

## **Theoretical considerations of the volume penalization immersed boundary method for turbulent flows**

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This letter explores the Volume Penalization-Immersed Boundary Method (VP-IBM) for turbulent flows from a more physically perspective. The VP approach consists of introducing a penalty source into the governing equations, resulting in a flow akin to a porous medium with low permeability. Although penalizing the turbulent equations conventionally involves adding a similar penalty source as in the original equations, this work reveals an alternative formulation that includes an additional term with physical meaning. The novelty of this letter is to consider the penalised flow with an additional property, the fluid resistance, establishing a cross-correlation with fluctuating velocity for further modelling.

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The Immersed Boundary Method (IBM)<sup>1</sup> is a numerical technique for embedding bodies with complex geometries within Cartesian-like meshes for fluid flow simulations. At present, IBM remains a current issue in the Computational Fluid Dynamics (CFD) community<sup>2</sup>. Volume Penalization (VP)<sup>3</sup> belongs to the IBM family, where the governing equation embodies a penalty force that is equivalent to a boundary condition applied in certain computational nodes of the mesh. For example, consider the incompressible Navier-Stokes (iNS) equations,

$$\frac{\partial u_i}{\partial x_i} = 0, \tag{1a}$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j} \left( u_i u_j - \nu \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho} p \delta_{ij} \right) = 0, \tag{1b}$$

where  $u_i$  is the velocity field,  $p$  is the pressure,  $\rho$  is the density, and  $\nu$  is the kinematic viscosity. Assume a rigid body is moving in the domain  $\Omega$  with a velocity  $u_{b,i}$ . The problem imposes the condition  $u_i(\cdot, t) = u_{b,i}(t)$  on the wall. Then the (standard) penalized iNS equations can be written as follows:

$$\frac{\partial u_{\eta,i}}{\partial x_i} = 0, \tag{2a}$$

$$\frac{\partial u_{\eta,i}}{\partial t} + \frac{\partial}{\partial x_j} \left( u_{\eta,i} u_{\eta,j} - \nu \frac{\partial u_{\eta,i}}{\partial x_j} + \frac{1}{\rho} p_{\eta} \delta_{ij} \right) + s_{\eta,i} = 0, \tag{2b}$$

where the penalty source  $s_{\eta,i} = \chi/\eta [u_{\eta,i} - u_{b,i}]$  drives  $u_{\eta,i}$  to  $u_{b,i}$  within the body region,  $\Omega_{\text{body}}$ , for small values of the penalized parameter  $\eta$ , i.e.  $0 < \eta \ll 1$ . Note that the application of  $s_{\eta,i}$  modifies the set of solutions, and therefore,  $(u_{\eta,i}, p_{\eta})$  is not the same as  $(u_i, p)$ . Angot, Bruneau, and Fabrie<sup>4</sup> (later by Carbou and Fabrie<sup>5</sup>) provided the convergence of the velocity of the penalized equation (2) when  $\eta \rightarrow 0$  to the solution of the velocity of the iNS equation (1) with no-slip boundary condition, i.e. the modelling error depends on the penalization parameter<sup>6</sup> as  $\|u_i - u_{\eta,i}\| \propto \eta^{\alpha}$  where  $\|\cdot\|$  is the  $L_p$ -norm and  $\alpha \in \mathbb{R}$  ( $\alpha = 1/2$  for Dirichlet boundary conditions). With regard to pressure, Angot, Bruneau, and Fabrie<sup>4</sup> only noted that there is a Darcy flow within the body at the order  $\eta$ . However, Basarić *et al.*<sup>7</sup> provided the convergence of the solution  $(\rho_{\eta}, u_{\eta,i}, T_{\eta})$ , and hence also of  $p_{\eta} = p_{\eta}(\rho_{\eta}, T_{\eta})$ , for the Navier-Stokes-Fourier equations (compressible viscous and heat-conducting flow).

The limit of the VP-IBM application will be given by the numerical aspect. Typical permeability values are  $\eta \in \{10^{-7}, 10^{-10}\}$  (see e.g. Ménez *et al.*<sup>8</sup>). This limitation is due to stability issues since small  $\eta$  results in very stiff source terms, which restrict the time step<sup>9</sup>.

On the other hand, the mask function  $\chi$  characterises the geometry of the body. Typically,

$\chi$  is selected as a step-like function (sharp mask):

$$\chi(x_i, t) := \begin{cases} 1, & \text{If } x_i \in \Omega_{\text{body}}(t) \\ 0, & \text{Otherwise} \end{cases}.$$

Nonetheless, this definition is not the sole option and continuous functions<sup>10–13</sup> (smooth mask) can be used, for example. In some cases of moving bodies, the mask function might be described by a transport equation<sup>14,15</sup>.

On the other hand, IBMs remain challenging for turbulent flows because of non-conforming meshes. In such high Reynolds numbers, the importance of friction is inevitable near the wall. Recent contributions in ghost cell<sup>16–18</sup>, direct forcing<sup>19–22</sup> and VP<sup>23,24</sup> enhance IMBs for turbulent flows; see Iaccarino and Verzicco<sup>25</sup> for an exhaustive review of turbulence in IBM. Nevertheless, when penalization is applied to turbulent flows, it is approached more from a numerical perspective than from a physical one. From a physical point of view, penalization involves modelling the body as a porous medium with permeability  $\eta$  approaching zero. Hence, for practical purposes, it is essential to know the contributions of turbulence within the specified region where the body is assumed to be located.

This letter aims to show a discrepancy when the volume penalization-immersed boundary method (VP-IBM) is applied for turbulence modelling. Articles dealing with VP-IBM for turbulent flow (e.g. Yu and Yu<sup>26</sup>) just simply take the turbulent equations and penalized the turbulent velocity field. This calls into a research question: Is this the only way to obtain a penalized version of the turbulent equations? To illustrate the aim of this letter, the Unsteady Reynolds-Averaged Navier-Stokes (URANS) equations are applied. It will show that two different formulations of the penalty source are achieved for the momentum equations.

When dealing with turbulent flows, handling the URANS equations in a penalty version becomes necessary in some form for VP-IBM. At first glance, one can proceed as follows: split each instantaneous quantity in the iNS equations (1) into its averaged and fluctuating components (Reynolds decomposition) and ensemble-averaging these equations,

$$\begin{aligned} \frac{\partial \bar{u}_i}{\partial x_i} &= 0 \\ \frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left( \bar{u}_i \bar{u}_j - \nu \frac{\partial \bar{u}_i}{\partial x_j} - R_{ij} + \frac{1}{\rho} \bar{p} \delta_{ij} \right) &= 0, \end{aligned}$$

where  $R_{ij} := -\overline{u'_i u'_j} = \nu_t \partial u_i / \partial x_j$  is defined as the Reynolds stress tensor with eddy viscosity  $\nu_t$ . These equations are the traditional URANS. Then one penalized the momentum equation, that is,

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0, \quad (3)$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \bar{\Pi}_{ij} + s_{\eta,i}^\dagger = 0, \quad (4)$$

being  $s_{\eta,i}^\dagger = \chi/\eta [\bar{u}_i - \bar{u}_{b,i}]$ . The subscript  $\eta$  is omitted from  $\bar{u}_i$  and  $\bar{p}$  for convenience.  $\bar{\Pi}_{ij} := \bar{u}_i \bar{u}_j - (\nu + \nu_t) \partial \bar{u}_i / \partial x_j + (\bar{p}/\rho) \delta_{ij}$  is the average total tensor. What is happening inside the solid region now needs to be investigated.

The idea behind VP-IBM is to quickly damp the solution in  $\Omega_{\text{body}}$ . The characteristic length and time scales of the domain are  $\mathcal{L}$  and  $\mathcal{T}$ , respectively, and the characteristic velocity and pressure scales are  $\mathcal{U}$  and  $\mathcal{P}$ , respectively. In convection-dominant problems (e.g. turbulent flows)  $\mathcal{P} \sim \rho \mathcal{U}^2$ . Introducing those scales in the momentum equation (2) and multiplying by  $\eta/\mathcal{U}$ , the resulting is

$$\begin{aligned} \frac{\eta}{\mathcal{T}} \frac{\partial u_{\eta,i}^*}{\partial t^*} + \frac{\eta}{\mathcal{T}_c} \frac{\partial}{\partial x_j^*} (u_{\eta,i}^* u_{\eta,j}^* + p_\eta^* \delta_{ij}) \\ - \frac{\eta}{\mathcal{T}_d} \frac{\partial^2 u_{\eta,i}^*}{\partial x_j^* \partial x_j^*} + \chi [u_{\eta,i}^* - u_{b,i}^*] = 0, \end{aligned} \quad (5)$$

where  $\mathcal{T}_c := \mathcal{L}/\mathcal{U}$  is a characteristic convection time,  $\mathcal{T}_d := \mathcal{L}^2/\nu$  is a characteristic diffusion time, and  $\phi^*$  is a dimensionless generic variable. The relation between convection and diffusion times is given by the Reynolds number:  $\mathcal{T}_d/\mathcal{T}_c = Re := \mathcal{U}\mathcal{L}/\nu$ .

Let's take a value of  $\eta$  small enough so that  $\eta \ll \mathcal{T}_c$  and  $\eta \ll \mathcal{T}_d$ . When the Reynolds number is large,  $\mathcal{T}_d \gg \mathcal{T}_c$  and the penalty condition yields

$$\eta \ll \mathcal{T}_c \ll \mathcal{T}_d. \quad (6)$$

This condition is equivalent to the intermediate damping regime described by Hester, Vasil, and Burns<sup>12</sup>. Hester, Vasil, and Burns<sup>12</sup> defined several volume-penalty regimes depending on the damping time scale  $\varepsilon_t$  ( $\eta/\mathcal{T}_c$  in Eqn. (5)), the damping length scale  $\varepsilon_l$  ( $\eta/\mathcal{T}_d$  in Eqn. (5)), and the Reynolds number. They show that to approximate the body, both  $\varepsilon_t$  and  $\varepsilon_l$  must be small; and for a high Reynolds number, the damping time scale dominates the damping length scale, whose interpretation is identical to the condition (6). Therefore, the

penalty source must dominate the spatial term of Eqn. (5). This penalty condition seems to hold even if the location of  $\chi$  is not known beforehand, as in deformable bodies<sup>27</sup>.

As a result, the governing equation within the body region is the following:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{1}{\eta} \bar{u}_i = \frac{1}{\eta} \bar{u}_{b,i}, \quad \forall x_i \in \Omega_{\text{body}}(t), \quad (7a)$$

with initial condition  $\bar{u}_i(x_i, 0) = \bar{u}_{b,i}^0$ . The analytical solution is

$$\bar{u}_i = e^{-t/\eta} \left[ \bar{u}_{b,i}^0 + \frac{1}{\eta} \int_0^t \bar{u}_{b,i} e^{\tau/\eta} d\tau \right], \quad (7b)$$

within  $\Omega_{\text{body}}$ . Upon employing the Integration-by-Parts (IbP) formula to evaluate the integral of equation (7b), the outcome is:

$$\int_0^t \bar{u}_{b,i} e^{\tau/\eta} d\tau = \eta \bar{u}_{b,i} e^{t/\eta} - \eta \int_0^t \frac{\partial \bar{u}_{b,i}}{\partial t} e^{\tau/\eta} d\tau - \eta \bar{u}_{b,i}^0.$$

Repetition of IbP to the new integral over and over again results in

$$\begin{aligned} \int_0^t \bar{u}_{b,i} e^{\tau/\eta} d\tau &= \eta \left[ \bar{u}_{b,i} e^{t/\eta} - \bar{u}_{b,i}^0 \right] \\ &+ \sum_{k=1}^{\infty} (-1)^k \eta^{k+1} \left[ \frac{\partial^k \bar{u}_{b,i}}{\partial t^k} e^{t/\eta} - \frac{\partial^k \bar{u}_{b,i}}{\partial t^k} \Big|_0^0 \right]. \end{aligned}$$

Substituting the latter into the solution (7b), the velocity field within  $\Omega_{\text{body}}$  can be written as follows,

$$\bar{u}_i = \bar{u}_{b,i} + \sum_{k=1}^{\infty} (-1)^k \eta^k \left[ \frac{\partial^k \bar{u}_{b,i}}{\partial t^k} - \frac{\partial^k \bar{u}_{b,i}}{\partial t^k} \Big|_0^0 \right] e^{-t/\eta}. \quad (7c)$$

The limit case shows that  $\lim_{\eta \rightarrow 0} \bar{u}_i = \bar{u}_{b,i} \quad \forall x_i \in \Omega_{\text{body}}(t)$ . This complements what Angot, Bruneau, and Fabrie<sup>4</sup> prove with greater rigour. The infinite sum can be understood as an artificial velocity arising from errors due to the modellization of the volume penalization.

On the other hand,  $\bar{u}_i \neq \bar{u}_{b,i} \quad \forall x_i \in \Omega_{\text{body}}(t)$  in a general case. Only if the body does not move ( $\bar{u}_{b,i} = 0$ ) or the body moves uniformly ( $\bar{u}_{b,i} \neq \bar{u}_{b,i}(t)$ ) then  $\bar{u}_i = \bar{u}_{b,i} \quad \forall x_i \in \Omega_{\text{body}}(t)$ . Even in the steady state, the result is  $\lim_{t \rightarrow +\infty} \bar{u}_i = \bar{u}_{b,i} + \mathbf{u}_i$  where  $\mathbf{u}_i$  is the remainder term of Eqn. (7c).

Let's rethink the penalization problem from a different perspective. First, the penalty source in penalized system (2) is rearranging as follows:

$$s_{\eta,i} = \mathcal{R}_\eta [u_i - u_{b,i}], \quad (8a)$$

where

$$\mathcal{R}_\eta(x_i, t) := \frac{\chi}{\eta} = \begin{cases} \frac{1}{\eta}, & \text{If } x_i \in \Omega_{\text{body}}(t) \\ 0, & \text{Otherwise} \end{cases}. \quad (8b)$$

The inverse of permeability is called resistance. Therefore,  $\mathcal{R}_\eta$  represents a piecewise-constant function of fluid resistance throughout the domain  $\Omega$ . Now, Reynolds decomposition and ensemble-averaging the penalized system (2) yields,

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0, \quad (9a)$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \bar{\Pi}_{ij} + \bar{s}_{\eta,i} = 0. \quad (9b)$$

In Equation (9b) we get the ensemble-averaged penalty source:

$$\bar{s}_{\eta,i} = \overline{[\mathcal{R}_\eta + \mathcal{R}'_\eta] [\bar{w}_i + w'_i]} = \overline{\mathcal{R}_\eta \bar{w}_i} + \overline{\mathcal{R}'_\eta w'_i}, \quad (9c)$$

where  $w_i = u_i - u_{b,i}$  is the relative velocity field. An extra term ( $\overline{\mathcal{R}'_\eta w'_i}$ ) arises because the body is moving. Why does  $\mathcal{R}_\eta$  split? Moving the body means in the VP-IBM problem that the fluid resistance changes.  $\mathcal{R}_\eta$  must be understood as a property of the fluid, such as density or viscosity, that changes. This allows it to fluctuate in the same nature as the flow; see Fig. 1.

The resistance fluctuation ( $\mathcal{R}'_\eta$ ) will occur mainly near the body interface. However, the assurance that  $\overline{\mathcal{R}'_\eta w'_i} = 0$  when  $\mathcal{R}'_\eta = 0$  away from the interface cannot be guaranteed due to correlation. In the case of a semi-infinite body, for example, once the resistance fluctuation is equal to zero,  $\overline{\mathcal{R}'_\eta w'_i}$  will decay to zero. However, within a finite body, a point enclosed by the body will be influenced by the entire interface, leading to the assumption that  $\overline{\mathcal{R}'_\eta w'_i}$  remains a non-zero value within  $\Omega_{\text{body}}$ .

At this point, the interpretation of the second term from Eqn. (9c) is probably of great interest because its physical interpretation is not straightforward. This fluctuating term should be related to an interaction between the fluid and the body. Cross-correlations involving this term ( $\mathcal{R}'_\eta$ ) cannot therefore be closed, like for the Reynolds stress tensor, for example (or the fluid-body interaction will have to be considered, and it is no longer a simple matter of solving the URANS equations). How could the term  $\overline{\mathcal{R}'_\eta w'_i}$  be applied in practice? A possible way could be the following.

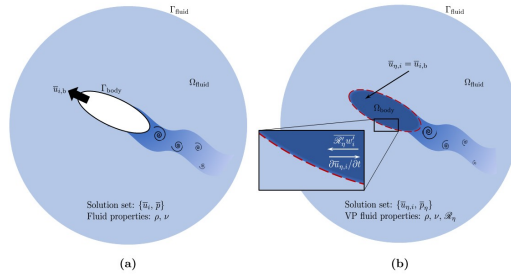


FIG. 1. A sketch of a body moving in a fluid flow. (a) classical problem: domain  $\Omega(t) = \Omega_{\text{fluid}}(t)$  and boundary  $\Gamma(t) = \Gamma_{\text{fluid}} \cup \Gamma_{\text{solid}}$ . (b) VP-IBM problem: domain  $\Omega = \Omega_{\text{fluid}}(t) \cup \Omega_{\text{solid}}(t)$  and boundary  $\Gamma = \Gamma_{\text{fluid}}$ , body interface in red dashed line.

Return to the same analysis as performed for Equations (7). The governing equations in the solid region for system (9) read as follows:

$$\frac{\partial \bar{u}_i}{\partial t} + \overline{\mathcal{R}_\eta \bar{u}_i} = \overline{\mathcal{R}_\eta \bar{u}_{b,i}} - \overline{\mathcal{R}'_\eta w'_i}, \quad \forall x_i \in \Omega_{\text{body}}(t), \quad (10a)$$

and its analytical solution,

$$\begin{aligned} \bar{u}_i &= \exp\left(-\int_0^t \overline{\mathcal{R}_\eta} d\tau\right) \\ &\times \left[\bar{u}_{b,i}^0 + \int_0^t \left[\overline{\mathcal{R}_\eta \bar{u}_{b,i}} - \overline{\mathcal{R}'_\eta w'_i}\right] \exp\left(\int_0^\tau \overline{\mathcal{R}_\eta} d\xi\right) d\tau\right]. \end{aligned} \quad (10b)$$

Now the question is: What would be the value of  $\overline{\mathcal{R}'_\eta w'_i}$  such that  $\bar{u}_i = \bar{u}_{b,i} \forall t > 0$ ? A straightforward calculation yields

$$\begin{aligned} \overline{\mathcal{R}'_\eta w'_i} &= \overline{\mathcal{R}_\eta \bar{u}_{b,i}} - \exp\left(-\int_0^t \overline{\mathcal{R}_\eta} d\tau\right) \\ &\times \frac{\partial}{\partial t} \left(\bar{u}_{b,i} \exp\left(\int_0^t \overline{\mathcal{R}_\eta} d\tau\right)\right). \end{aligned}$$

If the second term is expanded, then

$$\overline{\mathcal{R}'_\eta w'_i} = -\frac{\partial \bar{u}_{b,i}}{\partial t}. \quad (11)$$

The result is the acceleration of the body. The minus sign indicates that the acceleration of the fluid in the region of the body opposes the acceleration of the body.  $\overline{\mathcal{R}'_\eta w'_i}$  vanishes from Eqn. (9c) if and only if the body does not move or move uniformly. Therefore, the fluctuation term is an unsteady correction: a local force per mass acting on the fluid where the solid is supposed to be.

It is important to note that if the body does not move (i.e.  $u_{b,i} = 0$  and  $\mathcal{R}_\eta = \overline{\mathcal{R}_\eta}$ ), then  $\overline{s}_{\eta,i} = s_{\eta,i}^\dagger = \mathcal{R}_\eta \overline{u}_i$ . This means that “penalized the traditional URANS equations” and “averaging the penalized iNS equations” are indistinguishable procedures.

The system (9) with the new term (11) ends up as

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0, \quad (12a)$$

$$\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \overline{\Pi}_{ij} + \overline{\mathcal{R}_\eta} \overline{w}_i - \chi \frac{\partial \overline{u}_{b,i}}{\partial t} = 0. \quad (12b)$$

Body acceleration is multiplied by the mask function to apply the force per mass within  $\Omega_{\text{body}}$ . Together system (12a)-(12b) we impose, for convenience, the following set of boundary condition (BC) and initial value (IV), respectively,

$$\overline{u}_i = 0, \quad x_i \in \Gamma, t > 0 \quad (12c)$$

$$\overline{u}_i^0 = \chi \overline{u}_{b,i}^0, \quad x_i \in \Omega, t = 0 \quad (12d)$$

Now, the question arises of whether the new term (11) respects energy conservation, a fundamental principle of physical relevance. An energy stability analysis yields the following result:

**Theorem 1.** *Let  $\overline{u}_i$  be a solution to the system (12a)-(12b) with BC (12c) and IV (12d), then the energy norm of the solution is bounded by the body motion (boundary condition in the classical problem, Fig.1(a)) provided that the total (molecular and eddy) viscosity of the system does not become negative.*

*Proof.* Multiply Eqn.(12b) by  $\overline{u}_i$  and integrate over  $\Omega \times [0, T]$ ,

$$\underbrace{\int_0^T \int_\Omega \overline{u}_i \frac{\partial \overline{u}_i}{\partial t} d^3x dt}_{(I)} + \underbrace{\int_0^T \int_\Omega \overline{u}_i \frac{\partial \overline{\Pi}_{ij}}{\partial x_j} d^3x dt}_{(II)} + \underbrace{\int_0^T \int_\Omega \overline{u}_i \left[ \overline{\mathcal{R}_\eta} \overline{w}_i - \chi \frac{\partial \overline{u}_{b,i}}{\partial t} \right] d^3x dt}_{(III)} = 0. \quad (13)$$

The term (I): using the chain rule, applying Leibniz’s rule and integrating in time gives

$$\int_0^T \int_\Omega \overline{u}_i \frac{\partial \overline{u}_i}{\partial t} d^3x dt = \frac{\|\overline{u}(\cdot, T)\|_2^2 - \|\overline{u}_b^0(\cdot)\|_2^2}{2}, \quad (14a)$$

being the  $L^2$ -norm  $\|\phi\|_2^2 := \int_\Omega \phi^2 d^3x$  and  $\overline{u}^2 = \overline{u}_i \overline{u}_i$ .

The term (II): integrating by parts,

$$\int_\Omega \overline{u}_i \frac{\partial \overline{\Pi}_{ij}}{\partial x_j} d^3x = \oint_\Gamma \overline{u}_i \overline{\Pi}_{ij} n_j d^2x - \int_\Omega \frac{\partial \overline{u}_i}{\partial x_j} \overline{\Pi}_{ij} d^3x, \quad (14b)$$



the first integral of the right-hand side (RHS) becomes zero by BC (12c),  $n_j$  is the normal vector of  $\Gamma$ . Using mass conservation to the second integral of the RHS,

$$\int_{\Omega} \frac{\partial \bar{u}_i}{\partial x_j} \bar{\Pi}_{ij} d^3x = \frac{1}{2} \int_{\Omega} \frac{\partial (\bar{u}^2 \bar{u}_j)}{\partial x_j} d^3x - \int_{\Omega} (\nu + \nu_t) \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_i}{\partial x_j} d^3x. \quad (14c)$$

The first integral of the RHS became zero after applying the divergence theorem and BC (12c).

The term (III): This integral only exists within  $\Omega_{\text{body}}$ . In this region, we deduce that  $\bar{u}_i = \bar{u}_{b,i}$  ( $\bar{w}_i = 0$ ). Using the chain rule, applying Leibniz's rule and integrating in time gives

$$\int_0^T \int_{\Omega} \bar{u}_i \left[ \overline{\mathcal{R}_{\eta} \bar{w}_i} - \chi \frac{\partial \bar{u}_{b,i}}{\partial t} \right] d^3x dt = \frac{\|\bar{u}_b^0(\cdot)\|_2^2 - \|\bar{u}_b(\cdot, T)\|_2^2}{2}. \quad (14d)$$

Inserting (14) into (13) and reassigning gives

$$\|\bar{u}(\cdot, T)\|_2^2 = \|\bar{u}_b(\cdot, T)\|_2^2 - 2 \int_{\Omega} (\nu + \nu_t) \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_i}{\partial x_j} d^3x.$$

Assuming  $\nu + \nu_t \geq 0$ , the above integral is negative semi-definite, and therefore  $\|\bar{u}(\cdot, T)\|_2 \leq \|\bar{u}_b(\cdot, T)\|_2$ .  $\square$

The reach and applicability of the ideas proposed in this letter to other problems are investigated briefly. For example, let's assume the body not only moves but also has a fixed temperature gradient at the wall,  $\partial T / \partial n = q$  where  $\partial T / \partial n = n_k \partial T / \partial x_k$  with  $n_k$  the surface normal and  $q$  a heat flux. The inhomogeneous Neumann condition is enforced by applying an external force on the derivatives of  $T$  where the normal surface extends linearly within the body region<sup>28</sup>. This leads to the penalized heat equation  $\partial T / \partial t + \partial(u_j T + \kappa \partial T / \partial x_j) / \partial x_j + \mathcal{R}_{\eta_T} h = 0$  where  $\kappa$  is the thermal diffusivity (constant),  $\mathcal{R}_{\eta_T} := \chi / \eta_T$  is the thermal resistance, and  $h := \partial T / \partial n - q$ . In a similar analysis as above, the averaged governing equation within the body region is  $\partial \bar{T} / \partial t + \overline{\mathcal{R}_{\eta_T} \partial T / \partial n} = \overline{\mathcal{R}_{\eta_T} \bar{q}} - \overline{\mathcal{R}'_{\eta_T} h'}$ . After some mathematical manipulations, the following advection equation yields  $\partial \bar{h} / \partial t + \partial(\overline{\mathcal{R}_{\eta_T} \bar{h}}) / \partial n = -\partial(\overline{\mathcal{R}'_{\eta_T} h'}) / \partial n - \partial \bar{q} / \partial t$ . With an appropriate zero value of  $\bar{h}$  as both IV and BC, the gradient of  $\overline{\mathcal{R}'_{\eta_T} h'}$  in the direction of surface normal must balance the temporal variation of  $\bar{q}$  to achieve a null solution within the body region. Using the method of characteristics,  $\overline{\mathcal{R}'_{\eta_T} h'} = -\int \partial \bar{q} / \partial t d\xi$  with  $dx_k / d\xi = n_k$ .

Another application of these concepts concerns compressible flows. Now, the penalty source (8) is written  $s_{\eta,i} = \mathcal{R}_\eta \rho w_i$ . To obtain again an averaged form of the momentum equation, the penalized instantaneous momentum equation (2b) is assemble-averaged. Now, introducing the Favre decomposition ( $a = \tilde{a} + a''$  where  $\tilde{a} = \overline{\rho a} / \bar{\rho}$  is the density-weighted average) of  $w_i$  and the Reynolds decomposition ( $a = \bar{a} + a'$ ) of  $\mathcal{R}_\eta$  and  $\rho$  gives the following ensemble-averaged penalty source:  $\bar{s}_{\eta,i} = \bar{\rho} \widetilde{\mathcal{R}_\eta w_i} + \overline{\rho \mathcal{R}'_\eta w''_i}$ , where  $\mathcal{R}_\eta$  has been expressed in terms of a density-weighted average for convenience. The same analysis as in (10) results in  $\overline{\rho \mathcal{R}'_\eta w''_i} = -\partial(\bar{\rho} \tilde{u}_{b,i}) / \partial t$ . For the conservation equation in compressible flows, a Neumann condition is added<sup>29,30</sup>. Similarly to the previous thermal problem, the modelling of the new cross-correlation term can be achieved.

An important observation is that VP is highly dependent on the porous medium modelling approach. The penalization discussed in Eqn. (2) is referenced to as the “standard” VP, to distinguish it from the Characteristics-Based VP (CBVP)<sup>28,30</sup>. In CBVP, spatial terms undergo penalization but also the introduction of a penalty non-physical diffusion. Although the ideas in this letter can be applied to CBVP, the calculations might be less cumbersome if the penalization equation is expressed in a conservative form. In that case, the new diffusion coefficient would allow for fluctuation.

To conclude, this letter shows a discrepancy in the process of obtaining the penalized turbulence equations. The URANS equations were used for this purpose. This discrepancy arises from the way the turbulent solution is penalized: a new penalty source that penalized the mean flow or averaged the original penalty source. From a conceptual point of view, the traditional URANS equations were derived from the Navier-Stokes equations (1). If the URANS equations for a penalized flow are desired, the starting point should be the system (2) by applying Reynolds’ decomposition and ensemble averaging.

The main idea of the letter is to treat the coefficient  $\chi/\eta$  as a new property (namely, fluid resistance) of the VP-IBM flow problem. The average of the penalty source adds an additional term from the cross-correlation between the fluid resistance and the relative velocity field. To provide a physically interpretable explanation for the presence of this additional term, a study of the velocity field within the body region was proposed. By removing the modelling errors in this region, the body acceleration emerges as this additional term. If the body does not move or move uniformly, then both ways of proceeding with the penalty source lead to the same results, and the processes can be said to be indistinguishable.

If not, the body acceleration term remains as an unsteady corrector. Lastly, these ideas could be extrapolated to problems with other types of conditions or compressible flow.

The results of the present aim to demonstrate that deriving a penalized form of the turbulent equations without due care may lead to overlooking terms crucial for accurately modelling turbulence in such penalized flows.

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