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ABSTRACT

Ultrasound directed self-assembly (DSA) enables noninvasively aligning high aspect ratio particles in three-dimensional (3D) user-specified orientations, which finds application in a myriad of engineering applications, including manufacturing engineered materials. However, the number of ultrasound transducers and their spatial arrangement limit the accuracy of the particle alignment with any 3D user-specified orientation. We define a set of 3D user-specified orientations and use numerical simulations to quantitatively evaluate the effect of the number of ultrasound transducers, their spatial arrangement including a sphere, cube, and two parallel plates, and the size of the spatial arrangement on the orientation error of a high aspect ratio particle in a standing ultrasound wave field. We demonstrate that a spatial arrangement of ultrasound transducers with more than two unique wave propagating directions is required to orient a high aspect ratio particle in 3D, and we determine that the orientation error decreases with the increasing number of unique wave propagation directions. Furthermore, we show that in a spherical arrangement of ultrasound transducers, the orientation error is independent of the size of the arrangement of transducers. This knowledge facilitates using ultrasound DSA as a fabrication method for engineered composite materials that derive their function from the location and orientation of particle inclusions.
transducer operating parameters, and the “inverse” ultrasound DSA problem, which resolves the ultrasound transducer operating parameters required to assemble a user-specified pattern of particles. The forward ultrasound DSA problem is straightforward to solve analytically. However, solving the inverse ultrasound DSA problem often requires complex numerical optimization techniques. Several solutions exist to the inverse ultrasound DSA problem: user-specified patterns of spherical particles in 2D and 3D, and of high aspect ratio particles in 2D and 3D, where the solution also accounts for the particle orientation.

The number and spatial arrangement of ultrasound transducers limit the ultrasound standing wave patterns and, thus, the patterns of particles that can be assembled. For spherical particles, a pattern is feasible if we can establish an ultrasound standing wave where the ARP minima coincide with the user-specified particle locations, whereas for high aspect ratio particles, the ARP minima must additionally align with the user-specified orientation.

It is not well understood how the number and spatial arrangement of ultrasound transducers relate to the portfolio of feasible user-specified patterns. The literature documents that common user-specified patterns of particles result from a priori knowledge of patterns of particles that are intuitive to assemble, such as a line pattern between parallel ultrasound transducers, or a rectangular pattern between orthogonally oriented ultrasound transducers. Additionally, researchers use trial-and-error of the number and spatial arrangement of ultrasound transducers, until the desired user-specified pattern of particles is feasible to assemble, which is time consuming. Alternatively, Guevara Vasquez et al. theoretically showed that with a spherical arrangement of an infinite number of ultrasound transducers, any planar pattern of particles is feasible in the far-field, provided that the pattern of particles is a level-set of a 2D function with spatial frequency limited by the wavenumber.

However, even for feasible user-specified patterns, deviations may exist between the user-specified and experimentally assembled or simulated patterns of particles; for instance, because of constructive or destructive interference in the ultrasound wave field, reflections, and manufacturing tolerances or misalignment of ultrasound transducers. A pattern error quantifies the deviation between the user-specified and any experimentally assembled or simulated pattern of particles. For spherical particles, it accounts for the deviation between the user-specified and actual particle locations, whereas for high aspect ratio particles, the pattern error also accounts for the deviation between the user-specified and actual orientation.

Few researchers have attempted to measure or simulate how the number and spatial arrangement of ultrasound transducers define the portfolio of feasible user-specified patterns. For instance, Girenko et al. simulated that the area in which the location of a single spherical particle can be controlled increases with increasing number of ultrasound transducers arranged into a circle. Greenhall et al. simulated ultrasound DSA of complex 2D patterns of spherical particles, such as a block “U” pattern, with 200 ultrasound transducers arranged into a square, and also qualitatively concluded that the number of ultrasound transducers affects the geometric complexity of the pattern of particles that one can assemble. Prisbrey et al. also simulated ultrasound DSA of complex 3D patterns of spherical particles with 225 ultrasound transducers arranged into a sphere, confirming that Greenhall’s observations in 2D also apply in 3D.
in two orthogonal directions \(k_x\) and \(k_y\) simultaneously at multiple locations along \(e_z\).

The ARP in a fluid medium with density \(\rho_0\) and sound propagation speed \(c_0\) is given as:

\[
U = 2\Phi_1 \left( |P|^2 \right) - 2\Phi_2 \left( \left| \frac{\partial P}{\partial x} \right|^2 + \left| \frac{\partial P}{\partial y} \right|^2 + \left| \frac{\partial P}{\partial z} \right|^2 \right),
\]

with the acoustic contrast factors

\[
\Phi_1 = \frac{\pi r_p^3}{3} \left( \frac{1}{c_0^2 \rho_0} - \frac{1}{c_p^2 \rho_p} \right),
\]

\[
\Phi_2 = \frac{\pi r_p^3}{3} \left( \frac{\rho_p - \rho_0}{\rho_0 \rho_1 (\rho_0 + 2 \rho_p)} \right),
\]

where \(r_p\) is the length of the minor axis (thickness) of the high aspect ratio particle.

\[
P = \sum_{j=1}^{N_t} p_j
\]

is the total (complex) pressure at an arbitrary domain point \(x_0\), where we calculate the contribution of each \(j\)th ultrasound transducer (circular with radius \(a\)) as

\[
p_j = P_0 \left( \frac{I_1 (k_0 d \sin (\theta_j))}{d \sin (\theta_j)} \right) e^{j k_0 d \cos (\theta_j)}.
\]

\(k_0 = 2\pi/\lambda_0\) is the wavenumber, \(\lambda_0\) is the wavelength of the ultrasound wave field, \(I_1\) is the first order Bessel function of the first kind, \(P_0\) is an ultrasound transducer property (pressure amplitude in Pa per volt peak-to-peak (Vpp) square excitation signal at a distance from the ultrasound transducer) that relates the pressure amplitude to the voltage amplitude driving the \(j\)th ultrasound transducer, \(r_j\) is the Euclidean distance between the \(j\)th ultrasound transducer and a domain point \(x_0\) and \(\theta_j\) is the angle between the normal on the \(j\)th ultrasound transducer surface and \(x_0\).

Figure 1 also depicts a point cloud of acoustic trap locations \(x_i\) associated with the ultrasound wave field that results from applying \(\Phi\) to all \(N_t\) ultrasound transducers. Specifically, \(x_i\) are the locations where the acoustic radiation force \(F = -\nabla U\) acting on a high aspect ratio particle with density \(\rho_p\) and sound propagation speed \(c_0\) equals zero and points toward \(x_i\) in the surrounding region, and where \(U\) is locally minimum. A cluster of acoustic trap locations in close proximity locate and orient a single high aspect ratio particle in the orientation established by the ultrasound wave field. Thus, the major axis \(e_u\) (blue) of an ellipse fitted to the point cloud of acoustic trap locations \(x_i\) defines the 3D orientation of a high aspect ratio particle in the ultrasound wave field. Perfect alignment of the major axis of the high aspect ratio particle with the user-specified orientation exists when \(e_u = e_o\). Hence, we define the orientation error \(\gamma\) between \(e_u\) and \(e_o\) as

\[
\gamma = \arccos(e_u \cdot e_o).
\]

We only consider the orientation error because we always locate the high aspect ratio particle at \(\mathbf{0}\).

Figure 2 shows ultrasound transducers arranged into (a) a sphere, (b) a cube, and (c) two parallel planes and illustrates how we increase \(N_t\) from sparse to dense. We select these arrangements to represent configurations in which the primary wave propagation direction emitted from each ultrasound transducer is unique (sphere), points along three orthogonal axes (cube), and establishes a standing wave in one direction (parallel planes).

We maintain an equidistant ultrasound transducer spacing in the spherical arrangement, whereas in the cube and parallel plane arrangements, we ensure that the normal on the ultrasound transducer surface at the center of each plane array intersects \(\mathbf{0}\). For each spatial arrangement, we also vary the characteristic dimension \(C_{d_0}\) which we define as the radius of the sphere, the distance from the center \(\mathbf{0}\) to the planes of the cube, and distance from the center \(\mathbf{0}\) to each plane, respectively. We simulate ultrasound transducers with radius \(a = 4.5\) mm (type MURATA MA40S4S) with \(c_{\text{ph}} = 2\pi/40\) kHz, and orient a high aspect ratio expanded polystyrene (EPS) particle \((\rho_p = 25\) kg/m\(^3\)) with the average length of the major and minor axes being 4.2 mm and 2.1 mm in air.

We define 100 different user-specified orientations using combinations of \(\theta_u\) and \(\phi_u\) between \(0^\circ\) and \(90^\circ\) in \(10^\circ\) increments and determine the orientation error \(\gamma\). We select \(C_{d_0}/\lambda_0 = 3, 3.5, 10,\) and 13.5 for each spatial arrangement to determine the effect of the size. The minimum \(C_{d_0}/\lambda_0 = 3\) ensures that the center point \(\mathbf{0}\) resides in the far-field region of the ultrasound wave field. Furthermore, we vary \(N_t\) for the sphere between \(N_t = \{6, 99\}\), cube \(N_t = \{6, 1014\}\), and parallel planes \(N_t = \{2, 578\}\). Thus, we calculate 100 orientation errors for each spatial arrangement, for each characteristic dimension, and for each number of ultrasound transducers.

Figures 3(a)–3(c) show the average orientation error \(\gamma_o\) for the set of 100 user-specified orientations as a function of the number of
ultrasound transducers $N_t$ and characteristic dimension $C_d\lambda_0$ for ultrasound transducers arranged into (a) a sphere, (b) a cube, and (c) two parallel planes. The error bars represent one standard deviation of the orientation error. From Fig. 3(a), we observe that $\gamma_a$ is almost independent of $C_d\lambda_0$ but decreases with increasing $N_t$. The standard deviation of $\gamma$ also decreases with increasing $N_t$, indicating that the accuracy increases. From Fig. 3(b), we observe that the $\gamma_a$ increases with increasing $C_d\lambda_0$ and decreases with increasing $N_t$. Furthermore, the standard deviation of $\gamma$ is independent of $N_t$. From Fig. 3(c), we observe that the average and standard deviation of $\gamma$ does not vary significantly with $N_t$ or $C_d\lambda_0$. We also note the high $\gamma_a$ for the spatial arrangement of two parallel planes [Fig. 3(c)] compared to that of the sphere [Fig. 3(a)] and cube [Fig. 3(b)].

Figures 4(a)–4(c) show $U$ resulting from implementing $\bf v^*$ (from the solution to the inverse ultrasound DSA problem) in a square solution domain with length $2\lambda_0$ centered at $\mathbf o$ in the $xz$-plane, for $\theta_d = 0^\circ$ and $\phi_d = 30^\circ$ (indicated by $\mathbf e_d$ in red), respectively, and for the spatial arrangement of sphere [Fig. 4(a)], cube [Fig. 4(b)], and two parallel planes [Fig. 4(c)]. We maintain $N_t$ constant and vary $C_d\lambda_0$ to illustrate how the minima of $U$ (dark green), where a high aspect ratio particle aligns, evolve with increasing $C_d\lambda_0$.

We observe from Fig. 4(a) that there is no difference between $U$ for $C_d\lambda_0 = 3$ and $C_d\lambda_0 = 13.5$, which matches the observations of Fig. 3(a) that show that the $\gamma_a$ is independent of $C_d\lambda_0$. The minima (dark green) of $U$ at $\mathbf o$ result from ultrasound waves emitted from ultrasound transducers that have a unique propagation direction.

**FIG. 3.** Average orientation error $\gamma_a$ for ultrasound transducers arranged into (a) a sphere, (b) a cube, and (c) parallel planes as a function of the number of ultrasound transducers $N_t$ and characteristic dimension $C_d\lambda_0$.

**FIG. 4.** ARP $U$ in (a) sphere, (b) cube, and (c) parallel plane ultrasound transducer arrangements for $C_d\lambda_0 = 3$ and $13.5$ and for $\theta_d = 0^\circ$ and $\phi_d = 30^\circ$. 

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Thus, the ability to align a high aspect ratio particle in a user-specified orientation in a spherical arrangement of ultrasound transducers is independent of the size of the sphere. In contrast, we qualitatively observe from Figs. 4(b) and 4(c) that the width of minima of $U$ (dark green) increases in the $x$-direction, with increasing $C_d \lambda_0$. Furthermore, we observe that the inclination of the minima of $U$ approaches zero, despite imposing $\theta_d = 0^\circ$ and $\varphi_d = 30^\circ$ to the inverse ultrasound DSA solution. The Huygens principle causes the ultrasound waves emitted from each ultrasound transducer to approach a plane wave, with the increasing distance from the source. Hence, in spatial arrangements that comprise orthogonal or parallel-oriented plane arrays of ultrasound transducers, the ability to align a high aspect ratio particle in a user-specified orientation that is not parallel to the ultrasound transducers decreases with the increasing size. This explains the increasing $\gamma_a$ with increasing $C_d \lambda_0$ for the spatial arrangement [Fig. 3(b)]. The ability to orient a high aspect ratio particle with just two parallel arrays of ultrasound transducers is even more compromised as evidenced by the high $\gamma_a$ independent of $C_d \lambda_0$ and $N_t$ [Fig. 3(c)].

Figures 5(a)–5(c) show $U$ resulting from implementing $v^+$ (from the solution to the inverse ultrasound DSA problem) in a square solution domain with length $2\lambda_0$ centered at $\mathbf{a}$, in the $xz$-plane, for $\theta_d = 0^\circ$ and $\varphi_d = 30^\circ$ (indicated by $\mathbf{e}_p$ in red), respectively, and for the sphere [Fig. 5(a)], cube [Fig. 5(b)], and two parallel planes’ [Fig. 5(c)] spatial arrangement of ultrasound transducers. We maintain a constant $C_d \lambda_0$ and vary $N_t$ to illustrate how the minima of $U$ (dark green), where a high aspect ratio particle aligns, evolve with increasing $N_t$.

We qualitatively observe from Fig. 5(a) that increasing $N_t$ for the spherical arrangement improves the alignment of the minima of $U$ (dark green) at $\mathbf{a}$ with the user-specified direction $\mathbf{e}_p$. However, the improvement between $N_t = 6$ and $N_t = 50$ does not continue beyond $N_t = 50$. Thus, for a spherical arrangement with sufficient ultrasound transducers, $\gamma_a$ is independent of $N_t$. In contrast, we qualitatively observe from Figs. 5(b) and 5(c) that increasing $N_t$ in the cube and two parallel plane arrangements does not improve the alignment of the minima of $U$ (dark green) at $\mathbf{a}$ with $\mathbf{e}_p$. However, it decreases the width of the minima of $U$ (dark green) in the $x$-direction.

We have assumed that the ultrasound waves emitted from the ultrasound transducers do not reflect off nearby surfaces. However, reflections could affect a practical implementation and orientation error. While we assumed a massless particle, one must ensure that the curvature of $U$ is sufficiently large in the direction of gravity to support the particle, by maximizing the curvature of $U$ in the direction of gravity, in addition to optimizing the remaining terms in the objective function.

We conclude that to minimize the orientation error of a high aspect ratio particle, it is important to use an arrangement of ultrasound transducers with wave sources oriented in different directions because the Huygens principle causes the ultrasound waves emitted from each ultrasound transducer to approach a plane wave, with the increasing distance from the source. Hence, in spatial arrangements that comprise orthogonal or parallel-oriented plane arrays of ultrasound transducers, the ability to align a high aspect ratio particle in a user-specified orientation that is not parallel to the ultrasound transducers decreases with the increasing size. In contrast, in a spherical arrangement, each ultrasound transducer is oriented in a unique direction. For that reason, the orientation error is independent of the size and decreases with increasing ultrasound transducers.

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**DATA AVAILABILITY**

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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