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Improving the efficiency of parallel alternating directions algorithm for time dependent problems

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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. Our work is motivated by the need to improve the parallel efficiency of our supercomputer implementation of the parallel algorithm.

We are targeting the IBM Blue Gene/P massively parallel computer, which features a 3D torus interconnect. We study the impact of the domain partitioning on the performance of the considered parallel algorithm for solving the time dependent Stokes equation. Here, different parallel partitioning strategies are given special attention. The implementation is tested on the IBM Blue Gene/P and the presented results from numerical tests confirm that decreasing the communication time better parallel properties of the algorithm are obtained.

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 article is to analyze the performance of the MPI and OpenMP parallel codes which use a new fractional time stepping technique, based on a direction splitting strategy, developed to solve the incompressible Navier-Stokes equations.

Projection schemes were first introduced in [1, 2] and they have been used in Computational Fluid Dynamics (CFD) for the last forty years. During these years, these techniques have been evolving, 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 of projection methods). In terms of computational efficiency, projection algorithms are far superior to the methods that solve the coupled velocity-pressure system. This feature makes them the most popular techniques in the CFD community for solving the unsteady Navier-Stokes equations. The computational complexity of each time step of the projection methods is that of solving one vector-valued advection-diffusion equation, plus one scalar-valued Poisson equation with the Neumann boundary conditions. Note that, for large scale problems, and large Reynolds numbers, the cost of solving the Poisson equation becomes dominant.

The alternating directions algorithm proposed in [4] reduces the computational complexity of the action of the incompressibility constraint. The key idea is to modify the standard projection approach, in which the vector fields are decomposed into a divergence-free part plus a gradient part. In the new method the pressure equation is derived from a perturbed form of the continuity equation, in which the incompressibility constraint is penalized in a negative norm induced by the direction splitting. The standard Poisson problem for the pressure correction is replaced by series of one-dimensional second-order boundary value problems. This technique is proved to be stable and convergent [for details see 4]. Furthermore, the parallel performance of this technique is analyzed in [5, 6]. The aim of this paper is to study the impact of the domain partitioning on the performance of the algorithm for solving the 3D time dependent Stokes equation.

STOKES EQUATION

Let us start by defining the problem to be solved. We consider the time-dependent Navier-Stokes equations on a finite time interval $[0, T]$, and in a rectangular domain Ω . Since the nonlinear term in the Navier-Stokes equations does not interfere with the incompressibility constraint, we focus our attention on the time-dependent Stokes equations, written

in terms of velocity \mathbf{u} and pressure p :

$$\begin{cases} \mathbf{u}_t - \nu \Delta \mathbf{u} + \nabla p = \mathbf{f} & \text{in } \Omega \times (0, T) \\ \nabla \cdot \mathbf{u} = 0 & \text{in } \Omega \times (0, T) \\ \mathbf{u}|_{\partial\Omega} = 0, \quad \partial_n p|_{\partial\Omega} = 0 & \text{in } (0, T) \\ \mathbf{u}|_{t=0} = \mathbf{u}_0, \quad p|_{t=0} = p_0 & \text{in } \Omega \end{cases}, \quad (1)$$

where \mathbf{f} is a smooth source term, ν is the kinematic viscosity, and \mathbf{u}_0 is a solenoidal initial velocity field with a zero normal trace. In our work, we consider homogeneous Dirichlet boundary conditions on the velocity.

To solve thus described problem, we discretize the time interval $[0, T]$ using a uniform mesh. Finally, let τ be the time step used in the algorithm.

FORMULATION OF THE SCHEME

Let us describe the proposed parallel solution method. Authors of [4] introduced an innovative fractional time stepping technique for solving the incompressible Navier-Stokes equations, based on a direction splitting strategy. They used a singular perturbation of the Stokes equation with the perturbation parameter τ . The standard Poisson problem for the pressure correction was replaced by series of one-dimensional second-order boundary value problems.

The scheme used in the algorithm is composed of the following parts: (i) pressure prediction, (ii) velocity update, (iii) penalty step, and (iv) pressure correction. Let us now describe an algorithm that uses the direction splitting operator

$$A := \left(1 - \frac{\partial^2}{\partial x^2}\right) \left(1 - \frac{\partial^2}{\partial y^2}\right) \left(1 - \frac{\partial^2}{\partial z^2}\right).$$

- *Pressure predictor.* The algorithm is initialized by setting $p^{-\frac{1}{2}} = p^{-\frac{3}{2}} = p_0$. Next, for all $n \geq 0$, a pressure predictor is computed as follows

$$p^{*,n+\frac{1}{2}} = 2p^{n-\frac{1}{2}} - p^{n-\frac{3}{2}}. \quad (2)$$

- *Velocity update.* The velocity field is initialized by setting $\mathbf{u}^0 = \mathbf{u}_0$, and for all $n \geq 0$ the velocity update is computed by solving the following series of one-dimensional problems

$$\begin{aligned} \frac{\xi^{n+1} - \mathbf{u}^n}{\tau} - \nu \Delta \mathbf{u}^n + \nabla p^{*,n+\frac{1}{2}} &= \mathbf{f}^{n+\frac{1}{2}} = \mathbf{f}|_{t=(n+\frac{1}{2})\tau}, \quad \xi^{n+1}|_{\partial\Omega} = 0 \\ \frac{\eta^{n+1} - \xi^{n+1}}{\tau} - \frac{\nu}{2} \frac{\partial^2(\eta^{n+1} - \mathbf{u}^n)}{\partial x^2} &= 0, \quad \eta^{n+1}|_{\partial\Omega} = 0 \end{aligned} \quad (3)$$

$$\frac{\zeta^{n+1} - \eta^{n+1}}{\tau} - \frac{\nu}{2} \frac{\partial^2(\zeta^{n+1} - \mathbf{u}^n)}{\partial y^2} = 0, \quad \zeta^{n+1}|_{\partial\Omega} = 0 \quad (4)$$

$$\frac{\mathbf{u}^{n+1} - \zeta^{n+1}}{\tau} - \frac{\nu}{2} \frac{\partial^2(\mathbf{u}^{n+1} - \mathbf{u}^n)}{\partial z^2} = 0, \quad \mathbf{u}^{n+1}|_{\partial\Omega} = 0. \quad (5)$$

- *Penalty step.* The intermediate parameter ϕ is approximated by solving $A\phi = -\frac{1}{\tau}\nabla \cdot \mathbf{u}^{n+1}$. This is done by solving the following series of one-dimensional problems:

$$\begin{aligned} \theta - \theta_{xx} &= -\frac{1}{\tau}\nabla \cdot \mathbf{u}^{n+1}, \quad \theta_x|_{\partial\Omega} = 0, \\ \psi - \psi_{yy} &= \theta, \quad \psi_y|_{\partial\Omega} = 0, \\ \phi - \phi_{zz} &= \psi, \quad \phi_z|_{\partial\Omega} = 0, \end{aligned} \quad (6)$$

- *Pressure update.* The pressure is updated using the parameter $\chi \in [0, \frac{1}{2}]$.

$$p^{n+\frac{1}{2}} = p^{n-\frac{1}{2}} + \phi - \chi \nu \nabla \cdot \frac{\mathbf{u}^{n+1} + \mathbf{u}^n}{2} \quad (7)$$

PARALLEL ALGORITHM

In the proposed algorithm, we use a rectangular uniform mesh combined with a central difference scheme for the second derivatives for solving equations (3)–(6). Thus the algorithm requires only the solution of tridiagonal linear systems. The parallelization is based on a decomposition of the domain into rectangular sub-domains. Let us associate with each such sub-domain a set of integer coordinates (i_x, i_y, i_z) , and identify it with a given processor. The linear systems, generated by the one-dimensional problems that need to be solved in each direction, are divided into systems for each set of unknowns, corresponding to the internal nodes for each block that can be solved independently by a direct method. The corresponding Schur complement for the interface unknowns between the blocks that have an equal coordinate i_x , i_y , or i_z is also tridiagonal and can be therefore easily inverted directly. The overall algorithm requires only exchange of the interface data, which allows for a very efficient parallelization with an efficiency comparable to that of an explicit schemes.

MPI implementation

To solve the problem, a portable parallel code was designed and implemented in C, while the parallelization has been facilitated using the MPI library [7, 8]. In the code, we use the LAPACK subroutines DPTTRF and DPTTS2 [see 9] for solving tridiagonal systems of equations resulting from equations (3), (4), (5), and (6) for the unknowns corresponding to the internal nodes of each sub-domain. The same subroutines are used to solve the tridiagonal systems with the Schur complement.

This version of the code uses MPI functions for the exchange of the data. For solving of one dimensional problems new communicators were created using `MPI_Comm_split` function.

Hybrid implementation

Our work presents perspectives of the parallelization based on the MPI and OpenMP standards. The work is motivated by the need to improve the parallel efficiency of our implementation of the parallel algorithm. Essential improvements of the first version of the parallel algorithm are made by introducing two levels of parallelism: MPI and OpenMP.

Parallel code using MPI Cartesian topology functions

We study the impact of the domain partitioning on the performance of the considered parallel algorithm for solving the time dependent Stokes equation. Here, different parallel partitioning strategies are given special attention.

Last version of the code uses MPI functions, OpenMP directives, and functions which process topologies and are embedded in MPI standard. In order to obtain a better mapping of the processors to the physical interconnect topology, the function `MPI_Comm_split` was replaced by the following sequence:

```
MPI_Dims_create /* Creates a division of processors in a Cartesian grid */
MPI_Cart_create /* Makes a new communicator to which topology information has been attached */
MPI_Cart_get   /* Retrieves Cartesian topology information associated with a communicator */
MPI_Cart_sub   /* Partitions a communicator into subgroups which form lower-dimensional Cartesian
sub-grids */
```

First, a division of the processors in a 3D Cartesian grid is obtained via `MPI_Dims_create`. After that a communicator using the Cartesian topology is created using the function `MPI_Cart_create`. The `MPI_Cart_get` is used to retrieve the Cartesian topology information from the communicator and `MPI_Cart_sub` to partition the communicator into lower dimensional sub-grids.

TABLE 1. Execution time for solving of 3D problem on Galera.

n_x	n_y	n_z	nodes								
			1	2	4	8	16	32	64	128	256
MPI code											
120	120	120	348.39	155.49	67.51	32.28	15.01	7.07	3.71	3.35	4.15
120	120	240	733.36	348.81	150.16	71.35	32.85	14.92	7.09	3.65	1.99
120	240	240	1605.20	769.83	351.08	163.61	74.00	32.97	15.79	7.53	3.95
240	240	240	3358.13	1629.69	772.10	352.42	160.75	70.01	35.40	16.39	8.10
240	240	480	6930.82	3368.49	1620.76	740.29	360.66	153.15	77.78	34.60	16.82
240	480	480	14961.80	7246.11	3376.59	1597.62	792.48	357.68	175.76	77.33	35.69
480	480	480	30064.50	15348.10	7472.27	3378.68	1652.82	772.97	378.36	175.28	76.66
hybrid version											
120	120	120	137.07	70.70	32.27	16.62	8.76	5.36	3.59	3.41	6.39
120	120	240	281.44	142.45	66.43	34.16	16.77	8.79	5.48	3.51	2.62
120	240	240	582.03	299.33	144.26	71.72	36.15	17.41	10.31	6.31	4.20
240	240	240	1184.09	615.22	295.62	145.24	73.65	34.18	17.84	10.72	7.26
240	240	480	2400.45	1234.29	606.84	295.88	147.28	71.36	36.47	19.24	11.67
240	480	480	5026.87	2513.60	1242.79	610.62	311.91	152.58	76.43	41.41	21.77
480	480	480	10239.10	5000.12	2503.64	1248.92	636.52	323.14	154.45	86.88	42.93
MPI + OpenMP + topology											
120	120	120	137.18	68.63	34.45	16.84	10.08	5.60	4.93	3.31	4.18
120	120	240	281.57	139.53	70.26	34.50	19.46	10.05	5.38	3.60	2.66
120	240	240	580.60	293.03	146.05	72.80	40.75	20.00	10.34	6.69	4.41
240	240	240	1169.91	587.90	300.12	147.76	74.51	35.60	17.82	11.31	7.00
240	240	480	2358.86	1177.95	605.26	302.16	154.11	74.19	36.53	23.39	13.19
240	480	480	5005.15	2392.65	1264.05	629.31	324.81	154.27	76.05	52.20	26.36
480	480	480	10028.60	5174.94	2571.37	1277.57	643.94	309.76	153.88	86.71	45.43

EXPERIMENTAL RESULTS

We have solved the problem (1) in the domain $\Omega = (0, 1)^3$, for $t \in [0, 2]$ with Dirichlet boundary conditions. The discretization in time was done with time step 10^{-2} . The parameter in the pressure update sub-step was $\chi = \frac{1}{2}$, and the kinematic viscosity was $\nu = 10^{-3}$. The discretization in space used mesh sizes $h_x = \frac{1}{n_x-1}$, $h_y = \frac{1}{n_y-1}$, and $h_z = \frac{1}{n_z-1}$. Thus, the equation (3) resulted in linear systems of size n_x , the equation (4) resulted in linear systems of size n_y , and the equation (5) — in linear systems of size n_z . The total number of unknowns in the discrete problem was $800n_xn_yn_z$.

The parallel code has been tested on a cluster computer system Galera, located in the Polish Centrum Informatyczne TASK and on the IBM Blue Gene/P machine at the Bulgarian Supercomputing Center. 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_k in seconds using k nodes, the parallel speed-up $S_k = T_s/T_k$ where T_s is the execution time using sequential algorithm.

Table 1 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”. For solving the tridiagonal systems of equations using LAPACK subroutines we linked our code to Intel Math Kernel Library (see <http://software.intel.com/en-us/articles/intel-mkl/>).

The execution time obtained on the cluster shows significant improvement of the efficiency of the algorithm using OpenMP directives for shared memory multiprocessing. As it was expected, there is no significant improvement on the performance using `MPI_Cart_create` function on the cluster.

Table 2 contains the speed-up obtained on the cluster. The discrete problem with $n_x = n_y = n_z = 480$ requires 19 GB of memory. That is why we report the speed-up on Galera only for problems with $n_x, n_y, n_z = 120, 240, 480$. Specifically, for larger problems we could not run the code on a single computational unit and thus the speed-up could be calculated.

TABLE 2. Speed-up on Galera.

n_x	n_y	n_z	nodes								
			1	2	4	8	16	32	64	128	256
MPI code											
120	120	120	1.00	2.24	5.16	10.79	23.21	49.24	93.93	103.99	83.98
120	120	240	1.00	2.10	4.88	10.28	22.71	49.16	103.49	200.68	368.00
120	240	240	1.00	2.09	4.57	9.81	21.87	48.68	101.65	213.17	406.23
240	240	240	1.00	2.06	4.35	9.53	20.96	47.97	94.86	204.91	414.53
240	240	480	1.00	2.06	4.28	9.36	19.61	45.26	89.11	200.31	412.01
240	480	480	1.00	2.06	4.43	9.37	19.14	41.83	85.13	193.49	419.26
480	480	480	1.00	1.96	4.02	8.90	18.19	38.89	82.62	171.52	392.20
hybrid version											
120	120	120	2.54	4.93	10.80	20.97	39.77	65.00	96.93	102.09	54.50
120	120	240	2.61	5.15	11.04	21.47	43.72	83.47	133.90	208.67	279.94
120	240	240	2.76	5.36	11.13	22.38	44.40	92.22	155.73	254.36	381.81
240	240	240	2.84	5.46	11.36	23.12	45.60	98.26	188.19	313.30	462.70
240	240	480	2.89	5.62	11.42	23.42	47.06	97.12	190.06	360.23	593.66
240	480	480	2.98	5.95	12.04	24.50	47.97	98.06	195.77	361.30	687.17
480	480	480	2.90	6.01	12.01	24.07	47.23	93.04	194.65	346.05	700.27
MPI + OpenMP + topology											
120	120	120	2.54	5.08	10.11	20.69	34.55	62.26	70.63	105.22	83.37
120	120	240	2.60	5.26	10.44	21.26	37.69	73.00	136.32	203.62	276.14
120	240	240	2.76	5.48	10.99	22.05	39.40	80.27	155.19	240.03	363.61
240	240	240	2.87	5.71	11.19	22.73	45.07	94.34	188.42	296.95	479.52
240	240	480	2.94	5.88	11.45	22.94	44.97	93.42	189.75	296.26	525.59
240	480	480	2.99	6.25	11.84	23.77	46.06	96.98	196.73	286.64	567.60
480	480	480	3.00	5.81	11.69	23.53	46.69	97.06	195.37	346.71	661.74

Table 3 present 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”. For solving the tridiagonal systems of equations using LAPACK subroutines we linked our code to Engineering and Scientific Subroutine Library (ESSL) (see <http://www-03.ibm.com/systems/software/essl/index.html>).

The memory of one node of IBM supercomputer is substantially smaller than on Galera and is not enough for solving 3D problem with $n_x = n_y = n_z = 240$. We solved these problems on two and more nodes. The execution time obtained on the supercomputer shows improvement of the efficiency of the algorithm using OpenMP directives. The last version of the code is the fastest when we solve the problem on 64, 128, 256, and 512 nodes of the supercomputer.

Table 4 shows the speed-up obtained on the supercomputer. Because of smaller memory on one node of the IBM Blue Gene/P we calculated the speed-up only for $n_x = 120$ and $n_y, n_z = 120, 240$.

Finally, computing time on both parallel systems is shown in Fig. 1. Because of the slower processors, the execution time obtained on the Blue Gene/P is substantially larger than that on the Galera. 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.

CONCLUSIONS AND FUTURE WORK

We have studied parallel performance of the recently developed parallel algorithm based on a new direction splitting approach for solving of the 3D time dependent Stokes equation on a finite time interval and on a uniform rectangular mesh. The performance was evaluated on two different parallel architectures. In order to get better parallel performance using four cores per processor on the IBM Blue Gene/P (and future multi-core computers) we developed mixed

TABLE 3. Execution time for solving of 3D problem on IBM Blue Gene/P.

n_x	n_y	n_z	nodes										
			1	2	4	8	16	32	64	128	256	512	1024
MPI code													
120	120	120	1623.59	769.55	370.32	177.48	115.22	45.41	23.24	12.51	7.05	3.72	2.73
120	120	240	3248.27	1601.47	763.08	371.15	175.98	117.95	45.83	24.45	13.77	6.97	5.03
120	240	240	6582.40	3264.95	1621.69	781.96	351.38	178.79	117.66	48.48	26.31	13.63	9.57
240	240	240		6638.63	3318.05	1662.52	793.75	382.38	184.69	123.06	52.14	26.76	15.49
240	240	480			6634.37	3320.41	1647.09	787.36	383.79	189.97	147.75	51.74	29.97
240	480	480				6717.84	3355.70	1663.86	804.80	377.84	195.58	127.11	58.38
480	480	480					6783.02	3384.23	1700.44	829.58	406.70	199.71	135.32
hybrid version													
120	120	120	549.73	265.11	132.38	65.82	49.01	18.25	9.90	6.59	4.35	2.61	2.21
120	120	240	1126.59	553.89	273.40	134.04	67.09	48.61	18.31	11.09	7.41	4.49	3.02
120	240	240	2252.34	1100.37	561.77	269.62	134.44	69.12	49.28	20.99	12.44	7.78	5.26
240	240	240		2302.57	1165.82	569.95	278.79	141.25	70.60	55.56	23.60	13.53	9.37
240	240	480			2387.11	1163.34	576.29	288.13	142.08	75.37	57.33	24.36	14.90
240	480	480				2314.18	1141.05	585.53	283.22	149.53	80.80	59.24	27.63
480	480	480					2367.99	1204.88	592.13	305.63	162.97	85.47	66.98
MPI + OpenMP + topology													
120	120	120	549.17	262.83	131.94	65.97	49.04	17.84	9.85	6.53	4.23	2.56	2.25
120	120	240	1125.37	561.52	271.08	133.87	70.23	49.66	18.22	11.10	7.28	4.37	3.06
120	240	240	2247.47	1117.46	566.45	274.94	137.27	68.26	49.48	20.98	12.30	7.61	5.30
240	240	240		2278.33	1148.40	584.24	289.53	140.43	70.42	54.47	23.14	13.17	9.29
240	240	480			2298.72	1164.64	594.57	290.60	141.66	75.35	56.98	23.72	14.92
240	480	480				2323.60	1180.71	594.29	282.45	149.46	80.24	58.40	27.61
480	480	480					2383.30	1191.96	590.37	303.45	161.87	83.82	65.62

TABLE 4. Speed-up on IBM Blue Gene/P.

n_x	n_y	n_z	nodes										
			1	2	4	8	16	32	64	128	256	512	1024
MPI code													
120	120	120	1.00	2.11	4.38	9.15	14.09	35.75	69.87	129.82	230.43	435.96	594.70
120	120	240	1.00	2.03	4.26	8.75	18.46	27.54	70.88	132.86	235.95	465.97	646.38
120	240	240	1.00	2.02	4.06	8.42	18.73	36.82	55.95	135.78	250.18	482.82	687.72
hybrid version													
120	120	120	2.95	6.12	12.26	24.67	33.13	88.97	164.03	246.49	372.85	621.32	734.01
120	120	240	2.88	5.86	11.88	24.23	48.42	66.82	177.45	293.02	438.55	723.49	1074.37
120	240	240	2.92	5.98	11.72	24.41	48.96	95.23	133.57	313.66	529.22	846.59	1250.99
MPI + OpenMP + topology													
120	120	120	2.96	6.18	12.31	24.61	33.11	90.99	164.79	248.77	383.74	634.30	722.66
120	120	240	2.89	5.78	11.98	24.26	46.25	65.40	178.28	292.73	446.31	743.00	1062.03
120	240	240	2.93	5.89	11.62	23.94	47.95	96.44	133.02	313.68	534.95	865.49	1242.42

MPI/OpenMP code. Furthermore, we synchronized the decomposition of the computational domain into sub-domains with the topology of the compute nodes in the Blue Gene connectivity network. In such way the communication time in the parallel algorithm is minimized.

In the near future, it is our intention to consider and compare the performance of this algorithm to other efficient methods for solving of the time dependent Stokes equation.

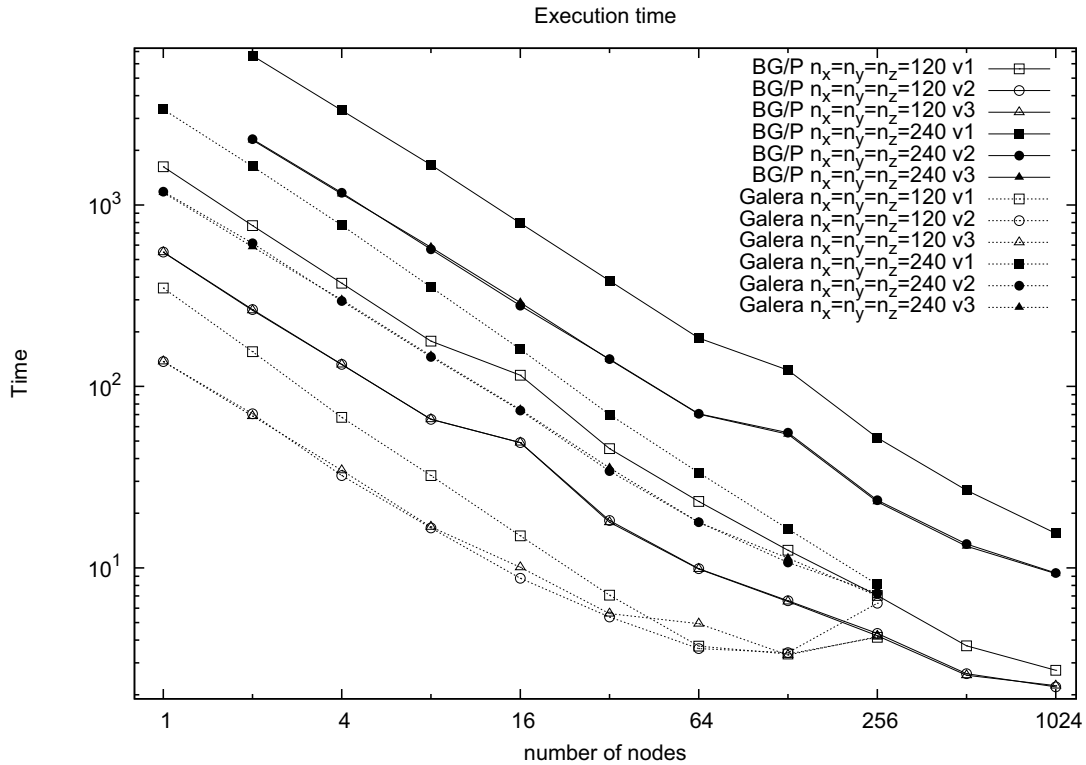


FIGURE 1. Execution time for 3D problem, $n_x = n_y = n_z = 120, 240$, v1 means MPI code, v2 — MPI + OpenMP, v3 — MPI + OpenMP + Cartesian topology functions

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