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Comparative Analysis of High Performance Solvers for Solving Stokes Equation

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Abstract. We consider the time dependent Stokes equation on a finite time interval and on a uniform rectangular mesh, written in terms of velocity and pressure. A parallel algorithm, based on a direction splitting approach is implemented. We are targeting the massively parallel computer as well as clusters consisting of many-core nodes. The implementation was tested on the IBM Blue Gene/P supercomputer and two Linux clusters. We compared the results from the direction splitting algorithm with the results from a state-of-the-art Finite Element software package for solving of Stokes equation.

Keywords: Navier-Stokes, time splitting, ADI, incompressible flows, pressure Poisson equation, parallel algorithm
PACS: 02.60.Cb, 02.60.Lj, 02.70.Bf, 07.05.Tp, 47.10.ad, 47.11.Bc

INTRODUCTION

The objective of this paper is to analyze (and compare between computers) the parallel performance of a novel fractional time stepping technique, based on a direction splitting strategy, developed to solve the incompressible Navier-Stokes equations.

Projection schemes were introduced in [1, 2] and they have been used in Computational Fluid Dynamics since. During these years, such techniques went through some evolution, but the main paradigm, consisting of decomposing vector fields into a divergence-free part and a gradient, has been preserved; see [3] for a review. In terms of computational efficiency, projection algorithms are far superior to the methods that solve the coupled velocity-pressure system, making them the most popular techniques for solving unsteady Navier-Stokes equations.

The alternating directions algorithm proposed in [4, 5] reduces the computational complexity of the enforcement of the incompressibility constraint. Here, the standard problem for the pressure correction is replaced by the series of one-dimensional second-order boundary value problems. This technique is proved to be stable and convergent (see [4, 5]). The aim of this paper is to experimentally investigate the parallel properties of the algorithm, for two-dimensional problems, on three distinct parallel computers.

STOKES EQUATION

We consider the time-dependent Navier-Stokes equations in a rectangular domain Ω, on a finite time interval $[0,T]$. Since the nonlinear term in the Navier-Stokes equations does not interfere with the incompressibility constraint, we henceforth focus our attention on the time-dependent Stokes equations written in terms of velocity with components (u,v) and pressure p:

$$\begin{cases} u_t - \nu\,(u_{xx}+u_{yy}) + p_x = f & \\ v_t - \nu\,(v_{xx}+v_{yy}) + p_y = g & \text{in} \quad \Omega\times(0,T) \\ u_x + v_y = 0 & \\ u|_{\partial\Omega} = v|_{\partial\Omega} = 0, \quad \partial_n p|_{\partial\Omega} = 0 & \text{in} \quad (0,T) \\ u|_{t=0} = u_0, \quad v|_{t=0} = v_0, \quad p|_{t=0} = p_0 & \text{in} \quad \Omega \end{cases}, \tag{1}$$

where a smooth source term has components (f,g); ν is the kinematic viscosity; and (u_0,v_0) is a solenoidal initial velocity field with a zero normal trace. The time interval $[0,T]$ was discretized on a uniform mesh and τ was the time step.

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TABLE 1. Compilers and libraries on the three computer systems

	Galera	HPCG	IBM Blue Gene/P
Compiler	Intel C Compiler 12.1.0	Intel C Compiler 12.1.0	IBM XL C Compiler 9.0
MPI	OpenMPI 1.4.3	Intel MPI 4.0.3.008	MPICH2
LAPACK	Intel Math Kernel Library 10.0	Intel Math Kernel Library 10.0	Engineering and Scientific Subroutine Library 5.1

PARALLEL ALTERNATING DIRECTIONS ALGORITHM

Guermond and Minev introduced (in [4]) a fractional time stepping technique for solving the incompressible Navier-Stokes equations, based on a direction splitting strategy. They used a singular perturbation of Stokes equation with a perturbation parameter τ. The standard Poisson problem was replaced by series of one-dimensional second-order boundary value problems.

The scheme used in the algorithm is composed of the following parts: pressure prediction, velocity update, penalty step, and pressure correction. For the complete description of the numerical scheme and the parallel implementation of the algorithm on distributed memory computers, consult [5, 6].

EXPERIMENTAL RESULTS

The problem (1) is solved in $\Omega = (0,1)^2$, for $t \in [0,2]$ with Dirichlet boundary conditions. The discretization in time is done with the time step 10^{-2}, and the kinematic viscosity $\nu = 10^{-3}$. The second order central differences were used for the discretization in space, on a rectangular mesh, with mesh sizes $h_x = \frac{1}{n_x - 1}$ and $h_y = \frac{1}{n_y - 1}$. The total number of unknowns in the discrete problem is $600\, n_x n_y$.

To solve the problem, a portable parallel code was designed and implemented in C, while the parallelization has been facilitated by applying the MPI and OpenMP standards [7, 8, 9, 10]. Here the OpenMP was used "within" multicore processors, while MPI was used to facilitate communication between such processors. We have used the LAPACK subroutines DPTTRF and DPTTS2 (see [11]) for solving tridiagonal systems in equations (4), (5), and (6) from [6] for the unknowns corresponding to the internal nodes of each sub-domain. The same subroutines were used to solve the tridiagonal systems with the Schur complement.

The parallel code has been tested on three computer systems: Galera, located in the Centrum Informatyczne TASK, on a cluster computer system HPCG located in the Institute of Information and Communication Technologies, and on the IBM Blue Gene/P machine at the Bulgarian Supercomputing Center. Table 1 summarizes the information about used compilers and libraries on the three computer systems. In our experiments, times have been collected using the MPI provided timer and we report the best results from multiple runs. In the following tables, we report the elapsed time T_p in seconds using m MPI processes and k OpenMP processes, where $p = m \times k$, and the parallel speed-up $S_p = T_1/T_p$.

Table 2 shows the results collected on the Galera. It is a Linux cluster with 336 nodes, and two Intel Xeon quad core processors per node. Each processor runs at 2.33 GHz. Processors within each node share 8, 16, or 32 GB of memory, while nodes are interconnected with a high-speed InfiniBand network (see also `http://www.task.gda.pl/kdm/sprzet/Galera`). Here, we used an Intel C compiler, and compiled the code with the option "-O3 -openmp". For solving the tridiagonal systems of equations using LAPACK subroutines we linked our code to multi-threaded layer Intel Math Kernel Library (MKL, see `http://software.intel.com/en-us/articles/intel-mkl/`).

The results obtained with an MPI (only) implementation of the alternating directions algorithm were reported in [6]. We observed slower performance using 8 cores on one node of the Galera using the MPI code. Now we used OpenMP and the multi-threaded layer Intel MKL for execution of the code on one node. We were unpleasantly surprised, because the new code has slower performance on 2, 4, and 8 cores, *e.g.*, for $n_x = n_y = 3200$ the execution time of the MPI-only code on 8 cores was 232 seconds, while the execution time of the OpenMP code on "the same" 8 cores was 550 seconds. We will investigate this fact further in the future.

For solving the problem with $n_x = n_y = 12800$ 18 GB memory is needed. The physical memory on a single node of Galera is not large enough for solving of twice larger discrete problems and we had to use two and more nodes of the cluster for such problems. However, observe that for the problems with size larger than $n_x = n_y = 12800$, a scaled speed-up can be calculated. Here, super-linear speed-up can be observed. For instance, for the largest problem, an

TABLE 2. Execution time for solving of 2D problem on Galera

n_x	n_y	processes											
		1	2	4	8	16	32	64	128	256	512	1024	2048
800	800	47.4	29.1	22.4	19.6	9.2	4.6	2.4	1.3	0.8	0.6	0.5	1.5
800	1600	96.7	58.3	44.5	39.8	19.3	9.4	4.7	2.5	1.4	0.9	0.8	0.6
1600	1600	201.3	119.7	91.7	82.9	38.6	19.7	9.6	4.8	2.6	1.5	1.1	0.9
1600	3200	437.2	263.4	212.9	200.0	79.3	39.5	19.8	9.8	5.0	2.7	1.8	1.2
3200	3200	1070.0	672.6	682.8	550.1	174.0	79.8	39.7	20.3	10.1	5.1	3.0	1.9
3200	6400	2525.6	1754.7	1920.2	1477.6	432.7	178.3	80.5	40.8	20.7	10.2	5.7	3.2
6400	6400	7418.9	4750.9	4007.3	3137.8	993.8	442.9	177.0	85.4	41.5	20.9	10.8	5.9
6400	12800	12650.0	8146.2	5823.4	4956.7	2188.2	1087.3	461.5	205.5	85.9	41.9	21.8	11.3
12800	12800	34804.7	21416.3	14318.1	11272.0	4985.2	2806.5	1111.4	556.6	209.2	86.4	42.7	22.0
12800	25600					10317.4	5035.7	2387.2	1547.4	543.7	211.0	92.3	43.2
25600	25600						11465.1	5126.7	3195.8	1582.4	567.8	214.1	88.6
25600	51200							10507.2	5292.6	3406.1	1596.8	559.3	214.7
51200	51200								11678.2	5220.0	3381.2	1620.5	582.8

TABLE 3. Execution time for solving of 2D problem on HPCG

n_x	n_y	processes							
		1	2	4	8	16	32	64	128
800	800	21.85	12.09	7.72	6.47	3.41	1.60	1.10	0.65
800	1600	46.79	25.27	15.98	13.29	6.94	3.67	2.03	1.13
1600	1600	95.89	50.63	31.53	25.43	13.87	6.65	4.16	2.20
1600	3200	194.19	100.66	63.58	50.56	29.60	13.52	7.96	4.23
3200	3200	400.59	206.77	129.85	106.50	51.77	28.20	14.97	8.25
3200	6400	901.91	470.02	299.95	240.32	116.79	53.55	29.97	17.34
6400	6400	1882.27	1108.73	696.65	562.38	253.67	113.27	71.79	35.34
6400	12800	4277.73	2323.90	1463.49	1113.83	562.59	337.00	153.85	72.42
12800	12800	8068.33	4748.90	3119.29	2761.58	1217.21	593.05	335.91	161.65

increase of the number of processors from 128 to 256 results in scaled speed-up of 2.13. This is a relatively standard effect related to extra improvement caused by reduction of sub-problem sizes.

Table 3 shows the results collected on the HPCG cluster. HP Cluster Platform Express 7000 enclosures with 36 blades BL 280c, dual Intel Xeon X5560 processors (total 576 cores). Each processor runs at 2.8 GHz. Processors within each blade share 24 GB RAM, while nodes are interconnected with non-blocking DDR Interconnection via Voltaire Grid director 2004 with latency 2.5 μs and bandwidth 20 Gbps (see also http://www.grid.bas.bg/hpcg/). Again, we used an Intel C compiler, and compiled the code with the option "-O3 -openmp". For solving the tridiagonal systems of equations using LAPACK subroutines we linked our code to multi-threaded layer Intel MKL.

Again, the somehow slower performance using 8 cores is clearly visible. There are some factors which could play role for the slower performance using all processors of a single node. Generally, they are a consequence of limitations of memory subsystems and their hierarchical organization in modern computers. One such factor might be the limited bandwidth of the main memory bus.

Table 4 presents execution time collected on the IBM Blue Gene/P machine at the Bulgarian Supercomputing Center. It consists of 2048 compute nodes with quad core PowerPC 450 processors (running at 850 MHz). Each node has 2 GB of RAM. For the point-to-point communications a 3.4 Gb 3D mesh network is used. Reduction operations are performed on a 6.8 Gb tree network (for more details, see `http://www.scc.acad.bg/`). We have used the IBM XL C compiler and compiled the code with the following options: "-O5 -qstrict -qarch=450d -qtune=450 -qsmp=omp". For solving the tridiagonal systems using LAPACK subroutines we linked our code to multi threaded Engineering and Scientific Subroutine Library (ESSL, see `http://www-03.ibm.com/systems/software/essl/index.html`).

Again, the new code has slower performance than the MPI code on 2 and 4 cores. The memory of one node of IBM supercomputer is substantially smaller than on clusters (2 GB vs. 24 or 32 GB) and the largest discrete problem in our experiments which can be solved on one node have $n_x = n_y = 3200$. Observe that also on this machine a slight superlinear scaled speed-up is observed (for the same reasons). For the largest problem, increasing the number of

TABLE 4. Execution time for solving of 2D problem on IBM Blue Gene/P

n_x	n_y	processes												
		1	2	4	8	16	32	64	128	256	512	1024	2048	4096
800	800	432.4	237.0	148.6	69.5	34.4	17.3	8.8	4.8	2.6	1.7	1.1	0.9	0.6
800	1600	879.2	505.1	305.8	144.0	69.8	35.5	17.3	9.5	4.9	3.2	1.8	1.6	1.0
1600	1600	1772.9	979.6	595.1	312.0	152.8	71.6	35.6	17.7	9.2	5.3	3.0	2.2	1.5
1600	3200	3600.3	2082.4	1295.4	633.9	313.1	148.4	72.0	36.5	18.0	10.3	5.5	3.9	2.4
3200	3200	7439.4	4281.1	2720.9	1324.2	608.7	320.8	157.3	73.0	36.5	18.7	10.0	6.1	3.7
3200	6400				2795.3	1327.1	651.0	321.7	151.1	73.3	38.0	19.1	11.7	6.5
6400	6400					2777.5	1354.1	625.4	323.7	160.1	74.9	37.9	20.3	11.2
6400	12800						2853.8	1357.3	656.4	325.0	154.2	75.7	41.0	21.0
12800	12800							2844.2	1362.2	628.7	329.2	163.7	78.4	40.5
12800	25600								2867.5	1365.6	666.7	330.9	160.8	79.5
25600	25600									2858.7	1376.7	639.1	335.9	168.9
25600	51200										2897.0	1381.0	679.0	338.5
51200	51200											2884.5	1390.8	649.2

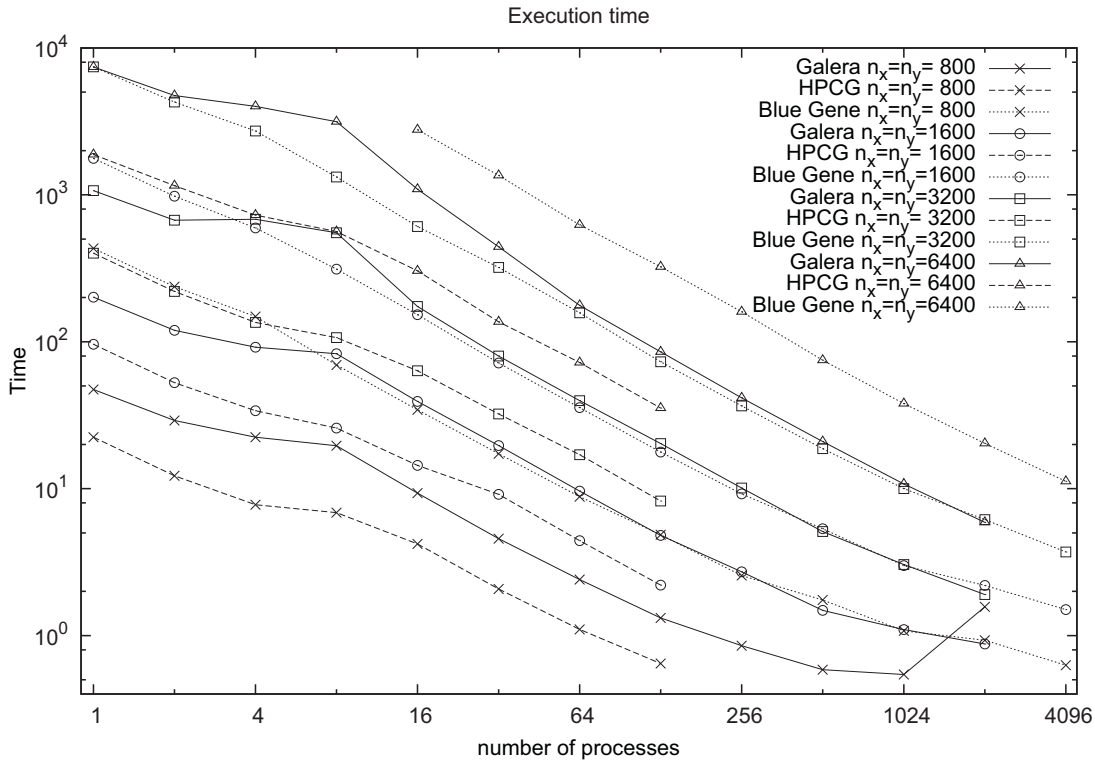

FIGURE 1. Execution time for 2D problem with $n_x = n_y = 800, 1600, 3200, 6400$

processors from 1024 to 2048 results in scaled speed-up of 2.07.

The execution time on the three parallel systems is shown in Figure 1. Because of the slower processors, the execution time obtained on the Blue Gene/P is substantially larger than that on the clusters. At the same time, the parallel efficiency obtained on a large number of nodes on the supercomputer is better. The main reason of this can be related to the superior performance of the networking infrastructure of the Blue Gene (recall, the extra networking infrastructure available there).

To round up the performance analysis of the alternating directions algorithm, the speed-up obtained on Galera is

TABLE 5. Speed-up on Galera

n_x	n_y	processes										
		2	4	8	16	32	64	128	256	512	1024	2048
800	800	1.63	2.12	2.41	5.08	10.38	19.71	35.94	55.46	81.01	87.16	25.33
800	1600	1.66	2.17	2.43	4.97	10.27	20.51	38.80	67.11	106.83	120.14	127.52
1600	1600	1.68	2.20	2.43	5.12	10.24	20.90	41.90	74.07	135.77	183.15	229.49
1600	3200	1.66	2.05	2.19	5.51	11.06	22.08	44.61	87.61	160.21	236.53	361.04
3200	3200	1.59	1.57	1.94	6.15	13.39	26.94	52.74	105.98	209.44	351.23	562.98
3200	6400	1.44	1.32	1.71	5.67	14.18	31.44	61.93	122.34	246.74	443.73	779.57
6400	6400	1.56	1.85	2.36	6.80	16.75	41.92	86.86	178.57	354.76	688.90	1259.92
6400	12800	1.55	2.17	2.55	5.78	11.63	27.40	61.53	147.18	301.45	580.05	1118.72
12800	12800	1.63	2.43	3.09	6.98	12.40	31.32	62.53	166.39	402.91	815.48	1584.34

TABLE 6. Speed-up on HPCG

n_x	n_y	processes						
		2	4	8	16	32	64	128
800	800	1.81	2.83	3.38	6.40	13.65	20.52	33.82
800	1600	1.85	2.93	3.52	6.74	12.76	23.04	41.47
1600	1600	1.89	3.04	3.77	6.92	14.43	23.05	43.55
1600	3200	1.93	3.05	3.84	6.56	14.37	24.39	45.87
3200	3200	1.94	3.08	3.76	7.74	14.20	26.76	48.58
3200	6400	1.92	3.01	3.75	7.72	16.84	30.09	52.01
6400	6400	1.70	2.70	3.35	7.42	16.62	26.22	53.26
6400	12800	1.84	2.92	3.84	7.60	12.69	27.80	59.07
12800	12800	1.70	2.59	2.92	6.63	13.60	24.02	49.91

reported in Table 5, while the speed-up on HPCG — in Table 6, the speed-up on the IBM Blue Gene/P — in Table 7, and the parallel efficiency — in Table 8.

In each case, when increasing the number of cores of the two clusters, the parallel efficiency decreases on 8 cores and after that it increases. As expected, the parallel efficiency on the IBM Blue Gene/P improves with the size of the discrete problems. The efficiency on 1024 cores increases from 39% for the smallest problems to 73% for the largest problems.

To compare the performance of the proposed approach with an existing method, we solved the same 2D Stokes problem using Elmer [12] Open Source Finite Element Software for Multiphysical Problems (see `http://www.csc.fi/english/pages/elmer`). Here, for the Elmer we used the following keywords in the input file:

Simulation
Coordinate System = “Cartesian 2D”
Simulation Type = Transient
Timestep intervals = 200
Timestep Sizes = 0.01
End

TABLE 7. Speed-up on IBM Blue Gene/P

n_x	n_y	processes											
		2	4	8	16	32	64	128	256	512	1024	2048	4096
800	800	1.82	2.91	6.22	12.57	25.05	48.99	89.10	168.67	247.90	401.65	465.48	687.32
800	1600	1.74	2.87	6.10	12.60	24.75	50.69	92.20	177.88	276.51	486.02	552.26	897.63
1600	1600	1.81	2.98	5.68	11.60	24.76	49.81	99.87	192.28	332.75	592.66	808.05	1180.51
1600	3200	1.73	2.78	5.68	11.50	24.26	49.97	98.57	200.07	349.59	651.68	923.50	1522.27
3200	3200	1.74	2.73	5.62	12.22	23.19	47.30	101.85	203.58	397.74	744.26	1209.29	2009.58

TABLE 8. Parallel efficiency

n_x	n_y	processes											
		2	4	8	16	32	64	128	256	512	1024	2048	4096
Galera													
800	800	0.813	0.529	0.302	0.321	0.324	0.308	0.281	0.217	0.158	0.085	0.015	
800	1600	0.829	0.543	0.304	0.314	0.321	0.320	0.303	0.262	0.209	0.117	0.076	
1600	1600	0.841	0.549	0.304	0.326	0.320	0.328	0.327	0.299	0.265	0.179	0.114	
1600	3200	0.830	0.513	0.273	0.345	0.346	0.345	0.348	0.342	0.313	0.231	0.176	
3200	3200	0.795	0.392	0.243	0.391	0.419	0.421	0.412	0.414	0.409	0.343	0.275	
3200	6400	0.720	0.329	0.214	0.365	0.443	0.490	0.483	0.477	0.481	0.433	0.381	
6400	6400	0.781	0.463	0.296	0.467	0.523	0.655	0.679	0.698	0.693	0.673	0.615	
6400	12800	0.776	0.543	0.319	0.361	0.363	0.428	0.481	0.575	0.589	0.566	0.546	
12800	12800	0.813	0.608	0.386	0.436	0.388	0.489	0.489	0.650	0.787	0.796	0.774	
HPCG													
800	800	0.904	0.708	0.422	0.400	0.426	0.321	0.264					
800	1600	0.926	0.732	0.440	0.421	0.399	0.360	0.324					
1600	1600	0.947	0.760	0.471	0.432	0.451	0.360	0.340					
1600	3200	0.965	0.764	0.480	0.410	0.449	0.381	0.358					
3200	3200	0.969	0.771	0.470	0.484	0.444	0.418	0.380					
3200	6400	0.959	0.752	0.469	0.483	0.526	0.470	0.406					
6400	6400	0.849	0.675	0.418	0.464	0.519	0.410	0.416					
6400	12800	0.920	0.731	0.480	0.475	0.397	0.434	0.461					
12800	12800	0.849	0.647	0.365	0.414	0.425	0.375	0.390					
IBM Blue Gene/P													
800	800	0.912	0.727	0.777	0.786	0.783	0.765	0.696	0.659	0.484	0.392	0.227	0.168
800	1600	0.870	0.719	0.763	0.787	0.773	0.792	0.720	0.695	0.540	0.475	0.270	0.219
1600	1600	0.905	0.745	0.710	0.725	0.774	0.778	0.780	0.751	0.650	0.579	0.395	0.288
1600	3200	0.864	0.695	0.710	0.719	0.758	0.781	0.770	0.782	0.683	0.636	0.451	0.372
3200	3200	0.869	0.684	0.702	0.764	0.725	0.739	0.796	0.795	0.777	0.727	0.590	0.491

```
Solver 1
Equation = Navier-Stokes
Procedure = "FlowSolve" "FlowSolver"
Variable = Flow Solution[Velocity:2 Pressure:1]
Flow Model = Stokes
Stabilize = True
Optimize Bandwidth = True
Stabilization Method = Stabilized
Linear System Solver = Iterative
Linear System Iterative Method = BiCGStab
Linear System Max Iterations = 500
Linear System Convergence Tolerance = 1.0e-6
Linear System Preconditioning = ILU2
Linear System ILUT Tolerance = 1.0e-3
End
```

Figure 2 shows the measured CPU time for solving the 2D Stokes problem using Elmer software, on the Blue Gene/P machine, for discrete problems with sizes $n_x = n_y = 100, 200, 400$.

As can be seen, the performance of the Elmer package is inferior to our approach. The first observation is related to the fact, that due to the differences in approaches, the Elmer requires much larger memory than our approach. This is the reason why we could not solve the problem using Elmer on smaller number of processors than 4 for the smallest problem; and 32 for the largest one. For similar reasons, the Elmer turned useless when attempted at being

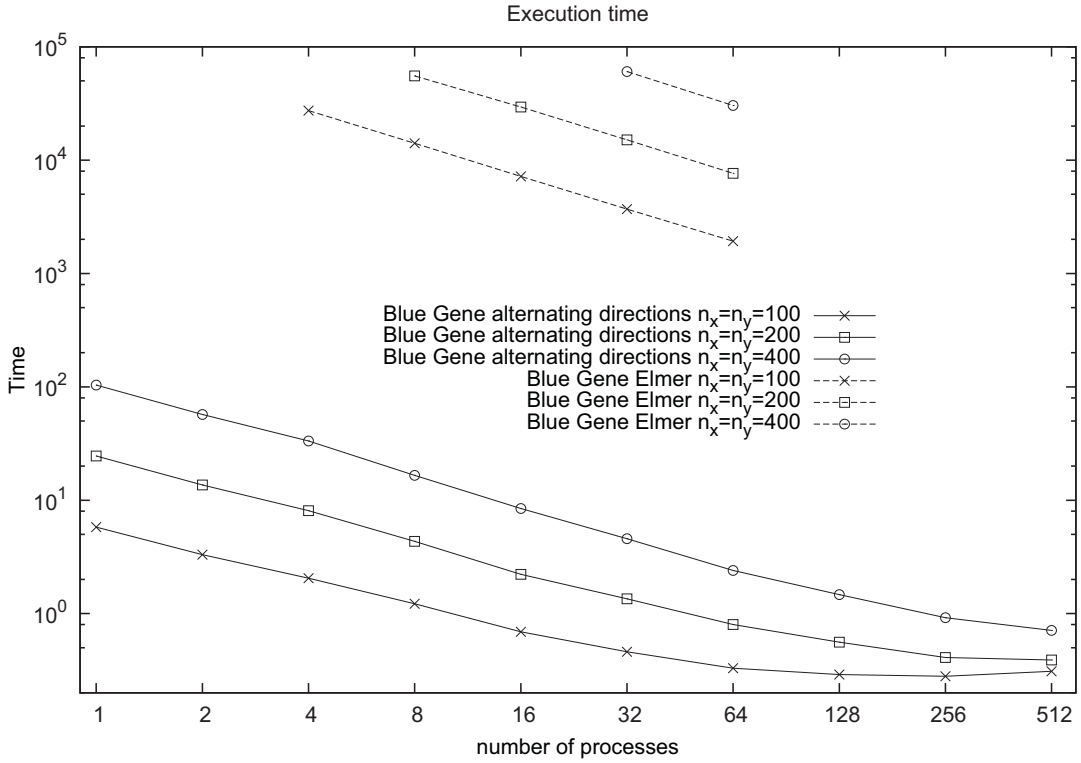

FIGURE 2. Execution time for 2D problem with $n_x = n_y = 100, 200, 400$

used on more than 64 processors. The second observation concerns execution times. Here, also, the proposed approach is superior to that available when using the Elmer package.

CONCLUDING REMARKS

In this paper we have considered parallel solution of time dependent Stokes equation using a direction splitting approach. We have studied performance of the parallel code, implemented using a hybrid approach based on OpenMP and MPI, when applied to a 2D model problem on a rectangular domain. The performance has been studied on two COTS clusters and on an IBM Blue Gene supercomputer. We have found that, against initial predictions, the hybrid solution method does not lead to the expected performance improvement. Second, the extra networking infrastructure available in the Blue Gene plays very important role when parallel efficiency is concerned. At the same time, processor speed and memory size make up for the networking "deficiencies" of the clusters, by allowing them to solve larger problems faster (in the sense of the wall-clock solution time). Finally, we have compared the performance of the proposed approach with that of the state-of-the-art Elmer package. We have found our method to be vastly superior both in terms of memory use and efficiency. In the next step we plan to make similar comparisons for the 3D problems and perform an in-depth study of the efficiency of the OpenMP-related part of code.

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