

Overview

The Problem

Many students learn about 3D structures of cells through a 2D medium. Traditional learning methods provide limited opportunities for interactive exploration of cellular structures.

Our Project

- Build an interactive digital twin of a human cell
- Two builds in parallel:
 - Whole-cell **compartmental model**
 - GPU-accelerated **spatial model**
- Python simulation backend + live web interface
- Our goal is to develop an **educational tool** for biology students to learn and interact with different components of the human cell

Development Plan

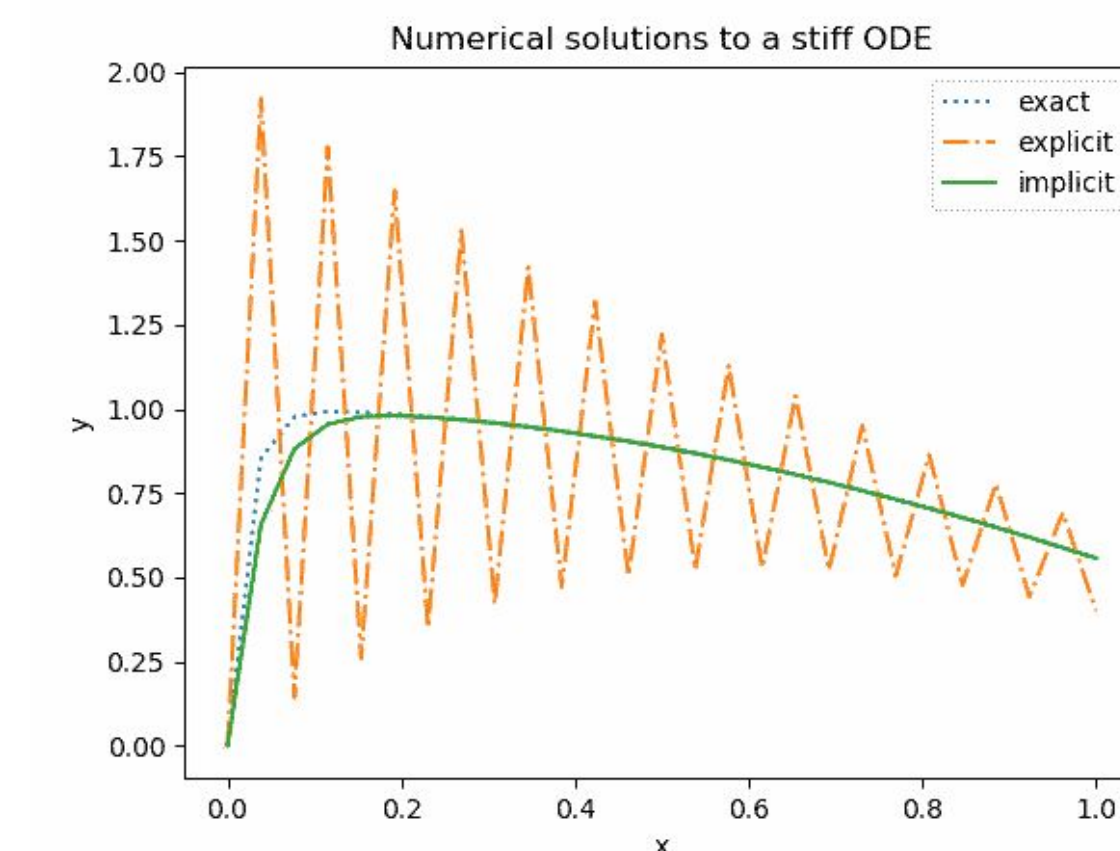
Application Concept

- Replaces static diagrams with a dynamic, interactive learning tool.
- Models metabolic shifts between **aerobic respiration** and **lactic acid fermentation**

Tech Stack

- **Python:** Handles mass-balance equations & stiff Michaelis-Menten ODE kinetics.
- **C++ / CUDA:** Powers 3D spatial diffusion on **P100/H100 GPUs** (up to ~800k voxels).
- **Web UI:** Interactive frontend for real-time slider controls (O₂, Glucose, ATP demand, etc.) and dynamic rendering.

Challenges

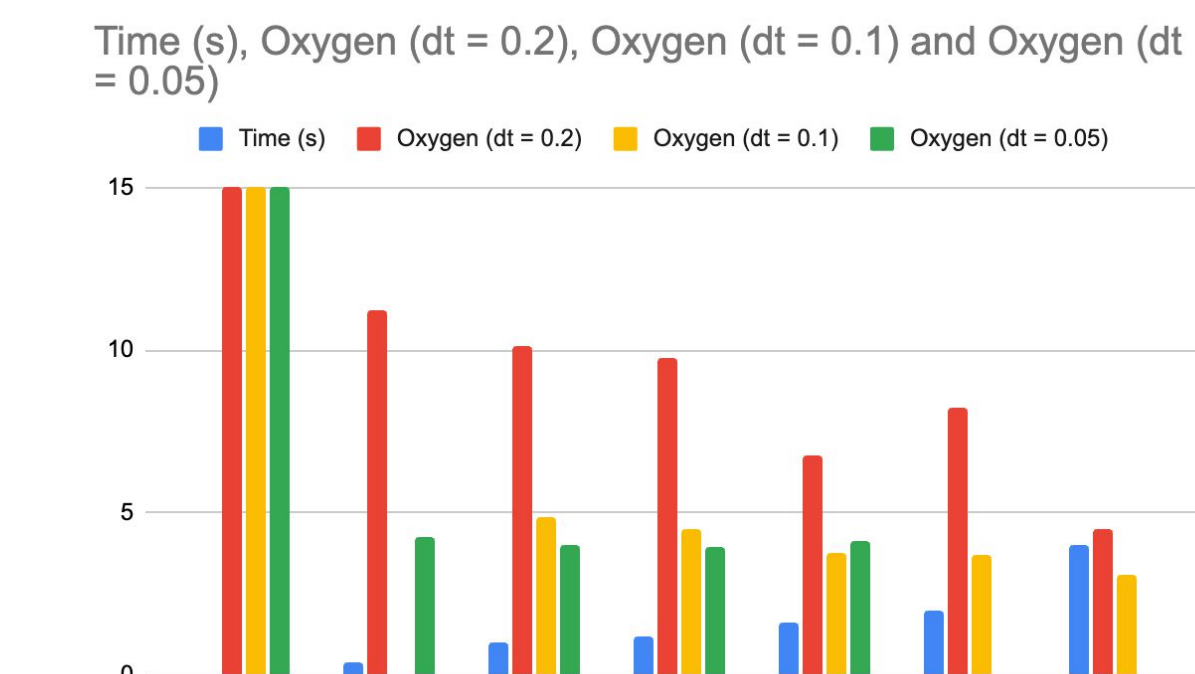


Stiff ODE Systems:

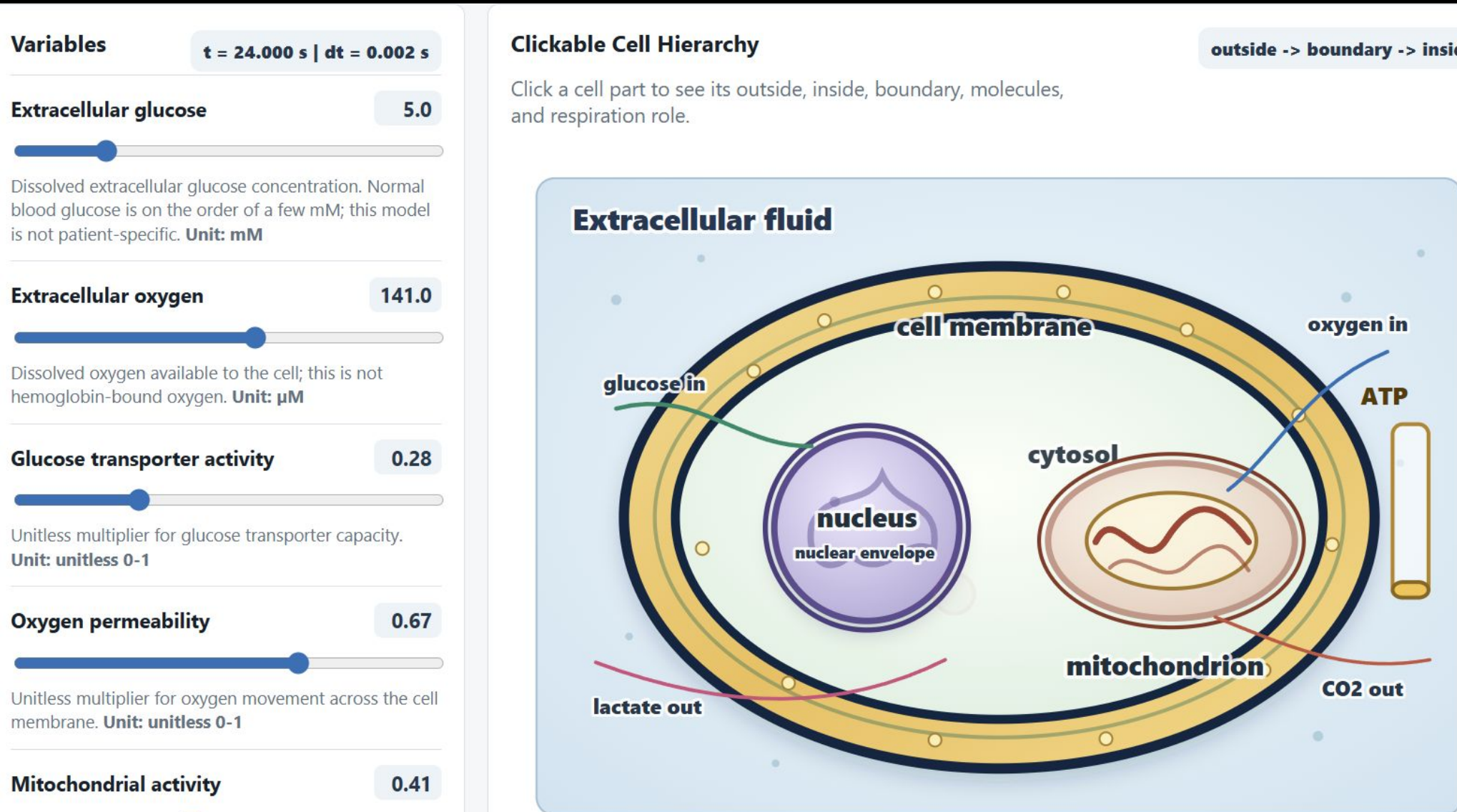
Biological processes (e.g., rapid cellular transport vs. slow metabolic consumption) operate across vastly different timescales, causing explicit solvers to oscillate or blow up.

Implicit Solvers

Required: Transitioning to implicit solvers restored numerical stability without forcing unrealistically tiny time steps (dt).



Compartmental Model



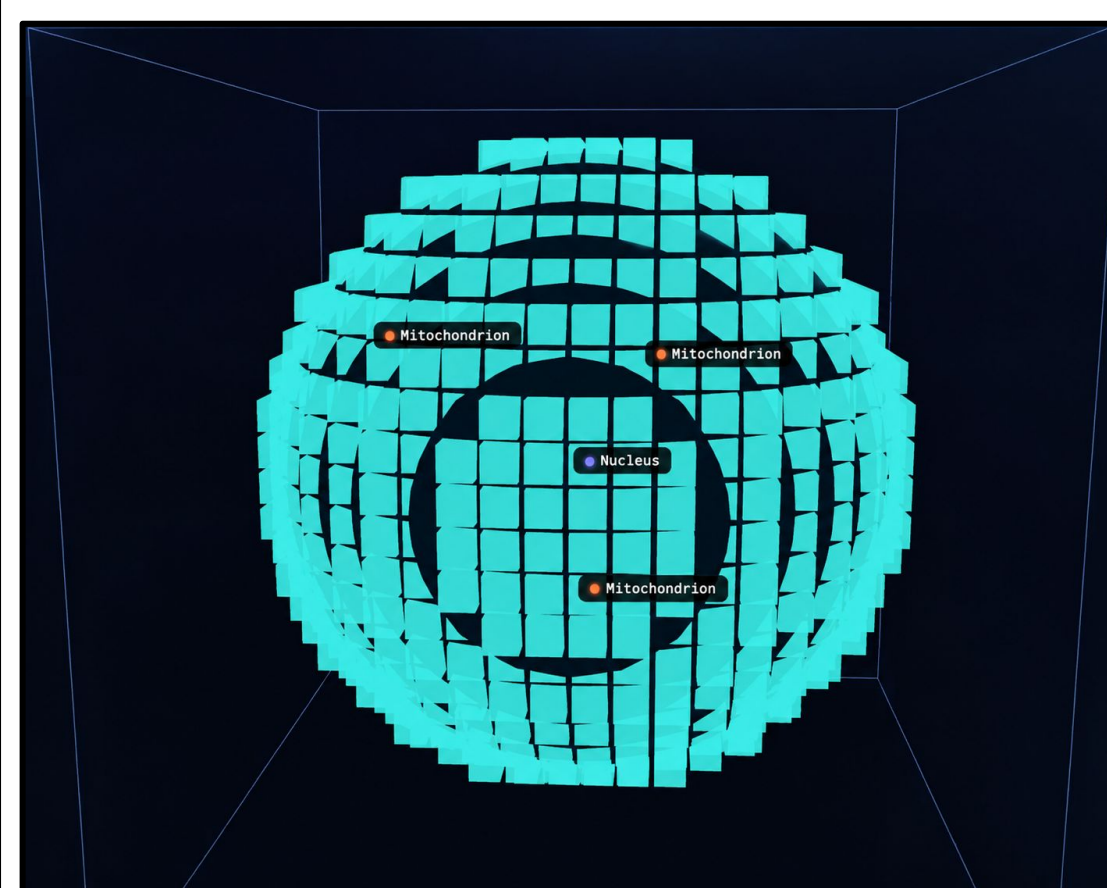
Interactive Web Interface: Enables real-time parameter tuning (e.g., glucose and oxygen levels).

Hierarchical Exploration: Allows users to click through cell regions (Outside → Boundary → Inside) to inspect local variables and biological processes.

Rapid Simulation: Provides fast, low-overhead computational feedback for immediate learning and experimentation.

Spatial Model

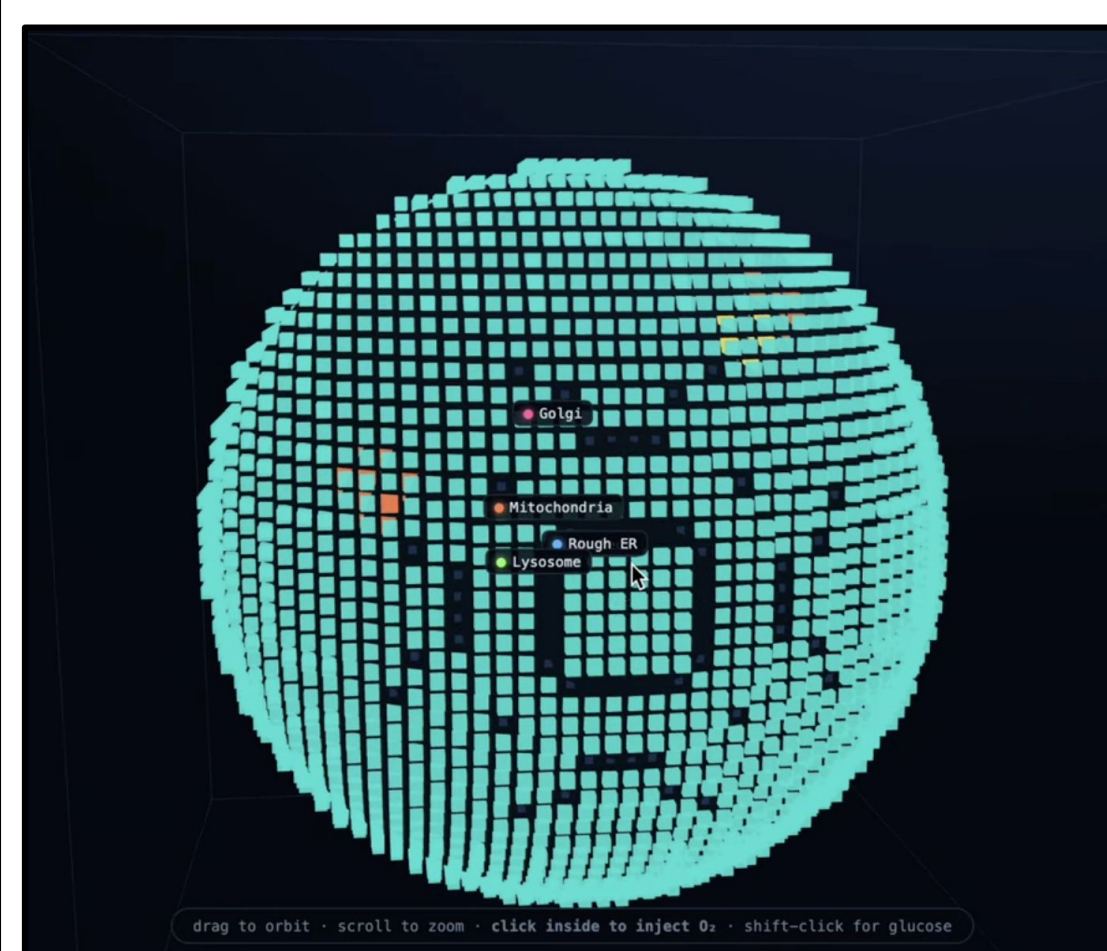
P100 GPU Early



A GPU-accelerated model that partitions the cell into a 3D grid of **voxels** (volumetric cells), each mapped to a specific organelle, to simulate molecular diffusion across cellular space.

Governed by **Fick's Second Law**, it resolves the spatial distribution of substances over time — capturing *where* molecules move, not only their concentration.

H100 GPU (Current)



Because each voxel updates independently, the computation parallelizes efficiently on the GPU; scaling from the P100 to the H100 advanced the model from a coarse proof of concept to a high-resolution, interactive simulation.

Results

- **Delivered two complementary models:** a whole-cell compartmental model (distributable executable) reproducing the aerobic–anaerobic metabolic transition, and a GPU-accelerated 3D spatial model
- **Achieved ~800,000 voxels in real time**, with migration from the P100 to the H100 GPU yielding a substantial gain in resolution
- **Resolved stiff-system instability** through adaptive time-stepping, eliminating oscillation artifacts

Acknowledgements

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Guidance from the **Chemical Engineering** team on the stiff ODE/numerical stability problem

