AN ELEMENTARY STUDY OF SPH-BASED SIMULATIONS FOR FREE SURFACE FLOWS WITH GRAVITY AND COMPRESSIBILITY EFFECTS IN CYLINDRICAL CONFINEMENT

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ABSTRACT

The design of nuclear pressure vessel requires the description of various dynamic effects, among which fluid-structure interaction. In some configurations, gravity effects (in the low frequency range) and compressibility effects (in the high frequency range) are of paramount importance and have therefore to be accounted for. The present paper is concerned with the description of free surface flows with gravity and compressibility effects, using a SPH (Smoothed Particle Hydrodynamics) method in circular confinement, with expected applications to the dynamic analysis of auxiliary nuclear component for naval propulsion. For the system under concern, the range of dynamic solicitation extends from low frequency (for seismic analysis of grounded prototype) to high frequency (for shock analysis of embarked reactors); it is therefore of particle interest to employ a numerical techniques which allows the description of linear and non-linear free surface effects, which can be expected in both cases. SPH method gives promising perspective for simulation of sloshing flows in various configurations; the present paper investigates the use of such a technique in the context of three-dimensional problems with cylindrical confinement.

INTRODUCTION

The design of nuclear pressure vessel requires the description of various dynamic effects, among which fluid-structure interaction. Many numerical methods can be employed to tackle fluid-structure interaction, some of which have been investigated by DCNS in the context of propulsion systems, in particular as far as nuclear propulsion is concerned [1-3]. In some configuration, coupling of an elastic structure with free surface flows has to be considered; this is the case in particular for some auxiliary nuclear component for naval propulsion reactors. Validation of fluid-structure interaction simulations can be performed on an elementary test case. The proposed test case, which is represented in Fig. 1, is representative of the structure under concern, yet sufficiently simple to allow for straightforward simulation using either numerical [4] or semi-analytical methods [5]. Validation of a coupled fluid-structure simulation with CFD-CSD numerical

procedures has been for instance performed on this configuration (see [6] and Fig. 2).

Fig. 1. An elementary test case for validation of coupled fluid-structure semi-analytical/numerical simulations

Fig. 2. Coupled fluid-structure simulation of the test case problem with CFD-CSD numerical procedure with VOF modeling of the fluid free surface [2]

As far as free surface fluid flows are concerned, CFD computations with VOF method are commonly resorted to for industrial applications. However, alternative approaches can be employed for free surface flows: it can be of particle interest to employ numerical techniques which allow the description of linear and non-linear free surface effects. SPH method gives promising perspective for simulation of free surface flows in various configurations.

Ecole Centrale de Nantes/HydrOcean have some years experience in the development and application of SPH-based methods for various industrial applications [7-10]. Applicability of the SPH method to tackle fluid-structure interaction is considered in the paper through SPH-based simulation on DCNS elementary test case depicted in Fig. 1. In such context, the present aims at evaluating various features of the SPH method – among which computational cost, and numerical precision – in order to perform coupled fluid-structure simulations on industrial problems [11]. The present study has to be understood as a first step in DCNS appropriation of the SPH method for future coupled simulations of FSI in the context of nuclear propulsion reactors. In this first step, simulation of a fluid problem solely is considered; coupled fluid-structure simulations will be addressed in future studies.

The paper is organised as follows: general principles of the SPH method are recalled in the first section; main features of the SPH code employed in the present – namely the SHP-Flow code, jointly developed and validated by Ecole Centrale de Nantes and HydrOcean – are presented in the second section; application of the SPH method on the test case is considered in the third section; comparison between simulation of free surface flow with non-linear SPH-based method and linear FEM-based method (using DCNS finite element code whose main features are recalled in appendix), are proposed in the last section.

1. SPH METHOD FOR FLUID FLOW SIMULATION

SPH is a particle method which can be used to solve the Navier-Stokes equations through a convolution-based discretisation [12]. This meshless and Lagrangian scheme is particularly well-fitted for complex free surface flow problems, involving high dynamics phenomena with strong non-linearities [13]. Note that viscous effects are neglected in the present paper, so that the equations to be solved reduce to the following Euler equations:

$$\mathbf{v} = \frac{d\mathbf{x}}{dt} \quad (1)$$

$$\frac{d\mathbf{v}}{dt} = \mathbf{g} - \frac{1}{\rho} \nabla p \quad (2)$$

$$\frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{v} \quad (3)$$

Note that, various SPH implementations exist for fluids, with compressible and incompressible formulation namely. In this paper, the compressible SPH method is used, in order to take

into account any compressible effects of liquids. This requires a specific equation of state to close the above set of equations. In order to approach the actual behaviour of water, the following Tait's equation of state is used:

$$p - p_o = \frac{\rho_o c_o^2}{\eta} \left(\left(\frac{\rho}{\rho_o} \right)^\eta - 1 \right) \quad (4)$$

where ρ_o , p_o and c_o correspond respectively to the nominal mass per unit volume, the reference pressure and the nominal speed of sound, and $\eta = 7$. Note that the use of the physical speed of sound of water ($c_o = 1,500$ m/s) leads to its actual compressible behaviour. But note also that for a wide range of applications where compressibility effects are negligible, the sound speed is often chosen low enough to limit the CPU time imposed by the CFL condition related to sound wave propagation, while respecting the weak-compressibility condition $M_a < 0.1$ everywhere in the fluid domain at anytime.

The main originality of the SPH method resides in the absence of mesh, providing a large flexibility. In this context, the interpolation of the differential operators applied to the pressure and velocity fields is achieved by a convolution of the discrete variables through a kernel function W :

$$f(\mathbf{r}) \approx \int_{\Omega} f(\mathbf{x}) W(\mathbf{x} - \mathbf{r}, h) d\Omega(\mathbf{x}) \quad (5)$$

where Ω is a compact spheroidal support for $\mathbf{x}$, and h its measure (smoothing length). The kernel function used in the model is a combination of cubic splines [12] defined as:

$$W\left(q = \frac{|\mathbf{r}|}{h}\right) = C \begin{cases} \frac{2}{3} - q^2 + \frac{q^3}{2} & 0 \leq q \leq 1 \\ \frac{1}{6} (2 - q)^3 & 1 \leq q \leq 2 \\ 0 & 2 < q \end{cases} \quad (6)$$

By extending (5) and by using integration by parts, the gradient of any function can be approximated applying:

$$\nabla f(\mathbf{r}) \approx \int_{\Omega} f(\mathbf{x}) \nabla W(\mathbf{x} - \mathbf{r}, h) d\Omega(\mathbf{x}) \quad (7)$$

in which the kernel gradient is known analytically. The surface integral neglected in (7) is zero inside the domain since the support Ω is chosen to be compact. Moreover, the above integrals are approached using the following quadrature formula:

$$\int_{\Omega} g(\mathbf{x}) d\mathbf{x} \approx \sum_i \omega_i g(\mathbf{x}_i) \quad (8)$$

where the subscript i refers to each interpolating point within the domain Ω . The weighting term ω_i corresponds to the discrete volume attributed to i , and evolves according to:

$$\frac{d\omega}{dt} = \omega \nabla \cdot \mathbf{v} \quad (9)$$

One can note from equations (3) and (9) that the product $\rho_i \omega_i$ remains constant, and corresponds to the mass of point i , justifying the concept of ‘particle’. Finally, the following SPH discretization for the Euler equation is applied [14] and integrated in time using a 4th order Runge-Kutta scheme:

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i \quad (10)$$

$$\frac{d\mathbf{v}_i}{dt} = \mathbf{g} - \sum_j m_j \frac{(p_i + p_j)}{\rho_i \rho_j} \nabla W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (11)$$

$$\frac{d\rho_i}{dt} = \rho_i \sum_j \frac{m_j}{\rho_j} (\mathbf{v}_i - \mathbf{v}_j) \nabla W(\mathbf{r}_i - \mathbf{r}_j, h) \quad (12)$$

Following Vila [15], it is possible to rewrite the SPH formalism in a slightly different manner inspired from the Finite Volume formalism. Following this process, the couples of particle to particle interactions (i, j) in equations (11) and (12) can be seen as the result of a flux acting at the middle of (i, j) , leading to:

$$\frac{dm_i}{dt} = -w_i \sum_j w_j 2\rho_E (\mathbf{v}_E - \mathbf{v}^o(\mathbf{x}_{ij})) \nabla W(\mathbf{r}_{ij}, h) \quad (13)$$

$$\frac{dm_i \mathbf{v}_i}{dt} = m_i \mathbf{g} - w_i \sum_j w_j 2(\rho_E \mathbf{v}_E \otimes (\mathbf{v}_E - \mathbf{v}^o(\mathbf{x}_{ij})) + p_E \mathbf{1}) \nabla W(\mathbf{r}_{ij}, h) \quad (14)$$

where $\mathbf{v}^o$ is a transport velocity, equal to the fluid velocity $\mathbf{v}$ in a Lagrangian framework and set to zero in an Eulerian framework. The terms ρ_E and $\mathbf{v}_E$ are the solution of the exact Lagrangian Riemann problem solved at the middle of each couple of particles i and j . Combined with the MUSCL (Monotone Upwind Centered Scheme for Conservation Law) extrapolation [16], this scheme provides some very stable and low-diffusive results, and appears as a very interesting alternative to the system (8) to (10). This scheme has been implemented in SPH-Flow, the 3D parallel SPH model developed by HydrOcean and Ecole Centrale Nantes, used in the present study.

2. SPH-FLOW SOFTWARE

2.1. Main features of the SPH-Flow solver

The research development of the solver *SPH-Flow* started seven years ago at Ecole Centrale Nantes, and led to the accomplishment of numerous PhD thesis and post-doctorates [7-9,17-18]. The main focus of these works targets the improvement of the accuracy of the solver (for example with Godunov-based scheme combined with MUSCL procedure, higher-order scheme [10], and the implementation of complex physical models such as fluid/structure interaction models. This platform is now a 3D parallel SPH solver with up to date pre- and post-processing capabilities, HydrOcean being responsible for its industrial development.

2.2. Parallelisation of the SPH-Flow solver

Due to the high sound speeds in the media to model (around 1500 m/s in water, and 5000 m/s in structures), the CFL condition leads to very small time steps, resulting in rather costly calculations. In order to decrease the CPU times, an efficient solution consists in the use of parallel calculations. The parallelization of SPH-Flow is based on a domain decomposition strategy, the inter-process communications being achieved via the MPI standard. The explicit feature of SPH provides lots of advantages concerning the parallelization of the model since each task is relatively independent from another, resulting in very nice parallelization performances. It is of interest to describe these performances through speed-up and efficiency of the parallelization, defined respectively as:

$$S_p(N) = \frac{t_{\text{ref}}}{t(N)} N_{\text{ref}} \quad (15)$$

$$E_r(N) = 100 S_p(N) / N \quad (16)$$

Considering a reference calculation time t_{ref} on a reference number of processes N_{ref} (in the present case, $N_{\text{ref}} = 2$), the speed-up $S_p(N)$ corresponds to the equivalent process number for N actual processes used, resulting in the calculation time $t(N)$. Thus a “perfect” speed-up would be obtained if $S_p(N) = N$ (corresponding to the black line in figure 1).

Figure 1 displays the result obtained for the present scalability study on up to 32 processes, for a calculation involving approximately 2×10^6 particles.

Fig. 3. Calculation speed-up for a problem involving 2×10^6 particles

This scalability study results in a calculation efficiency of about 80% on 32 processes, leading to a drastic computational time decrease [19].

3. APPLICATION TO A 3-D COMPRESSIBLE SLOSHING FLOW IN CYLINDRICAL CONFINEMENT

Application of the SPH method to calculate the fluid flow and the resulting fluid force on a rigid structure is considered within the framework of the elementary test case depicted in

Fig. 1. As recalled previously, this application is the first step of a collaborative study jointly undertaken by DCNS Propulsion and Ecole Centrale de Nantes/HydrOcean with the view to evaluating the applicability of SPH-based simulations for industrial application, for specific studies involving FSI. The free surface problem involves a cylindrical tank of radius $R'=0.2$ m and of height $L=1$ m. A central beam of radius $R=0.1$ m is fixed at the bottom of the tank, resulting in an annular liquid domain. As the study only focuses on fluid flow simulations, one will therefore consider in a first step that the internal elastic beam is fixed: in the test-case depicted in Fig. 1, boundary conditions are therefore those associated with a rigid wall (see Fig. 4 and appendix A). The annular space is filled with water ($\rho_o=1,000$ kg/m³), for which compressible effects are expected, defined by an imposed finite speed of sound c_o .

Fig. 4 Problem set-up in the SPH code

The quiescent column of fluid, of height $H=0.75$ m, is set into motion according to the following law of acceleration:

$$\gamma(t) = \begin{cases} \gamma_o \sin(2\pi t / \tau_o) & 0 \leq t \leq \tau_o \\ 0 & \tau_o \leq t \end{cases} \quad (15)$$

where $\gamma_o=500$ m/s² and $\tau_o=0.01$ s are the amplitude and duration of the imposed acceleration.

SPH simulations are performed with the SPH-Flow code (see previous sections); FEM computations on the same test-case are performed using 2D-axi symmetric finite element code, developed by DCNS (see [20] and appendix A). In the latter simulations, fluid gravity and compressibility effects are accounted for through linear equations.

Given the frequency range of interest in the case under study, compressibility effects are expected to be predominant on gravity effects; this poses no particular difficulties since the SPH and FEM approaches employed here are designed to tackle with compressibility effects

4. COMPARISON OF NON-LINEAR SPH-BASED SIMULATIONS AND LINEAR FEM-BASED SIMULATIONS

In the following SPH simulations, the SPH particles are initially set following a regular cylindrical distribution. The smoothing length (which corresponds to the space discretization parameter) is chosen as $h=0.006$ m, so that these calculations involve 600.000 particles.

Figure 5 compares the calculation of the fluid pressure force in the direction of the imposed acceleration obtained from the SPH-based and the FEM-based simulation.

Fig. 5. Fluid force on the inner structure (rigid and fixed beam). Comparison of SPH-based and FEM-based simulations

Fig. 6. Free surface deformations at time t=0 ms; t=2 ms; t=4 ms; t=6 ms; t=8 ms; t=10 ms

Note that, in the FEM-based simulation, the computed fluid force corresponds to an approximation of the continuous expression $\varphi(t) = -\int_0^{2\pi H} \int_0^1 p(R, \theta, t) R \cos \theta d\theta$ on a fixed fluid domain.

Figure 6 and 7 give a representation of the fluid free surface and a representation of the fluid pressure field at various time during the SPH-based simulation.

Fig.7. Visualisation of the SPH pressure field from time $t=0$ ms to $t=12$ ms

From the qualitative point of view, the SPH results suggest that the fluid response is largely dominated by the first symmetric fluid mode (modulation of the pressure field and free surface of $\cos\theta$ -type, see Eq. (g) in appendix A), as expected from the linear theory. However, a closer examination of the SPH results in terms of pressure field indicates that some secondary contribution of the lower order modes (of type $\cos 2\theta$, $\cos 3\theta$, etc...) are accounted for in the

simulation: this corresponds to three dimensional effects, which can result either from numerical and physical phenomenon. At this stage of the study, no significant explanation has been proposed to clarify this observation. This could also be one direction which would account for the discrepancy observed in the fluid force; Fig. 5 however indicated that wave propagation within the acoustic fluid cavity are accounted for by the SPH-simulation, at the expected acoustic frequency.

CONCLUSION

A numerical study on the dynamic behaviour of a fluid with free surface initially at rest in cylindrical confinement and subjected to an imposed dynamic loading has been reported in the present paper.

The proposed study aims at comparing SPH-based and FEM-based modelling of the considered problem, as a first step of a more general overview and benchmark of these numerical approaches for possible future industrial applications.

The proposed comparison yields good agreement between the two approaches from the qualitative point of view, although some questions have been raised from the quantitative point of view, as far as the fluid flow is concerned.

Fluid structure interaction simulation by coupling SPH (fluid) and FEM (structure) are also being tackle and yield quantitative agreement between FEM and SPH-based (fluid) simulations on the one hand and FEM FEM-based (fluid) simulations.

The study reported in the present communication corresponds to the initiation of a collaborative framework between ECN/HydrOcean and DCNS/Propulsion on the topic of fluid-structure interaction; ongoing studies aim at clarifying the qualitative interpretation of the SPH/FEM simulations in fluid as well as in fluid-structure interaction configurations.

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A. LINEAR FEM-BASED SIMULATIONS

FEM-based simulations are performed using a linear description of gravity and compressibility effects in the fluid problem. The governing equations of the dynamic problem are formulated in terms of pressure field in the fluid domain:

$$\frac{1}{c^2} \frac{\partial^2 p}{\partial t^2} - \Delta p = 0 \quad (a)$$

is the wave propagation equation which accounts for compressibility effects. The associated boundary conditions are formulated as:

$$\frac{\partial p}{\partial z} (z=0) \quad (b)$$

when considering the bottom as a rigid wall, and:

$$\frac{\partial p}{\partial r} (r=R) = \frac{\partial p}{\partial r} (r=R') = -\rho_o \gamma(t) \cos \theta \quad (c)$$

when considering the inner and outer surfaces as rigid wall subjected to the imposed acceleration.

The free surface condition can be described with or without gravity effects, that is:

$$p(z=h) = 0 \quad (d)$$

in the former case and:

$$\frac{\partial p}{\partial z} (z=h) = -\frac{1}{g} \frac{\partial^2 p}{\partial t^2} (z=h) \quad (e)$$

in the latter case.

The variational formulation of the fluid problem reads:

$$\begin{aligned} & \int_R^{R'} \int_0^{2\pi} \int_0^H \frac{1}{c^2} \frac{\partial^2 p}{\partial t^2} (r, \theta, z) \delta p(r, \theta, z) r dr d\theta dz \\ & + \int_R^{R'} \int_0^{2\pi} \frac{1}{g} \frac{\partial^2 p}{\partial t^2} (r, \theta, H) \delta p(r, \theta, H) r dr d\theta \\ & + \int_R^{R'} \int_0^{2\pi} \int_0^H \nabla p(r, \theta, z) \nabla \delta p(r, \theta, z) r dr d\theta dz \\ & = - \left(\rho_o \int_0^{2\pi} \int_0^H \delta p(R, \theta, z) R \cos \theta d\theta dz \right) \gamma(t) \end{aligned} \quad (f)$$

The discretization of the variational formulation is performed with a finite element approach. Since the coupled problem is geometrically axi-symmetric but the dynamic loading is non axi-symmetric, the pressure is expanded into a FOURIER serie as:

$$p(r, \theta, z) = p_0(r, z) + \sum_{s \geq 1} p_s(r, z) \cos(s\theta) + \sum_{a \geq 1} p_a(r, z) \sin(a\theta) \quad (g)$$

The 3D fluid problem (r, θ, z) is then turned into a 2D problem (r, z) . The two-dimensionnal fluid domain is meshed with four nodes linear finite element. Figure A gives a representation of the fluid reference element.

Fig. A. Linear 2D fluid finite element

The fluid shape functions are linear with respect to both local variables ξ, η :

$$N_i(\xi, \eta) = \frac{(1 + \xi_i \xi)(1 + \eta_i \eta)}{4} \quad (h)$$

The discretization of the integral form yields the mass and stiffness matrices:

$$\int_R^{R'} \int_0^{2\pi} \int_0^H \frac{1}{c^2} \frac{\partial^2 p}{\partial t^2} (r, \theta, z) \delta p(r, \theta, z) r dr d\theta dz \rightarrow \mathbf{\delta P}_s^T \tilde{\mathbf{M}} \mathbf{\ddot{P}} \quad (i)$$

$$\int_R^{R'} \int_0^{2\pi} \frac{1}{g} \frac{\partial^2 p}{\partial t^2} (r, \theta, H) \delta p(r, \theta, H) r dr d\theta \rightarrow \mathbf{\delta P}_s^T \overline{\mathbf{M}} \mathbf{\ddot{P}}_s \quad (j)$$

$$\int_R^{R'} \int_0^{2\pi} \int_0^H \nabla p(r, \theta, z) \nabla \delta p(r, \theta, z) r dr d\theta dz \rightarrow \mathbf{\delta P}_s^T \mathbf{K} \mathbf{P}_s \quad (k)$$

The final form of the dynamic problem is:

$$\mathbf{M} \mathbf{\ddot{P}}_s + \mathbf{K} \mathbf{P}_s = -\Gamma \gamma(t) \quad (l)$$

with $\mathbf{M} = \overline{\mathbf{M}} + \tilde{\mathbf{M}}$, $\mathbf{K} = \overline{\mathbf{K}} + s^2 \tilde{\mathbf{K}}$ and Γ standing for the boundary normal operator. The corresponding elementary matrices are defined by the following analytical expressions:

$$\bar{\mathbf{k}}(i, j) = ab r_0 \left[\frac{\xi_i \xi_j}{4a^2} \left(1 + \frac{\eta_i \eta_j}{3} \right) + \frac{\eta_i \eta_j}{4a^2} \left(1 + \frac{\xi_i \xi_j}{3} \right) \right] + \frac{a^2 \eta_i \eta_j}{12b} (\xi_i + \xi_j) \quad (m)$$

$$\tilde{\mathbf{k}}(i, j) = \frac{b}{8} \left[1 + \frac{\eta_i \eta_j}{3} \right] \times \left[2(\xi_i + \xi_j) - \frac{2r_0 \xi_i \xi_j}{a} + \left(1 - \frac{r_0 (\xi_i + \xi_j)}{a} + \frac{r_0^2 \xi_i \xi_j}{a^2} \right) \times \ln \left(\frac{r_0 + a}{r_0 - a} \right) \right] \quad (n)$$

$$\overline{\mathbf{m}}(i, j) = \frac{a}{g} \left[r_0 + \frac{r_0 \xi_i \xi_j}{3} + \frac{a(\xi_i + \xi_j)}{3} \right] \times \left[(1 + \eta_i)(1 + \eta_j) \right] \quad (o)$$

$$\tilde{\mathbf{m}}(i, j) = \frac{ab}{4c^2} \left[r_0 + \frac{r_0 \xi_i \xi_j}{3} + \frac{a(\xi_i + \xi_j)}{3} \right] \times \left[1 + \frac{\eta_i \eta_j}{3} \right] \quad (p)$$

The dynamic problem (l) is solved with a Newmark scheme and fluid forces are calculated from the fluid pressure node on the inner boundary ($r = R$).

Validation of the finite element code is performed through a comparison with analytical solutions in terms of fluid eigenmode calculation [4,].

- **Fluid sloshing modes** (gravity effects): Tab. A compares the computed frequency of some fluid sloshing modes with the expected analytical solution and validates the description of the gravity effects for the geometry under concern. The mode under concern correspond to the symmetric modes of order one – $s = 1$ in the Fourier development, Eq. (g).

Frequency	f_1	f_2	f_3	F_4
Analytical	0.9963	2.8519	3.9734	4.8513
Numerical	0.9965	2.8641	4.0398	5.0367

Table A. Elementary validation of the fluid finite element for sloshing modes in axi-symmetric problems

Fig. B. Fluid sloshing mode in pressure formulation

- **Fluid acoustic modes** (compressibility effects): Tab. A compares the computed frequency of some fluid sloshing modes with the expected analytical solution and validates the description of the compressibility effects for the geometry under concern. The mode under concern correspond to the symmetric modes of order one – $s = 1$ in the Fourier development, Eq. (g).

Frequency	f_1	f_2	f_3	F_4
Analytical	1617	1782	2205	2770
Numerical	1615	1781	2203	2767

Table B. Elementary validation of the fluid finite element for acoustic modes in axi-symmetric problems

Fig. B. Fluid acoustic mode in pressure formulation