

Blakemore, D. M., Govender, I., McBride, A. T. and Mainza, A. N. (2019) Multiple particle tracking in PEPT using Voronoi tessellations. *Chemical Engineering Science*, 207, pp. 780-789. (doi: <u>10.1016/j.ces.2019.06.057</u>)

There may be differences between this version and the published version. You are advised to consult the publisher's version if you wish to cite from it.

http://eprints.gla.ac.uk/189340/

Deposited on 1 July 2019

Enlighten – Research publications by members of the University of Glasgow <u>http://eprints.gla.ac.uk</u>

# Multiple Particle Tracking in PEPT using Voronoi Tessellations

DM Blakemore<sup>b</sup>, I Govender<sup>a,\*</sup>, AT McBride<sup>d</sup>, AN Mainza<sup>c</sup>

<sup>a</sup>School of Engineering, University of KwaZulu-Natal, Durban, 4041 <sup>b</sup>School of Clinical Medicine, University of KwaZulu-Natal, Durban, 4041 <sup>c</sup>Centre for Minerals Research, University of Cape Town, P/Bag Rondebosch, 7701 <sup>d</sup>Division of Infrastructure and Environment, University of Glasgow, United Kingdom

# Abstract

Many complex flow phenomena encountered in chemical engineering lack fundamental understanding. Central to this problem is the lack of non-invasive, in-situ measurement tools that can simultaneously track the motion and dynamics of different particle species across the entire phase space of the flow. To this end, a novel algorithm was developed for simultaneously tracking multiple particles using a Positron Emission Tomography scanner. The algorithm discretizes the back-to-back gamma rays emanating from multiple radio-labelled particles, and uses a Voronoi tessellation to create a density map of the points. The locations of the tracers are determined using a clustering technique. A series of experiments was performed to test the precision, robustness, and performance of the algorithm. Twenty tracers were successfully tracked, limited only by the amount of available sodium-22 isotope. The presented algorithm resulted in a RMSE of 1.26mm. The precision was found to be dependent on the level of discretization, and is robust in that the loss of a tracer (due to exiting the field of view, high acceleration, or tracer collision) is handled internally, with no need for human correction. The proposed algorithm can also be easily parallelized.

Keywords: PEPT, nuclear imaging, Voronoi, clustering

<sup>\*</sup>Corresponding author

*Email address:* indresan.govender@gmail.com (I Govender)

# 1. Introduction & Motivation

Positron Emission Particle Tracking, or PEPT, is a nuclear imaging technique developed at the University of Birmingham in the early 1990s (Parker et al., 1993). It makes use of Positron Emission Tomography (PET) scanners to track a single tracer, tagged with radioactive material, over time. The benefit of PEPT over other imaging techniques is that it can measure motion within complex opaque systems, allowing for accurate *in situ* measurements. PEPT has been used to measure flow fields of complex engineering systems (Parker et al., 1997; Fangary et al., 2000; Chang et al., 2011) and for validating numerical simulations (Hoomans et al., 2001; Govender et al., 2013).

A critical assumption to using single particle tracking of identical particles<sup>1</sup> is the ergodic hypothesis (Wildman et al., 2000): the time averaged behaviour (per volume of interest) of a single tracer is equivalent to the ensemble average under steady flow conditions. Simply put, given a sufficiently long measurement time, the tracer will sample the entire phase space spanned by the ensemble. However, most real granular flow systems (rotating drums, chutes, shear cells, inclined planes) exhibit a rich co-existence of flow regimes (Govender and Pathmathas, 2017) (quasi-static, dense and inertial) that are delineated by phase transition barriers, like the glass transition barrier between quasi-static and dense flows (Ni et al., 2013). In the absence of self-propulsion of particles—which is the case in most granular flow systems—a tracer particle found within the dense regime does not have sufficient energy to make the transition into the quasi-static regime, and it is only by a series of rare cage-breaking events (Pal et al., 2008) that this can happen. Consequently, most single particle PEPT experiments of realistic granular flow systems fail to meet the ergodic hypothesis, resulting in skewed residence time distributions (Wildman et al., 2000) that produce incorrect representations of the solids fraction distribution in the impenetrable zones, even in the simplest case of identical particles (Govender and Pathmathas, 2017). Extended tracking times can help; however, this does not guarantee that a cage-breaking event will occur. A practical solution for mono-sized granular flows is to have at least three tracers that are initially located within the three flow regimes. The problem is further exacerbated for realistic flow systems of n particle classes: 3n tracers (three tracers for each particle class) are required to minimally guarantee an ergodic representation of the flow

<sup>&</sup>lt;sup>1</sup>Identical particles constitute the simplest granular ensemble

for finite tracking times. The current approach (Govender and Pathmathas, 2017; Govender et al., 2017) to tracking mono-sized granular flows is to have multiple runs (at least three) of the same experimental configuration, and inserting the tracer into a separate flow regime each time. While this approach makes sense in theory, in practice it is difficult to guarantee placement of the tracer into a specific flow regime.

Beyond the ergodic problem encountered with single particle tracking, a granular mixture of n particle classes will also exhibit mixing and segregation. Industrial granular flows exhibit complex mixing phenomena caused by a range of competing factors (Hill, 2016) (buoyancy, kinetic stress gradients, inertia, pressure gradients, porosity gradients and convection) that currently resist fundamental understanding. To fundamentally model such industrial mixtures using PEPT requires two basic types of measurements: The time evolution of the mixture at the individual species level, and the steady state dynamics of the individual species. The single particle PEPT tracking strategies discussed above can be used to characterise the steady state dynamics of an *n*-particle system; however, the time evolution of the mixture is not accurately represented in such experiments. To achieve a meaningful time evolution of the individual species necessarily requires that the initial conditions be identical. This is best achieved with multiple tracer PEPT experiments where identical initial conditions are naturally guaranteed.

Multiple tracers could also be used to measure rigid body rotation as well as deformation of deformable materials: Simultaneous displacement-time measurements of multiple tracers placed in a coarse grid formation along (or within) a deformable material can provide key insights into the strain rates under loading. Combining this with material properties, it should be possible (in principle) to recover the underlying stress-strain constitutive relations governing the material deformation. Such measurements have value in validating/calibrating simulations of complex materials where the constitutive relations are not known. Finally, and most simply, using multiple tracers cuts down on experimental time, which would save time and expense.

The problem of multiple tracer tracking in PEPT was first explored by Gundogdu (2004) who tracked up to 8 tracers making use of intersecting lines of response along with a K-means clustering implementation (Mac-Queen et al., 1967). Yang et al. (2006, 2007) tracked three tracers using a modified version of the original Birmingham algorithm. They showed that tracking three tracers could allow for the rotation of a rigid body to be fully

described, given prior knowledge of the shape of the body. A drawback of the Birmingham method for multiple-PEPT was that each successive tracer had to be twice as active as the previous one, which quickly led to radioactive saturation of the PET scanner. Finally, Bickell et al. (2012) managed to track up to 16 tracers using the Line Density Algorithm, whereby the imaging space was discretized into voxels and tracers were located based on the radiation density within each voxel.

A common drawback to all of the existing multiple-PEPT techniques is that the number of tracers must be known in advance and kept constant throughout the experiment. Some workarounds have been implemented, but they require post-processing as well as some manual intervention. This can be a problem, since there may be multiple reasons for a tracer being lost: exiting the field of view, colliding with another tracer, or even moving with an acceleration that is high enough to make it difficult to track. Additionally, in some applications, like comminution in tumbling mills, the tracer may break up into two or more progeny particles.

This paper presents an algorithm which can be used to track multiple tracers, while being robust to tracer loss and number of tracers. The algorithm is termed the Voronoi-based Multiple Particle Tracking (VMPT) algorithm, and consists of multiple pre-existing and well-understood computing techniques. As the name implies, the algorithm is largely based on Voronoi tessellations (Aurenhammer, 1991), especially the fact that Voronoi cells become smaller in regions of high data point density. Since the data that are output from the PET scanner are noisy, outliers are determined using the Local Outlier Factor metric (Breunig et al., 2000). The remaining points are then clustered using the DBSCAN clustering method (Ester et al., 1996). DBSCAN was chosen because of its ability to automatically determine the number of clusters and the fact that it accounts for noise. Finally, a multiple target tracking technique is designed and implemented to track the located tracers.

# 2. PET, PEPT & Multiple Particle Tracking

Positron Emission Tomography (PET) is a medical imaging technique whereby positron-emitting radionuclides are used to observe biological processes *in situ*. The use of positron emission in medical imaging was first explored by Sweet (1951) and Wrenn et al. (1951) in the early 1950's. The radionuclides are attached to biologically active molecules, such as fludeoxyglucose (FDG), and introduced into the subject's body. A PET scanner is then used to generate concentration maps, which indicate the relevant tissue metabolic activity throughout the body. When using FDG, an analogue of glucose, the concentration map can show where melanomas may be present in the body, with areas of high glucose uptake indicated by "hot" spots on the map.

The radioistopes used are those with short half-lives, and include <sup>18</sup>F, <sup>11</sup>C, and <sup>68</sup>Ga, which all undergo  $\beta^+$  decay. The generic nuclear equation for  $\beta^+$  decay is

$${}^{A}_{Z}X \to {}^{A}_{Z-1}X' + e^{+} + \nu_{e}.$$
 (1)

This equation describes the decay of a proton within the nucleus to a neutron, with the emission of a positron and an electron neutrino. When the emitted positron slows to thermal energies and encounters an electron in the surrounding matter, the two particles annihilate, and the combined mass is transformed into two photons, each with an energy of 511 keV. To conserve energy and momentum, these two photons travel in a straight line at nearly  $180^{\circ}$  to each other.

The two photons are detected by the PET scanner. Most scanners consist of consecutive rings of detecting elements made from scintillator crystals. When these crystals are excited by ionizing radiation, they emit energy in the form of flashes of light. Through the use of photomultiplier tubes and the photoelectric effect, the flashes of light generate measurable currents, with the magnitude of the current proportional to the energy of the detected photon. When the scanner detects two photons within some small time window of each other (usually on the order of a few nanoseconds), they are considered to have originated from the same positron-electron annihilation event. Constructing a line joining the two detections creates a chord known as the *line of response* (LOR). In theory, the tracer would lie exactly along this LOR; in practice, the photons are not precisely 180° apart, so the LOR has a non-zero width.

In 1984, scientists at the Positron Imaging Centre at the University of Birmingham started exploring non-medical applications for PET scanners (Hawkesworth et al., 1991). The main purpose of this research was to develop Positron Emission Particle Tracking (PEPT), a technique used to dynamically track a single tracer over a period of time. Parker et al. (1993) developed the Birmingham algorithm in 1993, which was the first fully-functioning PEPT algorithm. The basic principle of the Birmingham algorithm relies on the fact that, ideally, a tracer will be located at the intersection of two LOR's. In reality it is very rare for two LOR's to intersect, due to tracer motion and erroneous line detection. The Birmingham algorithm therefore uses an iterative method to discard erroneous LOR's. Using the remaining LOR's, the tracer position is determined by calculating the point which minimises the sum of the perpendicular distances to each of the "true" LOR's.

Gundogdu (2004) was the first to develop an algorithm for tracking multiple tracers using PEPT. The algorithm made use of "intersecting" LOR's, with an intersection defined as two lines coming within some predefined perpendicular distance of each other.

Yang et al. (2006) developed a technique based on the original Birmingham algorithm, in that it incrementally removed erroneous LOR's. Once the first tracer was located, the discarded lines were used to find the next tracer. In order for the algorithm to effectively locate separate tracers, each tracer had to have twice the activity of the previous one. This put a hard cap on the number of tracers, as the total tracer activity quickly approached the saturation level of the scanner. This method was improved upon by Yang et al. (2007), by taking into account the sensitivity of the PET scanner over the length of the field of view.

Bickell et al. (2012) used a novel line density multiple tracer tracking technique. The algorithm discretized the field of view into a set of cubic voxels. Each voxel was assigned a density value based on the number of lines of response passing through them. The centroids of the voxels with the highest densities were used as the locations of tracers.

# 3. Algorithm Development

The VMPT algorithm is split into two major phases: the Location phase and the Tracking phase. The Location phase makes use of Voronoi tessellations, which are geometric constructs that divide a volume into nearestneighbour partitions, based on a set of discrete points called seeds (Aurenhammer, 1991). Each cell in a Voronoi tessellation includes a single seed point, and represents the set of points that are closer to the included seed than to any other seed. Voronoi tessellations are dual to Delaunay triangulations, and have seen use in fields such as biology (Sánchez-Gutiérrez et al., 2015; Li et al., 2012), computational mechanics (Springle, 2010), machine learning (Mitchell, 1997) and epidemiology (Borak, 2007).

# 3.1. Location

During the Location phase of the VMPT algorithm, the raw data from the PET scanner is broken up into *frames*, with each frame containing an equal number of consecutive LOR's. Since the time at which each LOR was detected is known, the timestamp of a frame is the mean of the timestamps of each LOR within that frame. For each frame, all of the tracers within the field of view of the scanner are located, and the positions and corresponding timestamps are saved to disk.

To locate the tracers in a single frame, the set of LOR's is first discretized, with each line transforming into a set of colinear, equidistant points. By describing a LOR with

$$\mathbf{x} = \mathbf{a} + \lambda(\mathbf{b} - \mathbf{a}) \tag{2}$$

where **a** and **b** are the end points of the line and  $0 \le \lambda \le 1$ , a point  $\mathbf{x}_i$  can be found by setting

$$\lambda \equiv \lambda_i = \frac{i\epsilon_{sep}}{|\mathbf{b} - \mathbf{a}|} \tag{3}$$

where  $\epsilon_{sep} = 5.0$  mm is the separation distance between consecutive points and  $i \in \mathbb{Z}, 0 \leq i \leq n_{points}$ . Here,  $n_{points}$  is determined by dividing the length of the line by  $\epsilon_{sep}$  and rounding, formally

$$n_{points} = \left\lceil \frac{|\mathbf{b} - \mathbf{a}|}{\epsilon_{sep}} \right\rceil,\tag{4}$$

where  $\lceil x \rceil$  is x rounded up to the nearest integer. It was found that a fixed separation distance of the order of the tracer radius (5 mm in the current experiments) performed close to optimally. Noting that not all LOR's are the same length, the fixed separation distance—as opposed to discretizing all lines into an equal number of points—led to a more reliable clustering and therefore better tracer location. Figure (6d) illustrates the RMSE for a range of separation distances investigated.

These points are then used as seeds for a 3D Voronoi tessellation. In the vicinity of a tracer, there will be a high density of these seed points. As such, the corresponding Voronoi regions will be smaller the closer they are to a tracer. To remove a large number of points from the data set, it is assumed that the point along a single LOR with the smallest corresponding Voronoi region is the point along that line which is closest to a tracer position. These points are determined and stored in a data structure, and will be referred

to as Points Under Consideration (PUC's). Since the true volume of an irregular polyhedron is computationally difficult to compute, a metric called the *mean vertex distance* (MVD) is used to determine the relative "sizes" of the polyhedra. The MVD is defined as the mean of the distances from the polyhedron centroid to each of the vertices, that is

$$\delta_{MVD} := \frac{1}{n} \sum_{i=1}^{n} |\mathbf{v}_i - \mathbf{c}| \tag{5}$$

where  $\mathbf{v}_i$  is the *i*th vertex of the polyhedron, and  $\mathbf{c}$  is the geometric centroid of the polyhedron, determined by

$$\mathbf{c} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{v}_i.$$
 (6)

It can be seen in figure (1) that the volumes of the polyhedra increase with the distance of the seed point from the tracer location. Therefore it can be assumed that the tracer location relative to some LOR is in the vicinity of the seed point on that line with the smallest volume (or mean vertex distance).



Figure 1: Voronoi diagram for seeds generated by two artificial tracers in 2D, with the colour of each polygon indicating the mean vertex distance,  $\delta_{MVD}$  in mm, of that polygon. The image on the right shows the logarithm of the volumes to more clearly indicate the differences.

It was found that the set of PUC's contained a considerable amount of noise. To remove the noisy data points, two filters are used. The first filter makes use of Local Outlier Factors (LOF's) (Breunig et al., 2000), using  $k_{lof} = 4$  as the nearest neighbour search parameter. LOF determination assigns a floating point number to each entry into a data set. This number indicates the degree of "outlier-ness" of an entry. Note that, as the name implies, the LOF determines the degree to which the entry is a *local* outlier, rather than a global outlier. This means each point is only compared to its neighbours, instead of the entire set. Because the LOF does not provide a binary measure of whether or not an object is an outlier, a cutoff value for the LOF must be chosen, with all objects having an LOF larger than the cutoff being outliers. By default, the algorithm discards all data points with an LOF value that falls in the top 50 % of the set of LOF's.



(a) Cumulative Distribution of LOFs indicates a Generalized Extreme Value distribution.

(b) Bimodal distribution of Voronoi cell mean vertex distances after LOF filter.

Figure 2: Distributions used to examine PUCs during filtering.

Since the LOF only examines *local* densities, further inspection of the PUC's after the LOF filter shows a bimodal distribution (see figure 2b) in the volumes of the surrounding Voronoi cells. The algorithm discards all points with a surrounding Voronoi volume in the greatest 40% of the remaining volumes based on trial and error: from the set of points still remaining after the LOF cleaning, those which have a volume of greater than the mean plus twice the standard deviation are discarded. This removes the far outliers which skew the data significantly. After this, a new mean and standard deviation are determined, and points with a volume larger than the mean

plus 0.2 times the standard deviation are discarded. Although heuristic this method was found through trial and error, it has shown to give consistent results.

Once filters have been applied, the remaining points are run through the DBSCAN clustering algorithm (Ester et al., 1996). The parameters used are k = 4 (the same nearest neighbour search parameter  $k_{lof}$  as used by the LOF) and  $\epsilon = \epsilon_{sep}$  (the same as the separation distance used in the discretization). At each time frame, the DBSCAN automatically counts the number of clusters, so the actual number of tracers in the frame does not need to be kept constant.

After clustering, for each cluster the geometric mean of the data points is calculated to determine the position of the centroid of the cluster, and this is defined as the location of a tracer.

#### 3.2. Tracking

Since the tracers are not distinguishable by any physical properties, a multiple target tracking method is used to associate the locations in a given time frame with the previous tracks. Multiple target tracking (MTT) is a computational technique used to track data points based only on their positions and velocities. The most popular MTT technique is the Multiple Hypothesis approach (Blackman, 2004). Other approaches include Monte-Carlo-based methods (Hue et al., 2002; Oh et al., 2004), particle filters (Särkkä et al., 2007) and multi-frame particle tracking velocimetry (Ouellette et al., 2006). The MTT technique used here is customized to accommodate large levels of inaccuracy in tracer location and erroneous or missing data points.

The position-time data generated by the Location phase is used to create multiple *tracks*, with each track illustrating the path of a single tracer. Due to a variety of factors, one tracer may have multiple tracks, so the number of tracks generated is on average larger than the number of tracers used in the experiment.

A track object stores all of the position-time entries for a particular tracer. The frames containing the positions detected in the Location phase are loaded in chronological order. Initially, each position is used to create a new *Track* object. As each successive frame is loaded, the following steps are followed:

• For each Track object, a number of previous entries in that Track are used to determine the location of the next entry, using a numerical extrapolation technique.

- The positions in the Location frame are matched to the predicted positions, and added to the end of the corresponding Track histories.
- Any detected positions not matched to a Track are used to initialize a new Track.
- Any Tracks with no associated detected position are assigned an empty place holder position.
- Any Track that has not had a detected position assigned to it in the last  $N_{skip,max}$  frames is terminated.

A linear least-squares fit is used to estimate the next position for each track. The most recent  $N_{ex} = 10$  entries in the history are used as the data points for the extrapolation.  $N_{ex}$  defines the number of points used to predict the next tracer location if the trajectory is not complex (linear or at most quadratic). If more complicated trajectories are anticipated, this value should be increased or modified. If there are fewer than  $N_{ex}$  entries in the history, all of the existing data points are used. Note that for the first entry the next position cannot be estimated. For a linear fit to yield the best results, the time interval between consecutive frames should be small enough such that a linear approximation is sufficient. When large accelerations or large time intervals are expected, a quadratic fit may be used, although in that case  $N_{ex}$  should be increased. It is not recommended that fits larger than second order be used, since larger order polynomials are more affected by variance.

To match the predicted positions to the tracks a custom similarity matrix  $\mathbf{D}$  was used. The entries in the matrix are the distances between each predicted track position and the new location entries in the current frame, that is

$$D_{ij} = |\mathbf{p}_i - \mathbf{x}_j|,\tag{7}$$

where  $\mathbf{p}_i$  is the predicted position of the *i*th existing track and  $\mathbf{x}_j$  is the position of the *j*th tracer in the frame under consideration.

From the similarity matrix, a "match matrix"  $\mathbf{M}$  is developed. Entries in the match matrix take on the value 1 or 0. An entry will be 1 if it is the smallest value in both its row and column, and represents a match between a track and a new entry. Physically, a location  $\mathbf{x}$  is matched to a predicted track's position  $\mathbf{p}$  if two conditions are met:

- 1.  $\mathbf{x}$  is closer to  $\mathbf{p}$  than it is to any other predicted position, and
- 2. **p** is closer to **x** than it is to any other new location.

Numerically, this can be determined by multiplying the corresponding entries from two matrices  $\mathbf{R}$  and  $\mathbf{C}$ , where

$$R_{ij} = \begin{cases} 1 & \text{if } D_{ij} = \min\left(D_{i,*}\right) \\ 0 & \text{otherwise} \end{cases}$$
(8)

$$C_{ij} = \begin{cases} 1 & \text{if } D_{ij} = \min\left(D_{*,j}\right) \\ 0 & \text{otherwise} \end{cases}$$
(9)

$$M_{ij} = R_{ij}C_{ij} \tag{10}$$

# 4. Experimental Procedure

A number of experiments were performed in order to test the performance, precision, and robustness of the VMPT algorithm. The experiments were performed at iThemba LABS using a Siemens EXACT3D PET scanner and 20 <sup>22</sup>Na tracers. Each tracer was made by drilling a hole in a 5mm diameter glass bead, inserting a small amount of <sup>22</sup>Na salt into the hole, and sealing it with resin. The initial activities of the tracers ranged from 49 to 74  $\mu$ Ci. Since <sup>22</sup>Na has a half-life of 2.6 years, the decrease in activity over the four weeks during which the experiments were performed was just over 2%.

A custom rig was designed to allow for controlled motion within the field of view of the scanner. It consisted of an aluminium shaft driven by an electric motor. Two polyethylene discs, shown in figure 3, were mounted on the shaft. Each of the discs had 24 holes machined into them in four radial columns of six holes each, spaced at 90° intervals.

Figure (4a) shows the custom experimental rig within the FOV of the scanner. Figure (4b) gives a closeup of the hole configuration.

The following is a description of each of the experiments performed.

## 4.1. Standard Rotation

A varying number of tracers were placed in the holes of the discs, which were rotated with a controlled circular motion. For each tracer configuration, two different velocities were used, with the velocity kept constant during each run. These experiments were performed mainly as a verification method, to check whether the algorithm could function on a basic level. Because the





(a) First disc, with column number 1 aligned with the keyway.

(b) Second disc, with columns rotated  $45^{\circ}$ .

Figure 3: Diagrams of polyethylene discs showing hole numbering system.

motion was known to be circular, the data gathered from these tests was used to analyse the precision of the tracer location.

#### 4.2. Erratic Rotation

The setup for these experiments was similar to the Standard Rotation setup. The only difference was that some of the tracers were attached to the discs using elastic bands. This caused an unpredictable bouncing motion in roughly half of the tracers caused by the elasticity of the attaching rubber bands, while the others were made to rotate with a controlled circular motion. The purpose of these tests was to observe how the algorithm would handle inconsistent and unpredictable motion. The bouncing also lead to higher accelerations and closer proximity between tracers. The data gathered from these tests was not examined quantitatively, but rather qualitatively.

# 4.3. Velocity Tests

To determine the effect of tracer velocity on the VMPT algorithm, the same setup was used as in the Standard Rotation experiments. However, in these tests, the number of tracers was kept constant, while a large range of velocities was used. The velocity was controlled by adjusting the rotational velocity of the motor. Since each tracer was kept at a constant distance from the centre of rotation, the linear velocity could easily be calculated. These tests were performed to assess the influence of the tracer velocity on the robustness and precision of the algorithm.



(a) CTI/Siemens EXACT3D model 966 PET scanner.



(b) View of assembled rig inside the PET scanner.

Figure 4: Custom rig used in VMPT experiments.

# 4.4. Z-axis Rotation

The tracers in the Standard Rotation experiments were made to rotate in the xy-plane; that is, the axis of rotation was aligned parallel to the longitudinal axis of the field of view of the camera. It is known from previous studies that the number of lines of response detected by the camera is dependent on the proximity of the tracer to the edge of the field of view. Therefore, tests were devised in which the tracers rotated in the xz-plane. This also allowed for tests in which one or more tracers completely exited the field of view. The data acquired from these tests was used to determine the effect of z-position on precision, and the robustness and reliability of the algorithm in the case of tracers leaving the field of view.

### 4.5. Tracer Impact

In real-world experiments, there is a significant chance that two or more tracers collide. In previous multiple tracer tracking algorithms, this was handled by halting the algorithm and restarting it after the collision. For the VMPT algorithm, it was desired that the algorithm run to completion without any manual intervention. As such, these tests were devised to qualitatively examine how the algorithm handled tracer impact. The tests involved two tracers suspended from a horizontal rod with lengths of string. They were pulled some distance apart and allowed to swing towards each other, causing them to impact and then move apart once again.

#### 5. Analysis & Results

#### 5.1. Precision

The precision to which the VMPT algorithm could locate a tracer was determined using a root mean square error (RMSE) method. This was done by plotting the x, y and z positions of the tracer versus time, as shown in figure 5. The Standard Rotation experiments described in Section 4.1 were used to determine the RMSE, since the motion in each dimension is predictably a sine curve. Being able to predict the motion of the tracers allows one to fit a best fit curve to the data. In the case of a single tracer moving in a circle in 3-dimensional space, the curve of best fit will take the form

$$\hat{x}(t) = A_x + B_x \sin(\omega t + \phi_x) \tag{11}$$

where  $\hat{x}$  is the predicted x-position of the tracer,  $A_x$  is the position around which the oscillation occurs,  $B_x$  is the amplitude of oscillation,  $\omega$  is the frequency of oscillation, t is the time, and  $\phi_x$  is the angular offset of the curve. The same equation holds for both the y and z dimensions.



Figure 5: Examples of plots generated by tracking four tracers moving with a controlled circular motion.

The RMSE is analogous to the standard deviation, in that it is a measure of the differences between measured and predicted values. The RMSE in each dimension is given by (for the case of the x-dimension)

$$RMSE_x = \sqrt{\frac{1}{n} \sum_{t=t_0}^{t_n} (x(t) - \hat{x}(t))^2}$$
(12)

where x(t) is the measured position at time t and n is the total number of measured data points. The total RMSE is then given by

$$RMSE = \sqrt{RMSE_x^2 + RMSE_y^2 + RMSE_z^2}.$$
 (13)

It should be noted that since the RMSE is a measure of the standard deviation, the precision is inversely proportional to the RMSE.

The RMSE was plotted against four variables, namely the number of tracers, the tracer velocity, the number of LOR's used per tracer in the location algorithm, and the spacing between consecutive seed points. These were the factors assumed to most affect the tracking precision, with velocity and tracer number being natural variables, while the LOR count and spacing are artificial variables.

Figure 6 shows the effect of the chosen variables on the RMSE. It can be seen that neither the tracer count nor the velocity have a significant effect on the average RMSE, but they both affect the variation. The RMSE is however highly dependant on both the spacing and the LOR count. Although the field of view is not specifically discretized into voxels, both the spacing and LOR count can be thought of as a measure of the degree of discretization, or voxel size. An increase in spacing and a decrease in LOR count both represent an increase in 'voxel size'. Figures 6c and 6d show that the RMSE decreases with a finer degree of discretization. Specifically, the RMSE decreases proportionally to  $1/\sqrt{n_{lines}}$ , where  $n_{lines}$  is the number of lines of response used per tracer. This is in agreement with previous studies done on a single tracer. This increase in precision does however come at a computational expense.

#### 5.2. Robustness

As a preliminary test of the robustness of the algorithm, the erratic motion experimental data was processed using the VMPT code. Figure 7 shows the results of the tracking. It can be clearly seen which tracers are experiencing controlled circular motion and which are bouncing due to the elastic attachment.



(a) RMSE versus number of tracers used.





(b) RMSE versus tracer velocity.



(c) RMSE versus number of LOR's per tracer.

(d) RMSE versus spacing between discretized points.

Figure 6: Plots showing the effect of tracer count, velocity, number of LOR's, and point spacing on the error in tracer location.

In certain physical situations, the VMPT algorithm can lose track of one or more tracers. The robustness of the algorithm is a measure of how the algorithm deals with these situations, and the level of human intervention needed to remedy them. As stated previously, there are three causes of tracer loss:

- Accelerations that are large enough such that the linear prediction used in the Tracking Step is not sufficient.
- One or more tracers exiting the field of view of the scanner.
- Two or more tracers colliding or coming so close to each other that



Figure 7: Eight tracers tracked, with four rotating in a controlled manner and four experiencing erratic motion.

they are indistinguishable.

It should be noted that although tracer count is itself not a direct cause of track loss, a larger tracer count increases the probability of a track being lost. This is because there are more LOR's to examine in a single frame, leading to larger noise levels.

Figure 8 illustrates the three sources of track loss. Figures 8a and 8b both show tracers with identical motion, the only difference being the number of tracers that were being tracked at the time. Although the plots only show small snapshots in time, the tracer in the experiment tracking only two tracers was successfully tracked over the entire experiment with no track loss, while the tracer in the experiment involving 20 tracers was lost multiple times. Figure 8c shows a set of five tracers, two of which periodically exit and re-enter the field of view. On return, the tracers are detected as new objects. Finally, Figure 8d shows the effect of tracer collision on the tracking. When the tracers come together they are detected as one for a short period of time, after which one is detected as a new object. It is impossible to predict which tracer will retain its identity; in some cases, *both* tracers are detected as new objects after collision. During the postprocessing analysis of the tracks, the time period over which the tracers merged is simply deleted from the data.



(a) Single tracer path in experiment using only two tracers. No track loss.



(c) Track loss due to tracers 1 and 2 exiting the field of view.



(b) Single tracer path in experiment using 20 tracers. Track loss at 18 s, 19.5 s and 27.5 s.



(d) Track loss due to collision between two tracers.

Figure 8: Plots showing track loss from multiple causes.

A drawback of all previous multiple tracer tracking algorithms is that the number of tracers had to be known at all times. This meant that the loss of a tracer had to be corrected manually by advancing the program to a point when the tracer reappeared. Because the DBSCAN clustering algorithm determines the number of clusters automatically, the VMPT algorithm is robust to tracer loss. This automatic correction for track loss is shown in Figure 8.

# 5.3. Computational Performance

When analysing the computational performance of the algorithm, the two main aspects to observe are processing time and memory usage<sup>2</sup>. The majority of the computational time was found to be used in the location section of the algorithm, and more specifically in the Voronoi tessellation. Since the speed of the tessellation is based on the number of seed points used, the total computational time can be considered to be dependent on the number of tracers used given constant discretization settings.



(a) Time taken to process a single frame (b) Memory needed of data. (b) Memory needed frame of data.

Figure 9: Computational performance of VMPT algorithm.

Figure 9 shows the relationship between performance and number of tracers being tracked. Although the performance is more strictly a function of the number of seed points in the Voronoi tessellation, one can use the tracer count as an independent variable because the number of seed points is directly related to the number of tracers. According to Aurenhammer (1991), the average runtime complexity of a Voronoi algorithm is  $O(n\log n)$ . A function of the form  $t(n) = n\log n$  was therefore fitted to the data points. Figure 9a shows that the curve of best fit is closely correlated to the data points, indicating the runtime of the algorithm is of the expected complexity.

To analyse the memory usage a similar method is used. Aurenhammer (1991) states that the Voronoi tessellation should on average use memory on

<sup>&</sup>lt;sup>2</sup>All code was written in Matlab version 2014b, and run on an Intel(R) Core(TM) i7-4500U, 1.80 GHz CPU with 4096 kB L2 cache and 6 GB memory.

the order of  $n^{d/2} = n^{1.5}$ , where d is the number of dimensions of the problem. As in the performance analysis, the curve of best fit shown in Figure 9b is closely correlated to the data, verifying the theoretical assumptions.

# 6. Conclusion & Recommendations

The VMPT algorithm was successful in tracking up to 20<sup>22</sup>Na tracers, although this does not appear to be the upper limit. To determine the precision of the tracking, the tracers were made to rotate in a circle at a constant velocity, and the data points gathered were fit to a sine curve using an iterative method. The root mean square error (RMSE) was determined for the fit, and used as a measure of the precision. It was found that the precision was mostly dependent on the level of discretization of the experimental volume, defined by both the number of LORs used per frame, and the separation distance between consecutive points on each LOR. The precision can therefore be increased by:

- decreasing the separation distance  $\epsilon_{sep}$
- increasing the number of LOR's used per frame

The RMSE was also determined for the original Birmingham tracking algorithm Parker et al. (1993) using a single tracer, and the two were compared. The Birmingham algorithm yielded an RMSE of 0.92 mm, while the VMPT algorithm yielded 1.26 mm, for an increase of 32 %.

The VMPT method was proven to be more robust than previous multiple tracer tracking methods, in that it automatically handles situations in which a tracer goes momentarily un-detected. Tracer loss can occur due to large accelerations, tracer collision, and a tracer exiting the field of view of the camera, and is exacerbated by the number of tracers within the field of view at any given time. Where previous algorithms needed manual intervention to skip past durations of tracer loss, the VMPT algorithm handles these occurrences automatically. Once a tracer is re-detected, it appears as a new, independent tracer.

The most reliable ways to decrease the chance of track loss are to:

- decrease the time interval between successive frames
- decrease the separation distance  $\epsilon_{sep}$

• increase the number of LOR's used per frame

Although the VMPT algorithm is robust, it is also computationally intensive and slow. Because a Voronoi tessellation is performed at every time step, the algorithm has a complexity of  $O(n\log n)$ , with n increasing linearly with tracer count. Tracking two tracers was found to take 1s per frame, while tracking twenty tracers took 14s per frame, with the time increasing according to the complexity. To decrease the time taken to process a given amount of data points, one can:

- increase the time interval between successive frames, thereby decreasing the total number of frames processed
- increase the separation distance  $\epsilon_{sep}$
- decrease the number of LOR's used per frame

It can be seen that the ways in which processing time can be decreased directly contradict those which can increase precision and robustness. The algorithm settings should therefore be changed based on how much the specific application values precision compared to performance.

As mentioned in Section 5.3, the Location Phase of the algorithm is inherently parallelizable. Adapting the code to run in parallel on multiple processors, can significantly reduce the processing time. Other ways to increase performance include writing the algorithm in a lower-level language such as C or Fortran and designing a dedicated Voronoi tessellation scheme.

# 7. Acknowledgements

The authors would like to thank the Centre for Minerals Research for funding the research.

We would also like to thank Michael van Heerden for assisting with the experimental setup, as well as iThemba LABS and PEPT Cape Town for use of the PET equipment.

- Aurenhammer, F., 1991. Voronoi diagrams a survey of a fundamental geometric data structure. ACM Computing Surveys (CSUR) 23, 345–405.
- Bickell, M., Buffler, A., Govender, I., Parker, D., 2012. A new line density tracking algorithm for pept and its application to multiple tracers. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 682, 36–41.
- Blackman, S. S., 2004. Multiple hypothesis tracking for multiple target tracking. Aerospace and Electronic Systems Magazine, IEEE 19 (1), 5–18.
- Borak, J., 2007. The ghost map: The story of london's most terrifying epidemic and how it changed science, cities, and the modern world.
- Breunig, M. M., Kriegel, H.-P., Ng, R. T., Sander, J., 2000. Lof: identifying density-based local outliers. In: ACM sigmod record. Vol. 29. ACM, pp. 93–104.
- Chang, Y.-F., Ilea, C., Aasen, Ø., Hoffmann, A., 2011. Particle flow in a hydrocyclone investigated by positron emission particle tracking. Chemical Engineering Science 66 (18), 4203–4211.
- Ester, M., Kriegel, H.-P., Sander, J., Xu, X., 1996. A density-based algorithm for discovering clusters in large spatial databases with noise. In: Kdd. Vol. 96. pp. 226–231.
- Fangary, Y., Barigou, M., Seville, J., Parker, D., 2000. Fluid trajectories in a stirred vessel of non-newtonian liquid using positron emission particle tracking. Chemical engineering science 55 (24), 5969–5979.
- Govender, I., Cleary, P., Mainza, A., 2013. Comparisons of pept derived charge features in wet milling environments with a friction-adjusted dem model. Chemical Engineering Science 97, 162–175.
- Govender, I., Pathmathas, T., 2017. A positron emission particle tracking investigation of the flow regimes in tumbling mills. Journal of Physics D: Applied Physics 50, 035601(10pp).
- Govender, I., Richter, M., Mainza, A., De Klerk, D., 2017. A positron emission particle tracking investigation of the scaling law governing free surface flows in tumbling mills. AIChE JOurnal 63 (3), 903–913.

- Gundogdu, O., 2004. Positron emission tomography particle tracking using cluster analysis. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 534 (3), 562–576.
- Hawkesworth, M., Parker, D., Fowles, P., Crilly, J., Jefferies, N., Jonkers, G., 1991. Nonmedical applications of a positron camera. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 310 (1), 423–434.
- Hill, K. H., 2016. Handbook of granular materials (editors: Scott V. Franklin and Mark D. Shattuck). CRC Press, Taylor and Francis Group.
- Hoomans, B., Kuipers, J., Salleh, M. M., Stein, M., Seville, J., 2001. Experimental validation of granular dynamics simulations of gas-fluidised beds with homogenous in-flow conditions using positron emission particle tracking. Powder Technology 116 (2), 166–177.
- Hue, C., Le Cadre, J.-P., Pérez, P., 2002. Sequential monte carlo methods for multiple target tracking and data fusion. Signal Processing, IEEE Transactions on 50 (2), 309–325.
- Li, H., Li, K., Kim, T., Zhang, A., Ramanathan, M., 2012. Spatial modeling of bone microarchitecture. Vol. 8290. pp. 82900P-82900P-9. URL http://dx.doi.org/10.1117/12.907371
- MacQueen, J., et al., 1967. Some methods for classification and analysis of multivariate observations. In: Proceedings of the fifth Berkeley symposium on mathematical statistics and probability. Vol. 1. pp. 281–297.
- Mitchell, T. M., 1997. Machine Learning (International Edition 1997 ed.). McGraw-Hill.
- Ni, R., Stuart, M. A. C., Dijkstra, M., 2013. Pushing the glass transition towards random close packing using self-propelled hard spheres. Nature Communications 4(2704), 1–7.
- Oh, S., Russell, S., Sastry, S., 2004. Markov chain monte carlo data association for general multiple-target tracking problems. In: Decision and Control, 2004. CDC. 43rd IEEE Conference on. Vol. 1. IEEE, pp. 735–742.

- Ouellette, N., Xu, H., Bodenschatz, E., 2006. A quantitative study of threedimensional lagrangian particle tracking algorithms. Exp. Fluids 40, 301– 313.
- Pal, P., O'Hern, C. S., Blawzdziewicz, E. R., Dufresne, E. R., Stinchcombe, R., 2008. Minimal model for kinetic arrest. Phys. Rev. E 78, 011111.
- Parker, D., Broadbent, C., Fowles, P., Hawkesworth, M., McNeil, P., 1993. Positron emission particle tracking-a technique for studying flow within engineering equipment. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 326 (3), 592–607.
- Parker, D., Dijkstra, A., Martin, T., Seville, J., 1997. Positron emission particle tracking studies of spherical particle motion in rotating drums. Chemical Engineering Science 52 (13), 2011–2022.
- Sánchez-Gutiérrez, D., Tozluoglu, M., Barry, J. D., Pascual, A., Mao, Y., Escudero, L. M., 2015. Fundamental physical cellular constraints drive self-organization of tissues. The EMBO Journal 35 (1), 77–88.
- Särkkä, S., Vehtari, A., Lampinen, J., 2007. Rao-blackwellized particle filter for multiple target tracking. Information Fusion 8 (1), 2–15.
- Springle, V., 2010. E pur si muove: Galilean-invariant cosmological hydrodynamical simulations on a moving mesh. MNRAS 401 (2), 791–851.
- Sweet, W. H., 1951. The use of nuclear disintegration in diagnosis and treatment of brain tumors. New England Journal of Medicine 245, 875 – 878.
- Wildman, R. D., Huntley, J. M., Hansen, J.-P., Parker, D. J., Allen, D. A., 2000. Single-particle motion in three-dimensional vibrofluidized granular beds. Physical Review E Volume 62, Number 3, 3826–3835.
- Wrenn, F. R., Myron, L., Handler, P., 1951. The use of positron-emitting radioisotopes for the localization of brain tumors. Science 113, 525 527.
- Yang, Z., Fryer, P., Bakalis, S., Fan, X., Parker, D., Seville, J., 2007. An improved algorithm for tracking multiple, freely moving particles in a positron emission particle tracking system. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 577 (3), 585–594.

Yang, Z., Parker, D., Fryer, P., Bakalis, S., Fan, X., 2006. Multiple-particle tracking - an improvement for positron particle tracking. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 564 (1), 332–338.