CONVERGENCE OF SPATIALLY RESOLVED PARTICLE DEPOSITION

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ABSTRACT

Lagrangian stochastic models are frequently used to model the turbulent dispersion of particles and predict their deposition. While there are methods to calculate uncertainty for spatially resolved properties, there is no standard method to ensure these properties are converged. This paper presents a methodology for the application of distance metrics to achieve quantifiably converged maps of spatially resolved deposition in a computationally efficient way. The methodology is insensitive to the choice of distance metric, provided the metric is valid for null values. The number of particles tracked is increased by both increasing the spatial resolution of particles injected, and aggregating the results of repeated injections at a fixed resolution. Established distance metrics are used to compare evolving spatially resolved particle deposition distributions generated from each approach. It is shown that when an insufficiently high spatial particle density is injected, turbulent dispersion will not necessarily redistribute particles through the domain sufficiently to achieve converged maps of deposition. Further, it is shown that monitoring bulk deposition statistics is insufficient for the evaluation of spatial convergence. For the test case used, the minimum spatial particle injection density for convergence of spatially resolved statistics is higher than that required for integral statistics.

KEYWORDS

PARTICLE DEPOSITION, TURBOPHORESIS, TURBULENT FLOWS, CONVERGENCE

NOMENCLATURE

\(d_p\) Particle diameter
\(D_{KL}\) Kullback-Leibler Distance
\(D_{\text{Hell}}\) Hellinger Distance
\(D_h\) Hydraulic Diameter (m)
\(N_S\) Number of samples
\(N_p\) Number of particles per sample
\(P\) Prior distribution
\(Q\) Posterior distribution
\(R_c\) Radius of Curvature (m)
\(s\) Sample number (m)
\(S\) Sample standard deviation
\(S\) Arc-length (m)
\(t_{N_S-1,\alpha}\) T-multiplier with \(\alpha\) confidence
\(U_g\) Bulk gas velocity (ms\(^{-1}\))
\(\delta\eta\) Absolute percentage difference (%)
\(\eta_s\) Deposition fraction of sample number \(S\) (%)
\(\bar{\eta}\) Mean deposition fraction (%)
\(\mu_g\) Gas kinematic viscosity (m\(^2\)s\(^{-1}\))
\( \rho \) Density (Kg m\(^{-3}\))

Re Reynolds Number (= \( \rho_g U_g D_h/\mu_g \))

\( R_0 \) Ratio of Curvature (= \( 2R_c/D_h \))

Stk Stokes Number (= \( \rho_g d_p^2 U_g/18 \mu_g D_h \))

CI Confidence Interval

KL Kullback-Leibler

CRW Continuous Random Walk

**INTRODUCTION**

Particle modelling has proven to be important for multiple engineering fields, from oral drug delivery optimisation to gas turbine degradation prevention. An estimated 10 tonnes of dust pass through an engine’s core during its lifetime, so the accumulation of even small impact fractions would be significant for its performance. Previous research (Vadgama *et al.*, 2020) shows that even when modelled integral deposition values are comparable to experimental validation data the spatial distribution of particles can be strikingly different. Thus, for the validation of particle tracking models accurate spatially resolved results are essential. Therefore, a precise understanding of where this deposition occurs, including small deposition fractions, can be important.

Whilst it is common for studies to show that the results, such as the fraction deposited from those injected, have become independent of the number of particles tracked it is often not clear how the required number and spatial distribution of particles is established (Graham and Moyeed, 2002; Berrouk and Laurence, 2008). Typically, predictions using increasing numbers of injected particles are compared in a method, analogous to mesh sensitivity studies for the continuous phase based on the number of cells. However, detail of the spatial density of injection and the number of repeated samples are not commonly reported. Further, convergence in one quantity is typically employed as a proxy for general convergence. (Graham and Moyeed, 2002; Reynolds, 1997)

To conduct particle tracking, the particles’ diameters, initial locations and velocities, and mass must be specified. For the particles’ locations, it is unrealistic to know the exact initial distribution of particles, and hence a uniform injection distribution is often considered with the aim of understanding all potential deposition.

Due to the complexity of the flow fields, low particle concentrations, and limited computing power, one-way coupled particle models have proven popular. These allow the à priori generation of a Reynolds Averaged Navier Stokes flow solution of the continuous phase into which the particles are injected. Lagrangian particle tracking through this steady state flow field would be spatially deterministic. Thus, in turbulent flows, a further stochastic model is required to capture turbophoretic effects, which are particularly important for small particles. With stochastic models, that calculate and apply the fluctuating turbulent velocities, the trajectories of identical particles with the same initial conditions are different for each injection (Legg and Raupach, 1982; Bocksell and Loth, 2006; Vadgama *et al.*, 2020). Thus, multiple injections \( (N_s>1) \) of the same spatial particle distribution can be combined to provide a probabilistic distribution. This paper focuses on this more complex case of stochastic models, with the results being equally applicable to deterministic models.

To demonstrate these issues, a test case of flow through a 90-degree bend where turbophoresis has been shown to be influential on the spatial distribution (Vadgama *et al.*, 2020) is introduced. For this paper a bespoke particle turbulent transport model has been applied, however, the technique is equally valid when using industry standard models such as the Direct Random Walk. It is shown that evaluating changes in integral deposition statistics using existing error estimation methods is insufficient to ensure a representative spatial deposition distribution. Measures of distance are introduced to quantify the difference between spatial distributions, and their robustness is assessed. These are then used to investigate the role of increasing the number of particles, both via further samples and a higher spatial density of particles per injection. The results show that a minimum sufficient density of particles and number of injected samples are required for convergence of the
spatial distribution. This leads to a clear practicable method for the generation of converged spatial distributions in an efficient way.

**METHODS**

In typical convergence strategies integral statistics are used, particle injection simulations are conducted using an arbitrary number of particles \(N_p\) on the injection plane. \(N_p\) is then increased until the mean impact fraction is found to be steady. In most cases this is confirmed using some user judgement (Pascal and Oesterlé, 2000; Graham and Moyeed, 2002). In such a process it is normal for a single injection \((N_s = 1)\) of the particle location distribution to be computed, rather than multiple samples \((N_s > 1)\). In the latter case, an average must be computed (Equation 1). Metrics used to monitor convergence are then the absolute percentage difference in impact fraction (Equation 2) and the confidence interval \((CI, \text{Equation 3})\). The user then sets two threshold criteria by which convergence is achieved: 1) the result is sufficiently close to the fully converged solution, \(< \text{ criterion 1} \); 2) that the uncertainty lies within acceptable limits, \(CI < \text{ criterion 2}\).

\[
\bar{\eta} = \frac{1}{N_s} \sum_{s=1}^{N_s} \frac{\eta_s}{100}
\]

Equation 1

\[
\delta \eta = 100 \times \frac{\eta_s - \bar{\eta}_{s-1}}{\bar{\eta}_s}
\]

Equation 2

\[
CI = 2t_{N_s-1,95} S/N_s
\]

Equation 3

This study is focused on ensuring the computed spatial distribution of deposit is representative. To the authors’ knowledge, no criterion has been proposed to assess the closeness of a spatially resolved result to the fully converged result in the existing open literature, thus this is the focus of this paper.

In order to compare the similarity of multi-dimensional data distributions, where new data are added to an existing set, there already exist a multitude of tests. Typically, they compare the prior distribution \((P)\) and posterior distribution \((Q)\), the former is the distribution before the current observed data are included and the latter after the newly observed data is included. In this study, the prior distribution \((P)\) and posterior distribution \((Q)\) are either different due to increased spatial density, or a further sample being used in the calculation of the posterior distribution.

One category of tests is distance or divergence metrics: a commonly used divergence measure being the Kullback-Leibler (KL) divergence (Equation 4). This, however, is unsuitable for the assessment of deposition as it fails when the probability changes from 0 in the prior to non-zero in the posterior, which is the most common change in probability state when little deposition occurs. An alternative measure is the Hellinger distance, Equation 5, which is more robust and thus is used in this remainder of this paper. The authors also propose Equation 6 as an alternative, with a form more similar to the familiar differingence formula used in Equation 2. The normalising factor, of \(\frac{1}{2}\), ensures this measure scales between 0 and 1 for true probability distribution functions (i.e. their integral is 1).

\[
D_{KL}(P||Q) = \sum_{x \in X} \sum_{y \in Y} P(x, y) \log \left( \frac{P(x, y)}{Q(x, y)} \right) , P(x, y), Q(x, y) > 0
\]

Equation 4

\[
D_{\text{Hell}}(P||Q) = \frac{1}{\sqrt{2}} \sqrt{\sum_{x \in X} \sum_{y \in Y} \left( \sqrt{P(x, y)} - \sqrt{Q(x, y)} \right)^2 , P(x, y), Q(x, y) \geq 0}
\]

Equation 5

\[
D(P||Q) = \frac{1}{2} \sum_{x \in X} \sum_{y \in Y} |P(x, y) - Q(x, y)| , P(x, y), Q(x, y) \geq 0
\]

Equation 6

An equivalent measure for the confidence interval can be calculated using the approach of Graham et al. (2002) who provide a method to characterise the uncertainty of spatially resolved results and
estimate the number of particles required to meet the required confidence interval (Graham and Moyeed, 2002). They found that the uncertainty is only dependent on the total number of particles injected ($N_s \times N_p$). Further, to increase the precision by an order of magnitude the number of particles must be increased by two orders of magnitude. Graham et al. (2002) suggest that in the region of interest the steps are:

1. Use a nominal number of particles ($N_p$) per sample and repeat the injection (i.e. increment $N_s$) until the maximum standard deviation at each location in the distribution of the aggregated results, $S(x,y)_{\text{max}}$, becomes a good estimation of the population’s maximum local standard deviation, $\sigma_{\text{max}}$, (i.e. $\sigma_{\text{max}}= S_{\text{max}}$ when $N_s \to \infty$, hence $\sigma_{\text{max}} \approx S_{\text{max}}$ when $N_s$ is large). This indicates the number of samples ($N_s$) that need to be used.
2. Increase the number of particles per injection, each time taking $N_s$ samples, until the trend in the injection location with highest standard deviation $S(x,y)_{\text{max}}$ is proportional to $N_p^{-1/2}$.
3. Calculate the confidence interval using Equation 3 replacing the sample standard deviation ($S$) with the local maximum sample standard deviation $(S(x,y)_{\text{max}})$. Decide on the precision required and use the trend identified to calculate the parameters needed to provide the required level of accuracy.

Test Case

To assess current approaches and the proposed approach, a simple but sufficiently complex case of interest is chosen. Pui et al. (1987) conducted experiments of deposition in a 90-degree bend of curvature ratio ($R_0$) 5.6-5.7 with a diameter of 8.51 mm. The flow characterised by ambient conditions and a Reynolds number (Re) of 6,000 - 10,000. Monodisperse liquid droplets of Uranine ($\rho_g = 925$ kg/m$^3$) with Stokes numbers ($\text{Stk}$) between 0.03 and 1.35 were dispersed in the flow. This liquid allowed experimentalist to mimic an all-stick condition, which eliminates the need for particle bounce-stick modelling.

A domain (Figure 1) and validated mesh (Figure 2) from a previous study by Vadgama et al (2020) is used. A linear pressure-strain Reynolds stress model with wall reflection effects and enhanced wall treatment was used, with the maximum $Y^+$ below one. Fluent 19.2 and ICEM 19.2 were used for the flow solution and the mesh generation respectively. The CRW model, as in its final implementation, from Vadgama et al. (2020) is used to model turbulent dispersion. In this paper, it is shown that there is sufficient turbophoresis to influence particle trajectory for the particles studied. The simulations simulate 6.4 μm diameter particles in a flow with Reynolds number 10,000, these particles showed most variation due to turbophoresis.

![Figure 1 Simulated domain of the Pui et al. (1987) 90-degree pipe bend experiment. Entry and exit are labelled with boundary conditions.](image-url)
Injections using 10 different spatial densities of uniformly distributed particles are compared, all located at the injection plane. For this study, particles are injected ten diameters upstream of the bend entrance, Figure 1. The spatial density is approximately doubled between injections, and described by Table 1 and shown in Figure 3. Each of these injections, with the particles located at the same initial positions for each sample, were simulated 50 times to create 50 samples.

**Table 1: Definition of the 10 different injections, with varying spatial density of particles.**

<table>
<thead>
<tr>
<th>Injection Reference</th>
<th>Density (# particles/m²)</th>
<th>Spacing (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.1E+06</td>
<td>6.86E-04</td>
</tr>
<tr>
<td>2</td>
<td>4.5E+06</td>
<td>4.71E-04</td>
</tr>
<tr>
<td>3</td>
<td>9.3E+06</td>
<td>3.28E-04</td>
</tr>
<tr>
<td>4</td>
<td>1.8E+07</td>
<td>2.36E-04</td>
</tr>
<tr>
<td>5</td>
<td>3.6E+07</td>
<td>1.68E-04</td>
</tr>
<tr>
<td>6</td>
<td>7.2E+07</td>
<td>1.18E-04</td>
</tr>
<tr>
<td>7</td>
<td>1.4E+08</td>
<td>8.38E-05</td>
</tr>
<tr>
<td>8</td>
<td>3.3E+08</td>
<td>5.50E-05</td>
</tr>
<tr>
<td>9</td>
<td>1.1E+09</td>
<td>2.96E-05</td>
</tr>
<tr>
<td>10</td>
<td>2.3E+09</td>
<td>2.09E-05</td>
</tr>
</tbody>
</table>

The simulations investigate both the integral and spatial distribution in the bend. The deposition fraction is calculated as the number of particles hitting the wall of the 90-degree bend divided by the
number of particles entering the 90-degree bend that are successfully tracked (either hit the wall or exit the domain). To generate a map of deposition fraction that can be easily presented, the bend wall is represented as a 2D surface with the two axes being the circumferential angle and arc length (θ and S respectively in Figure 1). The local deposition fraction is plotted, its integral is equal to the total deposition fraction.

While judicious choice of a kernel function could result in a continuous distribution, and possibly reduce the number of particles required, this introduces further degrees of freedom because this function needs to be specified. For this study, discontinuous distributions are used with a resolution of 92 (arc-length-wise) by 46 (circumferentially) to be consistent with the study by Berrouk and Laurence (2008).

RESULTS & DISCUSSION

Firstly, the impact fraction (equivalent to deposition fraction as all particles which impact also stick) of particles sticking on the bend wall is monitored. The mean impact fraction of 50 samples of is plotted in Figure 4. Injection 4 is seen to be sufficient to predict the percentage of particles impacting, with the mean of the highest density injection falling within the confidence interval. Further, Figure 5 shows that the absolute error by this point is, and remains, below ~1%.

![Figure 4 Average impact fraction from 50 samples with 95% confidence intervals. The horizontal line shows the mean impact fraction as per injection 10.](image)

![Figure 5 The absolute percentage error of impact fraction as calculated using Equation 2. The dotted horizontal line is at 1%, the chosen critical value.](image)

To test that only the total number of particles injected matters, as per Graham and Moyeed (2002), the confidence interval of the resultant spatial distribution is investigated. Following step 1 in the procedure described above, it was found that 50 injections were sufficient for the samples’ standard deviation (S) to become a good estimate of the population’s standard deviation (σ). As per step 2, Figure 6 shows the error becomes proportional to $N_p^{-1/2}$ for injection number 3 (Table 1) and above. Figure 7, as per Graham and Moyeed (2002), shows this error is only dependent on the total number of particles injected implying the calculation is correct. The 90% confidence interval using 50 samples of injection number 4 is $6.17 \times 10^{-7}$.

Figure 8 shows the spatial distributions for each of the injection cases. It is clear that the earlier injection cases are not converged for spatial distribution, with zero deposition in the lower density injection cases where there is significant deposition in the higher density injection cases. Figure 9 compares the spatial impact distribution from the lowest spatial density case that meets the criterion on integral deposition (injection 4) to the highest spatial density case (injection 10). It is shown that injection 10 does not fall within the distribution of injection 4 even after assuming a maximum deviation of the confidence interval. It is clear that the lack of particles is resulting in gaps in the distribution. Further calculations showed that even extremely low confidence intervals have the same
results. This appears obvious once we consider that this comparison is equivalent to comparing the integral results using injection 10 to that of injection 1, as we have not checked that the distribution is converged.

Figure 6 Maximum standard deviation (across the spatially resolved impact fraction distribution) with increasing density of particles on injection plane. $N_s = 50$. Lines $\propto N_p^{-1/2}$ are shown for comparison.

Figure 7 Confidence interval, using Equation 3, as a function of the total number of particles injected. Lines $\propto (N_p N_s)^{-1/2}$ are plotted for comparison.

Figure 10 shows the Hellinger distance between distributions calculated with an increasing density of particles. This is the equivalent of Figure 4, but for spatially resolved data. The number of samples used does not affect the ability to conclude when sufficient similarity has been established, therefore the required injection particle density can be found without conducting multiple samples. This is because, in this test case, turbophoresis is a second order effect compared to the variation introduced by increasing the spatial density of particles at the injection plane. There is no guarantee this is the case in geometries where stochastic mechanisms are present. Figure 11 shows the Hellinger distance between distributions calculated with an increasing number of samples, where injections with less particles take longer to converge. Whilst these statistics do give an impression of the information gain, it is difficult for an engineer to contextualise these numbers.

Figure 8 Spatially resolved impact fraction, I and O mark the inner and outer of the bend.
Figure 9 Comparison of spatially resolved deposition fraction resulting from injection 4 and 10, considering the estimated confidence interval. I and O mark the inner and outer of the bend.

Figure 10 Hellinger distance (Equation 5) between deposition distributions, each injection is compared to the previous lower spatial injection density with an equal number of samples.

Figure 11 Hellinger distance (Equation 5) between distributions using n-1 and n samples of injections with the same particle density on their injection plane.

Figure 12 shows the use of Equation 6 to measure the distance between two distributions. Comparing with Figure 10, it is clear the choice of metric has had little effect on the implied convergence. By normalizing the distance by the integral deposition fraction, context for the magnitude of this result can be made (Figure 13). This normalization makes the result equal to the distance between distributions to the percentage of deposited particles at each location. This creates a universal (non-case-dependent) and interpretable threshold for convergence to be set (chosen here at 10%). It also provides a similar graph to Figure 5 for spatially resolved data. For this threshold, 10 injections of the highest density were enough to ensure an accurate representation of the spatial distribution had been generated.
The confidence interval can be calculated as per normal statistical techniques, as done by Graham and Moyeed (2002). To justify the number of particles per injection and the minimum number of samples when investigating spatially resolved quantities, where the stochastic effects are likely to be heavily influential, it is recommended that one should iteratively compare converged distributions of increasing $N_p$ (using the required $N_s$ for distance to fall within acceptable limits each time) until the distance between these converged distributions fall below a converged limit. Where turbophoresis is not modelled or it can be assumed a secondary effect, considerable time saving can be achieved by using this methodology:

1. Measure distance using increasing $N_p$ with a single sample,
2. Measure distance using increased $N_s$ with the required $N_p$ from step 1

**CONCLUSIONS**

A measure of distance between particle deposition distributions is proposed, and a methodology for its use to ensure convergence is outlined. It is shown that in order to understand all potential deposition on a spatially resolved basis, a minimum spatial density of particle injection sites is required at the inlet, and that multiple repeated injection is insufficient to overcome the limitations imposed spatially. To achieve convergence this minimum density must first be increased while monitoring the distance metric until it lies beneath a maximum threshold. Further error measurement calculations can then be applied to repeated injections at this or higher particle densities. In this paper monodispersed particle injection has been used to establish the convergence procedure: the convergence criteria need not be updated in the event of injecting a size distribution, but the minimum number of repeated injections required to achieve a converged mass impact fraction distribution would increase.

This approach is applicable to turbomachinery components, the key challenge for more complex surfaces being the discretization of any deposition surface into sufficiently resolved sub-regions. It is likely that consideration of the requirement for the spatial distribution to be converged would increase the computational requirements, as significantly more particles must be tracked.
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