# Comsol Multiphysics Simulation Integrated into Genetic Optimization

INNOVATION MAKERS

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ENERGY, INDUSTRY & LIFE SCIENCES

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# OUTLINE

- Context & Objectives
- Thermoelectric Micro-Generators
- Genetic Algorithm
- Optimization Tool
- Results
- Conclusion

# CONTEXT & OBJECTIVES

## CONTEXT

industrial research program focused on the development of **thermoelectric micro-generators** (μTEGs) based on **innovative materials**

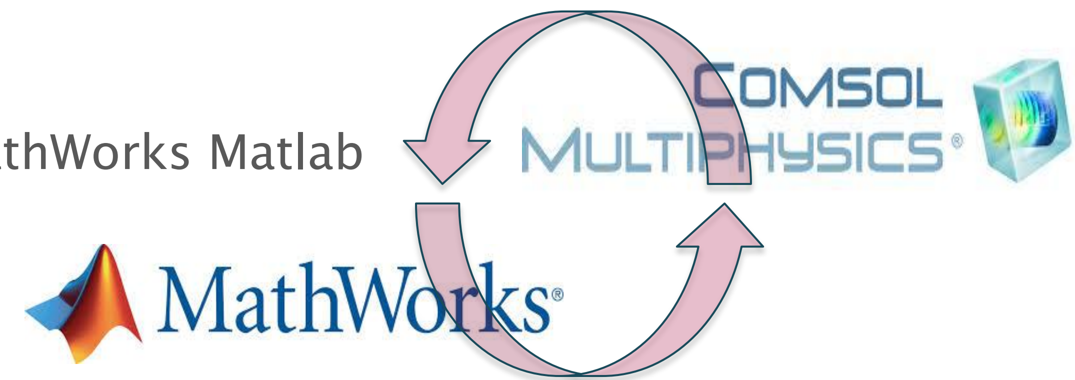
## GOAL

*innovative tool of modeling, simulation and optimization*

- ✓ **system performances improvement**
- ✓ **huge numbers of parameters and constraints**
- ✓ **wide range of applicability**

## APPROACH

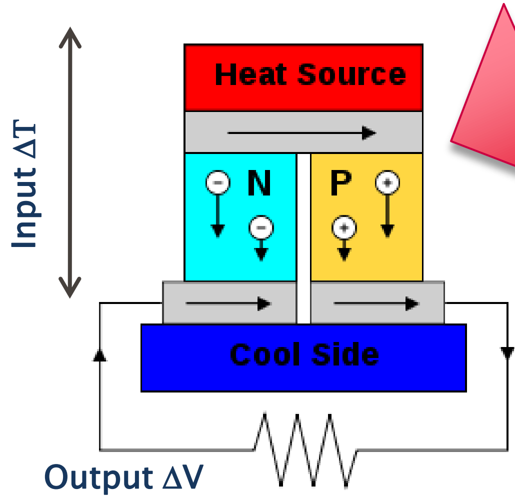
**interaction** between
Comsol Multiphysics and MathWorks Matlab



## DEFINITION

A thermoelectric micro-generator (μTEG) is a solid state device able to generate an electric potential when it is exposed to a temperature gradient due to the thermoelectric **Seebeck effect**

Thermoelectic generator scheme




**THERMOELECTRIC FIGURE OF MERIT**

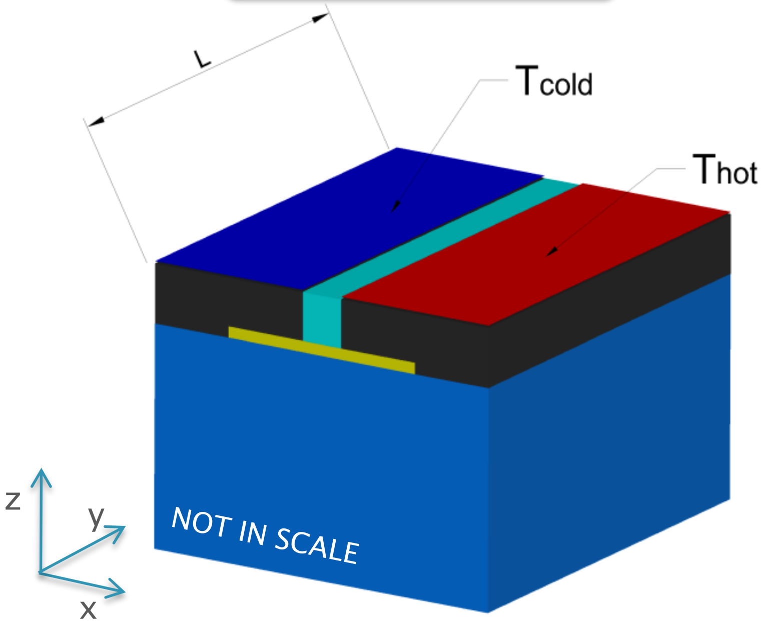
$$ZT = \frac{\alpha^2 \sigma}{k} T$$

α: Seebeck coefficient
σ: Electric conductivity
k: Thermal conductivity
T: Absolute temperature

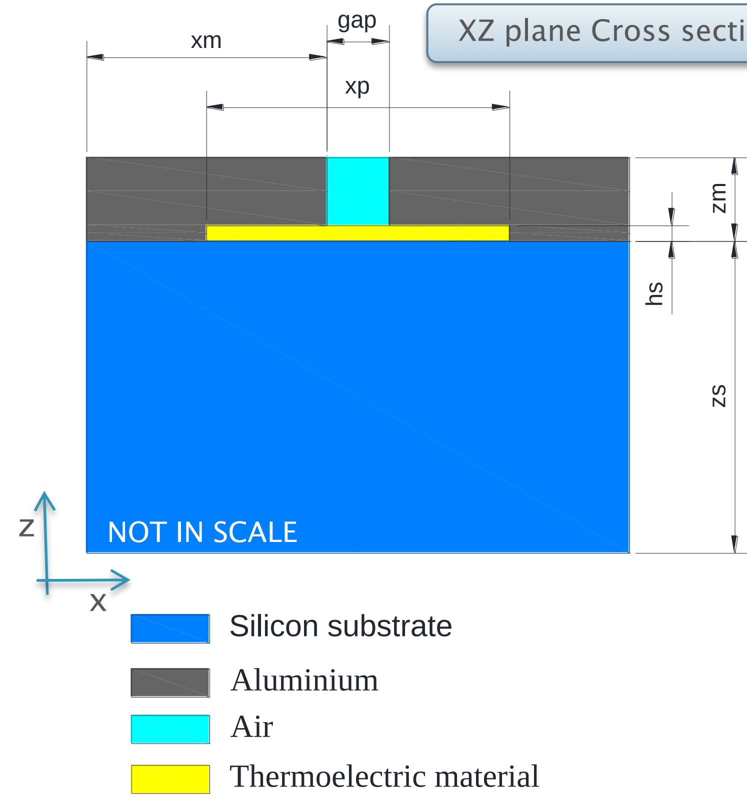
The possibility of using μTEGs to convert waste heat into electricity has recently regained interest as a consequence of the discovery of high ZT values in a certain range of materials, but in order to fabricate an **high efficiency μTEG**, it is necessary to design the **optimal geometry** of the μTEG's element!

# THERMOELECTRIC MICRO-GENERATOR – Geometry

Single TE element




XZ plane Cross section




Heat exchange surfaces:

T hot side = 493.15K

T cold side = 293.15K

Electric exchange surfaces:

Cold side: Potential ground

Hot side: Variable potential

| Variable | PROJECT VALUE |
|---|---|
| **xm** | 55 μm |
| **xp** | 7 μm |
| **gap** | 4 μm |
| **zm** | 6 μm |

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The main physical quantities are

- heat flux ( Q )
- electric current flux ( J )

$$\begin{cases} Q = \alpha T J - k \nabla T \\ J = \sigma E - \sigma \alpha \nabla T \end{cases}$$

Governing equation for thermoelectric effect are:

- Heat energy conservation
- Electric current balance

$$\nabla \cdot Q = J \cdot E$$

$$\nabla \cdot J = 0$$

Stationary case

$$\nabla \cdot [\alpha T(-\sigma \nabla V - \sigma \alpha \nabla T) - k \nabla T] = (-\sigma \nabla V - \sigma \alpha \nabla T) \cdot (-\nabla V)$$

$$\nabla \cdot (-\sigma \nabla V - \sigma \alpha \nabla T) = 0$$

COMSOL Physic Interface

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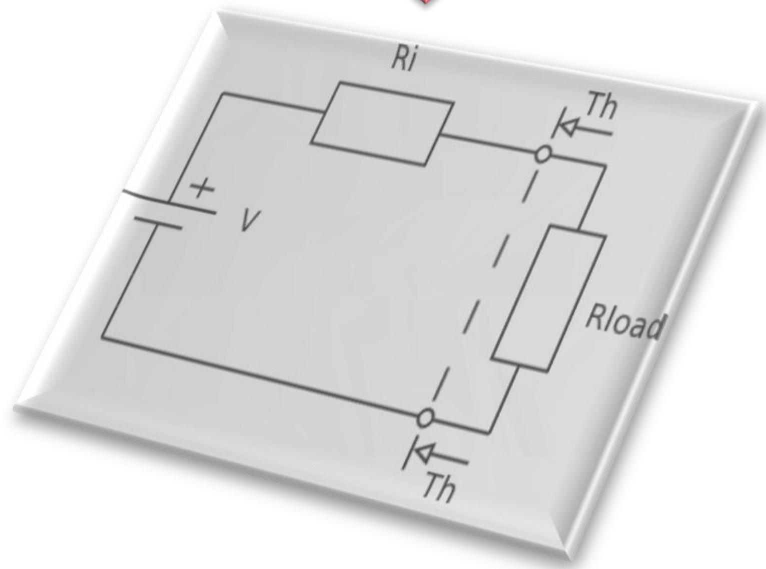
The single TE element can be schematized with an equivalent electric circuit.




## Calculation method

1° ru
Open Circu
$V_{oc}$

2
Short Ci it:
$I_{sc}$

**Post processing electric power evaluation**

$$P_{load} = \frac{V^2}{4{R_i}^2} = \frac{V_{oc} I_{sc}}{4}$$

Max power transfert

V: Seebeck generated voltage
$R_i$: Internal resistance of the TE generator
$R_{load}$: Load resistance

## OPTIMIZATION PROBLEM FORMULATION

**max** f(**x**) *objective function*

such that:

c(**x**) $\leq$ 0 *non– linear constraints*

*A* • ***x*** $\leq$ **b** *linear constraints*

***l*** $\leq$ ***x*** $\leq$ ***u*** *lower and upper bounds*

FIRST CHOICE → OBJECTIVE FUNCTION

**Electric Power Density = Electric Power/Area (Watt/cm$^2$)**

*In manufacturing processes*

- ✓ *maximize the electrical power*
- ✓ *minimize the area in order to reduce the probability of defect occurrence at wafer level*

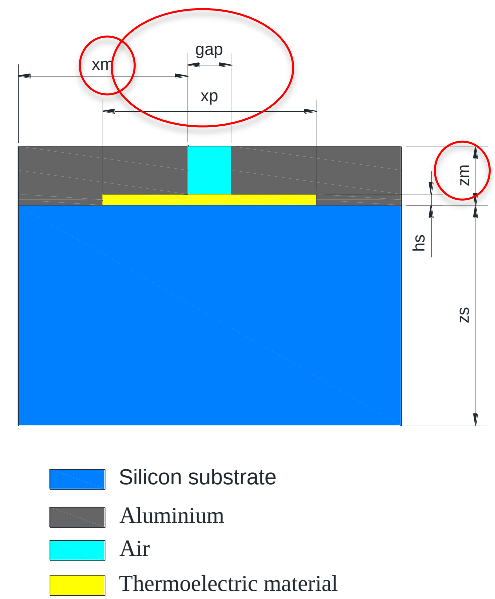
# GENETIC ALGORITHM – Problem Design (2)

## SECOND CHOICE → VARIABLES TO OPTIMIZE

**Upper & Lower Bound Definition**

| VARIABLES TO OPTIMIZE | | |
|---|---|---|
| NAME | LOWER BOUND | UPPER BOUND |
| xm | 10 µm | 60 µm |
| xp | 6 µm | 10 µm |
| gap | 4 µm | 5 µm |
| zm | 1 µm | 6 µm |

*Given by specialists*




## THIRD CHOICE → CONSTRAINTS DEFINITION

**Linear Constraint**

$$xp - gap > 2\mu m$$

*Technical constraint: lithography resolution*

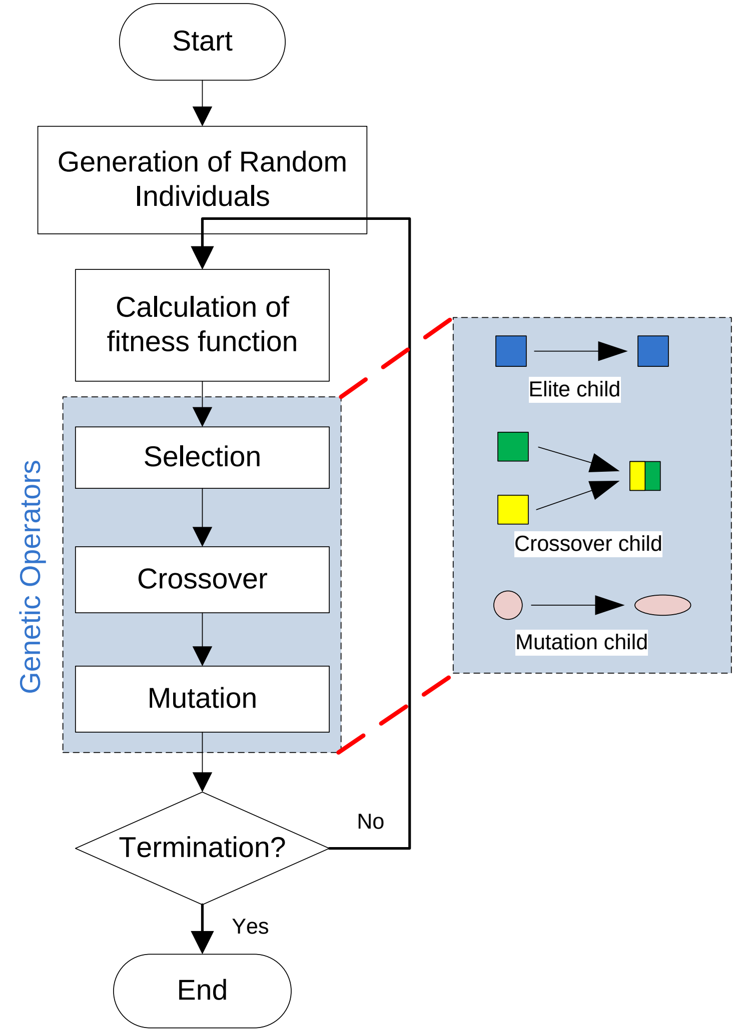
*GENETIC ALGORITHM: heuristic search that simulates the process of natural selection*

*The algorithm starts by creating a random initial feasible population; then it creates a sequence of new populations.*

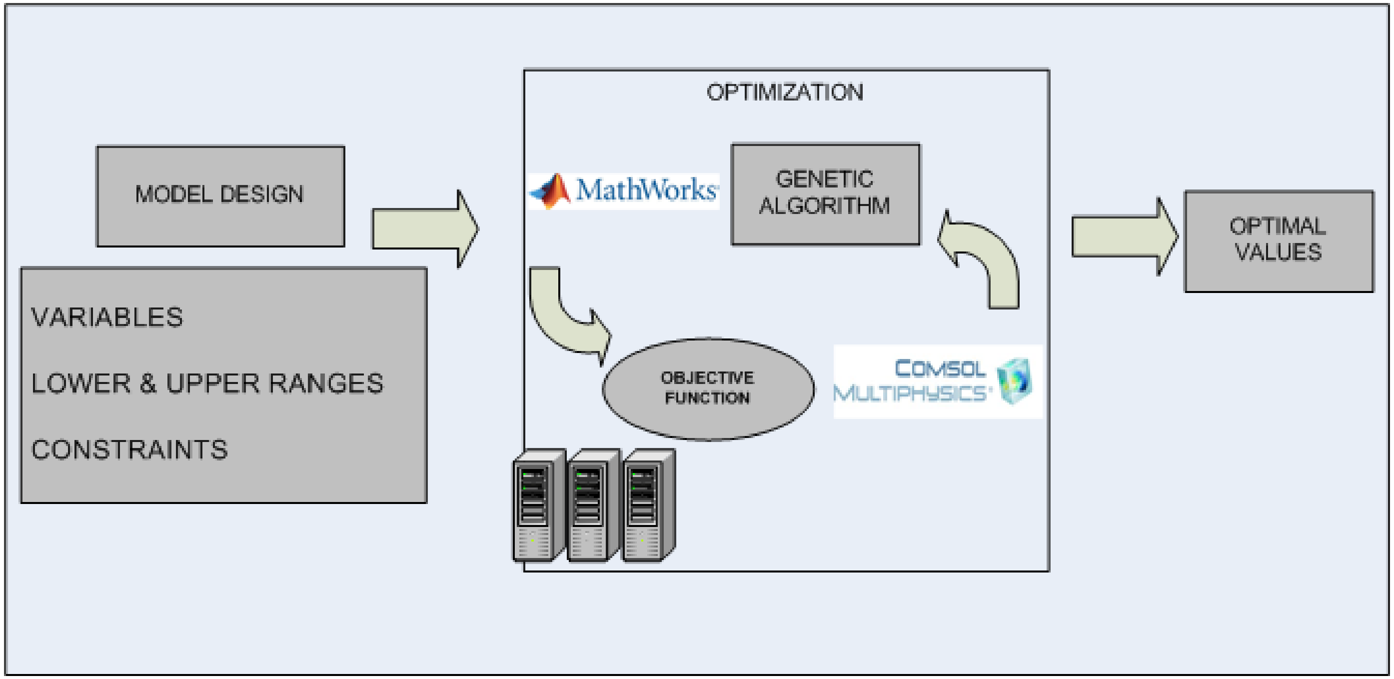
*At each step:*

- *It scores each individual of the current population by computing its fitness value*
- *It selects members, called parents, based on their fitness, in order to create the next population.*
- *It creates the new population from parents by means of selection, crossover and mutation*

*It stops when stopping criteria is met: average cumulative change over generations*



- Genetic Algorithm is implemented in MathWorks MatLab
- Electrical Power Density is the fitness function and its evaluation is performed by Comsol Multiphysics




At each generation, for each individual processed by genetic algorithm, MatLab sets new values into Comsol model's parameters and invokes Comsol simulations to evaluate fitness function

# NUMERICAL RESULTS (1)

Genetic Algorithm finds optimal values for each variable:

| Variable | PROJECT VALUE | OPTIMIZED VALUE |
|---|---|---|
| xm | 55 µm | 10 µm |
| xp | 7 µm | 7.36 µm |
| gap | 4 µm | 4 µm |
| zm | 6 µm | 2.12 µm |

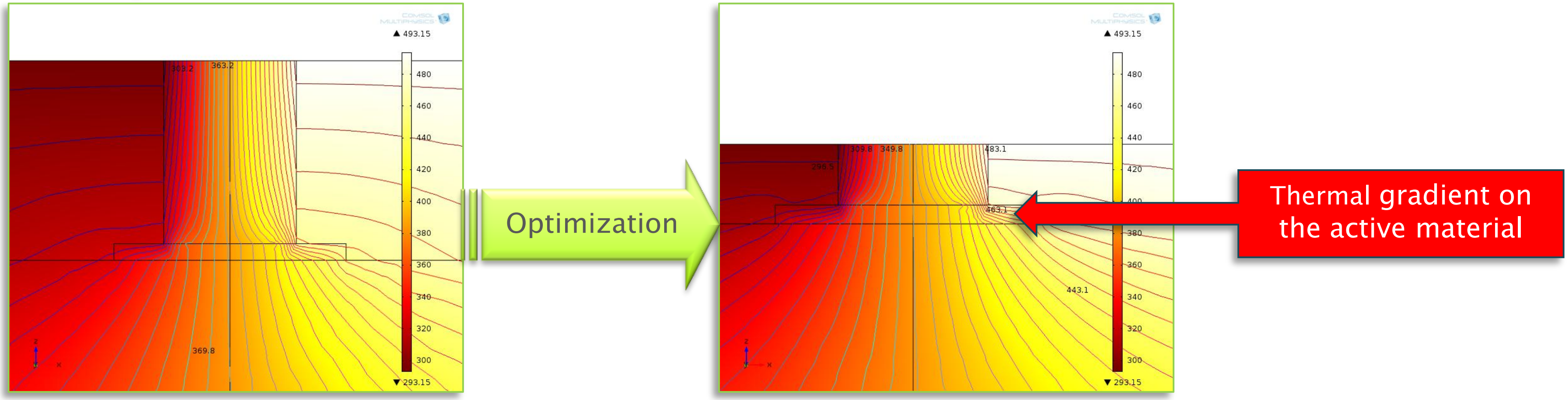
Optimization

Optimal values maximize electrical power density :

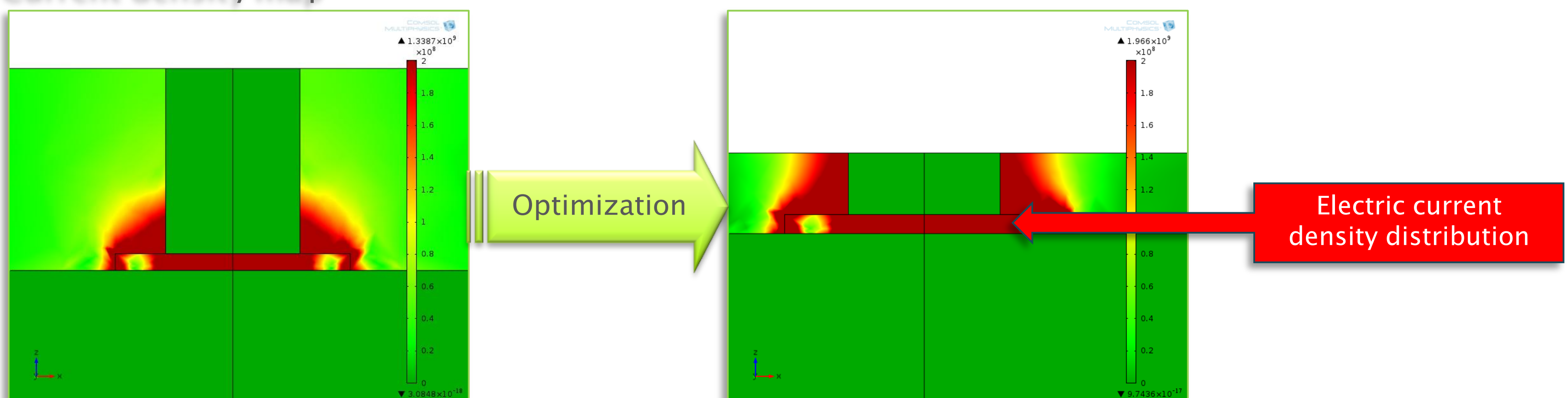
| FEATURE | PROJECT VALUE | OPTIMIZED VALUE |
|---|---|---|
| Horizontal area (S) | 2280 $\mu m^2$ | 480 $\mu m^2$ |
| Electric Potential (V) | 57.80 mV | 69.92 mV |
| Electrical Current (I) | 5.75 mA | 7.10 mA |
| Heat flux | 435.18 mW | 274.33 mW |
| Electric Power generated (Pload) | 0.08 mW | 0.12 mW |
| Electric Power Density (Pd) | 3.64 $W/cm^2$ | 25.86 $W/cm^2$ |

# RESULTS (2)

## Heat map




## Current density map



# CONCLUSION

- This work aims at demonstrating the power of interaction of multi-physics simulation with the optimization approach of genetic algorithms

- Numerical results must be considered demonstrative

- The tool greatly improves μTEG's performances

- More generally, this tool can be a precious contribution to device designers, especially when device models have many variables to take in account and many complex geometrical or technical constraints.

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