Parallel algorithms of implicit coupling in fluid-structure interaction problems*

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Abstract. The partitioned approach in fluid-structure interaction problems makes it possible to perform computations in fluid and structure independently of each other with implicit coupling at the interface boundary. Implicit coupling between physical problems involves solving a nonlinear interface system of equations. The article deals with quasi-Newtonian algorithms for solving nonlinear systems of equations. Comparison of efficiency is shown for solving fluid-structure interaction problems with different degrees of nonlinearity.

Keywords: Parallel computing · HPC · Fluid-structure interaction · Quasi-Newtonian methods · Nonlinear systems.

1 Implicit Coupling Schemes

The problems of numerical simulation of the interaction between a deformed solid and a fluid are actual. This is due to the development of methods, algorithms and computer systems. Fluid-structure interaction (FSI) problems are complex, as they require a joint solving both the equations of solid dynamics and the equations fluid dynamics.

Partition approach [1] of the solving FSI problems allows each problem to solve independently by the most appropriate method with using own parallelism model.

In this case, the system of equations of fluid dynamics is solved by arbitrary Lagrangian-Eulerian finite-volume methods within OpenFOAM [2]. Parallelization is carried out using MPI. The problem of deformation of a solid is solved by a finite-element packet FEStudio [3]. Within FEStudio, the stages of solving the problem are paralleled based on OpenMP and CUDA.

Fluid-structure interaction problem at the time $t + \Delta t$ with strong coupling approach in operator form is a solving of a nonlinear system ($\mathcal{N}$) and it is wrote as follows:

$$^{t+\Delta t}\mathbf{u}_S = \mathcal{S} \circ \mathcal{F}\left(^{t+\Delta t}\mathbf{u}_S^{(k+1)}\right),$$

where k — iteration number of the interface system solving on step Δt, $\mathcal{S}$ — dynamic problem of the solid mechanics, $\mathbf{u}_S$ — its solution, $\mathcal{F}$ — fluid dynamics problem.

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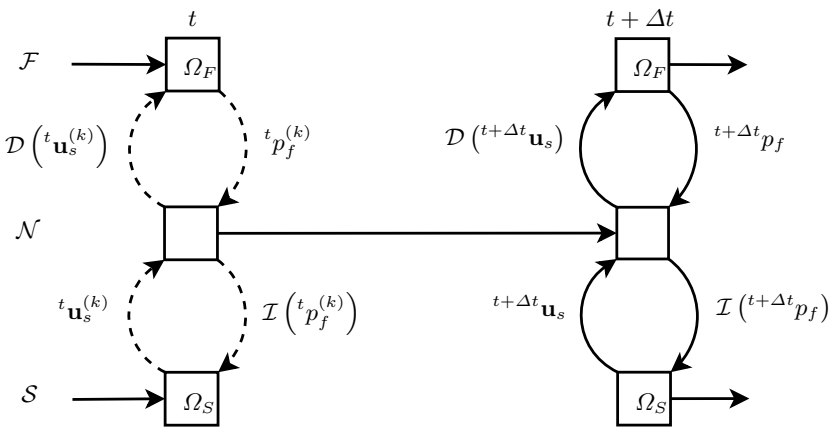

Fig. 1. Algorithm of the solving FSI problem in strong coupling approach

Matching solutions on interface border of two physical problems can be of two types: weak and strong. In the case of strong matching, several exchange are used on each integration time step. This provides a stronger couple between approximate solutions of physical problem. With this matching, a nonlinear interface system of equations must be solved (operator $\mathcal{N}$, fig. 1).

Usually, the solving of the nonlinear interface system of equations is carried out by classical iterative methods such as method of the fixed-point iterations with acceleration, Gauss-Seidel method or methods of Newtonian and quasi-Newtonian type. In this article, different quasi-Newtonian methods of the solve nonlinear systems are considered as well as ways to reduce computation effort and ways parallelizing the algorithm are represented.

Minimizing of costs on the solving interface system is achieved on the one hand through the use of effective algorithm for solving nonlinear systems of the equation (this reduce the number of arithmetic operations), on the other hand cutting computation time by parallelizing the operations of the algorithm.

2 Algorithms for solving the interface system

Each application of FSI program model uses own parallel model, an independent parallel implementation of the numerical methods and algorithms, and own requirements for a parallel execution environment. Therefore, the solving of the interface nonlinear system should be based on the reduction of the dependent components intended for solving physical problems. Based on the limitations associated with the independence of methods for solving problems in various physical domains, in this paper we consider several methods that satisfy these constraints: the fixed-point iteration method with the Anderson acceleration [4] and quasi-Newton methods (the Gauss-Seidel method and the generalized Broyden method).

As opposed to the Gauss-Seidel method, the generalized Broyden method is characterized by rapid convergence. Also, it use a several previous solutions for approximation of the Jacobian. This algorithms are described in [5,6].

Algorithm 1: Fixed-point iteration algorithm with Andersen acceleration

$u^{(k)} = u_0,\ m^{(k)} = 0,\ m^{max} > 0$
$u^{(k+1)} = \mathcal{S} \circ \mathcal{F}\left(u^{(k)}\right)$
$R^{(k)} = u^{(k+1)} - u^{(k)}$
while $||R^{(k)}||_2 > \varepsilon$ **do**
  $k = k + 1$
  $g^{(k)} = \mathcal{S} \circ \mathcal{F}\left(u^{(k)}\right)$
  $G^{(k)} = (g^{k-m^{(k)}}, \ldots, g^{(k)})$
  $f^{(k)} = g^{(k)} - u^{(k)}$
  $F^{(k)} = (f^{k-m^{(k)}}, \ldots, f^{(k)})$
  Compute QR factorization for $F^{(k)}$:
  if *k=1* **then**
    $F^{(1)} = QR,\ Q = f^{(0)}/\|f^{(0)}\|_2,\ R = \|f^{(0)}\|_2$
  if *k>1* **then**
    $F^{(k)} = QR$, where Q and R update as follows:
    for $i = 1$ *: $m^{(k)}$-1* **do**
      $R(i, m^{(k)}) = Q(\cdot, i)^T * f^{(k-1)}$
      $f^{(k-1)} = f^{(k-1)} - R(i, m^{(k)}) * Q(\cdot, i)$
    $Q(\cdot, m^{(k)}) = f^{(k-1)}/\|f^{(k-1)}\|_2,\ R = \|f^{(k-1)}\|_2$
  $\alpha = R^{-1} * Q^T * f^{(k)}$
  $u^{(k+1)} = \mathcal{S} \circ \mathcal{F}\left(u^{(k)}\right) - G^{(k)} * \alpha$
  $R^{(k)} = u^{(k+1)} - u^{(k)}$

Let's consider in more detail algorithm of the fixed-point iteration method with Anderson acceleration, adapted to the solving of the fluid-structure interaction problem (Algorithm 1). The most costly part of this algorithm is solving of the problem of minimizing the functional. Its solves by the least squares method, based on the QR factorization with the decomposition obtained by the Householder reflections.

The convergence rate of algorithms was compared on the tests systems presented in the work [7]. Obviously, the convergence depends both on the initial approximation and on the parameters used in the algorithms (the value of the relaxation parameter ω, the number of solutions used for the Jacobian approximation, etc.). In a number of systems, it was not possible to achieve significant convergence results for any of the considered algorithms and variations of their parameters (see (1)). This is primarily due to the high stiffness of the system of

equations (as a rule these are systems with logarithmic and exponential functions and their variations).

$$\text{Test 209} \qquad f_i = \begin{cases} x_i^2 - i, & i = 1; \\ x_{i-1}^2 + \ln(x_i) - 1, & i = \overline{2,n}. \end{cases} \qquad \text{Test 210} \qquad f_i = e^{\cos(i \sum_{k=i}^{n} x_k)},\ i = \overline{1,n}. \tag{1}$$

On the systems that are close in stiffness to the interface systems obtained in FSI problems (see (2)), a high rate of convergence showed by algorithm based on the fixed-point iteration method with Anderson acceleration. Thus, with the size of the problem is 10^3 equations, the error of the solution compose less then 10^{-8} for the test system "Test 212", based on this algorithm, was obtained in 8 iterations, based on the Gauss-Seidel method for 79 iterations, and the accuracy obtained by the Broyden method for 1000 iterations is about 10^{-2}.

$$\text{Test 202} \qquad f_i = \begin{cases} x_i - 0.1\, x_{i+1}^2, & i = \overline{1,n-1}; \\ x_i - 0.1\, x_1^2, & i = n. \end{cases} \qquad \text{Test 212} \qquad f_i = \begin{cases} x_i, & i = 1; \\ \cos(x_{i-1}) + x_i - 1, & i = \overline{2,n}. \end{cases} \tag{2}$$

An estimate of the rate of convergence for the "Test 202" system showed: the Anderson acceleration method – 5 iterations, the Gauss-Seidel method – 75 iterations, the Broyden method – 13 iterations.

Let's consider possibilities of parallelization of the considered algorithms. Let us compare the total time spent on solving the interface system of equations by the example of solving FSI with different degrees of nonlinearity.

3 Parallel effectiveness of algorithms and numerical simulations

In the considered algorithms, vector computations occupy a significant part. Parallelizing vector calculations such as multiplying a vector by a scalar, adding and subtracting vectors, dot product, the assignment operation involves using a loop over vector elements, which naturally allows them to be parallelized using OpenMP.

In the Anderson acceleration algorithm (Algorithm 1), QR factorization is constructed, this process is the most costly operation of this algorithm. However, the feature of the Anderson acceleration algorithm lies in the fact that the size of the matrix $F^{(k)}$, the factorization of which must be constructed, increases by one for each iteration and does not exceed m^{max}. This feature allows us to replace the factorization procedure for the matrix $F^{(k)}$ on each iteration, whose complexity is of the order of $O(2/3m^3)$ for the recalculation of the matrices Q and R (Algorithm 1, the line 10 – 13) whose complexity is $O(2m)$. Thus, the formation of the matrix $F^{(k)}$ and its decomposition into Q and R is carried out gradually, as the new components of the matrix $F^{(k)}$ are computed.

A comparison of the efficiency of the considered methods for solving a nonlinear system of equations was carried out on several problems with different stiffness. The first test problem describes the interaction of a nonstationary supersonic gas flow and a deformable cantilever in a shock tube. A detailed description of the problem, as well as the results of experimental and numerical studies can be found in [8,9].

Table 1 represents the number of iterations of the interface system solving, the average execution time of one iteration, and the total time of solving of one time step Δt.

Table 1. Average integration time of step Δt, $\rho_s/\rho_f = 7.8$

	Aitken acceleration	Time of iteration, s 1×thread	8×threads	Number of iterations	Total time, s 1×thread	8×threads
Gauss-Seidel	–	6.5	3.1	47	338.4	147.6
	+	6.9	3.2	42	310.8	132.2
Broyden	–	12.2	5.7	14	184.4	83.8
	+	12.5	5.9	13	175.5	85.3
Anderson	–	19.2	8.4	9	152.8	75.6

As can be seen from the Table 1, the use of Aitken's acceleration makes it possible to reduce the number of iterations, but increases the time spent per iteration due to additional vector computations. Despite this, a decrease of even one iteration reduces the overall solving time. The using of multithreading in vector operations also reduces the execution time of one iteration and the total time of the system solving. A small acceleration obtained with the use of eight OpenMP threads is explained by the small sizes of the vectors (about 10^3 equations).

In the second test, we considered the problem of interaction of flow of an incompressible viscous fluid flowing with a hollow cylinder fixed from two ends, described in detail in [10,11].

Table 2. Average integration time of step Δt, $\rho_s/\rho_f = 1.2$

	Aitken acceleration	Time of iteration, s 1×thread	8×threads	Number of iterations	Total time, s 1×thread	8×threads
Gauss-Seidel	–	16.8	4.1	50+	855.1	211.2
	+	17.3	4.4	50+	885.6	224.7
Broyden	–	17.7	3.9	36	651.6	147.3
	+	18.2	4.1	36	662.4	149.1
Anderson	–	28.1	6.9	19	533.9	131.1

The simulation results for the flow of an incompressible fluid flow in an elastic cylinder showed (Table 2) that the system solving based on the Gauss-

Seidel algorithm was carried out in more than 50 iterations. The system solving based on the generalized Broyden secant algorithm, when simulating the same problem, was performed on an average of 36 iterations. Despite the fact that the number of arithmetic operations in the Broyden algorithm is greater, reducing the total number of iterations leads to a reduction in the total computational time. Coupling based on the Anderson acceleration algorithm showed that, on average, the system solution was performed in 18–19 iterations. The acceleration obtained by using of eight OpenMP threads is about 4 times and more than 6 time from the Gauss-Seidel algorithm.

The considered algorithms for implicit coupling were used to numerical simulation of the physical experimental investigation of the interaction of the vibrating console plate with a layer of viscous liquid deposited on its surface [12]. Forced vibrations of a plate with a frequency of 4.5 kHz are excited by a piezoelectric element, with a cantilevered plate. The figure 2 a) shows the result of the experiment performed for the vacuum oil. At the excitation of vibrations, viscous liquids applied as a thin layer on the plate surface initially flow to the plate surface areas with the antinodes of vibrations taking a convex form. The coupled solution of the problems is carried out on hexahedral non-matching meshes with a size of 1300000 cells for the fluid dynamics problem and 23,000 cells for the dynamic problem of the solid.

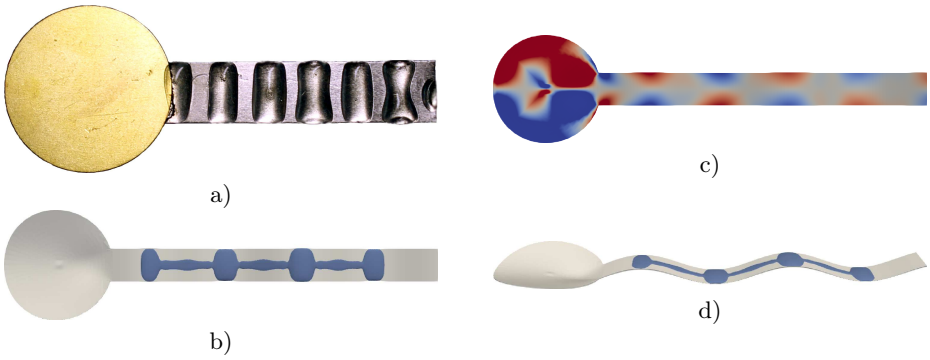

Fig. 2. a) the droplet of vacuum oil on the vibrating plate a) in one of the experiments described in [12], b) in numerical simulation; c) transverse distribution of displacement; d) longitudinal bending of the vibrating plate, at a scale of 20 in 1.

To describe the droplet dynamics, we used two immiscible incompressible fluids, the motion of each is described by the system of Navier-Stokes equations, with the conditions of dynamic equilibrium at the interface. The discretization is based on the use of the Volume of Fluid method [13]. To determine the dynamics of the interface boundary and its geometric characteristics solves the transfer equation for a scalar indicator function α be meaningful of volume concentration. Differential operators approximation is performed by the finite volume method using the front artificial compression method to calculating the α field.

The elastodynamic problem is solved by the finite element method taking into account geometric and physical nonlinearity. It is important to note that the vibrations of a thin plate in the form of the superpositions of longitudinal (see Fig. 2 d)) and transverse (see Fig. 2 c)) waves allow obtaining stable droplet patterns (see Fig. 2 b)) which cannot be formed on an underformed substrate.

The computational complexity of the fluid-structure interaction problem is determined by solving physical problems of the solid dynamics and, for the most part, solving the hydrodynamic problem. The solution of the elastodynamic problem is carried out by the explicit integration scheme, which ensures high parallel efficiency. However, the low parallel efficiency of the algorithms used in solving the hydrodynamic problem has a significant influence both on the solution time and on the overall parallel efficiency. Therefore, schemes of implicit coupling, with a reduced number of iterations, based on Broyden's algorithms and Anderson's acceleration, show high efficiency and significantly reduced the time for the solution matching. At the same time, the simulation results showed well matching of the obtained solution with the experimental data.

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