Oral presentation | Data science and AI

Data science and AI-II

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[10-C-02] Application of Graph Neural Networks to Accelerate Airflow and Pressure Prediction on 1D Human Airways

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Application of Graph Neural Networks to Accelerate Airflow and Pressure Prediction on 1D Human Airways

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1 Introduction

Computational fluid dynamics (CFD) has been a powerful tool to study airflows, and is recently engaged by biologist and pulmonologist to explore the mechanism of respiratory functioning. The low cost and riskless simulations replacing experiments on human subjects are major advantages of CFD which draw the attention of researchers. However, CFD simulations are often computationally expensive and time consuming, making them not eligible for a quick medical diagnosis. Many researchers move their attention to data-driven CFD, which could accelerate the prediction by generalizing information from old CFD data. Convolutional neural network comes as the most common approach, since it is easily done to convert CFD data from structured grid into two-dimensional images. Recurrent neural networks techniques are often used for transient flow data, which its occurrence emerges in most of CFD simulations. For unstructured grid, graph convolutional neural networks (GNN) is essential due to the complex procedure of converting grid data to sequence or image suited with regular neural networks models. In this study, we employed GNN model to predict CFD output on 1D network structure based on human lung airway. The 1D airways' meshes are derived from real human airway central line and 1D CFD simulations are performed to archive corresponded CFD data.

2 Problem Statement

The one-dimensional (1D) network structures of human lung were employed using QCT images during static breathing. A group of 20 healthy subjects and 20 cement dust exposed subjects were gathered, and the CT scans were obtained at both full inspiration and normal expiration. We employed 1D CFD scheme to estimate pressure and airflows in subject's 1D airways (Choi et al. [1]), which is based on an incompressible isothermal energy balance equation (Predley et al [2]).

$$\int_{\Gamma} \mathbf{u}_i \mathbf{n}_i dS = 0$$

$$\int_{\Omega} \left\{ \frac{\partial}{\partial t}\left(\frac{\rho U^2}{2}\right) + \nabla . \left[P\mathbf{u}_i + \frac{\rho U^2}{2}\mathbf{u}_i \right] - \mu \mathbf{u}_i \frac{\partial^2 \mathbf{u}_i}{\partial x_i \partial x_i} \right\} dV = 0$$

where $\mathbf{u}_i$, $\mathbf{n}_i$, ρ, U, P and μ are velocity vector, outward normal vector, fluid density, velocity magnitude, pressure and fluid dynamic viscosity, respectively. Flowrate was also computed using the formula $Q = \int_{\Gamma} \mathbf{u}_i \mathbf{n}_i dS$ at each branch's end. We employed the pressure and flowrate for the prediction of our model.

In this regard, we proposed a GNN-based model for the prediction of corresponding CFD output. The model could be decomposed into two separated components: a GNN to encode the 1D lung mesh features, followed by a GNN to predict the output field. A recurrent scheme which matched each time step's output to the next input is adapted to produce sequential prediction of CFD data. The preliminary results show an agreement on the trend of the predicted output to the ground truth CFD data (Figure 1). From our study, the correlation of predicted and ground truth data is stronger as it goes nearer to the terminal branch, which could be explain by the number of data points given were larger therein. We also observe that the prediction on peak inspiration and peak expiration were more identical between GNN and CFD data, address the importance of data scaling. The GNN model produces significantly faster result compares to CFD simulations (~30 seconds per prediction compares to ~15 minutes per CFD simulation), making it promising for more high level tasks.

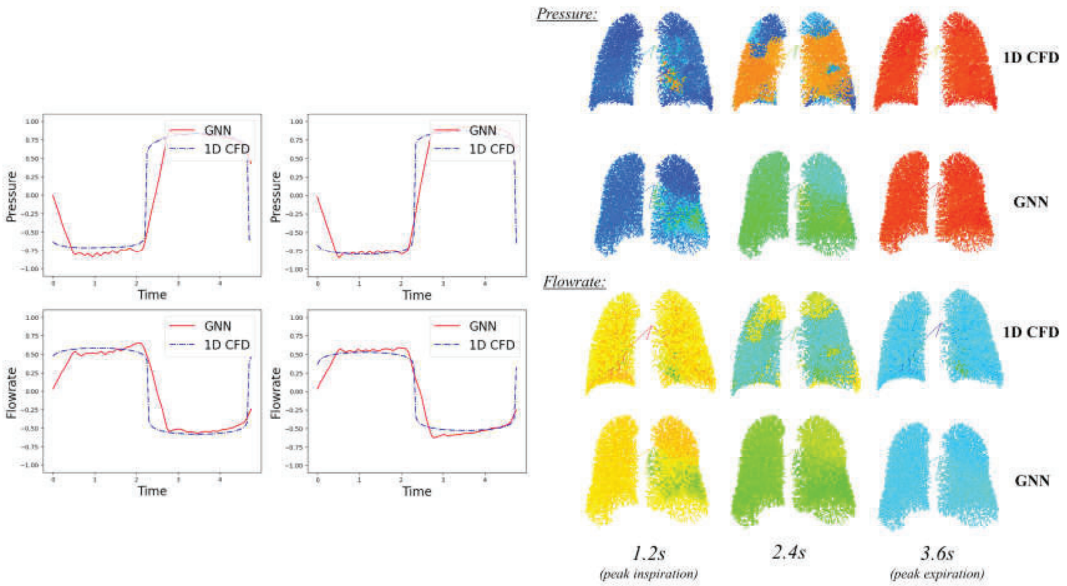

Figure 1: Compare the prediction of GNN surrogate model and 1D CFD.

References

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