1 Verification and Validation of the Existing Code

The existing code calculates the position and velocity of the particles but also includes a discrete element method (DEM) to simulate the collision of particles. The latter is computationally expensive and is not needed for the heat and mass transfer calculations. The DEM code can be "switched off" so the existing code solves just for the particle position and velocity. There are some checks that need to be done to ensure the code is solving the equations correctly and producing physical results.

The check that can be made is to find if the code produces statistically stationary conditions. This can be done by calculating the relative velocity. I.e. the difference between the particle velocity and the fluid velocity at different times. The particle velocity is a Lagrangian variable (only varying with time). Whilst the fluid velocity is an Eulerian variable as it varies with both space and time. To calculate the relative velocity between the particle and fluid a Lagrangian description is needed for velocity.

The averaging procedure to get the relative velocities is:

$$\bar{U}_{x,rel}(t) = \sum_{i=1}^{N} \frac{\left[U_{p_i}(t) - U_{f_i}(t)\right]}{N} \tag{1.1a}$$

$$\bar{V}_{y,rel}(t) = \sum_{i=1}^{N} \frac{\left[V_{p_i}(t) - V_{f_i}(t)\right]}{N} \tag{1.1b}$$

$$\bar{W}_{z,rel}(t) = \sum_{i=1}^{N} \frac{\left[W_{p_i}(t) - W_{f_i}(t)\right]}{N} \tag{1.1c}$$

Where for each velocity component the relative velocity is found for all particles and averaged to produce the mean velocity component. The behaviour of the mean relative velocity will be random initially but should converge to some value at a later point in time. This behaviour should be the same for the other statistical moments.

The Stokes number will dictate the behaviour of the particles. If it is $<< 1$ the particles are massless and should follow the flow. If the Stokes number is $>> 1$ the particles are essentially billiard balls and the flow field of the velocity has no bearing on the motion of the particles.

The default conditions the code uses for the simulation of a Taylor-Green vortex in a box are:

- Number of particles: 10000
- Particle density: 2000 kg/m^3
- Particle diameter: 0.05 m
- Fluid viscosity: 0.0193 Ns/m^2 (according to the report 1.040 should be used for a Stokes number of 1)

The distribution of starting conditions gives a mean particle speed of $1m/s$ and standard deviation of $0.1m/s$. With the particle directions evenly distributed.