Unbalanced Optimal Transport For Stochastic Particle Tracking

Kairui Hao[1], Atharva Hans[1], Pavlos Vlachos[1], Ilias Bilionis[1,*]

1: School of Mechanical Engineering, Purdue University, West Lafayette, IN, United States
*Corresponding author: ibilion@purdue.edu

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ABSTRACT

Non-invasive flow measurement techniques, such as particle tracking velocimetry, resolve 3D velocity fields by pairing tracer particle positions in successive time steps. These trajectories are crucial for evaluating physical quantities like vorticity, shear stress, pressure, and coherent structures. Traditional approaches deterministically reconstruct particle positions and extract particle tracks using tracking algorithms. However, reliable track estimation is challenging due to measurement noise caused by high particle density, particle image overlap, and falsely reconstructed 3D particle positions. To overcome this challenge, probabilistic approaches quantify the epistemic uncertainty in particle positions, typically using a Gaussian probability distribution. However, the standard deterministic tracking algorithms relying on nearest-neighbor search do not directly extend to the probabilistic setting. Moreover, such algorithms do not necessarily find globally consistent solutions robust to reconstruction errors. This paper aims to develop a globally consistent nearest-neighborhood algorithm that robustly extracts stochastic particle tracks from the reconstructed Gaussian particle distributions in all frames. Our tracking algorithm relies on the unbalanced optimal transport theory in the metric space of Gaussian measures. Specifically, we optimize a binary transport plan for efficiently moving the Gaussian distributions of reconstructed particle positions between time frames. We achieve this by computing the partial Wasserstein distance in the metric space of Gaussian measures. Our tracking algorithm is robust to position reconstruction errors since it automatically detects the number of particles that should be matched through hyperparameter optimization. Notably, our tracking algorithm also readily applies to the standard deterministic PTV case. Finally, we validate our method using an in vitro flow experiment using a 3D-printed cerebral aneurysm.

1. Introduction

Particle tracking velocimetry (PTV) is a fluid velocity field measurement technique that works by tracking the tracer particles (Maas et al., 1993; Malik et al., 1993). Multiple cameras record the three-dimensional motion of tracer particles in two-dimensional images. Then one uses a regression approach to build forward measurement models that map the physical space particles to the images (Maas et al., 1993; Malik et al., 1993). The two-dimensional projected particle images can be mapped back to the physical space using triangulation Maas et al. (1993); Wieneke (2012). Once physical space particle positions are reconstructed at each recorded frame, one uses tracking algorithms to obtain Lagrangian tracks Malik et al. (1993). Finally, the Eulerian velocity and pressure fields can be estimated from these Lagrangian tracks (Neeteson et al., 2016; Zhang et al., 2020; Virant & Dracos, 1997; Hagemeier et al., 2015).

Two crucial steps in PTV are the reconstruction of physical space particle positions from recorded images and the extraction of Lagrangian tracks from the reconstructed particle positions. One of the standard reconstruction methods is Iterative Particle Reconstruction (Wieneke, 2012; Jahn et al., 2021). To extract Lagrangian tracks, one uses tracking algorithms to identify the most probable tracks. The classic approach is the nearest neighbor searching (NNS) algorithm Malik et al. (1993) that finds the nearest particle to an individual particle or predictor location. Several subsequent improvements to the NNS algorithm have been developed. Dracos (1996) proposed to penalize large acceleration. Baek & Lee (1996) used iterative estimation of match probability and no-match probability. Okamoto et al. (1995) developed a spring model technique to match particle clusters. The method in Guezennec et al. (1994) finds the most likely particle tracks by minimizing a penalty function associated with each possible track. The objective is to use path coherence, such as smoothness of position and velocity to identify particle tracks. Li et al. (2008) used a regression method to predict future particle positions and the developed method is more robust to noisy input particle positions. Mikheev & Zubtsov (2008) added a term that accounts for particle diameters for enhancing pairwise matching. Cardwell et al. (2011) introduced a multi-parametric particle-pairing algorithm. Cierpka et al. (2013) uses a multi-frame high-order approach to pair particles. Instead of finishing reconstruction and tracking in two steps, the state-of-the-art method, shake-the-box Schanz et al. (2016), combines these two steps together to identify the Lagrangian tracks in time progressively.

Despite the great progress in the field, there still remain some open challenges. First, all current methods are deterministic and cannot account for uncertainties in PTV. In the reconstruction step, the reconstructed physical space particles are not fully faithful due to camera measurement noise, overlapping particles, and reconstruction algorithm errors. These errors subsequently propagate to the particle tracking phase. Deterministic approaches produce a single Lagrangian track, which is incapable of quantifying the errors. Second, all the tracking algorithms use NNS-type approaches that only utilize local displacement information to match particle pairs. This local matching strategy is not necessarily globally consistent since one particle might be identified as the nearest neighbor particle for multiple particles or predictors. Hence, further processing is required to identify the unique particle tracks. Last, it is still challenging for the current tracking algorithms to address the reconstruction errors, and robustly identify Lagrangian tracks from the potentially erroneous position reconstruction results. Robustly identifying the stochastic Lagrangian tracks against reconstruction errors is crucial to reconstruct the stochastic Eulerian velocity field using Physics-informed reconstruction algorithms (Alberts & Bilionis, 2023; Hao & Bilionis, 2023).

The objective of this paper is to develop a globally consistent nearest-neighborhood algorithm that robustly extracts stochastic particle tracks from the reconstructed Gaussian particle distributions in all frames. We use the unbalanced optimal transport (UOT) theory. Specifically, we solve the partial Wasserstein distance (PWD) (Chapel et al., 2020) formulation of UOT. Our method is the first PTV tracking algorithm to match reconstructed Gaussian position estimation and propagate uncertainties from stochastic particle positions to stochastic Lagrangian tracks. We achieve this by matching the Gaussian position estimation in the metric space of Gaussian measures, also known as the Wasserstein space.

The structure of this paper is as follows. In section 2 we review the Bayesian volumetric reconstruction method. In section 3, we develop our tracking algorithm. In section 4, we validate the algorithm with a cerebral aneurysm flow experimental example. In section 5, we conclude the paper.

2. Background on Bayesian volumetric reconstruction in PTV

We briefly review the Bayesian volumetric reconstruction (BVR) method developed in Hans et al. (n.d.). We consider U as a 3D flow domain and $r = (x, y, z) \in U$ as a position in the domain. BVR formulates a Bayesian inference problem to estimate the posterior distribution of the 3D physical space particle positions given observed camera images. Two ingredients are needed. First, a prior distribution of 3D particle positions $p(r_{1:N})$ that quantifies our belief of particle positions before observing the images. This is the users' choice and can be just a uniform distribution over U. The second ingredient is a likelihood function $p_\lambda(y_{1:M}|r_{1:N})$ defined by the parameter λ, which links the 3D particle positions to the observed images. Each y_m is the observed mth grayscale camera image.

Then we apply the Bayes' theorem to get the posterior distribution of particle positions:

$$p_\lambda(r_{1:N}|y_{1:M}) \propto p_\lambda(y_{1:M}|r_{1:N})p(r_{1:N}).$$

Jointly finding the posterior distribution and the optimal likelihood parameter λ analytically is intractable. So BVR uses variational inference (Jordan et al., 1999) and the training technique in variational auto-encoder (Kingma & Welling, 2013) to approximate the posterior distribution while finding the optimal parameter.

This is achieved by maximizing the evidence lower bound (ELBO) over the likelihood parameter λ and a family of parameterized distribution $q_\psi(r_{1:N})$ to approximate the posterior $p_r(r_{1:N}|y_{1:M})$. Mathematically, the ELBO is defined as

$$\text{ELBO}\,(\psi, \lambda|y_{1:M}) = \int \log\left\{\frac{p_\lambda\,(y_{1:M}|r_{1:N})\,p(r_{1:N})}{q_\psi(r_{1:N})}\right\} q_\psi(r_{1:N})\,dr_{1:N}.$$

To improve the computational efficiency, BVR chooses the diagonal multivariate normal distribution for each particle position as the guide:

$$q_\phi(r_{1:N}) = \prod_{n=1}^{N} \mathcal{N}\left(r_n | \mu_n, \mathrm{diag}\left(\sigma_n^2\right)\right),$$

where μ_n and σ_n are the three-dimensional mean and standard deviation vectors for the nth particle, respectively. To further improve the reconstruction accuracy, BVR adds a penalty term to the ELBO. This significantly helps to escape local minimums in the optimization. The parameters λ defined in the forward camera model and measurement function are also optimized while computing the posterior distribution. The reader can find the details in Hans et al. (n.d.).

3. Methodology

In this section, we use UOT to develop a stochastic particle tracking algorithm that can identify and extract stochastic particle tracks from the posterior particle distributions produced by BVR.

We work in the metric space of probability measures $(\mathbf{P}, d)$. A point in this metric space is denoted by π and a collection of probability measures from this metric space is denoted by $\{\pi_i\}_{i \in I}$. In the BVR case, $\mathbf{P}$ is the space of Gaussian measures, a point π is a Gaussian measure and the metric d can be the Wasserstein 2- distance (Takatsu, 2011). The BVR method reconstructs a diagonal covariance matrix for each particle and the Wasserstein 2- distance is

$$W_2\left(\mathcal{N}(m_1, \mathrm{diag}(\sigma_1^2)), \mathcal{N}(m_2, \mathrm{diag}(\sigma_2^2))\right)^2 = \|m_1 - m_2\|_2^2 + \|\sigma_1 - \sigma_2\|_2^2 .$$

Equipped with the notations above, we assume there are N number of reconstructed particle position estimates $\Pi^k = \left(\pi_1^k, \cdots, \pi_N^k\right)$ at time frame k, and M number of estimates $\Pi^{k+1} = \left(\pi_1^{k+1}, \cdots, \pi_M^{k+1}\right)$ at time frame $k+1$. It should be emphasized that N is not necessarily equal to M.

Our objective is to design an optimal transport plan in the space of probability measures $\mathbf{P}$. First, we write down the source mass:

$$\mu(\pi) = \sum_{i}^{N} \delta_{\pi_i^k}(\pi), \tag{1}$$

and the target mass:

$$\nu(\pi) = \sum_{i}^{M} \delta_{\pi_i^{k+1}}(\pi). \tag{2}$$

A graphic illustration of transporting Gaussian distributions from the source to the target is shown in Fig. 1.

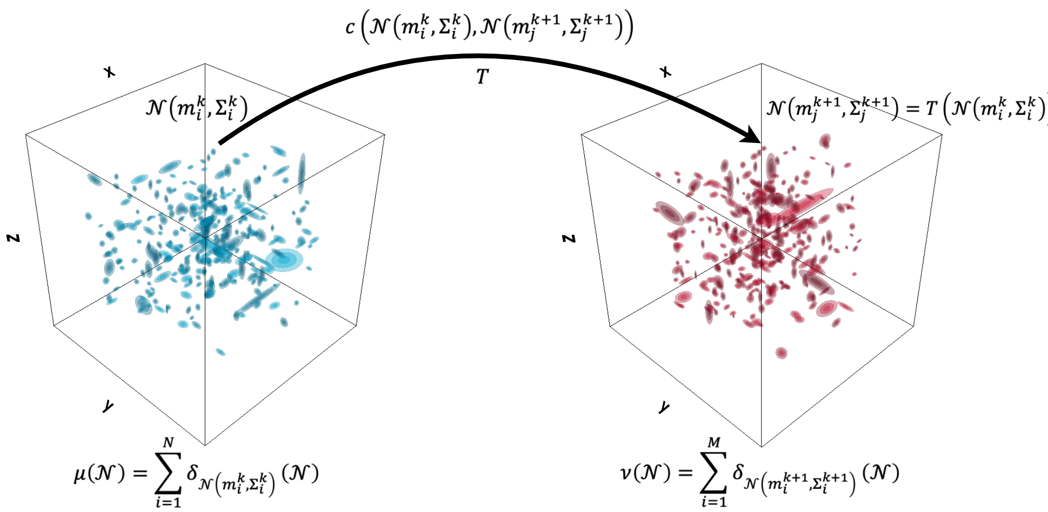

Figure 1. An illustration of unbalanced optimal transport of stochastic particle position reconstructions.

$$\begin{aligned}
\min_{\gamma} \quad & \langle \gamma, c \rangle_F \\
s.t. \quad & \sum_{j=1}^{M} \gamma_{ij} \leq 1, \text{ for } i = 1, \cdots, N, \\
& \sum_{i=1}^{N} \gamma_{ij} \leq 1, \text{ for } j = 1, \cdots, M, \\
& \sum_{i=1}^{N} \sum_{j=1}^{M} \gamma_{ij} = N_p \in \mathbb{N}^{+} \leq \min\{N, M\}, \\
& \gamma_{ij} \geq 0,
\end{aligned} \tag{3}$$

Since the source mass is not necessarily equal to the target mass, i.e., $N \neq M$, this problem is unbalanced in nature. We use the partial Wasserstein distance (PWD) formulation, shown in Eqs. 3, to find the optimal transport plan. This formation constrains the total transport number N_p. The first constraint states that the mass transported from the source should not be greater than the mass of the source. The second constraint states that the mass received by the target should not be greater than the mass of the target. The fourth binary constraint guarantees no mass split. In the third constraint, the positive integer N_p is the total mass to be transported. This is the hyperparameter that should be carefully chosen or optimized. In PTV particle matching, due to missing and overlapped particles, fluid flowing in and out of the observation volume and particle position reconstruction errors, the value of N_p is usually less than $\min\{N, M\}$. The number $N - N_p$ denotes our guess of the number of particles that do not have a matched particle pair in frame $k + 1$ due to position reconstruction errors or particles flowing out of the flow domain. Similarly, the number $M - N_p$ denotes our guess of the number of particles that do not have a matched particle pair in frame k.

4. Experimental example: cerebral aneurysm

We demonstrate our tracking algorithm using the experimental cerebral aneurysm dataset. Brindise et al. (2019) performed in-vitro experiments, where particle images were captured using four high-speed cameras with one center camera of 0° angle from the geometry plane and the other three of about 30° angles. 1216 $\times$ 1224 pixels time-resolved images were recorded at 2000 Hz. Lagrangian tracks were identified using the shake-the-box (Schanz et al., 2016) algorithm.

For our purpose, we first use the BVR algorithm (Hans et al., n.d.) to reconstruct the posterior distributions of particle positions at each frame using recorded images from the four cameras. Then, we identify stochastic Lagrangian tracks using our PWD formulation of unbalanced optimal transport. We showcase the reconstruction results in three plots. In Fig. 2, we plot the reconstructed particle position means using BVR in the left column, and the reconstructed track position and velocity means using PWD in the right column. Notice that the velocity means are plotted at the location of the position means. The identified tracks are visually reasonable compared to the reconstruted particle positions. In Fig. 3, we plot the total standard deviations, i.e., the squared root of the sum of the variances of x, y, and z coordinates. All standard deviations are plotted at the location of the position means. In the left column, we plot the result for the interior particles whose distances to the interior wall surface are greater than 1mm. The right column shows the result for the particles near the interior wall surface. We use pink color to emphasize high uncertainty. As the color in the right column is slightly higher than the left column color, the uncertainty of the reconstructed particle positions near the wall exhibits a slightly higher uncertainty. Usually, the reconstruction result shows more error and uncertainty in the regions that are closer to the wall, and our reconstruction result agrees with this fact. Fig. 4 plots the uncertainty of the velocities of the reconstructed Lagrangian tracks. As before, the left and right columns plot the result for the tracks that are greater and within 1mm distance to the interior wall surface, respectively. The velocity standard deviations are plotted at the location of the track means. We can observe a similar result that the velocity uncertainty near the wall is slightly higher than the uncertainty in the interior region.

5. Conclusions

In this paper, we develop a stochastic particle tracking method based on unbalanced optimal transport theory. The method optimizes a transport plan to move the reconstructed particles (represented by Gaussian distributions) between two frames in the most efficient manner. Since the

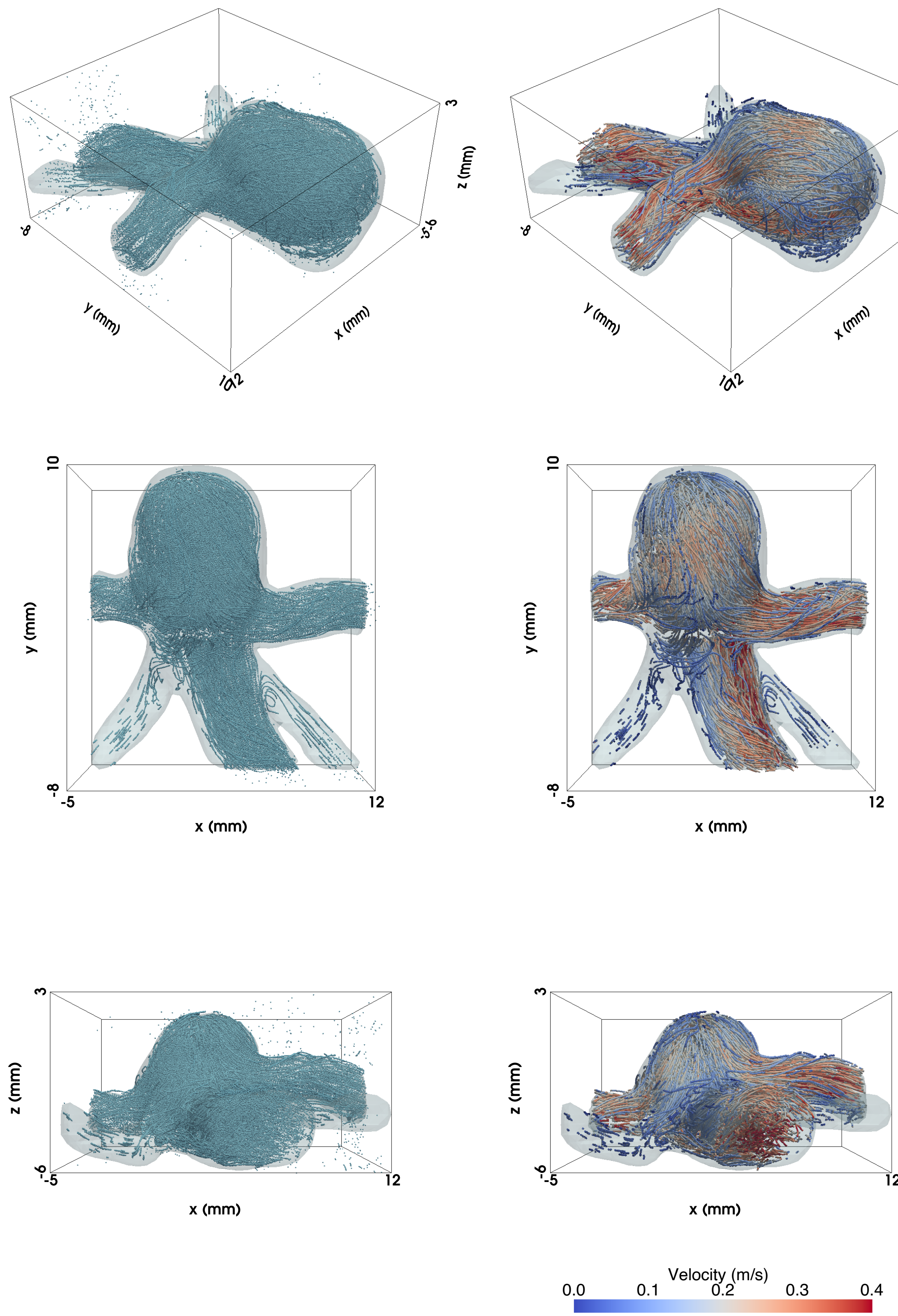

Figure 2. Cerebral aneurysm flow experimental data (Brindise et al., 2019). Left column: reconstructed particle position means across all frames using BVR. Right column: reconstructed track position and velocity means using PWD.

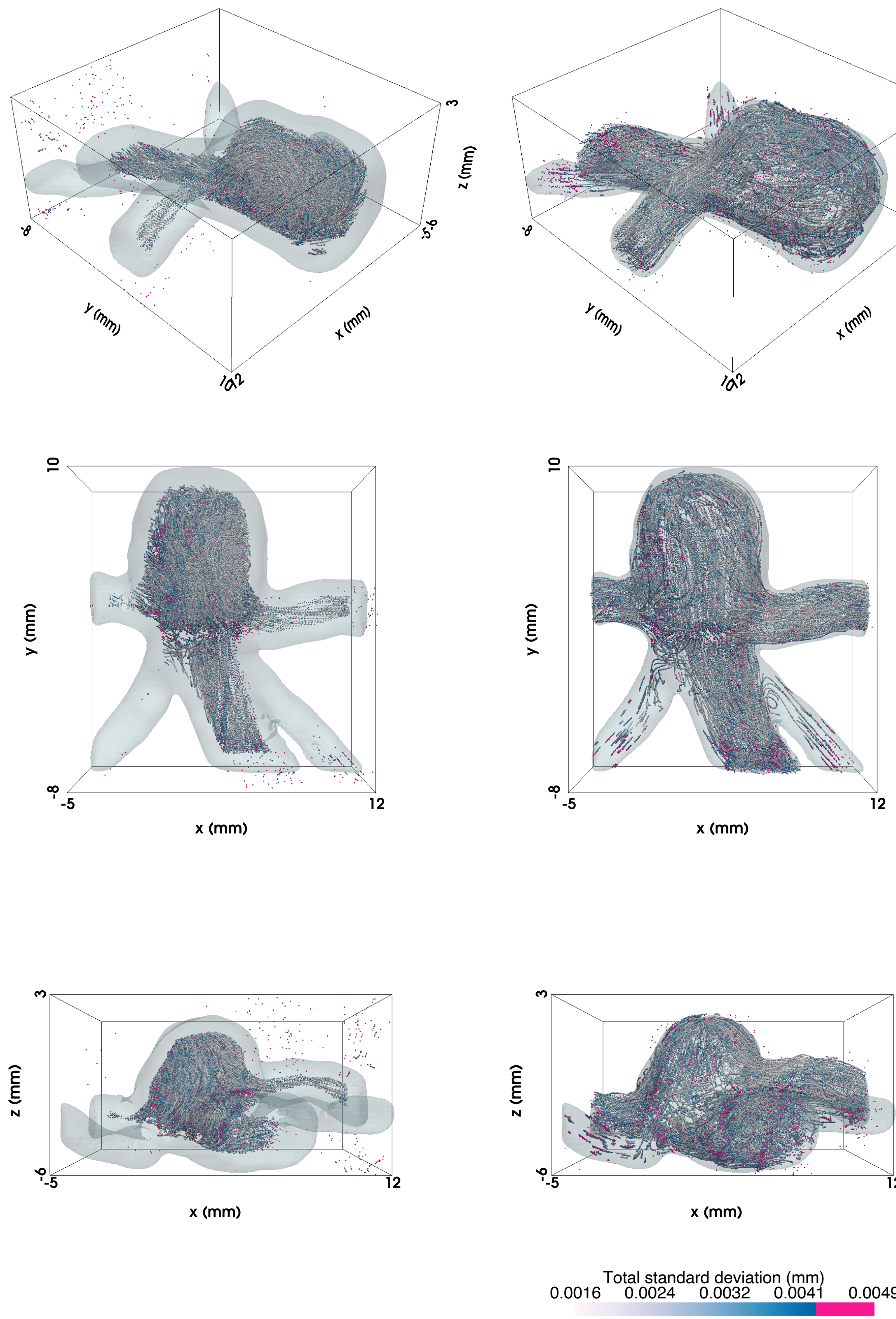

Figure 3. Cerebral aneurysm flow experimental data (Brindise et al., 2019). Left column: total standard deviations of the reconstructed particle positions across all frames using BVR in the interior region (particle distances to the wall are greater than 1 mm). Right column: total standard deviations near the wall (less than 1mm).

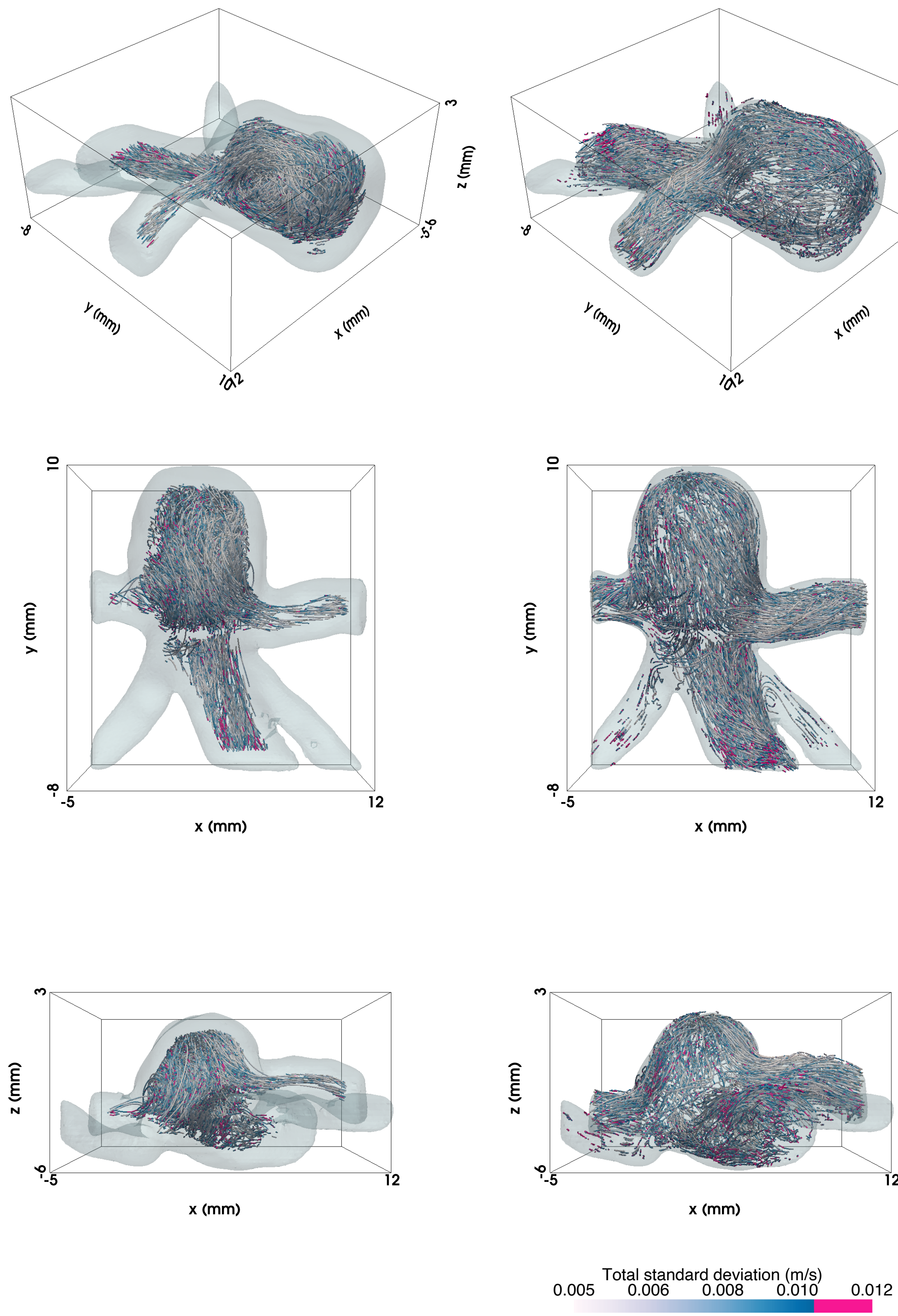

Figure 4. Cerebral aneurysm flow experimental data (Brindise et al., 2019). Left column: total standard deviations of the reconstructed track velocities using PWD in the interior region (track distances to the wall are greater than 1 mm). Right column: total standard deviations near the wall (less than 1mm).

numbers of reconstructed particles between two frames are rarely the same, we employ an unbalanced optimal transport formulation. Finally, we demonstrate and validate the developed stochastic particle tracking method using a cerebral aneurysm flow experimental example. In addition to showcase the reconstructed position and velocity means, we highlight the ability of our method to quantify the reconstruction uncertainty. In particular, we plot the velocity uncertainties in the interior region and near the interior wall surface region, respectively. The reconstruction result shows a slightly greater velocity uncertainty of the particles near the wall.

In summary, the developed method shows a convincing and promising capability to improve particle tracking accuracy and robustness. The method also adds an additional advantage of quantifying reconstructed position and velocity uncertainties over the conventional method.

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