C^2FD: A GPU based 3D Integrated Complex-fluids Toolkit for Moldeling Cellular Dynamics

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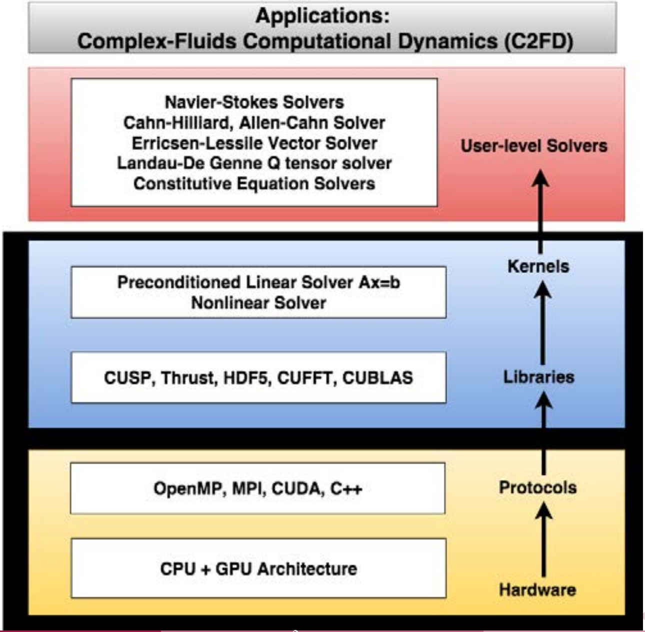
Outline

C^2FD: Computational Complex-Fluids Dynamics



Why GPU?

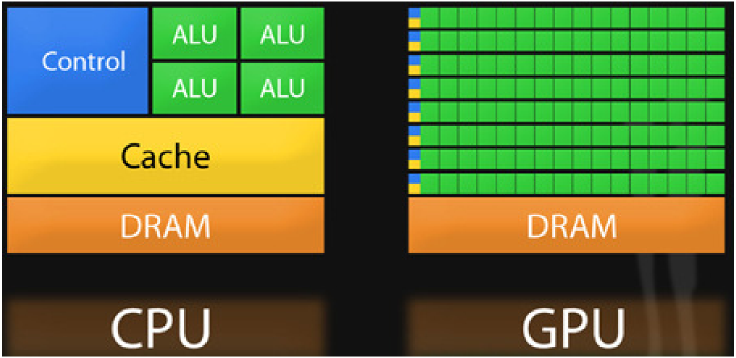


Figure : The GPU Devotes More Transistors to Data Processing.

What are Complex-fluids?

Complex fluids are fluids that are homogeneous at macroscopic scales and disordered at microscopic scales, but possess structure on a mesoscopic length scale. Mesoscopic scale dynamics or physics dominates the material's properties. [a]

[a] Gelbart and Ben-Shaul, JPC, 1996.

- A fluid made up of a lot of different kinds of stuff;
- Fluid mixtures with (micro)structure;
- polymers (thermoplastics, elastomers, composites), gels, colloidal fluids, suspensions, emulsions, foams, micelar and liquid-crystal phases, molten materials, etc.

Why model Cells as Complex Fluids?

' Everything flows! '

Heraclitus 535BC - 475BC [a]

[a] http://necspenecmetu.tumblr.com/image/24706611579

Continuum Theory

What is a continuum theory?

A theory that analyzes the kinematics and the mechanical behavior of materials modeled as a continuous mass rather than as discrete particles.

Navier-Stokes Equation

$$\begin{aligned}(\rho\mathbf{v})_t + \nabla\cdot(\rho\mathbf{v}\mathbf{v}) &= -\nabla p + \nabla\cdot\boldsymbol{\sigma} + \mathbf{f},\\ \rho_t + \nabla\cdot(\rho\mathbf{v}) &= 0,\end{aligned}$$

where ρ is the density, $\mathbf{v}$ is the velocity, p is the hydrostatic pressure, $\boldsymbol{\sigma}$ is the viscoelastic stress, and $\mathbf{f}$ is the external forces.

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Biological Background for Mitotic Cell Rounding

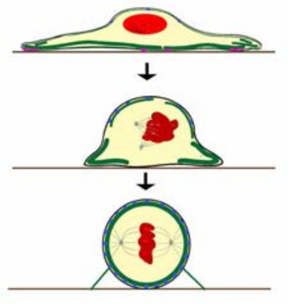

Figure : A Schematic Cartoon.

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Figure : Mitotic Cell rounding.

Homogeneous Mitotic Cell Rounding on Substrate

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Figure : Simulations of mitotic cell rounding on substrate.

Heterogeneous Mitotic Cell Rounding on Substrate

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(a)

load video

(b)

Figure : Mitotic Cell Rounding. (a) F-actin dynamics from Kapustina, UNC; (b) numerical simulation.

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Cytoplasmic flows accompany the traveling wave

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The nucleus is pushed around during oscillation

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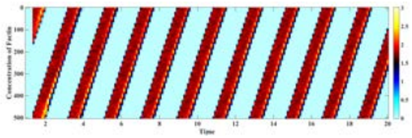
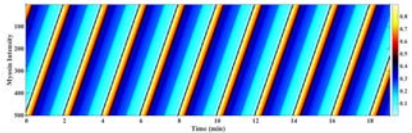
load video

Cortical Traveling Waves



(e) F actin



(f) Myosin

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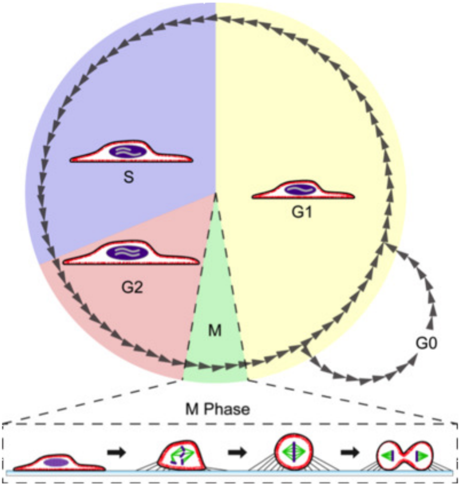
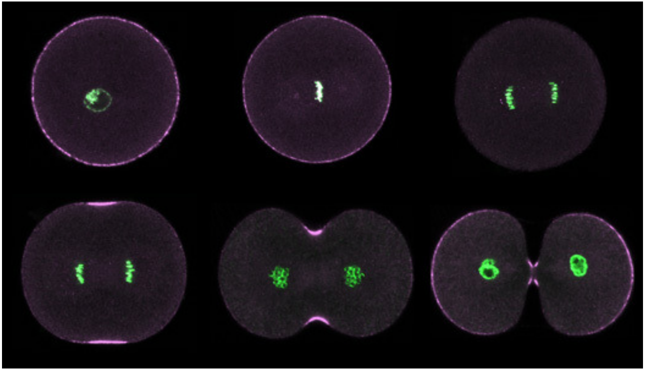
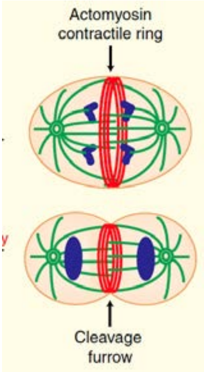
Cell Mitosis



Biological Background for Cytokinesis



(g) Actomyosin Distribution during cytokinesis



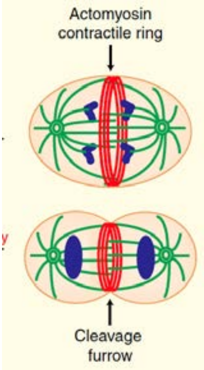
(h) Contractile Ring

Figure : Animal Cell Cytokinesis: (A) purple urchin zygotes during first mitosis, stained for DNA (green) and phosphorylated myosin II (magenta); (B) a cartoon of actomyosin contractile ring and cleavage furrow.

[1] Ann L. Miller, Current Biology, 21(24), 2011.

[2] http://php.med.unsw.edu.au/cellbiology/

Cell Cytokinesis



(a) Contractile Ring

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(b) 3D simulation of Cell Cytokinesis

3D Visualization of Contractile Ring Dynamics

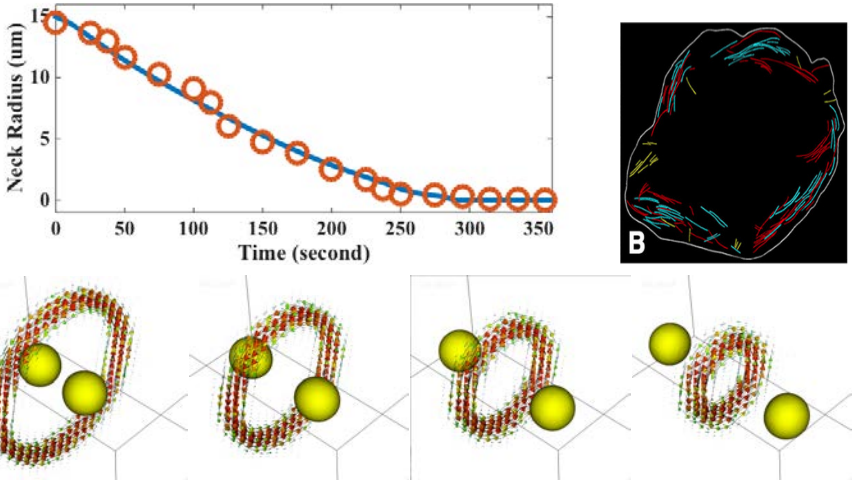
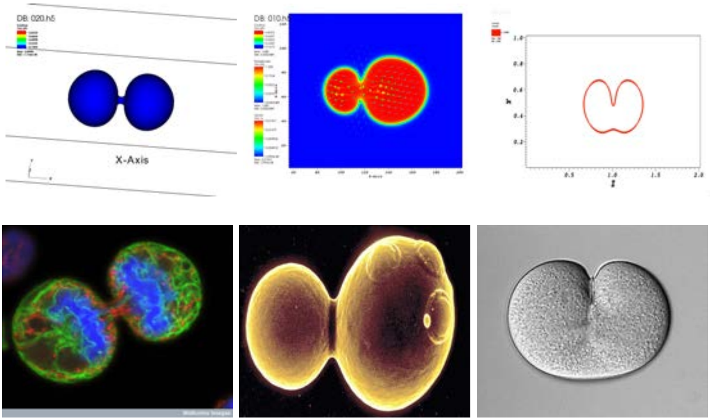


Figure : Arrangement of F-actin on the contractile ring at different stages.

[1] Kamasaki, Osumi and Mabuchi, Journal of Cell Biology, 178(5),2010.

Qualitative Comparison



(d) a melanoma cell before it divides completely

(e) a budding yeast

(f) Cleavage furrow in the jellyfish Aequorea

Figure : Qualitative Comparisons of asymmetric cytokinesis.

[1] http://php.med.unsw.edu.au/cellbiology/index.php?title=File:Melanoma-Cytokinesis.eps

[2] http://www.ppdictionary.com/fungi.htm

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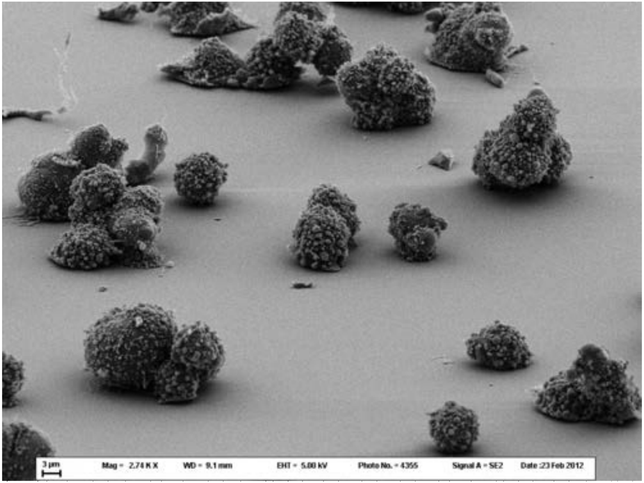
The plasm membrane after rounding is highly convoluted.



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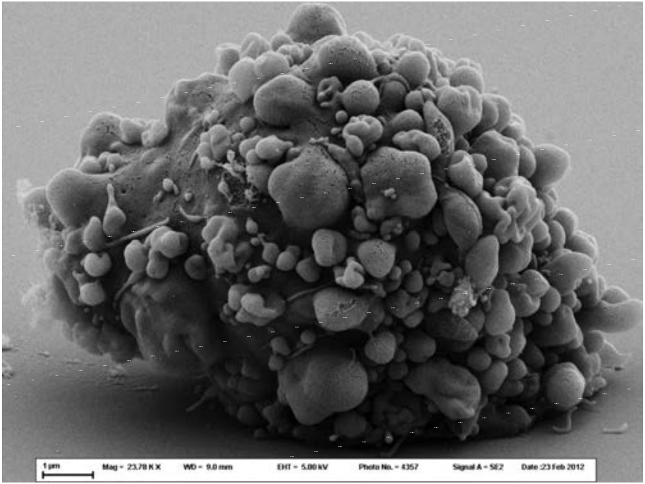
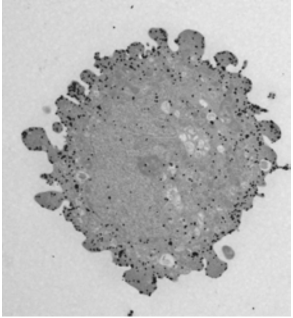


Bleb-like Protrusions



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Bleb-like Protrusions

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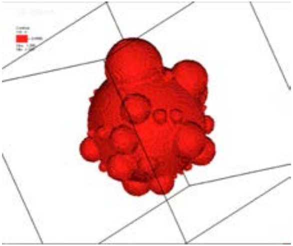

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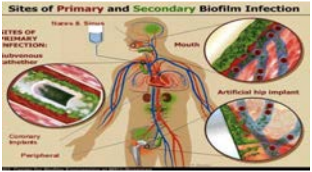
Biofilm Bacteria

(e) Dental Plaque

(f) Biofouling

(g) Streambed in Yellowstone



(h) Biofilm Infection

Figure : Biofilm Bacteria in Our Daily Life.

Biofilm Recovery After Antimicrobial Treatment

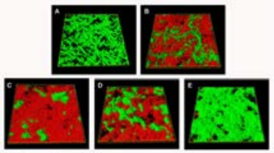


Figure : Biofilm recovery after 10-minute treatment with CHX-Plus.

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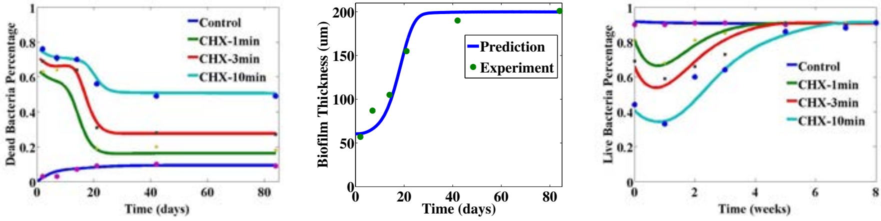
Figure : Numerical prediction of biofilm recovery.

Biofilm Treatment and Relapse



(a) (b) (c)

Figure : Model prediction and comparison with experiments of biofilm treatment and relapse. Here dots are experiment data, curves are predictions. (a) Percentage of dead bacterial cells at different times of biofilm recovery after being treated with CHX for 1, 3 and 10 minutes, respectively; (b) biofilm thickness; (c) Live bacteria percentage during biofilm recovery after CHX treatment.

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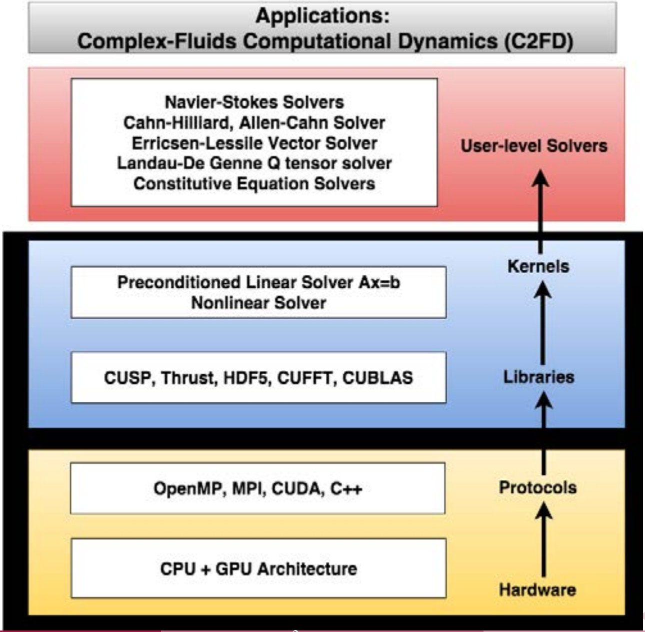

Acknowledgments

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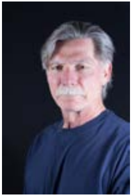
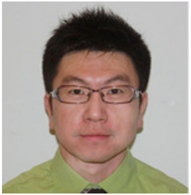


(a) Dr. Forest

(b) Dr. Wang



(c) Dr. Yang

(d) Dr. Jacobson

(e) Dr. Kapastina

(f) Dr. Shen