Hemodynamic Simulation with Lattice Boltzmann

Harvard IACS AC 290R

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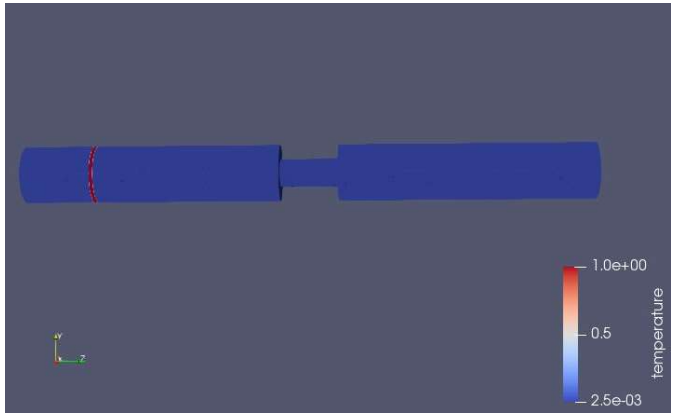
Module II in Context of AC 290R

- Goals of AC 290R: learn techniques in Extreme Computing applied to application domain of Fluid Dynamics
- Module I covered the continuum description and Navier Stokes; we simulated Rayleigh-Bénard Convection using the CPU-centric Drekar Code
- Module II shifted to the mesoscale description, which is well suited to the life sciences in particular
- We tackled a prototypical problem: a hemodynamics simulation
- We also learned about GPU computing
- While MUPHY can make good use of GPUs, our simulation ran on CPUs (1024 cores)

Problem Statement & Motivation

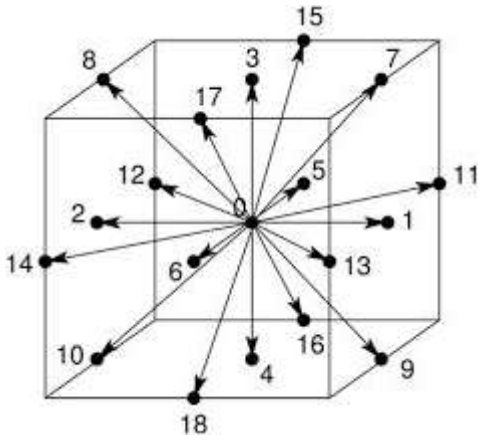
- We simulated the release of a therapeutic drug to treat a stenotic artery
- Stenosis is a narrowing of the artery, often caused by atherosclerosis
- We used an idealized geometry, modeling the artery as a cylinder with a narrowing in the stenotic region

- We wanted to model the dispersal of the drug agent into the stenotic region over a time scale in the range of 1-4 seconds (1 second is roughly 1 heartbeat)
- We attempted two simulations
  - Reynolds = 10
  - Hematocrit = 0,30%



Overview of Numerical Methods Used

- The Boltzmann Equation (Ludwig Boltzmann, 1872) is a triumph of classical thermodynamics and statistical physics
- The Lattice Boltzmann Method (LBM) is a CFD simulation technique based on the Boltzmann Equation
- The fluid is modeled as a distribution of *populations* of particles on a grid; each grid point tracks *p* counts of particles with different discrete velocities
- We used the common D3Q19 approach; 3D space is discretized into cubes
- Each cube has 19 neighbors: 1 at distance 0, 6 at distance 1, 12 at distance 2



Credit: research.tue.nl

Equations of Lattice Boltzmann

Bhatnagar-Gross-Krook Update Rule:

$$f_p(x + hc_p, t + h) = f_p(x,t) + \omega(x,t)h\left[f_p^{eq}(\rho, \mathbf{u} - f_p)(x,t) + w_p\frac{c_p \cdot \mathbf{g}}{c_s^2}\right]$$

Equilibrium Population:

$$f_p^{eq}(\rho, \mathbf{u}) = w_p\rho\left[1 + \frac{\mathbf{u}\cdot c_p}{c_2^2} + \frac{(\mathbf{u}\cdot c_p)^2 - c_s^2u^2}{2c_2^4}\right]$$

- f_p is the population with discrete velocity *p*
- u is the velocity
- c_p is the displace $\mathbf{u}(\mathbf{x},t) = \frac{1}{\rho(\mathbf{x},t)}\sum_p c_p f_p(\mathbf{x},t)$ discrete velocity, e.g. (1,0,0)
- ω is the relaxation frequency, related to viscosity by $\nu = c_s^2\left(\frac{1}{\omega} - \frac{1}{2}\right)$
- ρ is the density at this grid point, the sum of the f_p
- w_p are the LBM weights; ⅓, ⅙ and 1/18 for 0th, 1st and 2nd neighbors
- c_s is the lattice speed of sound, √3/3

Description of Code

- Workhorse is the back-end fluid simulator MUPHY/MOEBIUS
- MUPHY is a ~10 year old multi-physics simulator using LBM with an emphasis on biological applications; guest lecturer Simone Melchionna was a lead developer
- MOEBIUS is a commercial code developed by Dr. Melchionna's company Lexma
- MUPHY simulation engine written in C/C++ and Fortran for maximum speed
- Front end is in Python for convenience in specifying and running simulations
- `ShapePainter.py` generated the geometry for our problem; 8.6m points, 7.0m cells
- `run2.py` invokes the simulation in MUPHY, using MPI to run in parallel
- `runrbc.sh` is a shell script that runs our job on Odyssey with suitable parameters

Post-Processing: Visualization & Analysis

- Performance intensive visualization (e.g. Paraview) was run remotely on Odyssey due to huge size of simulation output (~2GB / frame)
- Analysis and plots carried out on a handful of frames were performed locally on frames downloaded every 100 ms from 0.1 to 1.0 seconds
- VTK outputs (.vtu and .pvtu) were converted to numpy using vtki library
- Drug volume was computing by summing concentration in cells
- Plots of velocity were made using points data with matplotlib
- Scratchlfs had slow performance over the weekend and on Monday; this made post-processing difficult (atypical problem)

Refactoring

- MUPHY/MAGIC: Backend library
- BUFFY: Each subdirectory represents each simulation with different RBC and Re
- Workflow: Create shapes in ShapePainter, copy the output files into their respective RBC_X_ReX folder, submit batch scripts
- Simulation attempts:
  - Re = 10: 0% RBC, 5% RBC (❌), 30% RBC (❌)
  - Re = 5: 5% RBC, 10% RBC (❌)

```
ac290ru1906@boslogin03:/n/scratchlfs/ac290r/blood_cells/MUPHY$ tree -L 2
.
└── MAGIC
    └── BACKEND

ac290ru1906@boslogin03:/n/scratchlfs/ac290r/blood_cells/BUFFY$ tree -L 2
.
├── RBC_0_Re10
│   ├── bgkflag.dat
│   ├── bgkflag.hdr
│   ├── bgkflag.xyz
│   ├── DIRDATA_BloodFlow
│   ├── DIRDATA_Bolus
│   ├── genparalleldomains.py
│   ├── jobgpu_parallel.slurm
│   ├── jobgpu_serial.slurm
│   ├── job.slurm
│   ├── RBC.xyz
│   ├── run2.py
│   └── runrbc_0.sh
├── RBC_5_Re5_NEW
│   ├── atom.inp
│   ├── bgkflag.dat
│   ├── bgkflag.hdr
│   ├── bgkflag.xyz
│   ├── genparalleldomains.py
│   ├── jobgpu_parallel.slurm
│   ├── jobgpu_serial.slurm
│   ├── job.slurm
│   ├── RBC.xyz
│   ├── runrbc.py
│   ├── runrbc.sh
│   └── wall.xyz
└── ShapePainter
    ├── all_mod.mod
    ├── atom.inp
    ├── bgkflag.dat
    ├── bgkflag.hdr
    ├── bgkflag.xyz
    ├── EXTRAS
    ├── __init__.py
    ├── preproc1.py
    ├── preproc2.py
    ├── preproc.sh
    ├── RBC.xyz
    ├── Re2
    ├── set_modules_vtk.sh
    ├── ShapePainter.py
    ├── ShapePainter.pyc
    ├── SP.stl
    └── wall.xyz
```

Parameters of the Simulation

- Simulation 1:
  - Dimensions: Re=10.0, Pe=10.0, Length L=1000.0, Radius =50.0
  - Red Blood Cells: 0%
  - Drug Release Time: 100000
- Simulation 2:
  - Dimensions: Re=5.0, Pe=10.0, Length L=500.0, Radius =25.0
  - Red Blood Cells: 5%
  - Drug Release Time: 50000
  - Blood Unfreeze Time: 2000 (3000)
- Density $\rho_0 = 1.0$
- Viscosity: $\nu = 0.1$
- Average Velocity: $\bar{u} = 0.01$

The “Odyssey”

Job Name	Run Time	Exit Code	Count	Diagnostic
RBC30RE10			2	MPI communications error.
RBC30RE10	10:30:32	1	1	Equilibration was not sufficiently long.
RBC10RE10	03:49:42	1	1	Segmentation fault (Address not mapped).
RBC10RE10		137	2	Segmentation fault (Address not mapped).
RBC30RE10	01:33:09	0	1	Node fail.
RBC10RE10	01:34:41	137	2	Releasing the cells is too abrupt.
RBC5RE10	02:56:34	1	2	Releasing the cells is too abrupt.
RBC5RE5		137	18	(MPI) InfiniBand retry count exceeded.
RBC5RE5		139	29	Segmentation fault when loading modules.
RBC5RE5	02:08:38	1	1	Adjusted cell release is still abrupt.
RBC5RE5	01:56:47		4	Corrupted double-linked list.
RBC0RE10	02:06:40		1	Segmentation fault when loading modules.

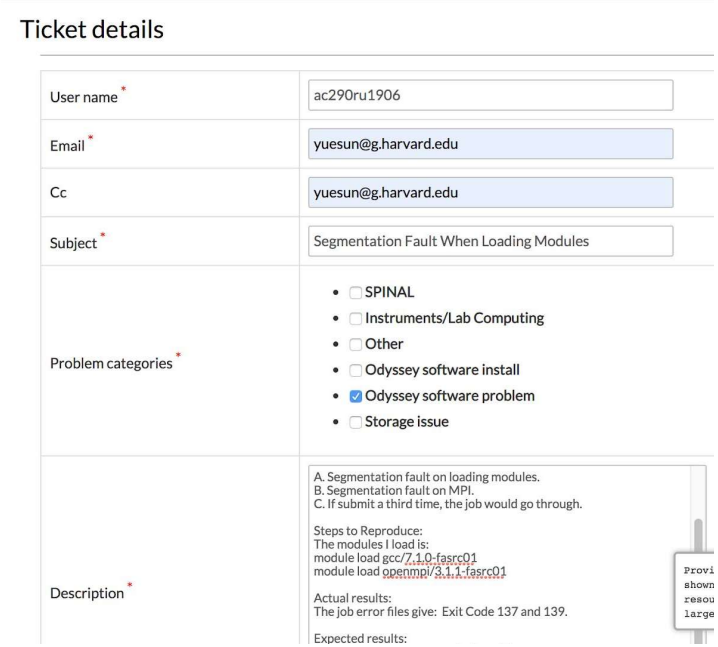
What Happened to the Re=5 RBC 5% Runs?

- When launching the job, received Segmentation Fault (Exit Code 139) pointing to the module loading section in the batch script. Relaunching the job, received Segmentation Fault (Exit Code 137) pointing to MPI processes communication error.
- After some resubmissions, the only scenario for the job to run was to: Receive Exit Code 139 → Receive Exit Code 137 →Job start.
- There were four jobs submitted successfully, and all of them ran for a while (10001/17201/21501/21501) of the total objective time steps (60000) and failed. The error logs point to a possible memory issue which we failed to trace back:

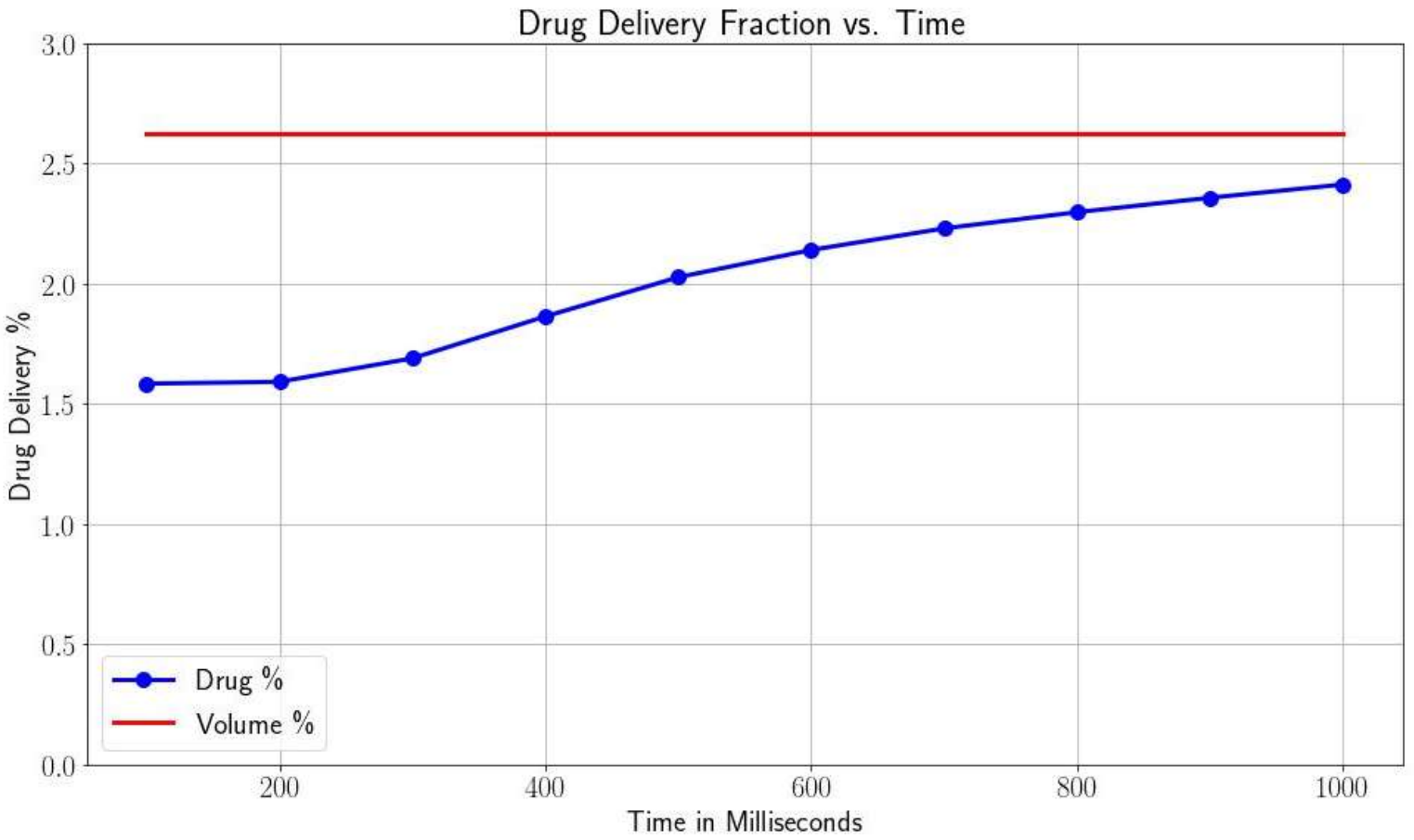
```
*** Error in `/usr/bin/python2': malloc(): memory corruption: 0x0000000004e6b460 ***
*** Error in `/usr/bin/python2': free(): invalid next size (normal): 0x0000000065e5780 ***
*** Error in `/usr/bin/python2': corrupted double-linked list: 0x0000000004af4770 ***
*** Error in `/usr/bin/python2': corrupted double-linked list: 0x000000000558fed0 ***
```

It’s Not A Perfect World...

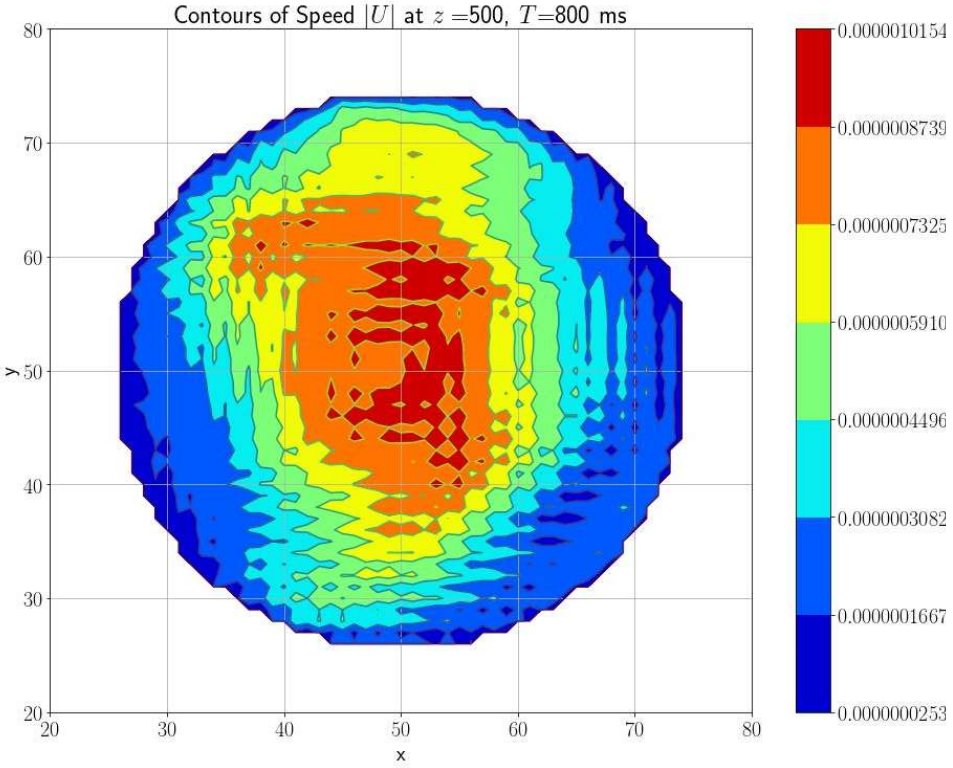
- Always run smaller test cases before launching the actual full-scale simulation
- Some errors are unexpected, and submitting jobs repeatedly may help. However, we need to be aware of the instability of highly distributed systems like this one.
- Data transfer from Odyssey is very time consuming and slow. Therefore, for post-processing we need to be aware of the size of files and the time of downloading.

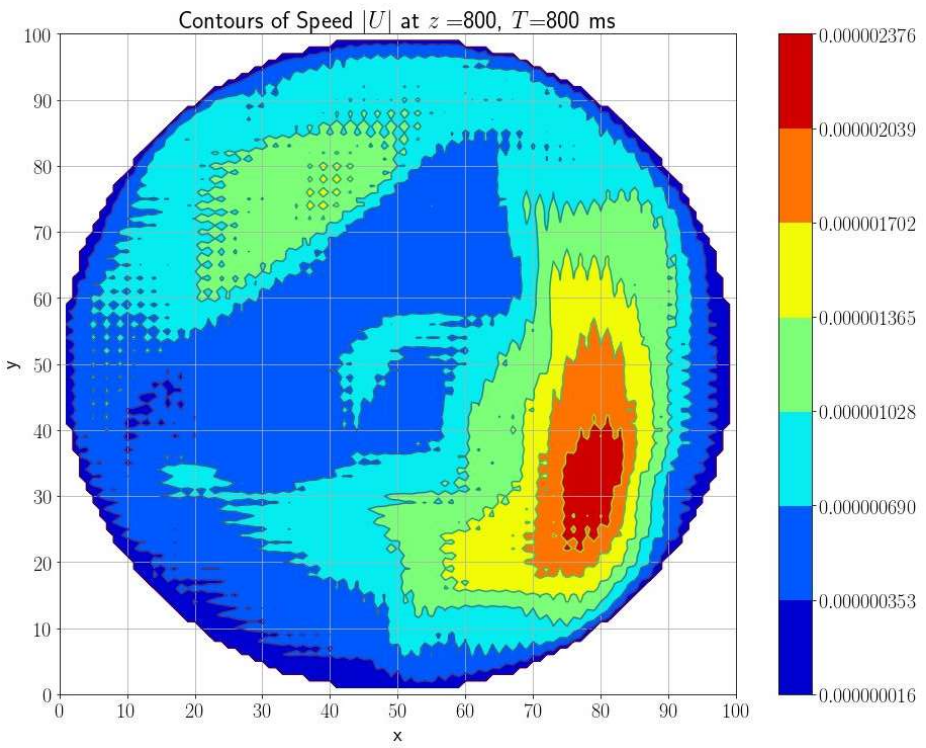


Drug Delivery Over Time

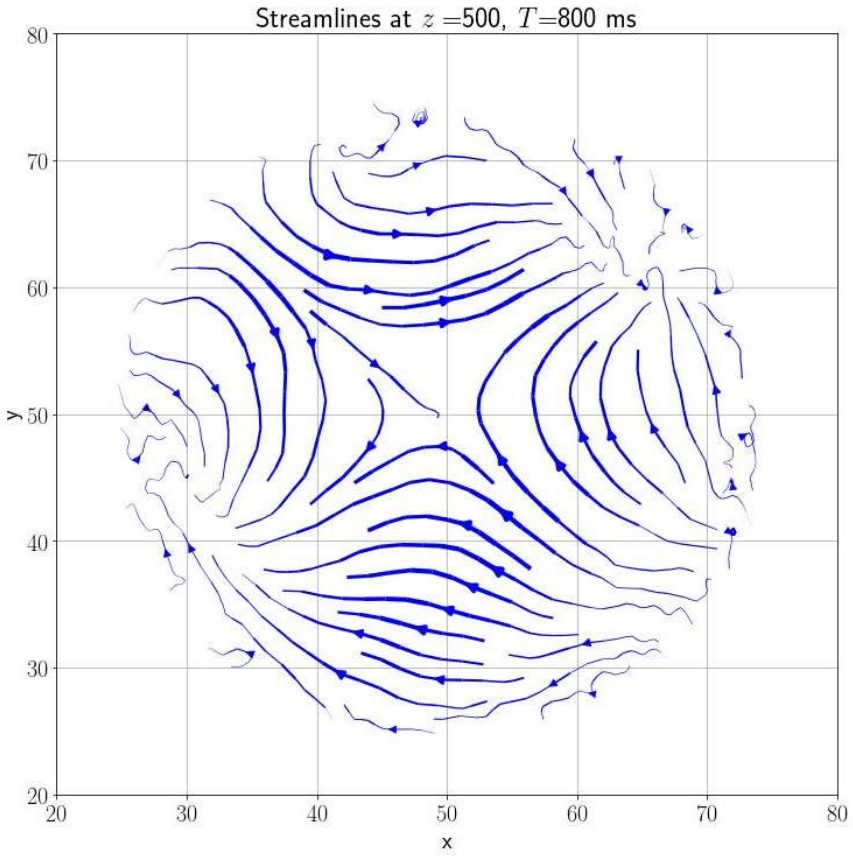


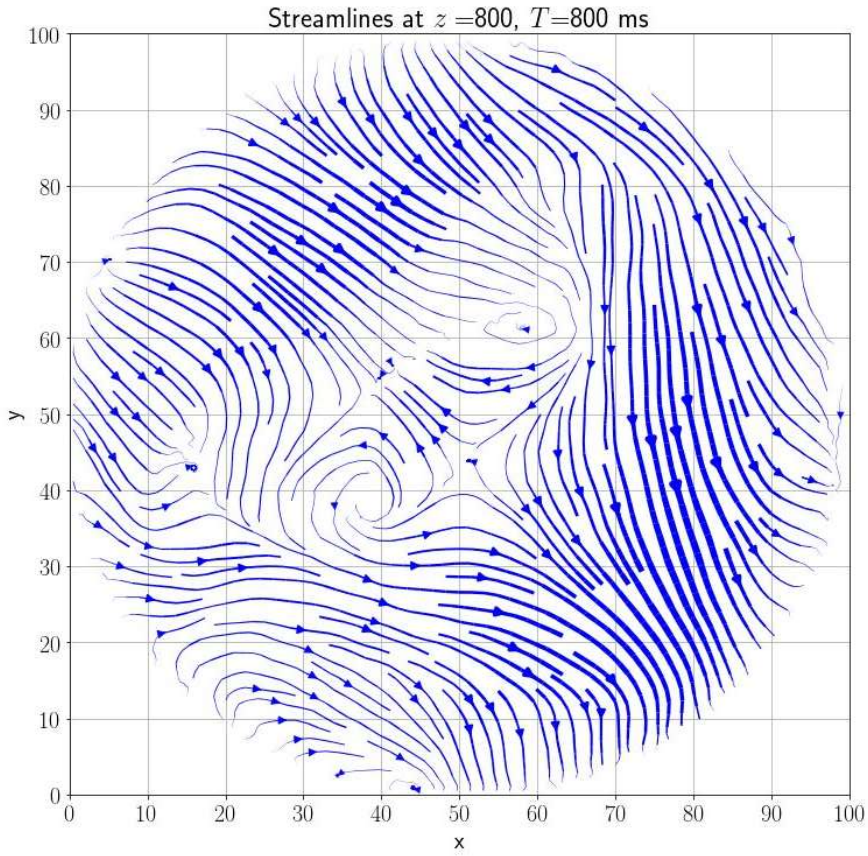
Contour Plots of Speed



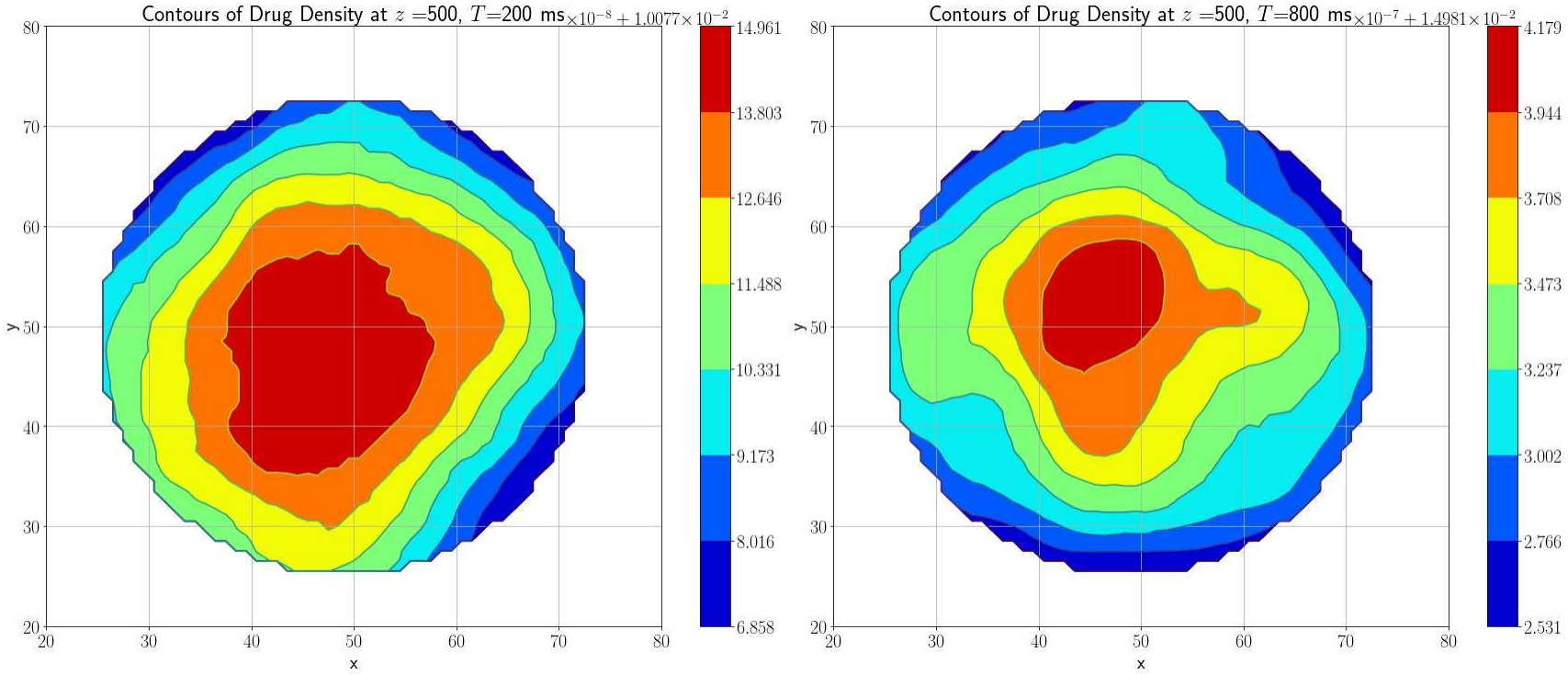


Streamlines

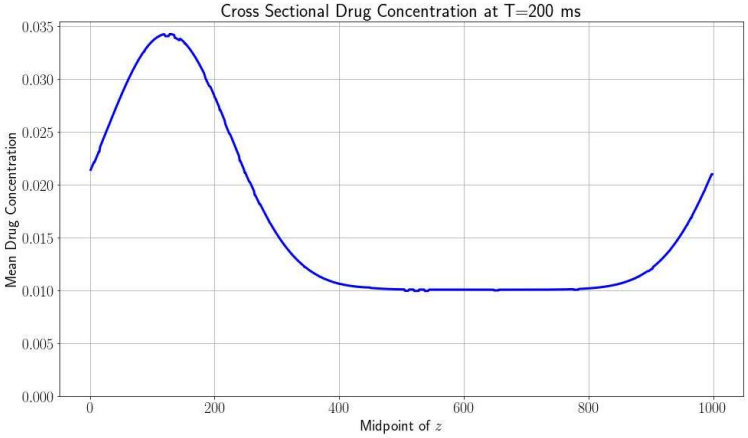


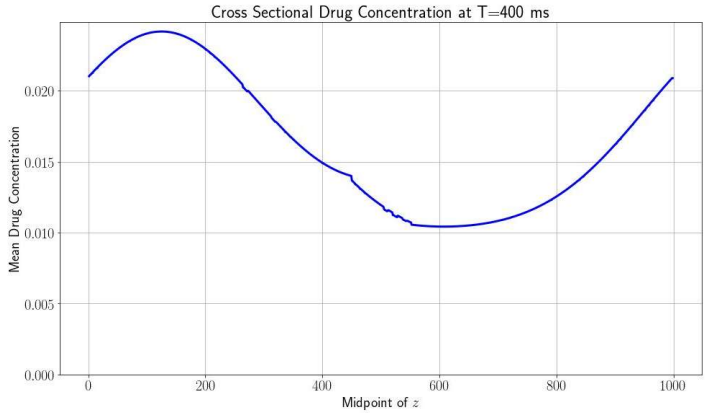


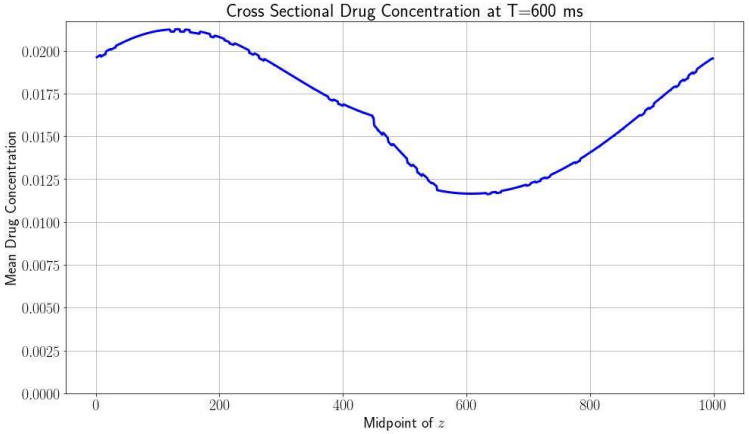
Contour Plot of Drug Density

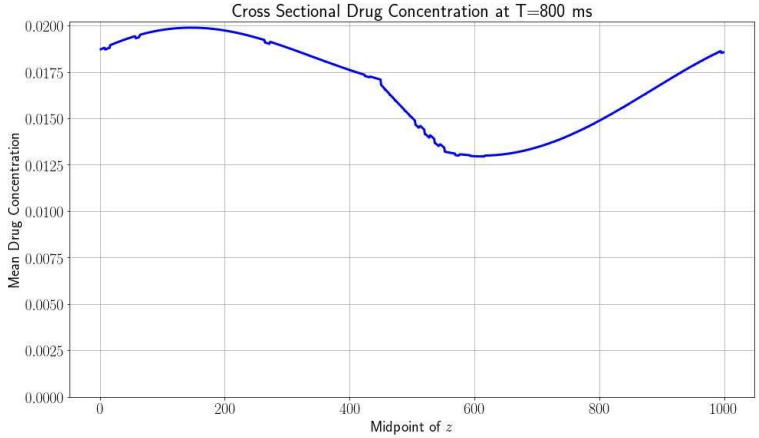


Longitudinal Drug Profile

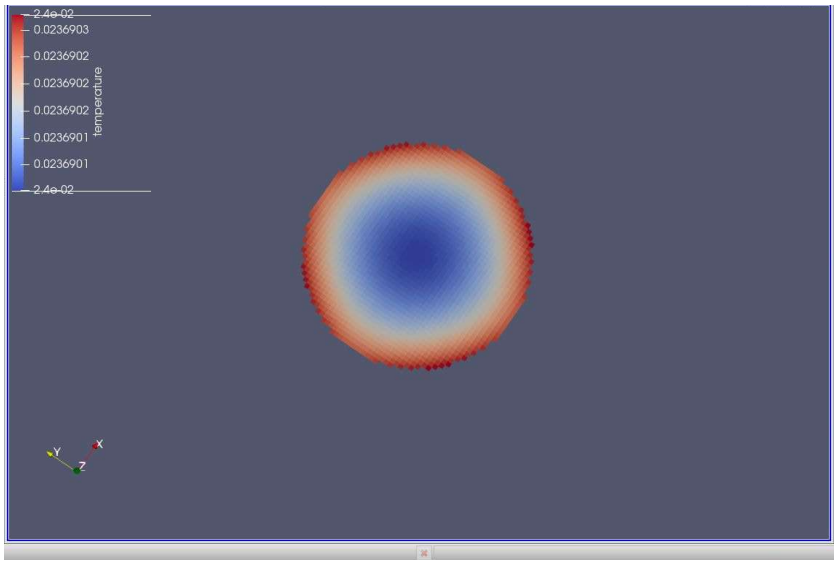




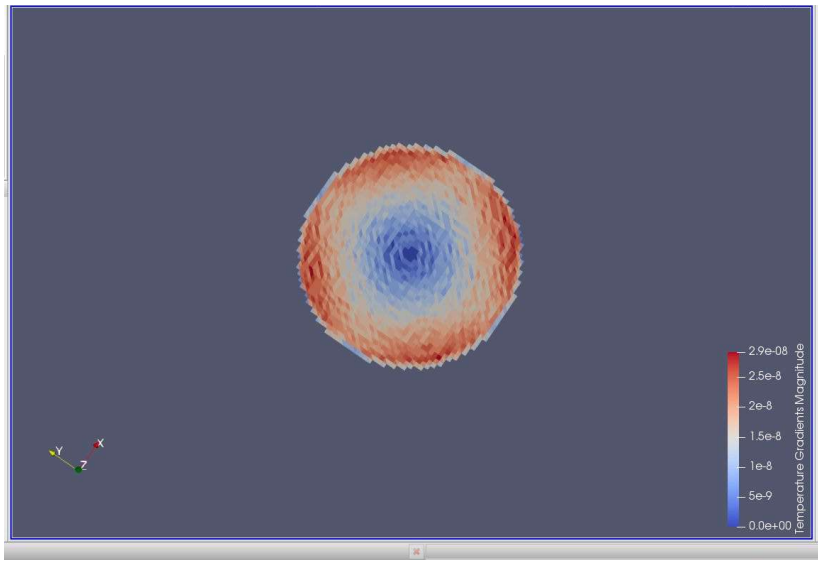




Schlierin



Temperature Field of Bolus
at Z = 457, T = 80000 for Re = 5, RBC = 0%



Temperature Gradient of Bolus
at Z = 457, T = 80000 for Re = 5, RBC = 0%

Schlierin & Color Palettes

Movie

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Conclusions: Hemodynamic System

- Baseline simulation suggests that the drug diffuses to equilibrium levels rapidly (~1 second) and specific geometry not too important
- Since the RBC runs failed, we couldn't learn about their effect on the simplified system, though we expect it to be small in a large artery
- To refine the simulation, we need a more accurate geometry, ideally a scan of a patient; probably more important than RBC for accuracy
- Suggested directions for future work:
  - More accurate geometry; replace period boundaries with heart & veins
  - Shift from CPU to GPU computing
  - More accurate biochemistry model

Conclusions: Extreme Computing

Grazie Mille, Grazie Ragazzi