An algorithm for fast DNS cavitating flows simulations using homogeneous mixture approach

A Žnidarčič¹, O Coutier-Delgosha¹, M Marquillie² and M Dular³
¹ Laboratoire de Mécanique de Lille, Boulevard Paul Langevin, 59655 Villeneuve d’Ascq, France
² Le Centre de Ressources Informatiques (CRI), Université de Lille 1, Cité Scientifique, 59655 Villeneuve d’Ascq, France
³ Laboratory for water and turbine machines (LVTS), Faculty of mechanical engineering, Askerčeva cesta, 1000 Ljubljana, Slovenia
E-mail: anton.znidarcic@ensam.eu

Abstract. A new algorithm for fast DNS cavitating flows simulations is developed. The algorithm is based on Kim and Moin projection method form. Homogeneous mixture approach with transport equation for vapour volume fraction is used to model cavitation and various cavitation models can be used. Influence matrix and matrix diagonalisation technique enable fast parallel computations.

1. Introduction
Cavitation-turbulence interactions raise many questions in cavitation research. Numerous experiments were performed to understand them better, with numerical work following and adding to the discoveries [1, 2].

Over the years, cavitation simulations improved significantly. Today, they are able to describe unstable [1, 2] or even compressibility effects [3]. Presently, the mostly used cavitation models utilise homogeneous mixture approach with incompressibly treated phases. Additional transport equation for vapour volume fraction is often introduced. Because of many simplifications in development of such models, and as RANS turbulence models normally accompany and interact with them, the accuracy of simulations with them is limited. Consequently also the possible models’ improvement and the knowledge about the mentioned interactions. To overcome this, cavitation-turbulence interactions in such simulations should be better analysed and DNS simulations seem a good tool for the task. There were some DNS simulations already performed, but their objectives were different [1, 2, 3] and their algorithms accepted only certain models [1, 2]. Therefore a new algorithm, capable of performing fast simulations with different models, is currently developed in our laboratory.

The aim of this paper is a brief description of the new algorithm. At first, the MFLOPS-3D code, representing a basis for our work, is described. Then, the new algorithm is presented through the equations, which up to now offered the most stable performance. At the end, some verification results are given.
2. MFLOPS-3D code

As intention is to use various cavitation models in computationally heavy simulations, a code capable of fast DNS simulations is needed. The MFLOPS-3D code performs fast DNS incompressible flow simulations and was therefore taken as a basis for our development. Here, a brief description of it follows and more information can be found in [4].

Governing equations solved in this code are non-dimensional Navier-Stokes continuity and momentum equations. Non-incremental form of Kim and Moin pressure correction projection method is used to form the algorithm. Simulations are performed in parallel, where influence matrix technique ensures continuity of solutions over whole domain, while systems of equations in sub domains are solved with matrix diagonalisation (eigendecomposition). As a result, the code solves only Helmholtz or Poisson equations which have constant left hand side. Consequently the most time consuming procedures of matrix diagonalisation and influence matrix technique are done only once, at the start of a simulation. Only a diagonal system of equations remains to be solved in each time step. All of this combined enables faster DNS simulations.

Code utilises structured and collocated grids. Spatial discretization is done with compact finite differences, while time derivatives are described with 2\(^{nd}\) order backward difference scheme (BDS). 2\(^{nd}\) order Adams-Bashforth scheme is used for some explicitly treated variables.

3. New algorithm for simulations of cavitating flow

3.1. The governing equations

Description of cavitation with homogeneous mixture approach uses Navier-Stokes momentum (1) and continuity (2) equations and transport equation (3) for vapour volume fraction \( \alpha \).

\[
\rho \left( \frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla) \vec{u} \right) = -\nabla p + \nabla \cdot (\mu (\nabla \vec{u}) + \mu(\nabla \vec{u})^T) - \frac{2}{3} \nabla (\mu (\nabla \cdot \vec{u})) \tag{1}
\]

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \tag{2}
\]

\[
\frac{\partial \rho_v \alpha}{\partial t} + \nabla \cdot (\rho_v \alpha \vec{u}) = S \tag{3}
\]

\( S \) in equation (3) is the source term, describing destruction or creation of \( \alpha \). It depends on pressure \( p \) and \( \alpha \). The relationship between the density \( \rho \) and viscosity \( \mu \) of the mixture and both present phases is given in equation (4). Subscripts \( v \) and \( l \) depict vapour and liquid phase.

\[
\rho = \alpha \rho_v + (1 - \alpha) \rho_l, \quad \mu = \alpha \mu_v + (1 - \alpha) \mu_l \tag{4}
\]

3.2. Developed algorithm for solving presented system of governing equations

Introduction of new governing equations demanded changes to the projection method in MFLOPS-3D code. The form of Kim and Moin method was retained, with the solution procedures for predictor velocity \( \vec{u}^* \) and intermediate variable \( \Phi \) heavily changed and additional step to obtain \( \alpha \) added. In this paper, only the most stable algorithm is described.

Firstly, \( \vec{u}^* \) is obtained. Equation for it is given in (5) and was, as in Kim and Moin method, developed from equation (1) by replacing \( \vec{u}^{n+1} \) in time derivative and viscous terms with \( \vec{u}^n \) [5].

\[
\left( \Delta - \frac{3\rho_l}{2\Delta t\mu_l} \right) \vec{u}^* = \rho^n - \frac{4\vec{u}^n + \vec{u}^{n-1}}{2\Delta t\mu^n} + \frac{\rho^n}{\mu^n} \left((\vec{u} \cdot \nabla)\vec{u} \right)^{n,n-1} - \frac{1}{\mu^n}(\nabla \mu^n) \cdot (\nabla \vec{u}^n) - \frac{1}{\mu^n}(\nabla \mu^n) \cdot (\nabla \vec{u}^n)^T - \frac{1}{3} \nabla (\nabla \cdot \vec{u}^n) + \frac{2}{3\mu^n} \nabla \mu^n (\nabla \cdot \vec{u}^n) + \frac{\nabla p^n}{\mu^n} + \left( \frac{3\rho^n}{2\Delta t\mu^n} - \frac{3\rho_l}{2\Delta t\mu_l} \right) \vec{u}_e^c \tag{5}
\]
Equation has many explicitly treated terms (n denotes time level and \( n, n-1 \) use of Adams-Bashforth scheme). To lower their amount and provide constant left hand side, Concus and Golub method (CG) is used [6]. This gives the last term on the right hand side of equation (5) and demands iterative steps until \( \bar{u}^n \) and its explicit value \( \bar{u}^n_e \) converge. Pressure term is included as the most stable procedure is based on pressure incremental form of projection method.

\( \Phi \) is solved next. Its equation is the difference between equations (1) and (5) and is given in equation (6) in most stable form (form, with \( \rho \) included in \( \Phi \), is also possible). Solving for \( \Phi \) proved to be the most difficult part and was specially formed because of the code’s demand for the constant left hand side. After applying divergence to equation (6), the unknown \( \nabla \cdot \bar{u} \) is, as in [7], replaced with \( S(1/\rho_v - 1/\rho_l) \), where \( S \) is linearised. The best solutions are obtained if \( S \) is linearised in regards to \( p \) and \( \alpha \), giving multiple terms including pressure change \( dp \) (also used in \( \partial S/\partial \alpha \)). \( dp \) is replaced with \( \phi \) using \( p-\Phi \) connection in equation (7). Finally, by using CG method again, this leads to more implicit and stable solving for \( \Phi \). Equation for \( \Phi \) solution is given in equation (8), where \( \sigma \) is the constant introduced by the CG method. The equation is solved until \( \Phi \) converges.

\[
\frac{3p}{2\Delta t}(\bar{u}^{n+1} - \bar{u}^n) = -\nabla \Phi
\]  

\[
p^{n+1} = \Phi + \mu \left( S \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right) - \nabla \cdot \bar{u}^n \right) + p^n
\]  

\[
(\Delta + \sigma) \Phi^{k+1} = -\frac{3}{2\Delta t} \left( (\bar{u}^k - \bar{u}^n) \cdot \nabla \rho^n + \left( \left( S^n + \frac{\partial S}{\partial \rho} dp + \frac{\partial S}{\partial \alpha} d\alpha \right) \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right) - \nabla \cdot \bar{u}^n \right) \right) + \sigma \Phi^k
\]

\( k \) in equation (8) denotes iteration level. \( \bar{u}^{n+1} \) is updated after each solution using equation (6). In linearised term \( S \), only \( \Phi \) values change between iterations, while \( S \) as a whole is updated with converged \( \Phi \). Next step is the solution of \( \alpha \) equation. This is solved in each point separately, as it cannot be reshaped into Helmholtz equation. Equation (9), obtained from equation (3), is used for this. Iterative steps are performed, in which \( \alpha^{n+1} \) and \( S^{n+1} \) are updated, \( k \) again denotes iteration level. Finally, \( \rho \) and \( \mu \) are updated using equation (4).

\[
\alpha^{n+1,k} = \frac{S^{n+1,k-1}}{\rho_v} + \frac{\alpha^n}{\Delta t} \left( \bar{u}^{n+1} \cdot \nabla \right) \alpha^{n+1,k-1} - \frac{1}{\Delta t} + S^{n+1,k-1} \left( \frac{1}{\rho_v} - \frac{1}{\rho_l} \right)
\]

Boundary conditions, especially for \( \Phi \), are an important factor. For \( \Phi \), MFLOPS-3D code originally uses von Neumann boundary conditions. These are unsuitable for cavitation as they impose compatibility condition for \( \Phi \). Mixed boundary conditions were implemented instead, in form of Dirichlet boundary condition as pressure value on the exit (using \( \Phi \) gave unstable simulations) and von Neumann conditions elsewhere. Boundary conditions for \( \bar{u}^n \) follow same logic as those in the original code, while \( \alpha \) demanded use of Dirichlet conditions.

4. Verification results
The algorithm was mainly tested with a verification procedure using the Method of Manufactured Solutions [8]. Analytical equations describing the flow with variable density and corresponding source term \( S \) were developed to see if the systems of governing equations are solved correctly. It was found that the algorithm indeed produces correct results. To test its limits, we compared it with an algorithm using Dirichlet boundary conditions for \( \Phi \), enabling ideal stability. It was found out that both algorithms have same stability. The only difference was in the speed, with the ideal conditions making the code faster by roughly 30 %.

An example of solutions, obtained with the presented algorithm, and comparison with analytical values, is given on figure 1. In this case, the range of \( \alpha \) was \( \alpha = \{0;1\} \) and \( S \) was
taken as $S = -\rho v \alpha p$. Used domain was a cuboid with $x \in \{-0.2; 0.2\}$ m, $y \in \{-0.2; 0.2\}$ m and $z \in \{-0.1; 0.1\}$ m. It was split into four sub domains, two in $x$ and two in $y$ directions. Grid was non-uniform with 41 points in $x$, $y$ directions and 11 points in $z$. 1800 time steps with increment $\Delta t = 0.014$ s were performed.

**Figure 1.** Comparison of analytical (above) and calculated (below) results for, from left to right, $u, v$ velocity, pressure $p$ and $\alpha$ at $z = 0$ m.

Results show very good agreement of analytical and calculated values. This case is actually limiting case still stably solved with described settings (coarser grid or longer time step result in unstable simulations). Errors were estimated using time averaged $L^2$ norm, where squares of the differences between analytical and computed values were divided (averaged) by number of points in the domain. Reported errors magnitudes are $10^{-3}$ for velocities, $10^{-1}$ for pressure and $10^{-2}$ for $\alpha$. Convergence tests show that MFLOPS-3D code with presented algorithm can reach 2nd order accuracy. In case of incompressible flow tests (original code), a bit better convergence is achieved, but accuracy still tends to 2nd order. This is mainly a consequence of using 2nd order BDS for time derivatives. We therefore conclude the algorithm is ready for real flow simulations.

5. Conclusion
A new algorithm for fast DNS cavitating flow simulations is presented. The algorithm is constructed to enable use of different cavitation models and it has proven to be able to solve the system of governing equations correctly. The algorithm will next be tested in real flow cases, which has not yet been done because of high CPU demands.

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