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Implementation of the Phase Field Method for Structural Topology Optimization in a FEM Framework Developed in C++

Guilherme T. Pimentel[1], Jeferson W. D. Fernandes[1], Marcelo Greco[1]

[1]*Department of Structural Engineering, Federal University of Minas Gerais*
Av. Antônio Carlos, 6627 – Pampulha Belo Horizonte 31270-901 – MG, Brazil
gui-teixeirapimentel@hotmail.com, jwdfernandes@ufmg.br, mgreco.dees.ufmg@gmail.com

Abstract. Topological optimization, specifically with a focus on compliance minimization, seeks the best material distribution within a design domain given different loading and constraints configurations. The Phase Field Method (PFM) offers a continuous and well-posed formulation from a mathematical point of view, naturally regularizing the problem by controlling the interface thickness, without the need for artificial filters. This paper presents the implementation of the PFM for topological optimization of structures in a finite element (FEM) framework developed in C++. The main objectives are to incorporate the PFM directly into a FEM code and compare its results with other methods, such as Solid Isotropic Material with Penalization (SIMP). The theoretical foundation of the study is based on a variational formulation, combining the structural equilibrium equation with the Allen–Cahn evolution equation to govern the material distribution. The coupling of the equations is made through a staggered scheme, this implies that each equation is solved separately and the outcome of each equation is iteratively exchanged to update the other. The results are used to confirm the successful implementation of the method and to demonstrate the phase field method ability to produce smooth and physically consistent topologies.

Keywords: Phase Field Method, C++, FEM, Topology Optimization, Compliance Minimization

1 Introduction

Structural topology optimization is a powerful computational design methodology for determining the optimal distribution of material within a given domain under prescribed mechanical loads, boundary conditions, and volume constraints. A central problem in this field is compliance minimization, where the objective is to maximize structural stiffness subject to a fixed amount of material. This problem has been extensively studied using density-based approaches such as SIMP (Solid Isotropic Material with Penalization), level-set methods, and heuristic strategies like the Evolutionary Structural Optimization (ESO) method as described by Yago et al. [1] and Cervera and Trevelyan [2].

In recent years, the Phase Field Method (PFM) has garnered growing attention in topology optimization due to its rigorous mathematical foundation and its inherent regularization of the material-void interface. Unlike SIMP or ESO, which often rely on artificial filters, projection schemes, or sensitivity modifications to suppress phenomena such as checkerboarding, gray elements, and mesh dependency, the phase field approach models material distribution through a continuous order parameter that transitions smoothly between void and solid. This transition is governed by a length-scale parameter (ϵ), which naturally enforces interface thickness and minimum feature size without requiring external filters as also discussed by Blank et al. [3] and Yago et al. [1].

Originating in materials science and image segmentation, phase field models have been adapted for structural optimization by reinterpreting the topology design problem as a variational energy minimization. The total objective functional commonly combines elastic strain energy with an interface penalization term, and material evolution is governed via gradient flow equations, most commonly the Allen-Cahn or Cahn-Hilliard dynamics, coupled with structural equilibrium equations solved via linear elasticity. These equations are often discretized and solved using a staggered scheme, alternating updates of the phase and displacement fields iteratively until convergence Blank et al. [3].

Despite the theoretical appeal of PFM, implementing it within custom finite element frameworks remains challenging many existing implementations rely on high-level or commercial environments, which can obscure numerical details and limit flexibility. In response, this work presents a complete integration of the Phase Field Method into a custom finite element code written in C++, allowing direct control over mesh discretization, interface

regularization, solver algorithms, and performance optimization strategies.

The primary objectives of this study are:

- To implement the phase-field formulation for compliance-minimization topology optimization within a C++ finite element framework;
- To validate this implementation on canonical 2-dimensional linear elasticity benchmarks;
- To compare the resulting topologies with those produced by the Solid Isotropic Material with Penalization (SIMP) method, analyzing differences in solution smoothness, mesh-independence, interface clarity, computational expense, and sensitivity to regularization parameters.

2 Theoretical and Numerical Formulation

2.1 Linear Elasticity and the State Equation

Under the assumption of small strains, the mechanical response of the structure follows the classical equations of linear elasticity. In the absence of body forces, the equilibrium equation expresses static balance of linear momentum:

$$\nabla \cdot \sigma = 0 \;\; in\, \Omega, \tag{1}$$

where σ is the Cauchy stress tensor and Ω the material design domain. For completenness, Dirichlet boundary conditions are prescribed on Γ_D and Neumann on Γ_N.

The constitutive law is Hooke's law with linear stress-strain relationship, considering Biot strain measure, extended by a phase-field interpolation:

$$\sigma(\phi) = C(\phi) : \epsilon(u) \quad \text{with} \quad \epsilon(u) = \frac{1}{2}(\nabla u + \nabla u^T). \tag{2}$$

Material interpolation uses:

$$C(\phi) = \phi^p C_0 + \eta C_0 \tag{3}$$

where C_0 is the elasticity tensor of base material, p (commonly 3) promotes near-binary material distributions, and $\eta \ll 1$ (e.g. 10^{-3}) avoids matrix singularity when $\phi \approx 0$.

2.2 Phase-Field Formulation for Topology Optimization

Topology optimization is formulated as minimization of a total energy functional that couples structural compliance and interface regularization:

$$J(\phi, u) = \int_\Omega \epsilon(u) : C(\phi) : \epsilon(u) d\Omega + \kappa \int_\Omega \left(\frac{\gamma^2}{2} |\nabla \phi|^2 + \frac{1}{\gamma} \psi(\phi) \right) d\Omega. \tag{4}$$

The first term is the mechanical compliance (to be minimized). The second term is the Modica-Mortola (Ginzburg-Landau) regularization, penalizing fine structural features and enforcing interface smoothness as presented in Xie et al. [4] and Blank et al. [5]. The double-well potential $\psi(\phi) = \phi^2(1-\phi)^2$ enforces ϕ close to $\{0, 1\}$. Parameters $\gamma > 0$ control interface thickness and $\kappa > 0$ weight the regularizer relative to compliance.

This variational formulation follows the foundational works by Bourdin and Chambolle [6], who rigorously established sharp-interface limit via Γ-convergence and showed that the phase-field regularization converges to perimeter-penalized shape optimization as $\epsilon \to 0$. Their earlier work also formulates compliance minimization via phase-field as a smooth approximation to classical topology design.

Gradient-flow dynamics yield an Allen-Cahn-type evolution:

$$\frac{\partial \phi}{\partial t} = -\frac{\delta J}{\delta \phi}, \tag{5}$$

which leads to the following partial equation differential equation:

$$\frac{\partial \phi}{\partial t} = \kappa \left(\gamma \delta \phi - \frac{1}{\gamma} \psi'(\phi) \right) + \epsilon(u) : \frac{dC(\phi)}{d\phi} : \epsilon(u). \tag{6}$$

The compliance-sensitivity term arises from $\frac{dC}{d\phi} = p\phi^{p-1}C_0$ (ignoring constant ηC_0).

2.3 Coupling Strategy and Time Integration

The optimization is solved via a staggered scheme:

1. Given ϕ^n , assemble the stiffness using $C(\phi^n)$ and solve equilibrium for u^n.
2. Compute compliance sensitivity.
3. Advance the Allen-Cahn equation to update ϕ^{n+1}.
4. Check for convergence and step to next pseudo-timestep.

This approach yields a robust, decoupled implementation that captures coupling between material distribution and mechanical response. Phase-field regularization ensures well-posedness, and delivers mesh-independent, checkerboard-free topologies with smooth feature definitions.

Numerical validation is often performed using classical 2D benchmark problems, notably cantilever-beam domains, bridge-like layouts, and inverter mechanisms, as extensively documented in the literature Chen et al. [7] Choi et al. [8] Gain and Paulino [9]. These serve as canonical tests to verify convergence, interface sharpness, and solution quality across mesh resolutions.

3 Numerical Implementation

We develop a hybrid FEM-FD framework, implemented in modular C++, to solve the coupled topology optimization problem by combining a structural FEM solver and a phase-field FD solver in a staggered fashion. The design emphasizes flexibility, performance, and numerical clarity.

3.1 Structural Problem: Finite Element Discretization

The weak form of the elastic equilibrium is discretized using a standard Galerkin FEM with quadrilateral or triangular elements. Element stiffness matrices are defined as:

$$K^e(\phi_e) = \int_{\Omega^e} B^T C(\phi_e) B d\Omega, \tag{7}$$

where B is the strain-displacement matrix and $C(\phi_e)$ the interpolated elasticity tensor at the element level, as detailed in Section 2.1. After assembling over all elements, the global equation:

$$K(\phi)u = f \tag{8}$$

is enforced. Dirichlet boundary conditions are imposed using elimination or penalty techniques, and the resulting sparse symmetric linear system is solved using multi-resolution sparse-direct or iterative solvers. In our C++ implementation, we can interface with PETSc (Portable Extensible Toolkit for Scientific Computation) for iterative linear solves and preconditioning support, providing both scalability and performance control. Element meshes are generated using Gmsh via .geo scripts offering both structured and unstructured discretizations.

3.2 Phase Field Evolution: Finite Difference Time-Stepping

We discretize the Allen-Cahn equation using an explicit Euler step in time and a second-order central finite-difference method in space on a uniform Cartesian FD grid. The semi-implicit scheme takes the form:

$$\phi_{i,j}^{n+1} = \phi_{i,j}^{n} + \Delta t \cdot - \left(\beta \frac{\partial C}{\partial \phi} \epsilon : \epsilon - \gamma \left[\xi \nabla^2 \phi^{n+1} - \frac{\partial w^m}{\partial \phi} \right] + \lambda^n \right) \tag{9}$$

where $\nabla^2 \phi$ is approximated by $\frac{\phi_{i+1,j}+\phi_{i-1,j}+\phi_{i,j+1}+\phi_{i,j-1}-4\phi_{ij}}{h^2}$ and $\frac{\partial w}{\partial \phi}$ is calculated using the standard double-well function as $2\phi(1-\phi)(1-2\phi)$. To ensure constant volume during optimization we use a Lagrange multiplier λ^n calculated per timestep as:

$$\lambda^n = -\frac{1}{|\Omega|} \int_\Omega \left(\beta \frac{\partial C}{\partial \phi} \epsilon : \epsilon - \gamma \left[\xi \nabla^2 \phi^{n+1} - \frac{\partial w^m}{\partial \phi} \right] \right) dx. \tag{10}$$

Coupling FEM with FD for topology optimization has been shown effective and widely adopted in Xie et al. [4]. The finite-difference approach applied to phase-field evolution is also used in other works where it proves effective in capturing interface dynamics with minimal oscillations as demonstrated also in Gain and Paulino [9].

3.3 Coupling via Mesh Superposition

To couple the unstructured FEM mesh with the uniform FD grid, we employ a mesh superposition strategy:

- The FD grid spacing h_{FD} is chosen such that FD nodes align with FEM element centroids or integration points.
- At each iteration, phase-field values ϕ^n at FD nodes are projected onto the FEM mesh to compute element-level elasticity tensors $C(\phi)$. We use bilinear interpolation for consistency or nearest-neighbor if grid alignment is perfect.
- After solving for u^n, we compute the strain-energy density $\epsilon(u) : C(\phi) : \epsilon(u)$ at each FEM integration point and interpolate it back to FD grid nodes.

This coupling strategy preserves energy consistency and material-void structure, while keeping the discretizations decoupled for flexibility.

4 Results and Discussion

To evaluate the performance and validate the implementation of the Phase Field Method (PFM) within the FEM framework, a numerical experiment was conducted on a benchmark problem in two-dimensional linear elasticity. The example chose is widely used in the topology optimization literature and allow for visual and quantitative assessment of the method's capacity to generate efficient, mesh-independent structural layouts. Additionally, comparisons are made with other methods to highlight key differences in solution quality, boundary definition, and computational cost.

All results presented in this section are obtained using quadrilateral finite elements for the structural problem and a Cartesian finite difference grid for the phase field evolution. Unless otherwise stated, material properties are normalized with Young's modulus $E = 1$ and Poisson's ratio $\nu = 0.3$, and the total volume constraint is imposed explicitly via the Lagrange Multipler λ. The interface thickness parameter γ, time step Δt, and penalization exponent p are selected based on numerical experimentation to balance convergence speed, interface definition, and computational stability.

4.1 Benchmark Problem: MBB Beam

The test case used is the classical Messerschmitt-Bölkow-Blohm (MBB) beam, a simply-supported beam loaded at its center and commonly used in compliance minimization studies. A schematic drawing of the problem is presented in Fig. 1. Only half of the domain is discretized by imposing symmetry boundary conditions. The design domain ends up with a length-to-height ratio of 3:1 and is discretized with 300 x 100 quadrilateral elements

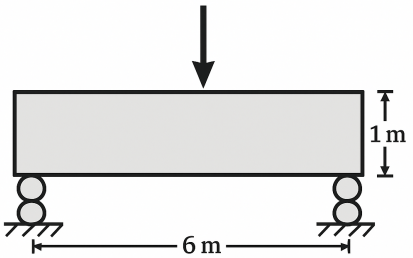


Figure 1. Schematic drawing of the MBB beam problem.

in FEM and 300 x 100 nodes in the finite difference grid. This mesh helps to couple the FEM and FD, as a nearest neighbor approach can be used in this case.

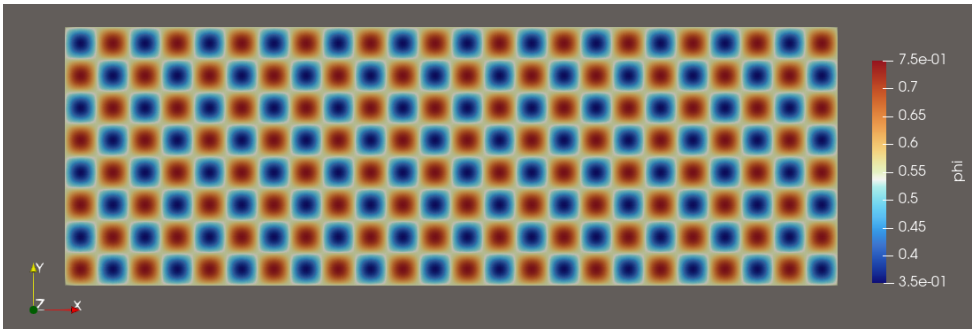


Figure 2. Initial condition for the phase-field problem.

The initial phase-field distribution is shown in Fig. 2. The total ammount of material, which is conserved through the use of the Lagrange Multiplier, is approximately 1.65. Mathematically, the function $\phi(x, y) = 0.55 + 0.2sin(8\pi x)sin(8\pi y)$ is used to construct the initial field.

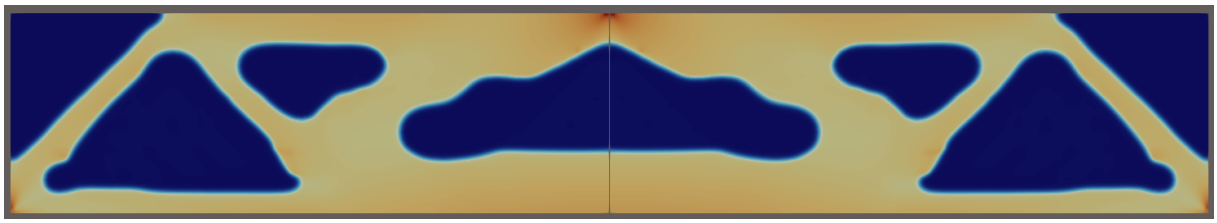


Figure 3. MBB result with parameters: $dx = 0.01$,$\beta = 1.5$, $\xi = 10^{-4}$, $\gamma = 16dx$ and $V_0 = V_f = 55\%$

4.2 Result and Comparison with other methods

The resulting topology, shown in Fig. 3, exhibits a smooth structure with clearly defined load paths. The material layout respects the structural symmetries and boundary conditions, with gradual transitions between solid and void regions near supports and loading zones. The interface between phases is well resolved, even at relatively coarse mesh resolutions, and no checkerboarding is encountered.

To compare the proposed approach with a different method, a solution for the same MBB beam using the Solid Isotropic Material Penalization (SIMP) technique is presented in Fig. 4.

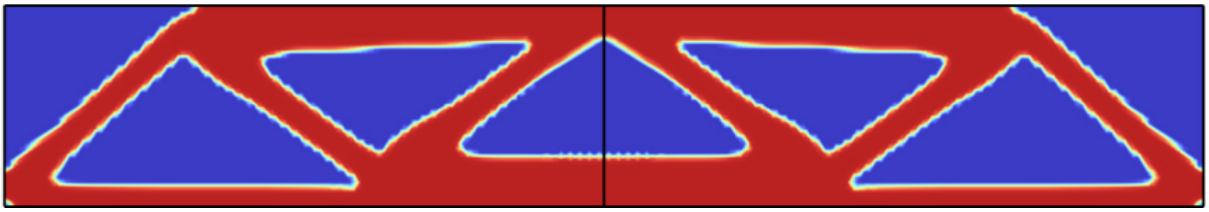


Figure 4. COMSOL MBB Topology Optimization using SIMP. Adapted from COMSOL [10].

The final layout obtained using SIMP with filters, shown in Fig. 4, resembles that of the phase field solution in terms of global topology. This shows that the method is indeed correctly distributing material along the design domain. From a computational perspective, the PFM incurs higher cost per iteration due to the solution of a nonlinear PDE and the need for finer phase field resolution to resolve interfaces.

4.3 Parameter Study and Sensitivity

A parametric study was conducted to investigate the influence of the regularization parameter on the resulting topologies. Three values were considered: $8dx$ (0.08), $16dx$ (0.16), and $32dx$ (0.32), where dx denotes the finite difference grid spacing.

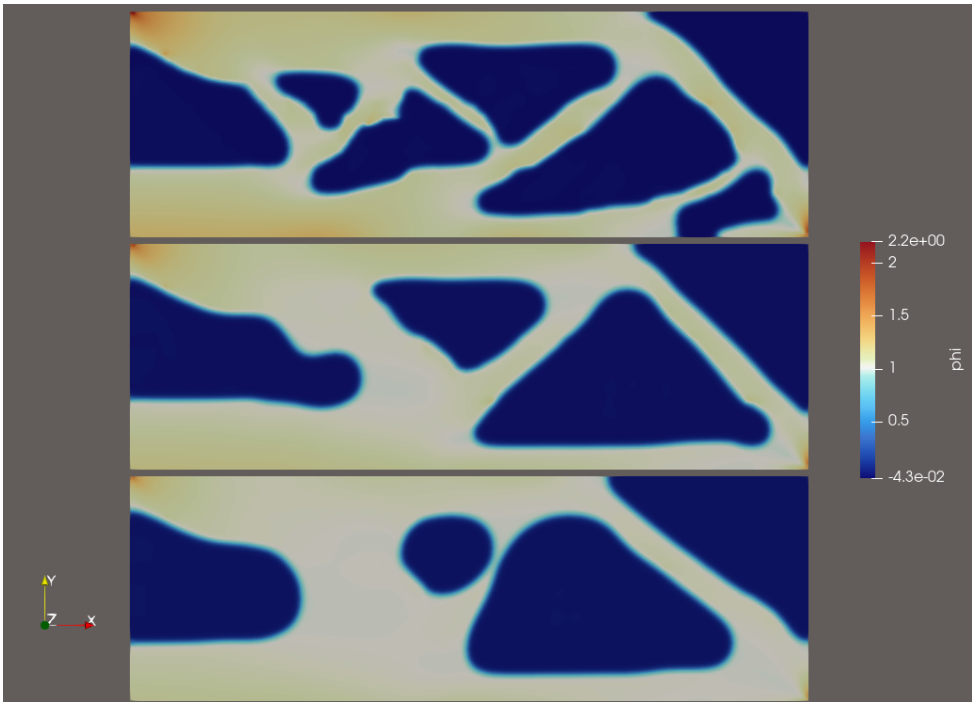


Figure 5. MBB results with parameters: $dx = 0.01$, $\beta = 1.5$, $\xi = 10^{-4}$ and $V_0 = V_f = 55\%$. The regularization parameter γ is varied as $8dx$ (0.08), $16dx$ (0.16), and $32dx$ (0.32).

The results shown in Fig. 5 reveal that smaller values of γ promote the formation of finer structural features, with a high level of detail and sharper edges, resembling the behavior of discrete methods without a filter radius when the mesh is refined. Intermediate values of γ produce features more consistent with commonly accepted optimal topologies, balancing detail and smoothness. For larger values of γ, the topology becomes more regularized, with rounded contours and smoother boundaries, as the diffuse interface suppresses small-scale features in favor of global structural coherence.

It is also important to highlight the lack of material in the bottom-right part of the first solution shown in Fig. 5. While the solution does satisfy the static equilibrium condition in eq. (8), such a void is undesirable in real-world applications, where robustness and manufacturability are essential. This outcome is partly related to the choice of parameters, as the case with $\gamma = 8dx$ can be considered sub-optimal, leading to features that are less consistent with commonly accepted MBB topologies.

The hybrid FEM-FD implementation, combined with mesh superposition and sensitivity projection, enables accurate and stable simulation of the coupled system. The staggered solution scheme decouples complexity and facilitates implementation.

5 Conclusions

The Phase Field Method (PFM) was successfully implemented within a custom finite element framework, yielding smooth, mesh-independent topologies with well-defined structural paths. When compared other methods, PFM demonstrated similar interface regularity and great robustness to mesh resolution.

A key outcome of this work is the identification of strong sensitivity to regularization parameters. The γ governs both the minimum feature size and the sharpness of the material interface; smaller values promote binary designs but require finer discretization.

These results confirm the method's potential for generating high-quality structural designs but also highlight the need for careful parameter tuning. Future work should explore adaptive parameter control, extensions to three-dimensional problems, and coupling with additional physical phenomena.

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