Computational Mathematics Research: Developments, Challenges and Opportunities

Jia Zhao

Assistant Professor of Mathematics
Department of Mathematics & Statistics
Utah State University

Motivation of This Lecture
From: *The Mathematical Science in 2025*

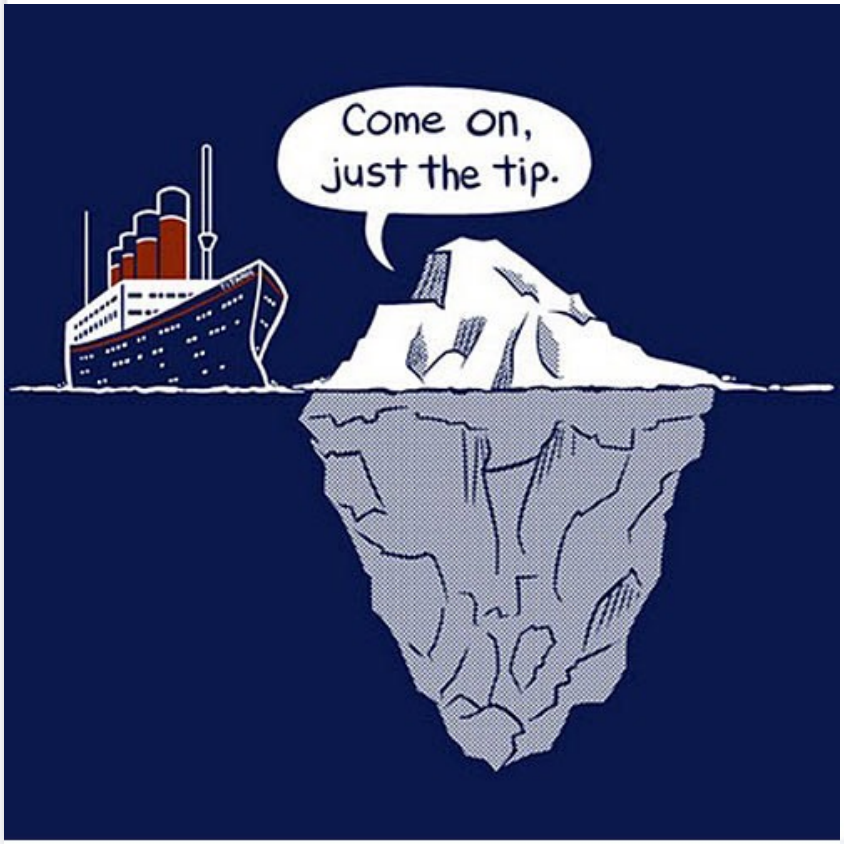
- This book "*explores the changes needed for the discipline to be in a strong position and able to maximize its contribution to the nation in 2025*".
- It emphasis an important trend in the mathematical sciences: "the mathematical sciences should more thoroughly embrace computing".
- We are forming a Committee at Dept. of Math & Stat, USU to design computing curriculum to better prepare our undergraduate/graduate students for the competitive market.

The Mathematical Science in 2025, by National Research Council, Division on Engineering and Physical Sciences, Board on Mathematical Sciences and Their Applications.

UtahState University

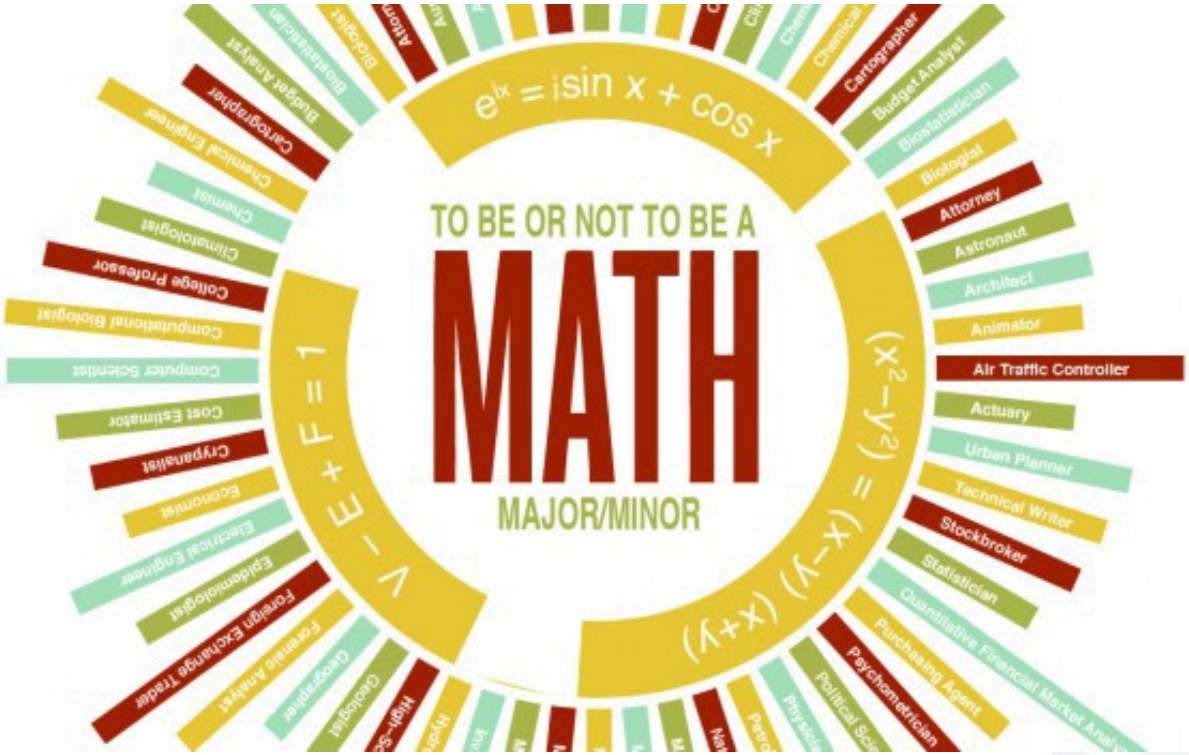
The Main Message

Learning Computational Skills is the Key to Jobs!



UtahState University

The mathematical sciences are part of nearly all aspects of every discipline.



Cartographer
Budget Analyst
Biologist
Attorney
Animator
Air Traffic Controller
Actuary
Urban Planner
Technical writer
Stockbroker
Statistician
Purchasing agent

https://www.math.uh.edu/~tomforde/

UtahState University

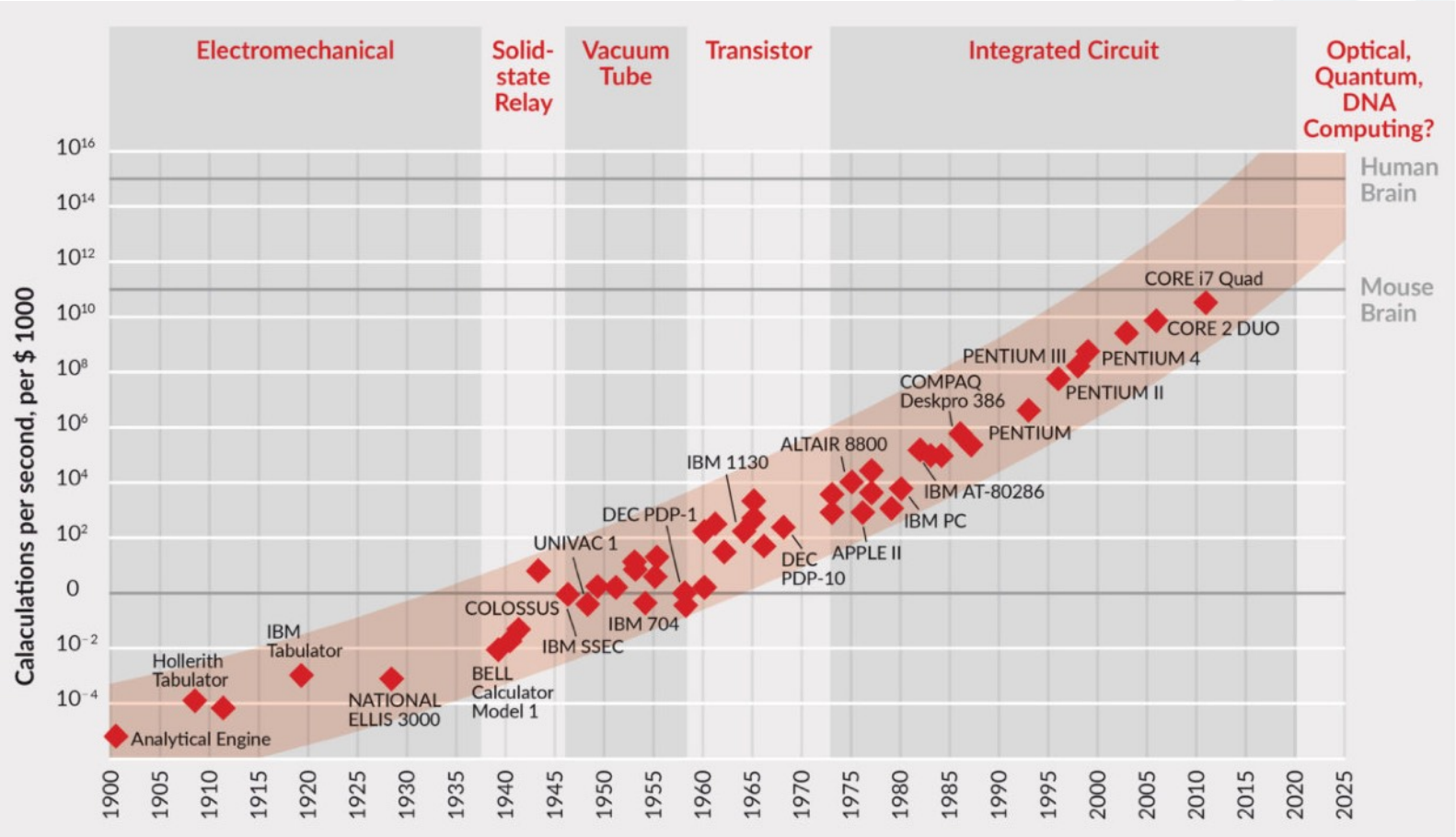
The computational mathematical sciences are part of nearly all aspects of every discipline.

Pick any field **X**, from archeology to zoology. There either is now a "**Computational X**" or there soon will be.

https://www.wired.com/2016/09/how-to-teach-computational-thinking/

UtahState University

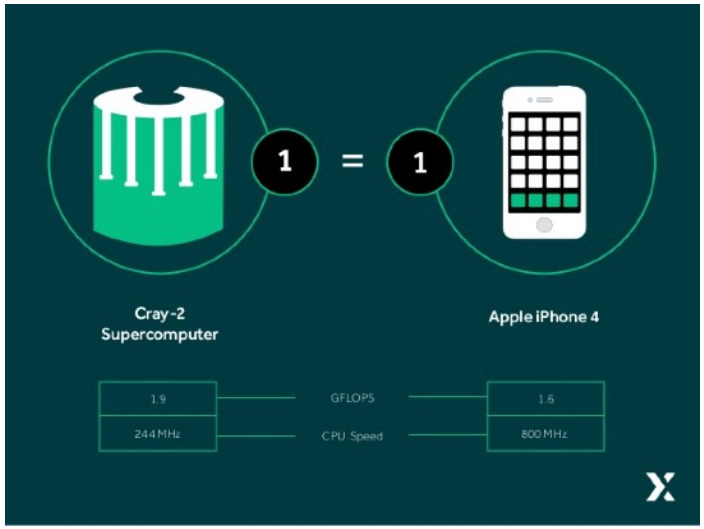
The Computing Power is Growing Exponentially



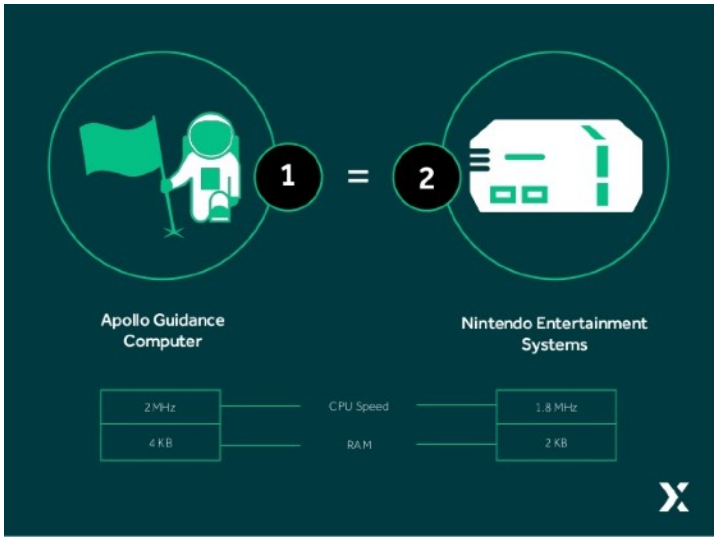
- In 2025, it will surpass brainpower of human.
- In 2045, it will surpass brainpower equivalent to that of all human brains combined.

UtahState University

The Computing Power is Growing Exponentially



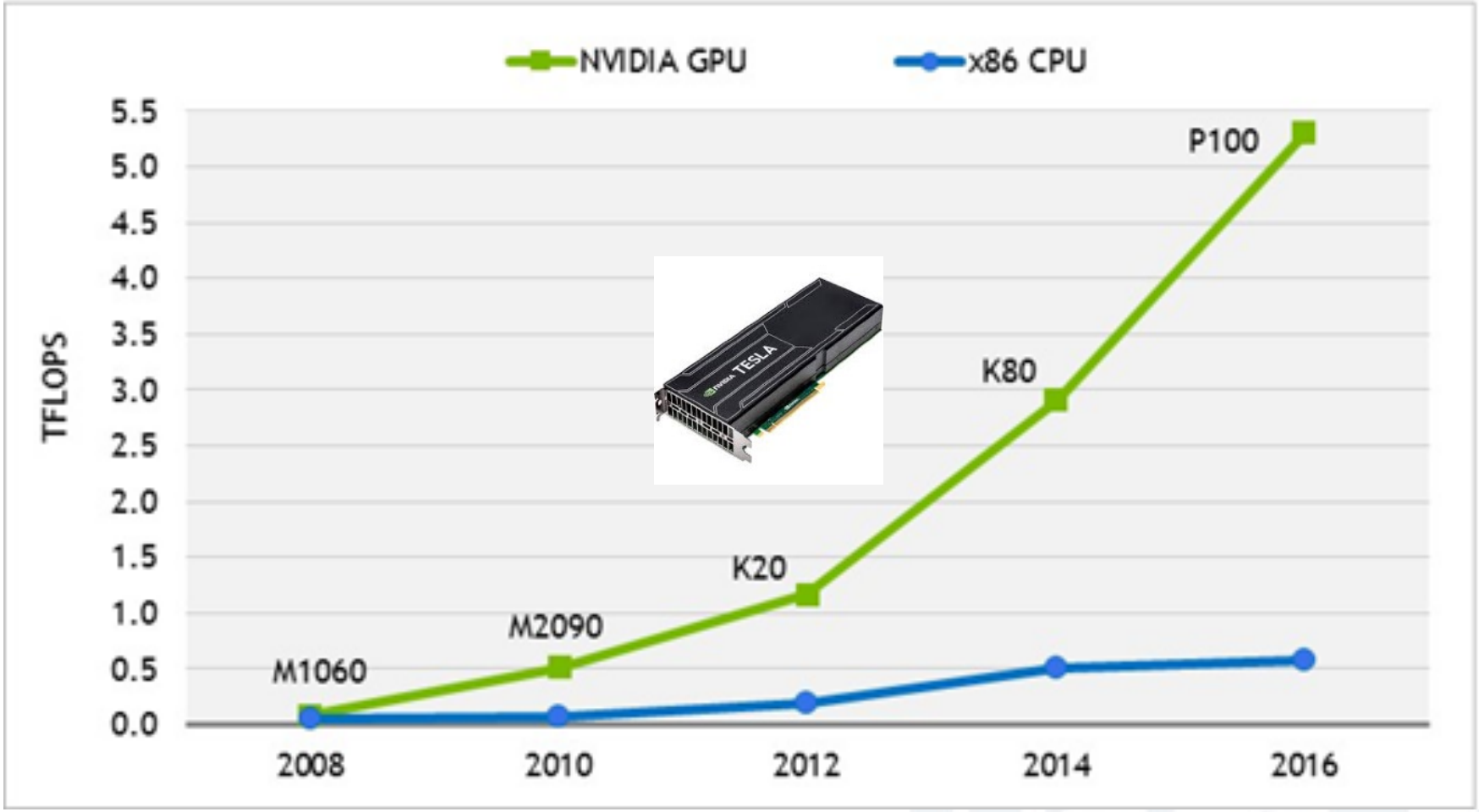
A single Apple iPhone 4 has 2.7 times the processing power than the 1985 Cray-2 supercomputer!



The NES contains half of the processing power as the computer that brought Apollo to the moon!

https://www.slideshare.net/Experts-Exchange/processing-power-compared

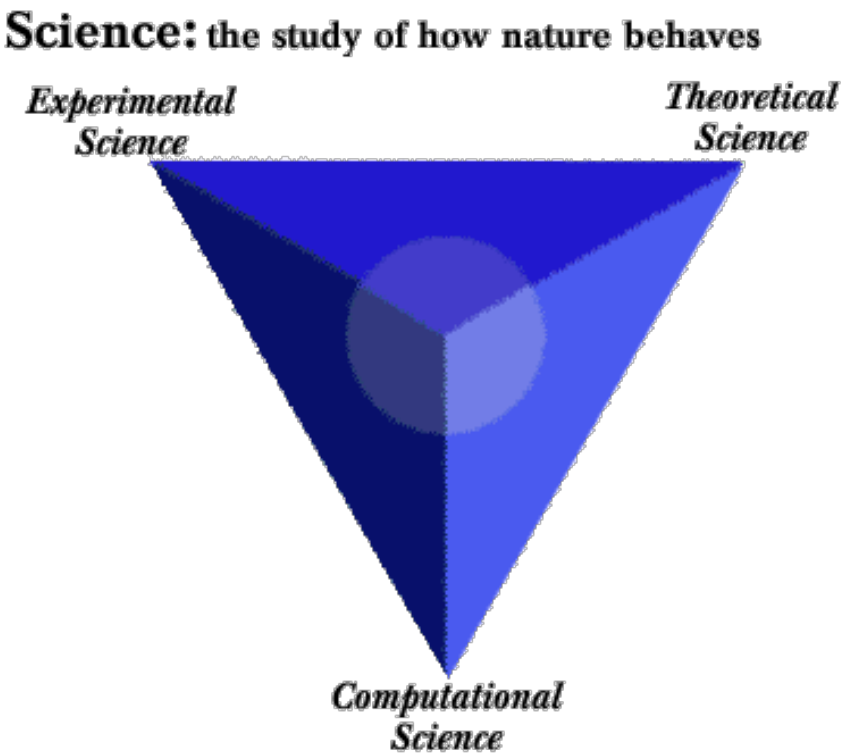
UtahState University

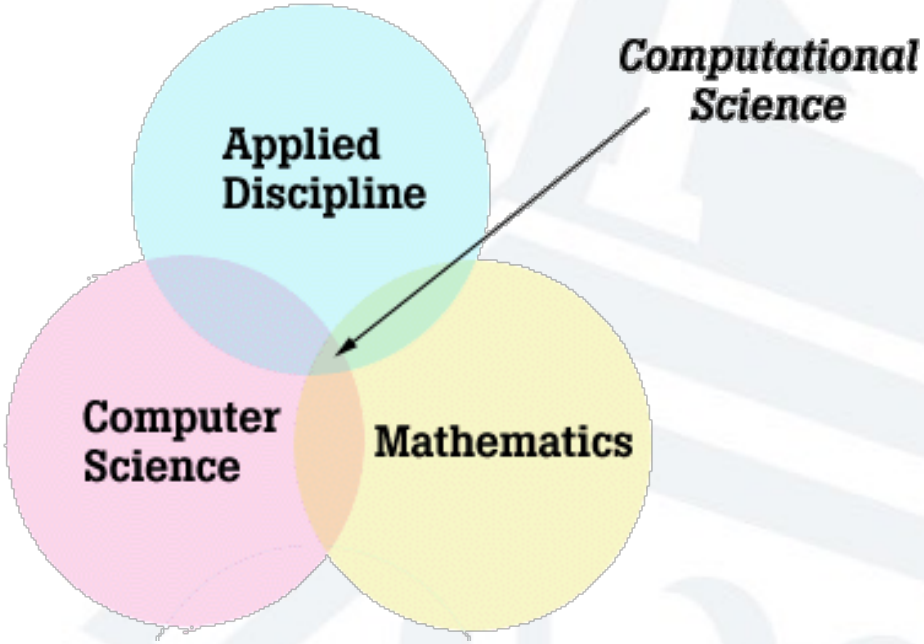


The GPU continues to deliver impressive gains in compute price/performance that far out-pace what is now possible with multi-core x86 CPUs. (Source: NVIDIA)

UtahState University

Where do “Computational Mathematics” stay?



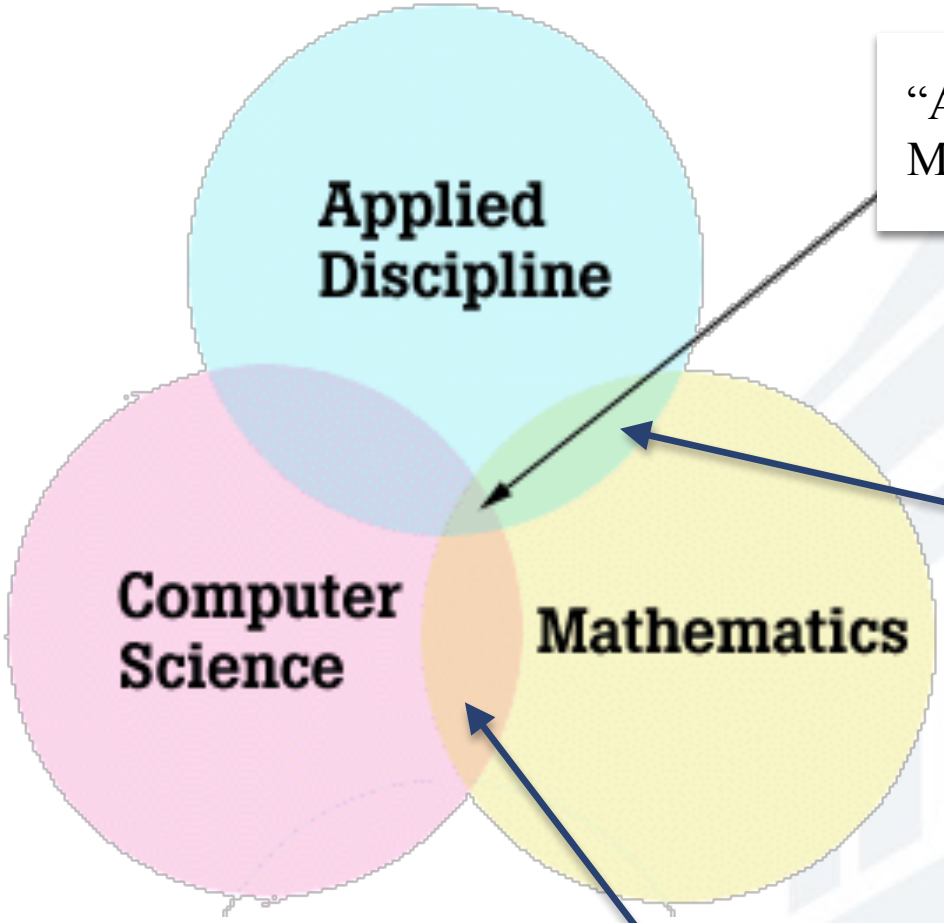


Computational Mathematics: concerned with the design, analysis, and implementation of algorithms for the numerical solution of problems that have no tractable analytical solution.

https://www.shodor.org/chemviz/overview/compsci.html

UtahState University

Where do “Computational Mathematicians” stay?



“Applied” Computational Mathematicians

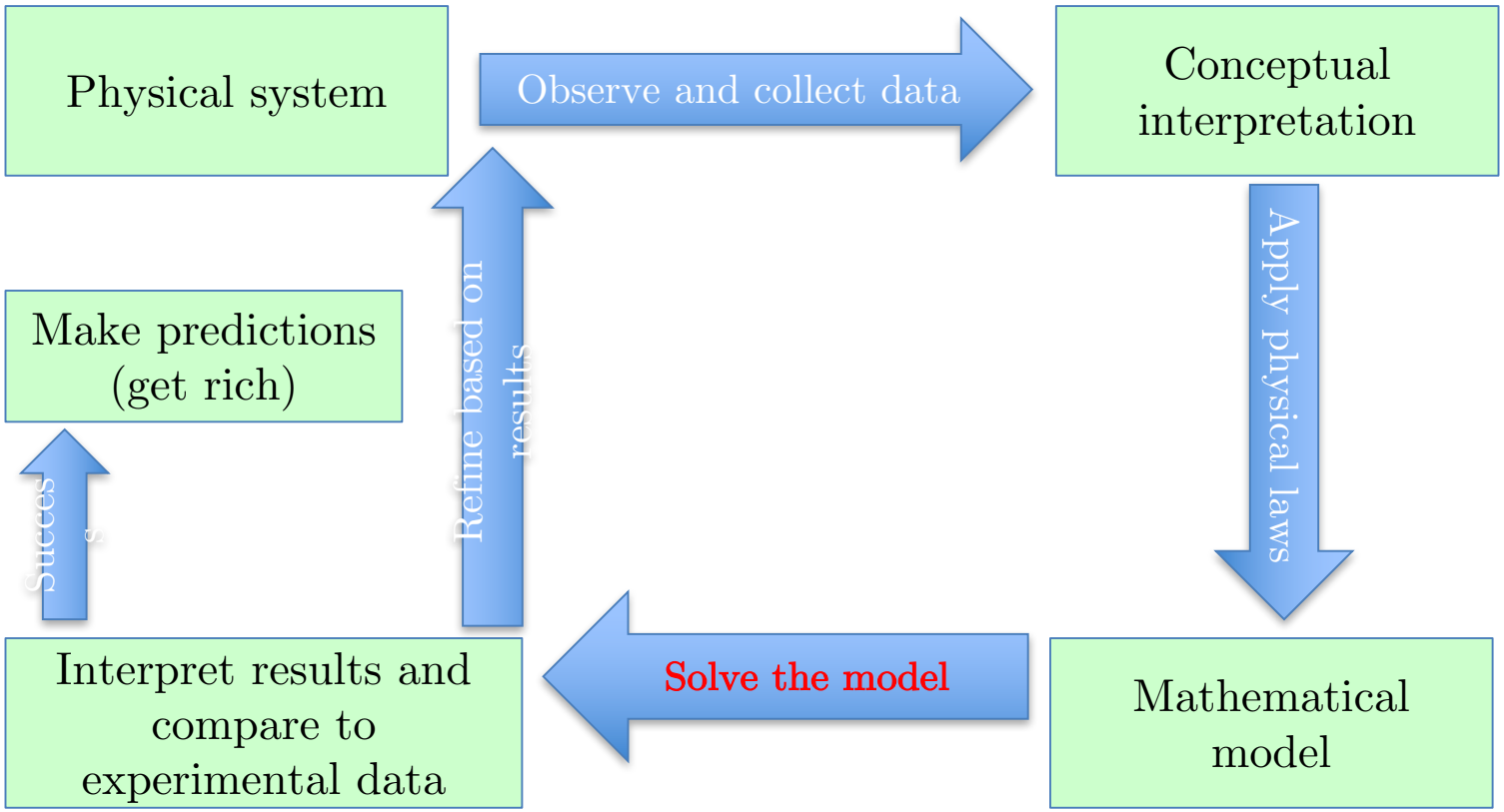
Applied Mathematicians

“Pure” Computational Mathematicians

UtahState University

Why is Computational Mathematics Important?

- Consider the following simplified model of the scientific process:

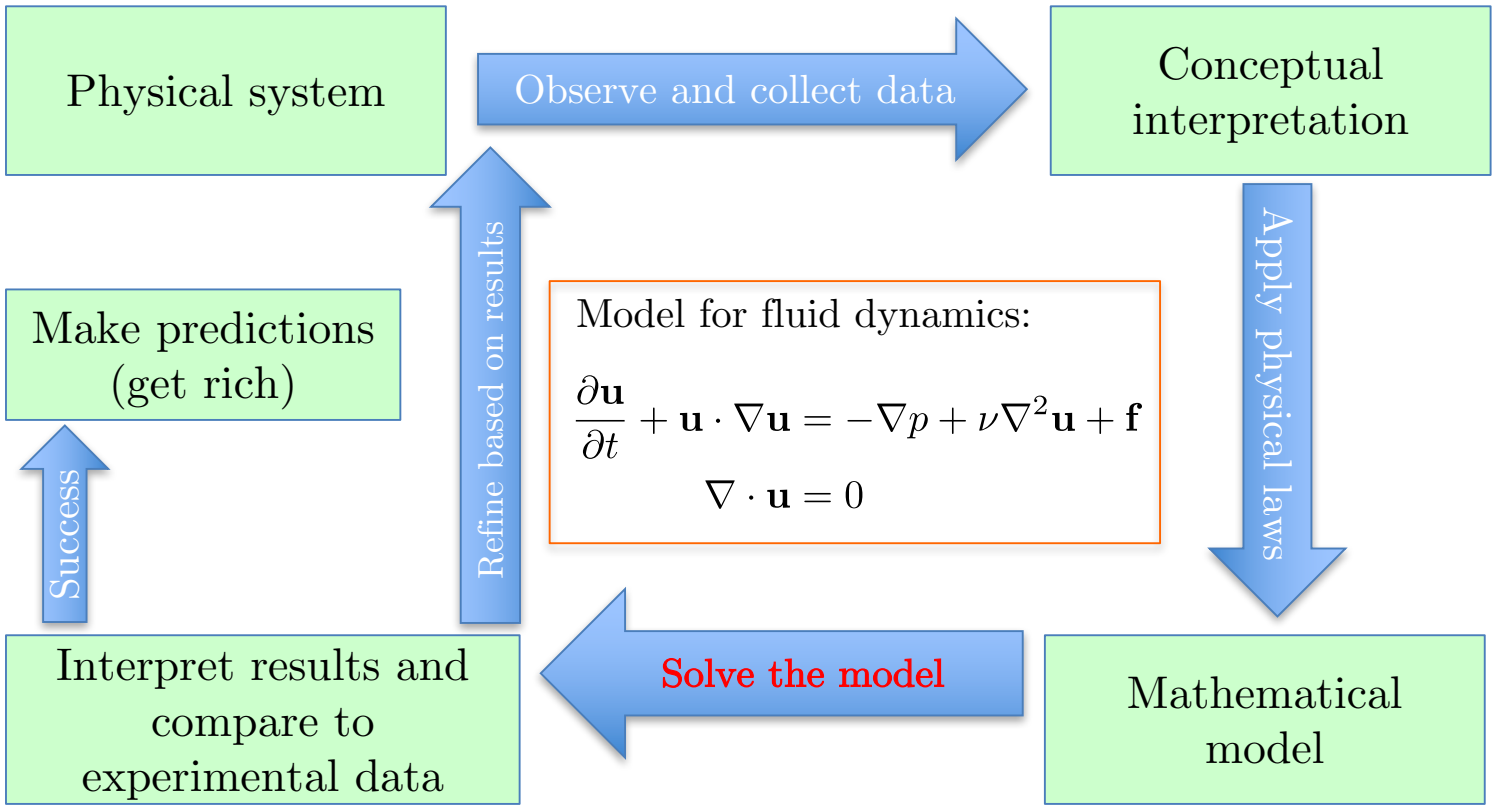


- Computational math fits in the solution phase, and often in the interpretation phase.

math.boisestate.edu/~wright/courses/m565/Introduction.pdf

Why is Computational Mathematics Important?

- Consider the following simplified model of the scientific process:



- Why: The resulting models can essentially never be solved completely using analytical (pencil and paper) methods.

UtahState University

Mathematicians V.S. Computational Mathematicians

Problem: solving a system of linear equations with n unknowns.

- We know Cramer's Rule gives an explicit formula for the solution.
- To use Cramer's Rule, we need calculate n+1 of n-th order determinant, where each n-th order determinant requires n! operations.
- If we have a computer with 3.0 GHz (300 billion per second) and n=20, the total time for is

$$\frac{21 \times 20!}{3 \times 10^{11} \times 60 \times 60 \times 24 \times 365} \approx 5.4$$ **Years**

UtahState University

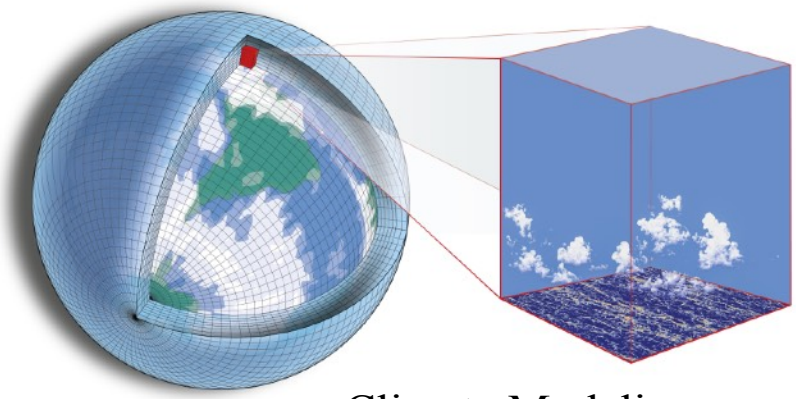
Computational Mathematics: Trends and Opportunities

The boundary of Computational Mathematics with other fields is becoming blur.

UtahState University

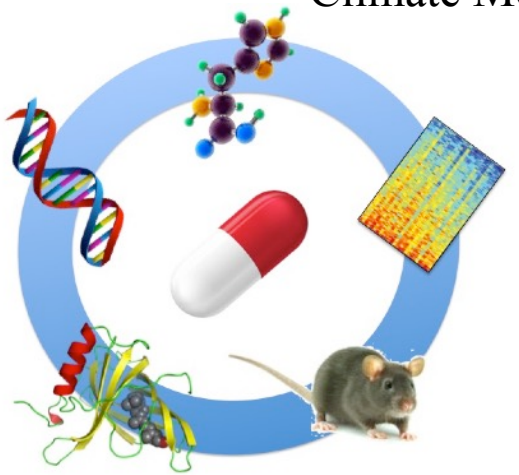
New Trends: Interdisciplinary Research

Multidisciplinary science is an ecosystem, not a battlefield.

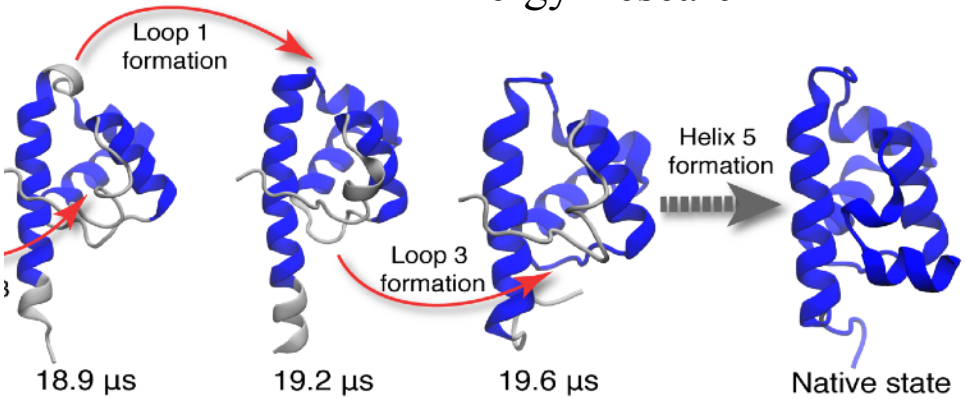


Climate Modeling

Energy Research



Drug Discovery



Protein Folding

UtahState University

Modeling, Computation and Analysis of Complex Fluids Flow with Applications in Engineering and Life Science

UtahState University

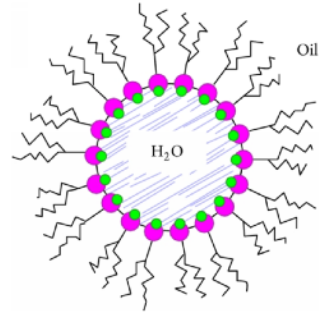
Complex fluids are fluids made up of a lot of different kinds of stuff (Gelbart et al., 1996)

Ketchup

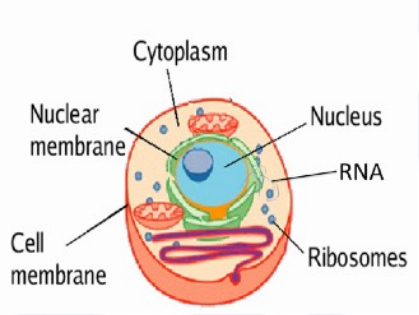
Dough

Egg (emulsion)

Foam

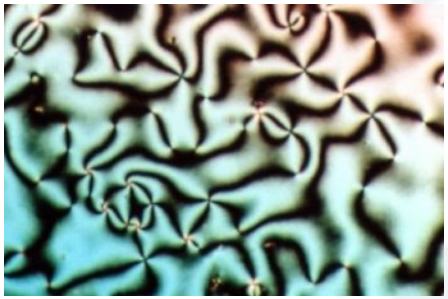


Micelles



Cytoplasm

Milk (colloid)



Liquid Crystals

Biofilms

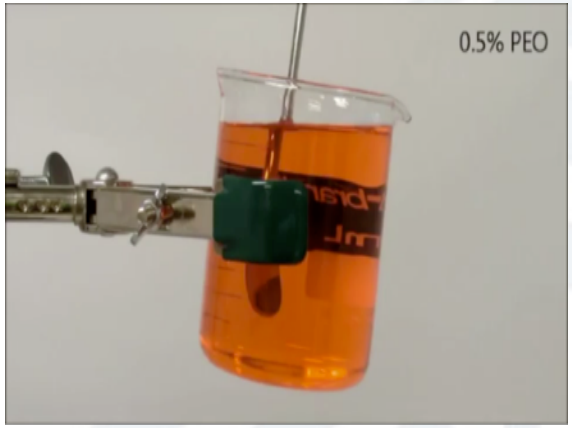
Images are from Google

UtahState University

Complex fluids have dramatically different properties

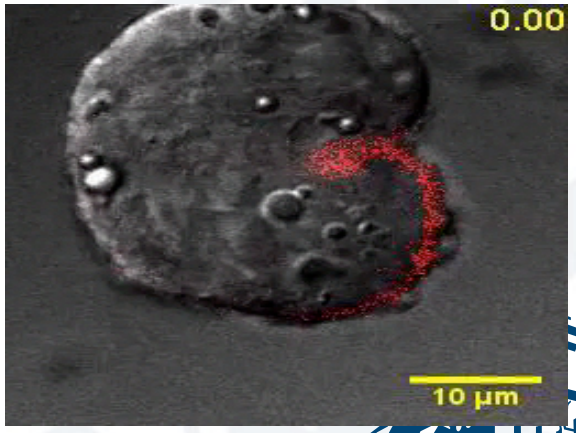
- Complex fluids consist of ”microstructure”, e.g., polymers, mucin molecules, actin filaments, liquid crystals.
- The microstructure stores and releases stress under deformation.

Weisenberg effect: rod climbing



Open siphon effect: dipping

Beads-on-a-string structures



Cytoplasm flow

UtahState University

Current Collaborators

Mathematical Modeling	
Numerical Analysis	
HPC Software	with graduate students
Interdisciplinary Applications	

Our Approach: Energy Variation + Onsager Principle

- We use **Energy Variation** to derive the rotation-invariant stress and translation-invariant stress, such that the model is **frame invariant**.
- We use **Onsager Principle** to derive the general flux, such that the model is **thermodynamically consistent**.

Consider viscoelastic fluids (one type of complex fluids) with total energy **E(v, C)**, where

- **v** is the velocity field, and
- **C** is the conformation tensor (a measure of microstructure deformation).

rotation invariant translation invariant

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \nabla \cdot (-\mathbf{CH} - \mathbf{HC} + \tau^s) - \mathbf{H}\nabla\mathbf{C}, \quad \mathbf{H} = -\frac{\delta E}{\delta \mathbf{C}}$$

$$\nabla \cdot \mathbf{v} = 0,$$

$$\partial_t \mathbf{C} + \mathbf{v} \cdot \nabla \mathbf{C} - \nabla \mathbf{v} \cdot \mathbf{C} - \mathbf{C} \cdot \nabla \mathbf{v}^T = \mathbf{G}.$$

UtahState University

A General Model for Complex Fluids Flow

$$
\begin{cases}
\rho\Big(\partial_t \mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}\Big) = -\nabla p + \nabla\cdot\Big(\frac{1}{2}(\mathbf{ph}-\mathbf{hp}) + (\mathbf{Q}\cdot\mathbf{H}-\mathbf{H}\cdot\mathbf{Q})\Big) \\
\quad +\nabla\cdot\tau_s - (\phi\nabla\mu + \nabla\mathbf{p}\cdot\mathbf{h} + \nabla\mathbf{Q}:\mathbf{H}), \\
\nabla\cdot\mathbf{v} = 0, \\
\partial_t\phi + \nabla\cdot(\mathbf{v}\phi) = -\nabla\cdot\mathbf{J}, \\
\partial_t\mathbf{p} + \mathbf{v}\cdot\nabla\mathbf{p} + \mathbf{W}\cdot\mathbf{p} = \mathbf{g}, \\
\partial_t\mathbf{Q} + \mathbf{v}\cdot\nabla\mathbf{Q} + \mathbf{W}\cdot\mathbf{Q} - \mathbf{Q}\cdot\mathbf{W} = \mathbf{G},
\end{cases}
\qquad
\begin{pmatrix} \tau_s \\ \mathbf{J} \\ \mathbf{g} \\ \mathbf{G} \end{pmatrix} = \mathcal{A}\begin{pmatrix} \mathbf{D} \\ -\nabla\mu \\ \mathbf{h} \\ \mathbf{H} \end{pmatrix}
$$

where $\mathbf{v}$ is the velocity, ρ is the density, ϕ is the volume fraction of one fluid, $\mathbf{p}, \mathbf{Q}$ are vector and tensor respectively to represent the microstructure arrangement, and $\mathbf{H} = -\frac{\delta F}{\delta \mathbf{Q}}$, $\mathbf{h} = -\frac{\delta F}{\delta \mathbf{p}}$, $\mu = \frac{\delta F}{\delta \phi}$.

L. Onsager. Physical Review, 37:405–426, 1931.

L. Onsager. Physical Review, 38:2265–2279,1931.

Yang, Forest, Wang, Soft Matter, 10:6758–6776, 2014.

Yang, Li, Forest and Wang, Entropy, 18(6):202, 2016.

Joanny et al., New Journal of Physics, 9:422, 2007.

UtahState University

Original Model

$$
\begin{cases}
\rho\Big(\partial_t \mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}\Big) = -\nabla p + \nabla\cdot\Big(\frac{1}{2}(\mathbf{ph}-\mathbf{hp}) + (\mathbf{Q}\cdot\mathbf{H}-\mathbf{H}\cdot\mathbf{Q})\Big) \\
\quad +\nabla\cdot\tau_s - (\phi\nabla\mu + \nabla\mathbf{p}\cdot\mathbf{h} + \nabla\mathbf{Q}:\mathbf{H}), \\
\nabla\cdot\mathbf{v} = 0, \\
\partial_t\phi + \nabla\cdot(\mathbf{v}\phi) = -\nabla\cdot\mathbf{J}, \\
\partial_t\mathbf{p} + \mathbf{v}\cdot\nabla\mathbf{p} + \mathbf{W}\cdot\mathbf{p} = \mathbf{g}, \\
\partial_t\mathbf{Q} + \mathbf{v}\cdot\nabla\mathbf{Q} + \mathbf{W}\cdot\mathbf{Q} - \mathbf{Q}\cdot\mathbf{W} = \mathbf{G},
\end{cases}
$$

$$
\begin{pmatrix} \tau_s \\ \mathbf{J} \\ \mathbf{g} \\ \mathbf{H} \end{pmatrix} = \mathcal{A} \begin{pmatrix} \mathbf{D} \\ -\nabla\mu \\ \mathbf{h} \\ \mathbf{H} \end{pmatrix}
$$

Equivalent Model

$$
\rho\Big(\partial_t \mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}\Big) = -\nabla\Pi + \nabla\cdot\tau_s + \nabla\cdot\Big(\frac{1}{2}(\mathbf{ph}-\mathbf{hp}) + (\mathbf{Q}\cdot\mathbf{H}-\mathbf{H}\cdot\mathbf{Q})\Big)
$$

$$
-(\phi\nabla\mu + \nabla\mathbf{p}\cdot\mathbf{h} + \nabla\mathbf{Q}:\mathbf{H}).
$$

$$
\nabla\cdot\mathbf{v} = 0,
$$

$$
\partial_t\phi + \nabla\cdot(\mathbf{v}\phi) = -\nabla\cdot\mathbf{J},
$$

$$
\partial_t\mathbf{p} + \mathbf{v}\cdot\nabla\mathbf{p} + \mathbf{W}\cdot\mathbf{p} = \mathbf{g},
$$

$$
\partial_t\mathbf{Q} + \mathbf{v}\cdot\nabla\mathbf{Q} + [\mathbf{W}\cdot\mathbf{Q} - \mathbf{Q}\cdot\mathbf{W}] = \mathbf{G},
$$

$$
\partial_t q_1 = \frac{\delta q_1}{\delta\phi}\partial_t\phi, \partial_t q_2 = \frac{\delta q_2}{\delta\mathbf{p}}\cdot\partial_t\mathbf{p}, \partial_t q_3 = \frac{\delta q_3}{\delta\mathbf{Q}} : \partial_t\mathbf{Q},
$$

$$
\partial_t q_4 = \frac{\delta q_4}{\delta\phi}\partial_t\phi + \frac{\delta q_4}{\delta\mathbf{p}}\cdot\partial_t\mathbf{p} + \frac{\delta q_4}{\delta\mathbf{Q}} : \partial_t\mathbf{Q}.
$$

$$
\begin{pmatrix} \tau_s \\ \mathbf{J} \\ \mathbf{g} \\ \mathbf{G} \end{pmatrix} = \mathcal{A} \begin{pmatrix} \mathbf{D} \\ \nabla\Big(\gamma_1\Delta\phi - \frac{\delta q_1}{\delta\phi}q_1 - \frac{\delta q_4}{\delta\phi}q_4\Big) \\ \gamma_2\Delta\mathbf{p} - \frac{\delta q_2}{\delta\mathbf{q}}q_2 - \frac{\delta q_4}{\delta\mathbf{p}}q_4 \\ \gamma_3\Delta\mathbf{Q} - \frac{\delta q_3}{\delta\mathbf{Q}}q_3 - \frac{\delta q_4}{\delta\mathbf{Q}}q_4 \end{pmatrix}
$$

University

Linear, Second-order Semi-discrete Scheme

$$
\begin{cases}
\rho\Big(\delta_t^+\mathbf{v}^n + B(\overline{\mathbf{v}}^{n+\frac{1}{2}}, \mathbf{v}^{n+\frac{1}{2}})\Big) = -\nabla\Pi^{n+\frac{1}{2}} + \nabla\cdot(\tau_s^{n+\frac{1}{2}} + \tau_e^{n+\frac{1}{2}} + \tau_a^{n+\frac{1}{2}}), \\
\nabla\cdot\mathbf{v}^{n+\frac{1}{2}} = 0. \\
\delta_t^+\phi^n + \nabla\cdot(\mathbf{v}^{n+\frac{1}{2}}\overline{\phi}^{n+\frac{1}{2}}) = -\nabla\cdot\mathbf{J}^{n+\frac{1}{2}}, \\
\delta_t^+\mathbf{p}^n + \mathbf{v}^{n+\frac{1}{2}}\cdot\nabla\overline{\mathbf{p}}^{n+\frac{1}{2}} + \mathbf{W}^{n+\frac{1}{2}}\cdot\overline{\mathbf{p}}^{n+\frac{1}{2}} = \mathbf{g}^{n+\frac{1}{2}}, \\
\delta_t^+\mathbf{Q}^n + \mathbf{v}^{n+\frac{1}{2}}\cdot\nabla\overline{\mathbf{Q}}^{n+\frac{1}{2}} + [\mathbf{W}^{n+\frac{1}{2}}\cdot\overline{\mathbf{Q}}^{n+\frac{1}{2}} - \overline{\mathbf{Q}}^{n+\frac{1}{2}}\cdot\mathbf{W}^{n+\frac{1}{2}}] = \mathbf{G}^{n+\frac{1}{2}}, \\
\delta_t^+ q_1^n = \overline{\frac{\delta q_1}{\delta\phi}}^{n+\frac{1}{2}}\delta_t^+\phi^n, \\
\delta_t^+ q_2^n = \overline{\frac{\delta q_2}{\delta\phi}}^{n+\frac{1}{2}}\delta_t^+\mathbf{p}^n, \\
\delta_t^+ q_3^n = \overline{\frac{\delta q_3}{\delta\phi}}^{n+\frac{1}{2}}\delta_t^+\mathbf{Q}^n, \\
\delta_t^+ q_4^n = \overline{\frac{\delta q_4}{\delta\phi}}^{n+\frac{1}{2}}\delta_t^+\phi^n + \overline{\frac{\delta q_4}{\delta\mathbf{p}}}^{n+\frac{1}{2}}\cdot\delta_t^+\mathbf{p}^n + \overline{\frac{\delta q_4}{\delta\mathbf{Q}}}^{n+\frac{1}{2}} : \delta_t^+\mathbf{Q}^n,
\end{cases}
$$

$$
\begin{pmatrix} \tau_s^{n+\frac{1}{2}} \\ \mathbf{J}^{n+\frac{1}{2}} \\ \mathbf{g}^{n+\frac{1}{2}} \\ \mathbf{G}^{n+\frac{1}{2}} \end{pmatrix} = \overline{\mathcal{A}}^{n+\frac{1}{2}} \begin{pmatrix} \mathbf{D}^{n+\frac{1}{2}} \\ \gamma_1\nabla\Delta\phi^{n+\frac{1}{2}} - \overline{\frac{\delta q_1}{\delta\phi}}^{n+\frac{1}{2}} q_1^{n+\frac{1}{2}} - \overline{\frac{\delta q_4}{\delta\phi}}^{n+\frac{1}{2}} q_4^{n+\frac{1}{2}} \\ \gamma_2\Delta\mathbf{p}^{n+\frac{1}{2}} - \overline{\frac{\delta q_2}{\delta\mathbf{q}}} q_2^{n+\frac{1}{2}} - \frac{\delta q_4}{\delta\mathbf{p}} q_4^{n+\frac{1}{2}} \\ \gamma_3\Delta\mathbf{Q}^{n+\frac{1}{2}} - \overline{\frac{\delta q_3}{\delta\mathbf{Q}}}^{n+\frac{1}{2}} q_3^{n+\frac{1}{2}} - \overline{\frac{\delta q}{\delta\mathbf{Q}}} q_4^{n+\frac{1}{2}} \end{pmatrix}
$$

UtahState University

Applications:
Computational Complex Fluids Dynamics (C2FD) Packages

User Level

Navier-Stokes Solver
Gradient Flow Solver
Constitutive Equation Solver
General Tensor Equation Solver

Fluid Structure Interaction (Immersed Boundary Method)

Kernels

Preconditioned Linear Solver
Newton-Raphson Nonlinear Solver

Deal.II Finite-Element Solver

Libraries

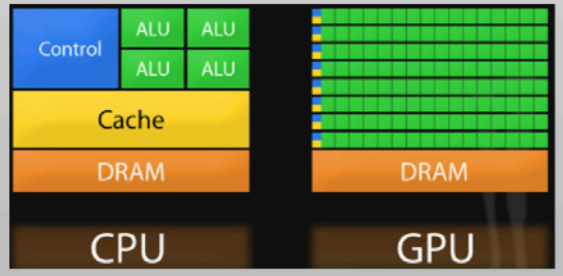
CUSP, Thrust, HDF5, CUFFT CUBLAS

Protocols

OpenMP, MPI, CUDA, C++

Hardware

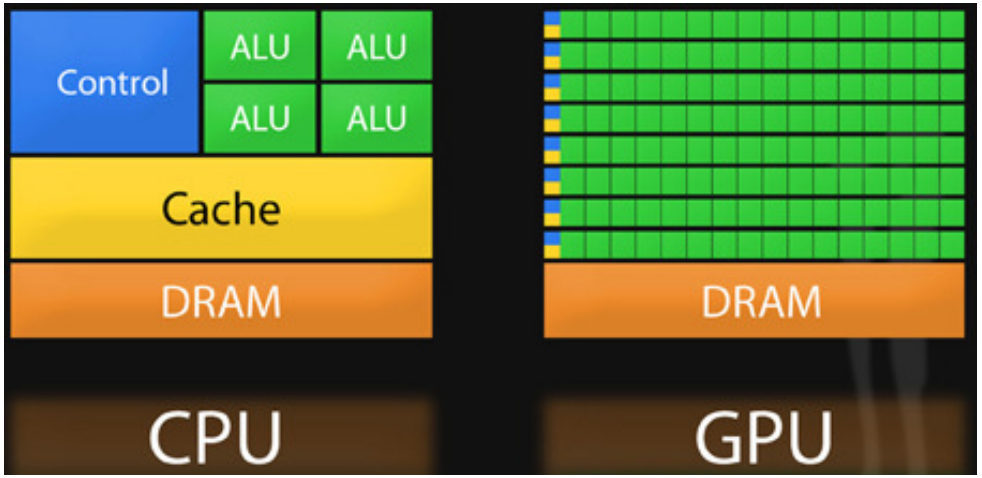
CPU + GPU Hybrid Architecture



www.c2fd.org

UtahState University

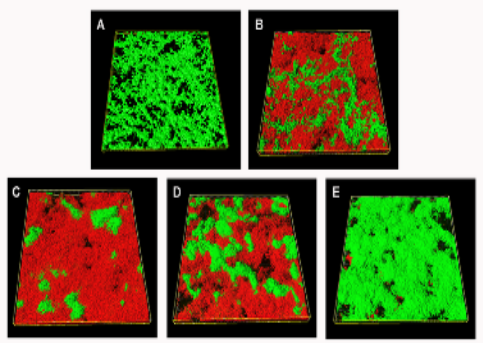
CPU vs. GPU



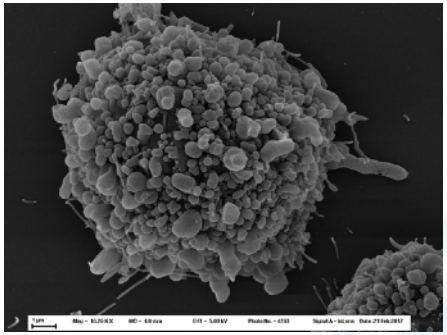
[redacted]

D: We work seamlessly with scholars from other disciplines

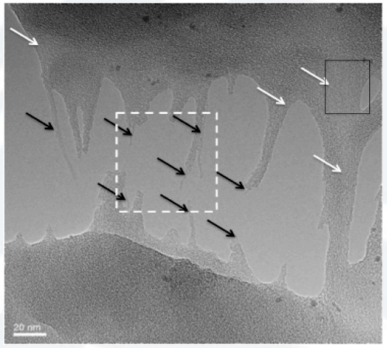
Biofilm Treatment
(with support from NSF)



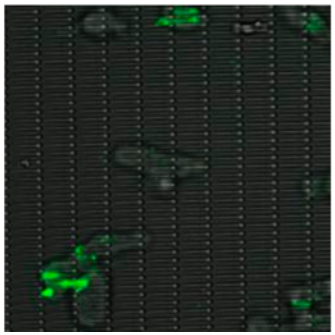
Cell Oscillations
(with support from NIH)



Carbon Nanotube Composites
(with support from ARO)

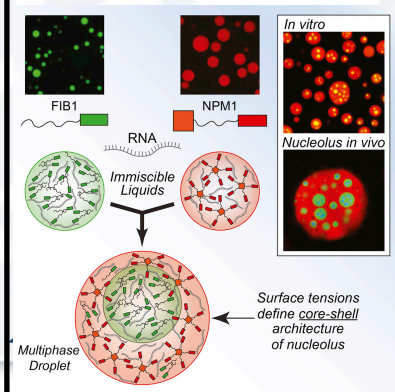


Cell Substrate Interaction
(pending grant)



Multiphase Complex-fluid
Soft-Structure Interaction (FSI)
(FRG Grant)

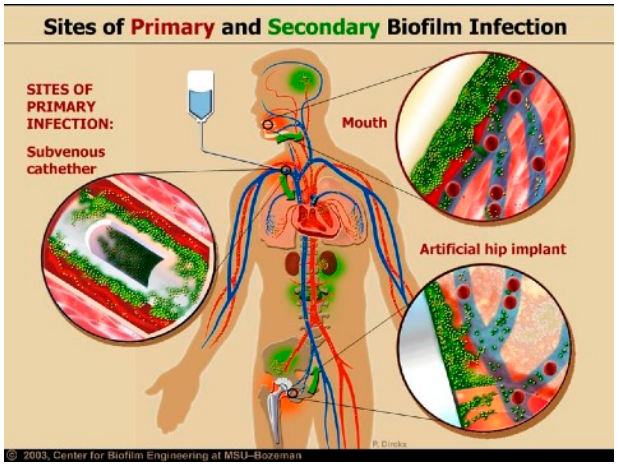
Phase Transition



State
iversity

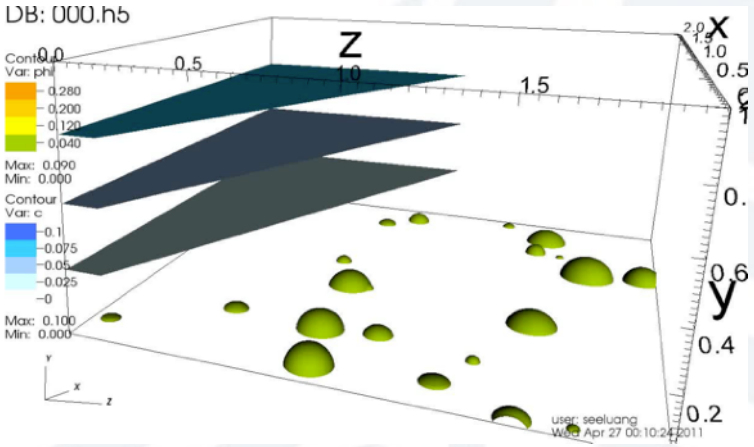
Biofilm Formation & Treatment

Biofilms are microorganisms in which bacteria stick to each other embedded within a self-produced matrix of extracellular polymeric substance (EPS).

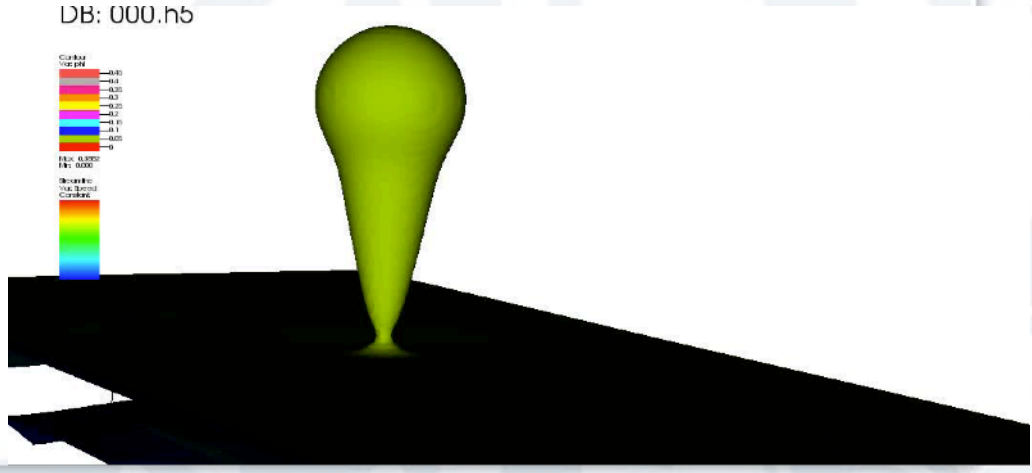


Once biofilm reach the bloodstream they can spread to any moist surface of the human body

Growth of Heterogeneous Morphology of Biomass



Sheared Single Growth Biofilm Colony (Pinching Off)

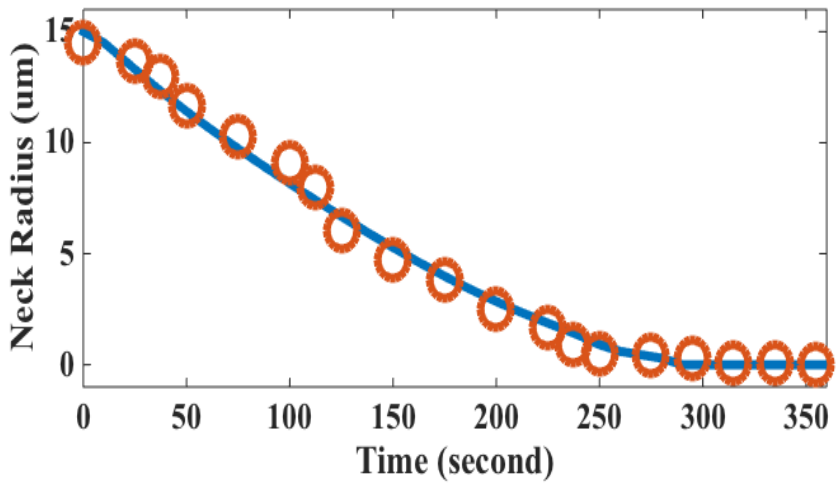


Zhao et al., J.Theor. Biol.,392:83-98,2016.

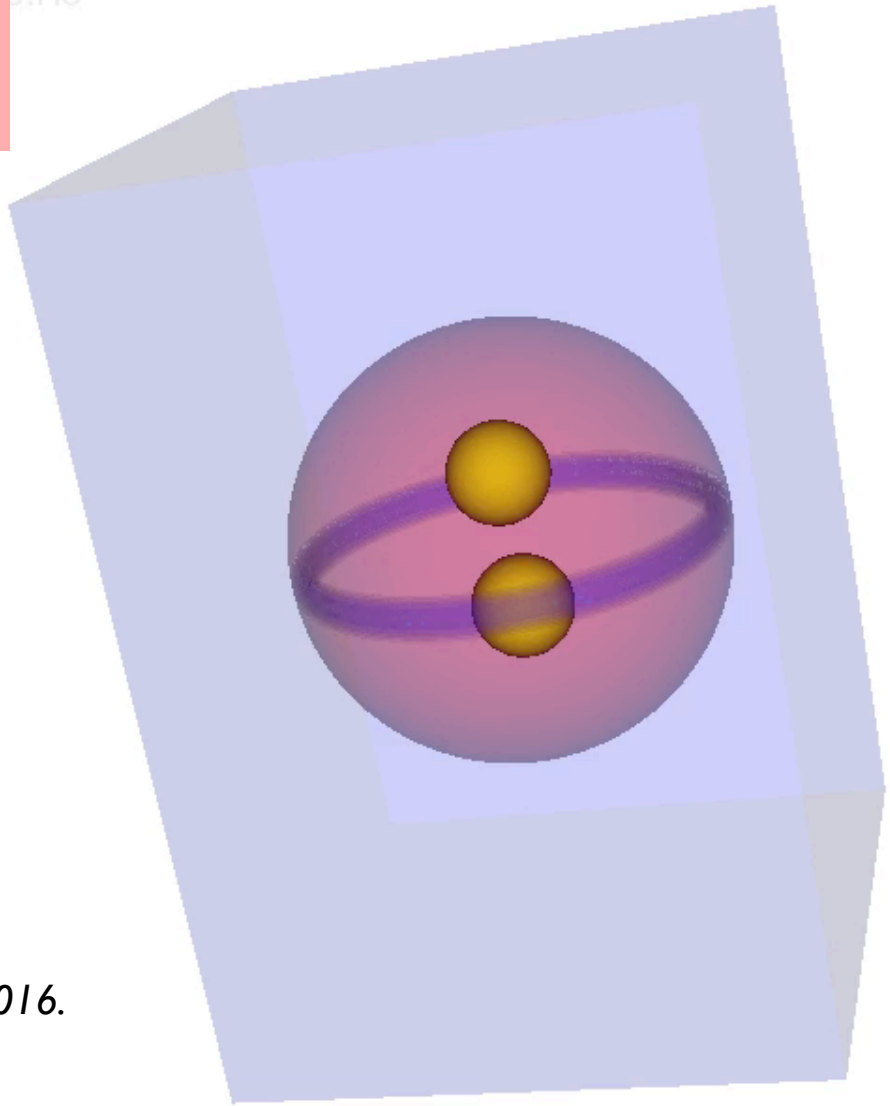
Zhao et al., Bull. Math. Biol. 79(4):884-919,2017.

Cell Cytokinesis Driven by F-actin Contractile Ring

Cytokinesis is the process during cell division in which the cytoplasm of a single eukaryotic cell is divided to form two daughter cells.



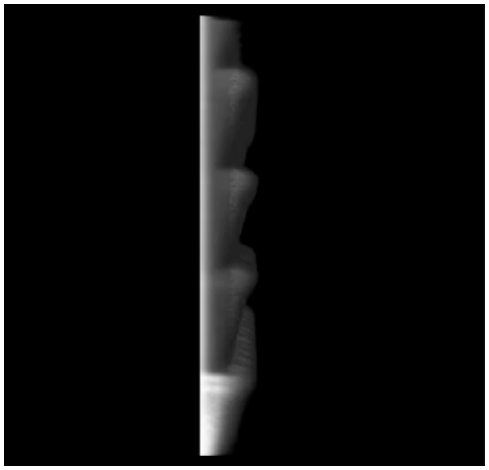
Dynamics of cytokinetic ring contraction



Zhao et al., Commun. Comput. Phys., 19(3):663-681, 2016.

Zhao et al.,submitted, 2017.

Cell Motions on Saw-teeth Patterned Substrate



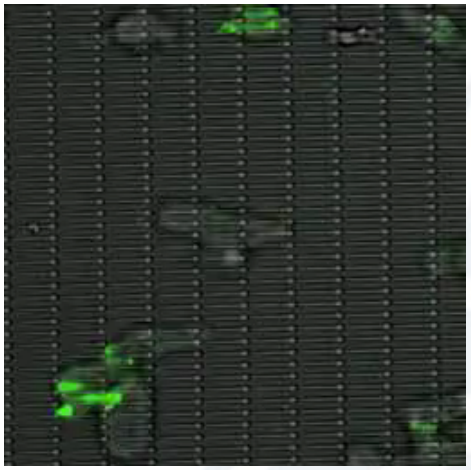
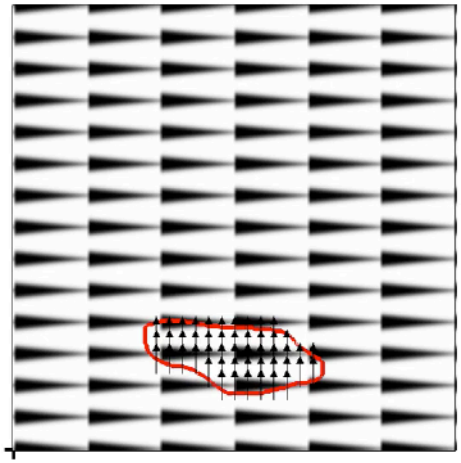
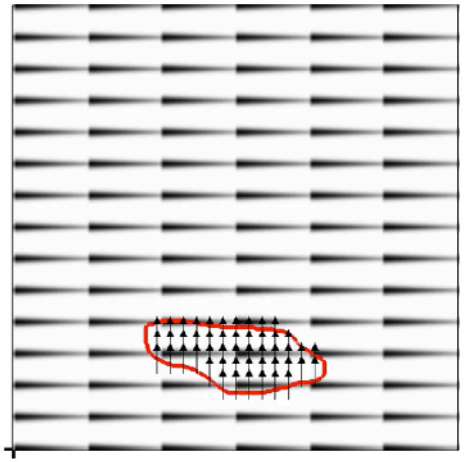


Figure: cells can be guided based on local asymmetries in nano microtopography on subcellular scales.





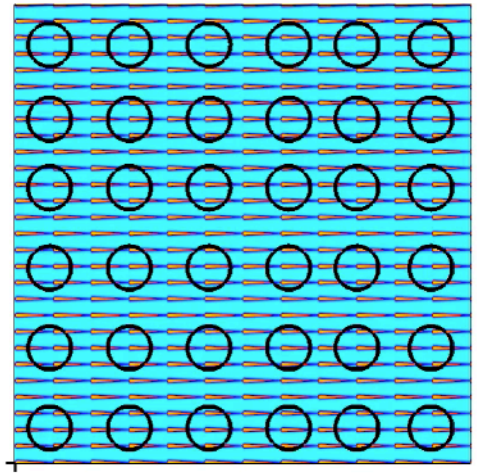
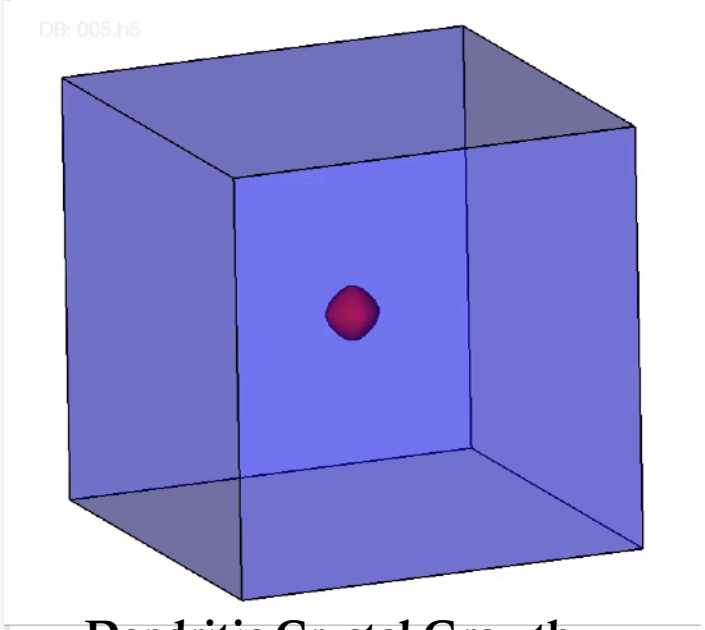
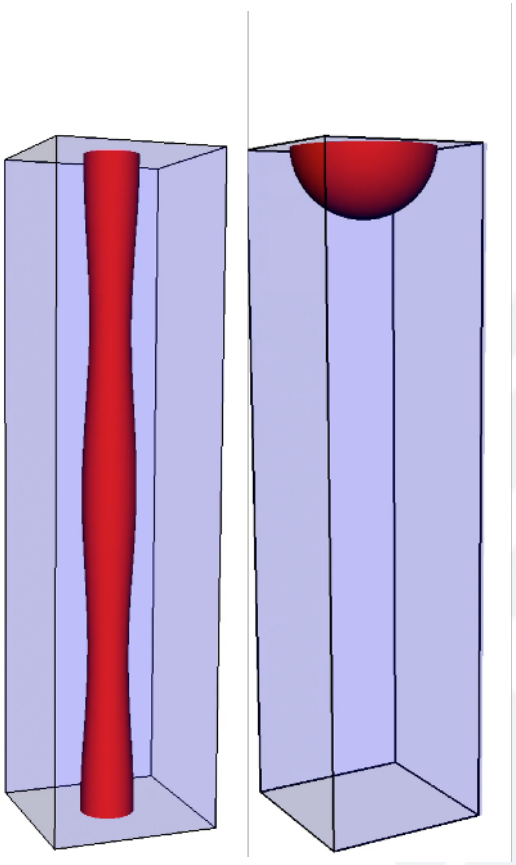


Figure: numerical simulations.

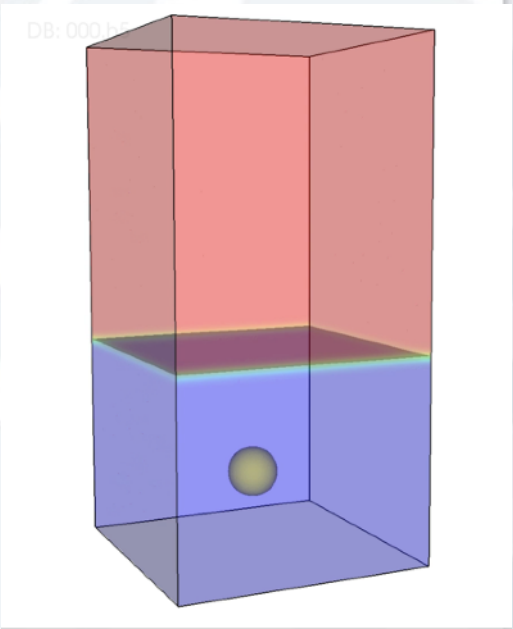
Applications in Engineering



Dendritic Crystal Growth



Liquid Crystal Drop



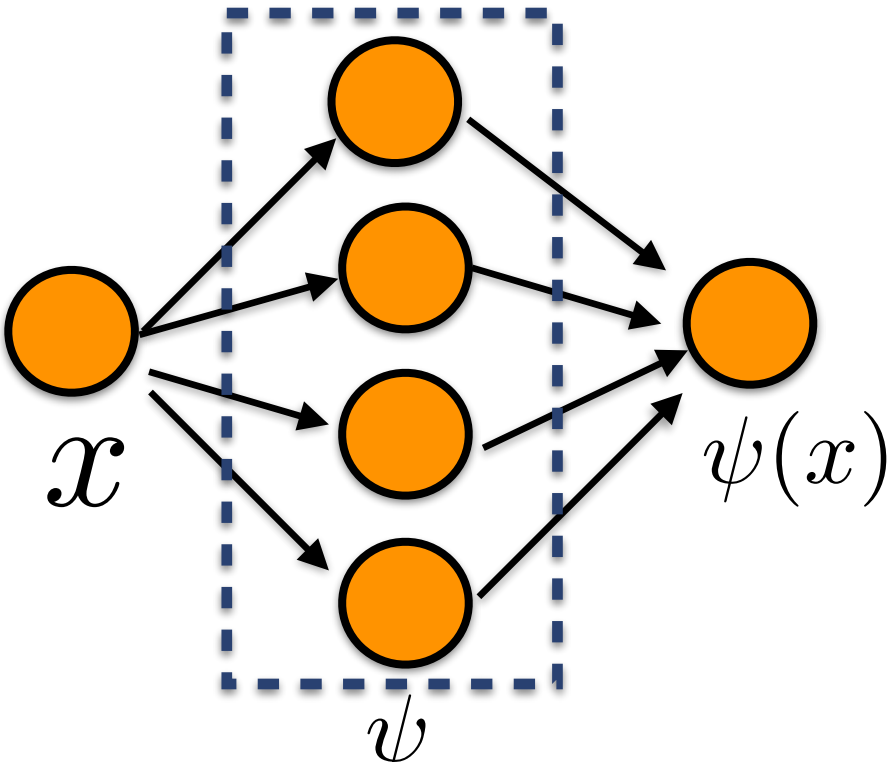
Multiphase Flow

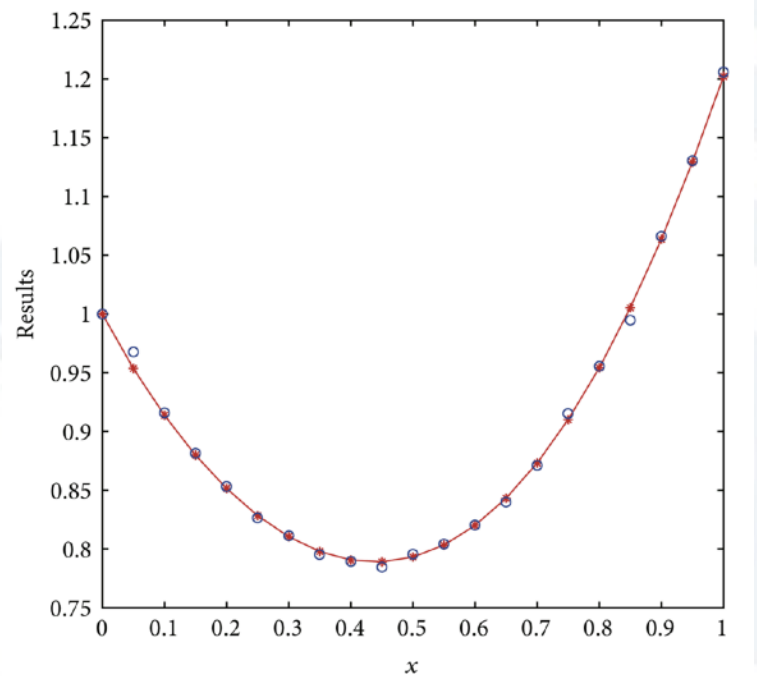
UtahState University

New Trends: Computational Deep Learning & Data Science

Example: using Neuron Network solving differential equations.

$$\frac{d\psi}{dx} + \left(x + \frac{1+3x^2}{1+x+x^3}\right)\psi = x^3 + 2x + x^2\frac{1+3x^2}{1+x+x^3}, \quad \psi(0) = 1.$$



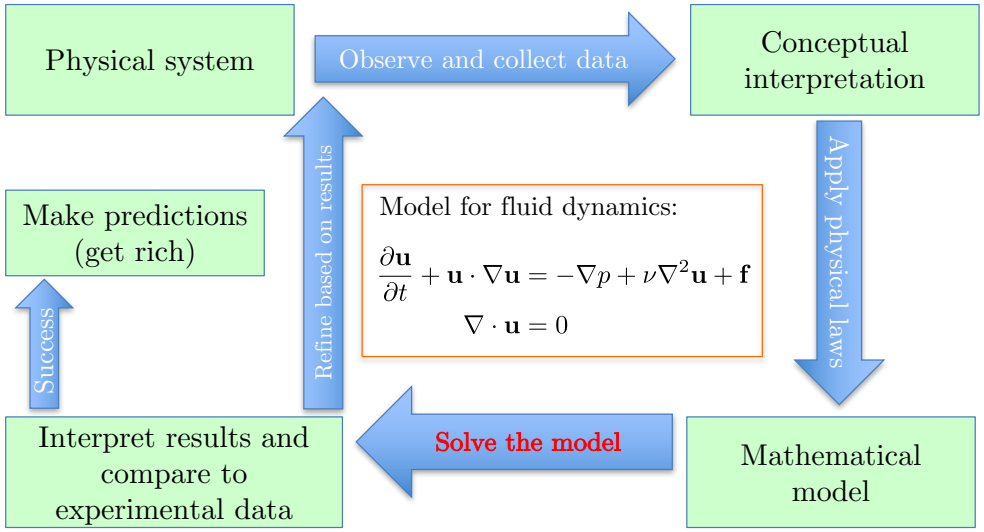


Universal Approximation Theorem

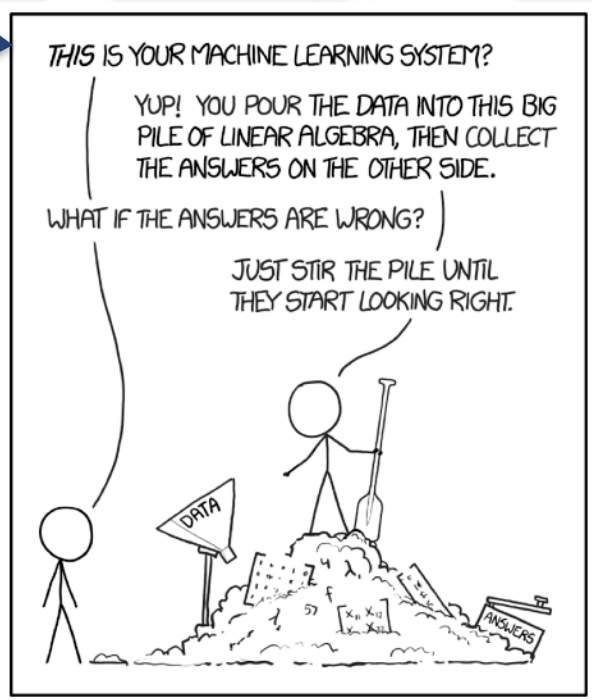
UtahState University

New Trends: Computational Deep Learning & Data Science

- Consider the following simplified model of the scientific process:



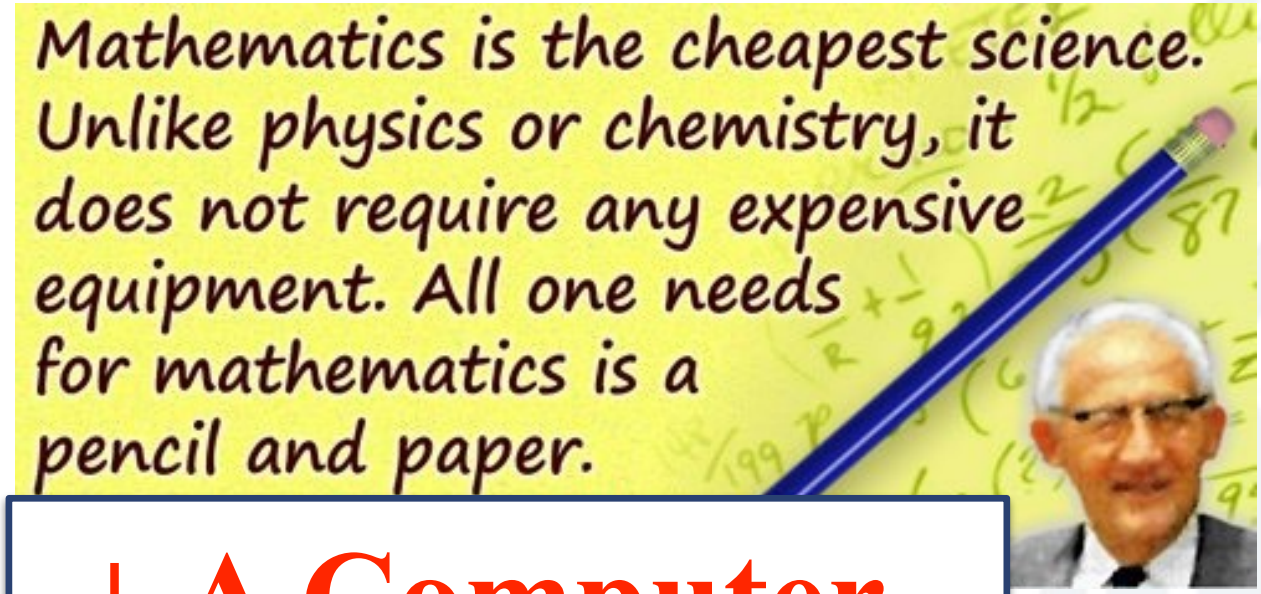
- Why: The resulting models can essentially never be solved completely using analytical (pencil and paper) methods.



TensorFlow

Conclusion

Learning computational skills is the key to jobs!



+ A Computer.

UtahState University

Position Openning

jia.zhao@usu.edu

- There are a few undergraduate research assistant (RA) positions opening.
- The RAs will be paid with flat rate $10 per hours and 10 - 20 hours per week, participating in one of my current research projects.

UtahState University

Acknowledgments

- NSF-DMS-1816783
- AMS-Simons Travel Grants
- The Research Catalyze grant from Utah State University
- NVIDIA GPU Grant with a Quadro P6000 GPU