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Multiscale Modeling of Drug Diffusion in Cardiovascular Collagen Networks Using Physics-Informed Neural Networks

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ABSTRACT

Cardiovascular disease (CVD) is the leading cause of mortality in Canada and worldwide, with serious complications such as atherosclerosis, stroke, and heart failure. These conditions often arise due to alterations in blood flow hemodynamics and progressive arterial degeneration. A key factor in arterial wall integrity is the hierarchical structure of collagen fibers, which provide mechanical strength while also influencing mass transport at multiple scales. Disruptions of collagen fibers can alter diffusive properties within the extracellular matrix (ECM), affecting nutrients delivery, drug transport, and pathological progression.

Modeling diffusion within collagen fiber networks presents significant challenges due to their multiscale nature, structural heterogeneity, and nonlinear interactions. Traditional computational fluid dynamics methods FEM/FVM capture macroscopic transport behavior but often require fine meshes and high computational resources at microscale. In this study, we propose a multiscale modeling framework that integrates physics-based homogenization techniques with data-driven approaches. Specifically, we employ physics-informed neural networks (PINNs) to solve diffusion equations efficiently while incorporating microscale structural features of collagen fibers. This meshless approach enhances computational efficiency while preserving essential multiscale interactions in collagen fiber diffusion modeling.

Drug diffusion in biological tissues happens at multiple spatial and temporal scales, where solute transport at the microscale influences macroscopic drug distribution. To bridge this multiscale gap, Physics-Informed Neural Networks (PINNs) are employed to infer effective diffusion coefficients by integrating microscale dynamics with macroscale transport models. PINNs incorporate governing physical laws directly into the loss function, enabling seamless coupling between scales. The loss function consists of: 1. PDE residuals from the advection-diffusion equation and Darcy's law to capture local solute dynamics within the ECM; 2. Boundary conditions at different scales; 3. Data-driven constraints: leveraging high-resolution diffusion data at small time and space scales to infer macroscale transport properties. Fibrous structures with high-porosity and low porosity ECM will be modeled to simulated cardiovascular tissues at healthy and disease states. The drug distribution results could provide valuable insights for optimizing nanoparticle drug design and delivery strategies.