NUMERICAL EXPERIMENTS WITH AN HOMOGENEOUS-FLOW MODEL FOR THERMAL CAVITATION

Edoardo Sinibaldi
Scuola Normale Superiore di Pisa
e.sinibaldi@sns.it

Maria Vittoria Salvetti
Dip. Ingegneria Aerospaziale, Università di Pisa
mv.salvetti@ing.unipi.it

ABSTRACT
An homogeneous cavitation flow model capable of accounting for both the effects of thermal cavitation and the concentration of the active nuclei is considered; the model results in a barotropic state law. The local presence of both incompressible zones (pure liquid) and regions where the flow may become highly supersonic (cavitating mixture) renders the problem particularly stiff from a numerical viewpoint. The continuity and momentum equations for compressible inviscid flows are considered together with the barotropic state law. They are discretized by a finite-volume formulation applicable to unstructured grids. A shock-capturing upwind scheme is proposed for barotropic flows. The accuracy of the proposed method at low Mach numbers is ensured by ad-hoc preconditioning, which only modifies the upwind part of the numerical flux; thus, the time consistence is maintained and the proposed method can also be used for unsteady problems. Finally, an implicit time advancing is proposed to avoid severe time-step limitations encountered with explicit schemes. The proposed CFD tool is validated by quasi-1D simulations of nozzle flow.

INTRODUCTION
The present work is a preliminary study towards the definition of an efficient numerical code for accurate simulation of cavitating flows typical of cryogenic propellants of rocket engines.

As for modeling, an homogeneous-flow cavitation model recently proposed by d’Agostino et al. [1] is adopted. It seems to be well suited for the applications of our interest since it is capable of accounting for thermal cavitation effects and the concentration of the active nuclei. The model results in a barotropic state law for the mixture [1]. Since body forces and viscous stresses are usually negligible with respect to the huge dynamic actions typical of modern hydraulic turbomachinery, the continuity and momentum equations for a compressible, inviscid and force-free flow are considered, together with the barotropic state law given by the adopted cavitation model.

As for numerical discretization, considerable difficulties are encountered despite the significant simplification provided by the previous assumptions. Indeed, both incompressible zones (pure liquid) and regions where the flow may easily become highly supersonic (liquid-vapor mixtures) are present in the flow and need to be solved simultaneously. The numerical stiffness of the problem is further increased both by the high liquid-to-vapor density ratio (which, for instance, is on the order of $10^5$ for water-vapor mixture at $20^\circ$C) and by the strong shock discontinuities occurring in the recondensation at the cavity clo-
the pressure as the flow transitions from a fully-wetted liquid to a two-phase cavitating mixture. It is evident that specifically designed numerical schemes must be set up in order to handle this situation. To this purpose, two opposite ways can be followed: adaptation to the compressible case of numerical methods suitable for incompressible flows or, conversely, adaptation to the low Mach number limit of compressible solvers.

The present approach belongs to the second class, i.e. compressible solvers preconditioned for low Mach numbers. Standard numerical methods for compressible flows are more efficient than the modified pressure-based schemes at high Mach numbers, but generally fail to compute the nearly incompressible limit of the flow equations. In this limit, two types of difficulties arise. Firstly, time-advancing of the standard schemes results inefficient due to the numerical stiffness of the equations having a very large disparity between acoustic and convective time-scales. Secondly, the spatial accuracy of the solution is lost as shown by e.g. Guillard et al. [2], who performed an asymptotic analysis in power of the Mach number of both the continuous and the discrete equations for gases characterized by a polytropic state law. In particular, it was shown that the discrete solution admits pressure fluctuations in space much larger than those of the analytical one. Turkel [3] proposed a class of time-preconditioners able to overcome the stiffness problem when converging to a steady-state solution. This preconditioning technique can also improve the accuracy of the steady-state solution as shown by Turkel et al. [4]. In addition, it can be extended to unsteady problems by introducing the preconditioner in such a way that the scheme remains consistent with the time-dependent equations [2-5]. Once again, an explanation of the success of the preconditioned formulation can be obtained by using an asymptotic analysis in power of the Mach number, as in [2].

In the present approach, the governing equations are discretized by a finite-volume formulation; fluxes are computed by an upwind scheme based on the definition of a Roe matrix [6] for the considered problem.

In a previous study [7] of the low Mach number asymptotic behavior of both the continuous and the discrete problem previously described, similar difficulties as for polytropic gases were found. Thus, the same kind of preconditioning procedure as in [2-5] is formulated for the case under consideration, which allows the resulting discrete solution to have an asymptotic behavior in agreement with the continuous one [7].

Finally, as for time advancing, a linearized implicit scheme is proposed, where the linearization is based on the properties of the Roe matrix. The implicit formulation is also extended to the preconditioned scheme and allows severe stability limitations of the time step to be overcome.

All of the proposed features have been validated in the case of a quasi 1-D nozzle flow of a cavitating liquid. Although in a simplified context, this test-case contains most of the numerical difficulties which characterize the simulation of cavitating flows of our interest.

CAVITATION MODEL AND GOVERNING EQUATIONS

The chosen cavitation model [1] is an homogeneous-flow model explicitly accounting for thermal cavitation effects and for the concentration of the active cavitation nuclei in the liquid. Thanks to these features, it can be effectively employed for performance predictions in space propulsion applications. According to this model, the mean flow behaves isentropically, so that it is possible to use the energy balance of the mixture in order to evaluate the mass interaction term accounting for evaporation/condensation phenomena between the two phases and ultimately derive a constitutive relation linking the density and the pressure of the cavitating mixture. As a result, it can be shown that the entire flow is barotropic [1], its constitutive relations being:

\[ p = p_{\text{sat}} + \frac{1}{\beta_{L}} \ln \left( \frac{\rho}{\rho_{L,\text{sat}}} \right) \]  

(1)

for the pure liquid (\( p \geq p_{\text{sat}} \)) and:

\[ \frac{1}{\rho} \frac{\partial \rho}{\partial t} = \frac{1}{\rho} \frac{\partial}{\partial x} \left[ \left( 1 - \varepsilon \right) \frac{p}{\rho_{\text{sat}}} \frac{\rho}{\rho_{\text{sat}}} \right] + \alpha \frac{\partial}{\partial p} \]

(2)

for the cavitation region (\( p < p_{\text{sat}} \)). While \( \beta_{L}, \gamma, \eta, p_c \) and \( \gamma_p \) are given constants depending only on the working liquid, \( p_{\text{sat}}, \rho_{L,\text{sat}} \) and \( \alpha_L \) are determined also by the liquid temperature \( T_L \), which is assumed to be constant and is fixed a priori: \( T_L = T_{\infty} \). Finally, the volume fraction of the liquid which is in thermal equilibrium with the bubbles is determined by \( \varepsilon_L (0 \leq \varepsilon_L \leq 1) \). It is given a function of the void fraction \( \alpha = p/p_{\text{sat}} - 1 \):

\[ \varepsilon_L = \left\{ \left[ \frac{\alpha}{1 - \alpha} \left( 1 + \frac{\delta_T}{\bar{R}} \right)^{-3} - 1 \right]^{-1/3} + 1 \right\} \]

where \( \delta_T/R \) is a free parameter accounting for thermal effects and the concentration of the active nuclei \( \varepsilon_L \). More precisely, from the theory of the thermally-controlled growth of a spherical bubble it is possible to write [1-8]:

\[ R^* \approx \frac{\varepsilon L \Sigma (T_{\infty})}{\varepsilon L \Sigma (T_{\infty})} \]

where the cavitation volume \( V_{\text{cav}} \) must be estimated (for example by means of a non-cavitating numerical simulation of the flow field), the concentration of the active nuclei \( n \) (of course, affected by \( T_{\infty} \)) is assigned a priori, and the parameter \( R^* \) may be evaluated as [8]:

\[ R^* \approx \frac{\delta_{L, \text{eff}} - \sigma U_{\text{eff}}^2}{\Sigma (T_{\infty})} \]

In this expression \( \varepsilon L \) can be estimated by means of a preliminary simulation of the flow field and the thermodynamic parameter \( \Sigma \) is given by [8]:

\[ \Sigma (T_{\infty}) = \frac{\rho_{L,\text{sat}}^2}{\rho_{\text{sat}}^2} \frac{H^2}{c_p L T_{\infty}} \frac{1}{\alpha_{L}^{1/3}} \]
In conclusion, once specified $T_\infty$ and $\delta_T/R$ or $n$, it is possible to (numerically) integrate eq. (2), thus obtaining a barotropic curve as shown in Figs. 1 and 2.

Consistently with the fact that body forces and viscous stresses are usually negligible with respect to the huge dynamic actions typical of modern hydraulic turbomachinery, the Euler equations for a force-free, inviscid fluid are considered, written here in 1D for the sake of simplicity:

$$\frac{\partial W}{\partial t} + \frac{\partial F(W)}{\partial x} = 0$$

(3)

where:

$$W = \begin{pmatrix} \rho \\ \rho u \\ F(W) = \begin{pmatrix} \rho u \\ \rho u^2 + p \end{pmatrix}$$

It should be noted that the present formulation is density-based (conservative form). The constitutive relation that closes the system is the barotropic law given by eqs. (1) and (2), in the form $p = p(\rho)$.

**NUMERICAL METHOD**

A finite-volume spatial discretization of eq.(3) is considered. More precisely:

$$\delta_t \frac{dW_i}{dt} + \Phi_{i(i+1)} - \Phi_{i(i-1)} = 0$$

(4)

where $\delta_t$ is the measure of the $i$-th cell, $W_i$ is the numerical approximation of $W$ in the $i$-th cell and the numerical flux $\Phi_{ir}$ between a left state $W_l$ and a right state $W_r$ is given by the Roe numerical flux function [6]:

$$\Phi_{ir} = \frac{F(W_l) + F(W_r)}{2} - \frac{1}{2} |A_{ir}| (W_r - W_l)$$

(5)

where the so-called Roe matrix $A_{ir}$ is the exact Jacobian $\partial F/\partial W(W^*)$ when both $W_l$ and $W_r$ tend to the same value $W^*$. Furthermore, it must be diagonalizable with real eigenvalues $\lambda_1$, $\lambda_2$: $A_{ir} = T \text{Diag}(\lambda_1, \lambda_2) T^{-1}$ and verify the following jump condition for any $(W_l, W_r)$:

$$\tilde{A}_{ir} (W_r - W_l) = F(W_r) - F(W_l)$$

The matrix $|\tilde{A}_{ir}|$ in (5) is then defined as: $|\tilde{A}_{ir}| = T \text{Diag}(\lambda_1, \lambda_2) T^{-1}$.

As far as the behavior in the low Mach number limit is concerned, an asymptotic study has been performed [7] in order to look for solutions to eqs. (3) and (4) of the form:

$$\Psi = \Psi_0 + M_\infty \Psi_1 + M_\infty^2 \Psi_2 + \cdots$$

where $M_\infty$ is a Mach number characteristic of the flow and $\Psi$ is a generic flow variable. In particular, for the continuous case $\Psi = \Psi(W(x, t)) = (\rho, u, p)^T$ while for the discrete one $\Psi = \Psi(W_i(t)) = (\rho_i, u_i, p_i)^T$. It has been shown that, when $M_\infty$ tends to zero, the continuous pressure field can be expressed as:

$$p(x, t) = p_0(t) + M_\infty p_1(t) + M_\infty^2 p_2(x, t)$$
while the discrete pressure field is of the form:

\[ \rho_i(t) = \rho_0(t) + M_s \rho_{ti}(t) \]

Thus, in the continuous case the leading term responsible for spatial oscillations of pressure is of order \( M^2_s \), while in the discrete case the dependence on the spatial (cell) distribution already appears in the linear term. As a consequence, the numerical solution may exhibit pressure fluctuations in space higher than the analytical one, thus causing a loss of accuracy. In order to overcome this problem, a preconditioning matrix \( P_{tr} = P(W_i, W_r) \) has been defined \([7]\) following \([2]\), which affects the numerical flux function as follows:

\[ \Phi_{tr} = \frac{F(W_i) + F(W_r)}{2} - \frac{1}{2} P_{tr}^{-1} [P_{tr} \tilde{A}_{tr}] (W_r - W_i) \]  

where:

\[ P_{tr} = \begin{pmatrix} \theta^2 & 0 \\ \tilde{u}(\theta^2 - 1) & 1 \end{pmatrix} \]  

and \( \theta \) is a given constant proportional to \( M_s \):

\[ \theta = \tilde{\theta} M_s \]

In \([7]\) an asymptotic analysis has been also performed for the preconditioned scheme. It has been shown that, in the low Mach number limit, the discrete solution provided by the preconditioned scheme shows pressure fluctuations in space of the order of \( M^2_s \), thus recovering the spatial accuracy of the continuous solution. It should be noted that the proposed preconditioning modifies only the upwind part of the numerical flux function \( (6) \) and therefore preserves the time-consistency of the scheme (i.e. it can be used also for unsteady flow simulations).

As far as the time integration of eq.(4) is concerned, a linearized implicit scheme has been proposed \([7]\) in order to avoid the severe time-step limitations imposed by an explicit advancing. More precisely, a fully implicit backward Euler scheme is considered:

\[ \frac{\delta_i}{\Delta n t} \Delta^n W_i + \Psi_{i+1}^{n+1} - \Psi_i^{n+1} = 0 \]  

where \( \Delta^n \Psi = \Psi^{n+1} - \Psi^n \) for any generic quantity \( \Psi \), \( n \) denotes the \( n \)-th temporal iteration level. By only exploiting the properties of the Roe matrix \( \tilde{A}_{tr} \), it is possible to introduce the following approximation \([7]\):

\[ \Delta^n \tilde{A}_{tr} \approx \tilde{A}_{tr}^{n+1} \Delta^n W_i + \tilde{A}_{tr}^n \Delta^n W_r \]  

where:

\[ \tilde{A}_{tr}^{n+1} = \frac{\tilde{A}(W^n_i, W^n_r)}{2} \]

By substituting \((10)\) into eq. \((9)\), the following linearized implicit scheme is obtained:

\[ M_{-1}^{i,n} \Delta^n W_{i-1} + M_0^{i,n} \Delta^n W_i + M_1^{i,n} \Delta^n W_{i+1} = \Delta_i \Phi^n \]

where:

\[
\begin{align*}
M_{-1}^{i,n} & = -\tilde{A}_{i-1}^{n+1}i \\
M_0^{i,n} & = \frac{\delta_i}{\Delta n t} I + \tilde{A}_{i+1}^{n+1} - \tilde{A}_{i-1}^{n+1}i \\
M_1^{i,n} & = \tilde{A}_{i+1}^{n+1}i \\
\Delta_i \Phi^n & = \Phi_i^{n+1} - \Phi_i^n
\end{align*}
\]

and \( I \) denotes the identity matrix. When the proposed preconditioning is applied, it is possible to introduce the same kind of linearization as in \((10)\), once \( \tilde{A}_{tr}^{n+1} \) have been replaced with \( (P_{tr})^{-1} (P_{tr} \tilde{A}_{tr})^{n+1} \) respectively \([7]\). As a result, the following scheme can be proposed for the preconditioned case:

\[ N_{i-1}^{n} \Delta^n W_{i-1} + N_0^{n} \Delta^n W_i + N_1^{n} \Delta^n W_{i+1} = \Delta_i \Phi^n \]  

where:

\[
\begin{align*}
N_{i-1}^{n} & = - (P_{n}^{i-1} \tilde{A})^{-1} (P_{n}^{i} \tilde{A}_{i}^{n+1} i)^+ \\
N_0^{n} & = \delta_i^{n+1} I + (P_{n}^{i} \tilde{A}_{i}^{n+1})^{-1} (P_{n}^{i+1} \tilde{A}_{i+1}^{n+1})^+ \\
& - (P_{n}^{i-1} \tilde{A})^{-1} (P_{n}^{i} \tilde{A}_{i}^{n+1} i)^- \\
N_1^{n} & = (P_{n}^{i+1} \tilde{A}_{i+1}^{n+1})^{-1} (P_{n}^{i} \tilde{A}_{i}^{n+1})^-
\end{align*}
\]

Once solved the block tridiagonal linear system given by eq. \((11)\) or eq. \((12)\), the unknowns at time level \( n + 1 \) are simply given by:

\[ W_i^{n+1} = W_i^n + \Delta^n W_i \]

1D NUMERICAL EXPERIMENTS

Problem description

The 1D inviscid flow in a nozzle is considered; a source term \( Q \) is added to the right-hand side of eq. \((3)\) to account for variations of the cross-sectional area \( A \) of the nozzle:

\[ Q = -\frac{1}{A} \left( \frac{dA}{dx} \right) \left( \frac{\rho u}{\rho u^2} \right) \]

In our simulations, the employed liquid is water at \( T_\infty = 20^\circ C \). The values of the various parameters in eqs. \((1)\) and \((2)\) are the following: \( \beta_{\text{at}} = 5 \times 10^{-5} \text{ Pa}^{-1}, \quad \rho_c = 2.2089 \times 10^3 \text{ Pa}, \quad g^* = 1.67, \quad \eta_0 = 0.73, \quad \gamma_1 = 1.28, \quad \rho_{\text{pad}} = 2339.953 \text{ Pa}, \quad \rho_{\text{L,at}} = 997.949 \text{ kg/m}^3, \quad a_L = 1415.7 \text{ m/s} \) and \( \delta_T / R = 0.1 \).

A convergent-divergent nozzle of non-dimensional length \( L = 21.4 \) is discretized with 360 cells. The cell width is refined by means of a geometric progression from the inlet towards the throat, where it reaches its minimum value \( \Delta x = 0.02 \); in the divergent part the grid is specular. The nozzle geometry and the cell distribution are illustrated in Fig. 3. Non-homogeneous Dirichlet conditions, \( \rho = \rho_\infty \) and \( u = u_\infty \) are imposed at the
Figure 3: Nozzle geometry and computational cell distribution

inlet section, while zero-gradient conditions are used at the outflow. These boundary conditions are numerically imposed by Steger-Warming decomposition [9]. Initially, the flow field is assumed to be uniform at inlet conditions, i.e. $\rho = \rho_\infty$ and $u = u_\infty$ and $Q = 0$ (constant section); then $Q$ is linearly increased to reach its actual value at a non-dimensional time $t_Q = 0.5$. Time-advancing is carried out either by an explicit 4-step Runge-Kutta scheme or by the implicit algorithm described in the previous section. In both cases a constant time step $\Delta t$ has been used for sake of simplicity. The simulations are advanced in time until a steady state is reached.

Finally, as for the preconditioning strategy proposed in the previous section, it is clear that it should be applied only to those regions where the flow is nearly incompressible, i.e. to the pure liquid. A first-stage implementation of a local preconditioning strategy has been based on the matrix (7) once $\theta$ has been replaced with the following local variable:

$$\theta_{l,\infty}(W_l, W_r) = \begin{cases} \theta & \text{if } \rho_l \geq \rho_{l,\text{sat}} \text{ and } \rho_r \geq \rho_{r,\text{sat}} \\ 1 & \text{otherwise} \end{cases}$$

where $\theta$ is the theoretical value given by (8) and $M_*$ in (8) is assumed to be equal to the inlet Mach number $M_\infty$.

**Results and discussion**

The various considered conditions are summarized in Tab. 1, where the cavitation number $\sigma$ is defined as follows:

$$\sigma = \frac{2 (p_\infty - p_{\text{sat}})}{\rho_\infty u_\infty^2}$$

and $p_\infty = p(\rho_\infty)$. In our simulations, cavitation phenomena occur in test-cases TC8, TC11 and TC13.

First, results obtained without preconditioning and with explicit time advancing are discussed. The anticipated lack of accuracy of the non-preconditioned solution in the incompressible limit (very low Mach numbers) has been observed in all the test-cases taken in consideration. For instance, the steady state solution for test-case TC9 is reported in Fig. 4: both density and pressure show an unphysical asymmetric behavior (the minimum should occur at the nozzle throat). An example for a cavitating flow (TC11) is given in Fig. 5. In this case the inaccuracy is evident in the behavior of the pressure in the convergent part, just before cavitation. The correct trend is recovered only in test-cases characterized by $M_\infty > 10^{-2}$ (not reported for sake of brevity), which correspond to conditions difficult to be reached for a liquid flow.

As for time advancing, all simulations are stable at $\Delta t = 10^{-5}$; since the steady state is reached within $t \approx 1$ to $t \approx 3$, CPU times (on a PC with 1200 Mhz processor and 256 Mb RAM) of about 150 s to 450 s are needed.

The proposed preconditioning technique appears to be effective in eliminating accuracy problems in all the test-cases taken in consideration. This is shown, for instance, in Figs. 6 and 7 for test-cases TC9 and TC11 respectively, where the unphysical behavior of pressure and density is completely eliminated. This *a-posteriori* supports the results of the asymptotic analysis and the proposed formulation. It may be worth remarking that the numerical results also validate the general structure of the preconditioner and, in particular, the assumption (8). Indeed, it should be noted that $\theta$ in Tab. 2 is derived from $M_* = M_\infty$ in Tab. 1 by essentially exploiting (8) with $\theta \approx 45$. However, the preconditioning procedure dramatically reduces the time step allowed by the stability of the explicit time advancing scheme, especially for the lowest Mach number cases and for cavitating flows, as shown in Tab. 2. In particular, it is clear from Tab. 2 that preconditioned explicit simulations would hardly be affordable in 3D.

The situation is remarkably improved by the proposed implicit time advancing: for the non-cavitating test cases the time step can be increased indefinitely and therefore the CPU time needed to reach the steady state becomes negligible. As for cavitating flows, for test-cases TC11 and TC13 $\Delta t$ can be increased up to $10^{-5}$ leading to simulations requiring a CPU time of about 120 s. Surprisingly, with implicit time-advancing,

<table>
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<th>Test-case</th>
<th>$p_\infty$ (atm)</th>
<th>$u_\infty$ (m/s)</th>
<th>$M_\infty$</th>
<th>$\sigma$</th>
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**Table 1:** Main features of the different considered test-cases
the simulation of test-case TC8 was not stable; this might be due to the unphysical transient (i.e. the artificial variation applied to the source term $Q$), which induces large oscillations of pressure when cavitation phenomena occur. This inconvenient might be overcome by ad-hoc variable $\Delta t$; however, in our opinion, this is beyond the scope of the present paper.

**CONCLUSIONS AND PERSPECTIVES**
The set-up and first validation of a density-based numerical method for simulating cavitating flows has been presented. As for modeling, an homogeneous-flow cavitation model capable of accounting for both the effects of thermal cavitation and the concentration of the active nuclei is considered. The governing equations are the continuity and momentum equations for a compressible, inviscid and force-free flow, together with the barotropic state law given by the adopted cavitation model.

Spatial discretization is based on a finite-volume formulation,
Figure 6: Steady state solution obtained for test-case TC9 with preconditioning; a) density; b) pressure; c) axial speed; d) Mach number.

A previous study of the low Mach number asymptotic behavior of both the continuous and the discrete problem showed that the numerical solution obtained from the above-mentioned discretization admits pressure oscillations in space much larger than those of the continuous one. In order to solve this problem, ad-hoc preconditioning is applied to the upwind part of the Roe scheme. The proposed preconditioned formulation is consistent with unsteady flow simulations and permits to obtain an asymptotic behavior in agreement with the continuous case. Finally, a linearized implicit time-advancing algorithm has been defined using the properties of the Roe matrix; the implicit formulation has also been extended to the preconditioned scheme.

All the proposed numerical features have been applied to a quasi-1D nozzle flow of a cavitating liquid. The results of the numerical experiments well illustrate the problems encountered in this type of applications and the effectiveness of the proposed
Table 2: Parameters of the preconditioned explicit simulations

<table>
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</tbody>
</table>

remedies. Indeed, it has been shown that, without preconditioning, the accuracy of the numerical solution is deteriorated for low Mach numbers, and this up to Mach number values that are hardly reachable in liquid flows. The proposed preconditioning technique seems to be able to eliminate this problem also at very low Mach numbers, of the order of $10^{-4}$-$10^{-6}$. However, preconditioning dramatically reduces the time step allowed by the stability of the explicit time-advancing; for the lowest considered values of the Mach number, the allowable $\Delta t$ is reduced by several order of magnitudes with respect to non-preconditioned simulations. From present results it is clear that 3D simulations of low Mach number barotropic flows would hardly be affordable. On the other hand, it has been shown that the proposed implicit time-advancing almost completely overcomes this problem. Indeed, for non cavitating cases, the $\Delta t$ can be increased almost indefinitely; when cavitation phenomena occur, although the gain is more limited because of the stiffness of the problem, the allowable $\Delta t$ is of the same order as that of explicit non-preconditioned simulations and, thus, the deteriorating effect of preconditioning on time stability is eliminated.

The next step of the present activity will consist in the implementation of the described numerical approach in a 3D solver based on a mixed finite-element/finite-volume formulation applicable to unstructured grids.

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