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SE(3)-equivariant hemodynamics estimation on arterial surface meshes using graph convolutional networks

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Abstract

Hemodynamic field estimation on the artery surface is valuable for patient-specific prognosis, diagnosis, and treatment of cardiovascular disease. Medical biomarkers like wall shear stress (WSS) can be obtained from computational fluid dynamics (CFD) simulation of the blood flow. Machine-learning methods could accelerate or replace the time-intensive CFD simulation. We propose a graph convolutional network (GCN) that predicts hemodynamic fields mapped to the vertices of a finite-element surface mesh. Our neural network is end-to-end SE(3)-equivariant and uses anisotropic convolution filters, as well as pooling layers, informed by the mesh structure. We generate a large dataset of CFD simulations in synthetic arteries which we use to train and evaluate our neural network. We show that our method can accurately predict WSS, up to two orders of magnitude faster than CFD.

Keywords: Geometric Deep Learning, Computational Fluid Dynamics, Wall Shear Stress

1. Introduction

Wall shear stress (WSS) on the coronary artery wall has been found to correlate with plaque development and arterial remodelling Samady et al. (2011); Hoogendoorn et al. (2019) which are key drivers of atherosclerosis, the number one cause of death. Clinical prognosis, diagnosis, and treatment planning could benefit from non-invasive WSS estimation based on medical images of the coronary arteries. Computational fluid dynamics (CFD) simulation can be used to quantify blood flow and derive WSS on the artery wall. However, CFD is compute- and time-intensive and which impedes certain time-critical applications, e.g. virtual surgery planning or shape optimisation of medical devices. Machine learning has been used as a replacement of CFD in hemodynamic-field estimation in coronary arteries. To this end, deep neural networks are trained on a dataset of geometric artery models, with hemodynamic fields mapped to their vertices, in an offline phase and then evaluated to produce estimations online within seconds. Previous works have used handcrafted parametrisation Itu et al. (2016); Su et al. (2020) of the artery wall together with convolutional neural networks (CNN). Ferez et al. (2021) have recently shown that graph

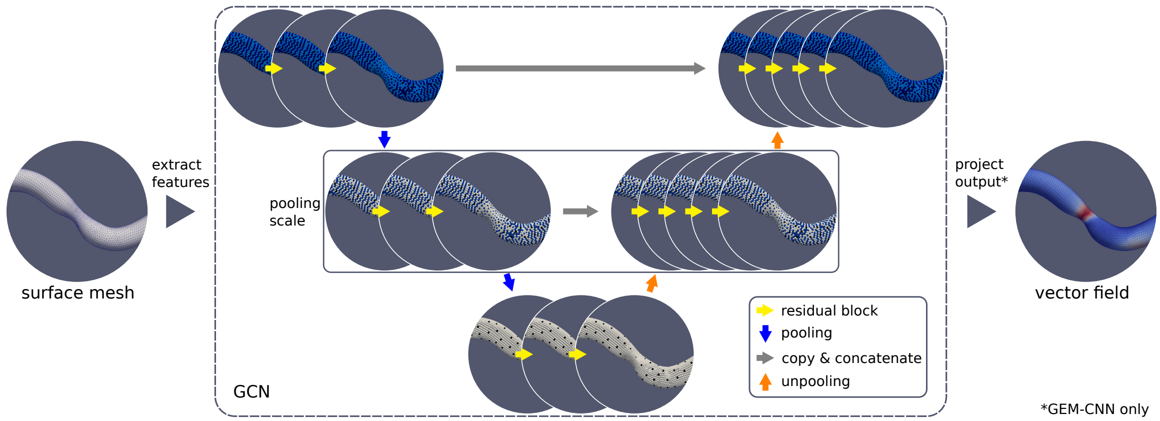

Figure 1: **Network architecture.** Gray vertices are deactivated on each pooling scale. Residual blocks consist of two convolution layers and a skip connection.

convolutional networks (GCN) outperfom previous approaches for the prediction of scalar endothelial cell activation potential in the left atrial appendage. We propose a method to estimate hemodynamic fields on an artery-wall surface mesh based on gauge-equivariant mesh (GEM) convolution de Haan et al. (2021). Our neural network uses anisotropic convolution filters and is end-to-end SE(3) equivariant. In particular, network outputs rotate according to the surface mesh and are independent of translation. In order to enable efficient message passing on large meshes, we use a hierarchical pooling scheme. This paper is a short version of our conference paper Suk et al. (2022) with updated numerical results.

2. Method

We use a three-level pooling scheme with convolution wrapped in residual blocks (Fig. 1).

2.1. Convolution

We use GEM convolution de Haan et al. (2021) on the mesh vertices $\mathcal{V}$:

$$(K * f)_p \coloneqq K_p f_p + \sum_{q \in N(p)} K_{p,q} \rho_{p,q} f_q, \qquad p \in \mathcal{V} \tag{1}$$

where $K_p, K_{p,q} \in \mathbb{R}^{c_{\text{out}} \times c_{\text{in}}}$ are trainable kernels, $f_p, f_q \in \mathbb{R}^{c_{\text{in}}}$, $\rho_{p,q} \in \mathbb{R}^{c_{\text{in}} \times c_{\text{in}}}$, $N(p)$ is a vertex neighbourhood, f_p is the feature vector mapped to vertex p, and $\rho_{p,q}$ performs parallel transport from q to p. Anisotropic filters depend on their neighbouring vertices q while isotropic filters are constant over $N(p)$.

2.2. Pooling

We create a hierarchy of vertex subsets $\mathcal{V}_1 \supset \mathcal{V}_2 \supset \mathcal{V}_3$ via farthest point sampling and find disjoint point clusters to map to vertices of the respective coarser set. We define pooling

		NMAE [%]			ε [%]			$\triangle_{\text{max}}$ [Pa]			$\triangle_{\text{mean}}$ [Pa]		
		mean	median	75th	mean	median	75th	mean	median	75th	mean	median	75th
Single Arteries $L_{\mathbf{max}} = 21.86$ [Pa] $L_{\mathbf{median}} = 2.03$ [Pa]	IsoGCN	2.2	2.0	2.6	32.4	30.0	37.0	10.41	7.80	14.65	1.11	1.01	1.32
	AttGCN	1.2	1.1	1.5	19.0	18.6	22.4	5.83	5.13	8.17	0.60	0.57	0.77
	GEM-GCN	**0.5**	**0.4**	**0.6**	**7.8**	**7.6**	**9.1**	**4.10**	**3.55**	**6.13**	**0.23**	**0.23**	**0.31**
	IsoGCN†	10.5	9.6	12.8	149.2	128.1	181.2	26.73	23.96	36.17	5.31	4.84	6.50
	AttGCN†	8.3	7.5	10.1	123.7	111.1	152.9	25.63	22.93	34.52	4.22	3.82	5.13
	GEM-GCN†	**0.5**	**0.4**	**0.6**	**7.7**	**7.5**	**9.2**	**4.10**	**3.50**	**5.79**	**0.23**	**0.22**	**0.31**
Bifurcating Arteries $L_{\mathbf{max}} = 7.16$ [Pa] $L_{\mathbf{median}} = 1.27$ [Pa]	IsoGCN	1.3	1.1	1.5	24.4	21.1	27.3	4.38	4.14	5.50	0.27	0.22	0.29
	AttGCN	1.2	0.9	1.3	20.7	18.1	22.3	4.10	3.72	4.77	0.23	0.19	0.25
	GEM-GCN	**0.6**	**0.6**	**0.7**	**11.9**	**11.3**	**13.0**	**3.38**	**3.25**	**3.92**	**0.13**	**0.11**	**0.13**
	IsoGCN†	7.3	6.9	9.6	117.4	115.2	151.3	8.60	8.29	10.10	1.45	1.37	1.91
	AttGCN†	7.4	7.4	10.1	119.6	117.1	161.1	8.39	8.33	9.78	1.48	1.47	2.01
	GEM-GCN†	**0.6**	**0.6**	**0.7**	**12.1**	**11.3**	**13.2**	**3.42**	**3.25**	**3.91**	**0.13**	**0.12**	**0.14**

†evaluated on randomly rotated test samples

Table 1: **Prediction accuracy** in terms of normalised mean absolute error (NMAE), approximation error ε, max vertex-wise difference $\triangle_{\text{max}}$, and mean vertex-wise difference $\triangle_{\text{mean}}$. Ground-truth label statistics $L_{\text{max,median}}$ for scale.

by averaging features vectors f_q in cluster $q \in C_p$ after parallel-transporting to p via $\rho_{p,q}$. Unpooling simply copies feature vectors back to each cluster element.

2.3. SE(3) equivariance

GEM convolution layers are SE3-equivariant if used with SO(3) input features. This is because we can restrict SO(3) features to SO(2) in planes tangential to the object surface, which rotate with the mesh by construction. We use linear combinations of relative vertex position and surface normal as input features. Additionally, we supply the vertex-wise geodesic distances to the artery inlet, which is an invariant scalar value.

3. Numerical experiments

We train our neural network by L^1-error regression on two datasets of 2,000 synthetic coronary artery simulations. The datasets consist of arteries with single inlet and outlet (around 8k vertices, 17k faces) and bifurcating arteries (around 17k vertices, 32k faces). For comparison, we introduce two baseline models by choosing $K_{p,q} = K_p$ and $\rho_{p,q} = \mathrm{I}$ ("IsoGCN") and $K_{p,q} = K_p$ and learned attention $\rho_{p,q} = \alpha(p, q)$ ("AttGCN") in (1). Quantitative evaluation (Table 1) shows GEM-GCN strictly outperforms the baseline models. We investigate rotation equivariance by randomly rotating meshes at test time. IsoGCN and AttGCN accuracy drops dramatically, in contrast to GEM-GCN accuracy.

4. Discussion

We show that our method can be a feasible CFD surrogate. Anisotropic graph convolution and SE(3) equivariance lead to improved performance and eliminate the need for roto-translational data augmentation. Hemodynamics estimation with GEM-GCN requires less than 5 s, compared to more than 10 min for CFD simulation in the same artery.

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