Deep Neural Network Surrogate Modeling for the Optimal Placement of Highly Conductive Capsules in Heat Transfer Systems

Master 2 or 5th-Year Engineering Internship

Expected starting date: as soon as possible

1 Context

Efficient heat transfer is a central challenge in many physical and engineering systems. In many situations, heat is initially concentrated in a limited region, and the objective is to distribute or extract it as efficiently as possible. From a physical point of view, this can be achieved either by allowing the system to evolve naturally toward thermal equilibrium, or by increasing the effective thermal conductivity of selected regions of the medium.

In this project, we consider the introduction of highly conductive inclusions, referred to as "capsules", into the system. These capsules locally enhance heat diffusion and may significantly accelerate thermal exchange (Bergman et al., 2011). A natural and important question then arises:

Where should these highly conductive capsules be placed in order to maximize heat extraction?

A first intuitive strategy would be to place the capsules close to the heat exchanger, since this is the region where heat is extracted. However, rigorously proving and optimizing such a strategy requires a precise characterization of the relationship between capsule position and the resulting heat flux. Directly evaluating this relationship for many possible capsule configurations using numerical PDE solvers can be computationally expensive.

The goal of this internship is therefore to develop a deep learning-based surrogate model capable of rapidly predicting the heat flux generated by a given capsule placement. Such a surrogate model would make it possible to perform fast optimization of the capsule location without repeatedly solving the full PDE problem (Karniadakis et al., 2021).

2 Mathematical Modeling

The physical system is modeled using the heat equation. As a first step, we consider a one-dimensional reservoir represented by the domain $\Omega = [-1, 1]$. A heat exchanger is located at one boundary, for instance at $x = -1$. A highly conductive capsule of width 2ε is placed at position α, defining the capsule region $C = [\alpha - \varepsilon, \alpha + \varepsilon]$. The thermal conductivity is assumed to be significantly larger inside the capsule than in the surrounding medium. The governing equations are therefore defined piecewise as follows:

- **Standard region $\Omega \backslash C$:** outside the capsule, the temperature $u(t, x)$ satisfies the standard heat equation:

$$\partial_t u - \partial_x^2 u = 0.$$

- **Capsule region C:** inside the capsule, the conductivity is multiplied by a large factor a, with $a \gg 1$, leading to:

$$\partial_t u - a\,\partial_x^2 u = 0.$$

The main quantity of interest is the heat flux extracted at the boundary by the heat exchanger, defined by

$$\mathrm{Flux}(\alpha) = -\partial_x u(-1).$$

The objective is to determine the optimal capsule location α^* that maximizes this extracted heat flux:

$$\alpha^* \in \arg\max_{\alpha} \mathrm{Flux}(\alpha).$$

3 Scientific Objectives and Expected Outcomes

1. Analytical Study of the Stationary Problem The first part of the internship will focus on the stationary case. By setting $\partial_t u = 0$, the problem reduces to a one-dimensional piecewise ordinary differential equation. The candidate will derive the analytical solution by hand, including the appropriate interface and boundary conditions. This will provide an explicit or semi-explicit characterization of the mapping $\alpha \mapsto \text{Flux}(\alpha)$. This analytical solution will serve as a reference solution and as a ground truth for the numerical and machine learning components of the project.

2. Numerical Data Generation Based on the analytical study, the candidate will implement a one-dimensional numerical solver, using finite differences or finite elements, to compute the heat flux for a broad range of capsule locations α. This step will produce a reliable dataset of input-output pairs $(\alpha, \text{Flux}(\alpha))$, which will be used to train and validate the surrogate models.

3. Neural Network Surrogate Modeling The candidate will then develop neural network-based surrogate models using PyTorch. The main tasks will include:

- Designing and training a feedforward neural network, such as a multilayer perceptron, to approximate the mapping
$$\mathcal{F} : \alpha \mapsto \text{Flux}(\alpha).$$
- Investigating Physics-Informed Neural Networks by incorporating the PDE structure, boundary conditions, and interface conditions directly into the loss function (Raissi et al., 2019).
- Assessing the predictive accuracy, robustness, and computational efficiency of the trained models by comparison with the analytical and numerical reference solutions.

4. Optimization and Possible Extensions Once a reliable surrogate model has been obtained, it will be used to perform rapid optimization of the capsule position. The objective will be to identify the optimal location α^* maximizing the extracted boundary flux. Depending on progress, possible extensions may include:

- the transient heat equation;
- multiple capsules;
- higher-dimensional geometries;
- more general conductivity distributions.

Expected Outcomes

At the end of the internship, the expected outcomes are:

- a rigorous analytical derivation of the one-dimensional stationary capsule problem;
- a validated numerical solver for generating reference data;
- a high-accuracy PyTorch surrogate model capable of predicting the boundary heat flux in real time;
- an optimization procedure for identifying the best capsule placement;
- scientific insight into whether placing highly conductive capsules near the heat exchanger is indeed optimal.

Required Skills

- Strong background in applied mathematics, numerical analysis, or scientific computing.
- Knowledge of partial differential equations, especially diffusion or heat equations.
- Basic knowledge of machine learning and neural networks.
- Programming experience in Python.
- Experience with PyTorch would be appreciated.
- Familiarity with finite difference or finite element methods would be an advantage.

Application Procedure

The internship will take place within the LMAC laboratory at the Université de Technologie de Compiègne, France. The internship will be jointly supervised by Faker Ben Belgacem and Mokhtar Z. Alaya, LMAC – UTC. Interested candidates should submit a motivation letter and a CV in PDF format to: `faker.ben-belgacem@utc.fr` and `alayaelm@utc.fr`.

Duration and Starting Date

The internship is expected to last approximately six months. The preferred starting date is as soon as possible. Due to funding constraints, the internship must end no later than December 2026.

References

Bergman, T. L., A. S. Lavine, F. P. Incropera, and D. P. DeWitt (2011). *Fundamentals of Heat and Mass Transfer* (7th ed.). John Wiley & Sons.

Karniadakis, G. E., I. G. Kevrekidis, L. Lu, P. Perdikaris, S. Wang, and L. Yang (2021). Physics-informed machine learning. *Nature Reviews Physics 3*(6), 422–440.

Raissi, M., P. Perdikaris, and G. E. Karniadakis (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics 378*, 686–707.