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Equilibrium Eulerian approach for predicting the thermal field of a dispersion of small particles

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Abstract

The equilibrium Eulerian method [J. Ferry, S. Balachandar, A fast Eulerian method for disperse two-phase flow, Int. J. Multiphase Flow 27 (7) (2001) 1199–1226] provides an accurate approximation to the velocity field of sufficiently small dispersed particles in a turbulent fluid. In particular, it captures the important physics of particle response to turbulent flow, such as preferential concentration and turbophoresis. It is therefore employed as an efficient alternative to solving a PDE to determine the particle velocity field. Here we explore two possible extensions of this method to determine the particle temperature field accurately and efficiently, as functions of the underlying fluid velocity and temperature fields. Both extensions are theoretically shown to be highly accurate for asymptotically small particles. Their behavior for finite-size particles is assessed in a DNS of turbulent channel flow ($Re_\tau = 150$) with a passive temperature field ($Pr = 1$). Here it is found that although the order of accuracy of the two extensions is the same, the constant factor by which one is superior to the other can be quite large, so the less accurate extension is appropriate only in the case of a very small mechanical-to-thermal response time ratio.

Keywords: Two-phase flow; Eulerian; Equilibrium Eulerian; Thermal advection; Turbulent channel flow; Direct numerical simulation

1. Introduction

When particles or droplets are advected in a turbulent flow the fluid conditions seen by the particles/droplets change over time and as a result their temperature, in general, will differ from that of the local surrounding fluid. To calculate the temperature of the disperse medium a variety of approaches have been used. For very large particles, it is necessary to solve for the temperature distribution within the particle, and in the region of fluid surrounding it. In this case it is often assumed that the temperature distribution within the particle is radially symmetric. When a particle is not as large, its temperature can be represented by a single value. In this *Lagrangian–Eulerian* approach, the particle temperature is evolved by assuming that there exists a representative fluid temperature at the particle position and a

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Nomenclature

C	specific heat
d	particle diameter
D/Dt	time derivative following the fluid ($\partial/\partial t + \mathbf{u}\cdot\mathbf{V}$)
d/dt	time derivative following a particle ($\partial/\partial t + \mathbf{v}\cdot\mathbf{V}$)
h	channel half-height
k	thermal conductivity
p	pressure
Pr	Prandtl number
Re	Reynolds number
T	temperature
t	time
$\mathbf{u}$	fluid velocity
$\mathbf{v}$	particle velocity
x	streamwise distance
y	spanwise distance
z	wall-normal distance

Greek symbols

μ	dynamic viscosity
ρ	density
τ	particle response time

Subscripts and superscripts

e	equilibrium Eulerian quantity
ee	equilibrium Eulerian with equilibrium Eulerian velocity
ef	equilibrium Eulerian with fluid velocity
ep	equilibrium Eulerian with (exact) particle velocity
f	fluid quantity
p	(exact) particle quantity
T	thermal
τ	wall-friction-based
+	wall units

characteristic conduction time between the particle and the surrounding fluid. When particles are so numerous that it becomes impractical to track each one, a continuum assumption is typically applied. Rather than evolving individual particles, one evolves a particle number density. It is then necessary to model the velocity and temperature of this particle continuum. A simple solution is to assume that the velocity and temperature of the particle field is equal to that of the fluid. This procedure is only valid in the case of extremely small particles, however. When accurate values are required, the traditional approach is to use the *Eulerian–Eulerian* method, where an additional system of PDEs (partial differential equations) is solved for the dispersed phase velocity and temperature fields.

There are a number of difficulties with the Eulerian–Eulerian method: (a) it is costly to evolve systems of PDEs, particularly for polydisperse particulate systems; (b) the boundary conditions for these PDEs are not well understood; (c) because of the time-step limitations imposed by the momentum and thermal response times of the particle, the equations to be solved are often stiff; and (d) it is necessary to add spurious diffusion terms to stabilize the PDEs for particle velocity and temperature. Of course, these difficulties may all be avoided by simply setting the particle field velocity and temperature to that of the fluid, but in doing so important physics is neglected. For example, particles evolved using the fluid velocity do not preferentially concentrate [1,2] or exhibit turbophoretic migration [3] towards or away from the walls.

On the other hand, the *equilibrium Eulerian* method captures the essential physics represented by the deviation of particle velocity from the fluid velocity, without requiring additional PDEs to be solved [4,5]. In this method the dispersed phase velocity field is explicitly expressed as an expansion in terms of the local fluid velocity field and its spatial and temporal derivatives, with the particle time-scale as the small parameter [6,7]. This expansion allows for the dispersed phase velocity field to be different from the local fluid velocity and thus enables essential physics, such as preferential concentration and turbophoresis, to be represented. Rani and Balachandar [8] have tested the equilibrium Eulerian approach by advecting a passive particulate concentration field in isotropic turbulence over long periods of time and comparing the results with the corresponding Lagrangian particulate distribution. Meynet and Dupays [9] compared the equilibrium Eulerian approach to the standard Eulerian–Eulerian method in a flow within a solid rocket motor, and found good agreement between the velocity fields computed. They also tested what would seem like a reasonable extension of the equilibrium Eulerian method to temperature field, but observed some disagreement with the results of the Eulerian–Eulerian method.

In this paper we will consider systematic extensions of the equilibrium Eulerian approach to include the thermal field as well. Three possible variants of the equilibrium Eulerian method will be identified and investigated in detail. These variants will be tested in a direct numerical simulation (DNS) of a passive temperature field advected by turbulent channel flow, with a one-way coupled, Lagrangian–Eulerian particle model. It is found that the method used by Meynet and Dupays [9] is not sufficient, but that excellent results are obtained with a carefully implemented variant.

2. The equilibrium Eulerian method for thermal fields

The equation of motion for a single spherical particle immersed in a fluid is rather complex, even in the low Reynolds number regime, where the particle-based Reynolds number is much less than 1, and the particle much smaller than the Kolmogorov scale of the fluid [10,11]. This equation may be used to model the behavior of a system of particles when the particle concentration is low enough that particle–fluid and particle–particle interactions can be neglected.

Here the method will be presented for the simple case of particle motion influenced only by drag. The neglect of other added-mass and history forces is appropriate for cases with a large particle-to-fluid density ratio. The equation of motion is then

$$\frac{\mathrm{d}v}{\mathrm{d}t} = \frac{\mathbf{u}-\mathbf{v}}{\tau}, \tag{1}$$

where $\mathbf{u}$ denotes the fluid velocity at particle location; $\mathbf{v}$, the particle velocity; $\mathrm{d}/\mathrm{d}t$, a time derivative following the particle; and τ, the particle response time, which is defined as follows:

$$\tau = \frac{\rho_\mathrm{p} d^2}{18\mu_\mathrm{f}}. \tag{2}$$

In this equation, μ_f is the dynamic viscosity of the fluid, ρ_p is the density of the particle material, and d is the particle diameter.

As noted by various authors [6,7], the particle velocity in (1) may be expanded formally in powers of τ. Such an expansion is valid for sufficiently small τ, since the particle velocity field then entrains exponentially quickly to a unique function of the fluid velocity field (and its spatial and temporal derivatives), independent of its initial condition [4]. In other words, there exists an equilibrium particle velocity field to which all solutions to (1) will entrain to provided τ is small. The equilibrium Eulerian expansion to particle velocity to $\mathrm{O}(\tau)$ accuracy can be expressed as

$$\mathbf{v}_\mathrm{e} = \mathbf{u} - \tau\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t}. \tag{3}$$

Here $\mathrm{D}/\mathrm{D}t$ denotes a time derivative following the fluid.

The energy equation for the evolution of particle temperature T_p can be written as [12]

$$\frac{\mathrm{d}T_\mathrm{p}}{\mathrm{d}t} = \frac{T_\mathrm{f}-T_\mathrm{p}}{\tau_\mathrm{T}}. \tag{4}$$

Here T_f is the fluid temperature, and τ_T is the particle's thermal response time

$$\tau_\mathrm{T} = \frac{C_\mathrm{p}\rho_\mathrm{p} d^2}{12k_\mathrm{f}}, \tag{5}$$

where k_f is the thermal conductivity of the fluid, and C_p is the specific heat of the particle.

To derive an equilibrium expansion for particle temperature based on (4), one begins by rewriting it as

$$T_\mathrm{p} = T_\mathrm{f} - \tau_\mathrm{T}\frac{\mathrm{d}T_\mathrm{p}}{\mathrm{d}t}. \tag{6}$$

The term $\mathrm{d}T_\mathrm{p}/\mathrm{d}t$ can then be replaced by substituting the expression in (6) for it, resulting in the expansion

$$T_\mathrm{p} = T_\mathrm{f} - \tau_\mathrm{T}\frac{\mathrm{d}T_\mathrm{f}}{\mathrm{d}t} + \mathrm{O}(\tau_\mathrm{T}^2). \tag{7}$$

Let T_ep denote the first-order truncation of this series

$$T_\mathrm{ep} = T_\mathrm{f} - \tau_\mathrm{T}\frac{\mathrm{d}T_\mathrm{f}}{\mathrm{d}t}. \tag{8}$$

In this equation the convective derivative $\mathrm{d}T_\mathrm{f}/\mathrm{d}t$ follows the exact particle velocity rather than some approximation to it.

To obtain a usable method, however, the convective derivative $\mathrm{d}T_\mathrm{f}/\mathrm{d}t$ in (8) must be approximated by a derivative following a velocity that can be computed. Using the approximation $\mathbf{v} = \mathbf{u} + \mathrm{O}(\tau)$, one obtains

$$T_\mathrm{ef} = T_\mathrm{f} - \tau_\mathrm{T}\frac{\mathrm{D}T_\mathrm{f}}{\mathrm{D}t} \tag{9}$$

as a possible method, and using $\mathbf{v} = \mathbf{v}_\mathrm{e} + \mathrm{O}(\tau^2)$, one obtains

$$T_\mathrm{ee} = T_\mathrm{f} - \tau_\mathrm{T}\left(\frac{\partial T_\mathrm{f}}{\partial t} + \mathbf{v}_\mathrm{e}\cdot\nabla T_\mathrm{f}\right). \tag{10}$$

The order of accuracy of the above approximations to T_p are

$$T_\mathrm{p} = T_\mathrm{f} + \mathrm{O}(\tau_\mathrm{T}), \tag{11}$$

$$T_\mathrm{p} = T_\mathrm{ef} + \mathrm{O}(\tau\tau_\mathrm{T}) + \mathrm{O}(\tau_\mathrm{T}^2), \tag{12}$$

$$T_\mathrm{p} = T_\mathrm{ee} + \mathrm{O}(\tau^2\tau_\mathrm{T}) + \mathrm{O}(\tau_\mathrm{T}^2), \tag{13}$$

$$T_\mathrm{p} = T_\mathrm{ep} + \mathrm{O}(\tau_\mathrm{T}^2). \tag{14}$$

For a fixed value of τ, the methods T_ef and T_ee are only first-order accurate in τ_T, which is the same as simply using the fluid velocity T_f. However, it is more useful to consider τ to be a fixed multiple of τ_T because their ratio depends primarily on the material properties of the particle and fluid media

$$\frac{\tau}{\tau_\mathrm{T}} = \frac{2k_\mathrm{f}}{3C_\mathrm{p}\mu_\mathrm{f}} \tag{15}$$

At low Reynolds numbers the value of this ratio for water droplets, glass particles, and copper particles, each immersed in cool air are 0.23, 1.13, and 2.44, respectively. Therefore, if the materials used for the particle and fluid are considered constant, both T_ef and T_ee can be considered second-order.

3. Description of the simulation

The accuracy of the three equilibrium methods for computing the particle temperature field, T_{ef}, T_{ee}, and T_{ep}, and of the simplest approximation of setting the particle temperature to be the local fluid temperature, T_f, are assessed by comparing these values to the exact particle temperature, T_p, for particles evolved in a turbulent flow. Here, the term *exact* refers to the temperature obtained from the Lagrangian–Eulerian method, although this itself is only another (albeit higher fidelity) model.

We consider the problem of pressure-driven, turbulent flow between two infinite parallel plates. Here the two plates are maintained at different, but constant, temperatures. The turbulent channel flow with the associated turbulent thermal field is chosen as the test bed for evaluating the above equilibrium approximations. The flow field and the passive thermal field are evolved according to the following continuity, momentum and energy equations

$$\nabla \cdot \mathbf{u} = 0, \tag{16}$$

$$\frac{D\mathbf{u}}{Dt} = -\nabla p + \frac{1}{Re_\tau}\Delta \mathbf{u}, \tag{17}$$

$$\frac{DT_f}{Dt} = \frac{1}{Pr\,Re_\tau}\Delta T_f. \tag{18}$$

The geometric and physical parameters for this flow have been chosen to match the numerical experiments of Piller et al. [13]. The Reynolds number based on the wall friction velocity and the channel half-height is $Re_\tau = 150$. The dimensions of channel are $1920 \times 300 \times 960$ wall units in the streamwise (x), wall-normal (y), and spanwise (z) directions, respectively. The DNS employs a pseudospectral algorithm on a grid of size $192 \times 128 \times 192$, fully de-aliased in the x and z directions. The effective grid resolution is therefore $128 \times 128 \times 128$. The velocity and thermal fields are evolved with a third-order Runge–Kutta time stepping method. The temperature field is constant at the top and bottom walls: $T = 1$ at $y^+ = 0$, and $T = -1$ at $y^+ = 300$. The Prandtl number is chosen to be the largest value considered by Piller et al. [13]: $Pr = 1$, and the mean and rms temperature fluctuations obtained agree with their results.

In this flow, twenty ensembles of 200,000 particles each were evolved, representing each combination of four response times ($\tau^+ = 0$, 0.03, 0.1, and 0.3), and five thermal response times ($\tau_T^+ = 0.03$, 0.06, 0.1, 0.2, and 0.3). The chosen values for τ_T^+ and τ^+ (other than $\tau^+ = 0$) span the range $0.1 \leqslant \tau/\tau_T \leqslant 10$, which is consistent with typical values for liquid or solid spheres in air at standard temperature and pressure (STP). For example, as mentioned above, the value of τ/τ_T is 0.23 for water droplets immersed in air. The values of τ^+ chosen correspond to water droplet diameters of 0, 1.76, 3.13, and 5.57 μm in the case of air (at STP) in a channel with half-height $h = 1$ cm. These diameters are well below the computational cell size except in the case of a cell bordering the wall, whose wall-normal extent is 3.06 μm. All values of τ^+ considered are small enough to lie in the regime in which the Maxey–Riley (or Gatignol) equation is valid: the particle-based Reynolds number is less than 0.07 for all values of τ^+ considered, whereas the ratio of the particle diameter to Kolmogorov length scale is everywhere less than 0.06. These values are for the case of water droplets, and are even lower for denser substances. The simplification of the Maxey–Riley equation to the Stokes-law equation (1) is valid because the particle-to-fluid density ratio is very high: 816 for the case of water in air. Similarly, the use of (4) is valid because of the small ratio of particle diameter to Kolmogorov length scale allows the thermal transfer to be viewed as a spatially uniform process, and the particle Reynolds number is small enough that the Nusselt number can be taken to be the constant 2. Finally, for the series expansion employed by the equilibrium Eulerian method to be accurate, one requires that τ and τ_T be smaller than the time scale of any eddy which acts on a particle. The Kolmogorov time scale is the smallest possible of such time scales, and in this case the largest value of τ or τ_T used is less than 15% of it everywhere in the channel.

The velocity and temperature of the particles are evolved according to (1) and (4). The particle velocity is then used to advance the particle position within the channel. Using periodicity, any particle exiting the computational domain is reintroduced into the channel. Particles colliding with the wall bounce elastically. This is not particularly realistic, but an accurate representation of near-wall effects is beyond the scope of this study.

A time step in wall units of $\Delta t^+ = 0.2$ was used to evolve the flow to a fully developed, statistically steady state after which particles are introduced into the flow. Although the above time-step was adequate for accurate resolution of all flow scales, a smaller time step of $\Delta t^+ = 0.02$ was used to accommodate the case of small particles with τ^+ and τ_T^+ equal to 0.03 in order to ensure numerical stability in the time integration of their equations of motion. (Note that this time-step restriction is, in fact, one of the very problems that the equilibrium Eulerian method is designed to remedy.) Particles were evolved for 1000 time steps to adjust to the flow, and then for another 20,000 time steps. Statistics were collected every 100th step. These Lagrangian results for the particles will be considered *exact*, and they form the benchmark against which other approximations will be compared.

Interpolation of quantities to particle locations is performed via Hermite interpolation [14]. This method

was desired not only for its accuracy, but, more importantly, for its smoothness (continuity of derivatives across cell boundaries). In the Lagrangian approach for evolving (1) and (4) the fluid velocity and temperature fields must be interpolated from the computational grid to the particle position. In practical application of equilibrium Eulerian approach no such interpolation is required, since the computation will remain entirely on the grid. In the present work, however, in order to evaluate their accuracy, the equilibrium Eulerian methods will be applied at the Lagrangian particle locations and this will require interpolation. For proper comparison the interpolation for T_p in the Lagrangian approach and for T_{ee}, T_{ep}, T_{ef} in the equilibrium Eulerian approaches must be performed carefully and consistently. Several points related to interpolation are discussed further in Appendix A.

4. Results

The $\tau^+ = 0$ case provides a convenient baseline because $\mathbf{u} = \mathbf{v}_e = \mathbf{v}$, so there is no distinction between the three methods used to compute the equilibrium particle temperature. In this case the notation T_e is used, since $T_e = T_{ef} = T_{ee} = T_{ep}$ for $\tau = 0$. Note, however, that in practice $\tau \to 0$ implies $\tau_T \to 0$. In the case of inertial particles ($\tau^+ > 0$), T_{ef}, T_{ee}, and T_{ep} will be distinct, in general.

Fig. 1 is a contour plot of the error $T_e - T_p$ in approximating the particle temperature with the equilibrium temperature versus the error $T_f - T_p$ in approximating the particle temperature with the local fluid temperature, for the case $\tau^+ = 0$, $\tau_T^+ = 0.03$. The data is collected over the x–z plane in a narrow region about $y^+ = 20$; temperature is normalized by the standard deviation of the fluid temperature fluctuation T_f' at $y^+ = 20$; and each contour line represents a factor of two increase in probability density.

Fig. 1 indicates that the equilibrium Eulerian method for temperature captures the exact particle temperature much better than its approximation as the local fluid temperature does $\tau_T^+ = 0.03$. Fig. 2 shows that the corresponding result for $\tau_T^+ = 0.3$, and it is evident that the equilibrium approximation still yields significant improvement over the local fluid temperature. The rms error of equilibrium Eulerian approximation is about 20% of the rms error when using the fluid temperature. From the location of the center the distribution it can be seen that for both $\tau_T^+ = 0.03$ and $\tau_T^+ = 0.3$ approximating the particle temperature with T_f results in a marked mean error, while the corresponding mean error is quite small for the equilibrium approximation. The contour plots indicate that the temperature statistics are similar to the velocity statistics presented in [4].

Figs. 1 and 2 indicate that the errors in T_f and T_e are statistically uncorrelated. This is largely true in the inertial case ($\tau^+ > 0$) as well, so the contour plots may be replaced by mean and rms statistics for each method. Fig. 3 shows the mean and rms of the error in equilibrium approximation T_{ep} plotted for against the nondimensional particle thermal response time, τ_T^+. Also plotted for reference is the corresponding mean and rms error in approximating the particle temperature with the local fluid temperature. The results are plotted for only the smallest and largest values of τ^+ considered (0 and 0.3)

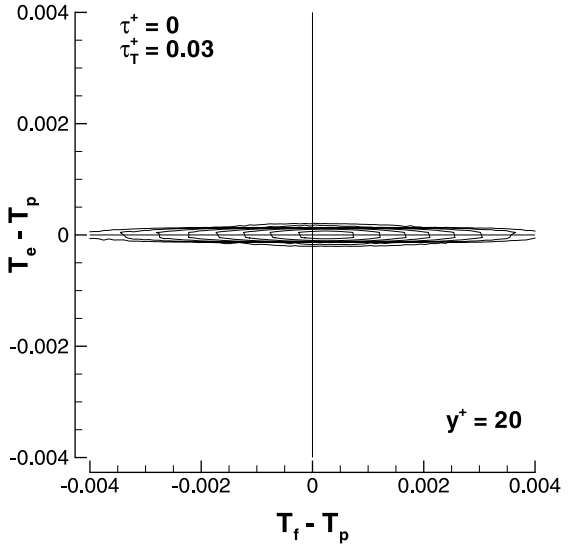

Fig. 1. Comparison of errors in T_e vs. T_f for fluid particles with $\tau_T^+ = 0.03$.

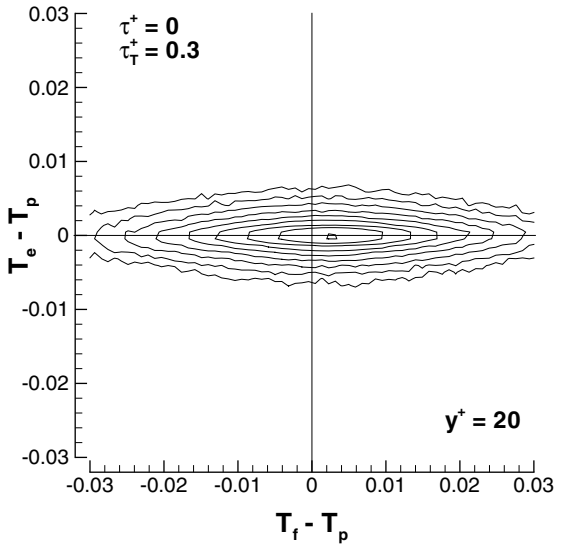

Fig. 2. Comparison of errors in T_e vs. T_f for fluid particles with $\tau_T^+ = 0.3$.

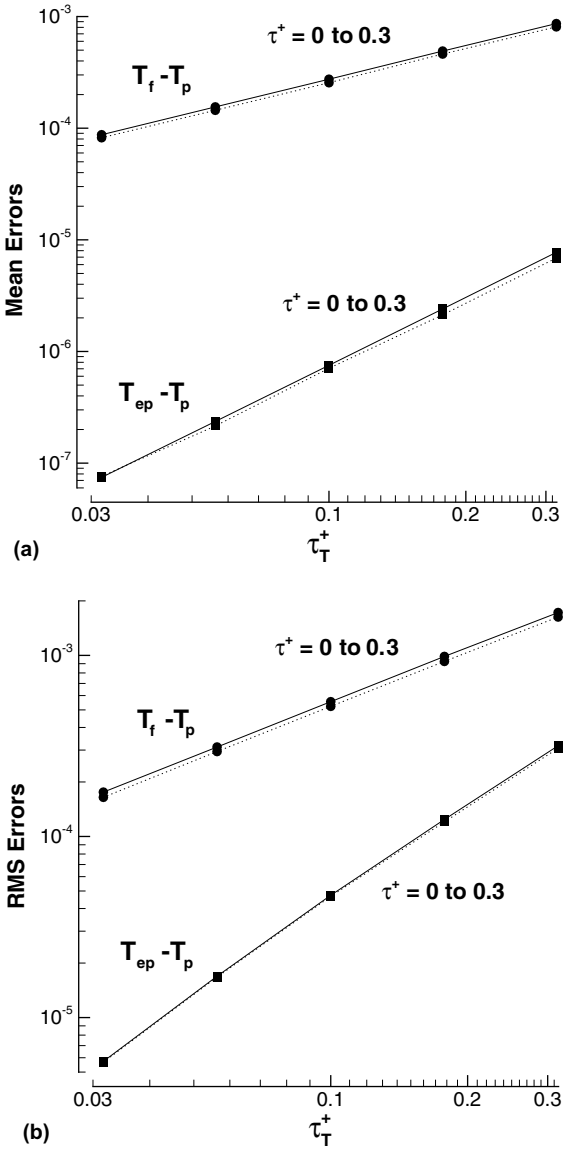

Fig. 3. (a) Mean and (b) RMS errors in T_f and T_{ep}.

as the results are clearly insensitive to τ^+. The errors for T_f are proportional for τ_T, but those for T_{ep} are proportional to τ_T^2, as expected. Over the entire range of τ_T^+ considered, the mean error in T_{ep} is more than two orders of magnitude lower than that in T_f. The corresponding difference in rms error is somewhat lower at one order of magnitude.

The equilibrium approximation using the exact convective derivative of fluid temperature following the particle, as in (8), was possible in the present simulation. However, in practical application of equilibrium Eulerian approach, the exact particle velocity will not be available and as a result the convective derivative of fluid temperature following the particle must be approximated. In other words, although T_{ep} is the best possible first-order equilibrium approximation to particle temperature, in practice it must be replaced by either T_{ef} or T_{ee}. Fig. 4 shows the mean and rms error for T_{ef}. Again the error for T_f is plotted for comparison. It is clear that the equilibrium approximation for particle temperature, even with a crude approximation to convective derivative, provides substantial improvement over T_f.

The asymptotic behavior of T_{ef} depends on the value of τ^+, however. In Fig. 4(a), even the smallest inertial particle ($\tau^+ = 0.03$) considered fails to perform as well

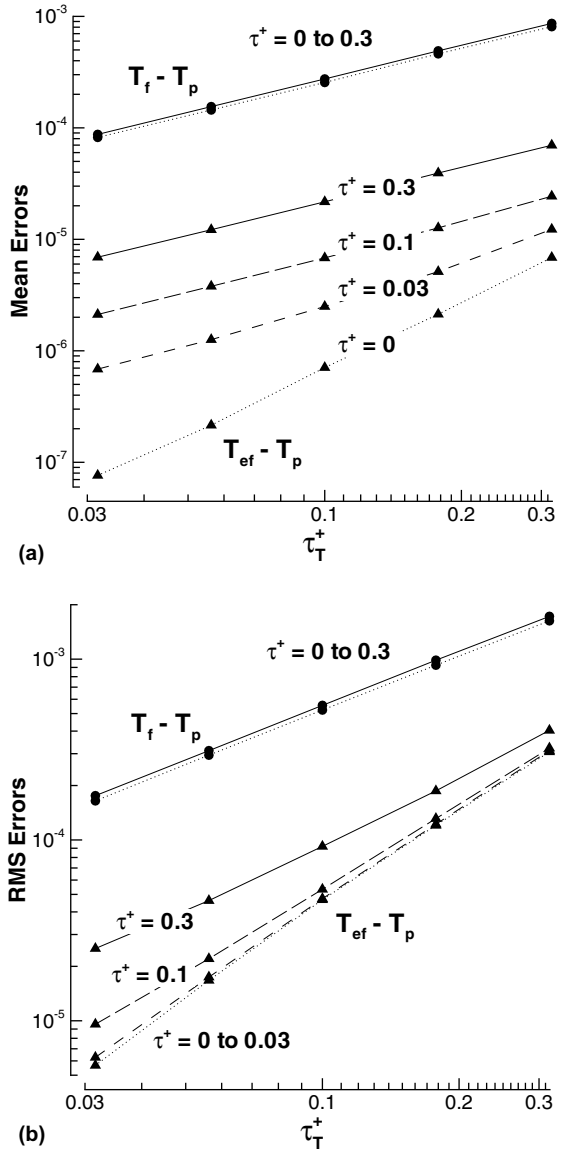

Fig. 4. (a) Mean and (b) RMS errors in T_f and T_{ef}.

as the $\tau^+ = 0$ particles. For $\tau_T^+ \gg \tau^+$ the mean error decreases as τ_T^{+2}, but for $\tau_T^+ \lesssim \tau^+$, only first order behavior is observed. These asymptotics are consistent with the order of accuracy indicated in (12). The rms exhibits a similar behavior, but less drastically.

The mean and rms error for T_{ee} are shown in Fig. 5. The error compares well with those shown in Fig. 3 for small values of τ^+. When the particle time scale increases much beyond the corresponding thermal time scale, a slight increase in both the mean and rms errors can be observed. But overall it can be seen that over the entire parametric range considered T_{ee} provides nearly as good an approximation to the particle temperature as T_{ep}.

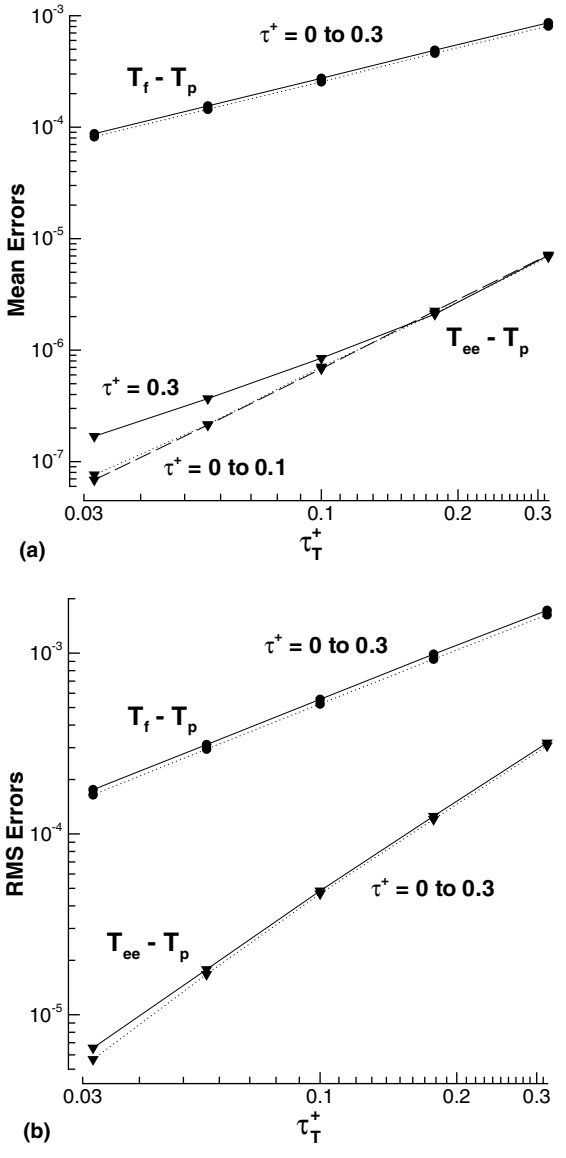

Fig. 5. (a) Mean and (b) RMS errors in T_f and T_{ee}.

There results are similar to those presented in [4] for velocity statistics. In that work, a further set of tests (which have no thermal analog) were carried out in which particles were allowed to move under the velocity prescribed by the equilibrium Eulerian method. The statistics of the resulting particle distribution showed a remarkable fidelity to the exact particle fields—results even better than what would be expected by considering the rms errors only. Rather, it was the small mean errors that accounted for the high fidelity. In this study the mean temperature statistics are better than those of the rms, just as in the velocity case.

5. Summary

The equilibrium Eulerian method is an efficient way to compute the velocity of sufficiently small particles in a turbulent flow. The authors have previously shown [4] that this method represents the particle velocity with $O(\tau^2)$ accuracy in turbulent flow. Two methods of generalizing the method to approximate the particle temperature field T_p have been explored in the current work, given by the formulas for T_{ef} and T_{ee} in (9) and (10). These are compared to the accuracy of using the fluid velocity T_f as an estimator, and to the ideal, but uncomputable, equilibrium method T_{ep} given in (8). The difference between the three equilibrium methods T_{ef}, T_{ee}, and T_{ep} is the velocity used to compute the convective derivative of temperature. The three methods use the fluid velocity, equilibrium Eulerian velocity, and exact particle velocity, respectively. It is found that the method T_{ef} does not suffice, in general. Fig. 4a highlights the degradation in the accuracy of T_{ef} as τ^+ increases. On the other hand, Fig. 5 shows that T_{ee} is an excellent approximation to the particle temperature, performing nearly as well as T_{ep}. Although T_{ee} is somewhat more complicated, with the correct implementation it would not be particularly costly because the equilibrium Eulerian velocity it requires will be anyway computed in order to obtain the particle velocity field.

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Appendix A. Interpolation

The exact representation of the velocity and temperature fields in a spectral simulation is given by a sum of sinusoidal functions. To compute the exact particle velocities and temperatures as the sum of these sinusoids

at a given instant requires work proportional to the product of the number of grid points and the number of particles, which is far too large to be practical. Therefore an efficient interpolation method is required. This appendix comments on the role of a chosen method's accuracy and smoothness, and emphasizes the need for consistent calculations in Lagrangian–Eulerian studies.

The method chosen in this study is total Hermite interpolation. To interpolate a function $f(x,y,z)$ with this method, one first locates the grid point (x_0,y_0,z_0) such that $x_0 \leqslant x < x_1,\ y_0 \leqslant y < y_1,\ z_0 \leqslant z < z_1$. Define $\Delta x = x_1 - x_0$, $\mathrm{x} = (x - x_0)/\Delta x$, and similarly for the y- and z-directions. Then define the following basis functions:

$$H_0^0(\mathrm{x}) = (1-\mathrm{x})^2(1+2\mathrm{x}),$$
$$H_0^1(\mathrm{x}) = (1-\mathrm{x})^2\mathrm{x}, \quad H_1^p(\mathrm{x}) = (-1)^p H_0^p(1-\mathrm{x}). \tag{A.1}$$

The interpolated function $F_{\mathrm{THI}}(x,y,z)$ is a linear combination of the values of f and all its first-order mixed partial derivatives at the eight surrounding gridpoints

$$F_{\mathrm{THI}}(x,y,z) = \sum_{i,j,k,p,q,r=0}^{1} H_i^p(\mathrm{x})H_j^q(\mathrm{y})H_k^r(\mathrm{z})f^{(p,q,r)}(x_i,y_j,z_k) \times (\Delta x)^p(\Delta y)^q(\Delta z)^r, \tag{A.2}$$

where $f^{(p,q,r)}$ is the result of taking p, q, and r derivatives of f in the x-, y-, and z-directions, respectively.

Hermite interpolation is fourth-order accurate, but it is important not to confuse order of accuracy with accuracy itself. The order of accuracy is a measure of how well a method interpolates low-wave-number components of a field, but Balachandar has shown [14] that the error for turbulent fields is dominated by the high-wave-number components. In this regard, Hermite interpolation is excellent, much better than sixth-order Lagrangian interpolation, for example.

Interpolation is a linear operator, so it commutes with summation and with temporal derivatives. That is, one gets the same results whether one interpolates a sum of terms, or interpolates each term individually and then sum. Products and spatial derivatives are another matter. To obtain values of the equilibrium Eulerian temperature at particle positions requires the interpolation of $\mathrm{D}T_{\mathrm{f}}/\mathrm{D}t$. There are various ways to compute this quantity at a particle location. Three of which are listed below for the same term $u_3\partial T_{\mathrm{f}}/\partial z$ that appears in $\mathrm{D}T_{\mathrm{f}}/\mathrm{D}t$

- Compute $u_3\partial T_{\mathrm{f}}/\partial z$ on the grid, then interpolate it;
- Interpolate u_3 and $\partial T_{\mathrm{f}}/\partial z$ individually, then multiply the results; or
- Interpolate u_3 directly and multiply it by the result of taking the z-derivative of (A.2) (with $f = T_{\mathrm{f}}$).

The first method gives the most accurate approximation of the projection of $u_3\partial T_{\mathrm{f}}/\partial z$ onto the spectral basis; the second gives the most accurate approximation of $u_3\partial T_{\mathrm{f}}/\partial z$ prior to projection. The third method is less accurate than the other two, but it is the correct choice for this study.

This may seems paradoxical but note that the Lagrangian dynamics of a particle evolved in an interpolated field are a function of that interpolated field, not of the original field. In a Lagrangian–Eulerian simulation, the only field which it is appropriate to study is the interpolated field. This is the only field the particles perceive. For example, if one wished to study the preferential concentration of particles with respect to an estimator of the divergence of the particle velocity field, then it would be important to recognize that even in the limit $\tau \to 0$, where the particle velocity approaches the fluid velocity, the divergence may not approach zero. The interpolated fluid velocity field may not be divergence-free, unless it incorporates all three components of velocity at once.

In the current study, various methods of approximating particle temperature are employed, and they are based on the spatial and temporal derivatives of the field perceived by the particle. It would therefore be misguided to attempt to minimize the error between the value of $u_3\partial T_{\mathrm{f}}/\partial z$ at a particle location and the exact, spectral value of that quantity. Instead, one just computes $u_3\partial T_{\mathrm{f}}/\partial z$ exactly, based on the interpolated field, and therefore introduces no interpolation error in the comparison between the evolved quantity T_{p} and directly computed quantities such as T_{ef}. It is simple to implement the computation of the derivatives of an interpolated field based on the basis functions H_i^p in (A.1). For example,

$$\frac{\partial}{\partial z}F_{\mathrm{THI}}(x,y,z) = \sum_{i,j,k,p,q,r=0}^{1} H_i^p(\mathrm{x})H_j^q(\mathrm{y}) \times \frac{\mathrm{d}}{\mathrm{dz}}H_k^r(\mathrm{z})f^{(p,q,r)}(x_i,y_j,z_k) \times (\Delta x)^p(\Delta y)^q(\Delta z)^{r-1}. \tag{A.3}$$

The choice of Hermite interpolation can now be explained. The main reason for this choice is not its accuracy, but its smoothness. Hermite interpolation guarantees the continuity of first derivatives across cell boundaries. Without this property, one cannot show that the rms errors of T_{ef} and T_{ep} are proportional to τ_{T}^2 as $\tau_{\mathrm{T}} \to 0$ (when τ is a fixed multiple of τ_{T}). This result would be obscured by numerical error. The discontinuity of the spatial derivative would introduce an small, but constant (in τ_{T}), error in $\mathrm{D}T_{\mathrm{f}}/\mathrm{D}t$ near cell boundaries, which would in turn manifest as an $\mathrm{O}(\tau_{\mathrm{T}})$ error in the difference between T_{p} and any equilibrium estimate (T_{ef}, T_{ee}, or T_{ep}). This error would decay within a small time ($\mathrm{O}(\tau_{\mathrm{T}})$), and hence would only exist over a small re-

gion (again, $O(\tau_T)$) of the cell. The net result would therefore be an additional $O(\tau_T)$ error over an $O(\tau_T)$ region of the cell, and although this results only in an additional $O(\tau_T^2)$ error in the mean, it results in an $O(\tau_T^{3/2})$ error in rms, which will dominate for sufficiently small τ_T.

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