Development of Fluid-Structure Interaction Program for the Mercury Target

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JAERI is developing the liquid mercury target as a neutron scattering experiment facility. The liquid mercury target is planned to receive MW class proton pulse beam and high intensity spallation reactions occur in the target generating neutrons. Under such condition, high density heat is released and consequently strong pressure wave is generated. It is considered that the pressure wave propagates through mercury and reflects on the container of target made of hard stainless steel, and the erosion of the wall might be caused by the cavitation. In fact, some experiments show that pit type scratch is created on the wall when strong pressure wave reflects on it. If the phenomenon happens in mercury target, it makes the life span of container shorter. Since the pressure wave propagation and the wall deformation have influence with each other in this phenomenon, a coupled simulation study is needed in order to reveal the process of the scratch generation. In this report, a simulation of the interaction between the pressure wave propagation of the liquid mercury and the wall deformation is carried out in order to investigate the possibility of the cavitation in the mercury target. In particular, we propose a method in which the bubble dynamics model is linked with the so-called weakly coupled method between the fluid model and the solid model. In particular, we propose a method in which the bubble dynamics model is linked with the so-called weakly coupled method between the fluid model and the solid model. In our project of the year 2004, the fluid-structure interaction program was developed for the fine meshes of the mercury target, for example, 10 million grid points. The large scale model was applied to simulate the interaction between the pressure wave propagation and the wall deformation.

Keywords: mercury target, neutron scattering, wall deformation, coupled simulation, fluid-structure interaction

1. INTRODUCTION

As a plan of the high power proton accelerator project, a mercury target used for a neutron source in a high intensity neutron scattering laboratory will be constructed. The structure of the mercury target is a pipe-like channel made of SUS316 as depicted in Fig. 1 and liquid mercury circulates inside the channel. Protons come from the perpendicular direction to the flow channel and collide with mercury atoms. Then the mercury emits neutrons due to a nuclear fission caused by collisions with protons, and high density energy release by the nuclear fission causes strong shock waves within the mercury target. Furthermore a recent experiment in the shock wave reflection at the liquid-solid interface reveals that the inside of the outer wall suffers fine damage due to the cavitation created after the deep impact by the shock wave into the wall. This research is to simulate the interaction among three physical phenomena such as pressure wave propagation, wall deformation and bubble dynamics in a mercury target in order to investigate the possibility of the cavitation in the mercury target.

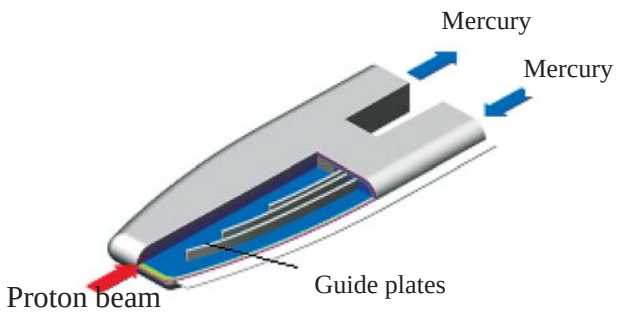

Fig. 1 Overview of the mercury target

2. SIMULATION MODELS

2.1. Fluid model

In our fluid program, the finite volume method is adopted in order to simulate dynamics of compressible thermal fluids. The mercury target geometry is discretized by a regular grid with three dimensional generalized coordinate. The

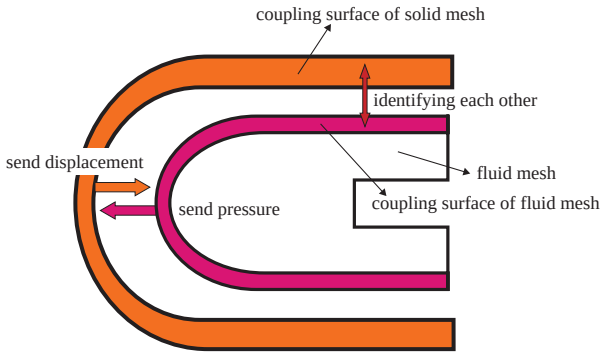

Fig. 2 Coupling surfaces of fluid and solid meshes

advective term is differenciated with three kind of algorithm such as the first order upwind scheme, the central difference scheme and the TVD scheme. The time integration is carried out by the HSMAC scheme and the BiCGSTAB iterative solver is implemented for solving the Poisson's equation for pressure. The complete set of equations are composed of the mass, the kinetic momentum and the energy conservation equations with the equation of state for liquid mercury. These basic equations can realize the phenomena in the mercury target.

2.2. Solid model

For dynamics of elastic solids, the finite element method is adopted in order to simulate dynamics of elastic solids. The geometry of the wall of the mercury target container is discretized by isotropic shell element with four nodes. The lumped mass matrix is adopted and the explicit time marching can be carried out by the central difference method. This solid model is described by the elastic body equation and kinetic boundary condition and geometric boundary condition.

2.3. Weakly coupling

In order to evaluate the effect of the interaction between the pressure wave propagation and the wall deformation, so called weakly coupling method is adopted here. The fluid program receives the displacements of nodes at the target wall from the solid program. After that, metrics of the generalized coordinate such as Jacobian and boundary flow velocity are renewed. On the other hand, the solid program receives the pressure of meshes near the target wall from the fluid program. The solid program transfers the pressure at the wall into the nodal loads. Such data communications between the fluid program and the solid program are executed every time step. These procedures are all implemented by the standard MPI libraries.

2.4. Bubble Dynamics Model

For the case of the radial motion of a bubble, an equation accounting approximately for the liquid compressibility was given by Keller in the following form as shown in [1] and [2].

$$\left(1-\frac{\dot{R}}{c}\right)R\ddot{R}+\frac{3}{2}\dot{R}^2\left(1-\frac{\dot{R}}{3c}\right) =\left(1-\frac{\dot{R}}{c}\right)\frac{1}{\rho_L}\left[p_B(t)-p_S\left(t+\frac{R}{c}\right)-p_\infty\right]+\frac{R}{\rho_L c}\frac{dp_B(t)}{dt} \quad (1)$$

where R is the radius of a bubble and ρ_L is the density of a host liquid and p_S is the nonconstant ambient pressure component and p_B is the liquid pressure on the external side of the bubble wall, which is related to the internal pressure by

$$p(t)=p_B(t)+\frac{2\sigma}{R}+4\mu_L\frac{\dot{R}}{R}.$$

The internal pressure p and temperature T of a bubble are described by the following equations.

$$\dot{p}=\frac{3}{R}\left\{(\gamma-1)K\frac{\partial T}{\partial r}\bigg|_{r=R}-\gamma p\dot{R}\right\}, \quad (2)$$

$$\frac{\partial\tau}{\partial t}+\frac{\gamma-1}{\gamma pR^2}\left(\frac{\partial\tau}{\partial t}-\frac{\partial\tau}{\partial t}\bigg|_{y=1}y\right)\frac{\partial\tau}{\partial t}-D\dot{p}=\frac{D}{R^2}\Delta\tau, \quad (3)$$

where γ, K, D and y is the ratio of the gas specific heats, the thermal conductivity, the gas thermal diffusivity and the normalized distance of the bubble wall respectively and $\tau=\int^T K(\theta)d\theta$. Three equations above are calculated by the Runge-Kutta integration scheme.

For the coupling simulation between the pressure wave and the bubble dynamics, the local fraction of volume occupied by the bubbles is introduced at every cell.

$$\beta(t)=\frac{4}{3}\pi nR(t)^3, \quad (4)$$

$$\alpha(t)=1-\beta(t), \quad (5)$$

where β is the local volume fraction of bubbles, α is the local volume fraction of liquid, n is a number of the bubbles per unit volume and R is the radius of the representative bubble. As shown in Fig. 3, a bubble cloud in a cell is represented by one bubble which is the mean of all bubbles in the cell. At every cell, the radial motion of the representative bubble is calculated by the Keller equation. Then, by substituting $\rho = \alpha\rho_L$ into the mass conservation equation, the effect of the bubbles is linked with the mass conservation

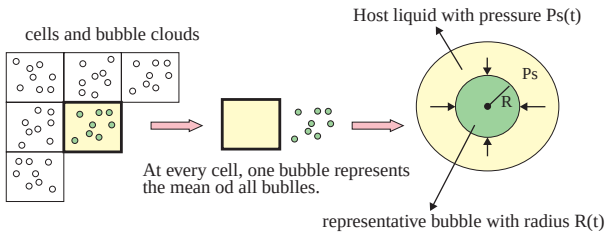

Fig. 3 Interaction between pressure wave propagation and bubble dynamics

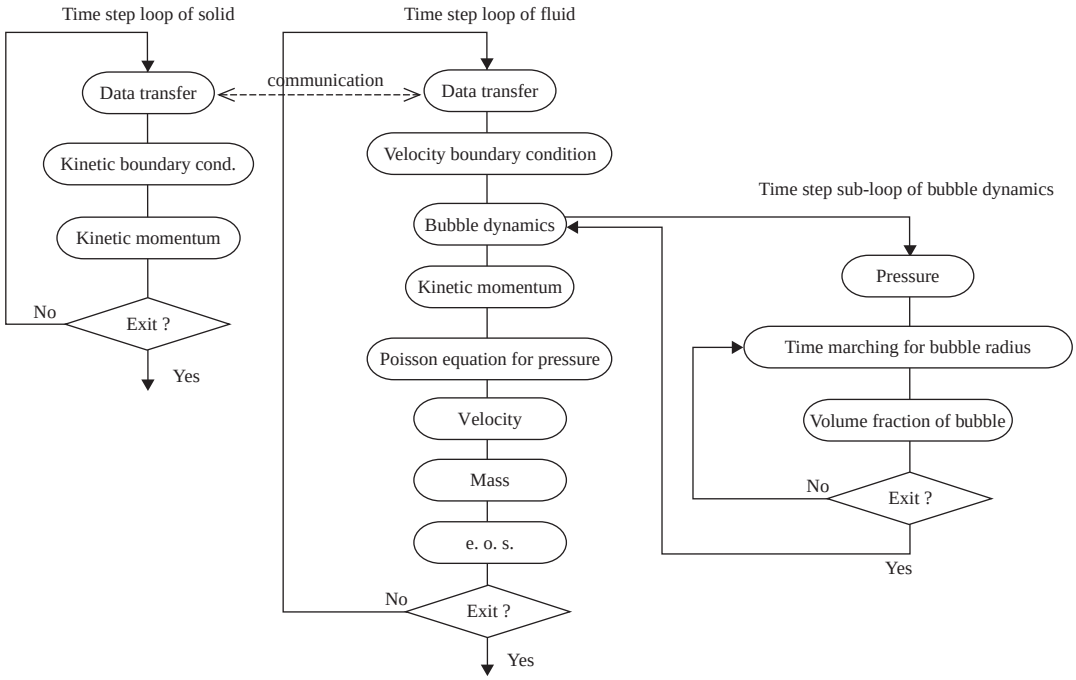

Fig. 4 Flow chart of our coupling procedure

equation as follows.

$$\frac{\partial(\rho_L|J|)}{\partial t}=\frac{1}{\alpha}\left\{-\sum_{k=1}^{3}\frac{\partial(\rho|J|U_k)}{\partial\xi_k}+4\pi n\rho_L|J|R^2\dot{R}\right\}. \quad (6)$$

The second term in the right hand side above is corresponding to the effect of the bubble dynamics.

Now, a relation between the time step loop for the fluid model and the time step loop for the bubble dynamics model should be mentioned here. As shown in the flow chart of our coupling procedure above (Fig. 4), the time step loop for the bubble dynamics model is nested within the time step loop for the fluid model. In other words one time step for the fluid model is divided into some substeps for the bubble dynamics model. And the bubble dynamics model receives the pressure p_S of a host liquid from the fluid model every time step and calculates the radial motion of a bubble by the Keller equation during its substeps and sends the volume fraction of bubbles to the fluid model. Then the fluid model moves its time step forward.

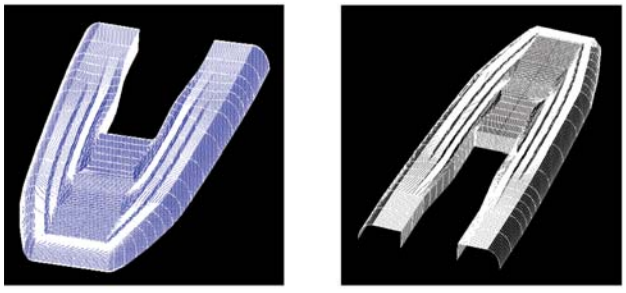

Fig. 5 Fluid mesh (left) and solid mesh (right)

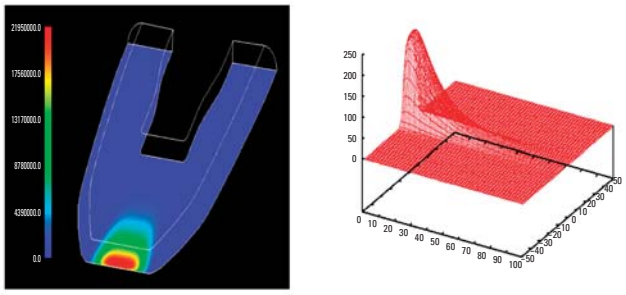

Fig. 6 Initial pressure distribution (left) and initial heat distribution (right)

3. COUPLED SIMULATION

The fine meshes of the mercury target were generated. Fig. 5 shows the mesh of fluid with 100,000 cells and the mesh of solid with 10,000 nodes. First of all, we started with a coupling simulation during 2.0 msec. to grasp a rough tendency of the interaction between pressure wave propagation and wall deformation in a mercury target. Here, the coarse meshes of fluid with 60,000 cells and of solid with 5,000 nodes were used in order to reduce the calculation time. Fig. 6 shows the iniail pressure distribution and initial heat distribution respectively.

Since the speed of the elastic wave in the wall is about 5,000 m/sec. and the speed of sound of liquid mercury is about 1,400 m/sec. and minimum mesh size is about 1.0mm, time step interval was set to be 1.0e-7sec. by the Courant number criteria.

By receiving high pressure, the target wall was deformed. Fig. 7 shows the wall deformations of x, y and z-directions respectively after 0.1 msec. In particular, the beam window,

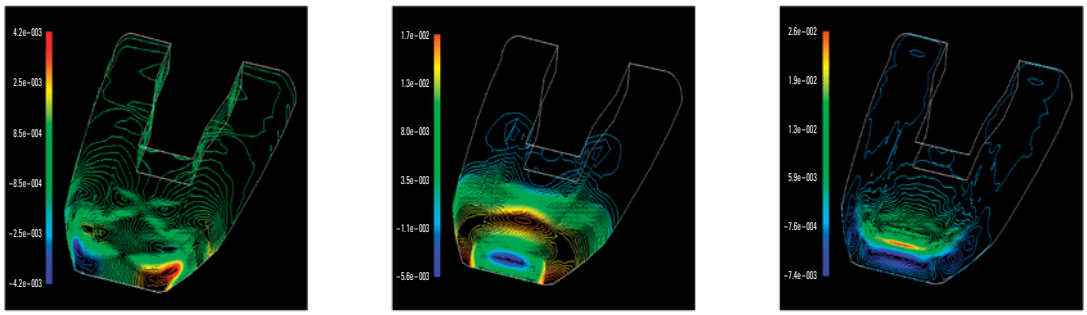

Fig. 7 Wall deformation after 1.0e-4 sec. (x-direction, y-direction and z-direction)

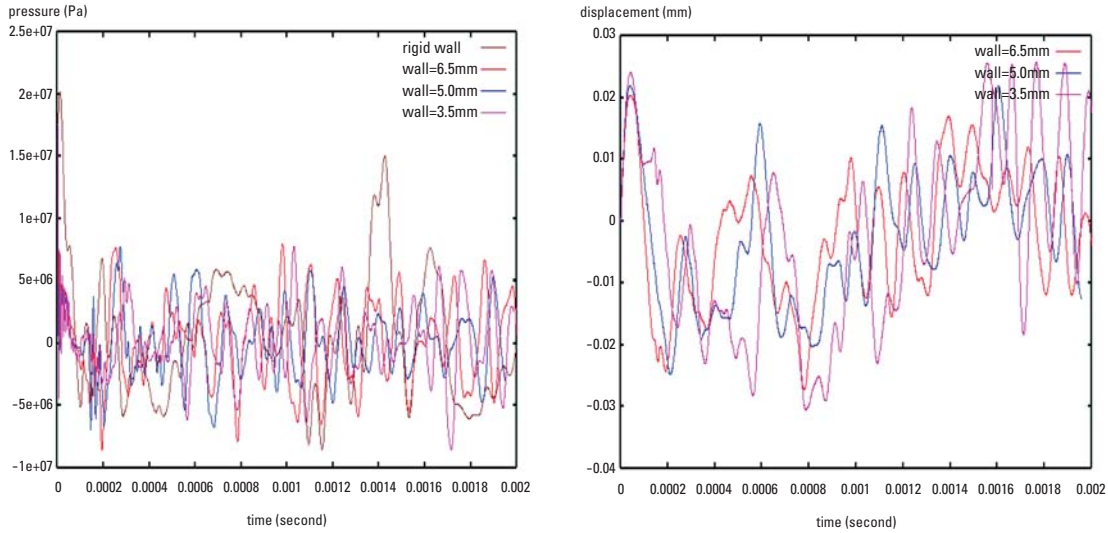

Fig. 8 Time histories of the pressure near the wall (left) and the displacement at the wall (right).

which is the front part of the wall, had the largest deformation.

By changing such parameter as thickness of the target wall, comparisons of the simulation results were performed. Fig. 8 shows the time histories of the pressure near the beam window and the displacement of the wall for 2.0 msec. Each line of colors in Fig. 8 means the difference of the wall thickness. By taking account of the deformation of the target wall, pressure near the beam window seems to be reduced rapidly immediately after the start of the simulation. In order to investigate the rapid reduction of pressure in more detail, only the first 2,000 steps are calculated in more cases of wall thickness. Here, the fine meshes of fluid with 120,000 cells and of solid with 7,500 nodes were used.

Furthermore, the finest meshes of fluid with over 1,000,000 cells were applied on the Earth Simulator in order to evaluate performances for the parallelization and the vectorization. The parallelization is implemented by the domain decomposition method and the vectorization is implemented by taking the vector length as long as possible. In particular, the Jagged diagonal storage, which is a storage format of matrix elements, was adopted in the solid program by using PARCEL (Parallel Computing Elements) which is a mathematical library for parallel computing developed by CCSE / JAERI. As a result, mean vectorized operation ratio of the fluid-structure program exceeds over 98% and vectorized ratio is beyond 0.97, where the fluid domain is decomposed into 32 blocks, 56 blocks and 64 blocks for 32 CPU's, 56 CPU's and 64 CPU's respectively.

Next, a simulation of the interaction among pressure wave propagation, wall deformation and bubble dynamics was carried out since the result above implies the possibility of the cavitation. From the preliminary simulation above, it is known that the time step interval for the coupling simulation between the pressure wave and the bubble dynamics needs to be chosen to be very small. So, the time step interval of the fluid model and the substep interval of the bubble model were set to be 1.0e-8 sec. and 1.0e-9 sec. respectively. Hence the bubble dynamics model was only introduced into some fluid meshes near the target wall, and coarse meshes of fluid with 30,000 cells and of solid with 4,000 nodes were used in order to shorten the calculation time.

Now, by changing such parameters as an initial bubble radius and an initial number of bubbles, the dependence of the initial amount of bubbles were investigated. As shown in Table 1, four cases with the different initial radius of bubble

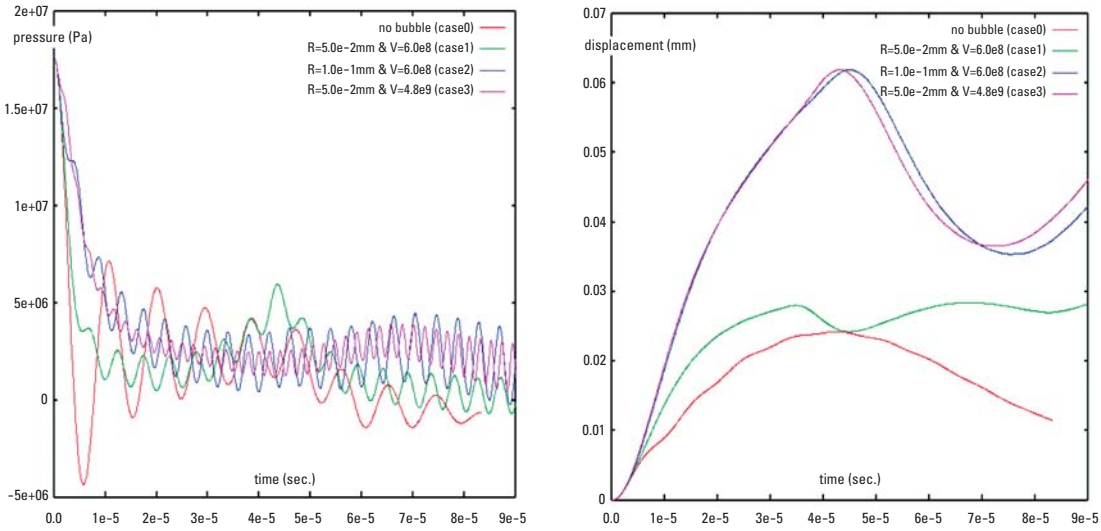

Fig. 9 Time histories of the pressure near the wall (left) and the displacement at the wall (right)

Table 1 A comparison of the initial conditions for bubbles

case	initial radius	number of bubbles	volume fraction
case0	—	no bubbles	0.00 %
case1	5.0e-2 mm	6e8	0.03 %
case2	1.0e-1 mm	6e8	0.25 %
case3	5.0e-2 mm	4.8e9	0.25 %

and the different initial number of bubbles were done. Fig. 9 shows time histories of the pressure near the wall and the displacement at the wall. Comparing the case of no bubbles (case 0) with the case that bubbles exist (case 1, 2, 3), it turns out that pressure reduction has become weaker and pressure value remains positive in the case that bubble dynamics model is coupled. In fact, pressure reduction in the case with initial volume fraction of bubbles of 0.25% is smaller than in the case with initial volume fraction of bubbles of 0.03% or 0.0%. Moreover it was observed that the amplitude of the oscillation of pressure value in the case 2 is bigger than in the case 3. This shows that the effect of the bubble radius is stronger than the effect of the bubble number. These results imply the necessity to take the coupling of bubble dynamics model into consideration in order to investigate the process of pressure reduction near the wall exactly. [3, 4]

4. SUMMARY

The coupling simulation among three physical phenomena such as pressure wave propagation, wall deformation and bubble dynamics in a mercury target was carried out. As results, it was found that the wall deformation causes a rapid reduction of pressure near the wall and that a negative pressure is reached there in the case that the wall thickness is smaller than 5.0 mm. Moreover it was observed that the pressure reduction becomes weaker and pressure value remains positive in the case that bubble dynamics model is coupled. From these results, it can be said that the coupling of bubble dynamics model is required in order to investigate the process of pressure reduction near the wall exactly.

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水銀ターゲットにおける液体水銀の圧力波伝播と容器壁の変形挙動と気泡成長の相互作用のシミュレーション

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核破砕タイプの高密度中性子源である水銀ターゲットの流れを、流体と構造の連成で大規模シミュレーションすることにより、その強度設計支援や、液体水銀内部で起こる現象を把握しターゲットの使用可能期間を延ばすことを可能にする定量的データを取得した。

本研究は日本原子力研究所と高エネルギー加速器研究機構が共同で開発している核破砕タイプの高密度中性子源である水銀ターゲットの開発に関するもので、最終目的は、水銀ターゲットの強度設計支援や、液体水銀内部で起こる現象を把握しターゲットの使用可能期間を延ばすことにある。シミュレーションに必要なデータは、設計を担当しているグループから提供を受け、有効な計算結果が得られた場合、その結果は設計担当グループに還元され利用される。中性子散乱実験は、たんぱく質の精密な構造決定など、科学の様々な分野で利用されるもので、より高密度の中性子源の開発が待たれている。水銀ターゲットの開発はその要望に答えるもので、特に、ターゲットの使用可能期間延長という目的のためには、地球シミュレータでなければ不可能な大規模な計算が必要となる。

これまでに開発したTVDスキーム組込み流体解析コードと構造解析コードとの弱連成コードに、新たにキャビテーションの挙動に関するマクロモデルを組み込み、液体水銀の圧力波伝播とターゲット容器壁の変形挙動と気泡成長の相互作用をシミュレーションすることで、容器壁面上の圧力変動を評価し、エロージョンとの関係を解析した。

連成コードに新たにキャビテーションの挙動に関するマクロモデルを組み込み、高速化したコードが正常に動作することを確認した。キャビテーションの導入によって、圧力波の伝播に遅延が生じ、またピーク高さが変化することを確認した。図1はキャビテーションが発生し、そのボイド率の変化による挙動の系統的な変化を示し、合理的な連成計算が実行されたことを意味する。なお、1000万メッシュ規模の問題を地球シミュレータで40+1分割（流体40、構造1分割、キャビテーション壁面1層）で計算し、ベクトル演算率が97.4%、並列化率が98.9%というパフォーマンスを得た。

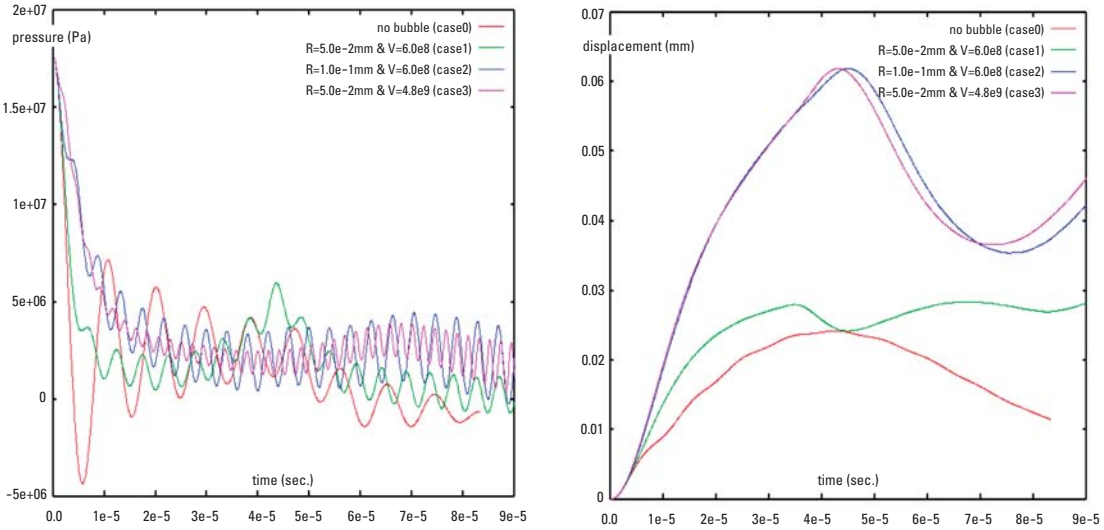

Fig. 1 キャビテーションが存在する場合の壁面近傍の圧力と変位の時間変化

キーワード：水銀ターゲット，核破砕，連成解析，キャビテーション