Metamaterials-by-Design

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Outline

• The “System-by-Design” Paradigm
• System-by-Design as applied to Metamaterials and Metasurfaces
• Design Examples
• Conclusions and Future Works

System-by-Design

• System-by-Design represent one of the major paradigm in upcoming international funding calls (Horizon2020, ESA, EDA, NSF, EPSRC, NIH,...)
• Basic idea:
  Task-oriented design, definition, and integration of system components to achieve desired performance with the minimum costs, maximum scalability, and reconfigurability

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**System-by-Design: How?**

Design a system so that it exhibits desired properties (e.g., in terms of electromagnetic propagation)

**Integrated approach**

1. Homogenization Techniques
2. Fast EM Simulation Tools
3. Optimization Algorithms

**EAs Suitable**

**Optimization Environment**

**How?**

1. Homogenization Techniques
2. Fast EM Simulation Tools
3. Optimization Algorithms

**EAs Open Issues**

**EAs Advantages:**
- Global search
- Hill-climbing features (no local “minima” problem)
- No differentiability
- Straightforward introduction of a priori information (or constraints)
- Discrete / continuous space
- Intrinsically parallel computing
- Hybridization with deterministic procedures

**EAs Recipe:**

1. Homogenization Techniques
2. Fast EM Simulation Tools
3. Optimization Algorithms

**Optimization Theorem**

The Lunch is No-Free... ... what’s the cost?

Let \( F = \{ \Phi_i | i = 1, ..., l \} \) be a functional space of \( p \)-differentiable functions over \( D \subset \mathbb{R}^N \) with bounded derivatives

\[
\left| \frac{d^p}{dt^p} \Phi(f + tu) \right| < \frac{\epsilon}{k} \quad f \in D, \quad |u| = 1
\]

and \( A \) a black-box algorithm which guarantees to find

\[
f^* = \arg\min_{f \in F} \Phi(f), \quad \Phi(f^*) < \varepsilon, \quad f^* \text{ being the global minimum.}
\]

Thus, there exist a function \( \Phi_A \), such that \( A \) will run for

\[
K \geq \left( \frac{P}{\varepsilon} \right)^p
\]

where \( P \) is the required iterations, \( K \) is the number of unknowns, \( \varepsilon \) is the confidence level, and \( \text{Confidence level} \)

\[\text{Confidence level} \geq \left( \frac{P}{\varepsilon} \right)^p\]

\[\text{Exponential growing with the Number of Unknowns}\]

**Optimization Costs**

Required number of cost function evaluations, weighted by the computational burden of a single evaluation, such that

\[ f : \Phi(f) - \Phi(f^*) < \varepsilon \]

**Cost** = \( K \times P \times \Delta t \)

- **K**: number of algorithm iterations
- **P**: number of agents per iteration
- **\( \Delta t \)**: time requested for a single functional evaluation
- **N**: number of unknown parameters

**Convergence rate**

**Computational load**

**How to mitigate?**

**How to obtain?**

---

**Material Homogenization**

**Objective**

Describe inhomogeneous medium in terms of homogeneous “equivalent” electromagnetic properties

**Input**

Permittivity/Permeability Tensors

**Output**

**Example:** Split Ring Resonator

**Example:** Graphene with electric/magnetic bias

**Example:** Fishnet structure
System-by-Design: How?

Design a material so that the device exhibits desired properties (e.g., in terms of electromagnetic propagation)

Integrated approach

1. Homogenization Techniques
2. Fast EM Simulation Tools
3. Optimization Algorithms

Objectives, Constraints

Traditional materials
Metamaterials
Graphene

How to?

Enabling Optimization through reduction of $\Delta t$

Cost $= K \times P \times \Delta t$

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Design a system so that it exhibits desired properties (e.g., in terms of electromagnetic propagation)

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Fast Electromagnetic Simulation

Objective

Compute electromagnetic propagation (e.g., field within structure) in a fast and accurate way

Permittivity/Permeability Tensors

Input

2$\pi f$ wave vector

Output

Field within device

How?

Full wave simulators (e.g., CST, HFSS, COMSOL, ...)
Application-specific numerical methods (e.g., modal analysis, grating lobe series, ...) [1][2]

Efficient, fast, valid for specific geometries

Predictors (LBE)

Fast Electromagnetic Simulation

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Optimization Costs – Remedies

(3) Reduction of $\Delta t$

Cost $= K \times P \times \Delta t$

Idea

Predict the values of $\Phi(f)$ or perform an approximate computation of $\Phi(f)$

Evaluation of $\Phi(f)$ can be very expensive (e.g., full-wave simulation of antennas, microwave components, or imaging systems)

Approach

Use of interpolation techniques or learning-by-example strategies

**Efficient evaluation of Φ(f)**

- **Open Issue**
  - Computationally-efficient methods

**Fast Direct Solvers**
- (small-medium problems)
  - customized solvers with limited range of application
  - no “training” needed
  - can be applied for small-medium problems

**Approximate Φ(f) computation**
- (large problems)
  - Φ(f) is predicted
  - need of a “training” phase
  - can be applied whatever the problem size

**What approaches?**

**Approximate Φ(f) computation (large problems)**

- Simple and efficient strategies
- Requires to a-priori know/estimate functional dependency (e.g.: polynomial, exponential, etc.)
- Low generalization capabilities
- Examples: linear interpolation, polynomial interpolation, spline interpolation

**Learning-by-Example Methods**
- Numerically efficient
- No a-priori knowledge required
- Good generalization capabilities
- Examples: support vector machines (SVM), artificial neural networks (ANN), gaussian processes (GP), Kriging

**How do LBE methods work?**

**Learning-By-Example Methods are formulated as two-step approaches**

**Training**

\[ \begin{align*}
& f \quad \text{known} \quad \text{LBE Algorithm} \quad \Phi(f) \quad \text{known} \\
& \text{Objective} \\
& \text{Give the LBE method a set of known input-output relations ([f, Φ(f)] computed pairs) to train it}
\end{align*} \]

**Testing**

\[ \begin{align*}
& f \quad \text{known} \quad \text{LBE Algorithm} \quad \Phi(f) \quad \text{unknown} \\
& \text{Objective} \\
& \text{Give the LBE method a set of inputs [f] and let it predict the output [Φ(f)]}
\end{align*} \]
**Smart Sampling Strategies**

**Problem**
How to efficiently sample a large dimensional space without considering all combinations?

**Aim**
- Reduced number of samples (experiments)
- Good coverage of the input space
- Good representation of parameters effect on output
- Investigation of interactions between input variables

**Approaches**
One-shot/adaptive techniques

**One-shot Sampling**
- Simple and efficient strategies
- Uniform or almost uniform sampling of the dimensional space
- Large number of samples
- Examples: grid (uniform) sampling, random sampling, orthogonal arrays, latin hypercube sampling (LHS)

**Iterative Adaptive Sampling**
- Computationally expensive
- Non-uniform/adaptive sampling of the solution space
- Reduced number of samples
- Examples: LOLA-Voronoi, MSE-based sampling, Expected Improvement for Global Fit (EIGF)

**Optimization Techniques: Resume**

**Problem**
How to minimize or maximize a function \( \Phi(f) \)?

**Approach**
Evolutionary Algorithms (GA, PSO, ACO, DE, ...)

- Evaluate \( \Phi(f) \)?
- Fast Direct Solvers (small-medium problems)
- Approximate \( \Phi(f) \) computation (large problems)
- LBE Methods
- Approximate \( \Phi(f) \)?
- Build training set?
- Interpolation
- Huge databases
- Smart Sampling

**System-by-Design: How?**

Design a material so that the device exhibits desired properties (e.g., in terms of electromagnetic propagation)

**How to?**
Integrated approach

1. Homogenization Techniques
2. Fast EM Simulation Tools
3. Optimization Algorithms

Objectives, Constraints
3 Optimization Algorithms

Aim
Derive optimal material features (unit cell structure) such that the overall EM objectives are met.

Desired EM performance

Geometrical/Electrical constraints

How?
Evolutionary optimization loop (integrated with material homogenization and fast EM solver)

Optimized Material

Optimization Algorithms: Approach

Input

Material configuration

Optimization Loop

Evolutionary Optimization Algorithm

Fast EM Simulation

Application objectives and constraints

Material parameters

EM performance (e.g., radiated field)

Homogenization Technique

Chosen material features

(e.g., fishnet structure, graphene, split ring resonators)

What paradigms?

3 Optimization Paradigms

“Which Algorithm is More Suitable for the Solution of an Optimization Problem?”

GAs
PSO
DE
ACO
MA
BF

“The Lunch is No-Free” [*]

3 EAs Recipe

Algorithm
GAs
PSO
DE
ACO
MA
BF

Problem
Unknown
Dimension Space

Continuous
Discrete
Low
High

Application?

**System-by-Design as applied to...**

**Metamaterials**
Artificial materials with positive/negative permittivity and permeability

Example: Microwave cloak based on square split rings

Example: Artificial chiral material at optical frequencies

**Metasurfaces**
Two-dimensional low-loss “metamaterial-like” structures

Example: Negative-permittivity surface

Example: Negative-permeability surface at THz

**Design Idea**
Unit cell (to be optimized) repeated over regular lattice to synthesize the metasurface with desired properties (defined by cost function)

**Basic Idea**

**Examples**

**Cost function?**
Depends on application

Terms in cost function?
- Polarization of transmitted wave
- Reflected power by absorber
- Far field pattern of antenna covered by radome
- Reflected/transmitted power vs. frequency
- Surface impedance mismatch vs. steering angle
- Antenna power pattern

**Examples?**

**System-By-Design: Application**

**Aim**
Task-oriented design of metamaterials/metasurfaces

No general purpose solution, design possible only for specific geometries allowing fast EM simulation

**Material-by-Design**

**WAIM**
specific geometries?

- Polarizer
- Absorbers
- Radome

**WAIM Design**
Wide Angle Impedance Matching

Artificial layer placed in front of phased array so that its input impedance matching is good for all steering angles and operative frequencies

**How to simulate?**
**System-by-Design Example: WAIM**

**Aim**
Minimize power reflection due to impedance mismatch by optimizing WAIM properties.

**Application objectives and constraints**

**Evolutionary Optimization Algorithm**

**Fast EM Simulation**

**Material configuration**

**System-by-Design**

**Output**

**Input**

**Problem definition**

\[
\left( \varepsilon_d, \mu_d, d \right)^{\text{opt}} = \arg \min \left[ \Phi \left( \varepsilon_d, \mu_d, d \right) \right]
\]

where \( \Phi \left( \varepsilon_d, \mu_d, d \right) \) depends on

**Degrees of Freedom**

- WAIM thickness
- \( \varepsilon_d, \mu_d, d \)
- Real-Valued Unknowns
- PSO Algorithm

**System-by-Design Example: WAIM**

**Objective**
Compute electromagnetic propagation (e.g., field within structure) in a fast and accurate way.

**WAIM Simulation**

**Permittivity/Permeability Tensors**

**Field within device**

**Fast solvers**

**Predictors (LBE)**

**Analytic methods**

**MODE MATCHING**

**System-by-Design**

**WAIM Optimizer Selection**

**Problem definition**

\[
\left( \varepsilon_d, \mu_d, d \right)^{\text{opt}} = \arg \min \left[ \Phi \left( \varepsilon_d, \mu_d, d \right) \right]
\]

where \( \Phi \left( \varepsilon_d, \mu_d, d \right) \) depends on

**Degrees of Freedom**

- WAIM thickness
- \( \varepsilon_d, \mu_d, d \)
- Real-Valued Unknowns
- PSO Algorithm
Numerical Validation
Circular Waveguides, Triangular Lattice

Array Parameters
- Lattice: Triangular
- Lattice size [mm]:
  - $s_y = 11.36 \times 10^{-3}$
  - $s_x = 9.86 \times 10^{-3}$

Antenna Parameters
- Type: Circular Waveguide
- Radius: 3.93 [mm]
- $e_{x,y} = 2.54$
- Fundamental Mode: TE11

Simulation Parameters
- Frequency: 15.25 [GHz]
- Feed admittance: $Y_{TE_{11}} = 1.663 \times 10^{-3}$ [Ω]

Mode Matching Parameters
- Number of guided wave modes: 6
- Number of Floquet terms: 81

Optimization Parameters
- Optimization ranges:
  - $e_{x,y,z}$
- PSO Parameters:
  - Population size: 7
  - Max iteration number: 500
  - Social acceleration: $C_s = 2.0$
  - Cognitive acceleration: $C_p = 2.0$
  - Inertial weight: $w = 0.4$

Optimized WAIM Parameters
- $d = 1.32 \times 10^{-3}$ [mm]
- $Y_{TE_{11}} = 4.99$
- $e_{x,y,z}$
- $\mu = 3.73$

Further constraints on fabrication yield thicker WAIM

Easier fabrication

Increased thickness $= 2.2 \times 10^{-3}$

Optimization Time: $\geq 4$ h
[3500 functional evaluations]

Numerical Validation
Circular Waveguides, Triangular Lattice

Synthesis of Wideband WAIM
Square Waveguides, Triangular Lattice

Array Parameters
- Lattice: Triangular
- Lattice size [mm]:
  - $s_y = 19.66 \times 10^{-3}$
  - $s_x = 9.83 \times 10^{-3}$

Antenna Parameters
- Type: Square Waveguide
- Side: 7.04 [mm]
- $e_{x,y} = 2.54$
- Fundamental Mode: TE10

Optimization Parameters
- Optimization ranges:
  - $e_{x,y,z}$
- PSO Parameters:
  - Max Iteration Number: 2000
  - PSO Population: 12

Optimized WAIM Parameters
- $d = 4.35 \times 10^{-2}$ [mm]
- $Y_{TE_{10}} = 14.5 – 15.5$ [GHz]
- Feed admittance: $Y_{TE_{10}} = f = 14.5 – 1.64 \times 10^{3} \times [1/\Omega]$
- $f = 15.5 – 2.14 \times 10^{3} \times [1/\Omega]$

Optimization Time: $\geq 4$ h
[3500 functional evaluations]

Synthesis of Wideband WAIM
Square Waveguides, Triangular Lattice

Layer Parameters
- Uniaxial Material
- Single Layer: N=1

Working Frequencies
- Frequency Band: 14.5 – 15.5 [GHz]
- Feed admittance: $Y_{TE_{10}} = f = 14.5 – 1.64 \times 10^{3} \times [1/\Omega]$
- $f = 15.5 – 2.14 \times 10^{3} \times [1/\Omega]$

Optimization Parameters
- Optimization ranges:
  - $e_{x,y,z}$
- PSO Parameters:
  - Social acceleration: $C_s = 2.0$
  - Cognitive acceleration: $C_p = 2.0$
  - Inertial weight: $w = 0.4$

Mode Matching Parameters
- Number of guided wave modes: 6
- Number of Floquet terms: 169

Further constraints on fabrication yield thicker WAIM

Easier fabrication

Increased thickness $= 2.2 \times 10^{-3}$

Optimization Time: $\geq 4$ h
[3500 functional evaluations]
**Synthesis of Wideband WAIM**

Optimized WAIM Parameters

\[ \begin{bmatrix} 2.07 & 0 \\ 0 & 2.07 \\ 0 & 0 \end{bmatrix}, \quad \phi = \frac{\pi}{4} \]

\[ d = 3.22 \text{ mm}, \quad \epsilon = \mu = 1 \]

**Transmission Coefficient**

\[ |\Gamma(\theta, \phi)|^2 \]

\[ f = 14.5 \text{ [GHz]} \]

**Good Matching in the whole frequency range!**

\[ f = 15.0 \text{ [GHz]} \]

\[ f = 15.5 \text{ [GHz]} \]

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**Next steps? Isoflux Metasurface Antennas**

Isoflux Pattern:

- Power received at ground is constant
- Antenna based on a metasurface composed by a dense texture of sub-wavelength (<\lambda>/10) metal patches on a grounded dielectric slab, excited by a surface wave generated by a coplanar feeder, aimed at exhibiting **isoflux pattern**

**Definition**

**Antenna based on a metasurface composed by a dense texture of sub-wavelength (<\lambda>/10) metal patches on a grounded dielectric slab, excited by a surface wave generated by a coplanar feeder, aimed at exhibiting isoflux pattern**

**How to design?**

Circularly-polarized feed

Metasurface made of small metallic patches with different size/orientation

**Isoflux Pattern**


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**PSO-Based Metasurface Optimization**

**Optimization Loop**

PSO-Based Evolutionary Optimization

\[ (p, \phi, \omega) \]

(trial solutions)

**Surface Impedance Homogenization**

Multilayer adaptive integral method (MLayAIM)

Surface impedance properties

**Surface Impedance**

\[ Z_{\text{surf}} \]

**EM performance (radiated field)**

**Metasurface parameters**

**Surface Impedance**

- Metasurface parameters
- Surface impedance properties
- Multilayer adaptive integral method (MLayAIM)
Conclusions

• The “System-by-Design” Paradigm
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