Interpolation error in DNS simulations of turbulence: consequences for particle tracking

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Abstract. An important aspect in numerical simulations of particle laden turbulent flows is the interpolation of the flow field. For the interpolation different approaches are used. Where some studies use low order linear interpolation others use high order spline methods. We compare several interpolation methods and conclude that interpolation based on B-spline functions has several advantages compared with traditional methods. First, B-spline interpolation can be executed very efficiently by optimal use of the pseudo-spectral code, only one FFT needs to be executed where Hermite spline needs multiple FFTs for computing the derivatives. Second, the smoothness of the interpolated field is higher than that of Hermite spline interpolation. Finally, the interpolation error almost matches the one of Hermite spline which is not reached by the other methods investigated. Further, we focus on estimating the interpolation error and compare it with the discretisation error of the flow field. In this way one can balance the errors in order to achieve an optimal result. Algorithms have been developed for the approximation of the interpolation error. As a spin-off of the theoretical analysis a practical method is proposed which enables direct estimation of the interpolation error from the energy spectrum, which may provide a quantitative indicator for this purpose.

1. Introduction

In recent years many studies on inertial particles in turbulence have focussed on the Lagrangian properties of these particles, see the review by Toschi & Bodenschatz (2009). Maxey & Riley (1983) among others introduced the equations of motion for small isolated rigid spherical particles in a non-uniform velocity field \( \mathbf{u}(\mathbf{x}, t) \). For such particles in turbulent flows it is required that the particle diameter \( d_p \) is much smaller than the smallest turbulent length scales, i.e., \( d_p < \eta \) with \( \eta \) the Kolmogorov length scale. An important assumption is that the particle Reynolds number \( Re_p = d_p |\mathbf{u} - \mathbf{u}_p|/\nu \ll 1 \), with \( \mathbf{u}_p \) the velocity of the particle and \( \nu \) the kinematic viscosity of the fluid. As we consider small particle diameters and small volume fractions of particles we ignore the effects of two-way and four-way coupling. Time integration of these equations to compute particle trajectories is an expensive, time- and memory consuming
task. In particular when particle-to-fluid density ratios are in the order of 1-5 (e.g. marine applications and sediment transport) the different contributions to the Maxey-Riley (MR) equation are relevant. The first hurdle is the computation of the Basset history force which can be computationally very expensive. However, a significant reduction can be obtained by fitting the diffusive kernel of the Basset history force with a sum of exponential functions, as recently shown by van Hinsberg et al. (2011a). Second, the interpolation step can be very time consuming and memory demanding as well, in particular when the other bottle-neck (computation of the Basset force) has been removed. There are several interpolation methods that can be used (Lekien & Marsden, 2005; Lalescu et al., 2010), which are compared in Section 3. Here one can see that the B-spline based interpolation method proposed by van Hinsberg et al. (2011b) has the most favorable properties when used in combination with a pseudo-spectral code. When choosing the B-spline interpolation method one has still the freedom of choosing the order of convergence of this method. High order methods are instead found to be computationally more expensive, therefore it is important that they give a significantly more accurate result (Homann et al., 2007). For efficient computations we need a quantitative indicator to choose both the interpolation recipe and the required resolution of the flow simulation (van Hinsberg et al., 2011c). In Section 4 we will show some error estimates of the interpolation. Finally, in Section 5 we will give concluding remarks.

2. Tracking of point-like particles in turbulence

Numerical codes evolving particles in a flow consists of two parts. First, the turbulent flow is approximated with an Eulerian approach by means of direct numerical simulations (DNS). The incompressible Navier-Stokes equations are solved on a triple periodic domain using a pseudo-spectral code. The pseudo-spectral code uses three-dimensional Fourier components and typically we use a resolution of $128^3 - 256^3$. Second, the particles are tracked by a Lagrangian approach. We consider particles with $(St \approx 1)$ as well as fluid parcels for which $(St = 0)$: for both all turbulent scales are important. The particle trajectories are obtained by using the Maxey-Riley equations. We consider particles with a particle-to-fluid density ratio of $\rho_p/\rho_f = 4$, for which all terms in the MR-equation are relevant (van Aartrijk & Clercx, 2010). For the Maxey-Riley equations the fluid velocity and its first derivatives must be known at the particles positions. In principle one could compute the velocity by exact summation of the Fourier waves at the position of the particles. Unfortunately, this would be far too expensive and in practice only small amounts of particles could be tracked in the order of hundreds. In order to avoid these Fourier summations, the velocity is usually transformed on a finite rectangular grid and an interpolation in real space should be carried out. In order to choose the most appropriate interpolation method for a particular case one needs to compare errors: the interpolation error is compared with the discretisation error of the flow field. In this way one can prevent unnecessary computations.

3. Comparison of interpolation methods

In this section four different interpolation methods are investigated. The criteria we are interested in are the following. First, the method must be fast, this is needed because many interpolations need to be carried out. Second, because a spectral code is used exponential convergence is expected for the fluid velocity. The interpolation methods do not have this exponential convergence and must have high order of convergence in order to keep the accuracy. Further, because we use a pseudo-spectral code, the computed velocity field is $C^\infty$ and therefore the interpolated function must have a high order of smoothness as well. Here, the order of smoothness is defined as the highest derivative that is still continuous. Finally, the method
must have small overall errors. In this way the interpolated field can also be used to find derivatives of the field which is needed for solving the MR equation.

The methods which we investigate are the following. First we have Lagrange interpolation where a polynomial function of degree \( N - 1 \) passes through \( N \) points (Faires & Burden, 1993). Second we investigate the spline interpolation proposed by Lalescu et al. (2010). Third, we have Hermite spline interpolation and finally the B-spline based interpolation method proposed by van Hinsberg et al. (2011b). In Table 1 some properties of the interpolation methods are given. All interpolation methods use piecewise polynomial functions of degree \( N - 1 \) to reconstruct the field. In Figure 1 we have shown the mode-dependent interpolation errors where the interpolation error of mode \( k \) with grid spacing \( \Delta x \) is given by

\[
\text{error} = \int_0^1 \left| U_k(x) - \tilde{U}_k(x) \right|^2 \, dx \quad \text{where} \quad U_k(x) = e^{2\pi i k x}
\]  

with \( \tilde{U}_k \) being the interpolant of \( U_k \) (for more details see van Hinsberg et al. (2011b)).

| method                   | \( n \) | order of smoothness | FFT | comment                  |
|--------------------------|--------|---------------------|-----|--------------------------|
| Lagrange interpolation   | \( N - 1 \) | 0                   | 1   | for even \( N \)         |
| spline interpolation     | \( N - 2 \) | \( (N - 2)/2 \)     | 1   | for odd \( N \)         |
| Lalescu et al. (2010)    | \( N - 2 \) | \( (N - 2)/2 \)     | 1   | only even \( N \)       |
| Hermite spline interpolation | \( N - 1 \) | \( (N - 2)/2 \)     | \( (N/2)^3 \) | only even \( N \)       |
| B-spline based interpolation | \( N - 1 \) | \( N - 2 \)         | 1   |                          |

**Table 1.** Overview of the interpolation methods investigated. Here \( N - 1 \) is the degree of the polynomial function. \( n \) is defined as the highest polynomial function for which the interpolation is still exact. For the order of smoothness to equal \( p \) the interpolated field must be continuous up to the \( p \)-th derivative. Further FFT denotes the number of FFTs needed for the interpolation.

When comparing the interpolation methods one can see that all methods have a weak point on one of our criteria except for the B-spline based method. The Lagrange interpolation, for example, is only continuous for even \( N \) and discontinuous for odd \( N \), see Table 1. Furthermore, the overall error is relatively high when compared with the other methods. The spline interpolation has a better degree of smoothness but has a lower \( n \) which results in a lower order of convergence. Here the order of convergence is taken in the limit of \( (\Delta x \to 0) \) and the order is equal to \( n + 1 \), see Figure 1. Also the overall error is relatively high compared with the other methods. Hermite interpolation on the other hand has an excellent overall error. The main disadvantage of this method is that multiple FFTs are needed which is very time consuming. The B-spline based interpolation does not have this problem, only one FFT needs to be executed. Additionally, this method reaches a much higher order of smoothness compared with the other methods. When looking at the overall errors in Figure 1, one can see that they almost match the one of Hermite interpolation, at variance with methods that have been investigated.

### 4. Error estimates of interpolation

In order to be able to compare the interpolation error with the discretisation error one needs a method to approximation the interpolation error. The relative interpolation error \( \epsilon \) in the \( L^2 \)-norm is given by

\[
\epsilon = \lim_{T \to \infty} \sqrt{\frac{\int_0^T |u - \tilde{u}|^2(x_p(t), t) \, dt}{\int_0^T |u|^2(x_p(t), t) \, dt}},
\]
where $x_p(t)$ denotes the center of a particle, $u$ is the flow velocity and $\tilde{u}$ is the flow velocity after interpolation. A practical method has been developed for the approximation of the this error by van Hinsberg et al. (2011c). This method uses the one-dimensional energy spectrum to compute this error. In Figure 2 it is shown how the energy spectrum is changed due to the interpolation. One can see that the modes close to $k_{\text{max}} = 21$ have lost energy due to the interpolation. Furthermore, modes with higher $k_{\text{max}}$ become energetic as an artifact of the interpolation. This undesirable behavior can be suppressed by using higher order interpolations. A first analysis shows that in conjunction with the applied interpolation method the choice of $k_{\text{max}} \eta$, which is a measure for the resolution of the viscous range, is critical to obtain similar interpolation and discretisation errors. For this reason high-order interpolations yield significantly improved results for increasing $k_{\text{max}} \eta > 1$.

5. Conclusions

We have compared several interpolation methods. For spectral codes the B-spline based interpolation method has several advantages compared with other traditional methods. The smoothness of the interpolated field is higher than that of Hermite spline interpolation and of the other methods investigated. Second, only one FFT needs to be done where Hermite spline needs multiple FFTs for computing the derivatives. Third, the interpolation error matches almost the one of Hermite splines, a property not reached by the other methods that have been investigated.

Additionally, we propose a practical method to estimate the interpolation error. Here, one uses the one-dimensional energy spectrum to compute the interpolation error. The proposed methods are validated by full turbulence simulations and it is shown that they give accurate results. In order to avoid unnecessary computations the discretisation and interpolation error

Figure 1. Interpolation error in $L^2$-norm. All methods are taken with $N = 4$ accept for the reference case of linear interpolation which has $N = 2$. 
Figure 2. Energy spectrum of the flow as obtained from the pseudo spectral code (solid line) and similar spectra after linear interpolation (dashed line) and high-order interpolation (dotted line).

should be of the same order of magnitude. The methods give a practical way of estimating the errors. Comparison of these errors shows that linear interpolation may not always be sufficient. Further, it is shown how the energy spectrum is modified due to the interpolation and its significance is discussed. This investigation opens the way for formulating a quantitative indicator to choose the appropriate interpolation recipe.

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