Organizing user-specified patterns of spherical and high aspect ratio particles in a fluid medium using ultrasound directed self assembly

Dissertation defense presentation
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Achievements (1)

• Journal publications

  - Google Scholar citations as of 04/13/2020:
Achievements (2)

- Conference presentations
  - M. Prisbrey, B. Raeymaekers, Ultrasound manipulation of 3D dynamic user-specified patterns of particles in air, *Proc. of 178rd ASA Conference*, San Diego, CA (USA), 2-6 December 2019
  - M. Prisbrey, B. Raeymaekers, Ultrasound manipulation of 3D dynamic user-specified patterns of particles in air, *Proc. of 176rd ASA Conference*, Victoria, BC (Canada), 5-9 November 2018
  - T. A. Ogden, M. Prisbrey, I. Nelson, B. Raeymaekers, S. E. Naleway, Freeze casting of bioinspired porous ring structures through ultrasound directed self-assembly; *Proc. of The Materials Science Conference*, Phoenix, AZ (USA), 11-15 March 2018
Overview

• Introduction
  - Polymer-matrix composite materials
  - Polymer-matrix composite material manufacturing methods
  - Directed self-assembly (DSA)

• Ultrasound directed self-assembly
  - Ultrasound DSA Process
  - Implementing ultrasound DSA in engineering applications
  - Ultrasound DSA background
  - Research objectives

• Results
  - Spherical particles: Static 3D user-specified patterns
  - Spherical particles: Dynamic 3D user-specified patterns
  - High aspect ratio particles: 2D user-specified patterns
  - High aspect ratio particles: 3D user-specified patterns

• Conclusions
  - Spherical particles
  - High aspect ratio particles
  - Implications
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Introduction: Polymer-matrix composite materials

- **Polymer-matrix composite materials**
  - Heterophase material consisting of a polymer-matrix and filler material (particles)
  - Properties of polymer-matrix composite material depend on the following design parameters:
    - Properties of polymer-matrix
    - Properties of filler material
    - Interaction between the matrix and filler materials
    - Shape and spatial arrangement of filler material
  - Tuning these parameters allows designing the properties of the polymer-matrix composite material
  - Can combine multiple functionalities [e.g. 1,2]

Introduction: Manufacturing methods

**Subtractive**
Based on etching channels on a substrate to fill with particles

- Requires layer stacking to create 3D structures
- Limited to creating nanoscale channels individually [3]
  - Long fabrication times
  - Not practically scalable

**Additive**
Based on stacking layers containing filler material

- Requires layer stacking to create 3D structures
- Limited material choices [4,5]
  - Photopolymer resin
  - Thermosetting resin
  - Polylactic acid (PLA)

**Directed self-assembly (DSA)**
Based on noninvasively organizing particles in fluid or on a substrate

- Three categories:
  1. Templated
  2. Template-free
  3. External field-directed

---

Introduction: Directed self-assembly

- Process by which particles or other discrete components organize due to interactions between the components and their environment, driven by internal or external forces

**Templated**
- Patterns constrained to micro/nanoscale areas/volumes
- Limited material choices

**Template-free**
- Patterns constrained to micro/nanoscale areas/volumes
- Limited material choices

**External field-directed**
- Patterns constrained to micro/nanoscale areas/volumes
- Typically requires high field strengths to work
- Limited material choices

- Does not require high field strengths
- Works independent of particle material properties

**In contrast to other manufacturing methods, ultrasound DSA enables:**
- Manipulating particles over macroscale areas/volumes (2D and 3D)
- Manipulating particles of any property

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Ultrasound directed self-assembly process

**Gor’kov’s acoustic radiation force:**
\[ \mathbf{F} = -\nabla U \]

**Acoustic radiation potential:**
\[ U = 2\Phi_1 \left( |P|^2 \right) - 2\Phi_2 \left( |\nabla P|^2 \right) \]

**Contrast factors:**
\[ \Phi_1 = \frac{\pi r_p^3}{3} \left( \frac{1}{c_0^2 \rho_0} - \frac{1}{c_p^2 \rho_p} \right) \]
\[ \Phi_2 = \pi r_p^3 \left( \frac{\rho_p - \rho_0}{\omega_0^2 \rho_0 (\rho_0 + 2\rho_p)} \right) \]

- \( P \): Pressure
- \( r_p \): Particle radius
- \( c_0 \): Fluid sound propagation speed
- \( \rho_0 \): Fluid density
- \( c_p \): Particle sound propagation speed
- \( \rho_p \): Particle density
- \( \omega_0 \): Angular frequency

**Particles organize where:**
- Acoustic radiation potential is locally minimum
- Acoustic radiation force is zero, points toward the particle in the surrounding region
Implementing ultrasound directed self-assembly

- Implementing ultrasound DSA for engineering applications requires knowing the relationship between the ultrasound transducer settings and the corresponding pattern of particles.

**Forward ultrasound directed self-assembly problem**

- User-specified ultrasound transducer settings
- Acoustic radiation potential
- Acoustic radiation force theory
- Resulting pattern of particles (white dots)

\[
\mathbf{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_{N_i} \end{bmatrix}
\]

\[
v_i = A_i e^{j\theta_i}
\]

**Inverse ultrasound directed self-assembly problem**

- User-specified pattern of particles
- Computed ultrasound transducer settings required to form user-specified pattern

\[
\mathbf{v}^* = \begin{bmatrix} v_1 \\ \vdots \\ v_{N_i} \end{bmatrix}
\]

*Inverse problem can be solved directly or indirectly*
Existing solutions to the inverse ultrasound DSA problem

- Inverse problem has been solved directly/indirectly previously to enable:

  **Static/dynamic ultrasound DSA**
  - Spherical particle(s) in 1D, 2D, 3D

  **Indirect alignment of high aspect ratio particles**

1D Static/Dynamic Indirect

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Research objective

- State-of-the-art ultrasound directed self-assembly methods for creating user-specified patterns of filler materials are:
  - Limited to two-dimensions
  - Do not explicitly account for the orientation of particles, limited to spherical particles

Thus, the research objective is twofold:

1. Test the hypothesis that ultrasound wave fields can be used to assemble user-specified patterns of spherical particles in three-dimensions

2. Test the hypothesis that ultrasound wave fields can be used to create user-specified patterns of high aspect ratio particles, thus explicitly accounting for the orientation of the particles
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Spherical particles: Static 3D user-specified patterns

- **Objectives:**
  - Theoretically derive a direct solution method to the inverse ultrasound DSA problem to calculate the ultrasound transducer settings required to arrange static 3D user-specified patterns of spherical particles
  - Experimentally validate the theoretical solution by creating static 3D user-specified patterns of carbon nanoparticles in water
Theory: Relating the ultrasound wave field and transducer settings

- Use the boundary element method (BEM) to compute the ultrasound wave field, acoustic radiation potential and force, as a function of ultrasound transducer settings.

Boundary element model of a 3D reservoir

**Acoustic radiation potential in terms of velocity potential**

\[
U = 2\pi r_p^3 \rho_0 \left\{ \frac{1}{3} k_0^2 \left[ 1 - \left( \frac{\beta_p}{\beta_0} \right)^2 \right] \langle |\varphi|^2 \rangle \right. + \left[ \frac{\rho_p - \rho_0}{2\rho_p + \rho_0} \right] \left\langle |\nabla \varphi|^2 \right\rangle \}
\]

**Acoustic radiation force**

\[
F = -\nabla U
\]

**Green’s 3rd identity**

\[
\varphi(x_i) = -\Omega(x_i) \int_{S} \left[ i k_0 Z G(q, x_i) + \frac{\partial G(q, x_i)}{\partial n(q)} \right] \varphi(q) \, ds(q) + \ldots
\]

\[
\ldots + \Omega(x_i) \int_{S} \nu(q) G(q, x_i) \, ds(q).
\]

**Variables:**
- \( \varphi \): Velocity potential
- \( G \): Green’s function
- \( k_0 \): Ultrasound wave number
- \( Z \): Transducer acoustic impedance
- \( \nu \): Transducer acoustic impedance setting
- \( \beta_p \): Particle compressibility
- \( \beta_0 \): Fluid compressibility
- \( \rho \): Density
- \( \rho_0 \): Reference density
Theory: Solving the inverse ultrasound DSA problem

- Link the ultrasound transducer settings to the resulting pattern of particles via the acoustic radiation potential

Ultrasound transducer settings

\[ \mathbf{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_N \end{bmatrix} \]

Boundary element method

Ultrasound wave field

\[ \varphi(x,y,z;\mathbf{v}) \]

Acoustic radiation force theory

Acoustic radiation potential

\[ U(x,y,z;\mathbf{v}) \]

- Solve the inverse problem using constrained optimization

3D User-specified pattern of particles

Pattern feature \((x_i, y_i, z_i)\)

Solve the optimization problem

\[ \mathbf{v}^* = \arg \min \frac{1}{N} \sum_{i=1}^{N} U(x_i, y_i, z_i; \mathbf{v}) \]

subject to \(|\mathbf{v}| = \alpha\)

Required ultrasound transducer settings

\[ \mathbf{v}^* = \begin{bmatrix} v_1^* \\ \vdots \\ v_N^* \end{bmatrix} \]
Experiment: Methodology

- Prescribe a user-specified pattern of particles
- Solve the inverse problem to find the ultrasound transducer settings required to create user-specified pattern
- Apply ultrasound transducer settings to experimental setup

\[
\mathbf{v}^* = \begin{bmatrix} v_1 \\ \vdots \\ v_{Ni} \end{bmatrix}
\]

User-specified pattern
Ultrasound transducers
Reservoir

Solve inverse problem
Apply settings

80nm carbon nanoparticles dispersed in water
Glass sheet
Function generator
Camera

Ultrasound transducers
Reservoir

Prescribe a user-specified pattern of particles
Solve the inverse problem to find the ultrasound transducer settings required to create user-specified pattern
Apply ultrasound transducer settings to experimental setup
Experiment: Pattern error calculation

- Quantify error between user-specified patterns and experimentally obtained patterns for vertical sheets, 3D grid, and horizontal columns patterns
- Measure feature error $\tilde{x}$ between user-specified and experimentally obtained pattern features

\[ E_{\text{pat}} = \frac{\text{Mean}(\tilde{x})}{\lambda_0/2} \]

- Calculate pattern error $E_{\text{pat}}$ for each pattern for prescribed pattern spacing $\lambda_0/2$
Experiment: Static 3D user-specified patterns

- Compare experimentally obtained patterns to user-specified and simulated patterns

- Results show good qualitative agreement between prescribed and experimental and simulated patterns
Experiment: Pattern error

- Pattern error $E_{pat}$ between user-specified (red) and experimentally obtained patterns (black)

### Sources of error:
- Misalignment of ultrasound transducers
- Non-ideal piston source ultrasound transducers

- Small $E_{pat}$ for all experimentally obtained patterns shows quantitative agreement between user-specified and experimentally obtained patterns
Summary: Static 3D user-specified patterns, spherical particles

- We theoretically derived a direct method of solving the 3D inverse ultrasound directed self-assembly problem to create a 3D user-specified pattern of particles in a fluid reservoir with arbitrary geometry and ultrasound transducer arrangement.

- We experimentally validated the theoretically derived method.

- We demonstrated good quantitative agreement by comparing user-specified patterns to those created in the experimental reservoir.
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  - **Spherical particles: Dynamic 3D user-specified patterns**
  - High aspect ratio particles: 2D user-specified patterns
  - High aspect ratio particles: 3D user-specified patterns

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  - Spherical particles
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Spherical particles: Dynamic 3D user-specified patterns

- **Objectives:**
  - **Theoretically derive** a solution to the inverse ultrasound DSA problem to calculate the ultrasound transducer settings required to manipulate the particles comprising a 3D user-specified pattern to follow a 3D user-specified trajectory
  - **Experimentally validate** the theoretical solution by creating dynamic 3D user-specified patterns of spherical expanded polystyrene (EPS) particles in air
Dynamic 3D user-specified patterns concept

1. User-specified trajectory for each particle in a pattern X

2. Discretized user-specified trajectory, with pattern locations $X_i (i=1,\ldots,m)$

3. Solve the inverse problem to compute required ultrasound transducer settings for each pattern location $X_i$

4. Apply ultrasound transducer settings in sequence ($i = 1,\ldots,m$) to move pattern from $X_1$ to $X_m$ along user-specified trajectory
Theory: Relating the ultrasound wave field and transducer settings

- Describe the relationship between the acoustic pressure in the solution domain as a function of the ultrasound transducer settings
  - Pressure at any solution domain point is the summation of the acoustic pressure contributed from each ultrasound transducer

**Phased array consisting of** $N_t$ **ultrasound transducers**

**Pressure due to ultrasound transducers**

$$ P = Bv $$

where each term in $B$ is computed as

$$ b_{ij} = 2P_0 J_1(k_0a \sin \theta_{ij}) e^{ik_0r_{ij}} / (k_0 a \sin \theta_{ij} r_{ij}) $$

**Ultrasound transducer settings**

$$ v^T = (A_1 e^{i\alpha_1}, ..., A_j e^{i\alpha_j}, ..., A_{N_t} e^{i\alpha_{N_t}}) $$

- $P$: Pressure
- $P_0$: Pressure amplitude
- $J_1$: First order Bessel function, first kind
- $k_0$: Ultrasound wave number
- $a$: Ultrasound transducer radius
- $v$: Ultrasound transducer setting
Theory: Relating the pattern of particles and transducer settings

- Relate the acoustic pressure to the user-specified pattern of particles using acoustic radiation force theory

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

\[ \Phi_1 = \frac{\pi r_p^3}{3} \left( \frac{1}{c_0^2 \rho_0} - \frac{1}{c_p^2 \rho_p} \right) \]
\[ \Phi_2 = \pi r_p^3 \left( \frac{\rho_p - \rho_0}{\omega_0^2 \rho_0 (\rho_0 + 2 \rho_p)} \right) \]

\[ \mathbf{F} = -\nabla U \]

\( \rho_0 \): Fluid medium density
\( c_0 \): Fluid medium sound speed
\( \rho_p \): Particle density
\( c_p \): Fluid medium sound speed
\( \omega_0 \): Ultrasound transducer operating frequency
Theory: Solving the inverse ultrasound DSA problem

- Link the ultrasound transducer settings to the resulting pattern of particles via the acoustic radiation potential

\[
v = \begin{bmatrix} v_1 \\ \vdots \\ v_N \end{bmatrix}
\]

\[
\begin{bmatrix} \mathbf{P}(x,y,z;v) \end{bmatrix} = \begin{bmatrix} P_0 \\ -P_0 \end{bmatrix}
\]

\[
\begin{bmatrix} U(x,y,z;v) \end{bmatrix} = \begin{bmatrix} U_{\text{max}} \\ U_{\text{min}} \end{bmatrix}
\]

- Solve the inverse ultrasound DSA problem to form a pattern of particles X

\[
v^* = \arg \min \frac{1}{N} \sum_{i=1}^{N} U(x_i, y_i, z_i; v)
\]

subject to \(|v| = \alpha\)

\[
v^* = \begin{bmatrix} v_1^* \\ \vdots \\ v_N^* \end{bmatrix}
\]

- Repeat process for each discrete pattern position in user-specified trajectory
Experiment: Method

- Prescribe a user-specified pattern of particles and user-specified trajectory
- Compute ultrasound transducer settings for the user-specified pattern of particles at each locations $X_i$ of the user-specified trajectory
- Apply ultrasound transducer settings to experimental and simulated setup

\[
\mathbf{v}_{seq} = \begin{bmatrix}
    v_1^* \\
    \vdots \\
    v_m^*
\end{bmatrix}
\]

Solve inverse problem for each pattern location $X_i$
Experiment: Pattern error calculation

- Quantify the accuracy of the solution of the inverse DSA problem for dynamic patterns of spherical particles
- Measure the difference between experimental and user-specified pattern locations

\[
E_{\text{pat}} = \frac{100}{N\lambda_0} \sum_{k=1}^{N} |d_k|
\]

Wavelength \(\lambda_0 = 8.65\) mm
Experiment: translation and rotation

- Translation demonstrates the ability to translate entire patterns of particles
- Rotation demonstrates the ability to specify a unique trajectory for each particle in the pattern

Experimental results

Initial user-specified pattern locations

User-specified pattern location

Simulated pattern location

Translation

Wavelength
\( \lambda_0 = 8.65 \text{ mm} \)

\( X_i \): \( i^{th} \) pattern location

Rotation

\( 8\lambda_0 \)

\( 2\lambda_0 \)

- Observe good quantitative agreement between user-specified and experimental and simulated pattern locations
Experiment: Scaling, shearing and translation/rotation

- Shearing, scaling demonstrates the ability to move subgroups of particles
- Translation/rotation demonstrates the ability to apply multiple simultaneous transformations

Initial user-specifed pattern locations  
Experimental results

Wavelength \( \lambda_0 = 8.65 \text{ mm} \)

\( X_i \): \( i^{th} \) pattern location

- User-specified pattern location
- Simulated pattern location

Scaling/shearing

User-specified pattern location, \( X_i \)

Translation/rotation

User-specified pattern location, \( X_i \)

- Observe good quantitative agreement between user-specified and experimental and simulated pattern locations
Summary: Dynamic 3D user-specified patterns, spherical particles

- We theoretically derived a direct inverse ultrasound DSA method that allows manipulating 3D user-specified patterns of particles along a 3D user-specified trajectory using standing ultrasound wave fields.

- We experimentally demonstrated that ultrasound DSA enables simultaneous translation, rotation, scaling, and shearing of patterns of particles.

- We quantified the pattern error between user-specified locations and simulated and experimental results and observe good agreement (error < 20% in 86% of pattern locations).
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High aspect ratio particles: 2D user-specified patterns

- **Objectives:**
  - **Theoretically derive** a direct solution to the inverse ultrasound DSA problem to calculate the ultrasound transducer settings required to arrange 2D patterns of high aspect ratio particles with user-specified locations and orientations
  - **Experimentally validate** the theoretical solution by creating 2D user-specified patterns of carbon microfibers in water

Direct solution method to the inverse ultrasound DSA problem EXPLICITLY accounting for orientation

Experimental ultrasound DSA demonstration

/ High aspect ratio particle

/ User-specified pattern
**Theory: Relating the ultrasound wave field and transducer settings**

- Use the boundary element method (BEM) to compute the ultrasound wave field, acoustic radiation potential and force as a function of ultrasound transducer settings

**Boundary element model of the reservoir**

**Acoustic radiation potential in terms of velocity potential**

\[
U = 2\pi r_p^3 \rho_0 \left\{ \frac{1}{3} k_0^2 \left[ 1 - \left( \frac{\beta_p}{\beta_0} \right)^2 \right] \left\langle |\phi|^2 \right\rangle - \left[ \frac{\rho_p - \rho_0}{2\rho_p + \rho_0} \right] \left\langle (\nabla \phi)^2 \right\rangle \right\}
\]

**Acoustic radiation force**

\[
F = -\nabla U
\]

**Green’s 3rd identity**

\[
\phi(x_i) = -\Omega(x_i) \int_S \left[ i k_0 \tilde{Z} G(q,x_i) + \frac{\partial G(q,x_i)}{\partial n(q)} \right] \phi(q) ds(q) + \ldots
\]

\[
\ldots + \Omega(x_i) \int_S v(q) G(q,x_i) ds(q).
\]

\(\phi\): Velocity potential

\(G\): Green’s function

\(k_0\): Ultrasound wave number

\(\tilde{Z}\): Transducer acoustic impedance

\(v\): Ultrasound transducer setting

\(\beta_p\): Particle compressibility

\(\beta_0\): Fluid compressibility
Theory: Solving the inverse ultrasound DSA problem

- Link the ultrasound transducer settings to the resulting pattern of particles via the acoustic radiation potential

\[ \mathbf{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_N \end{bmatrix} \]

Ultrasound transducer settings

Boundary element method

Ultrasound wave field \( \varphi(x,y;\mathbf{v}) \)

Acoustic radiation force theory

Acoustic radiation potential \( U(x,y;\mathbf{v}) \)

\[ U_{\text{max}} \quad U_{\text{min}} \]

- Solve the inverse problem using constrained optimization

User-specified pattern

Pattern feature \((x_i,y_i,\theta_i)\)

Solve the optimization problem

\[ \mathbf{v}^* = \arg \max \varphi \left( x_i, y_i, \theta_i; \mathbf{v} \right) \]

Required ultrasound transducer settings

Simulated acoustic radiation potential

\[ \mathbf{v}^* = \begin{bmatrix} v_1^* \\ \vdots \\ v_N^* \end{bmatrix} \]

**K** \( U \): Curvature of \( U \)

subject to \( |\mathbf{v}| = \alpha \)
Experiment: Method

- Prescribe a user-specified pattern of high aspect ratio particles
- Compute ultrasound transducer settings required to form the user-specified pattern
- Apply ultrasound transducer settings to experimental setup

\[ \mathbf{v}^* = \begin{bmatrix} v_1^* \\ \vdots \\ v_N^* \end{bmatrix} \]

User-specified pattern of high aspect ratio particles

Ultrasound transducers

Pattern of aligned carbon microfibers

Solve inverse problem

Apply settings

1 MHz PWM signals

FPGA signal generator

1 MHz PWM signals

Pattern of aligned carbon microfibers
Experiment: Pattern error calculation

- Quantify the accuracy of the solution of the inverse DSA problem for high aspect ratio particles

Position error

$$E_{pos} = \frac{100}{n\lambda_0} \sum_{i=1}^{n} |d_i|$$

Orientation error

$$\theta_{\text{diff}} = \frac{100}{\pi / 2} \left( \theta_{\text{des}} - \frac{1}{n-1} \sum_{j=1}^{n-1} \theta_j \right)$$
Experiment: Single user-specified orientation

- User-specified orientation between 0-90 degrees in 5 degree increments
- Good quantitative agreement between user-specified patterns and experimental results
**Experiment: Multiple user-specified orientations**

- Also create patterns with multiple, separate groups of microfibers with independent user-specified orientation.
Summary: 2D user-specified patterns, high aspect ratio particles

- We theoretically derived a direct inverse ultrasound DSA method that allows arrange high aspect ratio particles into organized 2D patterns with user-specified locations and orientations.

- We experimentally demonstrated that ultrasound DSA enables arranging single and multiple groups of high aspect ratio particles into patterns with independent, explicitly defined user-specified orientations.

- We quantified the pattern error between user-specified locations and simulated and experimental results and observe good agreement.
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High aspect ratio particles: 3D user-specified patterns

- **Objectives:**
  - Theoretically derive a direct solution to the inverse ultrasound DSA problem to calculate the ultrasound transducer settings required to arrange 3D patterns of high aspect ratio particles with user-specified locations and orientations.
  - Experimentally validate the derived solution by creating 3D user-specified patterns of high aspect ratio expanded polystyrene (EPS) particles in air.
Theory: Relating the ultrasound wave field and transducer settings

- Describe the relationship between the acoustic pressure in the solution domain and the ultrasound transducer settings
  - Pressure at any solution domain point is the summation of the acoustic pressure contributed from each ultrasound transducer

Phased array consisting of $N_t$ ultrasound transducers

Pressure due to ultrasound transducers

$$ P = Bv $$

where each term in $B$ is computed as

$$ b_{ij} = 2P_0 \frac{J_1(k_0a \sin \theta_{ij})}{k_0a \sin \theta_{ij}} e^{ik_0r_{ij}} $$

Ultrasound transducer settings

$$ v^T = (A_i e^{i\alpha_i}, ..., A_j e^{i\alpha_j}, ..., A_N e^{i\alpha_N}) $$

- $P$: Pressure
- $P_0$: Pressure amplitude
- $J_1$: First order Bessel function, first kind
- $k_0$: Ultrasound wave number
- $a$: Ultrasound transducer radius
- $v$: Ultrasound transducer setting
Theory: Relating the ultrasound wave field and transducer settings

- Relate the acoustic pressure to the pattern of particles using acoustic radiation force theory

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

\[
\Phi_2 = \frac{\pi r_p^3}{\omega_0^2 \rho_0 (\rho_0 + 2 \rho_p)}
\]

\[
F = -\nabla U
\]

\( \rho_0 \): Fluid medium density
\( c_0 \): Fluid medium sound speed
\( \rho_p \): Particle density
\( c_p \): Fluid medium sound speed
\( \omega_0 \): Ultrasound transducer operating frequency
Theory: Relating the ultrasound wave field and transducer settings

- Express the acoustic radiation potential as a function of the ultrasound transducer settings

\[ \mathbf{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_{N_t} \end{bmatrix} \]

Acoustic pressure \( P(x,y,z;v) \)

Acoustic radiation potential \( U(x,y,z;v) \)

Acoustic pressure

Acoustic radiation force theory

\( P_{\text{min}} \) \( P_{\text{max}} \)

\( U_{\text{min}} \) \( U_{\text{max}} \)
Solving the inverse problem

• Compute the required ultrasound transducer settings by:
  - Defining a pattern of high aspect ratio particles with a user-specified location and orientation
  - Compute the ultrasound transducer settings that maximize the objective function $f(v)$

\[
\mathbf{v}^* = \arg \max_v f(\mathbf{v}) \quad \text{subject to } |\mathbf{v}| = \alpha
\]

• The objective function here simultaneously optimizes curvatures in three mutually orthogonal directions, and minimizes $U$ at the user-specified location

\[
f(\mathbf{v}) = \kappa_U(\mathbf{x}_d, \mathbf{e}_i)\kappa_U(\mathbf{x}_d, \mathbf{e}_j) - \kappa_U(\mathbf{x}_d, \mathbf{e}_d)^2 + ... + \zeta \kappa_U(\mathbf{x}_d, \mathbf{e}_z)^2 - \delta U
\]
Experiment: Method

- Prescribe a user-specified pattern of high aspect ratio particles
- Compute ultrasound transducer settings required to form the user-specified pattern
- Apply ultrasound transducer settings to experimental setup

\[
v^* = \begin{bmatrix} v_1^* \\ \vdots \\ v_N^* \end{bmatrix}
\]

User-specified pattern of high aspect ratio particles

Solve inverse problem

Ultrasound transducer settings

Apply settings

Borescope camera

40 kHz PWM signals

High aspect ratio EPS particle

Ultrasound transducer

Arduino MEGA 2560

70 mm
Experiment: Pattern error calculation

- Quantify the accuracy of the solution of the inverse DSA problem for high aspect ratio particles using projections of the particle taken with the borescope cameras.

\[
\begin{bmatrix}
\cos(\theta_m) \\
\sin(\theta_m) \\
-\sin(\sigma_m)
\end{bmatrix}
\]

Measured orientation vector

\[
e_m = \begin{bmatrix}
\cos(\theta_m) \\
\sin(\theta_m) \\
-\sin(\sigma_m)
\end{bmatrix}
\]

Orientation error

\[
\gamma_e = \arccos(e_d \cdot e_m)
\]
Experiment: orientations in the $xy$-plane

- User-specified orientations in the $xy$-plane
  - Each row of results pertains to a single experiment

\[ \theta_d = 0 \text{ deg} \quad \sigma_d = 0 \text{ deg} \]
\[ \theta_d = 45 \text{ deg} \quad \sigma_d = 0 \text{ deg} \]
\[ \theta_d = 135 \text{ deg} \quad \sigma_d = 0 \text{ deg} \]

- Observe good quantitative agreement between user-specified and experimental patterns
Experiment: orientations out of the $xy$-plane

- User-specified orientations out of the $xy$-plane
  - Each row of results pertains to a single experiment

- Observe good quantitative agreement between user-specified and experimental patterns
Summary: 3D user-specified patterns, high aspect ratio particles

• We theoretically derived a direct inverse ultrasound DSA method that allows arrange high aspect ratio particles into organized 3D patterns with user-specified locations and orientations.

• We experimentally demonstrated that ultrasound DSA enables arranging single high aspect ratio particles with explicitly defined user-specified orientations.

• We quantified the pattern error between user-specified locations and simulated and experimental results and observe good agreement

• In contrast to the 2D method for high aspect ratio particles, a subset of ultrasound transducers must be used to levitate the particle, while the remaining ones orient the particle. From this, we observe a small increase in orientation error.
Overview

• Introduction
  - Polymer-matrix composite materials
  - Polymer-matrix composite material manufacturing methods
  - Directed self-assembly (DSA)

• Ultrasound directed self-assembly (DSA)
  - Ultrasound DSA process
  - Implementing ultrasound DSA in engineering applications
  - Ultrasound DSA background
  - Research objectives

• Results
  - Spherical particles: Static 3D user-specified patterns
  - Spherical particles: Dynamic 3D user-specified patterns
  - High aspect ratio particles: 2D user-specified patterns
  - High aspect ratio particles: 3D user-specified patterns

• Conclusions
  - Spherical particles
  - High aspect ratio particles
  - Implications
Conclusions: Spherical particles

- Spherical particles:

  - Theoretically derived a direct solution to the inverse ultrasound DSA problem to compute the ultrasound transducer settings required to arrange static 3D user-specified patterns of spherical particles.

  - Theoretically derived a direct solution to the inverse ultrasound DSA problem to compute the ultrasound transducer settings required to arrange dynamic 3D user-specified patterns of spherical particles.

  - Based on computing the ultrasound transducer settings that minimize the acoustic radiation potential associated with a standing ultrasound wave field at 3D user-specified locations.
Conclusions: High aspect ratio particles

- Theoretically derived a direct solution to the inverse ultrasound DSA problem to compute the ultrasound transducer settings required to arrange 2D patterns of high aspect ratio particles with user-specified locations and orientations.

- Based on computing the ultrasound transducer settings that maximize the curvature of the acoustic radiation potential associated with a standing ultrasound wave field at user-specified locations and orientations.

- Theoretically derived a direct solution to the inverse ultrasound DSA problem to compute the ultrasound transducer settings required to arrange 3D patterns of high aspect ratio particles with user-specified locations and orientations.

- Based on computing the ultrasound transducer settings that maximize an objective function that enforces specific behavior of the curvature of the acoustic radiation potential in multiple directions and minimizes the acoustic radiation potential simultaneously.
Conclusions: Engineering implications

- This work has implications for using ultrasound directed self-assembly to fabricate engineered polymer-matrix composite materials with designer properties that derive directly from the pattern of spherical or high aspect ratio particles embedded within the polymer matrix.

- Such composite materials may be functionalized for:
  - Structural components that self-detect damage [1]
  - Electrically conductive structural components with embedded wiring [2]
  - Structural components with electrical energy storage capabilities [15]

Questions?