3D LID DRIVEN CAVITY FLOW BY MIXED BOUNDARY AND FINITE ELEMENT METHOD

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Abstract. A numerical algorithm for the solution of the velocity-vorticity formulation of Navier-Stokes equations is presented. This formulation results in splitting of fluid flow into its kinematic and kinetic aspect. The Boundary Element Method (BEM) used for the solution of flow kinematics results in an implicit calculation of vorticity values at the boundary, whereas all transport equations are solved using Finite Element Method (FEM). The combination of both numerical techniques is proposed in order to increase the accuracy of computation of boundary vorticities, a weak point for a majority of numerical methods when dealing with velocity-vorticity formulation. Since the application of BEM results in fully populated system matrices, also the flow kinematics computation is done by combining BEM and FEM, the latter for computation of internal velocities, keeping the CPU time and computer storage requirements at the level close to Finite Element Method. To speed up the computation process and to distribute storage of integrals over several processors the algebraic parallelization of kinematics was performed. Lid driven flow in a cubic cavity was computed to show the robustness and versatility of the proposed numerical formulation. Results for Reynolds number value Re=100 and Re=1000 show good agreement with benchmark results.

1 Introduction

The velocity-vorticity formulation of the Navier-Stokes equations is gaining attention due to several advantages over other formulations, most notably primitive variables formulation, especially due to the absence of pressure term in the vorticity transport equation and accurate description of transport phenomena of higly vortical turbulent flows. However, there are several drawbacks of the formulation, most notably the problem with accurate computation of vorticity values at the solid walls and the high computational cost due to the solution of three transport equations for vorticity field. In this paper, the solution to the first problem, computation of boundary vorticity values, is solved by applying the Boundary Element Method to the solution of flow kinematics equation. In the field BEM-FEM numerical simulation with velocity-vorticity formulation of Navier-Stokes equations the contributions were made by Young et al. [1], where BEM was used to obtain boundary velocities and normal velocity fluxes implicitly and then explicitly the internal velocities and boundary vorticities were computed by derivation of kinematic integral equations. Slightly different approach was used by Brown and Ingber [2] and Brown et al. [3] where internal velocities were computed using regular form of generalized Helmholtz decomposition and boundary conditions for vorticity transport equation were applied using vortex sheet strengths. Vorticity transport equation was solved with Galerkin FEM. Combined algorithm was also developed by Zunič et al. [4] for planar geometries, where the detailed comparison of different approaches to computation of internal velocities was presented. In this contribution we develop the 3D boundary element integral representation of flow kinematics, with the vorticity values as unknowns in the system of equations, thus allowing the implicit computation of the boundary vorticity values, also on the solid walls. Since the application of the BEM technique to the solution of other transport equations including computation of internal velocities in flow kinematics, would lead to problems with computer memory requirements, the FEM was selected as approximation method for this part of the governing equations.

In the following, the derivation of integral representations of governing equations, using BEM and FEM, is explained, since these equations represent the starting point for discretisation and numerical solution. This is followed by explanation of parallel solution strategies for problems with large memory demands of the BEM part of computational algorithm. The contribution ends with the presentation of computational results for the 3D lid driven cavity flow.

2 Velocity-Vorticity formulation of Navier-Stokes equations

The dynamics of a viscous incompressible fluid flow is partitioned into its kinematic and kinetic aspect through the use of derived vector vorticity field function, see Škerget *et al.* [5] and Ravnik *et al.* [6].

Vorticity $\omega_i(r_j, t)$ is defined as a curl of the velocity field $v_i(r_j, t)$

$$\vec{\omega} = \vec{\nabla} \times \vec{v}, \qquad \vec{\nabla} \cdot \vec{\omega} = 0, \tag{1}$$

resulting in the following elliptic Poisson equation for the velocity vector

$$\nabla^2 \vec{v} + \vec{\nabla} \times \vec{\omega} = 0. \tag{2}$$

Vorticity kinetics is governed by vorticity transport equation, which is obtained as a curl of momentum equation and may be, in the case of incompressible viscous fluid flow, written as

$$\frac{\partial \vec{\omega}}{\partial t} + (\vec{v} \cdot \vec{\nabla})\vec{\omega} = (\vec{\omega} \cdot \vec{\nabla})\vec{v} + \nu\nabla^2\vec{\omega} .$$
(3)

We seek a solution of equations (2) and (3) in the domain Ω , which satisfies the initial conditions

$$\vec{v} = \vec{v}_0, \ \vec{\omega} = \vec{\omega}_0 = \vec{\nabla} \times \vec{v}_0 \quad \text{at } t = 0$$
(4)

and the boundary conditions

$$\vec{v} = \vec{v}_{\Gamma}, \ \vec{\omega} = (\vec{\nabla} \times \vec{v})|_{\Gamma} \quad \text{at } t \ge 0$$
(5)

on the boundary Γ of the domain Ω .

3 Boundary element integral representation of kinematics

The singular boundary integral representation of the kinematics can be formulated using the Green theorems for scalar functions or weighting residuals technique. The integral form of Poisson type equation (Wu and Thompson [7], Wrobel [8]) is used on the kinematic equation (2), yielding

$$c(\xi)\vec{v}(\xi) + \int_{\Gamma} \vec{v}(\vec{n}\cdot\vec{\nabla})u^{\star}d\Gamma = \int_{\Gamma} u^{\star}(\vec{n}\cdot\vec{\nabla})\vec{v}d\Gamma + \int_{\Omega} (\vec{\nabla}\times\vec{\omega})u^{\star}d\Omega, \tag{6}$$

with $u^* = u^*(\xi, S)$ denoting the elliptic Laplace fundamental solution, ξ is the source point on boundary Γ , S integration point in domain Ω (including Γ), $c(\xi)$ geometry coefficient and \vec{n} outward pointing normal to the boundary. Geometry coefficient can be generally computed as $\Theta/4\pi$, where Θ is the internal solid angle at point ξ in steradians. Laplace fundamental solution is

$$u^{\star}(\xi, S) = \frac{1}{4\pi r(\xi, S)},\tag{7}$$

where $\xi \in \Gamma$ is source point, $S \in \Omega$ is integration point and r distance between the source and the integration point.



Figure 1: Computational domain.

The final integral form of the kinematic equation, employing the derivatives of the fundamental solution, see also \check{S} kerget *et al.* [5] and Ravnik *et al.* [6], is

$$c(\xi)\vec{v}(\xi) + \int_{\Gamma} (\vec{\nabla}u^{\star} \cdot \vec{n})\vec{v} \, d\Gamma = \int_{\Gamma} (\vec{\nabla}u^{\star} \times \vec{n}) \times \vec{v} \, d\Gamma + \int_{\Omega} \vec{\omega} \times \vec{\nabla}u^{\star} \, d\Omega.$$
(8)

4 Finite element integral representations

In the computational algorithm, FEM will be used for the solution of transport equation as well as solution of velocity values away from boundary, in the interior of the computational domain.

In the case of flow kinematics, where FEM will be used for computation of internal velocity values, we derived the integral representation by following the Galerkin weighted residual method, Taylor and Hughes [9], Gresho and Sani [10], multiplying the equation (2) by the weighting function N and integrating it over the domain:

$$\int_{\Omega} N \,\nabla^2 \vec{v} \, d\Omega + \int_{\Omega} N \left(\vec{\nabla} \times \vec{\omega} \right) \, d\Omega = 0. \tag{9}$$

Next we apply Green's first theorem to the diffusion term to obtain a weak formulation of kinematic Poisson equation as

$$\int_{\Omega} \vec{\nabla} N \cdot \nabla \vec{v} \, d\Omega - \int_{\Gamma} N \left(\vec{n} \cdot \vec{\nabla} \vec{v} \right) \, d\Gamma - \int_{\Omega} N \left(\vec{\nabla} \times \vec{\omega} \right) \, d\Omega = 0.$$
(10)

Equivalent procedure can be performed to obtain weak formulation of vorticity transport equation. We multiply the equation (3) by the weighting function N and integrate it over the domain Ω , to obtain

$$\int_{\Omega} N \frac{\partial \vec{\omega}}{\partial t} \, d\Omega + \int_{\Omega} N \, (\vec{v} \cdot \vec{\nabla}) \vec{\omega} \, d\Omega = \int_{\Omega} N \, (\vec{\omega} \cdot \vec{\nabla}) \vec{v} \, d\Omega + \nu \int_{\Omega} N \, \nabla^2 \vec{\omega} \, d\Omega. \tag{11}$$

Replacing time derivative with first order backward finite differences approximation

$$\frac{\partial \vec{\omega}}{\partial t} = \frac{\vec{\omega} - \vec{\omega}_{\tau-1}}{\Delta t} \tag{12}$$

and applying Green's first theorem to the diffusion term, one can obtain a weak formulation of kinetic equation

$$\frac{1}{\Delta t} \int_{\Omega} N\vec{\omega} \, d\Omega + \int_{\Omega} N \, (\vec{v} \cdot \vec{\nabla}) \vec{\omega} \, d\Omega = \int_{\Omega} N \, (\vec{\omega} \cdot \vec{\nabla}) \vec{v} \, d\Omega$$
$$-\nu \int_{\Omega} \vec{\nabla} N \cdot \vec{\nabla} \vec{\omega} \, d\Omega + \nu \int_{\Gamma} N \, (\vec{n} \cdot \vec{\nabla} \vec{\omega}) \, d\Gamma + \frac{1}{\Delta t} \int_{\Omega} N \vec{\omega}_{\tau-1} \, d\Omega, \tag{13}$$

where Δt is the size of time step and subscript $\tau - 1$ denotes vorticity value in previous time step.

5 Parallel algorithm

Discretisation of the equation (8) followed by application of boundary conditions results in a system of linear equations Ax = b. System matrix A is fully populated and nonsymmetric.

In this system each row represents discretised equation that belongs to one boundary node. With the division of the matrix rows over the several processors we divide the boundary into equally sized patches.

System of equations divided between available processors is solved using a iterative solver with diagonal preconditioning.

There are four basic matrix and vector operations used in each iteration of iterative solver that need to be adopted for parallel execution:

1) matrix-vector product $\{y\} = [A]\{x\}$: prior to the multiplication the communication step (data exchange) is requested where the non-local data from vector x are obtained.

$$\{x\}^G = \text{allgatherv}(\{x\}^L)$$

$$\{y\}^L = [A]^L \{x\}^G ,$$
(14)

where subscript G and L means the global and local part of data;

2) vector update $\{y\} = \{w\} + \alpha\{x\}$: there are only local element by element operations present and no communication is needed

$$\{y\}^{L} = \{w\}^{L} + \alpha\{x\}^{L}; \qquad (15)$$

3) scalar (dot) product $\alpha = \{y\}^T\{x\}$: at first only local parts of vectors are multiplied and local sum is calculated and second all partial sums are summed together and global sum is sent to all processors (allreduce)

$$\alpha^{L} = \{y\}^{TL} \{x\}^{L} , \qquad (16)$$

$$\alpha^G = \text{allreduce}(\alpha^L) ; \tag{17}$$

4) preconditioning step $\{y\} = [Q]\{x\}$: when using a diagonal preconditioning only local part of operations occurs and no communication is needed

$$\{y\}^{L} = [Q]^{L} \{x\}^{L} .$$
(18)

With those four operations the iterative solver can be executed in parallel. For the data exchange the MPI message passing library was used [11].

6 Computational algorithm

First, the kinematic equation (8) is discretised using boundary element method and then rearranged to give boundary vorticities. We use the elliptic Laplace fundamental solution. Domain discretisation is obtained using 8 node trilinear domain cells, while boundary discretisation is obtained using 4 node bilinear boundary elements. Discretisation procedure of partial differential equation leads to the system of linear equations with fully populated non-symmetric matrix. This system is solved either directly with LU decomposition or iteratively with BiCGSTAB(L) iterative solver, Sleijpen and Fokkema [12], with diagonal preconditioning.

The kinematic equation (10) written in terms of internal velocities and kinetic equation (13) are discretised using finite element method. The finite element part is implemented using Galerkin weighted residual method. Boundary and domain interpolation functions were the same as for boundary element method. Discretisation procedure of partial differential equation leads to sparse system of linear equations. Matrices are stored in compressed row storage (CRS) form and are solved using BiCGSTAB(L) iterative solver with incomplete LU (ILU) preconditioning.

The solution algorithm can be described as follows:

- 1. Initialize parallel environment and divide boundary.
- 2. Choose initial velocity (\vec{v}_0) field, compute initial vorticity $(\vec{\omega}_0)$ field using equation (1), set initial time level $\tau = 0$, set initial nonlinear iteration level i = 0.
- 3. Compute local part of BEM integrals and FEM integrals. Form local BEM system matrix.
- 4. Time loop, $\tau := \tau + 1$.
- 5. Nonlinear iteration loop, i := i + 1.
- 6. Flow kinematics:
 - (a) Solve equations (8) by BEM for boundary vorticities, using internal vorticities from previous nonlinear iteration step (form local RHS vector and run parallel iterative solver).
 - (b) Solve equations (10) by FEM for domain velocities, using new boundary vorticities to form right hand side vector. It is also possible to use explicit BEM calculation, however this requires calculation and storage of a large number of integrals. Due to limited computer memory, we used FEM instead.
- 7. Flow kinetics, vorticity transport:
 - (a) Solve equations (13) by FEM for domain vorticities, using the new velocity field to evaluate convection contribution and use boundary vorticities from kinematics as boundary conditions.
 - (b) Use underrelaxation $0 < \phi \leq 1$ for computing new domain vorticity values $\vec{\omega}_{i+1} := \phi \vec{\omega}_{i+1} + (1-\phi) \vec{\omega}_i$.

- 8. Check convergence:
 - (a) Compute $error = ||\vec{\omega}_{i+1} \vec{\omega}_i||_2 / ||\vec{\omega}_{i+1}||_2$.
 - (b) If *error* is greater then predefined ε go to step 5.
- 9. Finish time loop:
 - (a) Store time step values $\vec{\omega}_{\tau} = \vec{\omega}_{i+1}, \ \vec{v}_{\tau} = \vec{v}_{i+1}$.
 - (b) If time step τ is less than maximum number of time steps NT go to step 4.
- 10. End of computation.

7 Parallel results

As a test example the lid driven flow in a cubic cavity was used. The Reynolds number value was defined on cavity size and was chosen Re = 100. Mesh nodes was equally distributed and the mesh size was $16 \times 16 \times 16$, which gives in total 4913 nodes. The total amount of memory storage for integrals was 245 MB.

NPR	CPU [s]	SPD	EFF
Integration			
1	346.24	1.00	1.00
4	86.15	4.02	1.00
8	47.95	7.22	0.90
16	24.50	14.13	0.88
Right hand side			
1	65.22	1.00	1.00
4	18.37	3.55	0.89
8	7.14	9.13	1.14
16	3.35	19.47	1.22
Solver			
1	86.16	1.00	1.00
4	23.60	3.65	0.91
8	12.44	6.93	0.87
16	10.32	8.35	0.52

Table 1: Speedup and efficiency factors. NPR is number of processors, CPU processor time in seconds, SPD speedup factor (SPD = CPU(1)/CPU(NPR)) and EFF efficiency factor (EFF = SPD/NPR).

In the Table 1 cpu times are presented for different number of processors. It can be observed that integration as well as right hand side vector formation are well parallelized operations since there is no need for any communication. The only source of efficiency loses is imbalance between domain sizes. In case of RHS vector formation we can observe a superlinear speedup, which can be explained with better usage of processor cache due to smaller vector sizes. Efficiency of the solver is gradually decreasing due to increased amount of communication.

8 Lid driven cavity

In our computation we used a cubic cavity with the edge size L = 1. The Reynolds number is based on the cavity's edge size and the top lid velocity, $Re = v_x L/\nu$, and was selected to be Re = 100 and Re = 1000. The mesh size used were $8 \times 8 \times 8$, $16 \times 16 \times 16$ and $32 \times 32 \times 32$ elements, all with maximum to minimum element length ratio of 8, with elements clustered near the walls.

Velocity boundary conditions were:

- z = 1: moving wall $(v_x = 1, v_y = v_z = 0)$,
- x = 0, x = 1, y = 0, y = 1, z = 0: no slip $(v_x = v_y = v_z = 0)$.

Prescribed convergence criterium for nonlinear iterations was $\varepsilon = 1 \cdot 10^{-6}$. Test case with Re = 100 was computed with time step $\Delta t = 2$ and underrelaxation factor $\phi = 0.2$, test case with Re = 1000 was computed with time step $\Delta t = 0.2$ and underrelaxation factor $\phi = 0.2$. For the prescribed time step size on the finest mesh test case with Re = 100needed 15 time steps to reach steady state and for Re = 1000, 375 time steps.

Both test cases were computed with initial conditions of $v_x = v_y = v_z = 0$. Prescribed tolerance for iterative solver was $\varepsilon_{slv} = 10^{-6}$. Results were compared to the results of Yang *et al.* [13].



Figure 2: Isosurface of magnitude of velocity $|\vec{v}| = 0.13$ for different Reynolds number values, Re = 100 left and Re = 1000 right.



Figure 3: Velocity vectors on center-planes for different Reynolds number values.

Figure 2 shows isosurfaces of absolute velocity $|\vec{v}| = \sqrt{v_x^2 + v_y^2 + v_z^2} = 0.13$ for different Reynolds number values. It can be seen, that the high speed core of the fluid becomes narrower with the increasing of the Reynolds number value.

Figure 3 shows comparison of velocity vectors on center-planes for different Reynolds number values.



Figure 4: Streamtraces for Re = 1000.



Figure 5: Velocity profiles along centerlines for different mesh sizes, Re = 100 top left, Re = 400 top right and Re = 1000 bottom.

It can be seen that in the z - y planes a pair of vortices appear near the centerline of the cavity and move out towards the lover corners as the Reynolds number increases. Additional two vortices appear in the top corners at Re = 1000. In the x - y plane fluid at first flows uniformly backwards and with the increasing of the Reynolds number value two vertical vortices appear. Similar behaviour of the velocity field was reported also by Yang *et al.* [13] and Wong and Baker [14].

Streamtraces are presented in figure 4 and qualitatively agrees well with the results of Li *et al.* [15].

The quantitative evaluation of the results is shown in figure 5, where we compare the v_x velocity along x = y = 0.5 centerline and v_z velocity along y = z = 0.5 centerline for different mesh sizes and different Reynolds number values. The mesh refinement shows that the coarsest mesh is too coarse, although it gives qualitatively reasonable results. The finest two meshes are in close agreement with the benchmark solution of Yang *et al.* [13].

9 Conclusions

The 3D BEM-FEM approach to the numerical solution of Navier-Stokes equations in velocity-vorticity formulation was presented. It consists of implicit calculation of boundary vorticities by means of Boundary Element Method and calculation of vorticity transport by means of Finite Element Method. For the computation of internal velocities the approach of solving the implicit system of equations, resulting from the Finite Element Method discretisation of elliptic Poisson velocity equation was used. Parallelisation of flow kinematics computation was done in order to speed-up the computations. Numerical testings of the algorithm on the 3D lid driven cavity flow for Re=100 and Re=1000 showed, that the proposed combination of BEM and FEM is an accurate computational tool for the numerical solution of 3-D incompressible Navier-Stokes equations.

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