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Graflow: A Neural Blood Flow Solver for Vascular Graph

Suprosanna Shit[1,2], **Chinmay Prabhakar**[2], **Johannes Paetzold**[1],
Martin Menten[1], **Bastian Wittmann**[2], **Ivan Ezhov**[1], **Bjoern Menze**[2]
[1]Technical University of Munich, [2]University of Zurich
suprosanna.shit@tum.de

Abstract

Simulating blood flow is paramount in identifying flow-based biomarkers for vascular-related diseases. A segmented vessel graph is used as a domain for the simulation. Traditionally, partial differential equations are solved with numerical methods. Here, we propose an alternative solver for the simulation of blood flow on a vascular graph leveraging geometric deep learning. Specifically, we reformulate the problem as an implicit function on the graph and learn the simulation by imposing the physics in the loss through a message passing layer. The resultant flow is accurate, fast, and applicable to various tasks.

Keywords: Geometric Deep Learning, Blood Flow Simulation, Vascular Graph

1. Introduction

Computational fluid dynamics provides a mathematical model of blood flow in our circulatory system. Given an inflow through a feeding artery and a computational domain (blood vessel geometry), we can solve the dynamic blood flow pattern. However, an accurate solution in the volumetric domain requires solving the Navier-Stokes equation and is compute-intensive Kissas et al. (2020); Shit et al. (2021).

On the brighter side, depending on the vessel's resolution, we can often approximate the vascular network with a graph structure with local properties (such as vessel length and thickness). These graphs lead to a drastic simplification of the flow simulation task and can be scaled up to a larger vascular region or fine capillaries. Conventionally, given a network, a numerical solver is used to solve the continuity equation Reichold et al. (2009); Schmid et al. (2017). This approach, however, requires external library and can not be used in an end-to-end pipeline to simulate flow from an image measurement.

With the advent of geometric deep learning, many emerging solutions have been proposed to leverage the geometric nature of vessel networks Li et al. (2021); Suk et al. (2021). These models take advantage of geometric deep learning algorithms to accelerate the flow simulation by exploring the geometric prior and constraints imposed by a differential equation. At the same time, current methods can directly infer vessel networks from image data Paetzold et al. (2021); Shit et al. (2022). Integrating a blood flow simulation into these inferred graphs calls for an end-to-end trainable feature on the flow solver.

This paper presents a novel blood flow solver based on an implicit function learned on graph. We particularly make use of the Pytorch-Geometric library to implement a message passing layer to impose physical constraint in the loss function. We show poof-of-concept results on a synthetic dataset, demonstrating our proposed solver's efficacy and applicability to a wide variety of tasks.

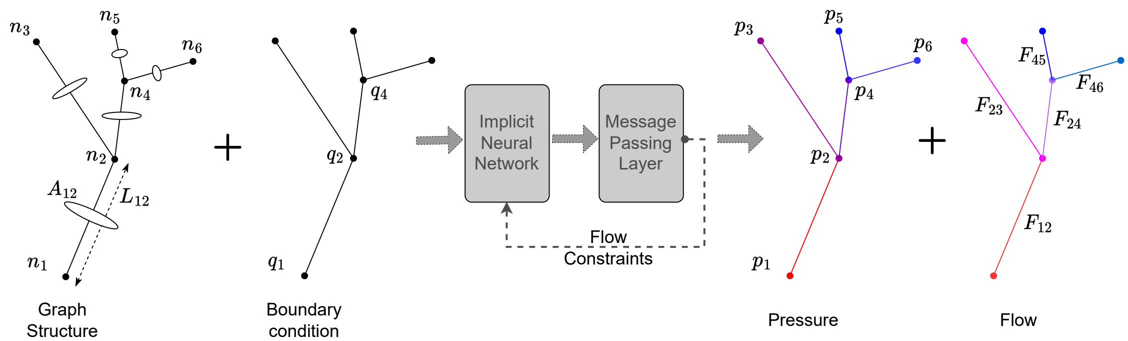

Figure 1: Overview of the Graflow solver.

2. Method

We first formulate the flow simulation problem and then detail the application of graph learning to obtain the solution.

2.1. Governing Equation

Let the vascular network be defined by an undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where $\mathcal{V}$ are the nodes and $\mathcal{E}$ are the edges. Each edge $e_{ij}|e_{ij} \in \mathcal{E}$ has two properties; area (A_{ij}) and length (L_{ij}). We consider a Dirichlet boundary condition on each node n_i as q_i (non-zero at inlet/outlet and zero elsewhere). Solving the flow requires mapping from the graph structure and its properties to pressure (p_i) at each node and flow rate (F_{ij}) at each edge. Given the physical properties of vessels and fluid properties of blood, we can construct the flow (F_{ij}) and conductance (G_{ij}) of each vessel as

$$F_{ij} = G_{ij}(p_i - p_j); \quad G_{ij} = \alpha \frac{\rho A_{ij}^2}{8\pi\mu L_{ij}}, \tag{1}$$

where μ and ρ are the dynamic viscosity and blood density, respectively. $\alpha = 1$ represents a perfectly cylindrical vessel, and $\alpha < 1$ accounts for deviation from the ideal scenario. Assuming rigid vessel walls, one needs to solve the following equation to obtain the pressure.

$$\sum_j G_{ij}(p_i - p_j) = q_i \tag{2}$$

2.2. Graflow

Clearly, the pressure distribution is a function of the geometrical structure and is driven by the boundary condition. Taking inspiration from implicit function learning Raissi et al. (2020); Sitzmann et al. (2020); Tancik et al. (2020) we model the pressure as an implicit function on the graph as

$$p = \boldsymbol{N}_\theta(\mathcal{G}), \tag{3}$$

where $\boldsymbol{N}_\theta$ is an implicit function with learnable parameter θ. Next, p goes through a message passing layer to obtain LHS of Eq. 2. Finally, we train the model with the following ℓ_2 loss

$$\mathcal{L} = \sum_{i|i \notin outlet} \| \sum_j G_{ij}(p_i - p_j) - q_i \|_2 + \sum_{i|i \in outlet} \|p_i\|_2 \tag{4}$$

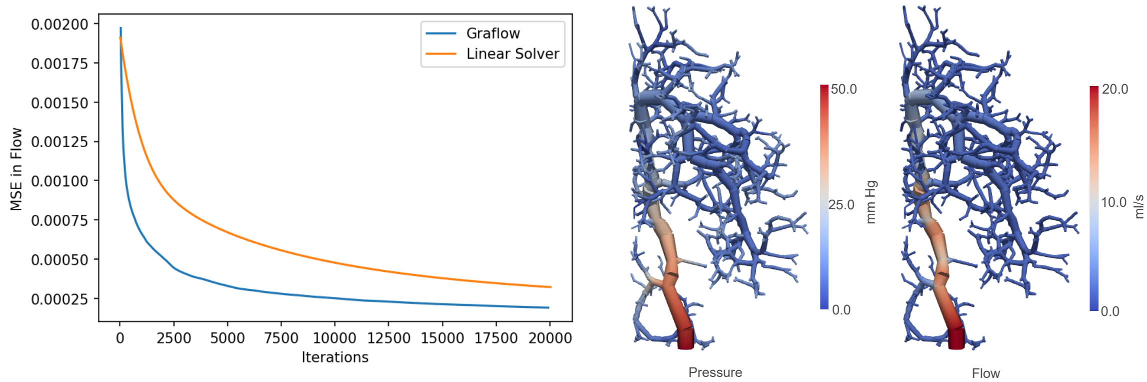

Figure 2: (**Left**) shows that Graflow converges faster to the correct solution. (**Right**) shows an exemplary visualization of the resultant pressure map and flow respectively.

The first part of the loss enforces the flow to be consistent with the *inlet* boundary condition and zero flow everywhere else except the outlet. The second part of the loss enforces zero pressure conditions at the outlet. We use Fourier features of the nodes as input features and the SIREN activation function. We use Adam with a second-order LBFGS optimizer with a learning rate of 1 for 20000 iterations. For simulation we assume the following values $\mu = 0.0015$ Pa.s and $\rho = 1060$ kg/M^3.

3. Experiment

In this paper, we present a proof of concept study to showcase our proposed solver's efficacy and general applicability. We compare against a LBFGS based constrained linear solver for comparison.

Dataset & Metric We used a synthetic vessel dataset Paetzold et al. (2021) and extracted 50 vessel trees with on average 1.7k nodes and 1.6k edges. We set the input flow at the largest feeding artery following Reichold et al. (2009); Lorthois et al. (2011).

Results We plot the mean-squared error of predicted flow in each node and their boundary condition in Fig. 2, demonstrating that the implicit neural solver converges faster than the constrained linear solver. Overall on average, for the whole dataset, we observe a ∼15% decrease in simulation time for Graflow, while the constrained linear solver reaches the same accurate solution in ∼12 min using a Quadro P6000 GPU. Qualitative visualization of the resultant flow and pressure demonstrates the accuracy of our solution, as shown in Fig. 2.

4. Conclusion

In this paper, we propose a novel implicit solver to simulate blood flow on the vascular graph. We show proof-of-concept results on a synthetic vessel dataset which suggests that our solver produces an accurate solution with reasonable reduction in simulation time. Future work will emphasize time-varying solutions on the graph by modeling the dynamic behavior of blood and vessel structures.

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