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Executive Summary of the Thesis

Verification and validation of quasi-static and dynamic VMS-LES methods for the numerical simulations of turbulent flows

Laurea Magistrale in Energy Engineering - Ingegneria Energetica

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1. Introduction

In this thesis we perform both verification and validation of the quasi-static and dynamic VMS-LES methods for the numerical simulation of turbulent flows. Turbulence is one of the most challenging topic of computational fluid dynamic, due to the random nature of the flow. Therefore, to solve the Navier-Stokes equations in turbulent regimes, mainly three approaches have been developed: Direct Numerical Simulations (DNS), Large-Eddy-Simulations (LES) and Reynolds Averaged Navier-Stokes (RANS). From the first to the last, we reduce the computational cost, but we lose accuracy [7, 10]. In this work we study the VMS-LES methods, which belong to the family of LES methods.
LES methods are based on the distinction between a coarse scale and a fine scale, which are put in relationship applying a filtering procedure. With the VMS-LES we still perform the distinction between the two scales, but we introduce a variational approach. In this regard, we split the solution into the direct sum of a coarse scale and a fine scale term, and we define the fine scale solution, such that it depends on the coarse solution [3, 8]. While the latter is approximated with traditional space discretization methods (we use Finite Element Method), for the fine scales it is possible to choose between many different definitions [1]. In this regard, we consider the quasi-static and the dynamic methods. The difference between these two is that in the first method the fine scale solution is time-dependent, since it depends on the coarse scale. On the other side, in the second method, we let the fine scale solution depend on time, computing it by solving an additional ordinary differential equation (ODE). This approach was introduced to solve the degeneration of the pressure stabilization parameter arising in the quasi-static method when lowering the timestep, wich possibly affects the quality of the solution. However, there are not many studies available in literature which compare these two methods numerically.
In this work, we aim to provide a quantitative overview of the performances of the two methods, performing verification and validation with a variety of physical and numerical differemt assumptions.
Verification and validation are two preliminary tests, which help to evaluate if a method is ready to be used on real applications. We perform verification to check if the implementation of our

methods is free of mistakes. For this purpos we use the Beltrami flow benchmark, for which the analytical solution is known, and we study the convergence of errors. On the other side, the aim of validation is to evaluate if the numerical model is able to represent the physics of the problem with the expected degree of accuracy [4]. Therefore, we employ the Taylor-Green-Vortex (TGV) fluid dynamic benchmark, which is a challenging test case representing all the main feature of turbulence. In the model validation we compare the numerical solution with the solution obtained from a DNS.
Finally, we conclude our thesis testing the quasi-static and dynamic VMS-LES methods on a real application, which is a patience-specific stenotic carotid.

2. Models for the Navier-Stokes equations: quasi-static and dynamic VMS-LES methods

In this section, we provide a brief overview of the equations governing the quasi-static and dynamic VMS-LES methods starting from Navier-Stokes problem [1, 3, 6, 8].
Let us consider a domain $\Omega \subset \mathbb{R}^d$ where $d = 3$, with a sufficiently regular boundary $\partial\Omega \equiv \Gamma$ such that $\partial\Omega = \Gamma_\mathrm{N} \cup \Gamma_\mathrm{D}$ and $\Gamma_\mathrm{N} \cap \Gamma_\mathrm{D} = \emptyset$. We define Γ_N the portion of the boundary where Neumann boundary conditions are applied and Γ_D the portion related to Dirichlet boundary data.
The Navier-Stokes equations for incompressible fluids read as follow:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \tag{1}$$
$$-\nabla\cdot\sigma(\mathbf{u},p) = \mathbf{f} \quad \text{in } \Omega \times (0,T), \tag{2}$$
$$\nabla\cdot\mathbf{u} = 0 \quad \text{in } \Omega \times (0,T), \tag{3}$$
$$\mathbf{u} = \mathbf{g} \quad \text{on } \Gamma_\mathrm{N} \times (0,T), \tag{4}$$
$$\sigma(\mathbf{u},p)\hat{\mathbf{n}} = \mathbf{h} \quad \text{on } \Gamma_\mathrm{N} \times (0,T), \tag{5}$$
$$\mathbf{u} = \mathbf{u}_0 \quad \text{in } \Omega \times \{0\} \tag{6}$$

We derive the weak formulation of the problem which, for the sake of coinciseness, we do not report here. We define the space of the solution as: $\mathcal{V}_g := \{\mathbf{v} \in [H^1(\Omega)]^d \;\; \mathbf{v} = \mathbf{g} \text{ on } \Gamma_\mathrm{D}\}$, $\mathcal{Q} := L^2(\Omega)$ and $\boldsymbol{\mathcal{V}}_g := \mathcal{V}_g \times \mathcal{Q}$, and the spaces of the test functions as: $\mathcal{V}_0 := \{\mathbf{v} \in [H^1(\Omega)]^d \;\; \mathbf{v} = \mathbf{0} \text{ on } \Gamma_\mathrm{D}\}, \mathcal{Q} := L^2(\Omega)$ and $\boldsymbol{\mathcal{V}}_0 := \mathcal{V}_0 \times \mathcal{Q}$.

2.1. The VMS-LES space discretization

We introduce the VMS-LES method by splitting the spaces into the direct sum of two subspaces, such that:

$$\boldsymbol{\mathcal{V}}_g = \boldsymbol{\mathcal{V}}_g^h \oplus \boldsymbol{\mathcal{V}}'_g, \tag{7}$$
$$\boldsymbol{\mathcal{V}}_0 = \boldsymbol{\mathcal{V}}_0^h \oplus \boldsymbol{\mathcal{V}}'_0. \tag{8}$$

The spaces $\boldsymbol{\mathcal{V}}_g^h = \mathcal{V}_g^h \times \mathcal{Q}^h$ and $\boldsymbol{\mathcal{V}}_0^h = \mathcal{V}_0^h \times \mathcal{Q}^h$ are the finite-dimensional spaces related to the coarse scales, approximated by the FEM theory:

$$\mathcal{V}_g^h = \mathcal{V}_g \cap [X_h^r]^d, \tag{9}$$
$$\mathcal{Q}^h = \mathcal{Q} \cap X_h^r, \tag{10}$$

where:

$$X_h^r = \{v_h \in C^0(\Omega) : v_h^k|_K \in \mathbb{P}_r, \forall K \in T_h\} \tag{11}$$

while $\boldsymbol{\mathcal{V}}'_g$ and $\boldsymbol{\mathcal{V}}'_0$ are the infinite dimensional spaces of the fine scales solution.
According to the VMS-LES method, if we define $\mathbf{U} = \{\mathbf{u}, p\}$, we have:

$$\mathbf{U} = \mathbf{U}_h + \mathbf{U}' \tag{12}$$

By plugging (12) in the weak formulation, we obtain the following weak problem:
Given $\mathbf{u}_0$, for any $t \in (0,T)$, find $\mathbf{U}^h = \mathbf{U}^h(t) = \{\mathbf{u}^h, p^h\}(t) \in \boldsymbol{\mathcal{V}}_\mathbf{g}^h$ such that:

$$\begin{aligned}
&\left(\mathbf{v}^h, \rho\frac{\partial \mathbf{u}^h}{\partial t}\right) + (\mathbf{v}^h, \rho(\mathbf{u}^h\cdot\nabla)\mathbf{u}^h) + \\
&+(\nabla\mathbf{v}^h, \mu\nabla\mathbf{u}^h) - (\nabla\cdot\mathbf{v}^h, p^h) + (q^h, \nabla\cdot\mathbf{u}^h) + \\
&+(\rho\mathbf{u}^h\cdot\nabla\mathbf{v}^h + \nabla q^h, \tau_M(\mathbf{u}^h)\mathbf{r}_M(\mathbf{u}^h, p^h)) + \\
&-(\nabla\cdot\mathbf{v}^h, \tau_C(\mathbf{u}^h) r_M(\mathbf{u}^h)) \\
&-(\rho\mathbf{u}^h\cdot(\nabla\mathbf{v}^h)^T, \tau_M(\mathbf{u}^h)\mathbf{r}_M(\mathbf{u}^h, p^h)) \\
&+(\rho\nabla\mathbf{v}^h, \tau_M(\mathbf{u}^h)\mathbf{r}_M(\mathbf{u}^h, p^h) \otimes \tau_M(\mathbf{u}^h)\mathbf{r}_M(\mathbf{u}^h, p^h)) \\
&= (\mathbf{v}^h, \mathbf{f}) + (\mathbf{v}^h, \mathbf{h})_{\Gamma_\mathrm{N}}
\end{aligned} \tag{13}$$

To introduce the quasi-static or the dynamic approximation of the fine scale, it is sufficient to change the definition of the fine scale variable:

$$\mathbf{U}' = \mathcal{F}'(\mathbf{U}^h, \mathbf{R}(\mathbf{U}^h, \mathbf{V}')) \tag{14}$$

where, different expressions of the functional $\mathcal{F}'$ lead to different VMS-LES methods [16].

2.2. Quasi-static and dynamic approximation of fine scales

In this section we first introduce the quasi-static and than the dynamic approximation of fine scales, for the VMS-LES method.

Quasi-static

In the quasi-static VMS-LES method we compute the fine scale solutions (pressure and velocity) as the product of the element-wise stabilization operators τ_C and τ_M and the residual of the coarse scale equations r_C and $\mathbf{r}_M$, respectively, such that:

$$p' \approx -\tau_C(\mathbf{u}^h) r_C(\mathbf{u}^h) \tag{15}$$

$$\mathbf{u}' \approx -\tau_M(\mathbf{u}^h) \mathbf{r}_M(\mathbf{u}^h, p^h) \tag{16}$$

accordingly, the stabilization parameters of pressure and velocity, respectively, are defined as:

$$\tau_C(\mathbf{u}^h) = (\tau_M(\mathbf{u}^h)\overline{\mathbf{g}} \cdot \overline{\mathbf{g}})^{-1} \tag{17}$$

$$\tau_M(\mathbf{u}^h) = \left(\frac{\sigma_t^2 \rho^2}{\Delta t^2} + \rho^2 \mathbf{u}^h \cdot \overline{\mathbf{G}} \mathbf{u}^h + C_r \mu^2 \overline{\mathbf{G}} : \overline{\mathbf{G}} \right)^{-\frac{1}{2}} \tag{18}$$

Notice that, when $\Delta t \to 0$ the pressure stabilization parameter τ_C tents to infinite. Therefore this method is inconistent.

Dynamic

In the dynamic VMS-LES method we keep the same expression for the pressure fine scale solution as in (15), but we compute the velocity fine scale solution by solving the following ODE:

$$\frac{\partial \mathbf{u}'}{\partial t} + (\widetilde{\tau}_M(\mathbf{u}^h))^{-1} \mathbf{u}' \approx -\mathbf{r}_M(\mathbf{u}^h, p^h), \tag{19}$$

Accordingly, deriving τ_C and τ_M in an analogous fashion as in the quasi-static method, we obtain:

$$\widetilde{\tau}_C(\mathbf{u}^h) = (\widetilde{\tau}_M(\mathbf{u}^h)\overline{\mathbf{g}} \cdot \overline{\mathbf{g}})^{-1} \tag{20}$$

$$\widetilde{\tau}_M(\mathbf{u}^h) = (\rho^2 \mathbf{u}^h \cdot \overline{\mathbf{G}} \mathbf{u}^h + Cr \mu^2 \overline{\mathbf{G}} : \overline{\mathbf{G}})^{-\frac{1}{2}} \tag{21}$$

We underline that the two stabilization parameters are now independent from Δt. Therefore, the inconsistency of (17) should be avoided.

3. Time discretization

The time-discretization of the problem is formulated according to the Backward Differentiation Formulas (BDF) of order σ_t [6, 11].
Let us consider a partition of the time domain $(0, T)$ into N_t subintervals of equal size $\Delta t = \frac{T}{N_t}$. The subscript n denote the time-step, such that $n = 0, ..., N_t$ and $\Delta t = t^{n+1} - t^n$.
We write the approximation of the time-derivative as:

$$\frac{\partial \mathbf{u}^h}{\partial t} \approx \frac{\alpha_{\mathrm{BDF}} \mathbf{u}^h_{n+1} - \mathbf{u}^h_{n,\mathrm{BDF}}}{\Delta t} \tag{22}$$

where $\mathbf{u}^h_n$ is the quantity $\mathbf{u}^h$ evaluated at the time t^n, while at the denominator we have the timestep.

We define $\mathbf{u}^h_{n,\mathrm{BDF}}$ as follows:

$$\mathbf{u}^h_{n,\mathrm{BDF}} = \begin{cases} \mathbf{u}^h_n \\ 2\mathbf{u}^h_n - \frac{1}{2}\mathbf{u}^h_{n-1} \\ 3\mathbf{u}^h_n - \frac{3}{2}\mathbf{u}^h_{n-1} + \frac{1}{3}\mathbf{u}^h_{n-2} \end{cases} \tag{23}$$

where from the first to the last row we have: BDF1 ($\sigma_t = 1$), BDF2 ($\sigma_t = 2$) and BDF3 ($\sigma_t = 3$) schemes, and $n \geq 1$, $n \geq 2$, $n \geq 3$, respectively.
Moreover, α_{BDF} reads as:

$$\alpha_{\mathrm{BDF}} = \begin{cases} 1 & \text{for } \sigma_t = 1 \\ \frac{3}{2} & \text{for } \sigma_t = 2 \\ \frac{11}{6} & \text{for } \sigma_t = 3 \end{cases} \tag{24}$$

To discretize in time the non linear term we apply either the implicit (25) or the semi-implicit (26) schemes.

$$(\mathbf{v}^h, \rho(\mathbf{u}^h_{n+1} \cdot \nabla)\mathbf{u}^h_{n+1}) \tag{25}$$

$$(\mathbf{v}^h, \rho(\mathbf{u}^h_n \cdot \nabla)\mathbf{u}^h_{n+1}) \tag{26}$$

In this regard, for the semi-implicit method we follow the Newton-Gregory approach, for which we address to [2].

4. Verification

In this section, we resume the crucial points of numerical and software verification.
For this purpose, we choose the Beltrami flow test case [5], a simple benchmark for which the analytical solution is known. To evaluate the performance of our methods, we perform

a mesh-refinement analysis and a consistency analysis of the stabilization parameters, applying the numerical setup of Table 1

Final time (T)	0.2s
Reynolds number (Re)	1 - 1000
FEM spaces	$\mathbb{Q}1 - \mathbb{Q}1$
BDF order	1

Table 1: Verification. Numerical setup

4.1. Mesh-refinement analysis

In the mesh-refinement analysis we fix the timestep (Δt) and we evaluate if pressure and velocity errors are converging when reducing the mesh size. For this purpose, we compute L_2 and H_1 errors by means of the definitions (27) and (28), respectively:

$$\|e\|_{L_2} = \sqrt{\int_\Omega e^2} \quad (27)$$

$$\|e\|_{H_1} = \left(\|e\|^2_{L_2} + \|\nabla \cdot e\|^2_{L_2}\right)^{\frac{1}{2}} \quad (28)$$

where $e = f - f_h$ is the difference between the reference (i.e. exact) solution f and the finite element solution f_h, for either pressure and velocity.

Numerical setup

We consider three different mesh size: coarse, medium and fine (Table 2).

N^{Ref}	h	N^{el}
2	0.25	64
3	0.125	512
4	0.0625	4096

Table 2: Mesh overview. N^{Ref} is the number of refinements, h is the size and N^{el} is the number of elements in the domain.

We fix the timestep as $\Delta t = 5 \cdot 10^{-3}$ s and we change the Reynolds number (Re) between 1 and 1000 by taking the density ρ equal to 1 or 1000 $\frac{kg}{m^3}$, respectively.

Numerical results

By testing the quasi-static and the dynamic VMS-LES methods with both implicit and semi-implicit time discretization, we obtain that:

- The dynamic, semi-implicit VMS-LES method is not converging when $Re = 1000$;
- the dynamic VMS-LES methods, when convergent, return lower errors with respect to the quasi-static;
- the convergence of velocity errors is in agreement with the finite element estimator, while pressure errors have different trends, when changing the numerical method and the Reynolds number.

These results suggest that there might be an implementation error in the dynamic, semi-implicit VMS-LES method. Moreover, since the convergence of pressure is affected by the choice of the method and the Reynolds number, the stabilization may influence pressure accuracy.

4.2. Consistency analysis

In the consistency analysis we want to numerically prove that the dynamic VMS-LES method is correcting the behaviour of the pressure stabilization parameter, which in quasi-static method goes to infinite when reducing the timestep. For this purpose we fix the mesh refinement as $N^{Ref} = 3$ and we change the Δt such that:

$$\Delta t = [10^{-2} \quad 10^{-3} \quad 10^{-4} \quad 10^{-5}]\ s \quad (29)$$

moreover, we fix $Re = 1000$ and the final time $T_f = 0.2$ s. In Figure 1 and 2 we report the space averaged stabilization parameters, normalized with respect to those ones computed for $\Delta t = 10^{-2}$ s, for visualization reasons.

As we see in the graphs, the numerical results are in agreement with theory. Indeed, the dynamic method is effectively correcting the inconsistency of the pressure stabilization parameter, which characterize the quasi-static VMS-LES method.

5. Model validation

We perform the model validation of the quasi-static and dynamic VMS-LES methods on the TGV fluid dynamic benchmark [15], which is a complex test case used to study the behaviour of

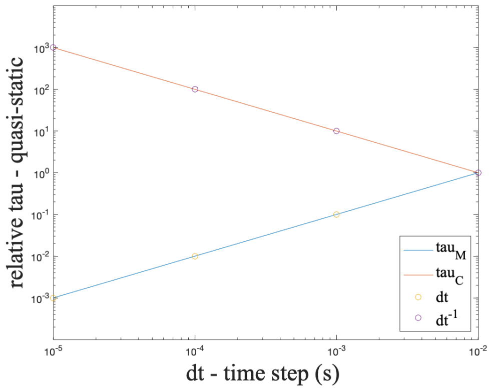

Figure 1: Relative τ. Quasi-static approximation of fine scale

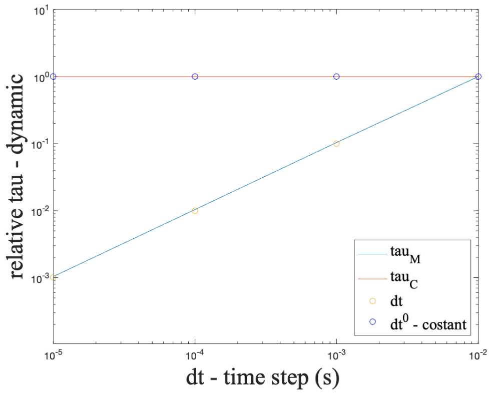

Figure 2: Relative τ. Dynamic approximation of fine scale

a numerical method with respect to turbulence. Indeed, the aim of this section is to evaluate if the methods we are validating appropriately represent turbulent flows. For this purpose, we compare with the reference data (retrived by a DNS) three physical quantities used to predict turbulence: space averaged kinetic energy (30), dissipation rate of kinetic energy (32) and enstrophy (31).

$$e_k(t) = \frac{1}{|\rho\Omega|}\int_\Omega \frac{1}{2}\rho\mathbf{u}(\mathbf{x},t)\cdot\mathbf{u}(\mathbf{x},t)d\Omega \tag{30}$$

$$e_\omega(t) = \frac{1}{|\rho\Omega|}\int_\Omega \frac{1}{2}\rho\boldsymbol{\omega}(\mathbf{x},t)\cdot\boldsymbol{\omega}(\mathbf{x},t)d\Omega \tag{31}$$

$$\epsilon(t) = -\frac{de_k(t)}{dt} \tag{32}$$

$$\epsilon(t) = 2\frac{\mu}{\rho}e_\omega(t) \tag{33}$$

Notice that, under the assumption of incompressible flow, we can write $\epsilon(t)$ as function of the enstrophy, such that (32) and (33) are equal.

Numerical setup

For the model validation we fix the numerical setup (Table 3) and we evaluate which method better represents the DNS solutions for $e_k(t), e_\omega(t)$ and $\epsilon(t)$ [14].

Final time (T)	5 - 2.3 s
Reynolds number (Re)	1600
FEM spaces	$\mathbb{Q}2 - \mathbb{Q}2$
BDF order	3
Mesh refinement	$N_{Ref} = 6$

Table 3: List of changing parameters

Numerical results

The results of validation show that the quasi-static VMS-LES methods give a satisfying approximation of the problem, while in some cases the dynamic semi-implicit and implicit VMS-LES methods are less accurate.
Going into details, we see that:

- In the dynamic semi-implicit VMS-LES method, $e_k(t), e_\omega(t)$ and $\epsilon(t)$ explode to infinite after few timesteps, confirming a possible implementation issue.
- The dynamic implicit VMS-LES method presents two inaccuracies in the kinetic energy results. First, an extra dissipation with respect to the DNS solution. Second, a wiggling behaviour, which is not retrieved by the reference data.
- Limited to enstrophy, we do not see any worsening of the solution.

According to these results, the dynamic methods seems to be not as accurate as the quasi-static. However, it is too early for such a statement and we believe that many more analyses still need to be done for a complete understanding (and improvement) of these methods.

6. Flow past a carotid bifurcation

In the last chapter of the thesis, we test the quasi-static and dynamic VMS-LES methods on a real application: a patience-specific stenotic carotid. Without entering into details of the medical aspects for which we address to [13], the stenosis we are considering is a reduction of the cross section of the vessel, caused by fat deposits, inflammatory cells, and scar tissue settle. Due to the high velocity and geometry, downstream the stenosis the blood flow may become turbulent. The swirling structures of turbulent flows bring negative effects caused by: extra shear stresses on vessels' walls, recirculation regions, and a possible interaction between eddies and blood elements due to the energy transfer that may take place if the two have a comparable scale [9]. Modelling the blood flow by means of numerical method can help specialists to prevent pathological situations.

6.1. Numerical setup

For a detailed description of the test case, we address to [12], we resume the main features.
In our simulation the domain discretization provides a mesh of tetrahedra made of about 1,5 million active cells with adaptive size. We set linear FE spaces ($\mathbb{P}1 - \mathbb{P}1$) for both pressure and velocity space approximation, and we perform the time discretization by means of the BDF3 scheme. Moreover, we fix the timestep as $\Delta t = 2 \cdot 10^{-3}$ s and we set a final time of $T_f = 2.2$ s. We consider an hearth period of 1.09 s, which means an heart frequency of 65 BPM, therefore, we simulate two hearth cycles. In this analysis we compare the quasi-static and dynamic implicit VMS-LES methods.

6.2. Numerical results

Downstream our simulations, we obtain similar results as model validation. We see that the solutions retrieved by the dynamic method, present an oscillatory pattern around a macroscopic trend, which does not arise with the quasi-static method. However, limited to the macroscopic trend, the solutions are overlapping.
By visualizing the solutions obtained with the dynamic method, we observe that downstream the stenosis it appears a region where velocity magnitude and direction are changing abruptly instant by instant, in agreement with the oscillation of the kinetic energy.
We think that this behaviour of velocity leads to the wiggles arising in the dynamic implicit VMS-LES method and it may be related to a purely numerical issue. However, we do not deepen this problem, which we believe to be an interesting topic for further researchers.

7. Conclusions

In this work we have presented a systematic analysis of the quasi-static and dynamic VMS-LES methods, with a special focus on comparing the performance of the second one with respect to the first one. By means of verification and validation we were able to evaluate: on the one hand implementation, accuracy and consistency, on the other hand the quality of the numerical solution, with respect to the physics of the problem, both on idealised cases. In the end, to provide an applicative counterpart of the study we have tested our methods on a realistic case.
Downstream our study, we observe that the dynamic VMS-LES method is solving the inconsistency arising in the quasi-static, but it retrieves "lower-quality" solutions. In particular, the semi-implicit version of this method may be affected by some implementation issues, while the implicit formulation has shown a worst representation of the physical quantities, with respect to the quasi-static.
To conclude this summary, we want to purpose a different perspective on the two methods.
According to literature, the dynamic VMS-LES method has been defined later than the quasi-static, to correct its inconsistency. Therefore, its the formulation is obtained from that one of the quasi-static, by simple changing the definition of the stabilization parameters. However, from a theoretical point of view, we may think the contrary and hence, that the quasi-static is a simplification of the dynamic. Indeed, the equation to define the velocity fine-scale solution is the same, but in the quasi-static method we assume $\frac{\partial \mathbf{u}'}{\partial t} = 0$. Following this perspective, we will have an additional term in the weak formulation of the dynamic VMS-LES method, which is now neglected. This may change the results of validation and verification.

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