Adaptive mesh refinement: Quantitative computation of a rising bubble using COMSOL Multiphysics®

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Abstract: The mesh is a key component in numerical simulations as it represents the spatial discretization of the model geometry. To accurately measure the variation of the unknowns, a relevant mesh should have a high density of degrees of freedom in regions where the norm of the gradient of the quantity of interest is significant. Fine meshes, on the other hand tend to induce long computational times, especially when complex 3D physics (fluid mechanics, electromagnetism …) are involved. Another sensitive point regarding meshes is the fact that regions with high gradients are likely to move during time dependent studies hence it can be difficult to define a fixed mesh that remains relevant with time.

The Adaptive Mesh Refinement (AMR) method implemented in COMSOL Multiphysics® can help to mitigate computational time while maintaining precision. Instead of using a fixed mesh throughout the simulation, the initial mesh is adapted to the solution while the simulation is computed. High gradients areas are identified through an indicator which, in this case, is the norm of the gradient. The indicator is defined on the initial coarse mesh, the mesh update is performed when the indicator threshold is reached and the first elements to be updated are those with the highest indicator value.

In this paper, the rising of a gas bubble in a liquid is modelled with the finite element (FE) software COMSOL Multiphysics® using a two-phase flow approach. Results from literature [1] are compared with results obtained using both fixed and adaptive meshes. The precision of the results and computational time are quantified to inform the FE analyst on the gain from using adaptive meshing. The results from the AMR method available in COMSOL Multiphysics® are then compared with results obtained with different software: NaSt3D and OpenFOAM [2].

Keywords: Adaptive mesh refinement, Two-phase laminar flow.

Introduction:

In order to assess the accuracy of the Adaptive Mesh Refinement (AMR) method implemented in COMSOL Multiphysics®, the classical physical phenomenon of a rising bubble of gas is studied. Moreover, this topic has been widely studied in the literature ([1] and [2]), enabling us to compare our numerical results obtained with COMSOL Multiphysics® with other software, like NaSt3D and OpenFOAM [2], both in time and accuracy. It is also suitable for the task because computational fluid mechanics models often present long computational times, especially in 3D. Moreover, two-phase flows simulations require a fine mesh around the interface for precision concerns. Therefore, the AMR method seems very efficiently by adapting the mesh, with a very fine mesh around the interface to achieve a high degree of precision, while having larger elements elsewhere to minimise the impact on computational time.

A quantitative comparison is made between the results from the AMR method, the fixed mesh case and the ones from literature [1] in 2D. Then, another comparison is established in 3D with the results from other software ([2]) to assess the efficiency of COMSOL Multiphysics® in the domain of computational fluid dynamics.

Governing equations and numerical model

1. Fluid mechanics

The Navier-Stokes equations describe the laminar fluid flow evolution. In the study, the fluid is assumed to be incompressible:

$$\begin{cases} \rho\left(\frac{\partial \vec{u}}{\partial t}+\left(\vec{u}\cdot\vec{\nabla}\right)\vec{u}\right)=\rho\vec{g}-\vec{\nabla}p+\mu\Delta\vec{u} \\ \vec{\nabla}\cdot\vec{u}=0 \end{cases} \quad (1)$$

where ρ and μ denotes respectively the mass density and dynamic viscosity of the fluid, $\vec{u}$ represents the velocity field vector, p the pressure field and $\vec{g}$ is the acceleration of gravity.

2. Phase-field approach

To represent the behaviour of the bubble inside the liquid, the phase-field method is used. This method consists in tracking a diffuse interface separating the immiscible phases with a dimensionless phase field variable denoted ϕ that can take values in [-1 , 1] according to the phase represented. In Figure 1, a schematic representation of the method is presented: each phase is characterised by a value of ϕ: -1 correspond to one phase and 1 to the other, while a value of 0 denotes the physical interface. The two phases are separated by a numerical interface, where ϕ varies in]-1, 1[.

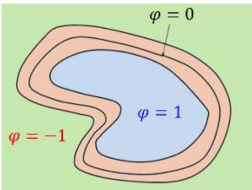

Figure 1. Visual representation of the phase field variable

A system of two 2nd order equations is used in COMSOL Multiphysics® to solve the Cahn-Hilliard equation, due to the presence of derivatives of 4th order:

$$\begin{cases} \frac{\partial \phi}{\partial t} + \vec{u} \cdot \vec{\nabla}\phi = \vec{\nabla} \cdot \frac{3\sigma\chi\varepsilon}{\sqrt{8}} \vec{\nabla}\psi \\ \psi = -\vec{\nabla} \cdot \varepsilon^2 \vec{\nabla}\phi + (\phi^2 - 1)\phi \end{cases} \quad (2)$$

With ϕ the phase field variable, σ the surface tension coefficient, and ε the interface thickness parameter. The symbols χ and ε represent the two numerical parameters of the phase-field method. The values assigned to these parameters as well as the mesh size h will be of paramount importance with regards to the convergence the model and the precision level of the results.

Linear relations are used to link the physical properties ρ and μ to the phase field variable ϕ and the physical properties of the two fluids:

$$\begin{cases} \rho = \rho_1 + (\rho_2 - \rho_1)\frac{1+\phi}{2} \\ \mu = \mu_1 + (\mu_2 - \mu_1)\frac{1+\phi}{2} \end{cases} \quad (3)$$

where subscripts 1 and 2 refer respectively to fluid 1 and fluid 2.

3. Geometry and boundary conditions

The 2D geometry and boundary conditions are presented in Figure 2, obtained from [1]. The bubble of fluid 2 is contained within a column of fluid 1. A no-slip condition is set on the upper and lower boundaries of the domains. On the vertical walls, a tangent slip is allowed. As the pressure only influences the Navier-Stokes equations through its gradient, it needs to be fixed at one point to ensure the uniqueness of the solution.

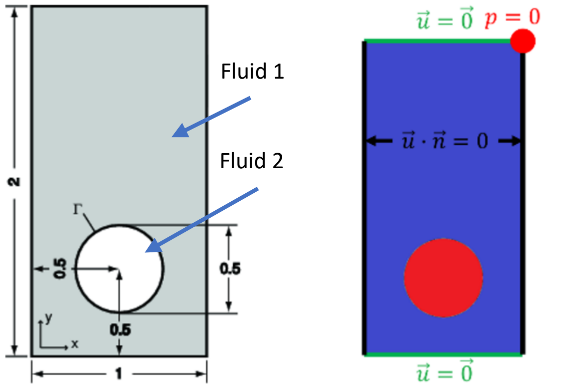

Figure 2. Geometry (left, from [1]) and boundary conditions (right) of the 2D model

A 3D model is built from the 2D one, extracted from [2]. The dimensions of the geometry are presented in Figure 3. The boundary conditions remain unchanged compared to that of the 2D model, apart from the non-slip condition, which is prescribed on the 6 walls of the domain.

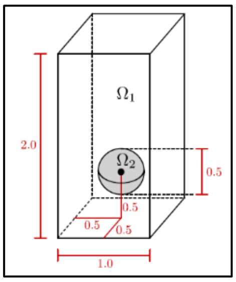

Figure 3. Dimensions and geometry of the 3D model obtained from [2]

4. Parameters of the study

The values of the different parameters used in the two models are presented in Table 1, extracted from [1]and [2].

ρ_1 (kg/m^3)	μ_1 $(Pa.s)$	ρ_2 (kg/m^3)	μ_2 $(Pa.s)$	g (m/s^2)	σ (N/m)
1000	10	1	0.1	0.98	1.96

Table 1. Material properties of the fluids and parameter values used in the studies

These numerical values have been roughly used to compare the results directly with the ones of [1] and [2].

The phase field parameter χ is set to 1 $m \cdot s/kg$ while ε is set to $\frac{1}{2}h$, where h is the size of the finest elements in the case of the adaptive mesh and correspond to the elements size in the case of the fixed mesh.

Simulation Results

1. Comparison criteria

To compare the results from the different cases, the following quantities are defined:

- The position of the centre of mass of the bubble: $\bar{y} = \frac{1}{|\Omega|}\int_{\Omega} y\, dX$
- The mean ascending velocity: $\bar{v} = \frac{1}{|\Omega|}\int_{\Omega} v\, dX$

Where the domain of the bubble Ω is defined as $\Omega = \{X \in \mathbb{R}^n \mid \phi(X) \geq 0\}$ and its measure is $|\Omega| = \int_{\Omega} 1\, dX$.

2. Modelling approach validation

To confirm the validity of the results, the fluid mass conservation is monitored during the study duration. In Figure 4, it can be seen that the mass variation is less than 0.03% which is considered negligible.

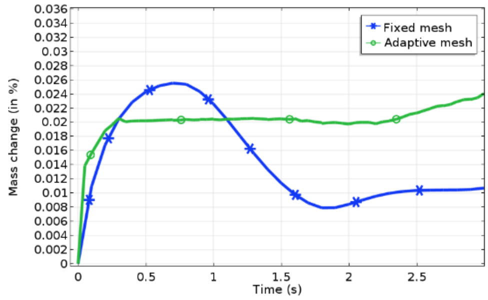

Figure 4. Mass change (in % of the initial mass) in the fixed mesh model and the adaptive one

The Navier-Stokes equations solved in the study assume a laminar flow. The Reynolds number *Re* should be small enough (<< 2000) to obtain the numerical convergence. *Re* is calculated *via* the formula

$$Re = \frac{\rho U L}{\mu} \qquad (4)$$

where U and L denote respectively a characteristic velocity and a characteristic length of the flow.

In Figure 5, the maximum values of *Re* are plotted with time, and it can be seen the maximum *Re* values are well below the threshold defined hence the laminar flow approach is validated.

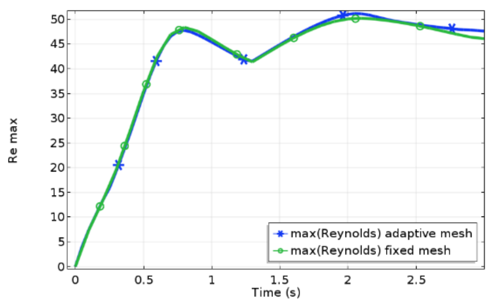

Figure 5. Maximum of Reynolds number value with time

3. Results from the 2D model

The shapes of the bubble domain from the fixed and adaptive meshes at $t = 3\ s$ are compared in Figure 6. It can be noticed that in both cases, the bubble has the same position, and the shapes of the bubbles show a satisfactory agreement which indicates a good coherence between the two techniques.

The presence of satellite bubbles falling off the main bubble can be noticed in the case where a fixed mesh is used. This can be explained by the fact that the coarse fixed mesh forces a coarse diffuse interface thickness as the latter is related to the parameter ε which is proportional to the mesh elements size h. In the case of the adaptive mesh, the refined elements are smaller than those of the fixed mesh hence the thin filaments can be represented.
The difference in the two shapes highlight a desirable feature of the AMR technique; details which would be omitted in the case of a coarse fixed mesh, and alternatively, would require a fine mesh in the entire domain are automatically captured.

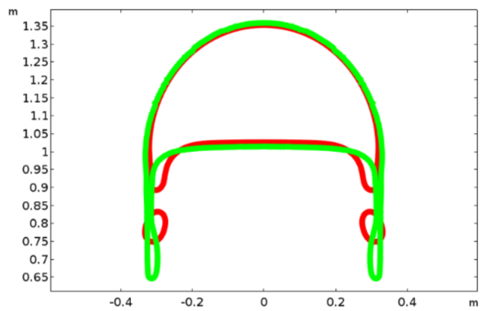

Figure 6. Shape of the bubble at $t = 3\ s$ with a fixed mesh (red) and adaptive mesh (green)

a. Reduction of computational time

In Table 2, the number of degrees of freedom (DOFs) i.e. number of unknowns solved for, and computational times for both mesh case studies are reported. It can be noticed that even though the two models have an equivalent number of DOFs, the AMR method reduced the computational time by a factor of 5.

	Number of DOFs	Computational time
Fixed mesh	260 000	75 mins
Adaptive mesh	250 000	15 mins

Table 2. Computational times of fixed mesh vs. adaptive mesh

b. Preservation of precision

The comparison criteria defined in section "Simulation Results-1" are used to compare the results from the benchmark [1] with the results from the 2D model using a fixed mesh and an adaptive mesh. The bubble centre of mass evolution with time is presented in Figure 7. It can be seen that the results from the three study correlate well. In Figure 8, the difference in the results is quantified through the position difference (in %) with the benchmark. The position difference is less than 0.8% for both meshes.

As mentioned in section "Results from the 2D model", the topography variation between the two studies is likely to be due to the difference in the diffuse interface thickness. Overall, the shape comparison is satisfactory, which confirms the AMR method does not distort the shape of the solution.

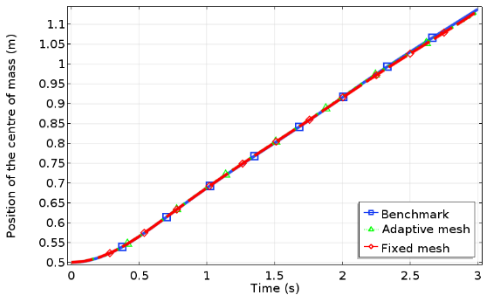

Figure 7. Position of the centre of the bubble evolution with time from the benchmark (blue), the fixed mesh (red) and adaptive mesh (green) FE model predictions

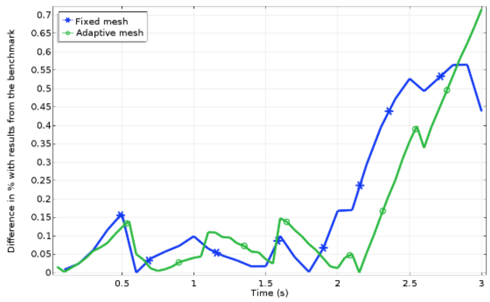

Figure 8. Difference of position of the bubble centre in % relative to the results from the benchmark and the fixed mesh case (blue) and the adaptive one (green)

In Figure 9, the mean rise velocity of the bubble is plotted for the three cases and it can be seen the three approaches predictions are in good agreement. For a more quantitative comparison, the difference in % relative to the results from the benchmark are shown in Figure 10. The difference between the results from the benchmark and those from the adaptive mesh is less than 4.5%. In the fixed mesh case, the relative error with the benchmark case results rises up to 7.5% at t=2s. This coincides with the separation of the satellite bubbles from the main one.

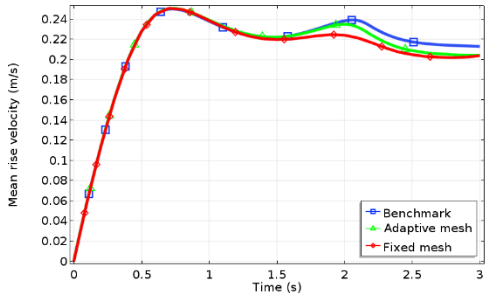

Figure 9. Mean rise velocity evolution with time from the benchmark (blue), the fixed mesh (red) and adaptive mesh (green) FE model predictions

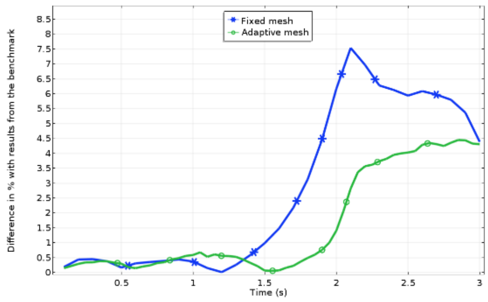

Figure 10. Difference of mean rise velocity in % relative to the results from the benchmark and the fixed mesh case (blue) and the adaptive one (green)

In this section, the 2D modelling of a rising bubble was presented using two meshing approaches. Results from a benchmark [1], a model using a fixed mesh and a model using an adaptive mesh were compared. It was found that the AMR method enabled reducing the computational time by a factor of 5 (compared with the fixed model) while improving the accuracy of the bubble shape.

4. 3D results

The AMR method proved to be effective in reducing the computational time on a 2D model. As the computational time of 3D models can be consequent, it would be attractive to use the AMR method on 3D models. However, the way the elements are refined changes when transitioning from 2D to 3D: in 2D, an element is refined in a regular pattern by creating smaller elements, homothetic relatively to the parent one. In 3D, an element is refined by splitting it in two along its longest edge. The AMR technique is applied on 3D models and the efficiency of the technique is assessed for both 2D and 3D cases.

The studied system being closed, the fluid mass conservation must be verified. The mass evolution of is plotted in Figure 11 and a variation lower than 0.15 % can be noticed, which is considered acceptable with regards to mass conservation.

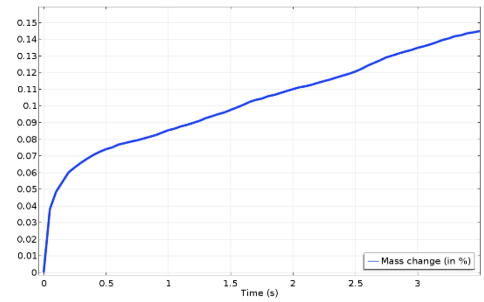

Figure 11. Mass change (in % of the initial mass)

As it was performed for the 2D case, the hypothesis of a laminar flow is checked by deriving the value of the Reynolds number along the study, as presented in Figure 12. The *Re* maximum value is indeed below the turbulent threshold (<2000) which confirms the laminar flow approach.

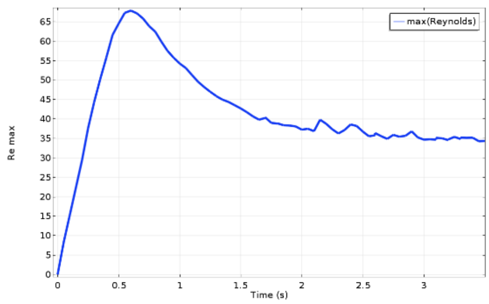

Figure 12. Maximum of Reynolds number value evolution with time

a. Gain in computational time

Two different computational fluid dynamic software are used in the [2]: NaSt3D which uses the finite difference method to solve the problem, and OpenFOAM which uses the finite volume approach. The computational times of the model using an adaptive mesh and the two models of the article [2] are presented in Table 3. Unlike the 2D case comparison, here it is not possible to quantify the gain in computational time from the AMR method in a quantitative way. This is due to the fact that the number of CPU and frequency do not allow a relevant comparison. However, with regards to the results, a notable gain in computational time is noticed.

Computational times	
COMSOL Multiphysics® with AMR method	22h on 2 CPU at 4.1 GHz
NaSt3D	1 week on 32 CPU at 2.226 GHz
OpenFOAM	60h on 32 CPU at 2.226 GHz

Table 3. Comparison in computational time with results from [2]

b. Preservation of precision

A comparison is made between the adaptive mesh method model and the two cases of the benchmark. The position of the centre of mass of the three models is shown in Figure 13. Excellent agreements are found, with a relative difference less than 1.1% between the results from the two software programs and those of the adaptive mesh case, as seen in Figure 14. This indicates the AMR method may enable saving computational time without leading to a drop-in accuracy.

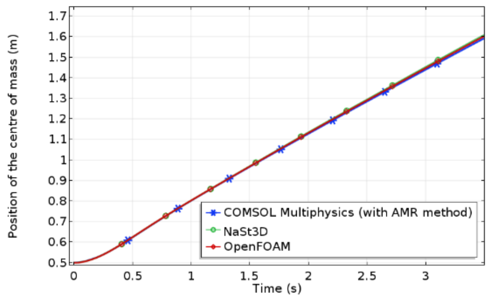

Figure 13. Position of the centre of the bubble evolution with time from the adaptive mesh (blue), NaSt3D (green) and OpenFOAM (red) FE model predictions

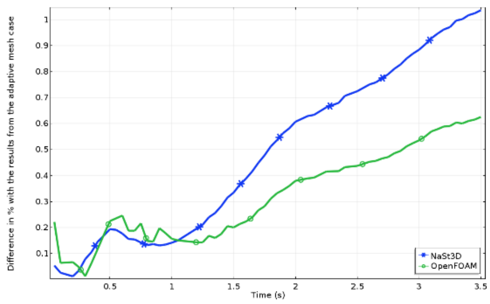

Figure 14. Difference of position of the bubble centre in % relative to the results from the adaptive mesh case and results from NaSt3D (blue) and OpenFOAM (green)

The mean rise velocity evolution with time is presented in Figure 15 for the three models. On the graph, it can be seen that the results match well. The difference relative to the results from the adaptive mesh case with NaSt3D and OpenFOAM is plotted in Figure 16. The maximum difference between the results is below 3% for NaSt3D less than 2% for OpenFOAM, which is considered negligible. This indicates once more the results from the model using the AMR method do not lose any accuracy compared to the model using a fixed mesh.

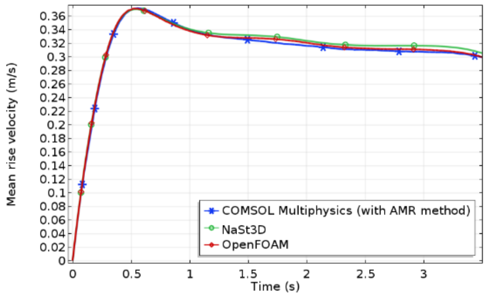

Figure 15. Mean rise velocity evolution with time from the adaptive mesh (blue), NaSt3D (green) and OpenFOAM (red) FE model predictions

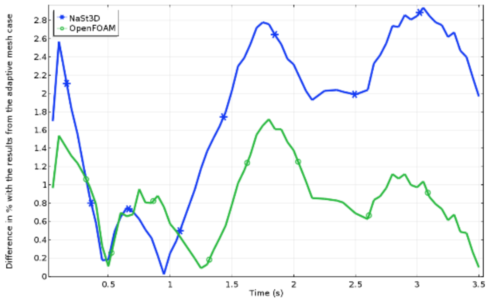

Figure 16. Difference of mean rise velocity in % relative to the results from the adaptive mesh case and results from NaSt3D (blue) and OpenFOAM (green)

The results from this study validate the AMR method in 3D, since the computational time is reduced in a consequent way while an equivalent precision is preserved.

Conclusions

2D and 3D validation studies consisting in a comparison between the results from a model using the AMR method, a model using a fixed mesh and results from literature. Satisfactory agreements were found, and it was highlighted that the AMR method provides a consequent reduction in computational time while preserving the numerical precision.

Even if comparisons between different methods are tough to establish, the 3D case underlined the fact that results from COMSOL Multiphysics® are equivalent in pertinence to those of others software, while having a much lower computational time. COMSOL Multiphysics® is then more than well suited for computational fluid dynamics models.

The efficiency of the AMR method is demonstrated here on the rise of a bubble to keep the physics involved simple enough. However, as the technique is particularly well suited for modelling problems involving high gradients in the field of interest, moving meshes and deformed geometry, it can be used on complex industrial cases such as numerical simulations of welding or additive manufacturing.

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