The impact and treatment of the Gibbs phenomenon in immersed boundary method simulations of momentum and scalar transport

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Abstract

Spectral discretization of quantities exhibiting abrupt shifts results in oscillations, or “ringing”, known as the Gibbs phenomenon. When spectral discretization is used to evaluate spatial gradients during numerical integration of the transport equations governing turbulent fluid flows, these oscillations can contaminate various flow quantities. A particularly relevant application where the emergence of Gibbs phenomenon is a well-recognized weakness is in the context of simulations using the immersed boundary method. In this paper, we examine the effect of the Gibbs phenomenon in such simulations in detail, and we propose a computationally efficient smoothing treatment to reduce the associated oscillations. The effectiveness of this treatment is demonstrated in *a priori* tests on functions with abrupt shifts, and in *a posteriori* tests in wall-modeled large-eddy simulations of incompressible flow and passive scalar transport over solid bluff bodies. Furthermore, the large eddy simulation results indicate that the Gibbs phenomenon’s impacts are significantly more detrimental

to the computations of the subgrid-scale quantities and of scalar transport close to the solid interface, as compared to their impact on computations involving the resolved velocity field.

Keywords: Gibbs phenomenon, immersed boundary method, immersed interface, large eddy simulation, spectral discretization

1. Introduction

Since the immersed boundary method (IBM) was first developed by Peskin [1], it has been successfully adapted and implemented for flows over various solid objects and complex surfaces [2-5]. The details related to implementing the IBM vary with the types of problems being dealt with [6], but the main advantage and appeal of this approach continue to be linked to the ability to use Cartesian (non-body conformal) grids and either continuous or discrete forcing to account for the force exerted by the bluff bodies on the flow, as summarized by Mittal and Iaccarino [6]. Furthermore, the method in general is straightforward to implement in existing codes, and only adds a relatively small computational overhead.

However, discontinuities in quantities of interest (eg. velocity, pressure, or temperature or density) often arise as a result of implementing the IBM. This can give rise to computational challenges, particularly for simulations of incompressible viscous flows

that use spectral discretizations (i.e. Fourier or Chebyshev collocation). Discontinuities (as in the case of a wall-modeled large-eddy simulation (LES)) in the computed variables arising from the IBM lead to a numerical artifact called the Gibbs phenomenon or Gibbs ringing [7], which refers to the characteristic oscillations in the truncated series expansion of the discontinuous function. The resulting unphysical oscillations associated with the function not being smooth and/or periodic can downgrade the numerical accuracy of spectral methods [8]; nevertheless, these methods are very appealing due to their ‘infinite order of accuracy’, provided the function is sufficiently smooth [9], and to their computational speed (i.e. quadrature in physical space versus Fourier space has $O(N^2)$ and $O(N \log N)$ operations, respectively). As such, it might not be always desirable to forego spectral methods to overcome the errors resulting from Gibbs ringing, particularly in mixed spectral/finite difference codes where Gibbs ringing error is usually restricted (along the direction using finite difference) to the region of the domain occupied by the solid. Therefore, assessing the impact of these errors on the simulated flow and transport, and developing approaches that can eliminate or at least mitigate them, are important challenges in numerical simulation of fluid flow and transport.

Avoiding or reducing Gibbs ringing is of both theoretical and practical interest. It has been extensively studied theoretically for problems that involve non-smooth or non-periodic functions that have analytical expressions [10-12]; however, the approaches proposed for treating the oscillations are not always directly transferable to numerical

solutions of discrete functions. For practical computational physics and engineering applications, the challenge imposed by the “oscillations” associated with the Gibbs ringing spans across different disciplines, such as environmental turbulent flows [13,14], aeroacoustics [15,16] and reactive chemical transport [17], and various strategies have been attempted to mitigate it.

Since Gibbs ringing is essentially related to the slow decay of Fourier coefficients, it is natural to test methods that attenuate the Fourier coefficients at the high frequencies that would be contaminated by the oscillations [18]. Applying spectral filters to accomplish that however removes the physical high wavenumber components, and it becomes difficult to assess the accuracy of this type of method in recovering the original function [19]. Goldstein et al. [20] noted that if the grid resolution is not high enough, more energy will be contained in the higher wavenumbers and thus spectral filtering could reduce the accuracy of the solution. As an alternative remedy, filtering/smoothing in the physical space can also reduce Gibbs ringing by allowing the spectral computations to be applied to a smoothed version/copy of the function. In the IBM implementation of Goldstein et al. [20], a ‘virtual’ force inside the bluff body was applied to obtain a smooth velocity field. Lamballais and Silvestrini [21] smeared the immersed boundary force over interfacial computational points by multiplying a Gaussian weight factor according to the distance from the interface. Although it reduces the oscillations, the location of the interface becomes diffuse. It is also worth noting that by using a sixth-order compact

scheme of ‘quasi-spectral’ accuracy, they observed non-negligible Gibbs oscillations that are usually not present with lower-order finite difference scheme. In addition, creating an internal flow field of no physical significance was also applied in direct numerical simulations (DNS) with quasi-spectral method coupled with IBM [22,23], which offered better regularity across the immersed boundary. Smoothing the velocity field in physical space can also be achieved using a radial basis function interpolation method, as illustrated by Fang et. al. [24], who successfully reduced Gibbs ringing using this approach. However, the computations needed to find the appropriate radial basis function representations and the iterative procedure in solving the Poisson equation for pressure combine to result in a high computational cost for this method. As a less expensive way to implement the physical space smoothing, Tseng et. al. [14] applied a Laplacian operator iteratively to the velocity field. However, the resulting smoothed field is sensitive to the initial values of the function and the number of iterations.

In general, the concept of ‘smoothing’ the original function via radial basis functions [24], adding a Laplacian operator [14], or through Fourier continuation analysis [25,26] have been demonstrated to be effective in reducing the Gibbs phenomenon whenever the function is non-smooth. However, given some of the challenges of these approaches mentioned above, the purpose of this paper is 1) to assess the influence of the Gibbs ringing errors on the simulated velocity and temperature fields in wall-bounded flows

over hot¹ bluff bodies to better understand the implications of these errors, and 2) to propose and test a new cost-effective and robust procedure to reduce the resulting oscillations and errors in simulations of high Reynolds number flows with IBM. The findings will be of significant value to the increasing number of scientists who are using the immersed boundary/interface method, combined with high-order numerical schemes, particularly given the relative scarcity of comparable studies that also address the problems of temperature or mass transfer. As we will show in this study, the consequence of Gibbs ringing is even more important for scalar exchanges at the solid-fluid interface. The outline of the paper is as follows. In the next section, we describe the new cost-effective smoothing procedure and show some *a priori* results of its effectiveness in reducing the “ringing” of the spectrally-computed derivatives of arbitrary discontinuous functions. In section 3, we briefly describe the implementation of the IBM in an LES code, along with the new smoothing approach. In section 4, we present two *a posteriori* LES test cases to illustrate the impact of Gibbs ringing on the velocity and temperature fields, and the improvement afforded by the smoothing procedure. Conclusions are drawn in the last section.

¹ For the purpose of this study, “hot” implies that the interfacial heat fluxes are from the solid to the fluid. We stress, however, that the associated thermal gradients are presumed to be sufficiently small that temperature can be treated as a passive quantity, with no influence on momentum transport.

2. Cubic Interpolation Smoothing

2.1 Gibbs phenomenon and order of accuracy

The Gibbs phenomenon refers to the nonuniform convergence behavior of a Fourier series approximation $\hat{f}(K)$ to the function $f(x)$ being approximated in the neighborhood of a discontinuity x_0 , in the limit of $K \rightarrow \infty$, where K is the wavenumber in the Fourier series [18] (in practice, $K > 2\pi/\Delta$, where Δ represents the computational mesh resolution). Two characteristics of Gibbs phenomenon are worth noting as summarized by Adomaitis [17]. The first one is that the Gibbs oscillations do not vanish with increasing number of terms N in the approximation series; instead, the magnitude of the oscillations asymptotically reaches a constant value of approximately 8.9% of the jump magnitude for a discontinuity of the type of a simple Heaviside step function [7]. The second one is that the oscillatory behavior extends beyond the discontinuity and influences the function approximation at all points in the physical space. Therefore, using spectral methods to calculate derivatives of quantities that are contaminated by these Gibbs errors will have a global impact on the model performance. To understand the origin of these errors, we point out that the order of accuracy of a spectral approximation of a derivative of order n of a function depends on the smoothness of its higher derivatives of order $> n$ [8]. The following theorem puts this in a more formal context:

Let $u \in L^2(\mathbb{R})$ have a q^{th} derivative ($q \geq 1$) of bounded variation, and let w be the q^{th}

spectral derivative of u on the discretized grid with spacing h , where $L^2(\mathbb{R})$ is the Hilbert space of complex square-integrable measurable functions, and h is assumed to be the spacing of a uniform mesh, without loss of generality. If u has $p - 1$ continuous derivatives in $L^2(\mathbb{R})$ for some $p \geq q + 1$ and a p^{th} derivative of bounded variation, then the absolute error in the spectral derivatives scales as $|w_j - u^q(x_j)| = O(h^{p-q}), h \rightarrow 0$, where $u^q(x_j)$ is the exact q^{th} derivative of u (for detailed proofs, please refer to [27] and [9]). Thus, if a function is not smooth at a point (e.g. the velocity at the solid-fluid interface which has a discontinuous first spatial derivative), its (exact) derivatives will not be continuous and the accuracy of their spectral approximation will therefore be adversely affected. As an example, if one is interested in the first derivative ($q = 1$), then attaining second-order accuracy for a spectral approximation requires that $p - q = 2$, which requires that $p = 3$ and $p - 1 = 2$; i.e. the function must have continuous first and second derivatives.

2.2 A priori tests of the cubic interpolation method

To obtain second-order accurate first derivatives with Fourier spectral method, the theorem above implies that continuity of the second derivative of a function is required [8]. An interpolation method across the discontinuity must therefore not only ensure continuity of the function itself, but also of its higher derivatives. For example, second-order accuracy of the first derivative near the neighborhood of the discontinuity

can be accomplished simply by applying a cubic interpolation to the function using two points in the fluid domain from each ‘side’ of the discontinuity as illustrated in Fig. 1. The resulting system is a four-by-four Vandermonde matrix, which is easy to solve. Thus, a uniquely determined cubic polynomial can be found with the four points. This is the interpolation scheme we apply and test *a posteriori* in this paper in numerical solutions of the Navier-Stokes equations. Note that different interpolation methods can be implemented as long as the continuity of the function and an appropriate number of higher derivatives at the interface is ensured. Also note that this method can be adapted to problems where a buffer region is introduced to make the simulation domain physically non-periodic along a direction over which spectral methods are used.

Fig. 1 A schematic picture showing the procedure of cubic interpolation smoothing, where two points (in the rectangular box) on each side of the discontinuity are used to construct the cubic polynomial $a_1x^3 + a_2x^2 + a_3x + a_4$ that is then used to construct a smoothed discrete function. The smoothed version of the function is then used in the spectral computations.

178 As an illustration, we consider the function $f(x) = (\sin(2x) + \sin(4x))(H(x_1') + H(x_2'))$,
 179 where H is the Heaviside step function, $x_1' = x - a$, and $x_2' = x - b$, where a and b are
 180 the left and right limits of the introduced discontinuity, respectively (see Fig. 2a.). Away
 181 from the discontinuity, $f(x)$ has finite well-defined analytical derivatives $g(x)$, but Fig. 2b
 182 shows that the derivatives obtained with a spectral method without any treatment are
 183 contaminated by Gibbs oscillations, near the discontinuity as well as away from it. These
 184 spectral derivatives depart significantly from the analytically computed $g(x)$. If the
 185 derivatives inside the discontinuity are not of interest (corresponding for example to
 186 velocity derivatives inside a solid region in a flow simulation with IBM), the cubic
 187 interpolation approach can be used to obtain second-order accurate derivatives in the
 188 region of interest (the fluid region). Fig. 2b demonstrates that the cubic interpolation
 189 smoothing procedure very effectively removes the Gibbs oscillations in the derivatives.
 190 Computation of the derivatives with a 4th order accurate finite difference scheme on the
 191 unsmoothed $f(x)$ are also shown and have larger errors than the spectral method with
 192 smoothing; this is consistent with the observation by other investigators (as mentioned in
 193 the introduction) that higher-order finite difference schemes are more adversely affected
 194 by the discontinuity of the function [21]. However, the errors in the finite difference
 195 gradients are related to their stencil, which becomes longer for higher-order schemes,
 196 extending into the solid, and are not exactly similar to the Gibbs phenomenon. Fig. 3

depicts another test for the function $f(x) = (10x^2)^{-1} (H(x_1') + H(x_2'))$. Similar to Fig. 2, the resulting Gibbs oscillation is effectively removed by the cubic interpolation smoothing. Again, the Fourier spectral method outperforms the 4th order finite difference method in achieving a higher accuracy.

Fig. 2 (a): $f(x) = (\sin(2x) + \sin(4x))(H(x_1') + H(x_2'))$, and a smoothed $f(x)$ where the values inside the discontinuity are interpolated using the cubic interpolation. (b): The first derivative of $f(x)$, $g(x)$, computed analytically, using 4th-order finite difference method, using the Fourier spectral method on the original $f(x)$ (No Smooth), and using the Fourier spectral method on the smoothed $f(x)$ (Smooth).

Fig. 3 (a): $f(x) = (10x^2)^{-1} (H(x_1') + H(x_2'))$, and a smoothed $f(x)$ where the values inside the discontinuity are interpolated using the cubic interpolation. (b): The first derivative of $f(x)$, $g(x)$, computed analytically, using 4th-order finite difference method, using the Fourier spectral method on the original $f(x)$ (No Smooth), and using the Fourier spectral method on the smoothed $f(x)$ (Smooth).

Recall from the theorem that the second-order accuracy was the lower limit for the spectral method, but the actual accuracy can be of higher order since the interpolation, while designed to ensure continuity of the second derivative, in practice might also yield continuity of higher derivatives. The higher order achieved by the smoothed spectral computation is illustrated in Fig. 4, which compares the maximum pointwise errors $\max(|g(x_i) - g_{sp,fd}(x_i)|)$, where $g(x)$ is the analytically-computed first derivative of $f(x)$ and $g_{sp,fd}(x)$ is the derivative calculated using a spectral or finite difference method. In Fig. 4a, one can also observe that the error decreases with N (the number of points used to discretize the function, or numerical resolution) if the cubic interpolation method is applied to the function before calculating the derivatives using Fourier spectral method,

226 second, and fourth order finite differences. The error of the unsmoothed spectral
227 computation on the other hand becomes worse with increasing resolution. Note that
228 unlike the previous figures (Figs. 2 and 3), the finite-difference gradients in Fig. 4a are
229 computed based on the smoothed function.

230 When the unsmoothed function is used (as in Figs. 2 and 3), the errors of the second and
231 fourth order finite difference methods increase in a similar way to the spectral method
232 without smoothing treatment, as shown in Figure 4b. While away from the discontinuity
233 the finite difference methods do not require a smoothing of the function since their error
234 is local, their maximum error occurs in the vicinity of the discontinuity when their stencil
235 extends into the discontinuity and their accuracy is thus reduced. The analysis in Fig. 4 is
236 only for $f(x) = (\sin(2x) + \sin(4x))(H(x_1') + H(x_2'))$, but a qualitatively similar trend is
237 obtained for $f(x) = (10x^2)^{-1}(H(x_1') + H(x_2'))$. Our proposed interpolation approach
238 hence also reduces these finite differencing errors near the discontinuity. This *a priori*
239 test illustrates that estimating the spatial gradient with a spectral method to an adequate
240 degree of accuracy is feasible near a discontinuity through interpolation of the function
241 into the discontinuous region, without any modification to the function outside of that
242 region, in a manner that ensures continuity of the second derivatives. While the
243 derivatives inside the discontinuity are not correct, we reiterate that with the IBM
244 approach this corresponds to regions inside the solid where regardless of the gradients

245 obtained, the velocity is reset to zero during time-advancement of the solution. Our
 246 method ensures that the computed gradients in the fluid regions are accurate, while
 247 maintaining the zero velocity in the solid region (for the pressure solver and wall model)
 248 to yield the correct forces on the fluid.

249 **Fig. 4. a)** The error between approximate values of $g(x)$ and the analytical result as a
 250 function of resolution N , i.e. the number of collocation points; the finite difference
 251 estimates are computed from the smoothed function. b) The errors when no cubic
 252 interpolation smoothing is implemented for the finite difference schemes; the errors
 253 increases with N for the finite difference methods similarly to the Fourier spectral method
 254 without smoothing.
 255
 256

257 As Lele [28] pointed out that comparing the Fourier coefficients of the derivative
 258 obtained from numerical scheme with the exact coefficients can give some interesting
 259 insights. Therefore, we look into the impact of smoothing on the Fourier transform of $g(x)$
 260 for $f(x) = (\sin(2x) + \sin(4x))(H(x_1') + H(x_2'))$ by computing the amplitude and phase
 261 of the Fourier coefficients of $g(x)$. We compared the amplitude and the phase of the
 262 analytical $g(x)$ with those of $g_{sp}(x)$ (with smoothing) and $g_{sp}^{usm}(x)$ (without smoothing).

A fast Fourier transform is applied to the various computed gradients to obtain the amplitude and phase information. Fig. 5(a) and (b) show the excellent agreement in terms of both amplitude and phase when the function is smoothed prior to computing the derivatives. On the other hand, the positive amplitude errors introduced in the high wavenumbers are clearly visible for $g_{sp}^{usm}(x)$ in Fig. 5(c); the phase errors also scatter across all wave numbers. Fig. 5 gives additional evidence that a cubic interpolation method in physical space will effectively rectify the amplitude error at high wavenumbers and correct for the phase error, which occurs for almost all wavenumbers. The large errors associated with the high wavenumbers (i.e. small spatial scales) when no smoothing is applied will have a profound impact in the subsequent *a posteriori* tests.

Fig. 4. Comparison of the amplitude (a) and phase (b) of the analytical result $g(x)$ and the one obtained from Fourier spectral method in which the original function $f(x)$ is treated with the proposed method $g_{sp}(x)$; the color bar represents the wavenumber. (c) (d): same as (a) and (b) but without cubic smoothing of the function $f(x)$.

Since eventually the goal is to apply this simple and effective cubic interpolation procedure to turbulent flow simulations, we tested the robustness of this method with the presence of a synthetic turbulent signal added to the original function $f(x)$. The turbulent perturbation signal $f_{\text{turb}}(x)$, which is added to the function, follows the $-5/3$ energy spectrum typical of Kolmogorov's inertial-range turbulence, with a turbulent length scale representative of the one resolved in turbulent simulations such as large eddy simulations. $f(x) + f_{\text{turb}}(x)$, with and without smoothing interpolation, are shown in Fig. 6. In this case, no analytical derivatives are available, but the figure clearly illustrates that near the

discontinuity, the Gibbs oscillations are effectively reduced and the FFT with smoothing agrees well with the 4th order finite difference derivatives (based on smoothed function).

Fig. 6 a) $f(x) + f_{turb}(x) = (\sin(2x) + \sin(4x))(H(x_1') + H(x_2')) + f_{turb}(x)$ and its smoothed version. b) The first derivative $d(f + f_{turb})/dx = g(x)$ using 4th order finite difference method with smoothing, Fourier spectral method without smoothing and with smoothing. For clarity, only the region close to the discontinuity is shown in b. However, the impact of artificial oscillations extends globally.

3. LES-IBM with cubic interpolation

While in the previous section we illustrated the effectiveness of cubic interpolation in reducing Gibbs ringing errors, the actual application of this method in a turbulent flow simulation code will likely raise additional challenges and it is unclear if the method will work equally well in *a posteriori* tests. It is also very important to assess the degradation in the quality of the flow simulation due to Gibbs errors, and the benefit of applying the interpolation treatment. To conduct these *a posteriori* tests, we will consider a

305 pseudospectral large eddy simulation (LES) code with an IBM scheme and apply it to
 306 simulate a viscous incompressible flow transporting a passive scalar emitted at the solid
 307 surface (e.g. heat from a building wall). We use the wall-modeled LES approach (see
 308 [29,30]), in which a discrete time momentum forcing is used to simulate the immersed
 309 boundary force, such that the velocity field inside the obstacle is zero. We select to test
 310 the method in a wall-modeled LES, since tests in DNS or wall-resolved LES are less
 311 challenging. The velocity in DNS and wall-resolved LES transitions more gradually to
 312 the no-slip condition near the wall, compared with the wall-modeled approach. A sharper
 313 transition (in wall-modeled LES) will result in more severe Gibbs ringing and if our
 314 proposed method is effective in reducing the Gibbs ringing in wall-modeled LES, we
 315 would expect an even better performance in wall-resolved simulations.
 316 A Lagrangian scale-dependent dynamic subgrid-scale model is used [31]. For details of
 317 the LES code, please refer to [32]. Here we give a brief description of the LES-IBM code,
 318 while detailing the cubic interpolation smoothing treatment. The LES code solves the
 319 resolved continuity, Navier-Stokes, and scalar conservation equations (we will omit the
 320 usual tilde above the variables that denotes filtering for simplicity, but all the variables
 321 we will discuss are the filtered resolved components solved in LES unless otherwise
 322 noted):

$$\frac{\partial u_i}{\partial x_i} = 0 \quad \mathbf{x}(1)$$

$$\frac{\partial u_i}{\partial t} + u_j \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) = -\frac{\partial p}{\partial x_i} + F_i - \frac{\partial \tau_{ij}}{\partial x_j} \quad (2)$$

$$\frac{\partial s}{\partial t} + u_i \frac{\partial s}{\partial x_i} = -\frac{\partial q_i^s}{\partial x_i} \quad (3)$$

where t denotes time, u_i is the resolved i^{th} component of velocity, p is a modified pressure, F_i is a body force (that excludes the IBM force but can include gravity and a constant driving pressure gradient for boundary layer flows, for example), τ_{ij} is the deviatoric part of the subgrid stress tensor. The density is assumed equal to 1 (all the equations are normalized so the numerical value of the density is irrelevant). In equation (3), s denotes the scalar quantity and q_i^s is the i^{th} component of the subgrid scale scalar flux. The Einstein convention is used here, where summation is implied for repeated indices. Since the code uses the second-order Adams-Bashforth time stepping method, the discretized form of equation (2) can be broken into two steps:

$$u^* = \Delta t \left(\frac{u_i^n}{\Delta t} + \frac{3}{2} RHS_i^n - \frac{1}{2} RHS_i^{n-1} + \frac{1}{2} \frac{\partial p^{n-1}}{\partial x_i} \right), \quad (4)$$

and

$$u_i^{n+1} = \Delta t \left(\frac{u_i^*}{\Delta t} - \frac{3}{2} \frac{\partial p^n}{\partial x_i} + f_i \right), \quad (5)$$

where u^* is an intermediate velocity, n refers to the number of the current time step, Δt is the time step; $RHS_i = -u_j \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) + F_i - \frac{\partial \tau_{ij}}{\partial x_j}$; F_i is the body force; and f_i is the immersed boundary force given by:

$$f_i = \begin{cases} 0 & \text{for points outside the immersed boundary (fluid),} \\ \frac{3}{2} \frac{\partial p^n}{\partial x_i} - \frac{u^*}{\Delta t} & \text{for points inside the immersed boundary (solid).} \end{cases} \quad (6)$$

In our code, the intermediate velocity u^* is set to zero inside the solid area, which simplifies the equation of the body force. Alternative approaches to the implementation of the IBM can be used (e.g. [24]), but here we adhere to the implementation detailed by Chester et al. in [13] since our focus is on the Gibbs phenomenon rather than the details of the IBM. Before solving Eq. (5) for u_i^{n+1} , we must obtain the pressure field, which is so far unknown for time step n . The divergence of Eq. (5) is taken and the resulting Poisson equation is solved for the modified pressure p , while imposing that $\frac{\partial u_i^{n+1}}{\partial x_i} = \frac{\partial f_i}{\partial x_i} = 0$ to yield a divergence free velocity field at time $n+1$. The resulting Poisson equation is

$$\frac{\partial^2 p}{\partial x_i^2} = \begin{cases} \frac{2}{3\Delta t} \frac{\partial u_i^*}{\partial x_i} & \text{for points outside the immersed boundary (fluid),} \\ 0 & \text{for points inside the immersed boundary (solid).} \end{cases} \quad (7)$$

It is also worth noting that if the Gibbs oscillations are present in the velocity gradients, such errors will also propagate spatially by solving the Poisson equation – an elliptic PDE – resulting in a global influence from these oscillations even along directions that do not use spectral discretization.

While vertical derivatives are computed using a second-order centered-difference scheme in the code (and hence no special treatment for the Gibbs phenomenon is required), the

Fourier-based pseudospectral method is used for calculation of the horizontal derivatives.

The horizontal partial derivatives for u_i are computed independently in the x and y directions following:

$$\frac{\partial u_i(x, y, z)}{\partial x} = \sum_{k_x} [\hat{u}_i(k_x, y, z)(ik_x)] e^{ik_x x} \quad (8)$$

and

$$\frac{\partial u_i(x, y, z)}{\partial y} = \sum_{k_y} [\hat{u}_i(x, k_y, z)(ik_y)] e^{ik_y y} \quad (9)$$

where $\hat{u}_i$ is the wavenumber space representation of u_i ; k_x and k_y are the wavenumbers in the x and y directions. Note that x and y in equations (8) and (9) correspond to the quadrature points, where u_i assumes its values. The cubic interpolation method described in the previous session is here applied independently in each of the x and y directions before obtaining the horizontal gradients spectrally using equations (8) and (9).

A level-set method [13] that uses a signed distance function is used to define or track the interface where cubic-interpolation smoothing is carried out. Similarly, this same procedure is applied to all other variables for which pseudospectral derivatives are calculated, namely: τ_{ij} in Eq. (2), and s and q_i^s in Eq. (3). It is also worth reemphasizing that the interpolated values inside the obstacle will not affect the values outside the obstacle since in the pressure solver and the wall model the zero velocity imposed by the IBM is used, while the smoothed functions are only used when taking the spectral derivatives of the variables indicated above. The desired velocity field will be

377 automatically generated by using the correct immersed boundary force f_i . The wall model
378 used in this study is an equilibrium log-law velocity and scalar concentration model to
379 account for the drag and scalar flux that the resolved obstacle surface applies to the
380 surrounding fluid. There is no wall model for a generalized geometry like the ones we use
381 here, but for the very high Reynolds numbers simulations considered here, the first grid
382 point will fall in the inertial layer [33,34], and thus the use of the equilibrium logarithmic
383 law is justified. Other approaches have been proposed in the literature but since this paper
384 is mainly concerned with the impact and reduction of Gibbs phenomenon, we do not
385 focus on improving or discussing the role of the wall model.

386 The current LES-IBM with the cubic interpolation approach only increases the
387 computational overhead by 3 to 5% in the following numerical tests. In general, it is
388 inexpensive to obtain the desired smoothed fields before the spectral method is used for
389 calculating horizontal derivatives. This is a major advantage of this approach.

391 **4. Numerical tests**

392 In this section we consider two test cases, one is the turbulent flow over a staggered array
393 of four cubes (in a periodic domain); the other is the scalar turbulent transfer problem
394 over a single wall-mounted cube. The impact of Gibbs ringing and the improvement in
395 the results associated with the cubic-interpolation IBM-LES are presented.

4.1 Flow over staggered cubes

The array of four staggered cubes of height h (used for normalizing the vertical distances from the wall) was selected since it is an extensively studied configuration. Experimental measurements, DNS and LES results under fully rough conditions are all available [35] [36], serving as a benchmark for detailed assessment of the impact of Gibbs phenomenon. Using the IBM-LES code described in the previous session, we simulated two test cases. The only difference is that smoothing treatment is applied to one of them. A horizontally periodic domain with free-slip impermeable top boundary condition is used for both simulations. The simulations are run for a warm-up period of 50 eddy turnover times defined as $L_z u_* / dt$, where L_z is the depth of the flow (here equal to the height of the domain), u_* the square root of the total kinematic surface stress generated by the simulation, and dt the time step. Statistics are computed over the next 50 eddy turnover times to ensure statistical convergence. Fig. 7 shows the configuration of the first test case; the points labeled from $x1$ to $x4$ are the locations where profiles of selected parameters were taken for comparison.

Fig. 8 shows the cross sections in x and y directions of the mean streamwise velocity u from the simulation with smoothing, showing no evidence of Gibbs ringing. The color scale indicates the magnitude of velocity. The mean velocity profiles for both smoothed and unsmoothed case, depicted in Fig. 9 show comparable results to Xie and Castro [36].

The means in this paper are taken in time, as surrogates of Reynolds averages, and are

denoted either by an overbar $\bar{}$ or by angle brackets $\langle \rangle$. The discrepancy resulting from the Gibbs ringing in the case without smoothing appears to be minimal. However, these profiles are relatively far from the immersed boundary and as shown in the previous section, the largest error introduced by Gibbs ringing is close to the first point near the discontinuity where the wall modeled stresses and fluxes in LES can be more significantly affected by these inaccuracies. Nevertheless, for this flow, the main surface drag is through the pressure/form drag, which does not seem to be very sensitive to the errors introduced by the Gibbs phenomenon near the wall.

Fig. 7 Configuration showing the geometry of four staggered cubes simulated in the two cases. Left: perspective view; right: top-view. Points marked with $x1$ to $x4$ are locations where the comparisons in subsequent figures were made. The flow enters from the bottom in right panel.

Fig. 8 The transects of mean streamwise velocity $\langle u \rangle$ along two vertical planes. The measurement points x_1 - x_4 indicated in Fig. 7 are labeled. The flow is coming from left to right in the top panel and into the page in the bottom panel. The color scale indicates the magnitude of the velocity.

Fig. 9 Comparison of the profiles of mean streamwise velocity $\langle u \rangle$ to the results of Xie and Castro [36]. These profiles were taken at points $x1$ (above); $x2$ (behind); $x3$ (in front); $x4$ (in between) labeled in Fig. 7. U_{ref} is a reference velocity taken at $z = 2h$.

To investigate the errors close to the discontinuity, a horizontal transect of both the vertical and horizontal mean velocities, $\langle w \rangle$ and $\langle u \rangle$, are plotted in Fig. 10 for the planes immediately below and above the top of the cube along the line that connects the points $x2$ and $x3$. These two planes are considered here because they include the most abrupt velocity change associated with the accelerating effect at the cube top, and feature the strongest oscillations. Although the vertical profile of $\langle u \rangle$ shows good agreement with

the benchmark results in Fig. 9, close to the interface, the presence of oscillations in Fig.
 10 is clear. This reaffirms that the impact of Gibbs ringing is more pronounced close to
 the interface. The smoothing is very effective for the plane below the top of the cubes ($z = 0.94h$) and results in velocity trends for both $\langle w \rangle$ and $\langle u \rangle$ that are significantly
 different (a difference of about 25% for $\langle u \rangle$ above the cube) from the simulation without
 smoothing. However, notice that for the planes above the top of the cubes $z = 1.06h — 1.12h$, the smoothing method cannot be applied since that plane has no
 immersed region. The sharp change in velocity there is indeed physical (as the flow goes
 past the top of the cube it changes its speed and direction very fast) and will result in
 some oscillations. Nevertheless, both $\langle w \rangle$ and $\langle u \rangle$ in Fig. 10 show less severe effect of
 ringing when smoothing is applied even above the cubes, especially for the wake region
 from $x/h=3 — 4$. The plane $z=0.94h$ displays significant ringing especially in the $\langle w \rangle$
 component, when no smoothing is done, but the ringing is effectively alleviated by the
 smoothing treatment.

Fig. 10 Profile of $\langle w \rangle$ and $\langle u \rangle$ along the line that connects x_1 - x_3 on planes close the top of the cube, where ringing is the most significant.

While the impact of Gibbs ringing on the mean parameters was moderate, the associated numerical oscillations would be expected to be more obvious and consequential for the second-order statistics. Gibbs ringing creates oscillations that can cancel out in the mean signal if spatial averaging is performed, thus leading to mean values close to the ones unaffected by the oscillations, but the second-order statistics can be more sensitive to these oscillations since their effect adds up and manifests itself as higher second-order moments in LES. Figs.11 and 12 show the comparisons of the LES-IBM simulated co-variances (stresses) and root-mean-square (rms) velocities to those from LES, DNS and experiments reported by Xie and Castro [36]. The second-order quantities in these figures represent the statistical characteristics of turbulence. Fig. 10 depicts a closer agreement between the total Reynolds stress (i.e. the

479 sum of resolved part and the SGS part) simulated with smoothing and those by Xie and
 480 Castro [36], compared to the simulations without smoothing, showing a more pronounced
 481 improvement than the mean profiles in Fig. 9. The unsmoothed simulations
 482 underestimate the stress near the top of the cubes at locations $x1$ and $x2$, and overestimate
 483 it at locations $x3$ and $x4$. The underestimations can be as large as about 30% of the peak
 484 value of the Reynolds stress. The overestimations in $x3$ and $x4$ are about 10% of their
 485 peak value. Note that we are not only comparing to the experimental results here, which
 486 could be contaminated by experimental errors, but also to the DNS and LES of Xie and
 487 Castro that use neither an IBM approach nor spectral numerical methods, and can be as
 488 such considered as the reference for these comparisons. At $x2$ the peak in the total
 489 Reynolds stress that occurs just above the top of the cube is better predicted when
 490 smoothing is applied. At $x3$, especially below the height of the cube, Fig. 11 shows that
 491 the simulation with smoothing accurately captures the increasing trend of $\langle u'w' \rangle$ below
 492 the first minima.

493 Fig. 12 shows the root-mean-square (rms) value of both streamwise velocity $\langle u \rangle$ and
 494 vertical velocity $\langle w \rangle$ at points $x2$ and $x3$. We should acknowledge that this comparison is
 495 a bit challenging since for the LES we are only showing the resolved rms velocities (we
 496 prefer not to attempt to model the SGS components since we are not certain about the
 497 accuracy of the available models in complex terrain), and since these quantities are more
 498 sensitive to the Reynolds number differences between experiments, DNS, and LES than

499 the mean velocities or stresses. But the comparison might still be informative. A slightly
 500 better agreement with the Xie and Castro simulations and experimental data is also found
 501 here when the smoothing treatment is applied, but the differences are not as significant as
 502 with the stresses. As stated previously, the surface drag is dominated by form drag. For a
 503 steady constant pressure gradient driven flow, the total wall friction velocity u_τ is set by
 504 the pressure gradient imposed (pressure forcing has to balance surface drag). The friction
 505 velocity u_* of the experimental/LES/DNS results of Xie and Castro is taken as $0.89u_\tau$.
 506 The value 0.89 is found for this geometry from theoretical argument given by [36,37]. It
 507 can be understood as an effective friction velocity of the rough channel flow. This u_* was
 508 used to non-dimensionalize the LES/DNS/Experimental results (Xie and Castro, 2006)
 509 that we compared with; therefore, we also adopted the same non-dimensionalization for
 510 our LES results. Despite the minor influence of the smoothing for these turbulent
 511 statistics, the agreement with the experimental/LES/DNS results away from the bottom
 512 wall validates the accuracy of our model, while the discrepancy at the bottom wall is
 513 related to the fact that the DNS and LES of Xie and Castro resolve the wall region and
 514 are therefore representing the trends in the buffer and viscous sublayer near the wall. On
 515 the other hand, our LES assumes a much higher Reynolds number, such that the first grid
 516 point above the bottom wall is already in the inertial log-region.

Fig. 11 Profiles of the Reynolds stress $\langle u'w' \rangle$ taken at points x1 (above); x2 (behind); x3 (in front); x4 (in between), as labeled in Fig. 7.

Fig. 12 Profiles of the rms streamwise and vertical velocities u and w taken at points x_2 (behind); x_3 (in front); labeled in Fig. 7.

The subgrid-scale (SGS) components are also some of the higher order moments that are expected to show sensitivity to Gibbs oscillations in LES. The SGS stress component τ_{13} is depicted in Fig. 13a along a streamwise line behind the cube (point x_4) at a height $z = 1.06h$, i.e. immediately above the top plane of the cube. The reduction of the oscillations when smoothing is applied is clear and demonstrates the effectiveness of this smoothing treatment in improving both the resolved and the subgrid scale components. Note the difference of about 100% in the magnitude of the SGS stress near the interfacial

533 computational points. Another key quantity in LES is the kinetic energy dissipation by
 534 the subgrid scales, which is often postulated to be the most important quantity an SGS
 535 model should reproduce [38]. Gibbs ringing can lead to excessive spatial gradients and
 536 thus to over estimation of the resolved strain rate S_{ij} , and this could contribute to an
 537 over-estimated SGS dissipation rate of resolved kinetic energy $\epsilon = -\langle \tau_{ij} S_{ij} \rangle$. As can be
 538 seen in Fig. 13b, the SGS dissipation rate of resolved kinetic energy, depicted along a
 539 streamwise line spanning the whole domain just beneath the top of the cube, is strongly
 540 overestimated and oscillates significantly when no smoothing is applied. The cubic
 541 interpolation smoothing almost eliminates the oscillations and reduces the magnitude of ϵ
 542 significantly. These observations are consistent with the *a priori* amplitude-phase
 543 analysis, such that the high wavenumber, i.e. small spatial scales, are more prone to the
 544 amplitude error. Note that the increase from the first point in front or behind the cube to
 545 the next point away from the cube is partially related to the transition from a wall model
 546 to an SGS model, and it is difficult to disentangle its effect from that of the Gibbs
 547 phenomenon in that region.

Fig. 13 a) The SGS stress component along a streamwise line directly behind (in the spanwise y direction) the center of the cube at a height $z = 1.06h$, i.e. right above the cubes. b) The SGS dissipation rate of resolved kinetic energy along a streamwise line spanning the whole domain at a height $z = 0.94h$, i.e. right below the top of the cubes.

To further analyze the details of Gibbs phenomenon on higher order statistics, we consider the radial power spectra of u and w shown in Figs. 14 and 15, respectively, both with and without smoothing. The radial power spectrum is obtained by time averaging 15 power spectra, each of which is constructed from the instantaneous velocity field in a horizontal plane (x - y plane). The radial wavenumber is defined as $k_r = \sqrt{k_x^2 + k_y^2}$. The horizontal axis is the radial wavenumber normalized by L_x , which is the streamwise length of the domain. The radial power spectrum will represent the contributions of ringing from both directions across different physical scales. For planes that are below the height of the cubes, the signature of the underlying geometry are shown as the periodic ‘bumps’ in the spectra, where the first bump corresponds approximately to the obstacle length scale (indicated by the vertical line) or the harmonics of that scale, and the subsequent bumps are all harmonics of the building length scale. Nevertheless, we

can identify the major impacts related to Gibbs phenomenon shown by the velocity spectra in Figs. 14 and 15. One impact is that the characteristic oscillations near the grid-scale (highest resolved wavenumber) that are clearly seen in the higher peak in the second to last point on the velocity spectra for the unsmoothed case. The w component shows a more pronounced effect, which is eliminated in the simulation with smoothing depicted in Fig. 15, thus confirming the successful removal of Gibbs oscillations. The other impact is variance in higher wavenumbers is reduced, as shown in Fig. 14. The variance of u distributed over the higher wavenumbers (above $k/L_z=0.1$) is larger in the case with cubic interpolation. Overall, the presence of Gibbs phenomenon does not change the distribution of energy in larger scales significantly, which explains why the mean and second-order moments were moderately affected by the associated errors. Hence, not much difference in the staggered cube case was found in Figs. 9, 11 and 12 when the mean quantities and second moments were compared with numerical simulations or experiments. On the other hand, the effect is the most significant at the smallest scales in the spectra, which explains the strong impact of the smoothing on the SGS quantities that are strongly tied to those smallest resolved scales. This also explains why that the stresses profiles show more improvement when smoothing is applied since the subgrid scale Reynolds stress can be highly contaminated by ringing.

Fig. 14 Radial power spectra F_{rad} of u without smoothing (left) and with smoothing (right) at four different heights below the obstacle. For clarity, only the higher wavenumber part ($k/L_x > 0.1$) of the spectra is shown.

Fig. 15 Radial spectra F_{rad} of w without smoothing (left) and with smoothing (right) at four different heights below the obstacle. For clarity, only the higher wavenumber ($k/L_x > 0.1$) part of the spectra is shown.

4.2 Passive scalar transfer of a single cube

Compared to velocity in incompressible high Reynolds number flows, the Gibbs

phenomenon will more detrimentally affect calculation of the transport of scalars (i.e. temperature with small thermal gradients or other passive substances). The reasons are two-fold: 1) the strongest influence from the ringing is near the boundary and thus introduce the highest error in the scalar boundary layers around the facets of the cube, where the transfer of scalars is occurring through turbulent diffusion in our wall-modeled LES (and through both viscous and turbulent diffusion in real flows), and 2) unlike momentum transfer that occurs through both viscous and pressure drag and that is dominated by pressure drag in high Reynolds number incompressible flows such as the one we simulate here, for scalars, the transfer is mainly through diffusive transport through the boundary layers and large errors associated with Gibbs ringing in those layers can become dominant.

The configuration and set up of the numerical test are similar to the one shown for multiple cubes in Fig. 7, but here we only have one hot wall-mounted cube. The cube is being heated from interior, where the wall-model of the LES is coupled to a one-dimensional heat conduction equation that assumes a constant core temperature. The fluid temperature initially is 273.15 K, the core temperature is fixed at 348.15 K, and the resulting surface temperature is around 318.15 K. Temperature in this case is modeled as a passive scalar for the purpose of demonstrating the impact of Gibbs phenomenon on scalars in general. The subgrid scale (SGS) model for momentum is the same as the simulation in previous session [31]. An eddy diffusivity model is implemented here as the

scalar SGS model, in which the SGS scalar flux is modeled as $q_i^s = -v_t / Pr_t$, where v_t is the eddy viscosity obtained from the momentum SGS model and Pr_t , the SGS turbulent Prandtl number set to 0.4. The warm up time is approximately over one eddy turn over time ($L_z u^* / dt$) only for this case since reaching a steady state is not essential. One additional eddy turn over time is used to obtain the averaged statistics. Similar to the previous simulations, two cases with and without the smoothing treatment were conducted. Fig. 16 depicts the time-averaged mean passive scalar field across a horizontal xy -plane. The Gibbs oscillation is almost completely removed in the case with smoothing treatment. More importantly, the development of the thermal boundary layer and thermal wake of the cube are hindered in the simulation with no smoothing due to the oscillations, while their development follows a more physically realistic pattern in the other simulation.

Fig. 16 Horizontal slice through the middle plane of the cube without smoothing (left) and with smoothing (right). Color scale is the temperature in Kelvin.

636 The two simulated cases were only ran for a relatively short period of time, such that the
 637 absolute difference in fluid temperature between them remained small. Therefore, we
 638 consider the quantity θ'' , defined as $\theta'' = (\theta - \theta_{init}) / (\langle \theta \rangle - \theta_{init})$, where θ_{init} is the
 639 initial air temperature, which is also the air temperature far from the wall, and $\langle \theta \rangle$ is the
 640 horizontally plane averaged fluid temperature of the case. θ'' represents the relative
 641 difference in the rate of heating between the two cases, from the initial conditions which
 642 are the same for both cases. Since the set up of this test is such that the temperature
 643 increases at closer distances to the cube surface, the decrease in the time-averaged
 644 temperature cross-sections in Fig. 17a near the cube from the case without smoothing
 645 follows a physically incorrect trend. The small oscillations for this case are also clearly
 646 visible. These problems are corrected by the smoothing. In general, Gibbs phenomenon
 647 results in to 40-50% less relative temperature increase near the wall. Fig. 17b depicts the
 648 vertical profile behind of the cube, showing significant differences between the
 649 simulations with and without smoothing. The most drastic change is near the top of the
 650 cube, where the temperature is expected to increase below the top and then steadily
 651 decrease. The results from the case with no smoothing are clearly contaminated by the
 652 Gibbs ringing, showing no appreciable increase in temperature. Thus, unlike the
 653 velocities shown in previous section, the accuracy of the mean profile of temperature can
 654 be more significantly degraded by the Gibbs errors. We have also plotted the radial
 655 power spectrum for temperature, but we do not show it here since it is quite similar to the

power spectra for the velocities depicted in Figs. 14 and 15. The cube-scale still imposes a characteristic signal in the spectra, and the simulation without smoothing yields a spurious increase in variance at small scales due to Gibbs ringing that is removed by the smoothing procedure applied to the other case.

Fig. 17 a) Normalized temperature θ'' cross-section along the x direction at the spanwise center of the cube and at $z/h=0.5$. b) The vertical temperature profile at the back of the cube, in the middle of the domain in the cross-stream direction, and at a streamwise distance to the interface of 3% of the size of the cube.

5. Conclusions

In this paper, we propose an approach for reducing the Gibbs phenomenon in simulations of incompressible flows in the context of the immersed boundary method. Compared to the previous solutions to this problem, we have demonstrated that this method is both effective and computationally efficient. The findings are particularly relevant for high Reynolds number incompressible flows in applications in engineering or environmental

fluid mechanics and mass transfer problems with the IBM approach.

After a proof-of-concept of the proposed method using *a priori* tests, the study analyzed and compared the effect of numerical errors caused by the Gibbs phenomenon in both turbulent momentum (where our results were compared to other experimental and numerical results) and scalar transfer problems. The mean velocities and second-order resolved statistics are moderately affected by the Gibbs phenomenon, with the co-variances being more sensitive to the errors than the variances or root-mean-square values. This was illustrated by comparing the various parameters at multiple points to experimental, DNS, and LES results from a code that does not use spectral computations or the IBM approach. The statistics related to the SGS scale were found to be significantly more sensitive to Gibbs errors, this is related to the larger impact of these errors on the smallest resolved scales (highest wavenumbers) as illustrated by both the *a priori* and the *a posteriori* tests.

Regardless of the magnitude of the impact of the Gibbs phenomenon, our proposed smoothing approach significantly improved the results for all parameters. The second-order resolved statistics showed better agreement with the results from the literature, and the trends were physically more realistic. These conclusions are also supported by the velocity spectra, which illustrated the spurious increase in energy at the smallest resolved scales due to the Gibbs ringing and thus explained why the SGS statistics are the most sensitive to the associated errors.

693 Compared to the impact on momentum, scalar transfer simulations can be much more
694 severely affected by the Gibbs ringing simply because of the nature of transfer
695 mechanism. Our simulations depicted the incorrect physical trend in the temperature
696 profile in the unsmoothed case near the boundary, and how the smoothing approach can
697 correct the problem. Moreover, the noted increase in computational overhead is more
698 than offset by the profoundly improved characterization of scalar fluxes. In general, we
699 can conclude that the Gibbs phenomenon associated with spectral method needs to be
700 assessed and mitigated more carefully when higher-order statistics and scalar transfer are
701 involved.

702 While we tested our method in a wall-modeled LES code, application to RANS,
703 wall-resolved LES or DNS should be very comparable and the benefits should be similar.
704 Finally, the cubic interpolation that we propose also resulted in more accurate
705 computations of derivatives using finite difference method at points where the stencils of
706 these methods would lie partially inside solid body.

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