Abstract—We address the challenge of controlling the density of particles in two dimensions by manipulating the electric field acting on the particles immersed in a dielectric fluid. An array of electrodes is used to control the electric field, which applies dielectrophoretic forces to achieve the desired pattern of particle density. To model the motion of a particle, we use a lumped, 2D, capacitive-based, and nonlinear model. We estimate the spatial dependence of the capacitances using electrostatic COMSOL simulations. We formulate an optimal control problem to determine the electrode potentials that will produce the desired particle density pattern. The loss function is defined in terms of the difference between the target density and the particle density at a specific final time. To estimate the particle density, we use a kernel density estimator (KDE) computed from the particle positions that vary with the electrode potentials. The effectiveness of our approach is demonstrated through numerical simulations that illustrate how the particle positions and electrode potentials change when shaping the particle density from a uniform to a Gaussian distribution.

I. INTRODUCTION

We aim to design and build a printer system for assembling micro-particles into engineered patterns. Micro-particles are submerged into dielectric fluid and their positions are controlled by manipulating the electric potential of a 2D array of electrodes. The particle positions are tracked by a high-speed camera and the control signals are generated by projecting images on photo-sensitive transistors attached to the electrodes. In [7], [12], [13], [14] we introduced control algorithms that act on individual particles. However, controlling and tracking of a large number of particles, at an individual level, is computationally expensive. It is more advantageous to control simultaneously large number of particles and shape them into a desired density. This is the problem we are addressing in this paper. At a conceptual level, we start with an initial particle density (e.g., uniform distribution) and we would like to converge to a target particle density (e.g., multivariate Gaussian distribution), over some time horizon, by varying the electrode potentials.

The problem addressed in this paper can be set in the larger context of optimal mass transport (OMT) theory that addresses the transport of mass from a source distribution to a target distribution with minimum effort. A review of OMT related problems and recent algorithms to solve such problems can be found in [5], [6]. A particular formulation of the OMT problem is the density control problem, where a cost function expressed in terms of the velocity field, is minimized while the density is constrained by the transport equation, together with boundary conditions. Our problem can be put in this context by viewing the particles as a discretization of the mass that needs to be transported. One fundamental difference in our formulation as compared to solutions proposed to solve the density control problem is that velocity field depends nonlinearly on the control variables: electrode potentials that shape the electric field. When using the electric potentials as optimization variables in an optimal control formulation, an analytic solution for the optimal control becomes illusive leading to the need to employ a numerical approach. Our problem formulation can also be seen from as an optimal control problem constrained by the Liouville equation. Controllability of the Liouville equation together with optimal control of its moments for some special cases (e.g., linear case) are discussed in [3]. In other related work [1], the authors introduce a dynamic output feedback control of the Liouville equations, applied to SISO discrete-time linear systems. Due to the nonlinear dependence of the electric potential field on the control inputs (electrodes potential), we cannot directly apply the approaches proposed in the previous references.

In this paper we use a practical, particle-based approach to approximate the particle density. In particular, we use a kernel density estimator (KDE) as a proxy for the particle density and solve the optimal control problem in terms of this quantity. Our objective is to compute a sequence of electrode electric potentials so that an initial particle distribution is shaped into a target distribution after applying this sequence over time. We define the optimal control cost function in terms of the $L_2$ metric used to compute the error between the particle density at the end of a time horizon and a target density. Another possible loss function is the KL divergence, but it is not the best choice for non-parametric densities since it is completely dominated by the tails of the densities. The KDE depends on the predicted trajectories of a set of particles, where the trajectory of a single particle is determined by a lumped, 2D, capacitive-based, nonlinear model describing its motion. We assume that there is no interaction between particles and that their motion is completely determined by the electric field generated by the array of electrodes. The electric field induces an accumulation of potential energy at the particles. We use automatic differentiation (AD) enabled by jax [8] to compute the forces (i.e., the gradient of the potential energy) that act on the particles, and the gradients of the loss and constraint functions that are passed to the optimization algorithm.

Notations: We denote scalars, vectors and random variables by Italic symbols, bold Italic symbols, and capital Italic
symbols, respectively. Let \( f(\mathbf{x}) \) be a multi-variable map, where \( \mathbf{x} = (x_i) \) is a vector of scalars. We denote by \( \nabla f \) the gradient of \( f \), and by \( \frac{\partial f}{\partial x_i} \) the partial derivative of \( f \) with respect to \( x_i \). For a vector valued function \( \mathbf{F}(\mathbf{x}) \), \( \frac{\partial \mathbf{F}}{\partial \mathbf{x}} \) denotes the Jacobian of \( \mathbf{F} \). For a function \( f(\mathbf{x}) \), with \( \mathbf{x} = (x_1, x_2) \), \( f(x_1, x_2) \) is an equivalent notation. The divergence operator applied to a vector-valued function \( \mathbf{F}(\mathbf{x}) \) is denoted by \( \nabla \cdot \mathbf{F} \). For a matrix \( A \), \( |A| \) denotes its determinant.

**Paper structure:** In Section II we introduce the experimental setup for controlling the micro-particles, and the single particle model of motion. We formulate the particle density control problem in Section III and showcase our approach through simulation results in Section IV.

II. PARTICLE MOTION CONTROL SETUP

We first introduce the experimental setup for controlling the particle density. Second, we describe the dynamical model for a single particle when actuated by an array of electrodes. Third, we generate a dynamical model for a single particle under the actuation of an arbitrarily large number of electrodes.

A. Experimental setup

The experimental setup is shown in Figure 1. The system has three hardware devices and three software modules. The hardware devices include: a high-speed camera for tracking the particle densities, an array of electrodes to generate a dynamic potential energy landscape for manipulating objects with dielectrophoretic (DEP) forces, and a video projector to actuate the array based on projected images. The software modules include: a module for image processing that estimates the particle density, a control module that compares the target particle density with the density at the end of the control horizon, and generates input signals to minimize the error between them, and an image generation module that maps the control inputs to images that are projected on the array. The projected images activate or deactivate electrodes, as indicated by the control inputs.

![Fig. 1: Diagram of the experimental setup: a high-speed camera tracks the particle density that is transmitted to the control module. A control module generates electrode potentials that minimizes the error between a target density and the particle density and the end of a time horizon. The control inputs (electrodes potential) are converted into images that are projected on the array. The light produced by the images powers the photo-transistors attached to the electrodes.](image)

B. Single particle dynamical model

By applying electric potentials to the electrodes, we generate DEP forces that act on the particles. A viscous drag force proportional to the velocity\(^1\) opposes the particle’s motion. Due to the negligible mass of the particle, the acceleration can be neglected. It follows that the particle dynamical model can be described by:

\[
\mu \dot{\mathbf{x}} = \mathbf{F}(\mathbf{x}, \mathbf{V}),
\]

where \( \mathbf{x} \) denotes the 2D particle position measured at its center of mass, \( \mathbf{V} = (V_{i,j}) \) are the electrode electric potentials, \( \mu \) is the fluid dependent viscous coefficient, and \( \mathbf{F}(\mathbf{x}, \mathbf{V}) \) is the vector of forces acting on the particle. The indices \((i, j)\) are associated to 2D electrode positions \( y^i_{i,j} \). We express the forces \( \mathbf{F}(\mathbf{x}, \mathbf{V}) \) as a function of the potential energy of the particle. We compute the potential energy using a capacitive-based electrical circuit that lumps the interaction between the electrodes and the particle (see Figure 2). The particle and the electrodes act as metal plates; hence the capacitances of these capacitors are dependent on the particle position.

The maximum values are attained when the particle’s position maximizes the overlap with the electrodes. To simplify the analysis, we limited our analysis to low frequency region only, where the dielectric constant is not frequency dependent. The vector of forces \( \mathbf{F} \) can be expressed as \( \mathbf{F}(\mathbf{x}, \mathbf{V}) = \sum_{i,j} C_{i,j}(\mathbf{x}) \nabla \phi(\mathbf{x}, \mathbf{V}) \), where \( C_{i,j}(\mathbf{x}) \) is the capacitance between the particle at position \( \mathbf{x} \) and electrode \((i, j)\), \( V_{i,j} \) is the electric potential of the electrode \((i, j)\), \( \phi(\mathbf{x}, \mathbf{V}) \) is the electric potential of the particle, and \( N \) is the number of actuated electrodes.

![Fig. 2: Capacitive-based model describing the interaction between particle and electrodes situated at positions \( y_j \).](image)

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Feedback control design requires explicit expressions for the capacitances between the particle and electrodes. We learn the capacitance model using COMSOL simulations. For symmetric particles (e.g., beads), we estimate the capacitances by simulating a 2D electrostatic COMSOL model, with the capacitance function of the form \( C_{i,j}(\mathbf{x}) = C(||\mathbf{x} - \mathbf{y}_{i,j}||) \), where \( \mathbf{x} = (x_1, x_2) \) denotes the particle 2D position,

\(^1\)The drag force is proportional to the velocity in non-turbulent flows, that is, when the Reynolds number is small.
and \( y_{i,j} \) is the fixed position of electrode \( i, j \). In the COMSOL model, a 16 \( \mu m \) width and 100 nm thickness copper object are surrounded by a dielectric with the same properties as the isopar-M solution. The capacitance matrix entries are computed from the charges that result on each conductor when an electric potential is applied to one of them and the other is set to ground, after electromagnetic simulations using partial differential equations. The COMSOL electrostatic model has as parameters, the diameter of the sphere, the electrode dimensions, the dielectric fluid constant (\( \varepsilon = 2 \)), the positions and material of the particle and the electrode. We fix the particle height at 5 \( \mu m \) and generate simulation results by varying its position on the \( x_1 \)-axis over the interval \([-1mm, 1mm]\). Note that due to the size of the particle versus the size of the electrodes, fringe effects (electric field distortions at the edges) are significant. The simulation results generate capacitances between the electrode and the particle for all considered positions. We parameterized the capacitance function using error functions: \( C(x) = \sum_{i=1}^{m} a_i \left[ \Phi \left( \frac{x + \delta}{\sigma} \right) - \Phi \left( \frac{x - \delta}{\sigma} \right) \right] \), where \( \Phi(x) = \frac{1}{\sqrt{\pi}} \int_{-x}^{x} e^{-t^2} dt \) is the error function, \( x \) is the distance between the center of the particle and the electrode center assumed at the origin, \( a_i \) and \( \sigma_i > 0 \) are scalars, and \( \delta \) is half of the electrode pitch (10 \( \mu m \) in our example). Figure 3 depicts \( C(x) \), the capacitance between the particle and the electrode as a function of the particle horizontal position, where the numerical values were fitted on the error function parameterization. For symmetric particles (e.g., sphere shaped), we can map the 1D model to a 2D model using the transformation \( x \rightarrow \sqrt{x_1^2 + x_2^2} \), which results in a capacitance function \( C(x_1, x_2) = \sum_{i=1}^{m} a_i \left[ \Phi \left( \frac{\sqrt{x_1^2 + x_2^2} + \delta}{\sigma_i} \right) - \Phi \left( \frac{\sqrt{x_1^2 + x_2^2} - \delta}{\sigma_i} \right) \right] \).

### C. From discrete to continuous electrode actuation

In this section, we demonstrate how to transform the particle motion model from a discretized actuation mechanism (discrete set of electrodes) to a continuous one. We start with the 1D case. We represent the particle electric potential as \( \nu(x, V) = \frac{1}{\sum_{i=1}^{N} \sum_{j=1}^{M} C_i(x)V_j}, \) and interpret \( \nu(x, V) \) as the expected value of a random function \( \mathcal{Y}(Y)|X = x \) over a discrete distribution \( p_i(x) = C_i(x)/\sum_{i=1}^{N} C_i(x) \). We represent the probability mass function \( p_i(x) \) as a conditional probability \( p_i(x) = Pr(Y = y_i | X = x) \), and hence the particle potential can be expressed as \( \nu(x) = E[\mathcal{Y}(Y)|X = x] \), where \( V_i = \mathcal{Y}(y_i) \) is a function that reflects the electric potential at each point \( y_i \). The discrete probability distribution can be seen as a discretization of a continuous probability distribution, i.e., \( p_i(x) = \int_{y - \delta}^{y + \delta} f(y|x)dy \), where \( \delta \) is half of the electrode pitch. The parameterization of the capacitance function in terms of the error functions tells us that the conditional probability density function (p.d.f.) is a mixture of Gaussian functions. For a sphere shaped particle, the mixture has only one term, and hence the capacitance is expressed as \( C_i(x) = 2a \int_{y - \delta}^{y + \delta} f(y|x)dy \), where \( f(y|x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y-x)^2}{2\sigma^2}} \). Therefore, the particle potential in the continuous representation can be expressed as \( \nu(x) = E[\mathcal{Y}(Y)|X = x] \), where the expectation is computed with respect to the conditional Gaussian distribution, \( \mathcal{N}(x, \sigma) \), and \( \mathcal{Y}(Y) \) is a function that assigns an electric potential to each point \( y \). The potential energy can now be represented as \( U(x) = aE[\mathcal{Y}(Y) - \nu(X)]^2|X = x] \), and, by combining (1) and (2), it follows that the 1D particle dynamics is given by the partial differential equation \( \dot{x} = \frac{\partial U(x)}{\partial x} \), where \( U(x) = aE[\mathcal{Y}(Y) - \nu(X)]^2|X = x] \), and \( \nu(x) = E[\mathcal{Y}(Y)|X = x] \).

**Extension to 2D case:** We denote by \( x = (x_1, x_2) \) the particle position and by \( y_{i,j} = (y_{i,1}^j, y_{i,2}^j) \) the position of electrode \((i, j)\). The particle dynamics becomes \( \dot{x} = \nabla U(x, V) \), where \( \mu \) is the viscous coefficient, and \( U(x, V) \) denotes the particle’s potential energy. The potential energy has a form similar to the 1D case, where \( \nu(x, V) \) denotes the particle electric potential, \( C_{i,j}(x) = C([|x - y_{i,j}|]) \) represents the capacitance between the particle at the position \( x \) and electrode \( i, j \) at position \( y_{i,j} \), and \( V_{i,j} \) represents the potential of electrode \((i, j)\). We assume that the capacitance \( C_{i,j} \) can be represented as the un-normalized discretization of a multi-variable Gaussian p.d.f., that is \( C_{i,j}(x) = 4a \int_{y_{i,1}^j - \delta/2}^{y_{i,1}^j + \delta/2} \int_{y_{i,2}^j - \delta/2}^{y_{i,2}^j + \delta/2} f(y|x)dy \), where the conditional density function \( f(y|x) \) is the multivariate Gaussian distribution \( \mathcal{N}(X, \sigma^2I) \). The potential energy is similar to the 1D case and it is given by \( U(x) = aE[(\mathcal{Y}(Y) - \nu(X))^2|X = x] \), where \( \mathcal{Y}(Y) \) is a map such that \( \mathcal{Y}(y_{i,j}) = V_{i,j} \).

**Remark 2.1:** Using a mean-field approximation argument (see for instance [4] in the context of the Cucker-Smale model) we can derive the Liouville equation for the evolution of the density of a large number of particles. We obtain a control input dependent PDE of the form \( \nabla \cdot (f(x, t)F(x, V(t))) + \frac{\partial f(x, t)}{\partial t} = 0 \), where \( f(x, t) \) denotes the particle density, and \( V(t) \) are the control inputs (i.e., the electrode potentials).

### III. Feedback control

The optimal control formulation is divided in two steps; first, we give an ideal formulation that introduces the control objective and optimization constraints in a continuous form. Second, we show how we map the continuous formulation...
into a discrete form that can be solved on a digital computer. As part of this discretization step, we use quadrature methods to evaluate the potential forces acting on the particles.

A. Optimal control: continuous form

The objective of the optimal control problem is to shape an initial density function \( f_0(x) = f(x,0) \) into a target density \( f_d(x) \). The ideal optimal control problem we would like to solve is: given a finite time horizon \([0, T]\), find the electric potentials \( \mathbf{V}(t) = (V_{ij}(t)) \) for \( t \in [0, T] \) such that \( f(x, T) \) equals the target density \( f_d(x) \). The main constraint of the optimization problem are the dynamics of the particle motion. The cost function is expressed in terms of a KDE for the particle density \( f(x, T) \). Let \( \{x(i)\}_{i=1}^n \) be a set of \( n \) particles. Then the KDE is given by \( \hat{f}(x,t) = \frac{1}{n} \sum_{i=1}^n K_H(x - x(i)) \), where \( H \in \mathbb{R}^2 \) is the symmetric, positive definite bandwidth matrix, \( K_H(x) = |H|^{-1/2} K(H^{-1/2}x) \), with \( K \) being the kernel function. Examples of commonly used kernels include: boxcar, Gaussian, Epanechnikov or tricube. In this paper, we use the standard multivariate kernel: \( K_H = \frac{1}{\sqrt{2\pi|H|}} e^{-\frac{1}{2}x^T H x} \), due to its smoothness.

Let \( \mathcal{X} \in \mathbb{R}^2 \) be a compact set that bounds the particle positions, and let \( V_{max} \) be the maximum magnitude of the electric potentials. We formulate the following optimal control problem:

\[
\min_{\mathbf{V}(t), x(i(t)), t \in [0, T]} \int_\mathcal{X} \left( \hat{f}(x, T) - f_d(x) \right)^2 dx
\]

s.t.
\[
\hat{f}(x, T) = \frac{1}{n} \sum_{i=1}^n K_H \left( x - x(i) \right) ,
\]
\[
|\mathbf{V}(t)| \leq V_{max}, \forall t \in [0, T],
\]
\[
x(i(t)) \in \mathcal{X}, \forall t \in [0, T],
\]
where \( x(0) \) are the initial particle positions. To numerically solve (3), we need to convert it into a discrete representation that employs discretization of both time and space.

B. Optimal control: discrete form

For the spatial discretization, we use an uniform mesh with cells that are centered at \( (x_i, t) \), each cell having area \( \Delta x^2 \). We discretize the time using a sampling period \( \Delta t \), resulting in a sequence of samples \( \{t_k\} \). We convert the continuous dynamics of the particle trajectories into discrete representations via a direct collocation method. In particular, we use the implicit trapezoidal rule to approximate the particle dynamics. Consequently, the optimization problem (3) becomes:

\[
\min_{\mathbf{V}(t_k), x(i(t_k)), t \in [0, T]} \sum_{i,j} \left( \hat{f}(x_{i,j}, T) - f_d(x_{i,j}) \right)^2
\]

s.t.
\[
x(i(t_{k+1})) = x(i(t_k)) + \frac{\Delta t}{2} \left[ f(x(i(t_k+1)), \mathbf{V}(t_k+1)) \right] \]
\[
+ \left[ f(x(i(t_k)), \mathbf{V}(t_k)) \right] , x(i(0)) = x(0)
\]
\[
\hat{f}(x_{i,j}, T) = \frac{1}{n} \sum_{i=1}^n K_H \left( x_{i,j} - x(i) \right) ,
\]
\[
|\mathbf{V}(t_k)| \leq V_{max}, \forall t_k \in [0, T],
\]
\[
x(i(t_k)) \in \mathcal{X}, \forall t_k \in [0, T],
\]

Potential force computation: To compute the potential force \( F(x, \mathbf{V}) \) in (4), we need to evaluate the expectations found in the expression of \( U(x) \), over the distribution \( \mathcal{N}(x, \sigma^2) \), with \( \sigma \) a parameter determined from the geometric properties of the spherical particle. We make use of Gauss quadrature rules [9], often found in the theory of generalized chaos polynomials (GCP) [15], [16], [18]. Gauss quadrature rules provide the means to accurately evaluate the conditional expectations, using a small number of points. Since the conditional probability distribution of \( Y | X = x \) can be expressed as product of two Gaussian distributions \( Y_i | X_i = x_i \sim \mathcal{N}(x_i, \sigma_i^2) \), with \( i \in \{1, 2\} \), we have that the expectation of \( V(Y) | X = x \) is given by \( \mathbb{E}[V(Y)|X = x] \approx \frac{1}{n} \sum_{i=1}^n w_i v_i \left( \mathbb{V}_{2} \sigma_{1} y_{1} + \mathbb{V}_{1} \sigma_{2} y_{2} \right) \), where \( n \) is the number of sample points, \( y_i \) are the roots of the physicists’ version of the Hermite polynomial \( H_n(y) \) and \( w_i \) are associated weights given by \( w_i = \frac{2^{n-1} n! \sqrt{\pi}}{n^n \rho_n (\rho_n + 1)^2} \). Similarly, the variance of \( V(Y) | X = x \) can be approximated as \( \mathbb{V}(x) = \mathbb{E} \left[ \hat{V(Y)} | X = x \right] \approx \frac{1}{n} \sum_{i=1}^n w_i v_i \left[ \mathbb{V}_{2} \sigma_{1} y_{1} + \mathbb{V}_{1} \sigma_{2} y_{2} - \mathbb{E}[\hat{V(Y)} | X = x]^{2} \right] \approx \frac{1}{n} \sum_{i=1}^n w_i v_i \left[ \mathbb{V}_{2} \sigma_{1} y_{1} + \mathbb{V}_{1} \sigma_{2} y_{2} \right] \).

We can interpret the electric potentials \( V_{ij} \) as evaluations of a continuous map \( V_{i,j}(t) = \mathcal{Y}(y_{ij}, t; \beta) \), where \( \beta \) is a vector of parameters that defines the map. Consequently, the optimal control problem is no longer dependent on the number of electrodes, but on the vector of parameters \( \beta \). We now have the final optimal control formulation for learning a continuous map of potentials over time:

\[
\min_{\beta(i)} \sum_{i,j} \left( \hat{f}(x_{i,j}, T) - f_d(x_{i,j}) \right)^2
\]

s.t.
\[
x(i(t_{k+1})) = x(i(t_k)) + \frac{\Delta t}{2} \left[ F(x(i(t_k+1)), \mathcal{Y}(\cdot, t_k; \beta)) \right]
\]
\[
+ F(x(i(t_k)), \mathcal{Y}(\cdot, t_k; \beta)) , x(i(0)) = x(0)
\]
\[
\hat{f}(x_{i,j}, T) = \frac{1}{n} \sum_{i=1}^n K_H \left( x_{i,j} - x(i) \right) ,
\]
\[
|\mathcal{Y}(\cdot, t_k; \beta)| \leq V_{max}, \forall t_k \in [0, T],
\]
\[
x(i(t_k)) \in \mathcal{X}, \forall t_k \in [0, T],
\]

Remark 3.1: Solving (5) requires a choice of representation for \( \mathcal{Y}(x; t; \beta) \). We can take a global approach to the map representation and get inspiration from spectral methods [17] to represent the map \( \mathcal{Y} : \mathcal{X} \times [0, T] \) in terms of a set of polynomial basis functions, namely \( \mathcal{Y} : \mathcal{X} \to \sum_{i=1}^M v_i(t) \phi_i(x) \), where \( M \) is the number of terms in the approximation, and \( \phi_i(x) = \phi_i(x_1) \phi_i(x_2) \), with \( \phi_i \) a set of polynomial basis functions (e.g., Chebyshev or Legendre polynomials). In this case the parameters \( \beta \) are the coefficients \( v_i(t_k) \) for all discrete time instances. Alternatively, we can use universal function approximators, such as neural networks (NNs) [10], and the parameters \( \beta \) are the weights and biases. This option has the advantage that \( \beta \) no longer depends directly on the number of time instances. Similar ideas can be used to represent the trajectory of the particles. For example, we can use NNs that take as input time and generate as output the particle position. Such approaches have already been used.
in the context of PDEs, where NNs are used to approximate PDE solutions \[2\]. Unlike more traditional methods though (e.g., finite elements, (pseudo-)spectral methods), the effects of the approximation errors are much more difficult to quantify.

Remark 3.2: The loss function in the optimal control formulation includes the KDE for the particle density at the final time only. It is well understood that the quality of the estimator depends on the choice of the bandwidth matrix \(H\). At the final time, we can use the statistics of target density to select \(H\). For example, using Silverman’s rule (Scott’s rule is identical for the 2D case), we can choose \(\sqrt{H_{ij}} = n^{-1/3} \sigma_i\), and \(H_{ij} = 0\), where \(\sigma_i\) is the standard deviations for the \(l^{th}\) variable, and \(i, j \in \{1, 2\}\). Since we select the target density, \(\sigma_i\) can be picked in relation with this density. For the intermediate particle densities, we do not have a good way to estimate \(\sigma_i\), hence we may end up computing under or over smooth estimates.

IV. RESULTS

We solved the optimal control (5) using global parameterizations for both the particle trajectories and electrodes electric potentials. In particular, the vector of positions \(Z : [0, T] \rightarrow \mathbb{R}^{2n}\), with \(Z = [x^{(1)}, \ldots, x^{(n)}]\), and the electric potentials \(V : \mathbb{R}^2 \times [0, T] \rightarrow \mathbb{R}\) are defined as NNs. One advantage of this type of parameterization is that we can use batch execution to evaluate the particle positions and the electric potential at a sequence of time instances and positions, jointly. Another advantage is that there is no need to explicitly discretize the particle dynamics since we can use AD to evaluate the time derivatives. To ensure scalability with the number of optimization variables, we use Adam [11], a first order gradient-based algorithm, and recast the optimization problem in primal-dual flavor. We minimize the loss function \(\sum_{i,j} \left( \frac{1}{n} \sum_{i=1}^n K_H \left( x_{i,j} - x^{(l)}(T) \right) - f_d(x_{i,j}) \right)^2 + \lambda \sum_{i=1}^n \sum_{k,l} \left( F(x^{(l)}(t_k), \psi(x_{i,j}, t_k)) \right)^2\), in terms of the weights and biases of the NNs, using Adam. The bounds constraints on the particle positions and electric potentials are imposed through projections. Periodically, the weight of the constraint \(\lambda\) is updated to reflect how far we are from satisfying the constraint, using a projected gradient step:

\[
\lambda \leftarrow \lambda + \alpha \left( \sum_{i=1}^n \sum_{k,l} \left( x_{i,j}^{(l)} - F(x^{(l)}(t_k), \psi(x_{i,j}, t_k)) \right)^2 - \varepsilon \right)
\]

for a positive stepsize \(\alpha\) and a small positive scalar \(\varepsilon\), playing the role of tolerance.

In our simulation results, we consider \(\mathcal{P} = 5mm \times 5mm\), and the electrodes are uniformly distributed, with 0.25 mm electrode pitch, resulting in 1680 electrodes. The maximum electrode potential magnitude is 400V. The particle capacitance is a multivariate, Gaussian distribution with mean at the particle position \(x\) and covariance matrix \(\sigma^2 I\), where \(\sigma = 0.25 \times 10^{-3}\). We consider a time horizon of 5 seconds and a sampling period of 0.05 msec. We assume that the camera is able to identify the positions of 450 particles and these positions will be used as initial conditions in the optimal control problem. We use two NNs to model each of the \(x_1\) and \(x_2\) directions of the particle positions. These NNs have one hidden layer of size 1500, using \(\tanh\) as activation function. The electric potential map \(\psi\) is modeled as a NN with a hidden layer of size 500 and \(\tanh\) as activation function. Note that while the complexity of the NN modeling the map \(\psi\) can remain constant, the complexity of the NNs modeling the particle positions over time will depend on the number of particles. We set the target particle distribution to a multivariate Gaussian distribution centered at zero, with covariance matrix \(\sigma^2 I\), where \(\sigma = 0.5 \times 10^{-3}\). The bandwidth parameter is chosen as \(h = 1.06 \sigma n^{-1/5}\), where \(n\) is the number of particles. In addition, we set the tolerance for satisfying the particle dynamics constraint to \(\varepsilon = 10^{-4}\). Note that this tolerance is significant considering that it is applied to the sum (not the average) of more than \(10^7\) residuals, when accounting for the number of particles, time samples, and grid points at which the electric potentials are evaluated. We start from a perfect uniform particle distribution. After solving the optimal control problem, the particle positions after 5 seconds are shown in Figure 4. The positions are computed by evaluating the trained NNs at the end of the time horizon. Figure 5 depicts a comparison between the target density and the KDE computed using the particle positions, at the end of the time horizon. The MSE between the KDE and the target density is \(6.7 \times 10^{-4}\). It is well in the range of errors obtained by sampling from the Gaussian distribution and computing the KDE using these samples.

Figure 6 shows the electric potential changes over the time horizon, for four time samples. The red and blue colors represent negative and positive potentials, respectively. The intensity of the colors is proportional to the magnitude of the potentials. Interestingly, the plots show a clockwise rotation of the potential distribution over time. The results for the electric potentials are not unique and depend on the type of parameterization we use. As we increase the complexity of the NN, we can model a larger class of control inputs while increasing the complexity of the optimization problem. The NN modeling the behavior of the electrode potentials over time has a total of 2501 parameters. Had we considered the
control inputs at each electrode and each time sample, we would have had more than $1.6 \times 10^4$ optimization variables just for the control input. The complexity reduction by using a NN (or other type of parameterization) is obvious. What is not obvious upfront is what NN architecture to start with. In our case, we used a parsimonious approach: we started with a simple, one hidden layer architecture and increased its complexity (i.e., the size of the hidden layer) until we obtain a satisfactory result. The same approach was used for modeling the particle positions.

V. CONCLUSIONS

We addressed the problem of shaping the distribution of particles immersed in a dielectric fluid, by manipulating an electric field controlled by an array of electrodes. We employed a KDE to approximate the particle density, where the dynamics of a particle was determined using a 2D capacitive-based model of motion. We provided a probabilistic view for interpreting the particle dynamics for an arbitrarily large number of electrodes. In addition, we showed how we can use Gauss-Hermite quadrature to accurately approximate the potential energy of the particle. We formulated an optimal control problem that minimizes the $L_2$ norm between the particle density at the end of a time horizon and a target density, having the particle dynamics as constraint. We used automatic differentiation to compute derivatives of physical quantities (e.g., potential energy) and the gradient of the cost and constraint functions. We demonstrated our approach by shaping the density of particles from a uniform to a Gaussian distribution. As future work, we will compare the KDE-based approach to an optimal control formulation that uses the Liouville equation, as dynamical constraint.

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