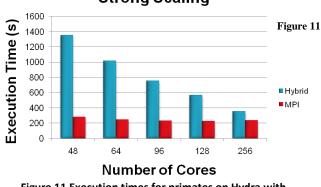


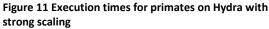
Figure 9 and Figure 10 show results after doing weak scaling with the primates dataset and the adh dataset on Hydra. These results show that hybrid MrBayes has a higher execution time than the MPI-only version.

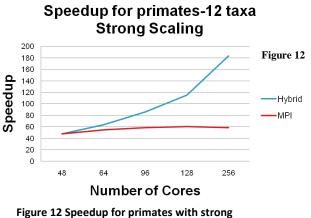
Figure 11 shows the results of executing the primates dataset on Hydra using the strong scaling technique. We were able to do strong scaling on this dataset since it is smaller with only 12 taxa. The results show that the hybrid version is much slower than the MPI version, but at 256 the execution times begin to get closer. Figure 12 shows the speedup of the primates dataset during the same run. This chart shows that hybrid experiences substantial speedup, whereas, MPI levels off. This is reflected in the chart of the execution times. The MPI version's execution time did not change substantially, but the hybrid version's execution time sees no substantial decrease in execution time suggesting that the additional cores are not necessary and actually introduce communication overhead.



Strong Scaling

Performance for primates-12 taxa





scaling on Hydra

# C. Energy Consumption on Dori

Table 3 shows energy consumption data collected with the primates dataset using Dori with 32 chains. The results in Table 3 show that the hybrid version has higher energy consumption than the MPI-only version for all number of cores except 32. With 32 cores, memory, hard drive, and motherboard all show lower energy values for hybrid MrBayes than that of MPI MrBayes. Also at 32 cores, hybrid MrBayes has a lower execution time.

The energy consumption data also show that 4 cores is the optimal number of cores for low energy consumption for both versions even though the time is higher than for 32 cores.

Tables 3-17 show the results for all datasets used.

#### V. CONCLUSIONS

The results of this research show that the MPI version of this application has a lower execution time than the hybrid version. The program benefits more from additional MPI processes than OpenMP threads. This is because OpenMP is not used as extensively as MPI. The different Markov chains 5

are distributed amongst the MPI processes. For example on Hydra-which has 16 cores per node-using strong scaling with the MPI version and 128 cores, the 512 chains were divided amongst the cores so that each core was given 4 chains. With the hybrid version in the same case, there are only 8 MPI processes to use. In the hybrid version each of the 8 MPI processes receives 64 Markov chains.

The results show that the hybrid version experiences a larger speedup than the MPI version. This suggests that the hybrid version would scale better on a larger multicore system. This is because the number of nodes increases as the number of cores increases, and the hybrid version uses nodes for MPI processes in contrast with the MPI-version which uses each core for MPI processes. So as the number of cores becomes larger the MPI-only version will begin to experience communication overhead which will increase the execution time, but the hybrid version will have more MPI processes to distribute the Markov chains amongst and will experience decreased execution time. This can be seen from the primates dataset using strong scaling on Hydra. The speedup and execution times show that with added cores, the hybrid version experiences increased speedup, whereas the MPI version stays almost the same. The hybrid version would experience lower execution time as well if more OpenMP directives were applied to other parts of the program rather than in one source file.

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# REFERENCES

[1] Message Passing Interface.

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- http://sc.tamu.edu/systems/hydra/hardware.php 3 Aug 2010
- [4] Huelsenbeck, J.P and F. Ronquist. 2004. Bayesian
- Analysis of Molecular Evolution using MrBayes
- [5] Huelsenbeck, J. P. and F. Ronquist. 2001. MRBAYES:
- Bayesian inference of phylogeny. Bioinformatics 17:754-755.

No. of Cores	Time (s)	System (kJ)	CPU (kJ)	Memory (kJ)	Hard Drive (kJ)	Motherboard (kJ)
2-hybrid	254.154	45.963065	27.30582	5.256297	2.103262	3.481821
2-mpi	214.611	39.263947	23.852611	3.997544	1.809655	2.966753
4-hybrid	178.418	37.648057	22.565793	3.875879	1.518767	2.486724
4-mpi	113.77	24.91126	14.459266	2.647337	0.972663	1.587298
8-hybrid	94.565	39.304558	22.842574	3.83381	1.545488	2.580222
8-mpi	67.301	28.043112	15.750636	2.833562	1.154268	1.855912
16-hybrid	56.887	45.89634	25.943368	4.370968	1.896912	3.085648
16-mpi	43.887	34.622904	18.566292	3.34392	1.378972	2.38708
32-hybrid	46.099	72.668664	40.61384	6.896368	3.023776	5.036632
32-mpi	46.651	71.06504	39.91648	7.145648	3.3108	5.181408

**Energy Consumption Primates-12 taxa on Dori** 

 Table 3
 Energy Consumption Hybrid MrBayes vs. MPI MrBayes from Dori

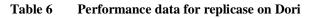
Primates on Dori			
Number of	Execution		
Cores	Time(s)	Speedup	Efficiency
2-hybrid	258.38	1.607129	0.8036
2-mpi	215.17	1.9299	0.9649
4-hybrid	179.27	2.3163385	0.5791
4-mpi	113.76	3.6502	0.9126
8-hybrid	94.99	4.3715128	0.5464
8-mpi	67.44	6.1573	0.7697
16-hybrid	57.04	7.279979	0.4550
16-mpi	44.57	9.3168	0.5823
32-hybrid	46.51	8.9281875	0.2790
32-mpi	46.28	8.9725583	0.2804

Anolis on Dori				
Number of	Execution	Speedup	Efficiency	
Cores	Time(s)			
2-hybrid	925.85	1.93260247	0.96630	
2-mpi	917.03	1.95119	0.97560	
4-hybrid	562.71	3.17979	0.79495	
4-mpi	501.72	3.56633	0.89158	
8-hybrid	300.37	5.95699	0.74462	
8-mpi	279.71	6.39698	0.79962	
16-hybrid	180.98	9.88673	0.61792	
16-mpi	164.31	10.88978	0.68061	
32-hybrid	136.7	13.08925	0.40904	
32-mpi	136.99	13.06154	0.40817	

Table 4Performance data for primates on Dori

 Table 5
 Performance data for anolis on Dori

Replicase on Dori				
Number of Cores	Execution Time(s)	Speedup	Efficiency	
2-hybrid	307.85	1.306903	0.65345	
2-mpi	207.10	1.94268	0.97134	
4-hybrid	263.39	1.52751	0.38188	
4-mpi	110.19	3.65124	0.91281	
8-hybrid	132.97	3.02572	0.37822	
8-mpi	63.73	6.31304	0.78913	
16-hybrid	77.46	5.19404	0.32463	
16-mpi	42.69	9.42446	0.58903	
32-hybrid	56.38	7.13604	0.22300	
32-mpi	45.59	8.82496	0.27578	



Adh on Dori				
Number of Cores	Execution Time(s)	Speedup	Efficiency	
2-hybrid	1146.35	1.242718	0.621359	
2-mpi	728.28	1.956102	0.978051	
4-hybrid	1000.65	1.423665	0.355916	
4-mpi	416.06	3.424001	0.856000	
8-hybrid	544.65	2.615606	0.326951	
8-mpi	237.47	5.999031	0.749879	
16-hybrid	332.97	4.278433	0.267402	
16-mpi	147.36	9.667413	0.604213	
32-hybrid	223.3	6.379713	0.199366	
32-mpi	114.3	12.4636	0.389488	

 Table 7
 Performance data for adh on Dori

Cynmix on Dori				
Number of Cores	Execution Time(s)	Speedup	Efficiency	
2-hybrid	1223.81	1.631479	0.815739	
2-mpi	904.27	2.207991	1.103995	
4-hybrid	994.69	2.007279	0.50182	
4-mpi	490.31	4.072158	1.01804	
8-hybrid	517.37	3.859172	0.482397	
8-mpi	312.62	6.386731	0.798341	
16-hybrid	303.51	6.578432	0.411152	
16-mpi	186.23	10.72126	0.670079	
32-hybrid	193.21	10.33394	0.322936	
32-mpi	155.66	12.8268	0.400838	

Avian on Dori					
Number of Cores	Execution Time(s)	Speedup	Efficiency		
2-hybrid	4834.53	1.799341	0.899671		
2-mpi	4477.48	1.942827	0.971414		
4-hybrid	3000.02	2.899637	0.724909		
4-mpi	2608.69	3.334612	0.833653		
8-hybrid	1579.85	5.5062	0.688275		
8-mpi	1488.91	5.842509	0.730314		
16-hybrid	922.3	9.431823	0.589489		
16-mpi	877.38	9.914712	0.619669		
32-hybrid	618.76	14.05871	0.439335		
32-mpi	659.04	13.19946	0.412483		

 Table 8
 Performance data for cynmix on Dori

Bglobin on Dori					
Number of Cores	Execution	Speedup	Efficiency		
	Time(s)				
2-hybrid	4259.39	2.23601267	1.11800633		
2-mpi	4669.53	2.03961641	1.0198082		
4-hybrid	2771.49	3.43643672	0.85910918		
4-mpi	2722.62	3.49811946	0.874530		
8-hybrid	1456.01	6.54119821	0.81764978		
8-mpi	1539.55	6.186256	0.773282		
16-hybrid	864.83	11.0126268	0.68828917		
16-mpi	983.56	9.683243	0.605203		
32-hybrid	626.83	15.193992	0.47481225		
32-mpi	690.18	13.7993712	0.43123035		

Table 10Performance data for bglobin on Dori

Table 9Performance data for avian on Dori

Primates on Hydra Weak Scaling Execution Time(s)			
Number of Cores Hybrid MPI			
16	132.05	23.22	
64	132.05	26.08	
96	138.61	29.58	
128	140.59	35.43	
256	160.55	73.38	

 Table 11
 Performance data for primates on Hydra

Replicase on Hydra Weak Scaling Execution Time			
Number of Cores Hybrid MPI			
16	261.16	21	
64	285.47	25.52	
96	291.27	27.96	
128	295.06	33.78	
256	319.34	72.84	

 Table 13
 Performance data for replicase on Hydra

Anolis on Hydra Weak Scaling		
Execution Time(s)		
Number of Cores	Hybrid	MPI
16	273.92	94.26
64	315.33	101.22
96	327.94	104.75
128	330.45	112.97
256	354.74	154.29

 Table 15
 Performance data for anolis on Hydra

Primates on Hydra Strong Scaling		
Execution Time(s)		
Number of Cores	Hybrid	MPI
48	1353.51	279.7
64	1014.44	244.64
96	755.75	230.18
128	564.64	221.99
256	353.48	232.23

Table 17Performance data for anolis on Hydra<br/>using strong scaling

Adh on Hydra Weak Scaling Execution Time(s)			
Number of Cores	Hybrid MPI		
16	1093.74	92.42	
64	1316.73	100.02	
96	1368.99	105.04	
128	1367.41	111.96	
256	1414.11	155.23	

 Table 12
 Performance data for adh on Hydra

Cynmix on Hydra Weak Scaling Execution Time(s)			
Number of Cores Hybrid MPI			
16	778.87	104.35	
64	858.44	114.75	
96	884.95	121.75	
128	888.95	131.37	
256	934.48	177.39	

Table 14	Performance	data for	cvnmix	on Hvdra
				011 11 010

Bglobin on Hydra Weak Scaling Execution Time(s)			
Number of Cores Hybrid MPI			
16	596.18	255.29	
64	711.13	271.96	
96	736.16	283.32	
128	742.76	293.92	
256	775.13	345.34	

 Table 16
 Performance data for bglobin on Hydra