Fictitious Domain Methods and Topology Optimization

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Geometric flexibility

- The geometric flexibility of the FEM an important reason for its success
- The FEM works well with **unstructured meshes**
- Unstructured meshes can be generated fast and automatically in many cases
**Typical FEM procedure**

Three distinctive steps:

- **Preprocessing:** Geometry definition (often from CAD) + generation of body-fitted mesh
- **Analysis:** Assembly of system matrices, solution of the algebraic equations
- **Postprocessing:** Visualization, qualitative and quantitative analysis of the solution
Limitations of the typical procedure

The clear separation between preprocessing and analysis sometimes problematic:

- The computational domain changes with time, e.g. fluid–structure interaction
- The geometry is a part of the solution of the problem, e.g. design optimization, free boundary problems

In those cases, can be an advantage to integrate geometry handling and analysis

Fictitious domain methods (also called domain embedding methods) accomplish this
Fictitious domain methods

Basic idea:

- A large (often square) computational domain $\hat{\Omega}$ covers “real”, physical domain $\Omega$
- The computational domain is meshed using a **fixed** (often regularly structured) mesh
- The equations are solved on the larger, computational domain
- The boundary conditions on the “real” domain becomes interior conditions in the computational domain
- The point with it all: easier to change the interior conditions than to remesh and interpolate on the new mesh
Fictitious domain methods

- The boundary conditions at the interior boundary have to be “forced” somehow.
- Two basic ways for this:
  - Through extra or modified boundary integrals in the variational form
  - Through extra or modified volume integrals in the variational form

Today: a basic (but very useful!) volume integral version.
Natural vs. essential boundary conditions

The three standard boundary conditions for second-order elliptic boundary-value problems:
(i) Dirichlet, (ii) Neumann, and (iii) Robin conditions

\[-\Delta u = f \quad \text{in } \Omega \]  \hspace{1cm} (1a)

(\text{Dirichlet}) \hspace{1cm} u = 0 \quad \text{on } \partial \Omega \]  \hspace{1cm} (1b)

(\text{Neumann}) \hspace{1cm} \frac{\partial u}{\partial n} = 0 \quad \text{on } \partial \Omega \]  \hspace{1cm} (1c)

(\text{Robin}) \hspace{1cm} \alpha u + \frac{\partial u}{\partial n} = 0 \quad \text{on } \partial \Omega \]  \hspace{1cm} (1d)

Note: Case (1c) requires \( \int_{\Omega} f \, dV = 0 \) for consistency.
Variational forms

Multiply equation (1a) with a test function $v \in H^1(\Omega)^+$, integrate, and use Green's formula:

$$
\int_{\Omega} vf \, dV = - \int_{\Omega} v\Delta u \, dV = - \int_{\partial\Omega} v \frac{\partial u}{\partial n} \, dS + \int_{\Omega} \nabla v \cdot \nabla u \, dV
$$

[Dirichlet BC: let $v \equiv 0$ on $\partial\Omega] = \int_{\Omega} \nabla v \cdot \nabla u \, dV

[Neumann BC: $\partial u/\partial n \equiv 0$ on $\partial\Omega] = \int_{\Omega} \nabla v \cdot \nabla u \, dV

[Robin BC: $\partial u/\partial n = -\alpha u$ on $\partial\Omega] = \int_{\partial\Omega} \alpha vu \, dS + \int_{\Omega} \nabla v \cdot \nabla u \, dV

$H^1(\Omega)$: the space of square-integrable functions with square-integrable derivatives
Variational forms

\( H^1_0 \): the subspace of \( H^1(\Omega) \) functions that vanish on the boundary

PDE with Dirichlet boundary condition

Var. form: **Essential** boundary condition

Find \( u \in H^1_0(\Omega) \) such that

\[
\int_{\Omega} \nabla v \cdot \nabla u \, dV = \int_{\Omega} v f \, dV \quad \forall v \in H^1_0(\Omega)
\]

PDE with Neumann boundary condition

Var. form: **Natural** boundary condition

Find \( u \in H^1(\Omega) \) such that

\[
\int_{\Omega} \nabla v \cdot \nabla u \, dV = \int_{\Omega} v f \, dV \quad \forall v \in H^1(\Omega)
\]

PDE with Robin boundary condition

Var. form: **Natural** boundary condition + bdy. integral

Find \( u \in H^1(\Omega) \) such that

\[
\int_{\Omega} \nabla v \cdot \nabla u \, dV + \int_{\partial \Omega} \alpha vu \, dS = \int_{\Omega} v f \, dV \quad \forall v \in H^1(\Omega)
\]
FE approximation & implementation

FEM: variational form solved in space $V_h \subset H^1(\Omega)$ of continuous, piecewise polynomial functions on a mesh with $N$ nodes.

Expanding in a nodal basis:

$$u_h(x) = \sum_{i=1}^{N} u_i \phi_i(x) \quad \text{for } u_h \in V_h \subset H^1(\Omega)$$

Essential boundary conditions are enforced explicitly on $u_h$.

Standard approach for $u_h = 0$ on the boundary, remove index for nodes on boundaries $I_{\text{int}} \subset \{1, \ldots, N\}$

$$u_h(x) = \sum_{i \in I_{\text{int}}} u_i \phi_i(x) \quad \text{for } u_h \in V_{h,0} \subset H^1_0(\Omega)$$
FE approximation & implementation

In contrast to essential boundary conditions, the natural conditions coming from Neumann boundary condition are **invisible** in the variational form!

\[
\int_\Omega \nabla v_h \cdot \nabla u_h \, dV = \int_\Omega v_h f \, dV \quad \forall v_h \in V_h
\]

Suggests a fictitious domain approach!
The “material distribution” approach

\( K_n \): the \( n \)th element in a mesh with totally \( M \) elements. For Neumann boundary conditions, the variational form can be written

\[
\sum_{n=1}^{M} \int_{K_n} \nabla v_h \cdot \nabla u_h \, dV = \sum_{n=1}^{M} \int_{K_n} v_h f \, dV \quad \forall v_h \in V_h
\]

Let \( \Omega \subset \hat{\Omega} \). Define the **element material indicator**

\[
\rho = \begin{cases} 
1 & \text{if } K_n \subset \Omega, \\
0 & \text{otherwise (} K_n \subset \hat{\Omega} \setminus \Omega \)
\end{cases}
\]

and extend the variational form into \( \hat{\Omega} \), meshed with \( \hat{M} > M \) elements:

\[
\sum_{n=1}^{\hat{M}} \int_{K_n} \rho \nabla v_h \cdot \nabla u_h \, dV = \sum_{n=1}^{\hat{M}} \int_{K_n} \rho v_h f \, dV \quad \forall v_h \in V_h
\]

or, equivalently

\[
\int_{\hat{\Omega}} \rho \nabla v_h \cdot \nabla u_h \, dV = \int_{\hat{\Omega}} \rho v_h f \, dV \quad \forall v_h \in V_h
\]
The material distribution approach

Solution $u_h$ undefined in $\hat{\Omega} \setminus \Omega$; stiffness matrix becomes singular. Cure: use modified material indicator:

$$\rho = \begin{cases} 1 & \text{if } K_n \subset \Omega, \\ \epsilon & \text{otherwise (} K_n \subset \hat{\Omega} \setminus \Omega) \end{cases}$$

($\epsilon \ll 1$, say $\epsilon = 10^{-6}$)

- Fixed mesh: the geometry is now defined by the values of function $\rho$
- An image (pixel) based geometry representation
- Very fine mesh needed for accurate geometry representation
Material distribution optimization

- The element material indicator $\rho$ has often a natural physical interpretation: local heat conductivity, thickness in depth direction, density of material, etc.

- **Material distribution optimization**: use the values of $\rho$ as decision variables in optimization

- Material distribution optimization perhaps the premiere application of this particular fictitious domain approach!
Example 1 (linear elasticity)

- Half of the material is cut out to obtain a structure as stiff as possible
- A so-called **topology optimization problem**: how the body is connected (the number of holes) is not given a priori

The problem is to divide a **ground structure** ($\hat{\Omega}$) into a **material region** ($\Omega$) and a **non-material (hole) region** ($\omega = \hat{\Omega} \setminus \Omega$)
Example 2 (the variable thickness sheet)

- A cantilever beam (sv. konsolbalk) is clamped to a wall and vertically loaded at the other side.
- The beam consists of a thin sheet of material of variable thickness $0 \leq \rho \leq 1$.
- Find the stiffest beam subject to

$$\int_{\hat{\Omega}} \rho \, dV \leq \gamma \int_{\hat{\Omega}} dV$$

for a given $\gamma \in (0, 1)$.

Results for $\gamma = 0.4$
Material distribution optimization for elasticity

- First numerical demonstration by Bendsøe & Kikuchi (1988).
- Intensely developed since then
- Used for advanced component design, particularly in the car and aeronautical industries
- Three applications of topology optimization carried out on the Airbus A380 aircraft is estimated to have contributed to weight savings in the order of 1000 kg per aircraft
Example 3 (acoustical “labyrinth”)

Fill the inside of a funnel-shaped device in order to maximize the transmitted sound energy.
From Wadbro & Berggren (2006):

Optimized for frequencies 400, 410, …, 500 Hz

Optimized for frequencies 150, 160, …, 300 Hz
Material distribution optimization with FEM

Conceptually, all three examples use a similar strategy:

- The material indicator function $\rho$ is used as decision variables in the optimization algorithm.
- With a crude mesh, the pixel image representation of the geometry is noticeable:

  Design variable $\rho \in [0, 1]$: $\rho$ represents thickness in normal direction.
  Design variable $\rho \in \{0, 1\}$: $\rho$ represents absence/presence of material.
Material distribution optimization with FEM

- For the optimization, we introduce an **objective function** $J$, a numerical performance measure. E.g. the elastic stiffness (example 1 & 2), or the acoustic transmission properties (example 3)
- The objective function is extremized (maximized or minimized) under constraints, e.g. $0 \leq \rho \leq 1$
- We use **gradient-based** optimization method. Needs to calculate $\partial J / \partial \rho_i$, where $\rho_i$ is the design value in element $i$.
- For the example problems above, gradients are easy to obtain by post processing of the numerical solution
- Iterative procedure: guess $\rho$ in all elements, calculate solution, calculate derivates, update $\rho$, etc…
The acoustical optimization problem: details

Outline:

1. Acoustics modeling
2. Material modeling
3. The optimization problem
4. Some additional results
The wave and Helmholtz equations

The **acoustic pressure** (pressure fluctuations) satisfies the wave equation

\[
\frac{\partial^2 P}{\partial t^2} - c^2 \Delta P = 0
\]

We consider time-harmonic solutions \( P(x, y, t) = e^{i\omega t} p(x, y) \) at angular frequency \( \omega \). The complex-valued amplitude function \( p \) then satisfies

\[
e^{i\omega t} \left( -\omega^2 p - c^2 \Delta p \right) = 0,
\]

that is, the **Helmholtz equation**

\[
-k^2 p - \Delta p = 0,
\]

where \( k = \omega/c \), the **wave number**
Plane wave solutions

Functions $p(x, y) = e^{\pm ikx}$ satisfy the Helmholtz equation.

Plane wave traveling towards increasing $x$:

$$P(x, y, t) = e^{i(\omega t - kx)} = e^{i\omega t} e^{-ikx}$$

Plane wave traveling towards decreasing $x$:

$$P(x, y, t) = e^{i(\omega t + kx)} = e^{i\omega t} e^{ikx}$$

- Plane waves occur in straight narrow channels (acoustic wave guides)
- Assume now that we put a conical-shaped horn at the end of a wave guide
The acoustic horn

\[ P(x,y,t) = e^{i\omega t}(Ae^{-ikx} + Be^{ikx}) \]

- Parts of plane wave in the wave guide is reflected back, parts is transmitted to free space
- When size of horn \( \geq O(\text{wavelength}) \), the reflection properties will be sensitive to horn shape
  - **Loudspeaker:** want low reflections at all transmission frequencies
  - **Brass instrument:** want the waves to be reflected with zero phase shift at certain pre-specified frequencies to build up standing waves in the feeding wave guide
- The horn directs the sound towards the front of the horn
Input/Output perspective

Input

\[ P_{\text{in}}(x,y,t) = e^{i\omega t} A e^{-ikx} \]

Output

\[ P(x,y,t) = e^{i\omega t} B e^{ikx} \]

Inviscid case:

\[ |A|^2 = |B|^2 + C \int_{0}^{2\pi} |p_{\infty}(\theta)|^2 \, d\theta \]
Loudspeaker optimization objectives

- **Transmission efficiency**: Minimize $|R|^2$, where
  $$ R = \frac{B}{A} = \frac{p|\Gamma_{in} - A}{A} $$
  is the *reflection coefficient*. Equivalent to maximizing total exterior output $C \int_0^{2\pi} |p_\infty(\theta)|^2 \, d\theta$

- **Directivity**: The angular distribution of sound in terms of the *far-field pattern* $\theta \mapsto p_\infty(\theta)$
2D Helmholtz equation, planar symmetry
Symmetric up/down with respect to boundary $\Gamma_{\text{sym}}$
The infinite domain truncated at $\Gamma_{\text{out}}$, located at radius $R_{\Omega}$. Need artificial boundary condition to absorb outgoing waves
A plane wave source in waveguide, at $\Gamma_{\text{in}}$, imposing a right-going wave with amplitude $A$
All other boundary parts, $\Gamma_n$, are sound hard. Constitute boundaries to solid materials
Boundary conditions

Condition of symmetry and presence of sound-hard boundaries enforced by

\[ \frac{\partial p}{\partial n} = 0 \quad \text{at } \Gamma_{\text{sym}} \text{ and } \Gamma_{n} \]

No pressure gradients at walls ⇒ no flow of air through wall.

Only plane waves in wave guide: \( p(x, y) = A e^{-ikx} + B e^{ikx} \). If \( \Gamma_{\text{in}} \) is located at \( x = 0 \), condition

\[ ikp + \frac{\partial p}{\partial n} = 2iA \quad \text{at } \Gamma_{\text{in}}, \]

sets amplitude \( A \) for the right-going wave and absorbs the left-going wave
Artificial boundary condition

The so-called first-order Engquist–Majda radiation condition

$$\left(ik + \frac{1}{2R_\Omega}\right)p + \frac{\partial p}{\partial n} = 0 \quad \text{at } \Gamma_{\text{out}}$$

absorbs reasonably well outgoing waves that travel perpendicular to $\Gamma_{\text{out}}$. 

The boundary-value problem

\[ - k^2 p - \Delta p = 0 \quad \text{in } \Omega \quad (2a) \]

\[ \left( ik + \frac{1}{2R_\Omega} \right) p + \frac{\partial p}{\partial n} = 0 \quad \text{on } \Gamma_{\text{out}} \quad (2b) \]

\[ ikp + \frac{\partial p}{\partial n} = 2iA \quad \text{on } \Gamma_{\text{in}} \quad (2c) \]

\[ \frac{\partial p}{\partial n} = 0 \quad \text{on } \Gamma_n \quad (2d) \]
Variational form

Recall: for the FE discretization, need to write the equations in variational form:

1. Multiply the PDE with a test function $q$ and integrate over the computational domain $\Omega$

2. Integrate terms with second derivatives by parts, utilizing Green’s identity

$$\int_{\partial \Omega} q \frac{\partial p}{\partial n} \, d\Gamma = \int_{\Omega} \nabla q \cdot \nabla p \, d\Omega + \int_{\Omega} q \Delta p \, d\Omega$$

3. Substitute the boundary condition expressions to get rid of $\partial p/\partial n$ terms
Variational form

Multiply (2a) with $q$ and integrate:

$$- k^2 \int_\Omega qp \, d\Omega - \int_\Omega q\Delta p \, d\Omega = [\text{Green’s identity}]$$

$$= -k^2 \int_\Omega qp \, d\Omega - \int_{\partial \Omega} q \frac{\partial p}{\partial n} \, d\Gamma + \int_\Omega \nabla q \cdot \nabla p \, d\Omega = [\text{Boundary conditions}]$$

$$= -k^2 \int_\Omega qp \, d\Omega + \left( ik + \frac{1}{2R_\Omega} \right) \int_{\Gamma_{\text{out}}} qp \, d\Gamma + ik \int_{\Gamma_{\text{in}}} qp \, d\Gamma - 2i \int_{\Gamma_{\text{in}}} qA \, d\Gamma$$

$$+ \int_\Omega \nabla q \cdot \nabla p \, d\Omega = 0$$
Variational form

Rewriting the expression yields that the solution $p$ satisfies

$$\int_{\Omega} \nabla q \cdot \nabla p \, d\Omega - k^2 \int_{\Omega} qp \, d\Omega + i k \int_{\Gamma_{\text{out}} \cup \Gamma_{\text{in}}} qp \, d\Gamma + \frac{1}{2R_\Omega} \int_{\Gamma_{\text{out}}} qp \, d\Gamma = 2i \int_{\Gamma_{\text{in}}} qA \, d\Gamma$$

for all test functions $q$ with square-integrable derivatives.

- The boundary conditions on $\Gamma_{\text{in}}$ and $\Gamma_{\text{out}}$ enters as boundary integrals
- As before: the Neumann boundary conditions at sound-hard (and symmetry) boundaries do not enter in the variational form!
- In particular, the material regions inside the horn is noticed only through its absence from the integrals!
Material modeling

- Extend the domain to $\hat{\Omega} = \Omega \cup \Omega_m$, where $\Omega_m$ is the sound-hard material region inside the horn.

- Here the material indicator $\rho : \hat{\Omega} \to \mathbb{R}$ signifies air or sound-hard material.

  $$\rho(x) = \begin{cases} 
  1 & \text{if } x \in \Omega \text{ (air)} \\
  \varepsilon & \text{if } x \in \Omega_m \text{ (sound hard)}
  \end{cases}$$

- Then the variational form can be written

  $$\int_{\hat{\Omega}} \rho \nabla q \cdot \nabla p \, d\Omega - k^2 \int_{\hat{\Omega}} \rho q p \, d\Omega + ik \int_{\Gamma_{\text{out}}} q p \, d\Gamma + \frac{1}{2 R_\Omega} \int_{\Gamma_{\text{out}}} q p \, d\Gamma = 2i \int_{\Gamma_{\text{out}}} q A \, d\Gamma$$

The function $\rho$ constitutes the **design variables**: the decision variables in the optimization algorithm.
Manipulating the design variable

- Optimization using $\rho \in \{\varepsilon, 1\}$ numerically difficult.
- Relax the feasible set to the interval $\rho \in [\varepsilon, 1]$. Allows gradient-based algorithms.
- To force either $\rho \approx \varepsilon$ or $\rho \approx 1$, penalize the objective:

$$J_\gamma(\rho) = \gamma \int_{\hat{\Omega}} (\rho - \varepsilon)(1 - \rho) \, d\Omega + \left| p|_{\Gamma_{in}} - A \right|^2$$

$\gamma > 0$: penalty parameter.
- To avoid microstructures on the element level, define $\rho$ indirectly through a filter:

$$\rho(x) = \int_{\mathbb{R}^2} k_R(x - y) \hat{\rho}(y) \, dV$$

where integral kernel $k_R$ has support only in a radius $R$ around point $x$. 

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Relaxation, penalty, filtering, sharpening
Minimizing reflection at 400 Hz

(Wadbro & Berggren 2006)

No penalty: $\gamma = 0$; $10^{-3} \leq \rho \leq 1$
Relaxation, penalty, filtering, sharpening
Minimizing reflection at 400 Hz

(Wadbro & Berggren 2006)

No penalty: $\gamma = 0; 10^{-3} \leq \rho \leq 1$

Penalty: $0 = \gamma_0 < \gamma_1 < \gamma_2 < \ldots$. Mesh dependent microstructures appear
Relaxation, penalty, filtering, sharpening
Minimizing reflection at 400 Hz
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Penalty and filter $\Rightarrow$ mesh independence (note the gray areas of size $R$!)
Relaxation, penalty, filtering, sharpening

Minimizing reflection at 400 Hz

(Wadbro & Berggren 2006)

No penalty: $\gamma = 0; \quad 10^{-3} \leq \rho \leq 1$

Penalty: $0 = \gamma_0 < \gamma_1 < \gamma_2 < \ldots$. Mesh dependent microstructures appear

Penalty and filter $\Rightarrow$ mesh independence (note the gray areas of size $R$!)

Sharpening: removing the filter and continue the iterations
Example 3 revisited

Simultaneous optimization over $N_{\text{freq}}$ frequencies:

$$J_\gamma(\tilde{\rho}) = \gamma \int_{\hat{\Omega}} (K_R * \tilde{\rho} - \epsilon)(1 - K_R * \tilde{\rho}) \, d\Omega + \sum_{n=1}^{N_{\text{freq}}} |p_{\omega_n}|_{\Gamma_{\text{in}}} - A|^2$$

Optimized for frequencies 400, 410, …, 500 Hz

Optimized for frequencies 150, 160, …, 300 Hz
Example 4: Interior layout of a reactive muffler

- Cylindrical symmetry
- Perforated pipe possibly running from inlet to outlet
- Placement of sound-hard material in $\Omega^d$ subject to design
- Reactive muffler: opposite objective to the horn: **minimize** the transmission through the muffler!
- With Esubalewe Yedeg and Eddie Wadbro
The making of a Helmholtz resonator

Minimizing transmission at 349 Hz, no pipe

(a) \[ \gamma = 0 \]

(b) \[ \gamma = 1/2 \] with filter

(c) \[ \gamma = 500 \] with filter

(d) \[ \gamma = 500 \] dropping filter

(e) after 2nd post processing
Multifrequency transmission minimization

20 frequencies, 200–1050 Hz. Exponentially spaced

(a) without pipe

(b) with pipe

(c) Transmission loss

--- without pipe

--- with pipe
Example 5: Interior layout of a subwoofer

- Design variables:
  - $1 \times 1 \times 60$ cm$^3$ voxels
  - air/sound hard material

- Maximize radiated power, fixed input voltage

- Hybrid model:
  - 3D Helmholtz models around driver (FEM) and exterior (BEM)
  - 2D Helmholtz in box
  - Mechanical and electrical circuits for driver
Preliminary results
Work in progress!