A Material Mask Overlay Strategy for Close to Binary Design-dependent Pressure-loaded Optimized Topologies

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Abstract
This paper presents a Material Mask Overlay Strategy topology optimization approach with improved material assignment at the element level for achieving close to black-and-white designs for pressure-loaded problems. Hexagonal elements are employed to parametrize the design domain as this tessellation provides nonsingular local connectivity. Elliptical negative masks are used to find the optimized material layout. The material dilation and material erosion variables of each mask are systematically varied in association with a gray-scale measure constraint to achieve designs close to 0-1. Darcy’s law in association with a drainage term is used to formulate the pressure field. The obtained pressure field is converted into the consistent nodal forces using Wachspress shape functions. Sensitivities of the objective and pressure load are evaluated using the adjoint-variable method. The approach is demonstrated by solving various pressure-loaded structures and pressure-actuated compliant mechanisms. Compliance is minimized for loadbearing structures, whereas a multicriteria objective is minimized for mechanism designs.

Keywords: Topology Optimization, Material Masks Overlay Strategy, Design-dependent pressure loads, Honeycomb tessellation, Compliant mechanisms

1 Introduction

Topology optimization (TO) is a numerical technique to find the optimized material layout within a given design domain experiencing external loads with boundary conditions by extremizing the objective subjected to a known set of constraints. External loads can be either constant (design-independent) or variant (design-dependent) with the design evolution during TO. A wide range of applications involving design-dependent pressure loadings can be found, e.g., in aircraft wings and fuselage, ships, wind and snow load experiencing houses, internal and external pressure-loaded pumps and containers, pneumatically and/or hydraulically actuated soft robots [1, 2]. However, treatment of design-dependent loads, e.g., fluidic pressure loads in a TO setting is challenging and involved [2]. This is because, a pressure load alters its magnitude, location and direction as design evolves in TO. The challenges increase further as one seeks optimized, black-and-white designs that are highly appreciated and desirable in TO [3]. The goal here is to present a Material Mask Overlay topology optimization approach with improved material assignment to get pressure-loaded designs close to binary solutions.

The Material Mask Overlay Strategy (MMOS), initially conceived in [4], employs masks to assign material to a group of hexagonal finite elements (FEs) used to parameterize the design domains. Edge-connectivity provided by hexagonal FEs subdued checkerboard patterns/point connections in optimized topologies without additional singularity suppression schemes [5–9]. To our best knowledge however, there is

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Compliant mechanisms (CMs) are monolithic designs that utilize their flexible (compliant) members to perform their tasks in response to input actuations and can find various applications with/without pressure loads in [15–17] and references therein. Only a few TO approaches for pressure-actuated CMs can be found [2] and in those, none of them yet is presented to achieve such optimized mechanism with 0-1 designs. With above improved material assignment for a mask, we not only seek geometrical singularities free, close to black and white pressure-actuated CMs but also, pressure-loaded structures. For the former, a multi-criteria [18] objective is minimized, whereas compliance is minimized for the latter. Figure 2 illustrates schematic diagrams for a pressure loadbearing structure and a pressure-actuated CM. It can be seen that pressure loading surface has moved from its initial surface $\Gamma_p$ to the final surface $\Gamma_{pb}$ (cf. Fig. 2a and 2b). Next, we summarize existing approaches in TO for pressure-loaded designs.

The first TO approach involving pressure loads was presented by Hammer and Olhoff [1] for designing loadbearing structures by minimizing compliance. Du and Olhoff [19] further modified the method presented in [1]. Fuchs and Shemesh [20] employed additional variables for pressure loading boundaries. An element-based approach was presented by Zhang et al. [21]. Lee and Martins [22] presented an approach which does not require a priori data of starting and ending points for pressure curves. Li et al. [23] presented a regional contour tracking algorithm in conjunction with digital image processing. Ibhadode et al. [24] presented an approach with boundary identification and load evolution. One can also find approaches using the level set methods in [25–27].

Instead of locating pressure loading contour explicitly, different alternate approaches were also presented. A fictitious thermal loading concept was used by Chen and Kikuchi [28]. Chen et al. [29] used the method in [28] to design pressure-actuated CMs. A three-phase material (solid, void, and fluid) definition was used by Bourdin and Chambolle [30]. Sigmund and Clausen [31] employed the mixed finite element method\(^1\) with three-phase material description. A pseudo electrical potential technique was employed by Zheng et al. [33]. Vasista and Tong [34] employed the SIMP (Solid Isotropic Material Penalization) and MIST (Moving Isosurface Threshold) methods with the mixed displacement-pressure FE formulation. Panganiban et al. [35] used the displacement-based nonconforming FE approach with three-phase

\(^1\)Needs to satisfy the Babuska-Brezzi condition [32]
material description, and de Souza and Silva [36] employed method presented in [31] in their approach. Kumar et al. [2] used Darcy’s law in association with a drainage term to design both pressure-loaded structures and pressure-actuated CMs. Herein, we adopt the method presented in [2] for pressure-field modeling.

In summary, the current manuscript offers following new aspects:

- A Material Masks Overlay Strategy topology optimization approach to achieve optimized, close to black-and-white pressure-loaded structures and pressure-actuated compliant mechanisms,
- Formulation of negative elliptical masks with material erosion and dilation variables to assign material density within each hexagonal FE,
- Implicitly detecting pressure loading surface using the Darcy law with hexagonal element description of the design domain in line with [2]
- Explicitly using a gray-scale measure constraint to ensure pressure-loaded topologies close to 0-1 solutions.

The remainder of the paper is organized as follows. Section 2 describes density material modeling using negative elliptical masks for an FE. Section 3 presents pressure modeling including methodology, finite element formulation, calculation of the nodal forces and verification problems. Topology optimization formulation, objective functions employed for the loadbearing structures and CMs under used volume and gray scale constraints and sensitivity analysis are presented in Section 4. Section 5 reports numerical examples for structure and CM designs, and pertaining discussions. Lastly, conclusions are drawn in Section 6.
2 Material density modeling

In a typical TO setting with regular FE discretization descriptions, each FE is assigned a material density $\rho$. Such variables (ideally) attain either 0 or 1 values at the end of optimization and thus, help decide the final material layout of the optimized designs. Herein, a set of negative elliptical masks are employed to determine material density of hexagonal FEs which are used to describe the given design domain. The final position, shape, size, orientation, material dilation and erosion variables of masks determine the optimized material layout wherein the density of the $i^{th}$ hexagonal FE with respect to the $j^{th}$ elliptical mask, i.e., $\rho_{ij}$ is computed using the logistic approximation of Heaviside function as

$$
\rho_{ij}(\alpha_j) = \frac{1}{1 + \exp(-\alpha_j d_{ij})},
$$

(1)

where $d_{ij}$, a Euclidean distance measure, determines position of the centroid of the $i^{th}$ FE with respect to that of the $j^{th}$ mask (cf. Fig. 2). $\alpha_j$, material dilation variable, influences the binary nature of the solutions (Fig. 1b). Mathematically, $d_{ij}$ is evaluated as (Fig. 2)

$$
d_{ij} = \left(\frac{X_{ij}}{a_j}\right)^2 + \left(\frac{Y_{ij}}{b_j}\right)^2 - 1,
$$

(2)

with,

$$
\left(\begin{array}{c}
X_{ij} \\
Y_{ij}
\end{array}\right) = \left[\begin{array}{cc}
\cos \theta_j & \sin \theta_j \\
-\sin \theta_j & \cos \theta_j
\end{array}\right] \left(\begin{array}{c}
x_i - x_j \\
y_i - y_j
\end{array}\right),
$$

(3)

where $(x_i, y_i)$ and $(x_j, y_j)$ are center coordinates of the $i^{th}$ hexagonal FE and $j^{th}$ elliptical mask. $a_j$ and $b_j$ represent the semi-major and -minor axes of the mask and $\theta_j$ is its orientation with respect to the horizontal direction. Note that the lower and upper limits for $a_j$ and $b_j$ can be defined based on the dimension of an FE and design, and $\theta_j \in [-\pi/2, \pi/2]$.

In view of $m_n$ such masks, one writes the material density of the $i^{th}$ FE as

$$
\rho_{i}(\alpha_j, \gamma_j) = \prod_{j=1}^{m_n} \left[\frac{1}{1 + \exp(-\alpha_j d_{ij})}\right]^{\gamma_j},
$$

(4)

where $\gamma_j$, material erosion variable, $\in [\gamma_l, \gamma_u]$ and $\alpha_j \in [\alpha_l, \alpha_u]$. $\alpha_j$ and $\gamma_j$ together, can steer the material density of an FE towards either 0 or 1 and thus, helping to ensure crisp final solutions. $\gamma_l$ and $\gamma_u$ are user defined lower and upper bounds on $\gamma_j$. Likewise, $\alpha_l$ and $\alpha_u$ represent lower and upper limits for $\alpha_j$. Let $\psi_j = \{x_j, y_j, a_j, b_j, \theta_j, \alpha_j, \gamma_j\}$. Negative masks can also be used to generate contact surfaces within them while designing contact-aided designs [37, 38].

3 Pressure loads modeling

Darcy’s law in association with a volumetric material-dependent pressure loss, i.e., drainage term, is employed to relate the pressure field with material density vector $\rho$. The associated PDE is solved using the standard finite element formulation using Wachspress shape functions [39]. The formulation facilitates implicit detection of the pressure loading surface and conversion of the obtained pressured field into the consistent hexagonal FE nodal forces.

3.1 Methodology

We describe the Darcy law, the drainage term and associated parameters in brief, and of that a detailed description can be found in [2]. The Darcy law that helps finding pressure field through a porous medium

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2In case of irregular FE discretization, in general, nodal design variables are preferred to avoid favoring one FE over others by TO.
is adopted wherein the Darcy flux $q$ depends upon the pressure gradient $\nabla p$, the fluid viscosity $\mu$ and permeability of the medium $\kappa$ as

$$q = -\frac{\kappa}{\mu} \nabla p = -K \nabla p,$$  \hspace{1cm} (5)

where $K$ represents the flow coefficient that refers to the ability to allow fluid to pass through a porous medium. To cater for a TO setting, each material-phase of an FE is also associated with one flow coefficient, and the actual flow coefficient of an FE is determined by performing interpolation between those associated to its solid and void material states using a smooth Heaviside projection function as

$$K(p_t(\psi_j)) = K_V(1 - (1 - \epsilon)) H_K(p_t(\psi_j), \eta_K, \beta_K),$$  \hspace{1cm} (6)

where $\epsilon = \frac{\kappa_s}{\kappa_v}$ is the flow contrast [40] wherein $K_s$ and $K_v$ are the flow coefficients for solid and void phased FEs, respectively. $H_K(p_t, \eta_K, \beta_K)$ indicates a smooth Heaviside projection function defined as

$$H_K(p_t(\psi_j), \eta_K, \beta_K) = \left( \frac{\tanh(\beta_K \eta_K) + \tanh(\beta_K(p_t - \eta_K))}{\tanh(\beta_K \eta_K) + \tanh(\beta_K(1 - \eta_K))} \right),$$  \hspace{1cm} (7)

where $\eta_K$ and $\beta_K$ help control position of the step and slope of $K(p_t(\psi_j))$ respectively. $p_t(\psi_j)$ is evaluated using Eq. (4) indicating that the defined flow coefficient $K(p_t(\psi_j))$ depends upon the position, shape, size, orientation, material dilation and erosion variables of the masks employed in TO. In a typical TO setting, using Darcy’s law alone may fail to ensure the desired pressure field for a reasonable design as it provides pressure gradient throughout the design domain (see Fig. 5a). Therefore, a drainage term conceptualized in [2] is employed to ensure a sharp and continuous pressure drop as soon as pressure loads encounter a solid FE while TO progresses (see Fig. 5d and Fig. 5e), i.e., drainage term becomes active when pressure loads faces solid FEs otherwise remains inactive. $Q_{\text{drain}}$ is defined as

$$Q_{\text{drain}} = -D(p_t(\psi_j))(p - p_{\text{ext}}),$$  \hspace{1cm} (8)

where the pressure field and external pressure are indicated via $p$ and $p_{\text{ext}}$, respectively and $D(p_t)$ is the drainage coefficient defined using a smooth Heaviside function as

$$D(p_t(\psi_j)) = D_s H_D(p_t(\psi_j), \eta_D, \beta_D),$$  \hspace{1cm} (9)

where $\eta_D$ and $\beta_D$ are adaptable parameters and $H_D(p_t(\psi_j), \eta_D, \beta_D)$ is analogous to that mentioned in Eq. (7). $D_s$ is the drainage coefficient of a solid hexagonal FE that controls the pressure-penetration depth and is determined in terms of $K_s$ as [2]

$$D_s = \left( \frac{\ln \frac{r}{\Delta s}}{\Delta s} \right)^2 K_s,$$  \hspace{1cm} (10)

where $r = \frac{p|_{\Delta s}}{p_{\text{in}}}$; $\Delta s$, a penetration parameter, is set to equal to width/height of a few FEs, and $p_{\text{in}}$ and $p|_{\Delta s}$ are input pressure and pressure at $\Delta s$ respectively.

### 3.2 Finite element formulation for pressure loading

The basic balance equation for Darcy’s law in conjunction with $Q_{\text{drain}}$ and incompressible fluid flow assumptions can be written as [2]

$$\nabla \cdot q - Q_{\text{drain}} = 0,$$  \hspace{1cm} (11)

In view of Eq. (5), Eq. (11) yields to

$$\nabla \cdot (K \nabla p) + Q_{\text{drain}} = 0.$$

The PDE in Eq. (12) is solved to evaluate pressure field using the Galerkin method of finite element formulation as

$$\sum_{i=1}^{N_{el}} \left( \int_{\Omega_i} \nabla \cdot (K \nabla p) \mathrm{d}V + \int_{\Omega_i} Q_{\text{drain}} \mathrm{d}V \right) = 0,$$  \hspace{1cm} (13)
where \( Nel \) indicates the total number of hexagonal FEs employed to describe the design domain \( \Omega \), \( Nel_{i=1, 2, 3, \ldots} \) represent hexagonal FEs, \( dV \) is the elemental volume, and \( G \) is determined using the same basis functions that are employed for interpolating pressure. For a hexagonal FE

\[
p = N_p \mathbf{p}_i, \quad \text{and} \quad G = N_p \mathbf{G}_i,
\]

(14)

where \( \mathbf{p}_i = [p_1, p_2, p_3, p_4, p_5, p_6]^{T} \) are the hexagonal nodal pressures and \( N_p = [N_1, N_2, N_3, N_4, N_5, N_6] \) are the Wachspress shape functions (see Appendix A). Using integration by parts, divergence theorem term are converted into the nodal force using Eq. 17.

\[
\int_{\Omega_i} \left( K \mathbf{B}_p^T \mathbf{B}_p + D N_p^T N_p \right) dV \mathbf{p}_i = \int_{\Omega_i} D N_p^T \mathbf{p}_{\text{ext}} dV - \int_{\Gamma_i} N_p^T \mathbf{q}_r \cdot \mathbf{n}_i \ dA
\]

(15)

where the flux through the boundary \( \Gamma_i \) is represented via \( \mathbf{q}_r \), \( \mathbf{B}_p = \nabla N_p \), \( \mathbf{n}_i \) indicates the outward normal to the surface \( \Gamma_i \), and \( dA \) is the elemental area. Eq. (15) transpires in global sense to

\[
\mathbf{A}_i \mathbf{p}_i = \mathbf{f}_i
\]

(16)

The global flow matrix \( \mathbf{A} \), the global pressure vector \( \mathbf{p} \) and the global loading vector \( \mathbf{f} \) are obtained by assembling corresponding elemental \( \mathbf{A}_i \), \( \mathbf{p}_i \) and \( \mathbf{f}_i \), respectively. In this work, \( \mathbf{p}_{\text{ext}} \) and \( \mathbf{q}_r \) are set to zero, therefore, \( \mathbf{A} \mathbf{P} = \mathbf{0} \) is solved to evaluate pressure field with given pressure loads at input locations. Each node has only one degree of freedom corresponding to pressure load and thus, it is computationally cheap to solve. The global hexagonal nodal forces \( \mathbf{F} \) are determined as

\[
\mathbf{F} = -\mathbf{T} \mathbf{p},
\]

(17)

where \( \mathbf{T} \) is a transformation matrix evaluated by assembling elemental \( \mathbf{T}_i \) determined as [2]

\[
\mathbf{T}_i = -\int_{\Omega} N_u^T \mathbf{B}_p \ dV,
\]

(18)

where \( N_u = [N_1 \mathbf{I}, N_2 \mathbf{I}, N_3 \mathbf{I}, N_4 \mathbf{I}, N_5 \mathbf{I}, N_6 \mathbf{I}] \), \( N_l_{l=1, 2, \ldots, 6} \) are Wachspress shape functions and \( \mathbf{I} \) is the identity matrix in \( \mathbb{R}^2 \). Integrations in Eqs. (15) and (18) are evaluated using the quadrature rule mentioned in Appendix B.

### 3.3 Pressure modeling verification

To demonstrate of the employed pressure modeling scheme (Sec. 3) with hexagonal FEs simulated using Wachspress shape functions, we consider two design domains: DDomain I (Fig. 4a) and DDomain II (Fig. 4b) with respective pressure and structural boundary conditions (Fig. 4). Each hexagonal FE of DDomain I is assigned low material density \( \rho = 0.01 \). DDomain II is with two solid material regions which are introduced to illustrate behavior of the drainage term (Eq. 9). \( \rho = 0.01 \) is assigned to each FE associated to the remaining domain of DDomain II. The bottom edge of DDomain I experiences pressure loading, whereas its remaining edges are kept at zero pressure loading. In DDomain II, the top and bottom edges experience zero and full pressure loading, respectively. Other specifications are indicated in Table 1. The employed scales for material density field and pressure field in this paper are plotted in Fig. 3a and Fig. 3b, respectively. Plane-stress conditions are considered herein for all other design problems reported in this paper.

The pressure field obtained by solving Eq. (15) is depicted in Fig. 5a for DDomain I, and that for DDomain II without and with drainage term are plotted in Fig. 5b and Fig. 5d, respectively. Fig. 5c and Fig. 5e indicate the pressure field with solid material layers. One notices that pressure gradient exists throughout within DDomain I, which is expected as per Darcy’s law. The material density for each FE in DDomain I is kept low (\( \rho = 0.01 \)) consequently, drainage term (Eq. 9) remains always inactive. One notices without drainage term the obtained pressure field is not realistic for DDomain II (Fig. 5b and Fig. 5e), whereas Fig. 5d and Fig. 5e indicate the desired pressure field and thus, the conceptualized drainage term is indeed essential. The obtained pressure fields of DDomain II with and without drainage term are converted into the nodal force using Eq. 17.
Figure 3: Scales for the material density field and pressure field are displayed in (a) and (b), respectively, that are employed in this paper to show the optimized results and final pressure field. \( p_{\text{max}} = 1 \) bar and \( p_{\text{min}} = 0 \) bar unless otherwise stated.

Figure 4: Design domains DDomain I and DDomain II are depicted in (a) and (b), respectively. Material density of each FE in (a) is set to 0.01. \( L_x = 0.2 \cos\left(\frac{\pi}{6}\right) \) m, and \( L_y = 0.2 \sin\left(\frac{\pi}{6}\right) \) m, designs are parameterized using \( 80 \times 60 \) FEs. DDomain II has two solid FE (dark) layers of width \( 0.1L_y \) separated by \( 0.2L_y \). Fixed locations, pressure and zero pressure loadings edges are shown.

Figure 5: Pressure fields for DDomain I and DDomain II are displayed. (a) DDomain I pressure field (b) DDomain II pressure field without drainage term is plotted without solid regions (c) DDomain II pressure field without drainage term with solid regions, (d) DDomain II pressure field with drainage term without solid regions and (e) DDomain II pressure field with drainage term with solid regions. One notice that the gradient of pressure field gets confined as soon as it faces the first solid region in DDomain when using the drainage term (Fig. 5d and Fig. 5e), however the same is not noted without the drainage term (Fig. 5b and Fig. 5c).

4 Optimization problem formulation

This section presents the optimization problem formulation and pertaining sensitivity analysis of the objectives employed for designing pressure loadbearing structures and pressure-actuated CMs.

Let \( \psi \) be the design vector stacks seven variables \( (x_j, y_j, a_j, b_j, \theta_j, \alpha_j, \gamma_{j, j=1,\ldots, m_n}) \) which define each mask. The material densities of all FEs stacked in a vector, as per Eq. 4 a function of \( \psi \), is denoted via \( \rho \). The following optimizations problem are solved:
with respect to design vector optimization problems, therefore one requires to have sensitivities of the objective(s) and constraint(s) respectively.

The method of moving asymptotes (MMA) [42], a gradient-based optimizer, is used herein to solve the optimization problems. One notes (Eq. 19), objectives \(SE\) and \(MSE = \sqrt{\psi}\) are determined using \(K(\rho(\psi))u = F\), and \(v\) evaluated employing \(^3K(\rho(\psi))v = F_d\), are the global displacement vectors corresponding to the forces \(F\) and \(F_d\). \(F_d\) is a dummy unit force applied in the direction of the desired output deformation of the CMs, whereas \(F\) is evaluated using Eq. (17). \(K\) is the global stiffness matrix of the design domain evaluated by assembling elemental stiffness \(k_i = [E_{\min} + \rho_i(\alpha_j, \gamma_j)(E_1 - E_{\min})]k_0\). \(E_1\) and \(E_{\min}\) are the Young’s moduli of a solid and void FE, respectively, \(\rho_i(\alpha_j, \gamma_j)\) is the material density of the \(i^{th}\) FE (Eq. 4) and \(k_0\) is the elemental stiffness matrix for a solid FE at unit elastic modulus. Further, \(\chi\), a consistent scaling factor, is primarily employed to adjust sensitivities of the objective pertaining to CMs [18]. \(g_1\), an inequality constraint, guides to achieve the optimized design with the permitted resource volume. \(V(\rho(\psi))\) and \(V^*\) indicate the current and permitted volumes of the design domain, respectively. \(g_2\) is the gray scale indicator [41] constraint and \(\delta\) is a user defined (very) small positive number. This constraint is applied to ensure that optimized designs get motivated towards 0-1 solutions with \(\alpha_j\) and \(\gamma_j\) as additional design variables. \(A, T\) and \(p\) represent the global flow matrix, global transformation matrix, and global pressure loads vector, respectively. \(\psi_{\min}\) and \(\psi_{\max}\) are the lower and upper limits on the design vector \(\psi\) respectively.

4.1 Sensitivity analysis

The method of moving asymptotes (MMA) [42], a gradient-based optimizer, is used herein to solve the optimization problems. Therefore one requires to have sensitivities of the objective(s) and constraint(s) with respect to design vector \(\psi\) for the optimization. One notes (Eq. 19), objectives \(SE\) and \(-\frac{MSE}{SE}\) and constraints are function of the material density vector \(\rho\) and that depends upon \(\psi\), therefore a chain rule is employed for determining the sensitivities, which is described below.

Let \(\psi_j\) represents any one of the \(\{x_j, y_j, \alpha_j, \beta_j, \gamma_j\}\) and \(\psi_j = \{\psi_j, \alpha_j, \gamma_j\}\). Using Eq. (4), derivative of \(\rho_i\) with respect to \(\psi_j\) can be evaluated as

\[
\frac{\partial \rho_i(\alpha_j, \gamma_j)}{\partial \psi_j} = \gamma_j \rho_i(\alpha_j, \gamma_j) \left[ 1 - \frac{1}{1 + \exp(-\alpha_j d_j)} \right] \frac{\partial d_j}{\partial \psi_j}.
\]

where \(\frac{\partial d_j}{\partial \psi_j}\) are evaluated using Eq. 2 and Eq. 3 as

\(^3K(\rho(\psi))v = F_d\) is solved only while designing CMs.
Therefore, as \( \lambda \) is sensitivities of the objectives with respect to the material density vector \( \rho \), derivatives of \( \partial \rho \) in (a) and (b) respectively.

\[
\frac{\partial d_{ij}}{\partial x_j} = 2 \left[ \left( \frac{X_{ij}}{a_j} \right) \cos \theta_j + \left( \frac{Y_{ij}}{b_j} \right) \frac{1}{b_j} \right] \\
\frac{\partial d_{ij}}{\partial y_j} = -2 \left[ \left( \frac{X_{ij}}{a_j} \right) \sin \theta_j + \left( \frac{Y_{ij}}{b_j} \right) \frac{1}{b_j} \right] \\
\frac{\partial d_{ij}}{\partial a_j} = -2X_{ij}^2 \frac{1}{a_j^2} \\
\frac{\partial d_{ij}}{\partial b_j} = -2Y_{ij}^2 \frac{1}{b_j^2} \\
\frac{\partial d_{ij}}{\partial \theta_j} = 2 \left( \frac{X_{ij}Y_{ij}}{a_j^2} - X_{ij}Y_{ij} \right)
\]

Derivatives of \( \rho_i(\alpha_j, \gamma_j) \) with variables \( \alpha_j \) and \( \gamma_j \) can be found as

\[
\frac{\partial \rho_i(\alpha_j, \gamma_j)}{\partial \alpha_j} = \gamma_j d_{ij} \rho_i(\alpha_j, \gamma_j) \left[ 1 - \frac{1}{1 + \exp(-\alpha_j d_{ij})} \right],
\]

\[
\frac{\partial \rho_i(\alpha_j, \gamma_j)}{\partial \gamma_j} = \rho_i(\alpha_j, \gamma_j) \log \left( \frac{1}{1 + \exp(-\alpha_j d_{ij})} \right).
\]

Therefore, \( \frac{\partial \rho_i}{\partial \gamma} = \left[ \left[ \frac{\partial \rho_i}{\partial \alpha} \right]^T \left[ \frac{\partial \rho_i}{\partial \gamma} \right]^T \left[ \frac{\partial \rho_i}{\partial \gamma} \right] \right] \). The adjoint-variable method is used to evaluate sensitivities of the objectives with respect to the material density vector \( \rho \). One writes the following overall performance functions \( \mathcal{L}_s \) for loadbearing structures as

\[
\mathcal{L}_s = f_s^0 + \lambda_{s1}^T (Ku + Tp) + \lambda_{s2}^T (Ap),
\]

where \( \lambda_{s1} \) and \( \lambda_{s2} \) are the Lagrange multiplier vectors. Likewise, the performance function \( \mathcal{L}_{CM} \) for CMs is

\[
\mathcal{L}_{CM} = f_{CM}^0 + \lambda_{CM1}^T (Ku + Tp) + \lambda_{CM2}^T (Ap) + \lambda_{CM3}^T (Kv - F_d),
\]

where \( \lambda_{CM1}, \lambda_{CM2} \) and \( \lambda_{CM3} \) are the Lagrange multiplier vectors. These multipliers can be determined as [2]

\[
\lambda_{CM1} = -\frac{\partial f_{CM1}}{\partial u} K^{-1} = \chi \left( \frac{u^\top M}{SE} - u^\top \frac{MSE}{SE} \right) \]

and

\[
\lambda_{CM2} = -\lambda_{CM1}^\top TA^{-1} = -\chi \left( \frac{u^\top M}{SE} - u^\top \frac{MSE}{SE} \right) TA^{-1},
\]

\[
\lambda_{CM3} = -\frac{\partial f_{CM3}}{\partial v} K^{-1} = \chi \left( \frac{v^\top M}{SE} \right)
\]

for CMs.
Using Eqs. (24), (25), (26) and (27), sensitivities of the objective functions with respect to $\rho$ can be written as
\[
\frac{d f_{s}^{0}}{d \rho} = \frac{\partial f_{s}^{0}}{\partial \rho} + \lambda_{\beta}^{s} \frac{\partial K}{\partial \rho} u + \lambda_{\gamma}^{s} \frac{\partial A}{\partial \rho} p = -u^{T} \frac{\partial K}{\partial \rho} u + 2u^{T} TA^{-1} \frac{\partial A}{\partial \rho} p
\]

and
\[
\frac{d f_{CM}^{0}}{d \rho} = \frac{\partial f_{CM}^{0}}{\partial \rho} + \lambda_{\beta}^{CM} \frac{\partial K}{\partial \rho} u + \lambda_{\gamma}^{CM} \frac{\partial A}{\partial \rho} p + \lambda_{\gamma}^{CM} \frac{\partial V}{\partial \rho} v = \chi \left[ u^{T} \frac{\partial K}{\partial \rho} \left( MSE \left( \frac{SE}{2} + \frac{v}{SE} \right) \right) \right] + \chi \left[ MSE \left( \frac{SE}{2} + \frac{v}{SE} \right) \right] \left[ \frac{1}{TA} \frac{\partial A}{\partial \rho} \right]
\]

Finally, one employs a chain rule in view with Eqs. (20) and (28) to determine derivatives of the objective functions with respect to design vector \( \psi \) as
\[
\frac{d f_{i}^{0}}{d \psi} \bigg|_{\tau = S, CM} = \frac{\partial f_{i}}{\partial \rho} \frac{\partial \rho}{\partial \psi}
\]

and thus, the associated load sensitivities get evaluated computationally cheaply. Likewise, sensitivities of the constraints are determined.

5 Numerical examples and discussion

We solve design problems related to loadbearing structures (arch and piston) and CMs (inverter and gripper) involving pressure loads to demonstrate the presented approach. The design domains with known boundary conditions for pressure loading and displacements are depicted in Fig. 6a and Table 1 indicates the design parameters employed. The area the design loadbearing structures and CMs, respectively. \( \Gamma_{p} \) and \( \Gamma_{po} \) denote the full and zero pressure loading boundaries, respectively. Optimization parameters and other specifications of the problems are tabulated in Table 1 and any digression is reported in the associated problem definition section. Implementation of the MMA with hexagonal FEs and elliptical masks is same as standard, except that after every MMA iteration one determines the new mask vector/variable as
\[
\psi_{new} = \psi_{old} + S \left( \psi_{current} - \psi_{old} \right)
\]

where \( \psi_{new} \), \( \psi_{old} \), and \( \psi_{current} \) represent the new, old and current mask design variables. Note \( \psi_{current} \) is the solution obtained from the MMA optimizer using \( \psi_{old} \). \( S \) indicates length of a step one requires to multiply that may depend upon types of the problems to be solved. In our experience, \( S \in [0.01, 0.1] \) can be a good choice. For all the problems solved, dimensions in \( x \)- and \( y \)-directions are denoted by \( L_{x} \) and \( L_{y} \), respectively. The number of FEs in \( x \)- and \( y \)-directions are indicated by \( N_{ex} \) and \( N_{ey} \) respectively. That for masks are denoted by \( N_{mx} \) and \( N_{my} \) respectively.

5.1 Internally pressurize arch

The problem for internally pressurized arch first presented in [1] is solved herein. The design specification is mentioned in Fig. 6a, and Table 1 indicates the design parameters employed. The area the design domain is set to \( L_{x} \times L_{y} = 0.2 \times 0.1 \) m². The domain is parameterized using \( N_{ex} \times N_{ey} = 100 \times 50 \) hexagonal FEs. \( N_{mx} \times N_{my} = m_{x} = 20 \times 10 \) elliptical masks are taken for optimization.

5.1.1 Qualifying \( \alpha_{j} \) and \( \gamma_{j} \) as design variables

We present a study to indicate that considering \( \alpha_{j} \) and \( \gamma_{j} \) as additional design variables can help achieve close to 0-1 optimized designs. To demonstrate, four cases are conceptualized, CASE I: \( \alpha_{j} = 1 \) and \( \gamma_{j} = 1 \), CASE II: \( \alpha_{j} = 1 \) and \( \gamma_{j} \) are included in the design variables with lower and upper bounds 1 and 10 respectively, CASE III: \( \gamma_{j} = 1 \) and \( \alpha_{j} \) are included in the design variables with 1 and 20 as lower and upper bounds respectively, CASE IV: \( \alpha_{j} \) and \( \gamma_{j} \) are considered design variables with bounds
(a) CASE I: $\alpha_j = 1$, $\gamma_j = 1$

(b) CASE II: $\alpha_j = 1$, $\gamma_j$ as design variables

(c) CASE III: $\gamma_j = 1$, $\alpha_j$ as design variables

(d) CASE IV: $\alpha_j$ and $\gamma_j$ as design variables

Figure 8: Results for four cases are displayed after 400 MMA iterations. (a) $f_0s = 5.261$ N m, $V = 20.33\%$, $GS_I = 35.2\%$ (b) $f_0s = 6.82$ N m, $V = 15.16\%$, $GS_I = 19.72\%$ (c) $f_0s = 6.35$ N m, $V = 15.96\%$, $GS_I = 6.15\%$ and (d) $f_0s = 6.46$ N m, $V = 16.30\%$, $GS_I = 5.80\%$. $GS_I$ indicates gray scale indicator.

Figure 8 depicts results for all the four cases with respective final normalized compliance values, volume fractions and gray scale indicators $GS_I$. Results are displayed after 400 MMA iterations. One notices that CASE IV indicates the lowest $GS_I$ value suggesting that the corresponding optimized design has lower gray FEs than others. Though CASE I gives lower final strain energy value, it is difficult to realize that continuum as it has many gray (fictitious material) FEs. To get solutions close to 0-1, we solve the problems henceforth with an additional gray scale indicator $GS_I$ constraint, i.e., with $g_2$ constraint (Eq. 19).

5.1.2 Arch design

In addition to above design parameters and variables, constraint $g_2$ (Eq. 19) is considered with $\delta$ set to $10^{-3}$, i.e., the desired $GS_I$ is 0.1%.

Figures 9, 10a and 10b indicate the optimized designs and convergence history plots for objective, volume fraction and gray scale indicator after 400 MMA iterations respectively. The final shape, size and orientation of masks are displayed with optimized material layout in Fig. 9a and 9b wherein thickness of the masks boundaries are directly proportional to their $\gamma_j$ and $\alpha_j$, respectively. Masks with higher $\gamma_j$ can have lower $\alpha_j$ and vice versa. The exclusive optimized material layout and that with pressure field are shown in Fig. 9c and 9d respectively. Final optimized designs are similar to those obtained in [1, 2]. The optimizer helps achieve the final design such that it can contain the applied pressure loading with minimum compliance. The obtained final normalized compliance, volume fraction and gray scale indicator are 5.34 N m, 0.20% and 0.54% respectively. The volume constraint is satisfied and active
Figure 9: Optimized design for internally pressure loaded arch after 400 MMA iterations (a) Optimized material layout with final elliptical masks whose thickness are proportional to their $\gamma_j$, (b) Material layout with final elliptical masks whose thickness are proportional to their $\alpha_j$, (c) Optimized material layout with $GS_1 = 0.54\%$ and (d) Optimized material layout with final pressure field.

Figure 10: Objective and constraints history for the arch problem.

(Fig. 10b), however gray scale constraint is not satisfied to its desired value of 0.1%. We solve the problem with different gray scale constraint ($\delta$) values (Eq. 19) using same parameters and variables with $100 \times 50$ and $200 \times 100$ FEs to indicate their effect on the final solutions and tabulate in Table 2. One notes that although a lower $\delta$ helps obtain continua closer to 0-1 solutions, the corresponding gray scale constraint does not get satisfied. One also notes from Table 2 that chances of achieving close to the desired/specified $\delta$ can increase with mesh refinement. Note that the solutions stays close to the specified constraint boundary. This may be because material density of each FE is a cumulative effect of all mask shapes, sizes, positions and orientations (see Eq. 4). After a limit for a given problem setting with $GS_1$ constraint, it may be difficult for the optimizer to move forward towards a better solution. Further, in view of Fig. 8d and 9c, one notices that using the material dilation and erosion variables alone do not necessarily yield a close to binary solution (Fig. 8d), and that one may need an explicit gray
scale constraint to achieve the same (Fig. 9c). Nevertheless, it can be inferred that the lower gray scale indicator constraint while keeping $\alpha_j$ and $\gamma_j$ as additional design variables helps in achieving close to 0-1 solutions. In this regard, we prefer to use $\delta = 0.001$ for all the problems. Fig. 10a and 10b illustrate the convergence plots for the objective, volume fraction and gray scale indicator constraint with the MMA iterations. At the end of the optimization, the plots have converging nature that is desirable, and the volume constraint remains active.

Table 2: Gray scale constraints for the arch problem

| Target $\delta$ (%) | 1.0 | 0.7 | 0.5 | 0.4 | 0.2 | 0.1 | Number of FEs |
|---------------------|-----|-----|-----|-----|-----|-----|---------------|
| Achieved $\delta$ (%) | 1.34 | 0.96 | 0.89 | 0.81 | 0.64 | 0.54 | 100 × 50      |
|                     | 1.25 | 0.71 | 0.67 | 0.65 | 0.44 | 0.44 | 200 × 100     |

Figure 11: A symmetrical half optimized design for piston design after 400 MMA iterations (a) Optimized material layout with final elliptical masks whose line widths are proportional to their $\gamma_j$, (b) Material layout with final elliptical masks whose line widths are proportional to their $\alpha_j$, (c) Optimized material layout with $GS_I = 0.78\%$ and (d) Optimized material layout with final pressure field.

5.2 Piston design

The pressure-loaded design for piston loadbearing structure was first presented in [30], which is taken herein as a second structure problem. The design domain specification with dimension $L_x \times L_y = 0.12 \times 0.04m^2$ is displayed in Fig. 6b. A vertical symmetry line exists for the design domain that is used herein to solve only a symmetrical part of the domain.

We use $N_{ex} \times N_{ey} = 100 \times 50$ hexagonal FEs and $N_{mx} \times N_{my} = 20 \times 10$ elliptical negative masks to
parametrize and determine the optimized material layout of the symmetrical design, respectively. Volume fraction and gray scale constraint are set to 0.25 and 0.001 respectively. The upper bound on $\alpha_j$ is set to 30. The maximum number of MMA iterations is set to 400. $S = 0.05$ is set for mask variable movement. We refer to Table 1 for other design parameters.

![Optimized material layout with final elliptical masks whose line widths are proportional to their $\gamma_j$](a)

![Material layout with final elliptical masks whose line widths are proportional to their $\alpha_j$](b)

![Optimized material layout with $GS_I = 1.37\%$](c)

![Optimized material layout with final pressure field](d)

Figure 12: A symmetrical half optimized design for inverter mechanism after 600 MMA iterations (a) Optimized material layout with final elliptical masks whose line widths are proportional to their $\gamma_j$, (b) Material layout with final elliptical masks whose line widths are proportional to their $\alpha_j$, (c) Optimized material layout with $GS_I = 1.37\%$ and (d) Optimized material layout with final pressure field.

![Objective convergence history](a)

![Volume fraction and gray scale indicator](b)

Figure 13: Objective and constraints convergence plots for the inverter mechanism.

A symmetrical half optimized piston design is displayed in Fig. 11. Plots with masks considering the values of $\gamma_j$ and $\alpha_j$ proportion to the line widths of masks are depicted in Fig. 11a and 11b respectively. One notices that $\alpha_j$ and $\gamma_j$ vary differently as noted in the arch problem result too. Specifically, nearly all masks whose boundaries define the contour of the continuum seem to have higher $\alpha_j$, as expected, since this helps boundary FEs attain states close to the solid state. However, not all $\gamma_j$ are high for the same masks. This suggests that selective dilation/erosion may be occurring at the continuum boundaries.
in an attempt to satisfy the gray scale constraint. The optimized piston design resembles the previously obtained results for the same problem \[2,30\]. The final normalized compliance, volume fraction and \( GS_1 \) are 10.97 N m, 0.25 and 0.78%, respectively. The volume constraint is satisfied and active at the end of optimization, however gray scale constraint is close to though not quite satisfied. Reasons could be as mentioned in the Section 5.1.2. Next, we solve pressure-actuated compliant mechanisms.

### 5.3 Pressure-actuated CMs

Pressure-actuated inverter and Gripper CMs are designed using a multi-criterion objective (Eq. 19) with volume and gray scale indicator constraints.

The symmetric half designs for inverter and gripper mechanisms are depicted in Fig. 7a and 7b, respectively. \( L_x \times L_y = 0.02 \times 0.01 \text{ m}^2 \) is set for each mechanism. Figures also depict the output location and the direction of movement for each mechanism using red thick arrows. For the inverter mechanism, an inverse motion with respect to the pressure loading direction is sought, whereas a perpendicular gripping motion is desired in case of the gripper mechanism. To provide a proper seat for the workpiece, a void passive region having dimension \( L_x \times L_y \) is provided and for gripping jaws (solid passive regions) dimension \( \frac{L_x}{2} \times \frac{L_y}{3} \) are set. Springs with stiffness \( k_s = 1 \times 10^5 \text{ N m} \) are attached at the output location of inverter and gripper mechanisms. These springs represent the workpiece stiffnesses at the output locations. \( N_{ex} \times N_{ey} = 120 \times 60 \) FE are employed to describe the design domains. The number of elliptical masks is set to \( N_{mx} \times N_{my} = 20 \times 10 \) for both. Volume fraction for each mechanism is set to 0.30. \( \delta \) for \( GS_1 \) is chosen as 0.001. The maximum number MMA iterations is set to 600. The upper bounds on \( \alpha_j \) and \( \gamma_j \) for the inverter mechanism used are 20, while for the gripper mechanisms those are 25 and 10, respectively. Step lengths (Eq. 30) for inverter and gripper are 0.01 and 0.025 respectively.

![Figure 14: A symmetrical half optimized design for gripper mechanism after 600 MMA iterations (a) Optimized material layout with final elliptical masks whose line widths are proportional to their \( \gamma_j \), (b) Material layout with final elliptical masks whose line widths are proportional to their \( \alpha_j \), (c) Optimized material layout with \( GS_1 = 0.81\% \), and (d) Optimized material layout with final pressure field.](image)

The optimized designs for inverter and gripper mechanisms are depicted in Fig. 12 and 14 respectively. Masks with optimized CMs with \( \gamma_j \) and \( \alpha_j \) represented by their line thickness are plotted in Fig. 12a, 14a and Fig. 12b, 14b, respectively. Fig. 12c and 14c show the optimized results with pressure field.
Figure 15: Deformed profiles for inverter and gripper mechanisms are displayed in (a) and (b) respectively. The actual deformation is magnified by 10 times for visibility purpose.

The final volume fraction for inverter and gripper mechanisms are 0.266 and 0.261, respectively and the final recorded gray scale indicator are 1.37% and 0.81% respectively. In both cases volume constraints are satisfied, however GS1 constraints do not satisfy. The optimized CMs with pressure field for the inverter and gripper mechanisms are depicted in Fig. 12d and 14d, respectively. One notes that to contain the pressure loads, the optimizer provides a chamber like inflated design at the input locations. The objective and constraints convergence plots for the optimized inverter mechanism are displayed in Fig. 13a and 13b respectively. At the end of the optimization process, these plots converge smoothly. The deformed profiles for the inverter and gripper mechanisms with their pressure field are illustrated in Fig. 15a and 15b respectively. The obtained motions of the output nodes of the mechanisms are as they are designed for.

6 Closure

The presented Material Mask Overlay Strategy (MMOS) topology optimization approach gives pressure-loaded structure and pressure-actuated compliant mechanism designs close to black and white. The final output displacements of these mechanisms are as expected. Negative elliptical masks are used, and for each mask, in addition to its position, size and orientation, logistic variable and exponent are posed as design variables. High value of the logistic variable leads to material addition near the mask boundary. In contrast, large value of the exponent results in material erosion inside and outside the boundary. By optimally determining their values for each mask, finite element densities can be controlled indirectly, leading to near black and white topologies, especially in presence of an explicit, gray scale constraint.

Hexagonal elements (honeycomb tessellation) are used to describe the design domains, which provide edge-connectivity and thus, point-connections and checkerboard patterns get automatically vanished from the optimized designs. To relate pressure field with the material density vector, Darcy’s law with a drainage term is employed wherein the flow coefficient of each element is interpolated using a smooth Heaviside projection function. The formulation facilitates determining of pressure loading surfaces/curves implicitly as the topology optimization evolves wherein the span of pressure gradient alters with topology optimization iterations. The pressure field is then transformed into nodal forces using Wachspress shape functions employed to model hexagonal elements. The importance of drainage term with hexagonal elements is demonstrated using a design domain containing multiple solid finite elements layers.

The approach provides automatic and computationally inexpensive evaluation of the load sensitivity terms while determining objective sensitivities using the adjoint-variable method. The optimized pressure-actuated compliant mechanisms are designed with small deformation mechanics assumptions. Extending the approach for large deformation problems for soft (compliant) robotic designs will have additional challenges, e.g., treating the pressure loads as follower forces, and thus, it needs a dedicated and detailed investigation, which can be one of the interesting future directions. Extending the proposed methodology to three dimensions can be another prospective study.
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Appendix

A Wachspress shape functions

A hexagonal element with vertices \(V_i, i = 1, 2, 3, \ldots, 6\) in \(\xi\) co-ordinates system is depicted via Fig. 16. \(C_c\) is the circumscribing circle with radius 1 unit. One finds the coordinates of \(V_i\) as \(\left(\xi_i, \eta_i\right) \equiv \left(\cos\left(\frac{2i-1}{6}\pi\right), \sin\left(\frac{2i-1}{6}\pi\right)\right)\). Let \(N_i\) be the Wachspress shape function corresponding to node \(i\), i.e., vertex \(V_i\) (Fig. 16). Using coordinate geometry, one writes the equations of straight lines \(l_i\) as

\[
egin{align*}
    l_1(\xi) & \equiv \xi_1 + \sqrt{3}\xi_2 - \sqrt{3} = 0 \\
    l_2(\xi) & \equiv -\xi_1 + \sqrt{3}\xi_2 + \sqrt{3} = 0 \\
    l_3(\xi) & \equiv 2\xi_1 + \sqrt{3} = 0 \\
    l_4(\xi) & \equiv \xi_1 + \sqrt{3}\xi_2 + \sqrt{3} = 0 \\
    l_5(\xi) & \equiv -\xi_1 + \sqrt{3}\xi_2 + \sqrt{3} = 0 \\
    l_6(\xi) & \equiv 2\xi_1 - \sqrt{3} = 0
\end{align*}
\]

and likewise, one finds the equation of circle \(C_a\) (cf. Fig. 16, passing through \(P_{i+2}\)) as

\[
    C_a(\xi) \equiv \xi_1^2 + \xi_2^2 - 3 = 0.
\]

Note that straight lines \(l_i\) and \(l_{i+2}\) intersect at point \(P_{i+2}\) (Fig. 16). The shape function of node 1, i.e., \(N_1\) is determined as \([39]\)

\[
    N_1 = s_1 l_2(\xi)l_4(\xi)l_5(\xi)/C_a(\xi),\quad (A.3)
\]

where \(s_1\), a constant, is extracted using the Kronecker-delta property of a shape function, which is defined as

\[
    \delta_{ij} = \begin{cases} 
        1, & \text{if } i = j \\
        0, & \text{if } i \neq j
    \end{cases}.
\]

Now, in view of co-ordinates of node 1, i.e., \((\xi_1, \xi_2)\), Eqs. (A.3) and (A.4), one finds

\[
    s_1 = \frac{C_a(\xi_1, \xi_2)}{l_2(\xi_1, \xi_2)l_4(\xi_1, \xi_2)l_5(\xi_1, \xi_2)} = \frac{1}{18}.
\]

Likewise, one can find Wachspress shape functions corresponding to the remaining nodes, respective constants which can be summarized as

\[
\begin{align*}
    N_1(\xi) & = \frac{-\xi_1 + \sqrt{3}\xi_2 - \sqrt{3}}{18(\xi_1^2 + \xi_2^2 - 3)}(2\xi_1 + \sqrt{3})(\xi_1 + \sqrt{3}\xi_2 + \sqrt{3})(-\xi_1 + \sqrt{3}\xi_2 + \sqrt{3}) \\
    N_2(\xi) & = \frac{2\xi_1 + \sqrt{3}}{18(\xi_1^2 + \xi_2^2 - 3)}(\xi_1 + \sqrt{3}\xi_2 + \sqrt{3})(-\xi_1 + \sqrt{3}\xi_2 + \sqrt{3})(2\xi_1 - \sqrt{3}) \\
    N_3(\xi) & = \frac{-\xi_1 + \sqrt{3}\xi_2 + \sqrt{3}}{18(\xi_1^2 + \xi_2^2 - 3)}(-\xi_1 + \sqrt{3}\xi_2 + \sqrt{3})(2\xi_1 - \sqrt{3})(\xi_1 + \sqrt{3}\xi_2 - \sqrt{3}) \\
    N_4(\xi) & = \frac{-\xi_1 + \sqrt{3}\xi_2 + \sqrt{3}}{18(\xi_1^2 + \xi_2^2 - 3)}(-\xi_1 + \sqrt{3}\xi_2 - \sqrt{3})(\xi_1 + \sqrt{3}\xi_2 - \sqrt{3})(2\xi_1 + \sqrt{3}) \\
    N_5(\xi) & = \frac{2\xi_1 - \sqrt{3}}{18(\xi_1^2 + \xi_2^2 - 3)}(-\xi_1 + \sqrt{3}\xi_2 - \sqrt{3})(\xi_1 + \sqrt{3}\xi_2 - \sqrt{3})(2\xi_1 + \sqrt{3}) \\
    N_6(\xi) & = \frac{-\xi_1 + \sqrt{3}\xi_2 - \sqrt{3}}{18(\xi_1^2 + \xi_2^2 - 3)}(-\xi_1 + \sqrt{3}\xi_2 - \sqrt{3})(\xi_1 + \sqrt{3}\xi_2 + \sqrt{3})
\end{align*}
\]

\[4\xi_1 = \cos\left(\frac{\pi}{6}\right), \quad \xi_2 = \sin\left(\frac{\pi}{6}\right)\]
Figure 16: Definition of the shape functions for a regular hexagonal element with vertices \( V_i \mid i = 1, 2, \ldots, 6 \) and circumscribing circle \( C_c \) with radius 1 unit. The co-ordinates the vertex \( V_i \) are \( (\xi_1, \xi_2) \equiv \left( \cos\left(\frac{(2i-1)\pi}{6}\right), \sin\left(\frac{(2i-1)\pi}{6}\right) \right) \). Straight lines \( l_i \) as depicted pass through vertices \( V_i V_{i-1} \). Straight lines \( l_i \) and \( l_{i+2} \) intersect at point \( P_{i+i+2} \). A circle \( C_s \) passing through points \( P_{i+i+2} \) is drawn, whose radius is equal to \( \sqrt{3} \) units.

**B Numerical quadrature points**

Numerical quadrature rule is employed to find the integration pertaining to the finite element formulation for solving PDEs corresponding to fluid and mechanical balanced equations. As per [43], quadrature points for a hexagonal element are tabulated below (Table 3) and a function can be integrated as

\[
\int_{\Omega_j} f dV \approx w_0 f(0, 0) + \sum_{k=2}^{k_{\text{max}}} \sum_{i=1}^{6} w_k f\left( r_k, \alpha_k + \frac{i\pi}{3} \right). \tag{B.1}
\]

In Table 3, \( N \) is the number of integration points having co-ordinates \( (\xi_1^i, \xi_2^i) = (r_k \cos(\alpha_k + \frac{i\pi}{3}), r_k \sin(\alpha_k + \frac{i\pi}{3})) \). \( i = 1, 2, 3, \ldots, 6 \), if \( k > 1 \), and \( i = 1 \), if \( k = 1 \), corresponds to single integration point at center \((0, 0)\). For \( k > 1 \), six integration points lie on the a circle with center at \((0, 0)\) and radius \( r_k \). \( w_k \) indicate the weights for these Gauss points. We have used \( k = 2 \), i.e, \( N = 7 \) quadrature points in this paper. Note that the quadrature rule is invariant under a rotation of 60° for a hexagonal FE [43].
Table 3: Quadrature points for a hexagonal element

| Cases | $r_k$ | $\alpha_k$ | $w_k$ |
|-------|-------|-------------|-------|
| 1, $k = 2$, $N = 1 + 6(k - 1) = 7$ | 0.0000 | 0.0000 | 0.255952380952381 |
|       | 0.748331477354788 | 0.0000 | 0.124007936507936 |
| 2, $k = 3$, $N = 1 + 6(k - 1) = 13$ | 0.0000 | 0.0000 | 0.174588684325077 |
|       | 0.657671808727194 | 0.0000 | 0.115855303626943 |
|       | 0.943650632725263 | 0.523681372148045 | 0.021713248985544 |
| 3, $k = 4$, $N = 1 + 6(k - 1) = 19$ | 0.0000 | 0.0000 | 0.11082657258661 |
|       | 0.792824967172091 | 0.0000 | 0.037749166510143 |
|       | 0.537790663359878 | 0.523598775598299 | 0.082419705350590 |
|       | 0.883544457934942 | 0.523598775598299 | 0.028026703601157 |
| 4, $k = 5$, $N = 1 + 6(k - 1) = 25$ | 0.0000 | 0.0000 | 0.08705549094808 |
|       | 0.48778213872069 | 0.0000 | 0.071957468118574 |
|       | 0.820741657108524 | 0.0000 | 0.027500185650866 |
|       | 0.771806696813652 | 0.523598775598299 | 0.045248932131663 |
|       | 0.957912268790000 | 0.523598775598299 | 0.007459692497607 |

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