Neural Networks for Structured Grid Generation

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Keywords

Neural Network, Curvilinear Coordinate System, Structured Grid, Partial Differential Equation, Finite Difference Method, Physics-Informed Neural Network, Geometric Modelling

TL;DR

A modern method for creating structured grids using neural networks, which serves as a specific instance of PINN solvers for the Winslow equation.

Introduction

We investigate a novel neural network (NN) - based approach to generate 2-dimensional body-fitted curvilinear coordinate systems (BFCs) that allow to stay on regular grids even when the complex geometry is considered. We describe a neural network as a geometric transformation that can represent a diffeomorphism under certain constraints and approximations, followed by the ways of training it to create BFCs. We show that the optimization system is similar to a physics-informed neural network (PINN) – based solution of Winslow equations. Unlike in classical BFC generation, NN provide a differentiable mapping between spaces, allowing to change an interior nodes distribution without the need of recreating the whole mapping.

Objectives

- Outline theoretical basis of Neural Networks as geometric transformations
- Discover optimization algorithms to perform BFC generation
- Outline the methods to make generated grids regular
- Find a network architecture that will benefit from the specificity of the task relative to usual PINN setup

Process & Methods

The methodology involves using a feed-forward and residual neural networks to represent geometric transformations that can map simple computational grids to curved physical domains. The training is processed by using non-convex optimization algorithms such as SGD or Adam. The paper discusses two main approaches:

1. non-PINN approach focuses on minimizing a point-wise loss function to ensure the boundary predictions fit the physical domain with additional constraints on weights of the network, ensuring that each transformation between two consecutive layers is a bijective map. It lacks expressiveness as obtained formulas were derived only for constant-width neural network with just two neurons per hidden layer, so many complex geometries are out of capabilities of such a setup.
2. PINN approach adds an interior loss term to make grid distribution conformal by minimizing the Winslow functional. It shows better convergence, however, in some cases the discretized nature of optimization process leads to degeneracies.

$$L_{\text{boundary}} = \frac{1}{B}\sum_i \|x\left(\xi_{(i)}\right) - x_{(i)}\|_2^2,$$

$$\xi_{(i)} \in \partial\Omega_C, \quad x_{(i)} \in \partial\Omega_P, \quad i = \overline{1..B}$$

Formula 1: data loss term that matches boundaries

$$L_{\text{int}} \approx \frac{1}{P}\sum_p \left(\frac{g_{11}+g_{22}}{\sqrt{\det g}}\right)_{(p)}$$

Formula 2: discretized Winslow functional, physical loss term

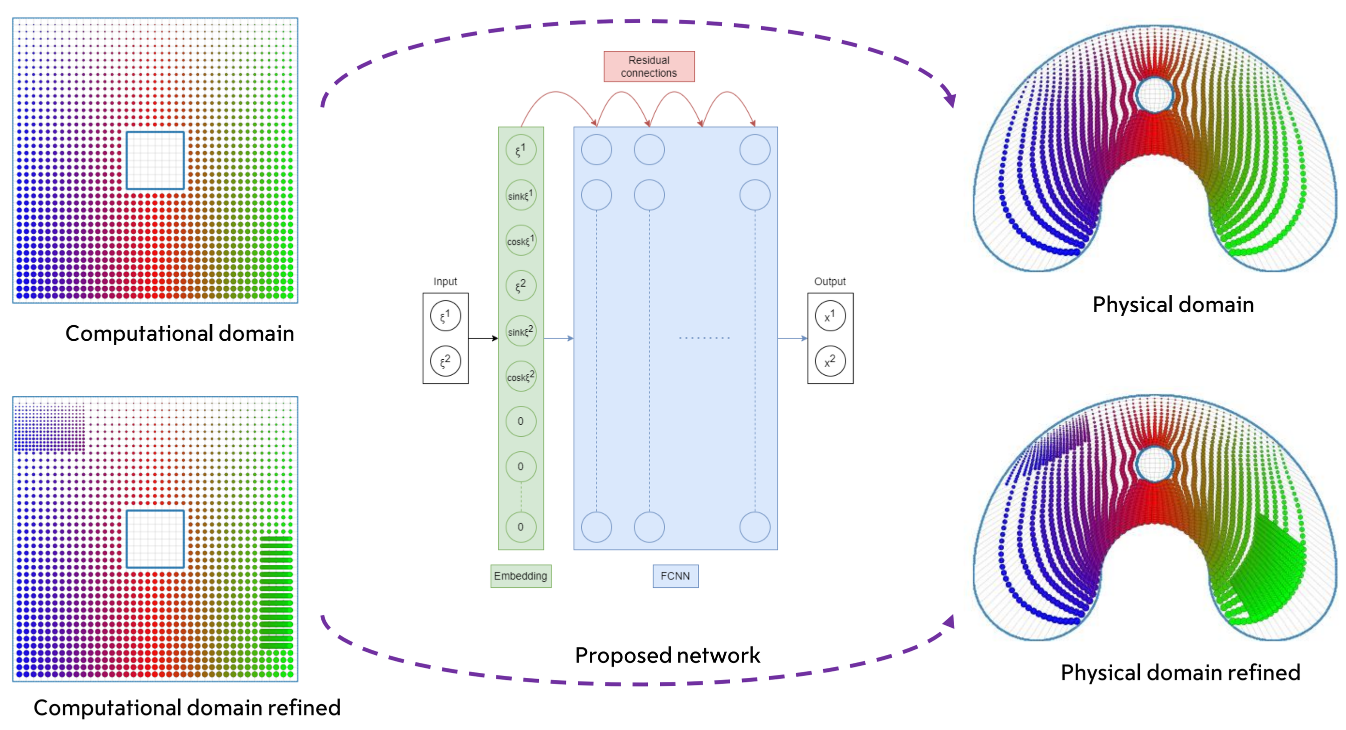

Fig 1.: mesh refinement as a single forward pass through a proposed neural network architecture

Conclusions

It was shown that a neural network can be used for body-fitted curvilinear coordinate system generation with further application to finite-difference solvers of partial differential equations.

While usually neural networks are considered black-box functions, several methods can be used to constraint Jacobians through weights control and mesh loss functions. Benefits of such a grid generation relative to discrete schemes of Winslow equations and others, are that it allows to vary the interior points distribution on the computational domain and compute metric tensors exactly, leading to better representations of differential operators. The use of BFC can be justified, for example, in inverse problem to find estimations of parameters on sparse grids, because it is fast and captures the boundary much better than a staircase approximation.

Still, the grid generator is far from being robust in terms of convergence in a soft loss setup. Further investigation implies the analysis of hard-constrained PINN solvers and interpretations of neural network in that case. Also, such features as 3D domain processing and time-dependent boundaries are to be investigated and still remain an open question.

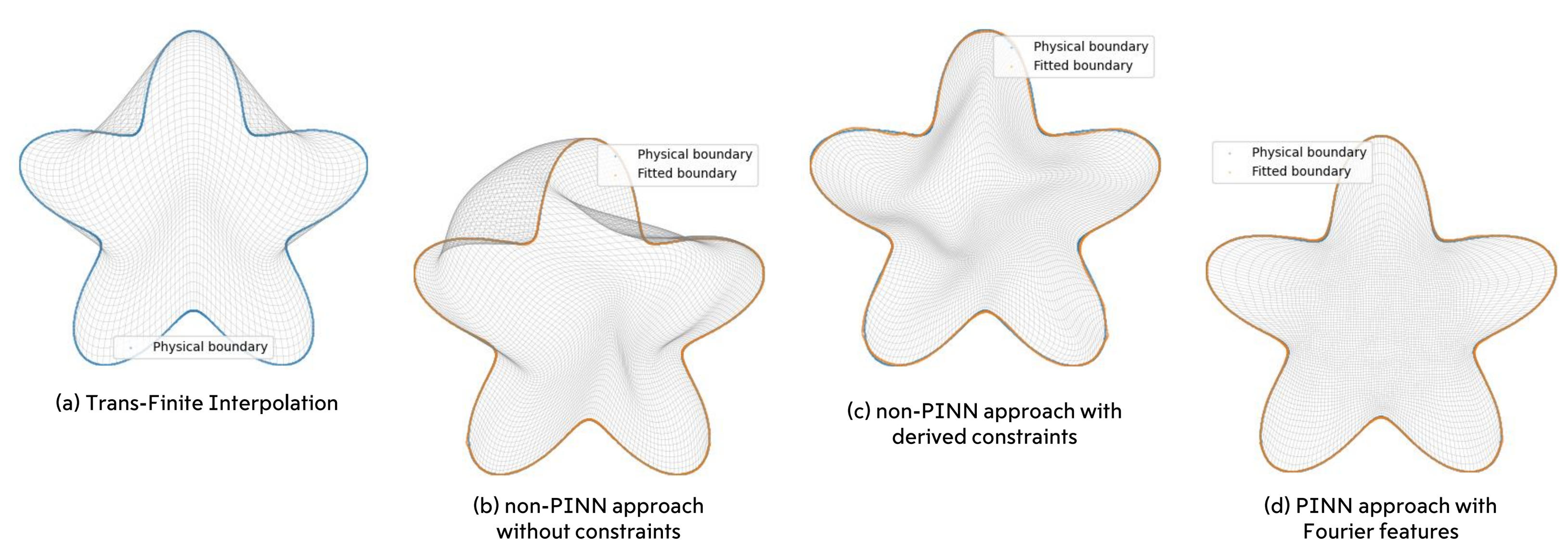

Fig 2.: grids generated with different methods for a single shape

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