AI-enabled Engineering

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**Abstract**

The optimization of artificial hearts presents a critical endeavour in the field of medical technology, aiming to enhance functionality while minimizing energy consumption and adhering to various constraints. In this study, we address the optimization challenge posed by a MedTech start-up preparing for human trials of the novel artificial heart in 2024. Our objective was to optimize both the pump and housing components to reduce energy consumption while satisfying all requisite constraints.

The complexity of this task stemmed from the necessity to account for diverse blood damage mechanisms, including shear stresses, complex flows, and heating, within a transient simulation framework. Existing simulations exhibited prolonged computational times (48-96 hours) and yielded inaccurate results, constraining optimization efforts.

To overcome these limitations, we employed fully automated computational fluid dynamics (CFD) coupled with advanced artificial intelligence (AI) technology. Through iterative simulation and optimization, we achieved notable improvements, enhancing shut-off pressure by 42% and efficiency by 15%. Remarkably, our optimization endeavours facilitated the removal of the connecting wire between the artificial heart and the battery, enabling wireless operation and significantly enhancing patient quality of life.

Our approach leveraged an AI-based optimization workflow integrated with a Large Physics Model (LPM) trained on simulation data, achieving 97% model accuracy with a single GPU over a span of 2 days. Utilizing a geometry generation engine comprising parametric computer-aided design (CAD) and advanced mesh morphing techniques, alongside the optimization engine, we established an end-to-end loop encompassing geometry generation, performance assessment, and optimization.

The efficiency of our methodology facilitated rapid iteration, with each geometry generated, assessed, and optimized in under 1 second. Over a 5-day period, our iterative loop generated approximately 1,000,000 geometries on a single Nvidia A100 GPU, ultimately converging to the global optimum within a high-dimensional design space. Overall, our study demonstrates the efficacy of automated simulation coupled with AI-driven design in optimizing artificial heart systems, offering promising implications for advancing medical technology and patient care.

# Introduction

Artificial hearts, or ventricular assist devices (VADs), serve as crucial therapeutic options for patients with end-stage heart failure, offering a lifeline while awaiting heart transplantation or even as an alternative to a transplant. However, the efficacy and safety of these devices hinge upon their design, particularly regarding energy efficiency, hemocompatibility, and patient quality of life.

In response to the growing demand for advanced cardiovascular therapies, a MedTech startup embarked on the development of a novel artificial heart system. With the ambitious goal of conducting the first human trials in 2024, the startup sought to optimize both the pump and housing components.

Main optimisation objectives are as follows:

* **Increase efficiency –** enables wireless charging, longer battery life and/or smaller batteries
* **Better flow performance** – higher shut-off pressure enables a reduced overall pump size, unlocking use in children while not requiring replacement as they grow up
* **Blood damage reduction** – no damaging of red blood cells (Haemolysis), increased survival rate, better life quality and fewer hospital visits

A diagram of a heart

Description automatically generated

1. Left-Ventricular Assisted Device (LVAD)

# CFD simulation setup

The simulation setup was underpinned by a number of challenges, chiefly centered around the intricate interplay between fluid dynamics, blood damage mechanisms, and device geometry. We leveraged state-of-the-art CFD tolling, best practices and smart physics and pre-processing choices to fully automate this workflow, which was later integrated into an CFD-based optimization loop.

Further details on the simulation setup:

* Fully automated STAR-CCM+ workflow using simulation operations & macro’s
* 12 operating points (2x RPMs, 6x mass flow) per geometry, leveraging   
  warm-start for faster convergence
* Blood damage metric: Normalized Index of Haemolysis (NIH), power law function of shear stress (𝜏) and residence time (Δt)
* Switched from transient RBM & lagrangian particle tracking to steady state MRF simulation & eulerian approach at very similar accuracy,   
  blood modelled as non-newtonian fluid
* Linked parametric CAD model via STAR-NX CAD client,   
  automated pre-preprocessing and meshing, 5 million polyhedral mesh elements
* >50 reports, including axial & radial rotor forces

# CFD-based optimization

In our study, CFD-based optimization served as a cornerstone of our iterative design refinement process, enabling the exploration of a wide range of design parameters to enhance the performance of the artificial heart system. Several key aspects characterized our CFD-based optimization approach, including parameterization, simulation setup, and computational efficiency. Some key optimization metrics below:

* 15 CAD parameters, reduced based on sensitivity & smart combination
* 1500 simulations runs over 12 operating points, solved on 4x128 cores in 4 weeks
* After 4 weeks of time consuming CFD optimization, limited performance improvement was found

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| --- | --- |
| **Metric** | **Improvement compared to baseline configuration** |
| Flow Performance (Δp) (higher is better) | +23% |
| Blood Damage (NIH) (lower is better) | +8% |
| Pump Efficiency  (higher is better) | -5% |

1. CFD based optimization - Improvement compared to baseline

The CFD-based optimization fell short due to the vast design space and slow simulation speeds. Despite efforts to streamline parameters and use parallel computing, exploring all configurations proved challenging. Limited computational resources hindered thorough exploration, leading to suboptimal results over the 4-week period. To overcome these limitations, we are exploring AI-driven techniques for faster, more efficient optimization.

# Deep Learning Surrogate (DLS) based optimization

The AI-driven optimization approach represents a paradigm shift from traditional methods, offering a more efficient and effective means of exploring the complex design space of the artificial heart system. Leveraging advanced deep learning algorithms and optimization techniques, the AI-driven optimization methodology aims to overcome the limitations of CFD-based approaches, particularly in terms of computational efficiency and scalability.

A diagram of a diagram

Description automatically generated

1. DL-based optimization workflow

Compared to a conventional parameter-based machine learning approach, the deep learning model encodes geometry in shape of the mesh (not only geometric parameters) and predicts 3-dimensional (flow) fields. This makes the DLS agnostic to parametrization changes or even the geometry creation approach itself. As the input to the model is the mesh, we were even able to deploy a non-parametric mesh-morpher for faster and free-shape geometric optimization. At the same time, due to the DLS also learning from the (flow) fields and not only scalar outputs, there was a lot more information to learn from for each single CFD sample. This leads to drastically reduced training data requirements at very high model accuracy. This DLS was only trained on 85 CFD runs achieving accuracies of ~97% for pressure and >94% for shear stress on unseen geometry. Furthermore, these DLS models benefit from much better extrapolation and even generalisation capability than normal ML models.

Further detail on the deep learning model used:

Model type: Geometric deep learning (GDL) architecture

Inputs:

* Pump housing & rotor surface mesh (400k mesh elements)
* RPM & mass flow

Outputs:

* Pressure & shear stress fields on surfaces
* Volumetric shear stress on coarse grid
* Scalars for NIH, rotor forces etc.

Training effort:

* DL model trained in 2 days including data conversion, training, tuning  
  (2h per training on single Nvidia A100 GPU)
* Trained on 85 CFD runs

Accuracy - on unseen geometry:

* Pressure - MAE <1mmHg (<1%), >97% R^2
* Blood shear stress - MAE <10Pa (<3%), Peak <100Pa (<10%), >94% R^2

A diagram of different colored circles

Description automatically generated with medium confidence

1. Comparison of CFD (left) vs DLS (right) surface field predictions

**DL-based optimization**

* Full 30 CAD parameter space used for optimization
* DL model trained on ~85 CFD runs including data conversion, training, tuning in 2 days (2h per training on single Nvidia A100 GPU)
* After ~8 hours and >100.000 configurations, the AI found the optimum pareto front and design

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| --- | --- |
| **Metric** | **Improvement compared to baseline configuration** |
| Flow Performance (Δp) (higher is better) | +42% |
| Blood Damage (NIH) (lower is better) | -7% |
| Pump Efficiency  (higher is better) | +15% |

1. Improvement compared to baseline configuration

The comparison between CFD & DLS based optimization shows the clear offset and performance impact of the DLS based workflow. In only 8 hours (+2 days of DLS training) the model was able to find the optimum pareto front for this problem, while the CFD based workflow didn’t get even close, even after 4 weeks and >1500 compute intensive CFD simulations.

A graph showing the difference between pareto and pareto

Description automatically generated

1. Optimization pareto front comparison

Final CFD validation shows very good correlation and again validates the exceptional extrapolation capability of the model used:

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| **Metric** | **Improvement compared to baseline configuration** |
| DLS Prediction of optimum geometry (Flow performance) | +43.7% |
| CFD Simulations of optimum geometry (Flow performance) | +42.3% |
| Prediction Error | 1.4% |

1. Improvement compared to baseline configuration