Modeling of Circulating Cancer Cells

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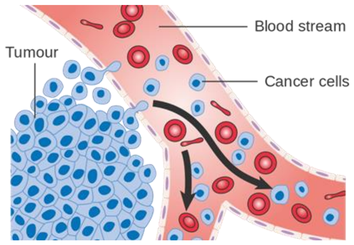
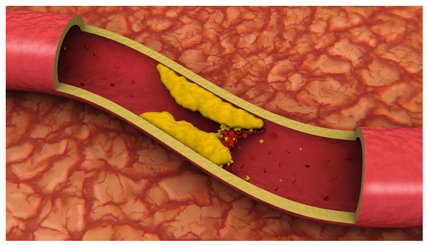
Background – Why Simulate Blood?

There are many Deadly Aliments that are Bloodborne in Origin:

Metastatic Cancer – Cancer Cells that break off larger tumors and travel in the blood flow



Vascular Disease – Such as Myocardial Infarctions
- **Mainly Caused by build up in vessels**



Together Cancer and Vascular Disease Cause ~1.3 Mil Deaths per year in the USA (according to cdc.gov)

Number of deaths for leading causes of death

- Heart disease: 647,457
- Cancer: 599,108
- Accidents (unintentional injuries): 169,936
- Chronic lower respiratory diseases: 160,201
- Stroke (cerebrovascular diseases): 146,383
- Alzheimer's disease: 121,404
- Diabetes: 83,564
- Influenza and pneumonia: 55,672
- Nephritis, nephrotic syndrome, and nephrosis: 50,633
- Intentional self-harm (suicide): 47,173

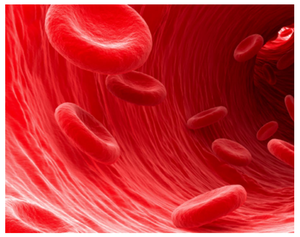
Increase Pace of Development
- In Medicine Experiments can take days or weeks
- In Simulations this time can be cut down drastically

Avoids Human and Animal Testing
- Simulation may replace the testing that is currently performed on animals and humans

It Is Becoming More Accessible
- As Personal Computing Power increases more and more complex systems become viable to simulate

Background – Blood

- **Normally Blood is ~50% Red Blood Cells (RBC) by volume, most of the remaining volume is water.**
  - The RBC's contribute the majority of the mechanical properties to the blood as a whole
  - Due to this Simulations of Blood Focus on RBC's
  - **RBC's are different from most cells:**
    - Lack Nucleus; Free Floating; No Division
- **RBC's are also similar in many ways:**
  - Lipid Bilayer Outer Membrane ; Cytoskeleton



Background – Cancer

- **Cancer is a leading Cause of Mortality and Costly Healthcare worldwide**
- **According to (cancer.org) ~ 1.7 Mil New Cases per Year**
- **Most Dangerous Behavior of Cancer:**
  - **Metastasis – The process of Tumor Cells entering the bloodstream by separating from a Main Tumor**
  - **So Dangerous because Cancer may spread around the body; Potentially to Vital Areas : Brain, Heart**

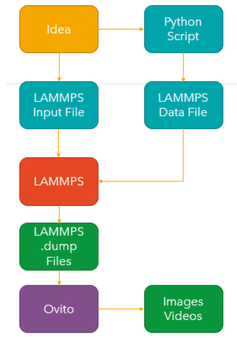
Background – Simulation

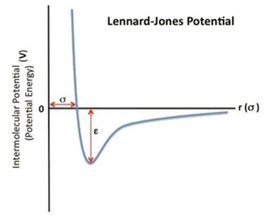
- **To Perform Simulation follow these Simple Steps:**
  - **1. Create Simulation – Specify Inputs:**
    - Simulation Parameters
    - Initial Geometry
    - Data Output Commands
  - **2. Run Simulation –**
    "Environment" setup around the simulation needs to be set correctly
  - **3. Analyze Results – Raw Data is Often Hard to Read**
    - Use Analysis tools to create:
      - Graphs
      - Tables
      - Images
      - Videos

Simulation Software : LAMMPS

- **(Large-scale Atomic/Molecular Massively Parallel Simulator)**
- **A Good Choice for Molecular Dynamics (MD) Code**
  - Open Source ; Well Documented
  - Large User Support Base
  - Simulates down to Atomic level
  - Growing Biomolecules Support

Generalized LAMMPS Workflow





$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

Important LAMMPS Input Parameters

Pair_style – Sets how different particles interact with one another; Governed by Potentials
- **Refer to Graph above:**
  - When particles close HIGH REPULSION
  - When particles far apart LOW ATTRACTION

Velocity – Sets Velocity of Particles
- Can be set Directionally or Randomly

Neighbor – Sets the area around each particle in which other particle interactions accounted for

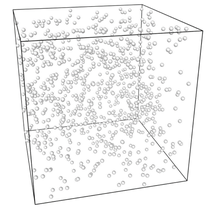
Dump – Writes data from the simulation to a .dump file
- Dump files can be converted to many forms
  - Images
  - Videos
  - Graphs, etc.

Software Tools

- **Python – Open Source; Programming Language**
  - **Used to write Lammps.data file**
- **Ubuntu – Open Source; Shell Operating System**
  - **Used to Edit, Compile and Run LAMMPS**
- **Ovito – Open Source ; Visualization Tool**
  - **Used to Produce Movies and Images from data files**

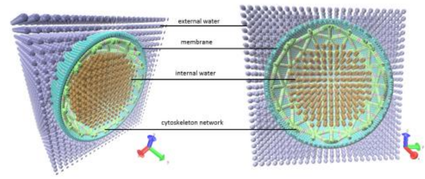
Example Simulations

- **JQ-Random – An Example I made for this Poster**
  - **1000 Water Atoms ;**
  - **Randomly Assigned Velocity and Positions**



Cell Simulations

- **Currently I am working on Producing a more Refined model of RBC and then to use this to make a Cancer Cell model**
- **Made up of 3 parts:**
  - **Lipid Bi-Layer Membrane**
  - **Spectrin Cytoskeletal Network**
  - **Water Molecules Within and outside**



- **Cancer Cell Model is modeled by taking the RBC Model and altering it slightly**
  - **Because Cancer cells have similar properties**
- **Once these are both built the "Detection" Simulation will be made to sort out the Cancer and RBC's**
  - **This will function by a couple possible methods**
    - **Micro Fluidics Channel**
    - **Induction of Mechanical Stress**
  - **Both of these methods can be verified by using Published Experimental Data**

References and Acknowledgments

References and all Project Files Can be found at:
https://github.com/jqstudy2019/lammpsfiles

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Thanks for Looking! If you have any questions:

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