Enhancing PEPT: high fidelity analysis with augmented detection

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Abstract. The Positron Emission Particle Tracking (PEPT) technique allows for the tracking of a radioactive tracer particle at high spatial resolution over time, from which its trajectory can be reconstructed with uncertainty. The uncertainty budget when working with higher order measurands, such as velocities and accelerations, is complex and poorly understood, which can be problematic in the case of derived quantities. The uncertainties involved in calculations with these quantities become large as numerical derivatives are computed. To solve this, an alternative filtering and data processing method is investigated, enabling numerical differentiation of the measured trajectories while maintaining useful uncertainty bounds on results. This new method is the Savitzky-Golay filter, a local polynomial least squares fitting technique which is adapted to incorporate propagation of measurement uncertainties applicable to the PEPT technique. This new method is benchmarked against systems of known motion to place confidence limits on the results obtained. These results are then compared to the existing method, and the Savitzky-Golay filter is found to outperform the existing method in both its precision and accuracy across all tested regimes of motion. This potentially improves the uncertainty budget in PEPT analysis, enabling higher precision measurements to be performed.

1. Introduction

The Department of Physics at the University of Cape Town (UCT) runs a dedicated facility for Positron Emission Particle Tracking (PEPT) at iThemba LABS, South Africa. The PEPT technique allows for the tracking of a radioactive tracer particle to high spatial and temporal resolution over an extended time, from which the trajectory (position as a function of time) of the particle can be accurately reconstructed with an associated uncertainty. PEPT enables the non-invasive study of many important dynamical systems, with applications in a range of fields from engineering to medicine [1, 2, 3]. From the trajectories of the tracer particles, first and second order time derivatives can be computed numerically to determine dynamic parameters of the motion, such as velocities and accelerations, from which bulk system behaviours can be inferred. However, the uncertainty budget involved in these calculations is complex and poorly understood, and the application of numerical differentiation is typically accompanied by a loss of dynamic information, leading to greater uncertainties in the computed results. To extend the capabilities of the PEPT technique to enable higher precision analysis, alternative filtering and data processing methods are required to allow for the numerical differentiation of the relevant trajectories while maintaining useful uncertainty bounds on results. In this paper a new differentiation method, applicable to data obtained from the PEPT technique, is formally benchmarked against systems of known motion.

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2. The PEPT technique and detector systems

The mechanism of tracking used in PEPT relies on a radioactive tracer particle being a positron emitter. When a positron is emitted, it annihilates with a free electron within a short displacement of the tracer to produce two approximately back-to-back ($180° \pm 0.5°$) annihilation gamma photons with an energy of 511 keV each [4]. If these two photons are detected in coincidence, a line of response (LOR) can be defined linking the two detectors in three dimensional space. Ideally, an LOR can then be used to define the line along which the annihilation event occurred, which, when combined with one or more additional LORs, can be used to identify the location of the tracer at a given time. Of course, not every coincidence detection corresponds to the same annihilation event from the tracer, due to effects such as random or scattered coincidences. To deal with this, an iterative least squares minimisation (triangulation) routine [1] is used to find the most likely location of the tracer at a given time, producing the position $\langle x, y, z\rangle$ and time t with corresponding uncertainties.

Two physical systems were used for the PEPT measurements of tracer trajectories in this paper, being the Siemens HR++ PET scanner, housed at iThemba LABS, and the H3D small-animal PET system, currently housed at UCT. The HR++ camera, as described in [2], consists of 432 bismuth germanate (BGO) block detectors, each segmented into an 8 x 8 grid of independent detector elements, with a total of approximately 28000 detector elements. The block detectors are arranged into a ring in order to facilitate coincidence measurements, giving an axial field of view (FOV) of 23.4 cm with a ring diameter of 82.0 cm. The H3D PET system is comprised of four Polaris generation detector modules [5] arranged into a square, with each module containing four $(20\times20\times10)$ mm CdZnTe (CZT) semiconductor crystals giving a central FOV of $(77 \times 77 \times 42)$ mm. While the BGO crystals of the HR++ camera have a much greater intrinsic efficiency leading to higher event rates, the significantly improved spatial and energy resolution of the semiconductor H3D system allows for the acquisition of the tracer emissions to a higher precision. The contrast between these two systems is therefore useful in testing the limits of the applied differentiation method.

3. Differentiation methods

3.1. The 6-point method

In previous research using the PEPT technique, differentiation methods have always been required for analysis, with the most commonly used method being the 6-point method [3].

When considering the output of measurements being of the form $(t_i, \overrightarrow{P_i}, \overrightarrow{u_i})$, with $\overrightarrow{P_i}$ being the vector position of the particle at time t_i with three dimensional uncertainty $\overrightarrow{u_i}$, the simplest way to estimate the velocity $\overrightarrow{v_i}$ of the tracer at time t_i is to use a difference quotient, which is nothing but the spatial difference between two measured positions divided by their relevant measured times. The 6-point method can be considered as a weighted average of six difference quotients, with specific weights and positions chosen for the differences.

The uncertainty on each computed velocity is then calculated by simply propagating the measured position uncertainties through the method. To determine accelerations from the calculated velocities, the 6-point method can be applied again, using the computed velocities as inputs rather than the measured positions. Since the uncertainties must be propagated again through the method, it is expected that they will rise significantly, leading to the desire for an alternative method.

A additional challenge arises when trying to numerically differentiate PEPT data, as the time resolution is low with tracked locations recorded to a precision of 1 ms, meaning that often consecutive locations have the same time stamp and division by zero issues can occur. Therefore, the 6-point method (which is symmetric about the particular point of interest) offers the benefit of increasing the statistics by using non-consecutive data points in division. This method has been shown to produce an unbiased approach, but introduces some smoothing of the instantaneous velocity as a result of the need for consecutive locations. Under conditions of high accelerations the method also suffers, as even consecutive points can have different dynamics.

3.2. The Savitzky-Golay filter

Here, we replace the conventional numeric approach of the 6-point method with a more advanced filtering method known as the Savitzky-Golay filter [6], which is a particular type of low-pass filter historically used for data smoothing [7]. However, this filter offers the calculations of velocities and accelerations of a tracer particle with potentially significantly reduced uncertainties. The filter assumes that, at least locally in some narrow window of the data, the trajectory of the tracer can be approximated by a polynomial of some degree. Since PEPT measurements are discrete spatial positions with timestamps, a window of the data is a selection of several consecutive discrete positions along the trajectory of the tracer, with the width of the window being the number of selected positions. To apply the polynomial approximation assumption, a weighted least squares fitting routine is used over a moving window of the trajectory of the tracer to simultaneously smooth the measured positions and enable differentiation, which is made simple by the polynomial approximation. The details of this process can be seen as described in [7], and particularly useful results are quoted here.

Consider a design matrix $\mathbf{X}$ of dimension $n \times (m+1)$, containing all the timing information of a selection of the measured positions along the tracer's trajectory, a weight matrix $\mathbf{W}$ of dimension $n \times n$, containing all the corresponding uncertainty information, and a position vector $\vec{y}$ of dimension $n \times 1$, containing all the consecutive measured positions corresponding to the selections in the previous matrices. Using these matrices and vectors, an m^{th} order polynomial can be fit to a window of the data of width n using the normal equations [8] to extract the best fitting coefficients of the polynomial, given by $\hat{\beta} = (\mathbf{X^T W X})^{-1}\mathbf{X^T W}\vec{y}$, with $\hat{\beta}$ being a vector containing each consecutive fitted polynomial coefficient. Similarly, the uncertainties on these parameters can be extracted using $E_\beta = (\mathbf{X^T W X})^{-1}$, with E_β defining a covariance matrix of the calculated coefficients.

On a case by case basis, the fitting polynomial degree m can be adjusted to better represent the motion of the tracer according to theoretical or experimental expectation. For example, with a tracer falling under gravity the motion is theoretically described by a second degree polynomial, but when a radial coordinate in circular motion is considered a polynomial of a greater degree may better describe the sinusoidal motion. If the calculation of acceleration is desired, the minimal polynomial degree that can be used is 2.

When implementing this filter, the design matrix is typically redefined with a coordinate transformation which places the data point central to the window at the local position $t = 0$. This is useful since with a polynomial of the form $y = \beta_1 + \beta_2 t + ... + \beta_m t^m$, to determine any filtered value central to the window, being a smoothed version of the same data or even the m^{th} derivative, only a single coefficient needs to be extracted since all others give no contribution following the coordinate transformation. In other words, to determine the values of the m^{th} derivative of the data, the data point central to the window is replaced with the value of $m!\beta_m$, which can then be translated in time back to its absolute position along the trajectory of the tracer particle, simplifying the calculation of the filtered values and uncertainty analysis.

4. Experimental proof of concept

4.1. Interpolation

In addition to the new differentiation method, the effects of interpolation on the smoothing of noise in the data was tested as a precursor to the main filtering. In the interpolation procedure, new events were inferred from measured data, however, as the events arrive randomly in time and are not uniformly distributed in time or space, this becomes an additional source of uncertainty to be propagated carefully.

In this paper, a first step in applying interpolation was the use of a moving average to smooth the data, replacing each measured position at time t_i with the mean of the surrounding 11 events, reducing some of the variation in the data due to noise. Following this, a weighted linear least squares fitting procedure was applied to the smoothed data, using a moving timing window of selected size Δt from which the position with uncertainty at the interpolation time can be extracted. The uncertainty is of course propagated through both the moving average and the linear fitting methods in typical fashion.

A critical assumption for this interpolation is that the event rate or the spacing between the events is small relative to the changes in the motion, such that no adverse effects are seen, which can be controlled to some degree with the choice of the Δt parameter. This limits applicability in cases where the dynamics of the tracer particle are rapidly changing, with time scales on the order of Δt, for example in turbulent flow.

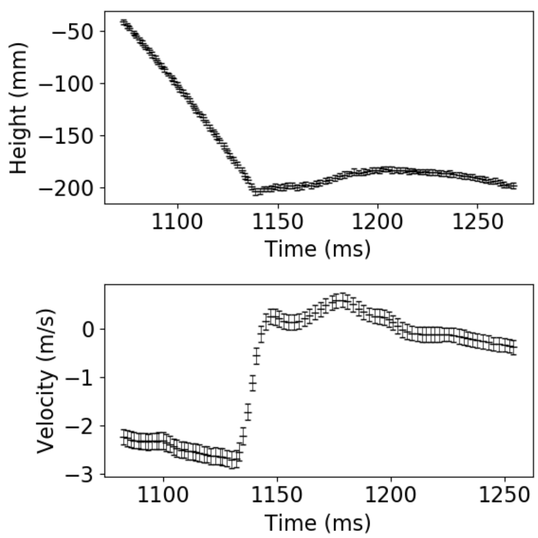

Figure 1. The height and velocity (calculated with the 6-point method) of a tracer falling and bouncing under the effects of gravity.

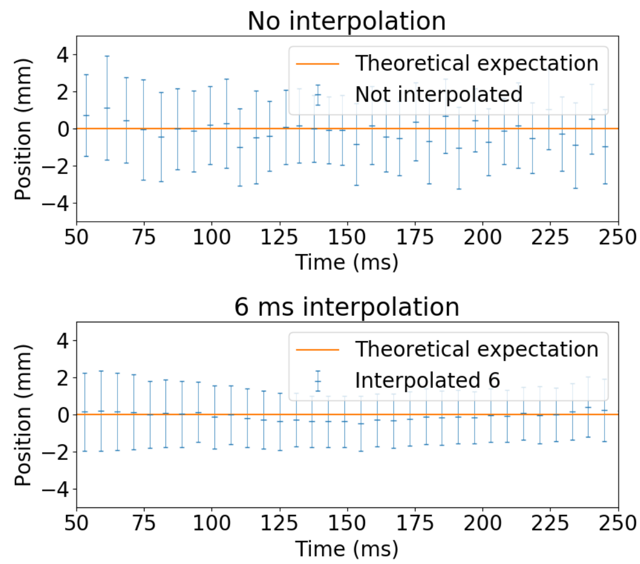

Figure 2. The effects of interpolation on the positions of a falling tracer, with residuals plotted showing the difference between measured values and theoretical expectation.

In testing this interpolation scheme, typical effects seen were an overall reduction in the mean uncertainties in each position, including a reduction in the overall deviation of the positions from the expected theoretical motion when working with benchmark systems of known motion. Figure 1 shows typical motion of a tracer falling under the effects of gravity, upon which a theoretical expectation for the motion can be built. Figure 2 shows the interpolation scheme applied to the falling tracer, with residuals calculated from the measured motion in figure 1 and the theoretical expectation obtained from the motion.

4.2. Results

The Savitzky-Golay filter was applied to measured data of a tracer particle undergoing standardized motion including remaining stationary, falling under the effects of gravity, and undergoing circular motion. In all cases the HR++ camera was used to perform these measurements, besides for a case of circular motion where the H3D system was used with a rotation speed of around 1 mm/s, showing its applicability to systems of small-scale motion.

The Savitzky-Golay filter was on average $30\% - 50\%$ slower than the 6-point method in computing the velocities and accelerations of the motion, but since these computation times reached only tens of seconds when applied to many hours worth of measured data, the time difference between the methods used was not considered in comparisons.

For stationary motion, in all cases the Savitzky-Golay filter was found to outperform the 6-point method, offering optimized mean uncertainty reductions for a moving window of the trajectory with a width of 25 consecutive events and a fitting polynomial degree of 2. This polynomial degree was selected as stationary motion is theoretically described by a 0^{th} order polynomial, but to calculate the acceleration from the filter a minimum degree of 2 had to be used as to test the method itself.

In comparison with the 6-point method, a 77% reduction of the mean uncertainty was seen in the computed velocities while maintaining an equivalent representation of the theoretical motion as the 6-point method. The representation of the theoretical motion was quantified by taking the sum of the squares of the differences between the discrete computed positions, velocities or accelerations and the corresponding theoretical prediction, with a lower value better representing the theoretical model. In the accelerations, a mean uncertainty reduction of 81% was seen with a 75% reduction, or improvement, in the representation of the motion in comparison to the results of the 6-point method.

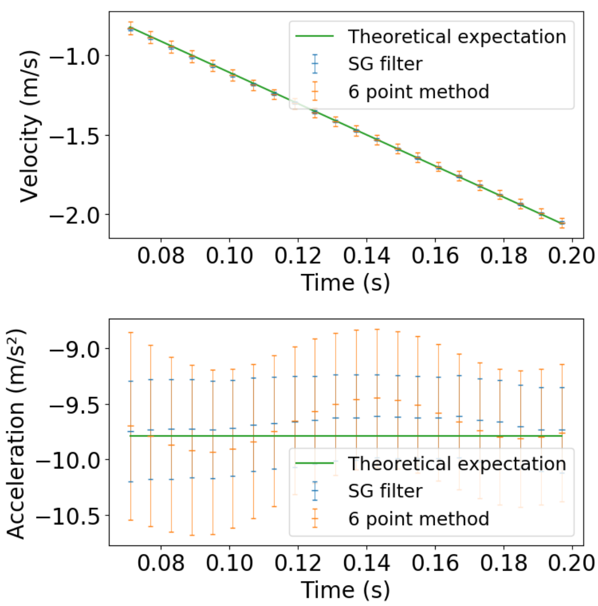

Figure 3. Velocities and accelerations of a tracer falling under gravity computed by the Savitzky-Golay filter, 6-point method, and theoretical expectation, measured by the HR++ camera. Both methods and expectation are in agreement. Note a clear reduction in uncertainties computed by the Savitzky-Golay filter.

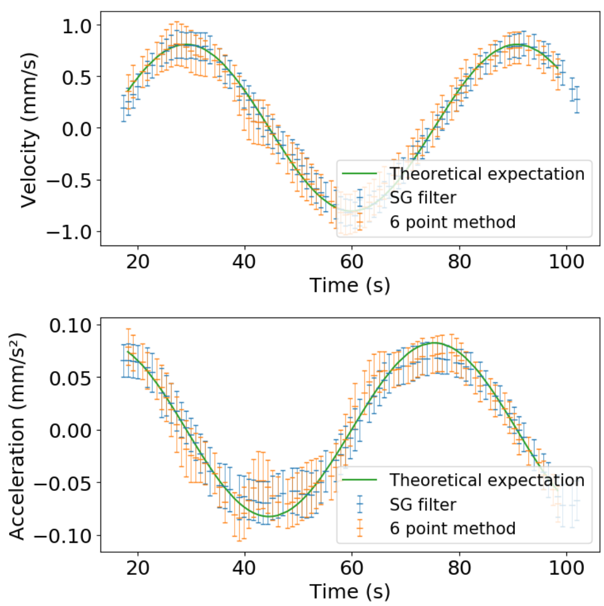

Figure 4. Velocities and accelerations of a tracer undergoing circular motion computed by the Savitzky-Golay filter, 6-point method, and theoretical expectation, measured by the H3D system. Both methods are in agreement, but a loss of accuracy at the extremes of the motion can be seen, leading to underestimates of the absolute velocities and accelerations.

When looking at the falling tracer, very similar effects were seen as in the stationary case, using the same window length and polynomial degrees, and in figure 3 the overall reduction in mean uncertainties in comparison to the 6-point method can be seen. In the case of the velocities, a 76% reduction of the mean uncertainty and a 53% improvement of the representation of motion was seen. With accelerations, a 40% reduction of the mean uncertainty and a 50% improvement of the representation of motion was seen. Interestingly, with the improvements offered by the Savitzky-Golay filter, we note that the deviations of the accelerations from the expected theoretical motion are all in the same direction in the Savitzky-Golay filtered results of figure 3, indicating that it may be possible to discern the effects of air resistance, but further analysis would be required to confirm this.

In circular motion, rapid changes in the extremities of a particular radial coordinate, i.e. the peaks of the sinusoidal motion of a particular coordinate, were underestimated by lower order polynomials and longer timescales. In this case, the fitting window of the data was reduced in size and the polynomial degree was increased on a case by case basis to account for the more rapid changes in the motion.

Using the circular motion as measured by the H3D system as an example, shown in figure 4, we see qualitatively that the mean uncertainties of the computed velocities and accelerations are approximately of the same order, with quantitative comparisons critical for analysis. To account for the underestimates of the extremities of the motion, the window width was reduced to 21 consecutive events with a fitting polynomial degree of 3. In the velocity a reduction of the mean uncertainty by 28% was seen, with a 67% improvement of the representation of the theoretical motion. In the acceleration, a 12% reduction of the mean uncertainty was seen, with a 52% improvement in the representation of the theoretical motion.

When looking at the results of the H3D system in figure 4, we note that the velocities and accelerations being computed are small, but with the uncertainties on these quantities remaining at least a factor of 6 smaller than the maximal velocity and a factor of 3 smaller than the maximal acceleration, with the uncertainty of the acceleration being of the order of 20 $\mu m.s^{-2}$. This will hopefully permit deeper analysis into small-scale systems of motion in the future.

5. Conclusions

A novel technique for PEPT, being the application of the Savitzky-Golay filter for smoothing and differentiation, was investigated to enhance the uncertainty budget involved when discussing PEPT analysis. The Savitzky-Golay filter was benchmarked, with the results from measured data compared to systems of known motion, and found to outperform existing methods on standardized data sets, offering generally decreased uncertainties on measured positions and derived velocities and accelerations, while also improving the representation of the theoretical motion by the filtered experimental results. However, this was only a proof of concept investigation, and a formal analysis of the uncertainty budget would be needed to quantify the improvements offered by the Savitzky-Golay filter on arbitrary data, but in doing this analysis the enhanced filtering method may lead to an improved quality of future PEPT analyses, particularly in terms of describing the quality of the inferences made from measured data.

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