They are not third parties: solutes and polymers in fluid-structure interaction

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07/11/2016

Molecular and Integrative Physiology
University of Michigan

Cardiac differentiation

Dendritic spine motility

The Immersed Boundary Method

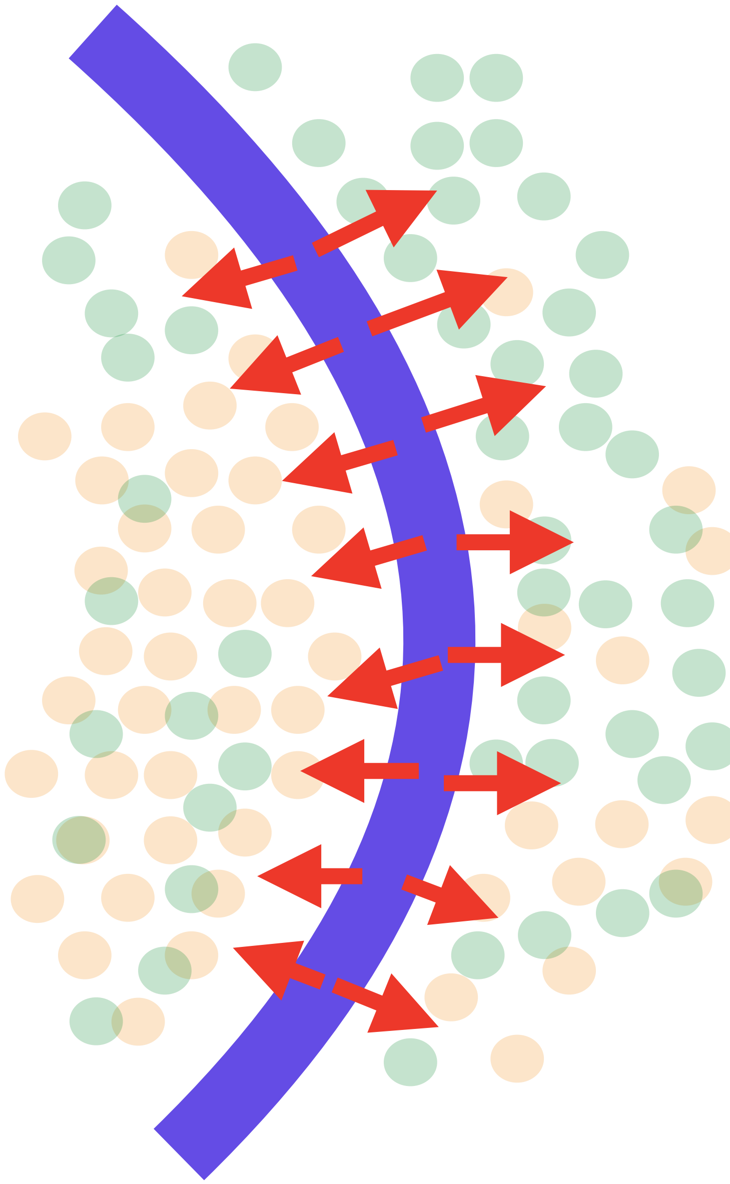
i) Advection-electrodiffusion

ii) Two-phase viscoelastic fluids and gels

Renal peristaltic concentration

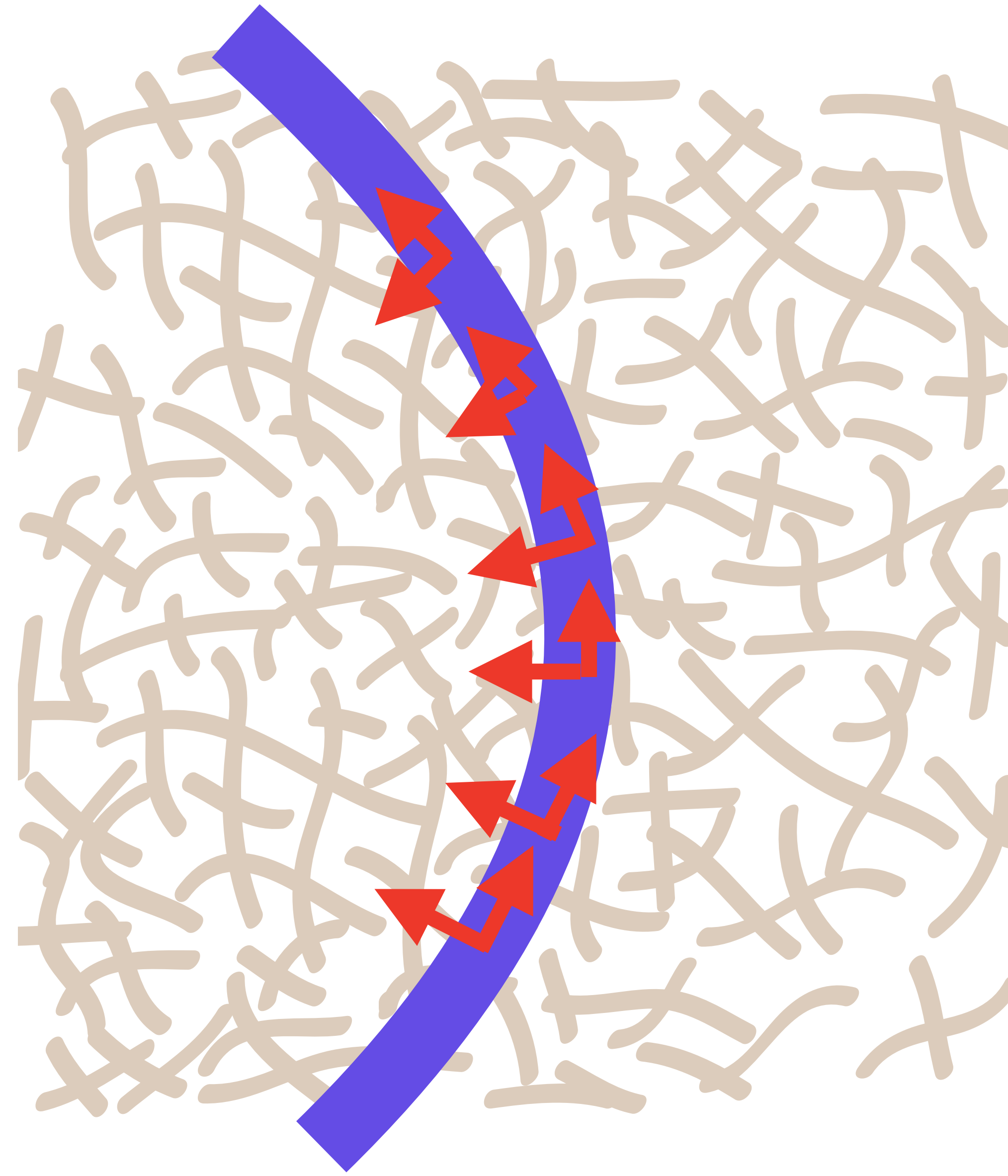
Non-Newtonian swimming

Fluid-structure interaction with solutes/polymers



$$-\frac{\delta E}{\delta \mathbf{X}} = \mathbf{F}_{\mathrm{ms}} + \mathbf{F}_{\mathrm{mf}}$$

Chemical potential barrier



$$-\frac{\delta E}{\delta \mathbf{X}} = \mathbf{F}_{\mathrm{mp}} + \mathbf{F}_{\mathrm{mf}}$$

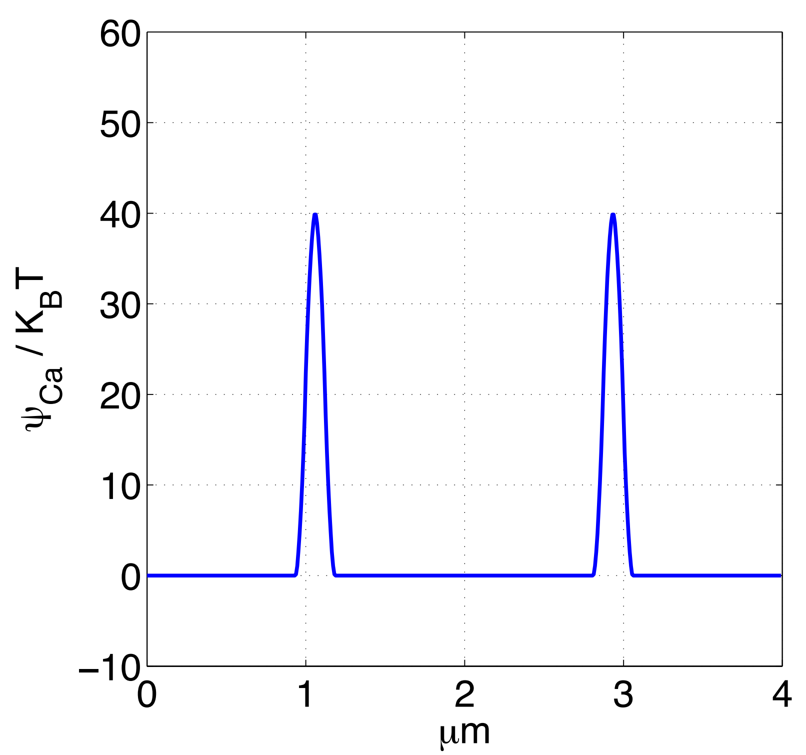
Resistive drag

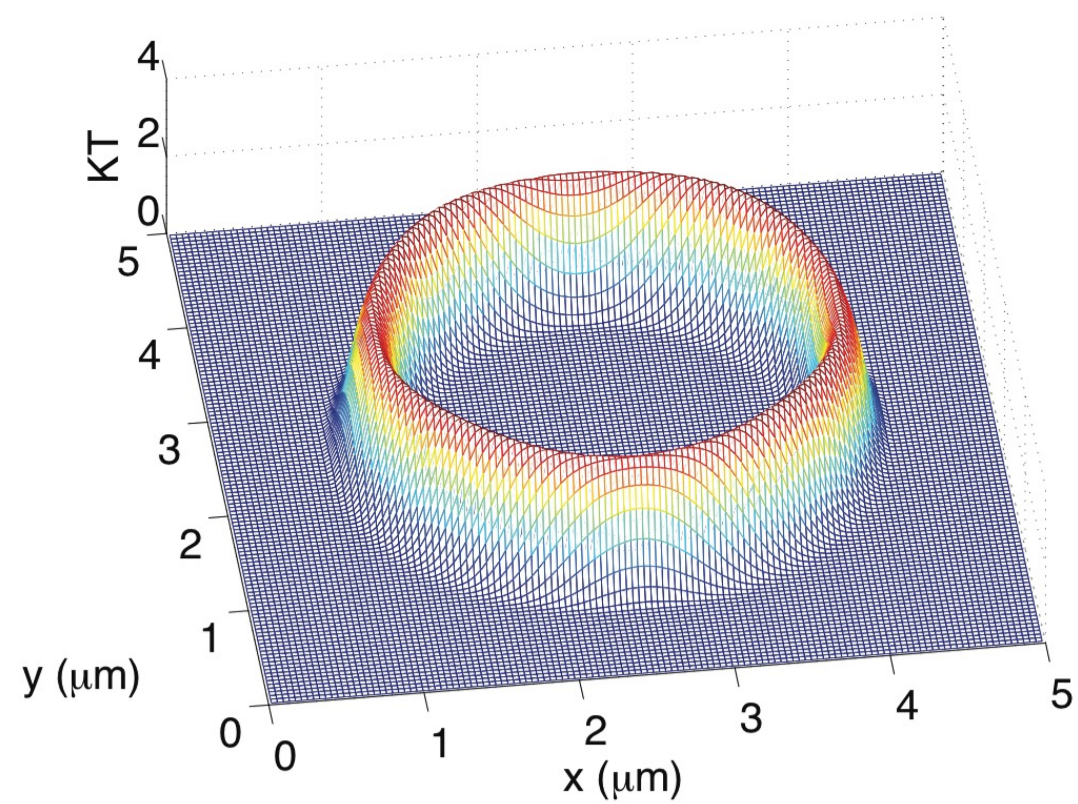
IB method for advection-electrodiffusion

Chemical potential barrier

$$\psi_i(\mathbf{x},t) = \int_{\Omega_\mathrm{L}} \Psi(\mathbf{x}-\mathbf{X}(s,t))A_i(s,t)ds$$

$$\mathbf{F}_\mathrm{ms}(s,t) = \int_{\Omega_\mathrm{E}} \sum_k (-\nabla\Psi(\mathbf{x}-\mathbf{X}(s,t))A_k(s,t)c_k(\mathbf{x},t)d\mathbf{x}$$



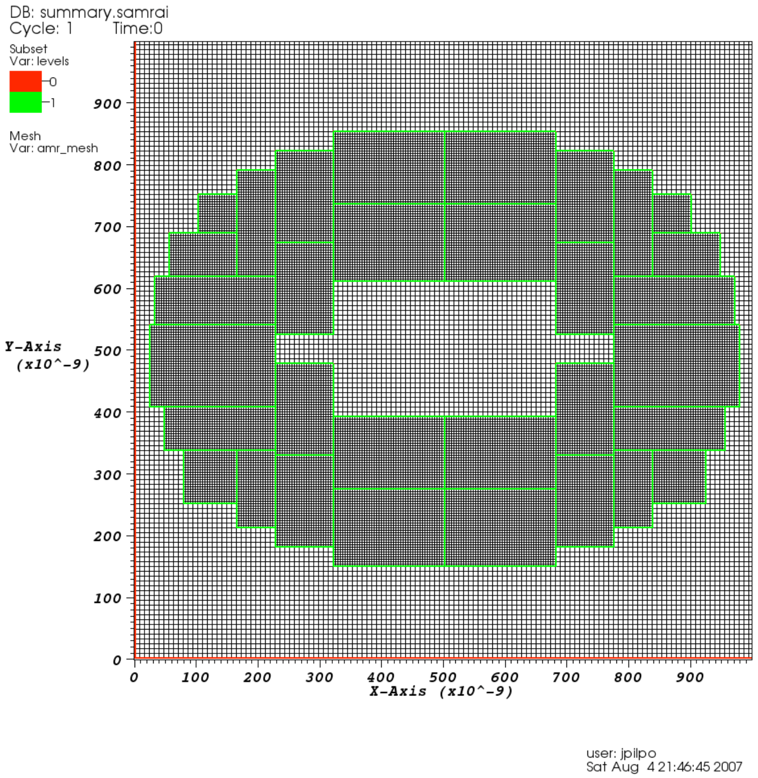


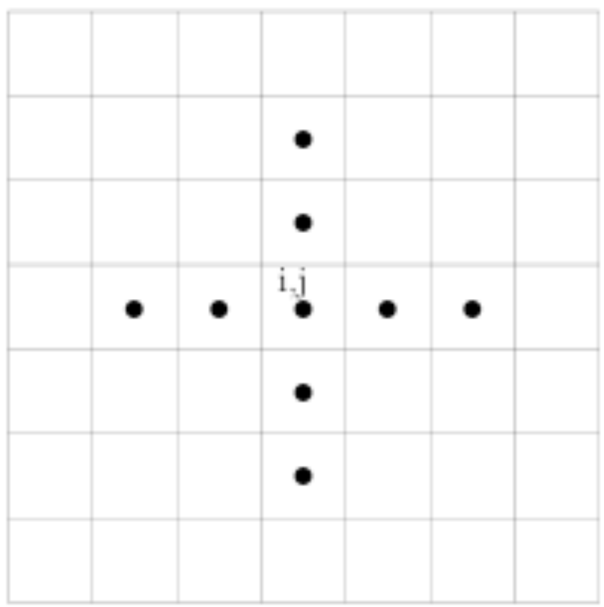
Lee, Griffith, and Peskin, JCP, 2010

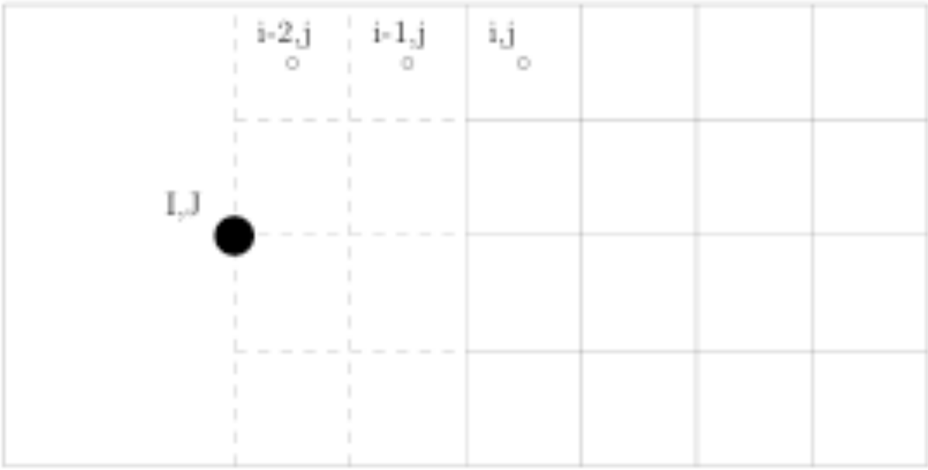
IB method for advection-electrodiffusion

Fast composite multigrid

- PETSc
- SAMRAI - multilevel adaptive mesh refinement
- Hypre - algebraic multigrid







Lee, Griffith, and Peskin, JCP, 2010

IB method for advection-electrodiffusion

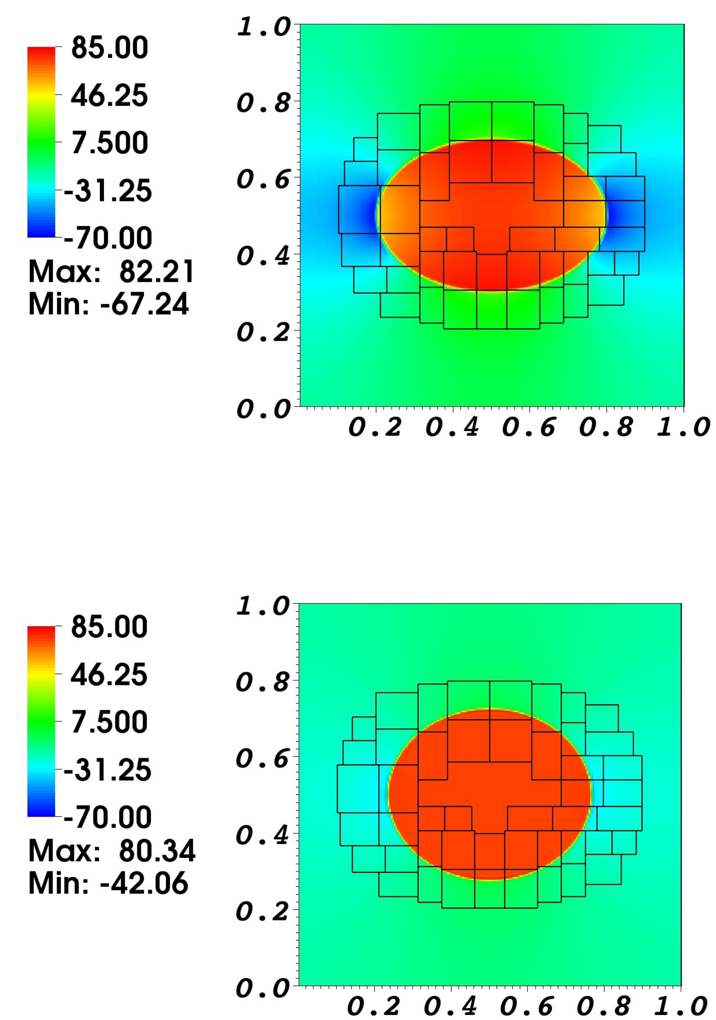
The Stokes equations with permeable membrane

$$\rho \frac{\tilde{\mathbf{u}} - \mathbf{u}^n}{\Delta t} + \mathbf{D}_h p^{n-\frac{1}{2}} = \mu L_h \frac{\tilde{\mathbf{u}} + \mathbf{u}^n}{2} + \mathbf{S}_n \mathbf{F}_{\mathrm{mf}}^{n+1} + \mathbf{f}_{\mathrm{b}}^n$$

$$\mathbf{u}^{n+1} = P\tilde{\mathbf{u}}$$

$$\zeta\left(\frac{\mathbf{X}^{n+1} - \mathbf{X}^n}{\Delta t} - \frac{\mathbf{U}^{n+1} + \mathbf{U}^n}{2}\right) = (\mathbf{F}_{\mathrm{mf}}^{n+1} \cdot \mathbf{N}_n)\mathbf{N}_n$$

$$p^{n+1/2} = p^{n-1/2} + \left(\frac{\rho}{\Delta t} L^{-1} - \frac{\mu}{2} I\right)\mathbf{D}_h \cdot \tilde{\mathbf{u}}$$



- Fast adaptive composite (FAC) method: preconditioner
- One layer of ghost cells, bottom solver (PFMG)
- Krylov subspace GMRES: main solver
- Cell-centered approximate projection method

Lee, Griffith, and Peskin, JCP, 2010

IB method for advection-electrodiffusion

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + \mathbf{D}_h \cdot \mathbf{J}_i^{n+1} = 0$$

$$\mathbf{J}_i^{n+1} = -D_i(D_h c_i^{n+1}) + [\frac{D_i}{K_\mathrm{B}T}(-qz_i D_h \varphi^n - D_h \psi_i^n) + \mathbf{u}^n]c_i^{n+1}$$

$$-L_h \varphi^n = (\sum_i q z_i^n c_i^n + \rho_\mathrm{b})/\epsilon$$

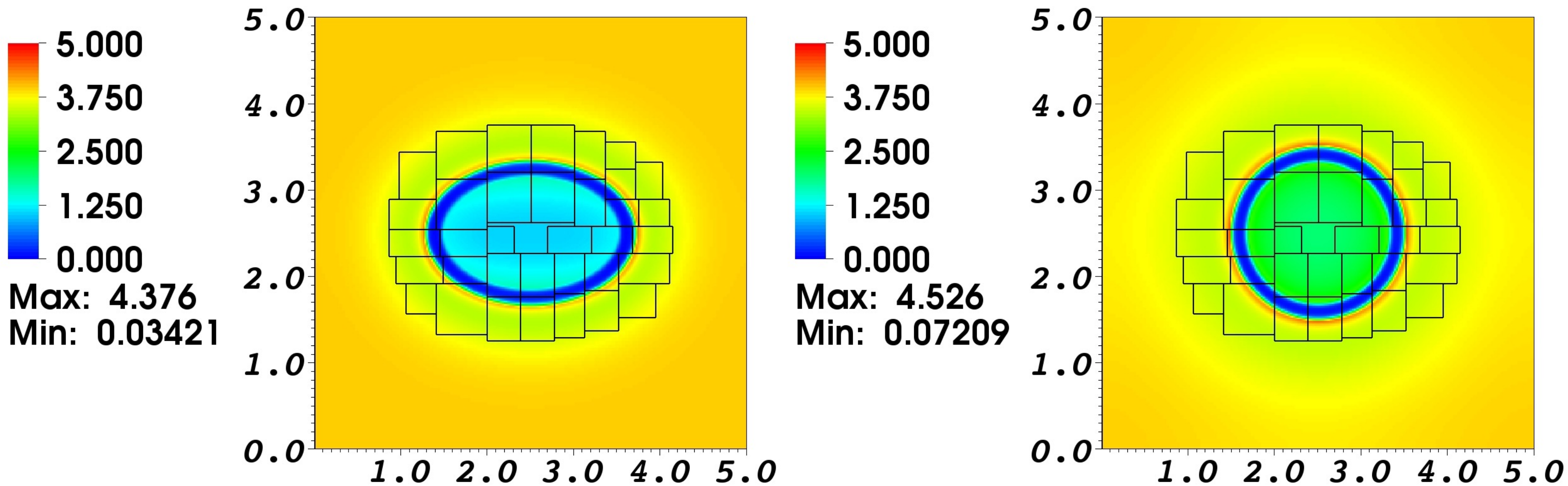
$$L_i^n c_i^{n+1} = c_i^n$$

$$L_i^n = L(\mathbf{u}^n, \varphi^n, \psi_i^n)$$

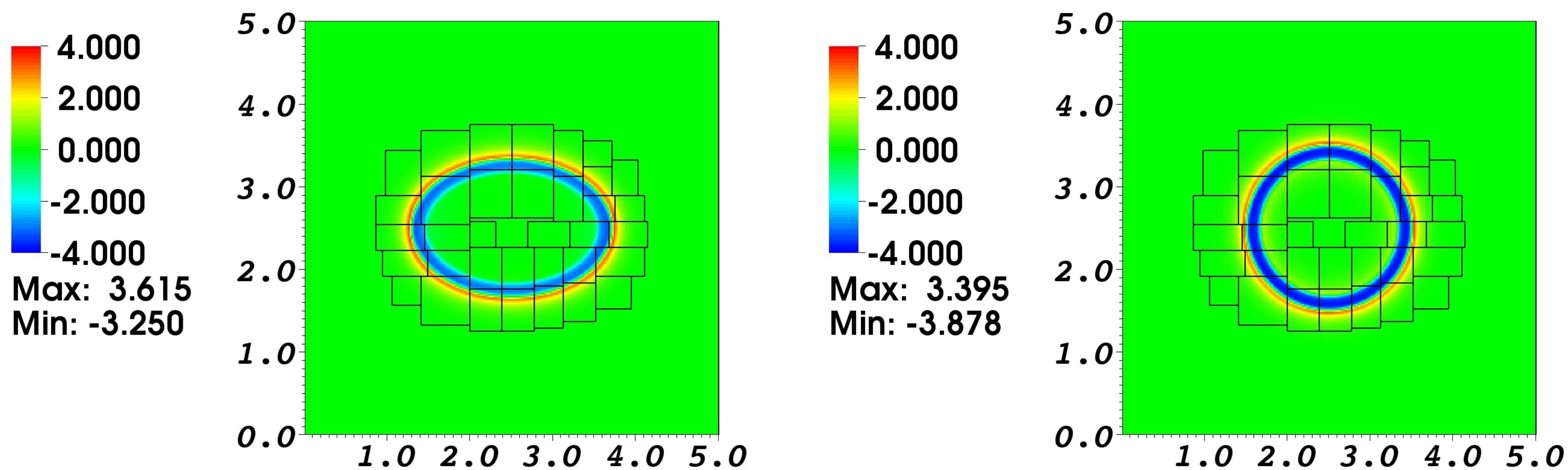
- Fast adaptive composite (FAC) method, preconditioner
- two layers of ghost cells
- bottom solver (PFMG), first order upwind
- GMRES, main solver

Lee, Griffith, and Peskin, JCP, 2010

IB method for advection-electrodiffusion



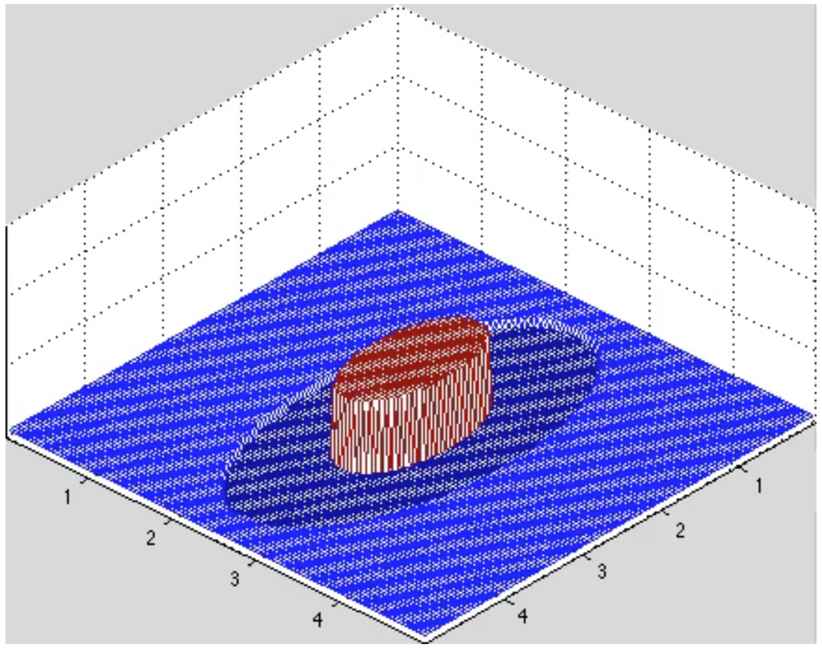
[Ca++] distribution



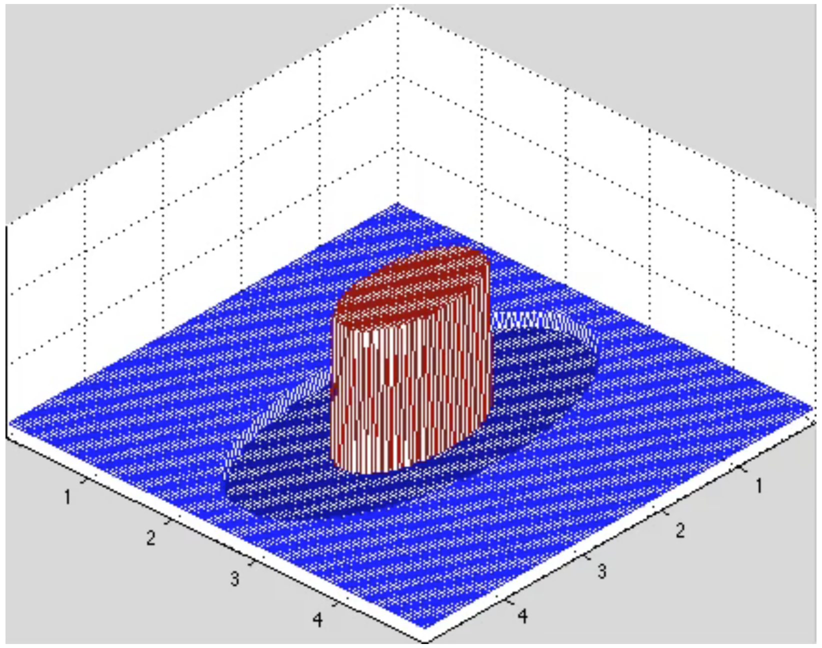
Electrical charge density distribution

Lee, Griffith, and Peskin, JCP, 2010

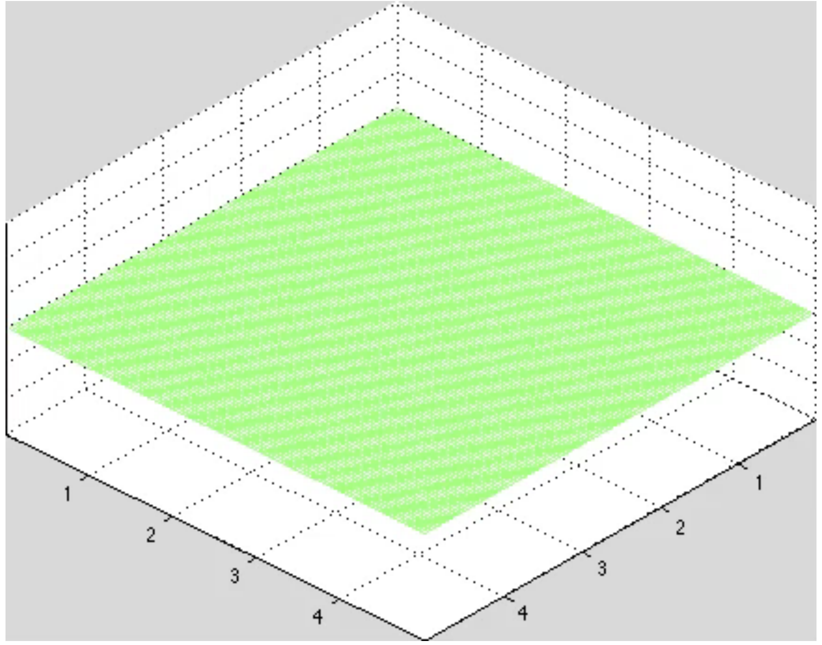
Concentration dependent contraction



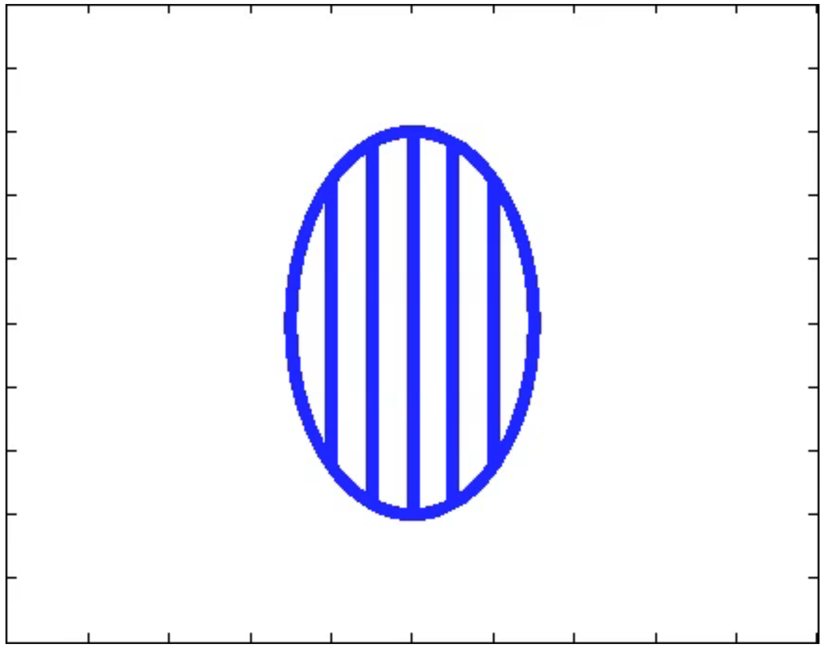
[Ca++] spatial distribution



[Cl-] spatial distribution

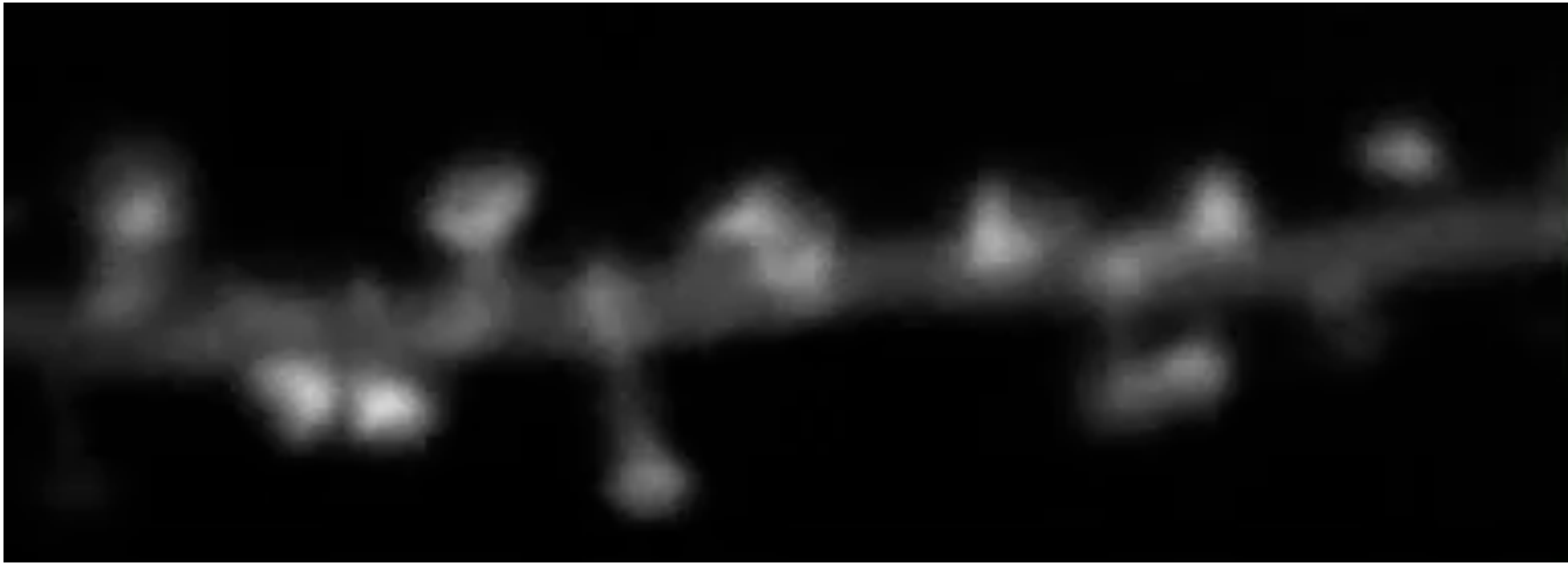


Electrical charge density spatial distribution



Contraction of actomyosin fibers

Dendritic spine motility and dendritic integration

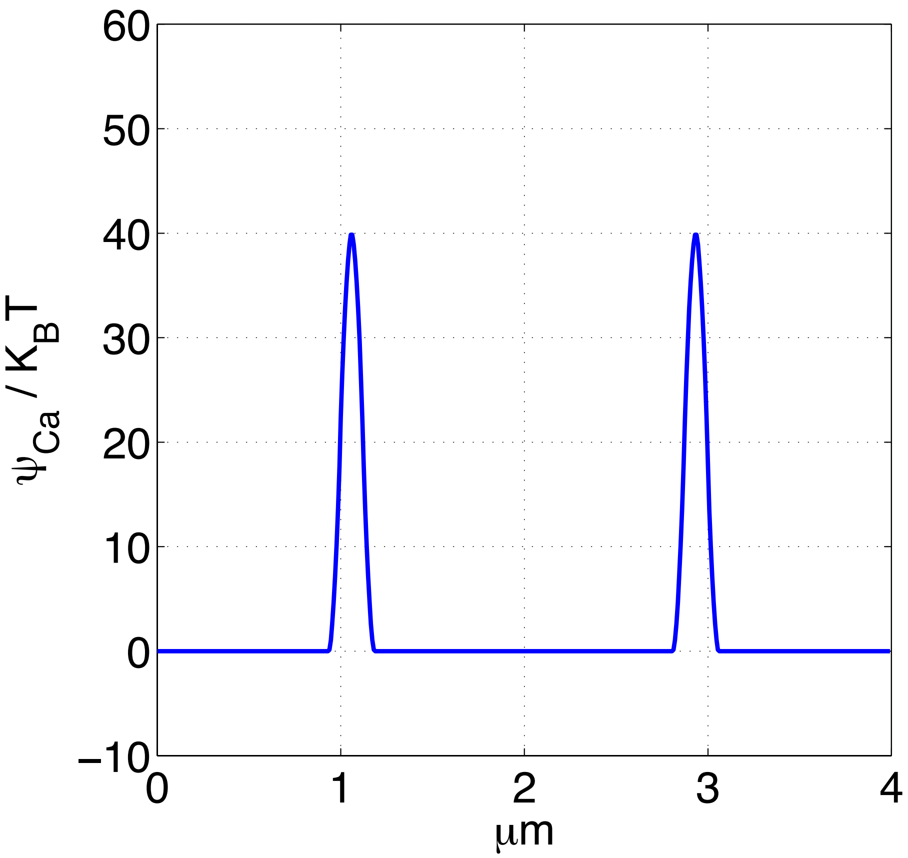


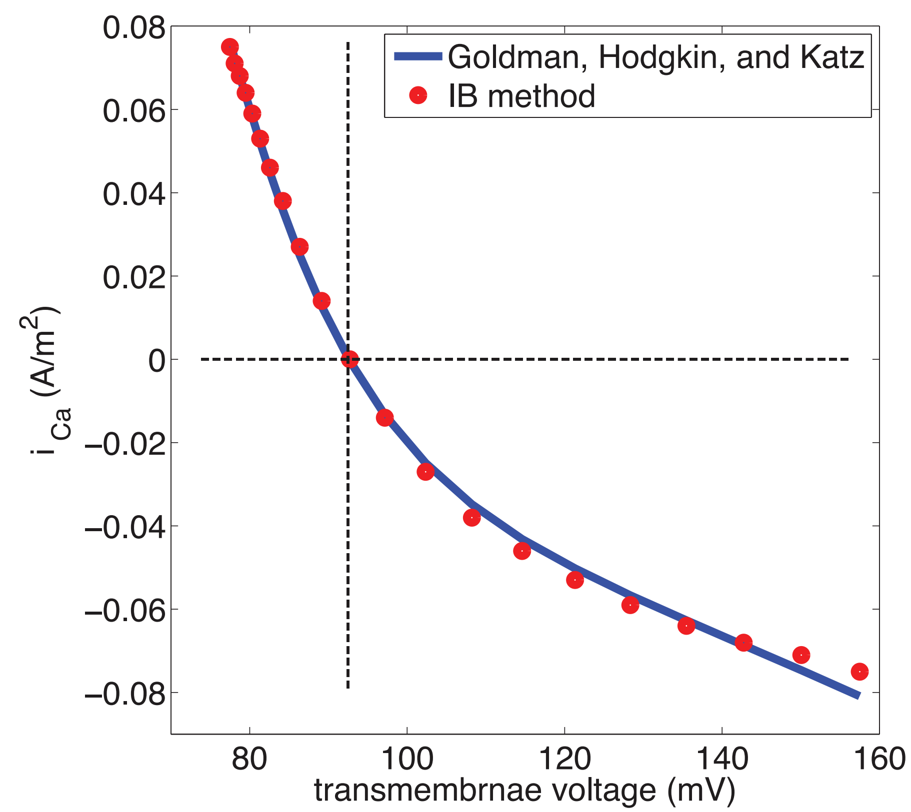
Matus, et al. 2006

How the following signals in dendritic spines change calcium dynamics and structural plasticity in dendrites and functionality in neural circuits?

- Myosin II activation
- Wnt signaling
- Amyloid beta aggregation

Voltage sensitive calcium ion channels in a dendritic spine





Membrane physiology
Interface boundary condition → Chemical potential barrier

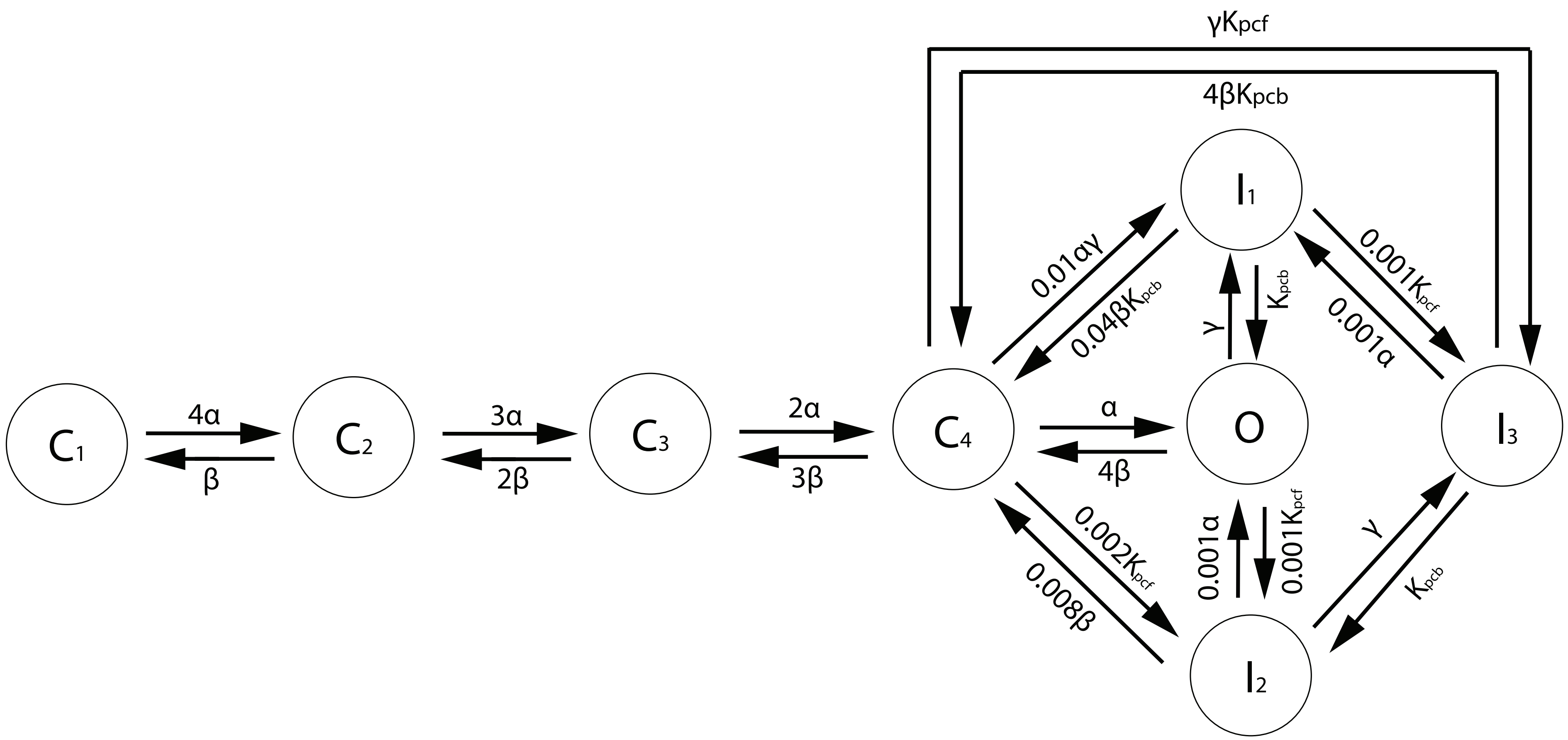
Lee, Sobie, Peskin, JTB, 2013

Voltage sensitive calcium ion channels in a dendritic spine

Continuous-time Markov process

$$P(S(t+dt)=S_j|S(t)=S_i)=r_{i,j}dt$$

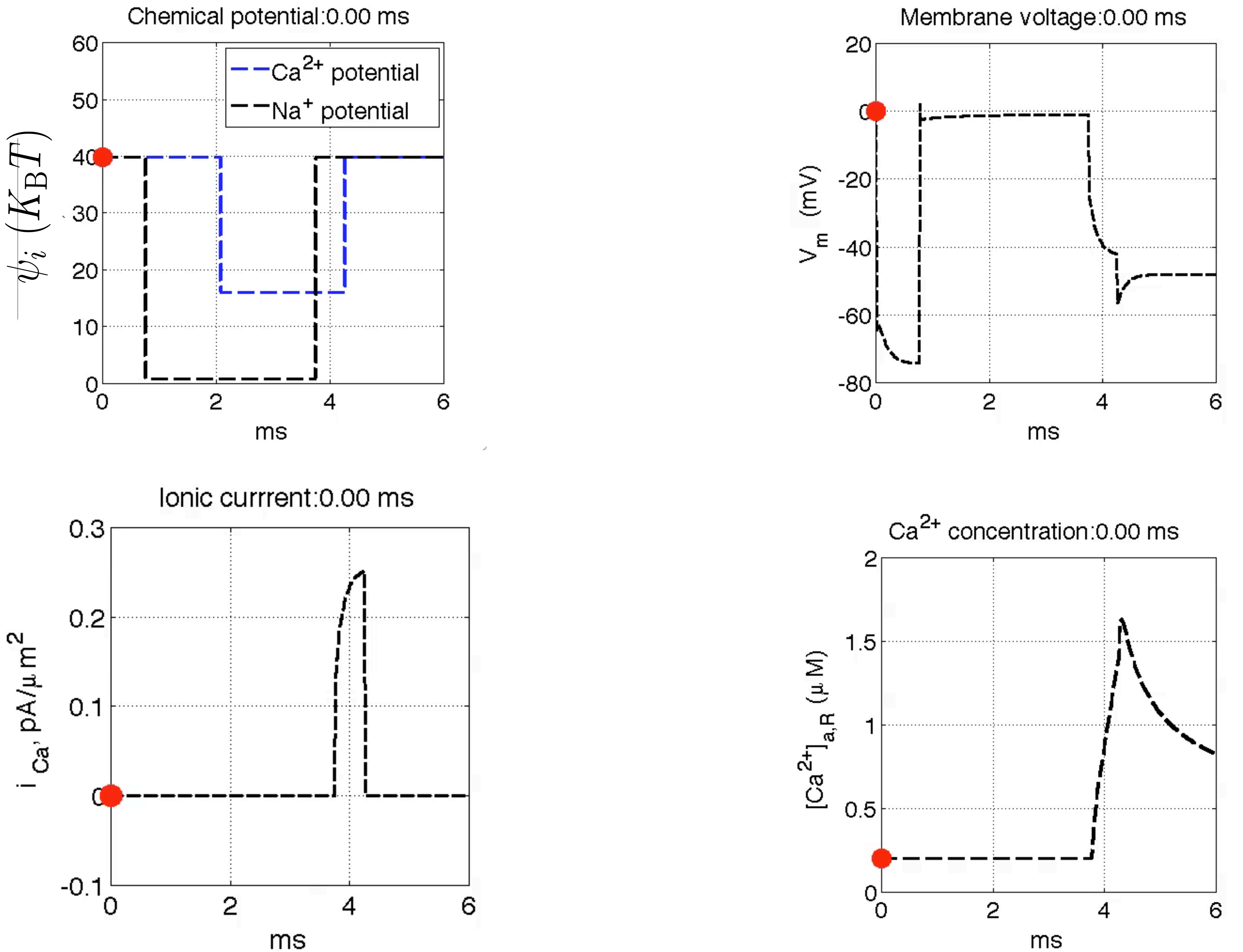
Markov chain of calcium ion channel,
Bondarenko et al. 2004



- 4 subunits
- voltage dependent activation
- intracellular calcium and voltage dependent inactivation

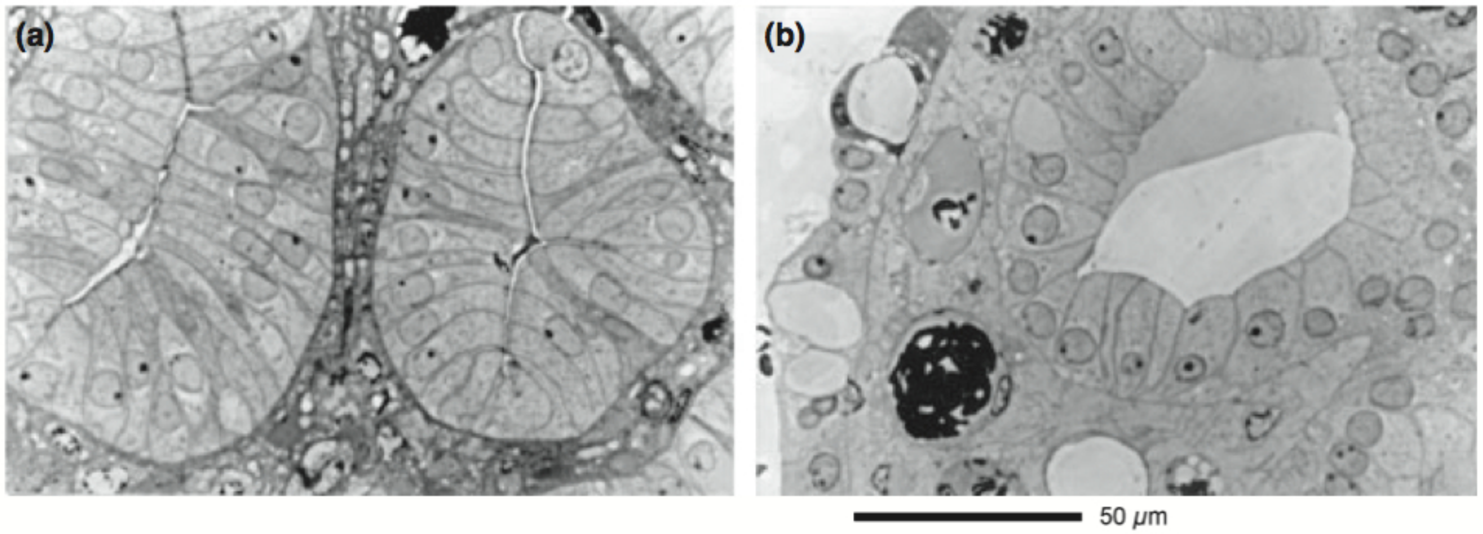
Lee, Sobie, and Peskin, JTB, 2013

Voltage sensitive calcium ion channels in a dendritic spine

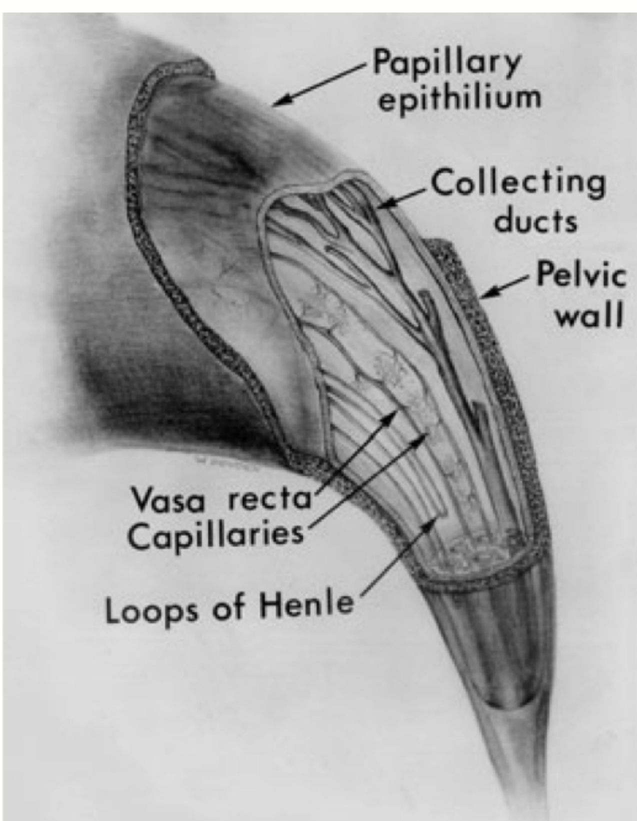


Lee, Sobie, and Peskin, JTB, 2013

Renal peristaltic concentration



A cross-section of papilla 300 micron above the tip, collecting ducts (a) closed with peristaltic contraction and (b) open with peristaltic relaxation



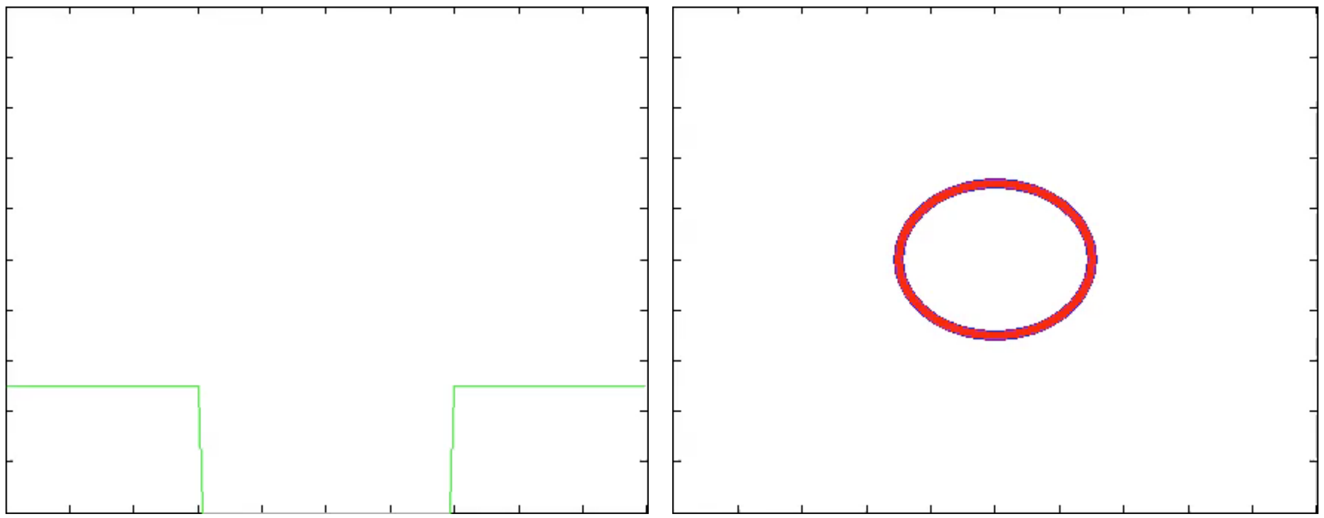
(Lower left) Schematic drawing of a hamster papilla

Peristalsis moves the green colored urine in waves through collecting ducts in the renal papilla

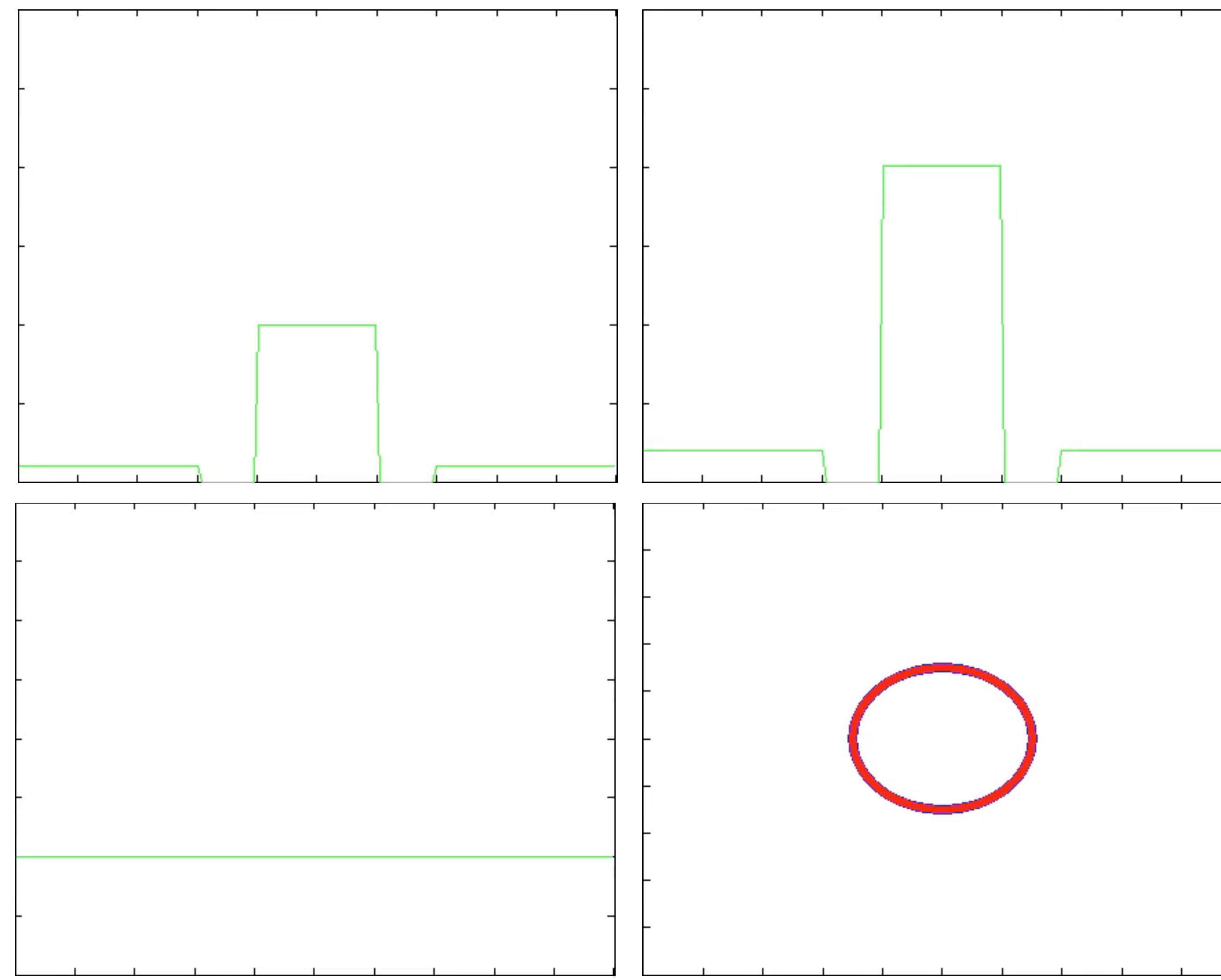
B. Schmidt-Nielsen and B. Graves 1982

Osmotic volume change

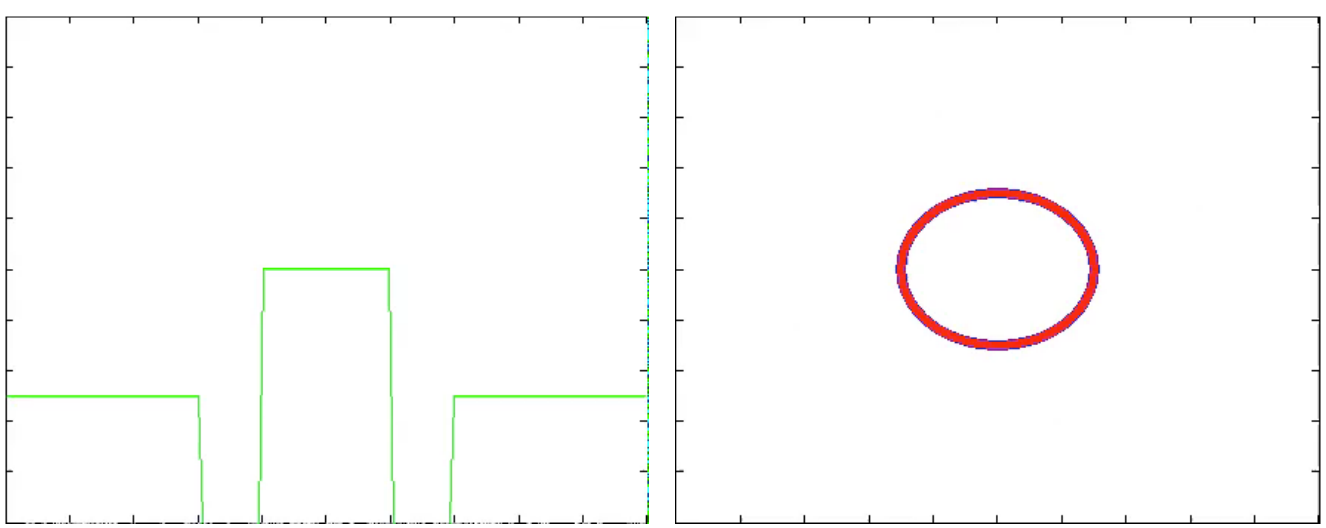
I. Water semi-permeable vesicle with hypotonic distribution



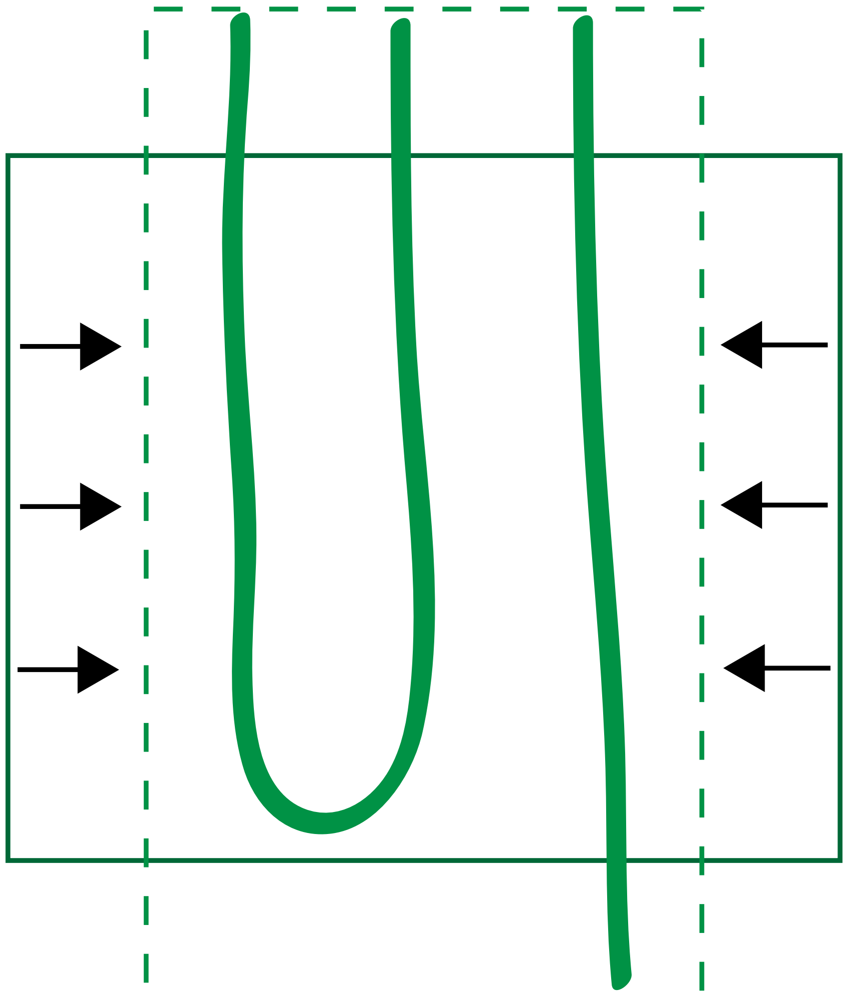
III. Water semi-permeable vesicle with hypertonic distribution

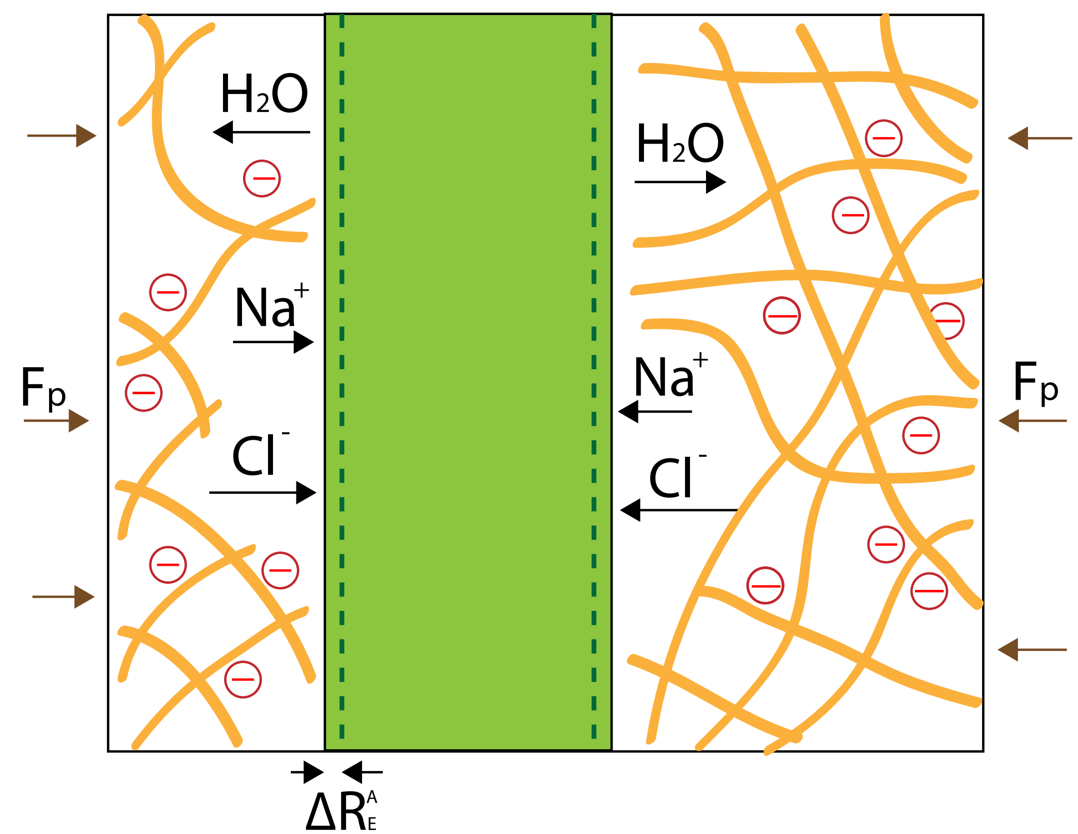


II. Water semi-permeable vesicle in equilibrium



Renal peristaltic concentration

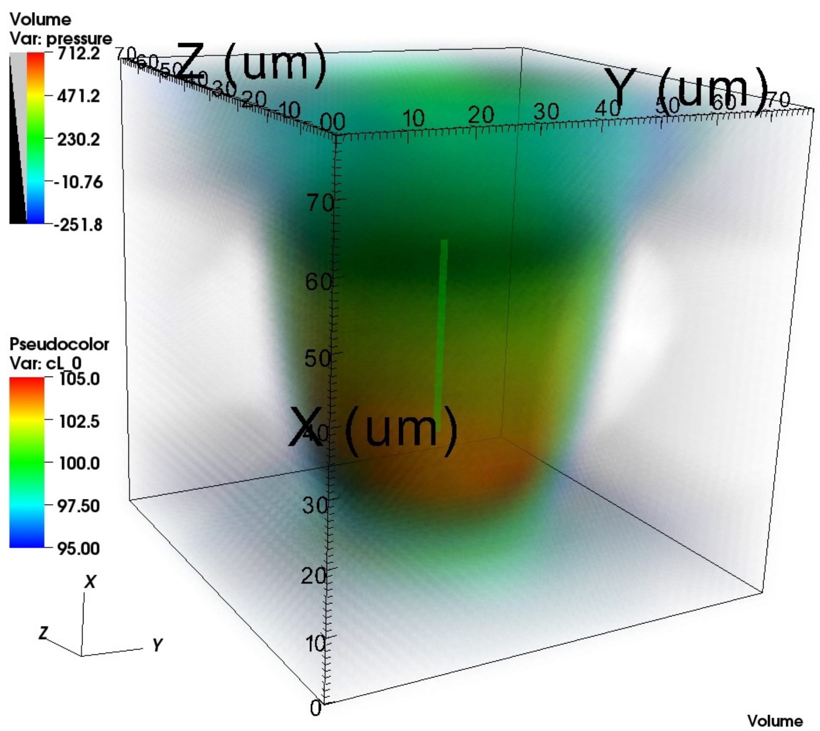




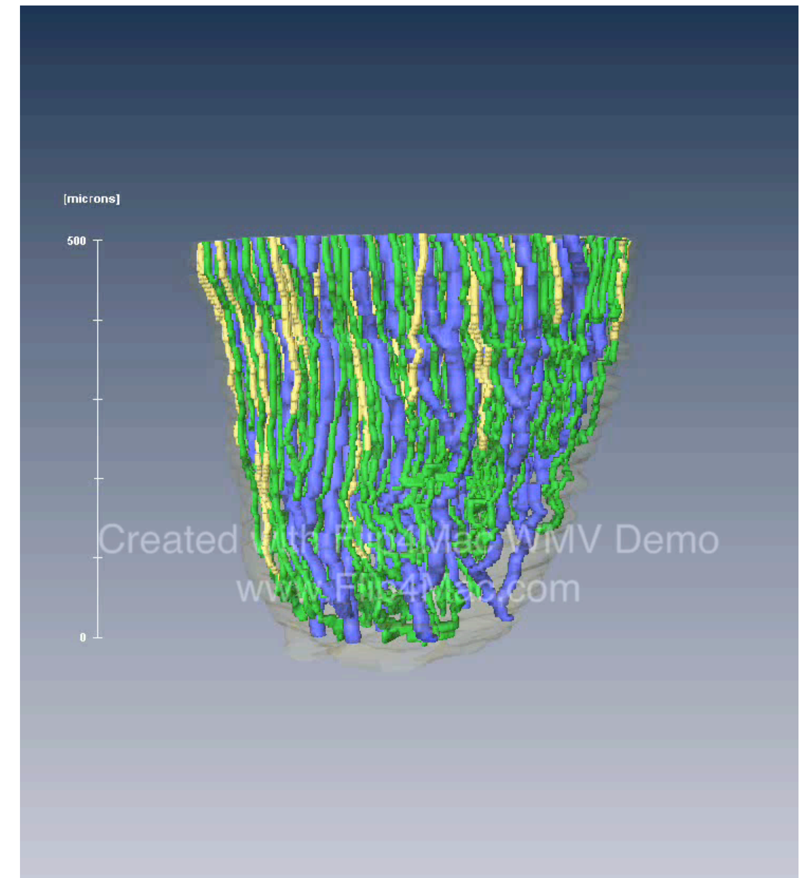
Hypothesized mechanisms of **rectified transport** of ions across epithelial layer via i) **electrically charged** and ii) **viscoelastic extracellular matrix**

Lee and Beard, 2013 EB

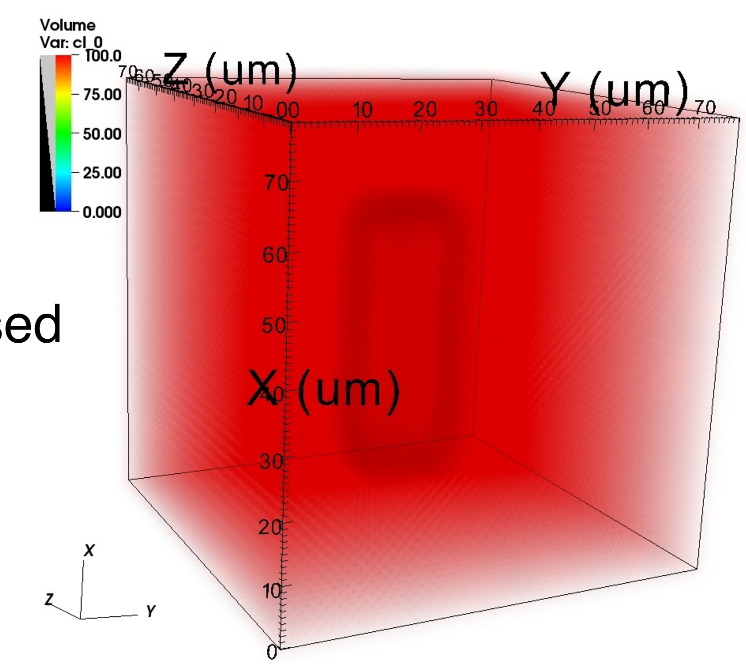
Renal peristaltic concentration



3D hydrostatic pressure distribution from peristaltic contraction and the luminal concentration in collecting duct



3D solute concentration in interstitium using the immersed boundary method with **chemical potential barrier**



3D reconstruction of all papillary collecting ducts (AQP2, blue), ascending thin limbs (ClC-K1, green), and descending thin limbs (AQP1-null, yellow) in a kidney.

T.L. Pannabecker and W.H. Dantzler, 2007

The way to go is to take realistic 1D tubules in 3D, and combine counter-current and peristaltic mechanisms in the renal concentration.

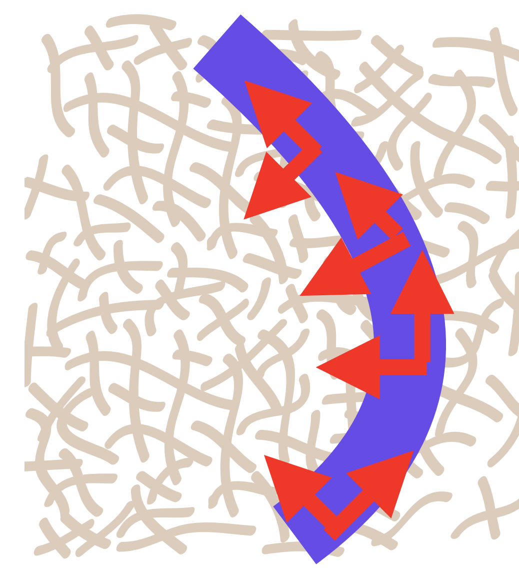
Lee and Beard, 2013 EB

IB method for two-phase fluids and gels

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (\phi \boldsymbol{v}_{\mathrm{p}}) = 0$$

$$\rho_{\mathrm{f}} \frac{\partial \boldsymbol{v}_{\mathrm{f}}}{\partial t} + \Gamma(\boldsymbol{v}_{\mathrm{f}} - \boldsymbol{v}_{\mathrm{p}}) = -(1-\phi)\nabla p + \eta_{\mathrm{f}} \nabla \cdot (\nabla \boldsymbol{v}_{\mathrm{f}} + \nabla \boldsymbol{v}_{\mathrm{f}}^{\mathrm{T}}) + S\boldsymbol{F}_{\mathrm{f}}$$

$$\rho_{\mathrm{p}} \frac{\partial \boldsymbol{v}_{\mathrm{p}}}{\partial t} + \Gamma(\boldsymbol{v}_{\mathrm{p}} - \boldsymbol{v}_{\mathrm{f}}) = -\phi \nabla p - \sigma_0 \nabla \phi$$
$$+ \eta_{\mathrm{p}} \nabla \cdot (\nabla \boldsymbol{v}_{\mathrm{p}} + \nabla \boldsymbol{v}_{\mathrm{p}}^{\mathrm{T}}) + \mu \nabla \cdot (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\mathrm{T}}) + S\boldsymbol{F}_{\mathrm{p}}.$$



$$\frac{d\boldsymbol{u}}{dt} = \frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{v}_{\mathrm{p}} \cdot \nabla \boldsymbol{u} = \boldsymbol{v}_{\mathrm{p}}$$

$$\nabla \cdot \{(1-\phi)\boldsymbol{v}_{\mathrm{f}} + \phi \boldsymbol{v}_{\mathrm{p}}\} = 0$$

$$\boldsymbol{F}_{\mathrm{p}} \cdot \boldsymbol{T} = \Xi_{\mathrm{T}} S^* (\boldsymbol{v}_{\mathrm{f}} - \boldsymbol{v}_{\mathrm{p}}) \cdot \boldsymbol{T}$$

$$\boldsymbol{F}_{\mathrm{p}} \cdot \boldsymbol{N} = \Xi_{\mathrm{N}} S^* (\boldsymbol{v}_{\mathrm{f}} - \boldsymbol{v}_{\mathrm{p}}) \cdot \boldsymbol{N}$$

$$\boldsymbol{F}_{\mathrm{f}} + \boldsymbol{F}_{\mathrm{p}} = -\frac{\delta E}{\delta \boldsymbol{X}}$$

Lee and Wolgemuth, POF, 2016

IB method for two-phase fluids and gels

Semi-implicit approximate projection approach

STEP I) without volume conservation condition

$$\frac{\phi^{n+\frac{1}{2}} - \phi^n}{\Delta t/2} + D_h \cdot (\phi^n \boldsymbol{v}_\mathrm{p}^n) = 0 \qquad \mathscr{L}_h = L_h + G_h D_h \cdot$$

$$\rho_\mathrm{f} \frac{\boldsymbol{v}_\mathrm{f}^* - \boldsymbol{v}_\mathrm{f}^n}{\Delta t} + \Gamma(\boldsymbol{v}_\mathrm{f}^{n+\frac{1}{2},*} - \boldsymbol{v}_\mathrm{p}^{n+\frac{1}{2},*}) = -(1-\phi^{n+\frac{1}{2}}) G_h p^{n-\frac{1}{2}} + \eta_\mathrm{f} \mathscr{L}_h \boldsymbol{v}_\mathrm{f}^{n+\frac{1}{2},*} + S_{n+\frac{1}{2}} \boldsymbol{F}_\mathrm{f}^{n+\frac{1}{2},*}$$

$$\rho_\mathrm{p} \frac{\boldsymbol{v}_\mathrm{p}^* - \boldsymbol{v}_\mathrm{p}^n}{\Delta t} + \Gamma(\boldsymbol{v}_\mathrm{p}^{n+\frac{1}{2},*} - \boldsymbol{v}_\mathrm{f}^{n+\frac{1}{2},*}) = -\phi^{n+\frac{1}{2}} G_h p^{n-\frac{1}{2}} - \sigma_0 G_h \phi^{n+\frac{1}{2}} + \eta_\mathrm{p} \mathscr{L}_h \boldsymbol{v}_\mathrm{p}^{n+\frac{1}{2},*} + \mu \mathscr{L}_h \boldsymbol{u}^{n+\frac{1}{2}} + S_{n+\frac{1}{2}} \boldsymbol{F}_\mathrm{p}^{n+\frac{1}{2},*}$$

$$\frac{\boldsymbol{u}^{n+\frac{1}{2}} - \boldsymbol{u}^n}{\Delta t/2} + \boldsymbol{v}_\mathrm{p}^n \cdot G_h \boldsymbol{u}^n = \boldsymbol{v}_\mathrm{p}^n$$

$$\boldsymbol{v}_\mathrm{f}^{n+\frac{1}{2},*} = \frac{\boldsymbol{v}_\mathrm{f}^n + \boldsymbol{v}_\mathrm{f}^*}{2}, \qquad \boldsymbol{v}_\mathrm{p}^{n+\frac{1}{2},*} = \frac{\boldsymbol{v}_\mathrm{p}^n + \boldsymbol{v}_\mathrm{p}^*}{2}$$

$$\boldsymbol{F}_\mathrm{p}^{n+\frac{1}{2},*} = \Xi_\mathrm{T}(\boldsymbol{v}_\mathrm{f}^{n+\frac{1}{2},*} - \boldsymbol{v}_\mathrm{p}^{n+\frac{1}{2},*}) \cdot \boldsymbol{T}^{n+\frac{1}{2}} \boldsymbol{T}^{n+\frac{1}{2}} + \Xi_\mathrm{N}(\boldsymbol{v}_\mathrm{f}^{n+\frac{1}{2},*} - \boldsymbol{v}_\mathrm{p}^{n+\frac{1}{2},*}) \cdot \boldsymbol{N}^{n+\frac{1}{2}} \boldsymbol{N}^{n+\frac{1}{2}}$$

$$\boldsymbol{F}_\mathrm{f}^{n+\frac{1}{2},*} = -\frac{\partial E}{\partial \boldsymbol{X}^{n+\frac{1}{2}}} - \boldsymbol{F}_\mathrm{p}^{n+\frac{1}{2},*}$$

$$\frac{\boldsymbol{X}^{n+\frac{1}{2}} - \boldsymbol{X}^n}{\Delta t/2} = S_n^* \boldsymbol{v}_\mathrm{f}^n$$

Lee and Wolgemuth, POF, 2016

IB method for two-phase fluids and gels

Semi-implicit approximate projection approach

STEP II) with approximate projection

$$\frac{\phi^{n+1}-\phi^{n}}{\Delta t}+D_h\cdot(\phi^{n+\frac{1}{2}}\boldsymbol{v}_{\mathrm{p}}^{n+\frac{1}{2}})=0$$

$$\rho_{\mathrm{f}}\frac{\boldsymbol{v}_{\mathrm{f}}^{n+1}-\boldsymbol{v}_{\mathrm{f}}^{n}}{\Delta t}+\Gamma(\boldsymbol{v}_{\mathrm{f}}^{n+\frac{1}{2}}-\boldsymbol{v}_{\mathrm{p}}^{n+\frac{1}{2}})=-(1-\phi^{n+\frac{1}{2}})G_h p^{n+\frac{1}{2}} +\eta_{\mathrm{f}}\mathscr{L}_h\boldsymbol{v}_{\mathrm{f}}^{n+1}+S_{n+\frac{1}{2}}\boldsymbol{F}_{\mathrm{f}}^{n+1}$$

$$\rho_{\mathrm{p}}\frac{\boldsymbol{v}_{\mathrm{p}}^{n+1}-\boldsymbol{v}_{\mathrm{p}}^{n}}{\Delta t}+\Gamma(\boldsymbol{v}_{\mathrm{p}}^{n+\frac{1}{2}}-\boldsymbol{v}_{\mathrm{f}}^{n+\frac{1}{2}})=-\phi^{n+\frac{1}{2}}G_h p^{n+\frac{1}{2}}-\sigma_0 G_h\phi^{n+\frac{1}{2}} +\eta_{\mathrm{p}}\mathscr{L}_h\boldsymbol{v}_{\mathrm{p}}^{n+1}+\mu\mathscr{L}_h\boldsymbol{u}^{n+\frac{1}{2}}+S_{n+\frac{1}{2}}\boldsymbol{F}_{\mathrm{p}}^{n+1}$$

$$\boldsymbol{F}_{\mathrm{p}}^{n+1}=\Xi_{\mathrm{T}}(\boldsymbol{v}_{\mathrm{f}}^{n+1}-\boldsymbol{v}_{\mathrm{p}}^{n+1})\cdot\boldsymbol{T}^{n+\frac{1}{2}}\boldsymbol{T}^{n+\frac{1}{2}} +\Xi_{\mathrm{N}}(\boldsymbol{v}_{\mathrm{f}}^{n+1}-\boldsymbol{v}_{\mathrm{p}}^{n+1})\cdot\boldsymbol{N}^{n+\frac{1}{2}}\boldsymbol{N}^{n+\frac{1}{2}}$$

$$\boldsymbol{F}_{\mathrm{f}}^{n+1}=-\frac{\partial E}{\partial\boldsymbol{X}^{n+\frac{1}{2}}}-\boldsymbol{F}_{\mathrm{p}}^{n+1}$$

$$(1-\phi^{n+1})\mathbf{v}_{\mathrm{f}}^{n+1}+\phi^{n+1}\mathbf{v}_{\mathrm{p}}^{n+1}= (I-G_h L_h^{-1}D_h)\,(1-\phi^{n+1})\boldsymbol{v}_{\mathrm{f}}^{*}+\phi^{n+1}\boldsymbol{v}_{\mathrm{p}}^{*}\}$$

$$\frac{\boldsymbol{u}^{n+1}-\boldsymbol{u}^{n}}{\Delta t}+\boldsymbol{v}_{\mathrm{p}}^{n+\frac{1}{2}}\cdot G_h\boldsymbol{u}^{n+\frac{1}{2}}=\boldsymbol{v}_{\mathrm{p}}^{n+\frac{1}{2}}$$

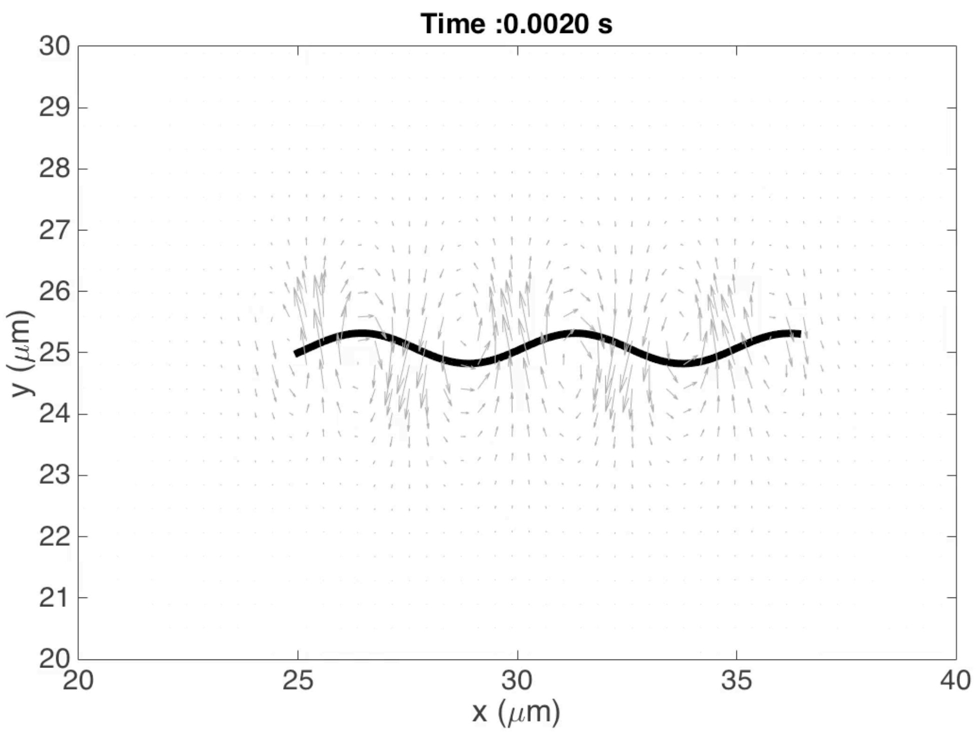
$$\frac{\boldsymbol{X}^{n+1}-\boldsymbol{X}^{n}}{\Delta t}=S_n^{*}\boldsymbol{v}_{\mathrm{f}}^{n+\frac{1}{2}}$$

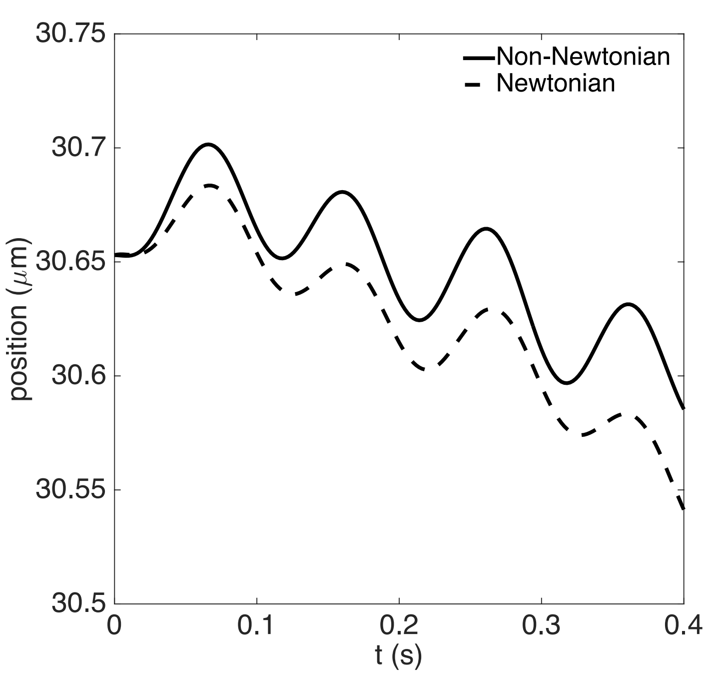
$$p^{n+\frac{1}{2}}-p^{n-\frac{1}{2}}=L_h^{-1}D_h\cdot\{\rho_{\mathrm{f}}\frac{\boldsymbol{v}_{\mathrm{f}}^{*}-\boldsymbol{v}_{\mathrm{f}}^{n+1}}{\Delta t}+\rho_{\mathrm{p}}\frac{\boldsymbol{v}_{\mathrm{p}}^{*}-\boldsymbol{v}_{\mathrm{p}}^{n+1}}{\Delta t} +\eta_{\mathrm{f}}\mathscr{L}_h(\boldsymbol{v}_{\mathrm{f}}^{n+1}-\boldsymbol{v}_{\mathrm{f}}^{n+\frac{1}{2},*})+\eta_{\mathrm{p}}\mathscr{L}_h(\boldsymbol{v}_{\mathrm{p}}^{n+1}-\boldsymbol{v}_{\mathrm{p}}^{n+\frac{1}{2},*})\}$$

Lee and Wolgemuth, POF, 2016

IB method for two-phase fluids and gels

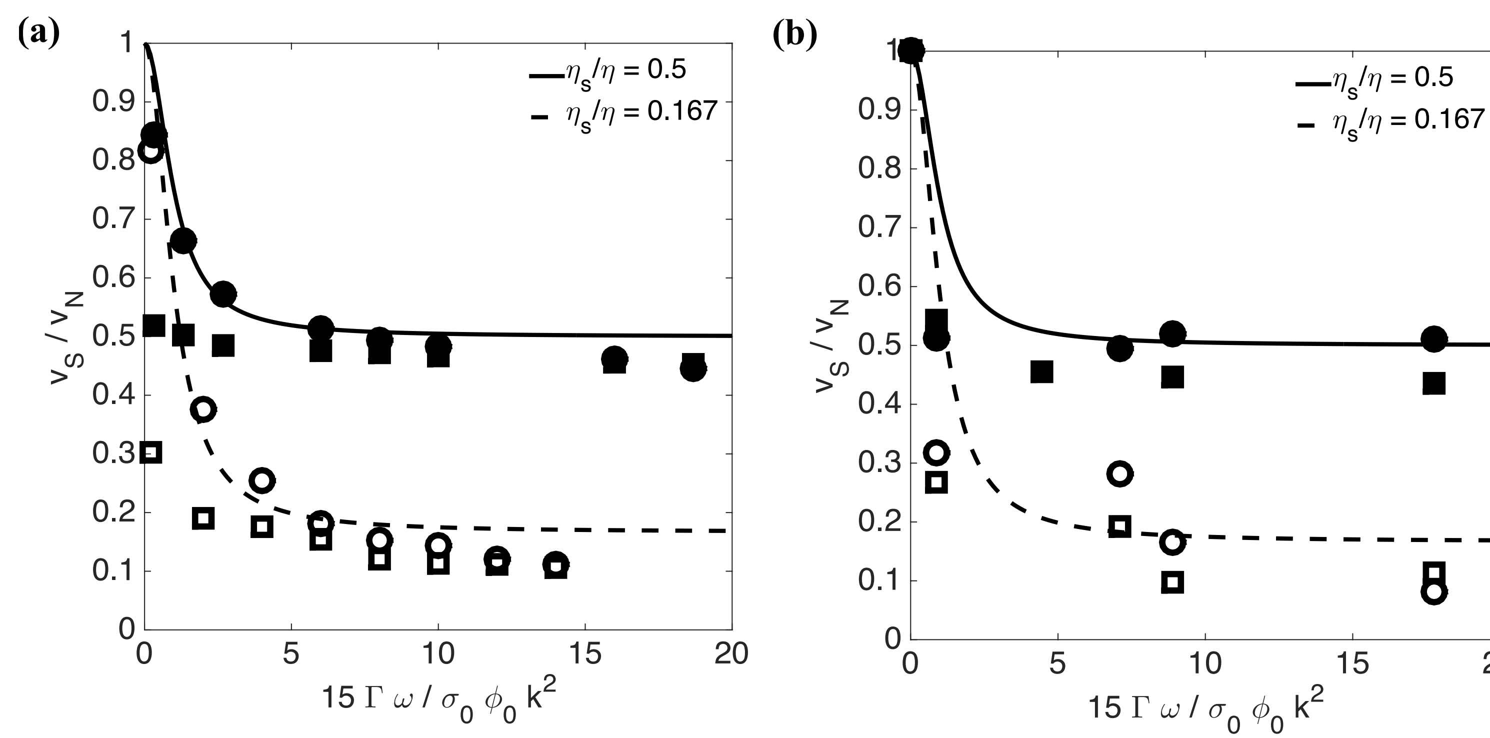
Two phase vs. single phase / Oldroyd B





$$V_S/V_N = \frac{1 + \eta_S/\eta \; De^2}{1 + De^2}$$

Lauga, 2007



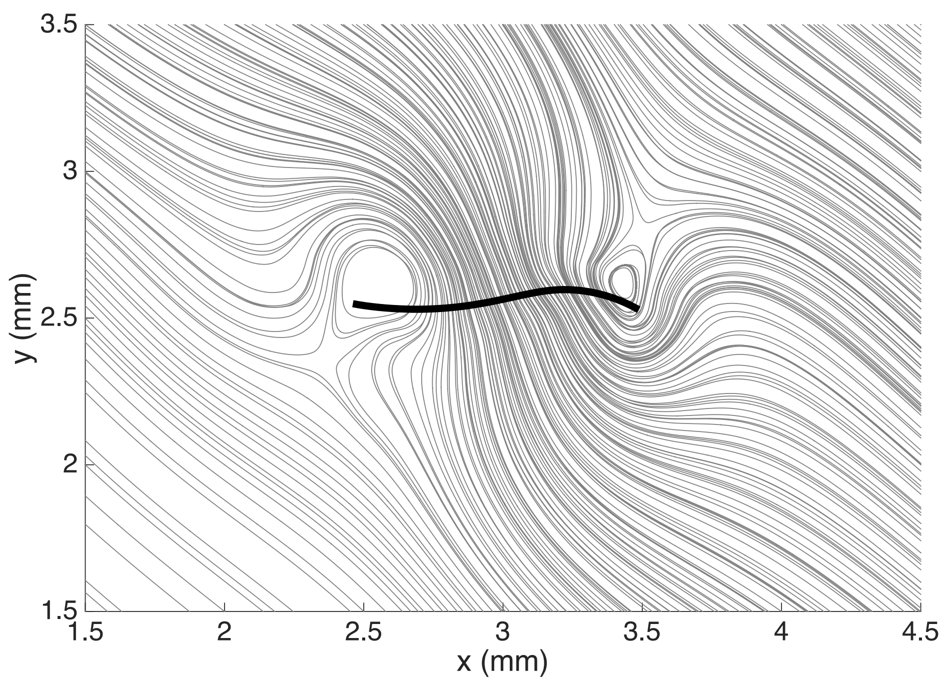
(a) small amplitude, infinite

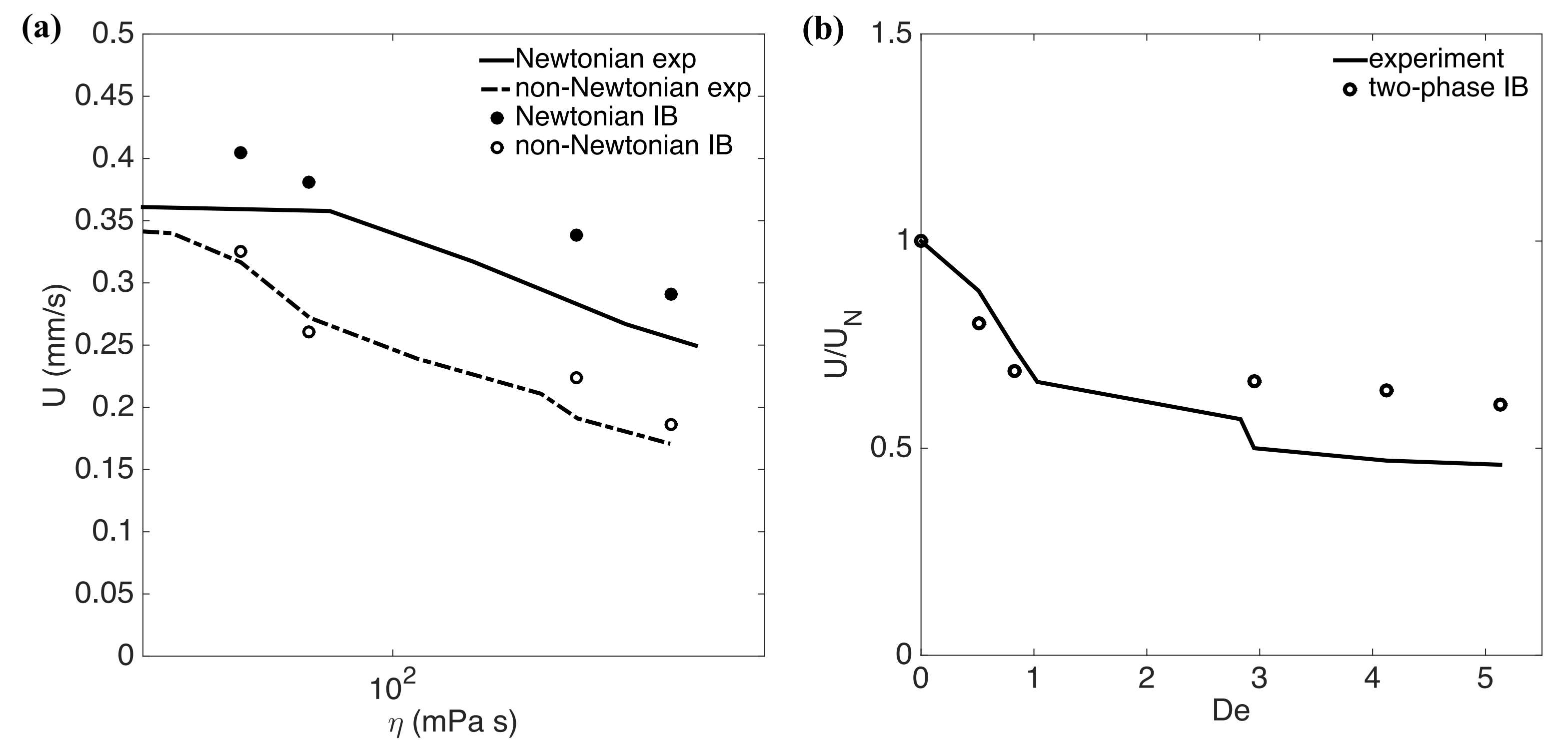
(b) finite length swimmer

Lee and Wolgemuth, POF, 2016

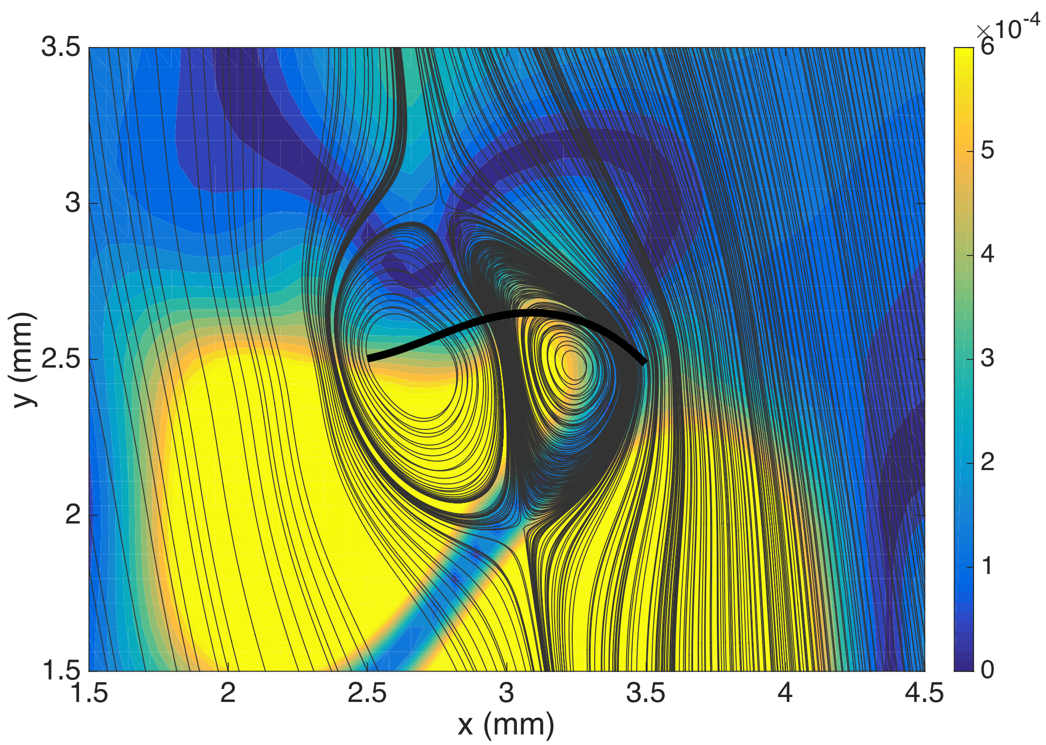
IB method for two-phase fluids and gels

C. elegans swimming / hyperbolic extensional flows





Experiments: Arratia lab



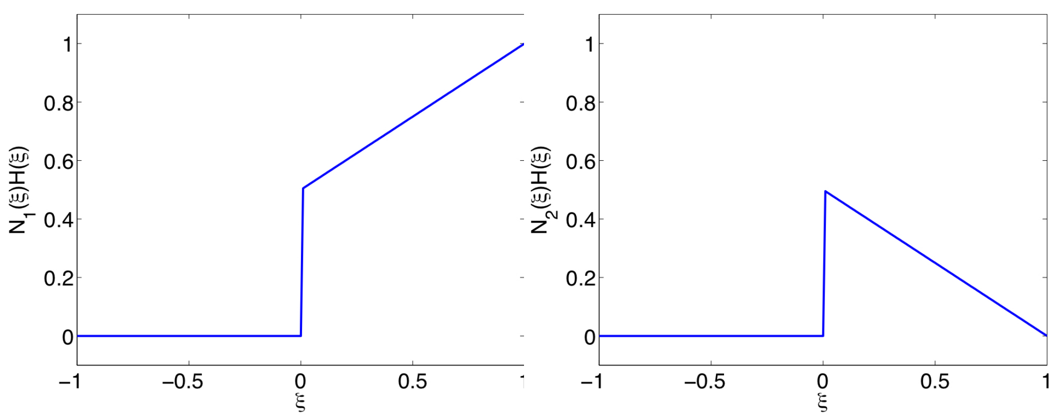
Flow streamlines about a swimming *C. elegans*. The colormap shows the magnitude of the trace of the elastic stress.

Lee and Wolgemuth, POF, 2016

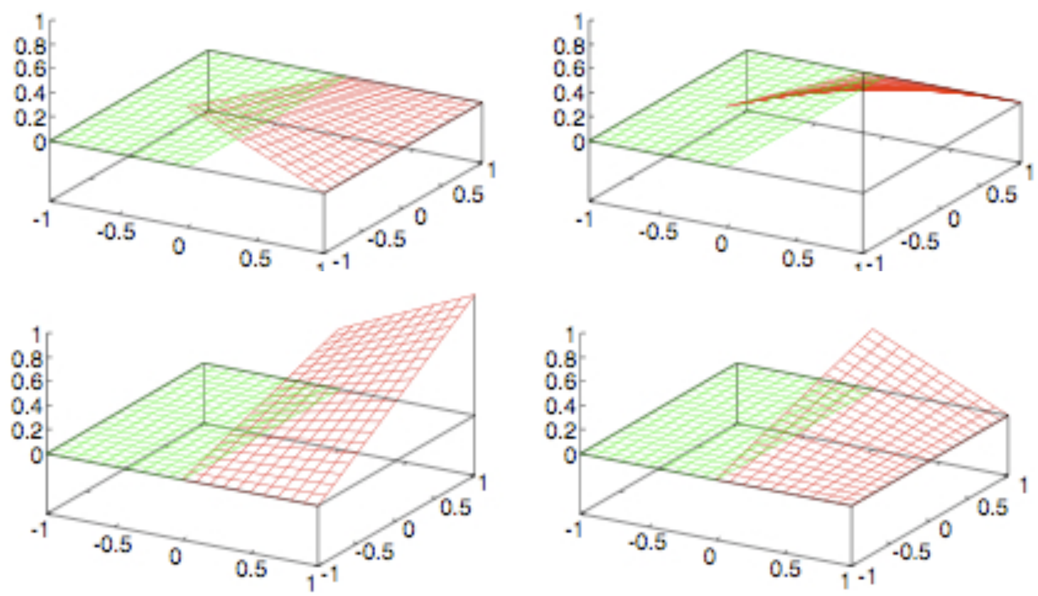
Future work

IB for advection-electrodiffusion with DG/XFEM

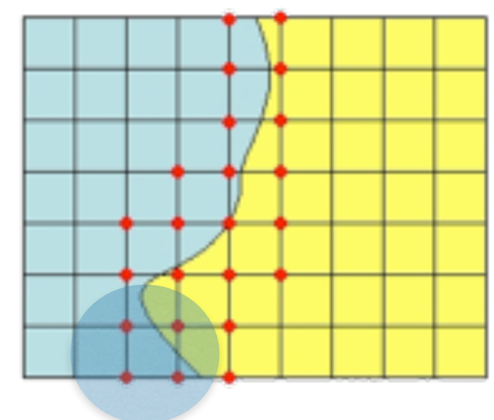
extended shape function 1D

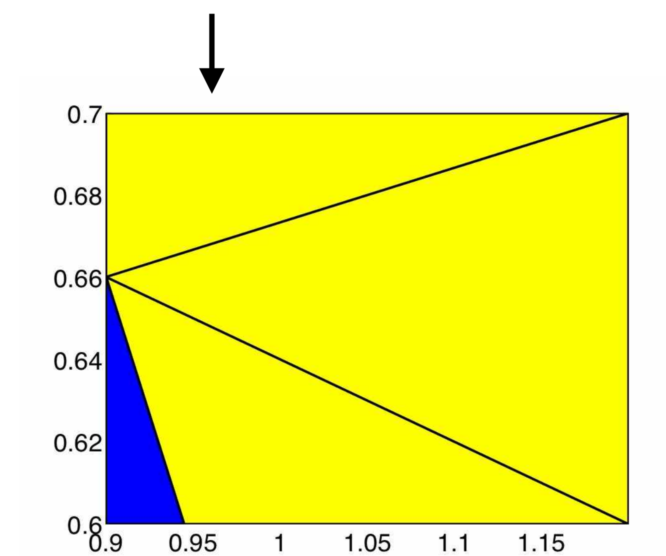


extended shape function 2D



enriched nodes





Integration by Delaunay trianguralization

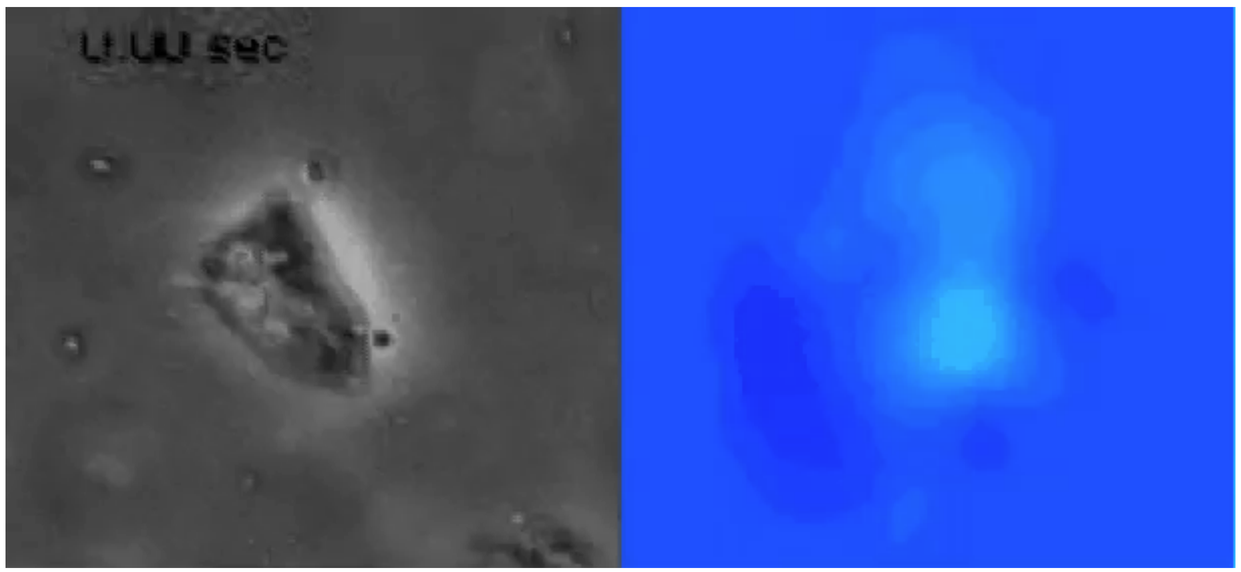
IB for two-phase viscoelastic fluids

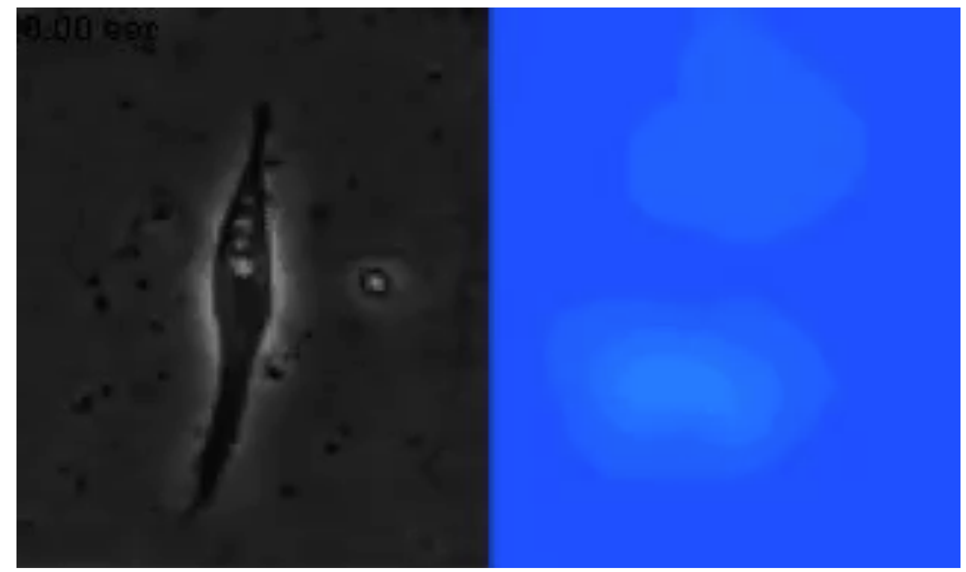
Fast composite multigrid as preconditioner

Exact projection method, MAC scheme

Mechano-sensing of cardiac differentiation

Embryonic cardiac myocytes contraction vs. microenvironment





Engler, et al. 2008 soft gel strain stiff gel strain

How the following developmental mechanisms are influenced by mechanical microenviorонment?

- myofibrillogenesis
- biogenesis
- calcium handling
- mitochondria PTP gating and volume regulation

Acknowledgement

Charles Peskin, Courant Institute, New York University
Boyce Griffith, University of North Carolina
Charles Wolgemuth, University of Arizona
Daniel Beard, University of Michigan

Eric Sobie, Mount Sinai School of Medicine
Paul Arratia, University of Pennsylvania

NIH P50 GM094503
NIH R01 GM072004