The immersed boundary method for advection-electrodiffusion

Matus, et al. 2006

University of Michigan

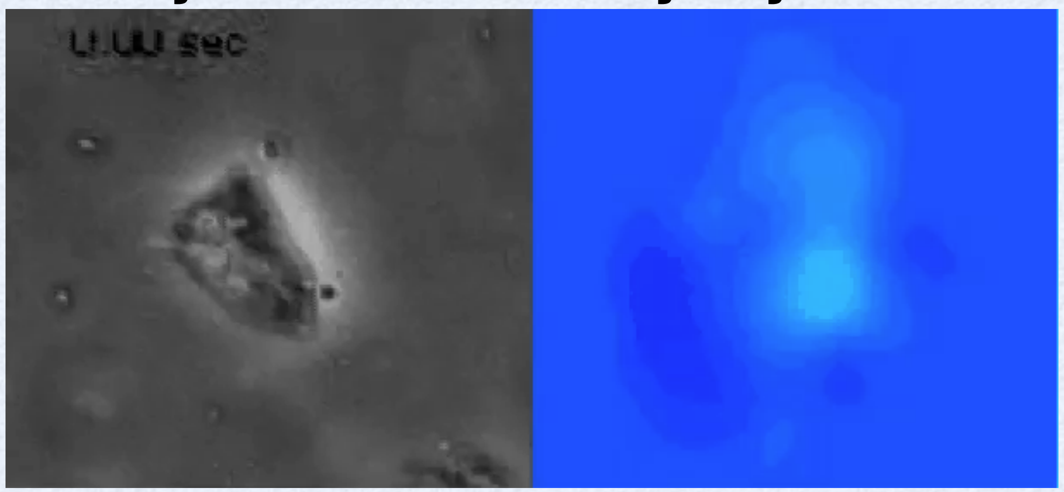
Pilhwa Lee

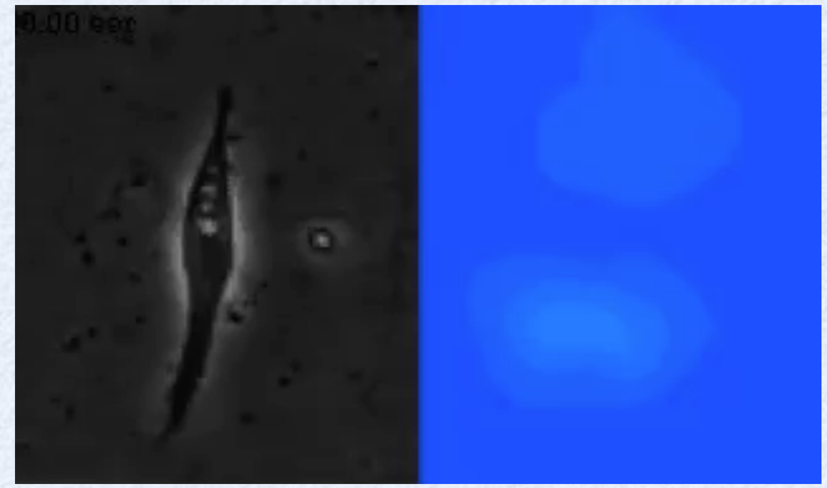
PETSc 20 workshop

The Virtual Physiological Rat Project

Free boundary problems in physiology

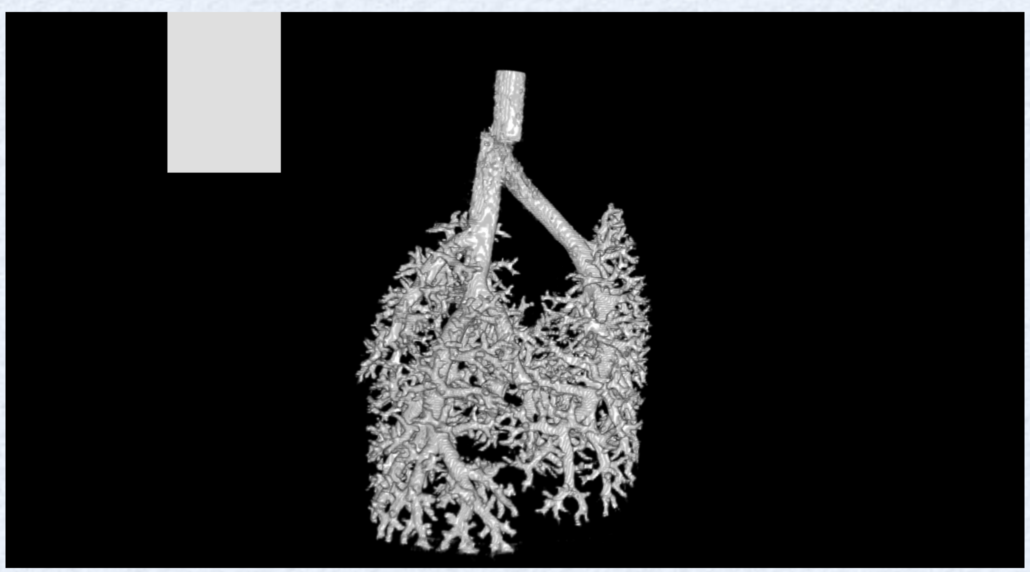
Embryonic cardiac myocytes contraction vs. microenvironment





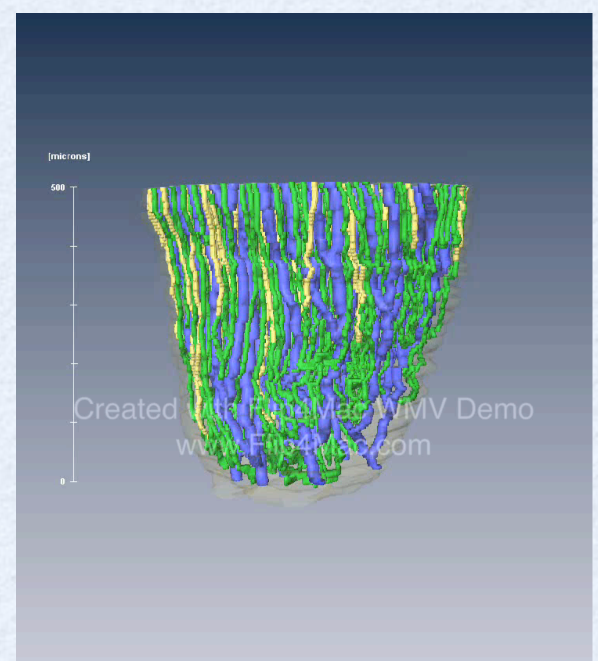
Engler, et al. 2008

Pulmonary arterial network, blood flow profiling



Vanderpool, et al. 2011

Renal inner medulla, solute concentration



Pannabecker and Dantzler, 2007

The immersed boundary method

Charlie Peskin and David McQeen

Fluid-structure interaction

3D distributed memory parallel computing

Boyce Griffith

Adaptive mesh refinement

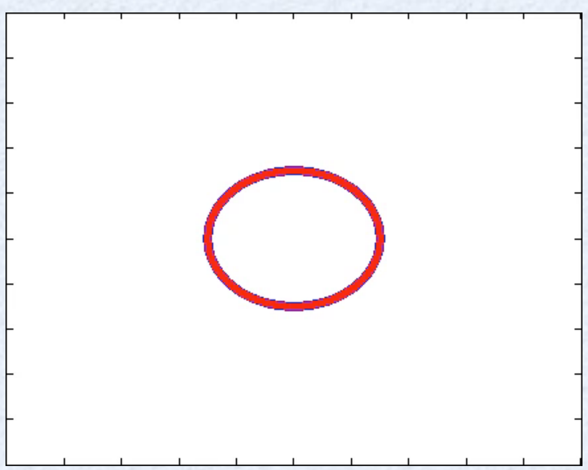
http://www.math.nyu.edu/faculty/peskin/myo3D/config12_animation.html

The immersed boundary method with advection-electrodiffusion

Fluid-solute-structure interaction Osmotic effects

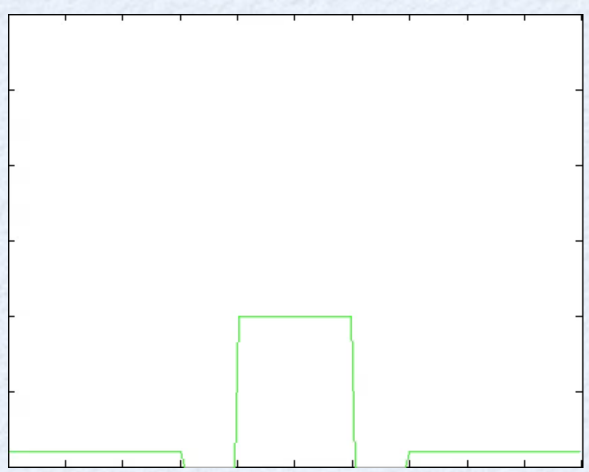
Electrodiffusion Electroneutrality - space charge layer

Membrane swelling

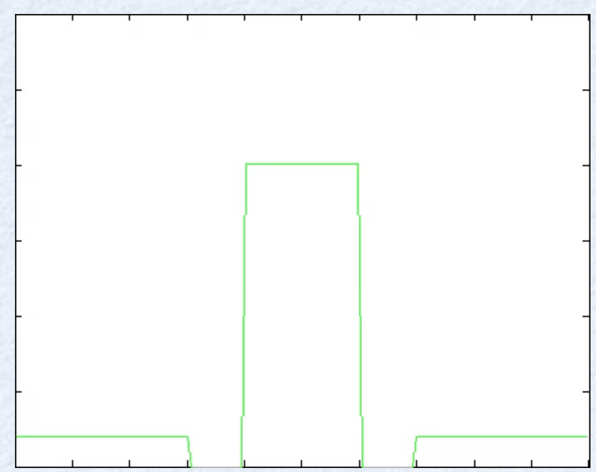


hypertonic

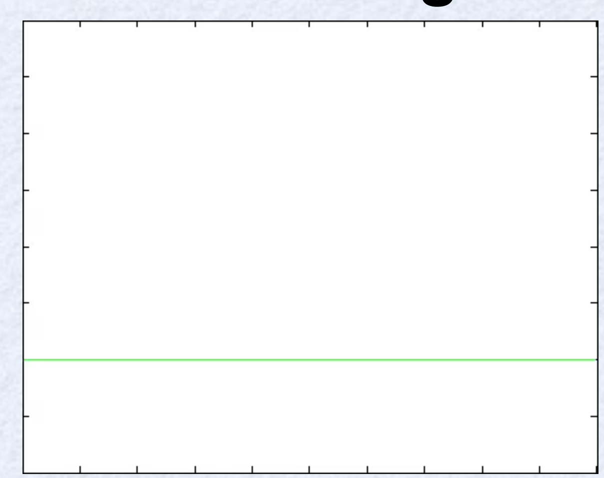
Ca++,impermeable



Cl-,semi-permeable



Electrical charge density



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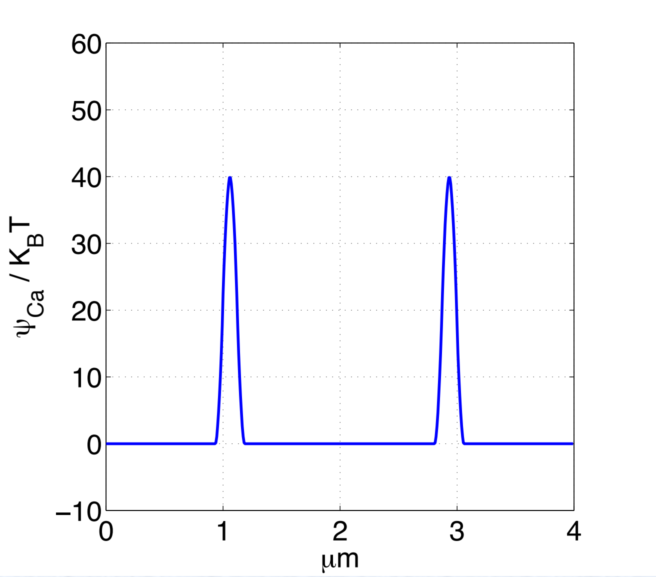
Computational issues

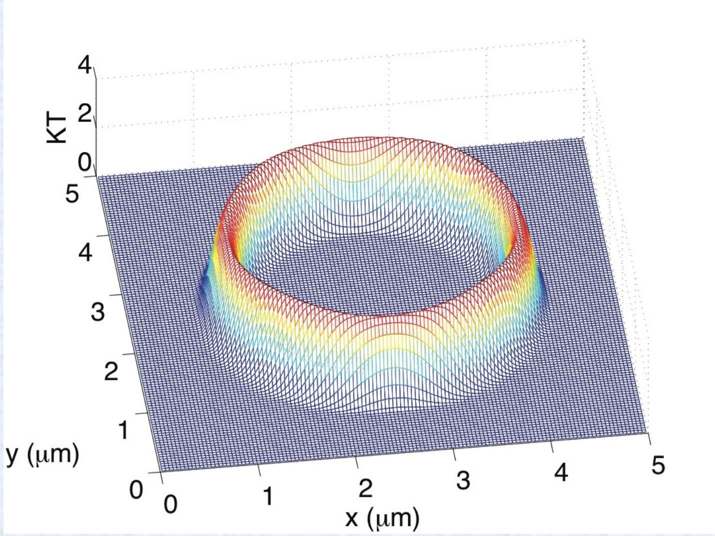
Immensely stiff in hyperbolic system

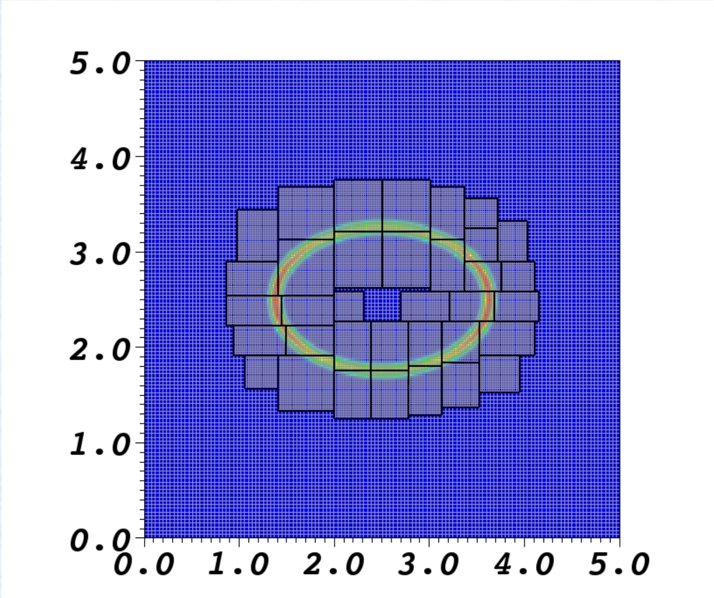
Thin membrane, local mesh refinement

Semi-implicit time stepping

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



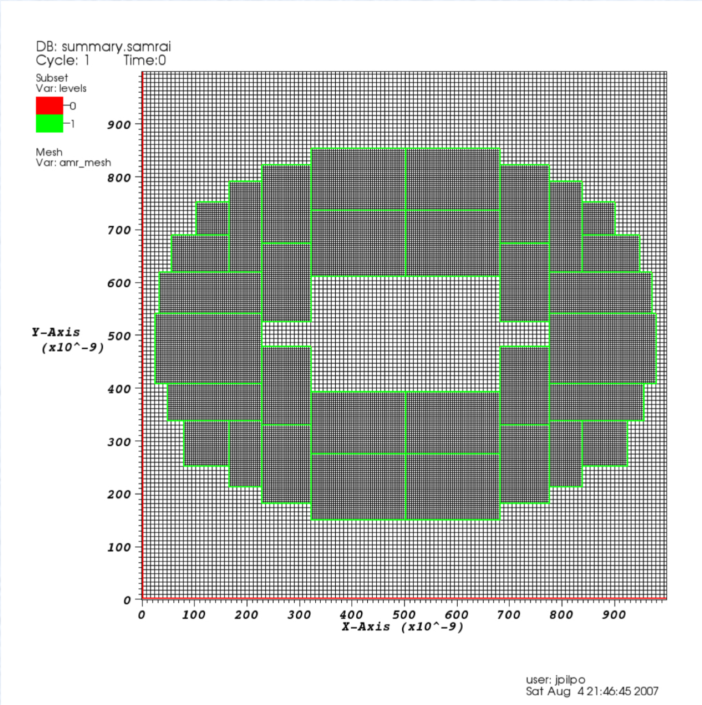


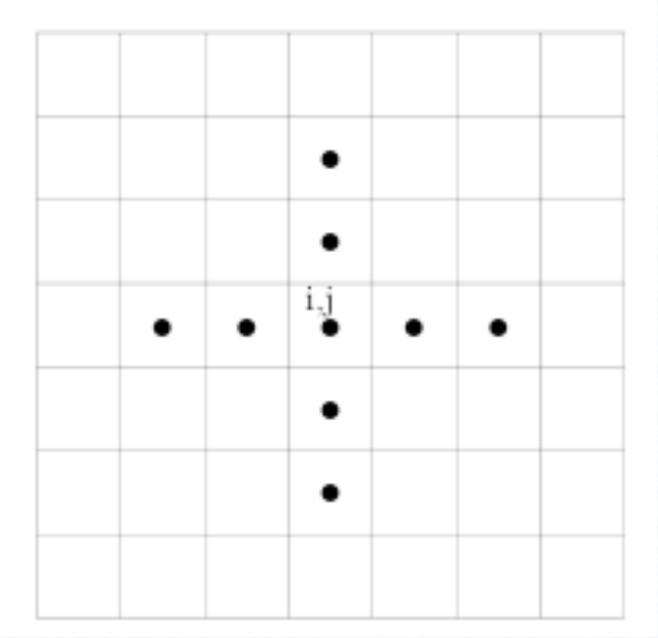


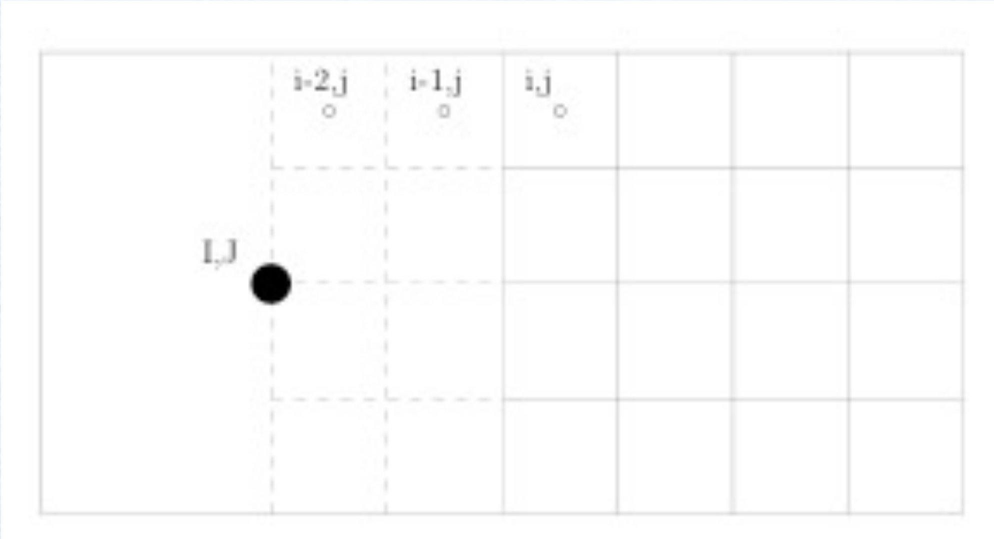
Lee, Griffith, Peskin, J. Comp. Phys. 2010

Numerical architecture

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







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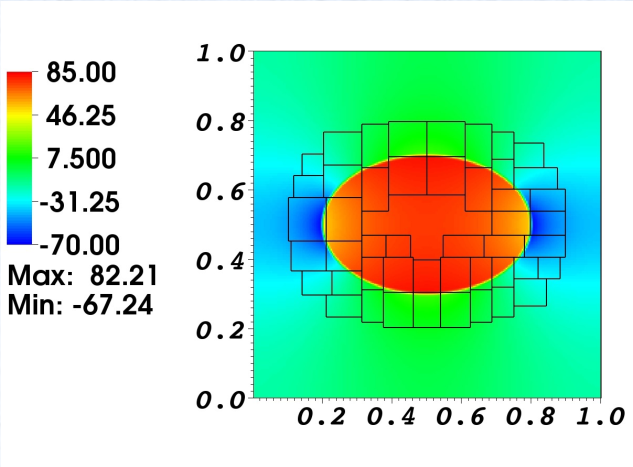
The Stokes equations with permeable membrane

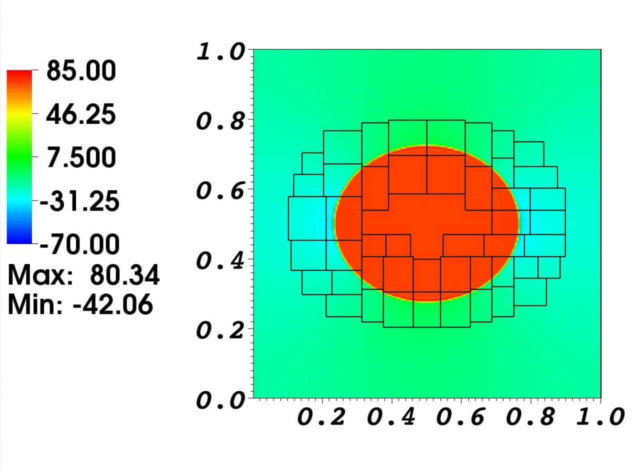
$$\rho\frac{\tilde{\mathbf{u}}-\mathbf{u}^n}{\Delta t}+\mathbf{D}_h p^{n-\frac{1}{2}}=\mu L_h\frac{\tilde{\mathbf{u}}+\mathbf{u}^n}{2}+\mathbf{S}_n\mathbf{F}_{\mathrm{mf}}^{n+1}+\mathbf{f}_{\mathrm{b}}^n$$

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

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

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





- Fast adaptive composite (FAC) method: preconditioner

  one layer of ghost cells, bottom solver (PFMG)
- Krylov subspace GMRES: main solver
- Cell-centered approximate projection method

Advection-electrodiffusion with immersed boundary

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

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

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

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

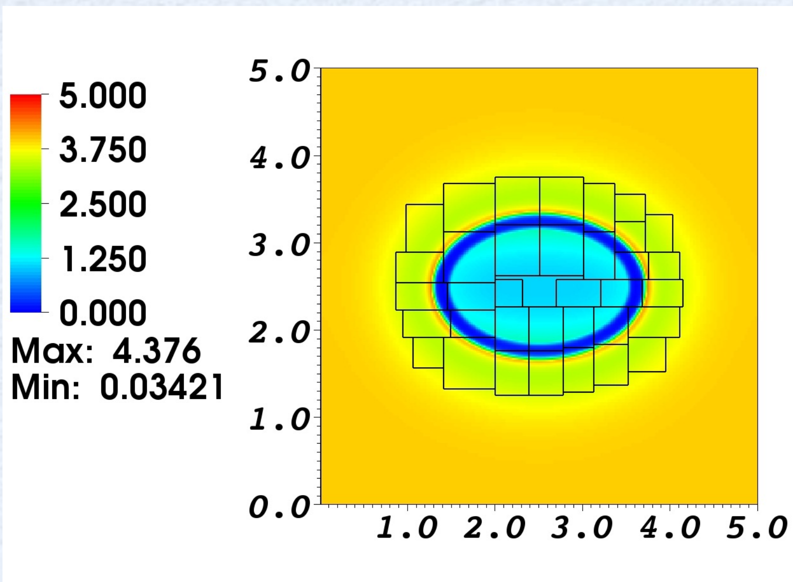
$$L_i^n = L(\mathbf{u}^n, \varphi^n, \psi_i^n)$$

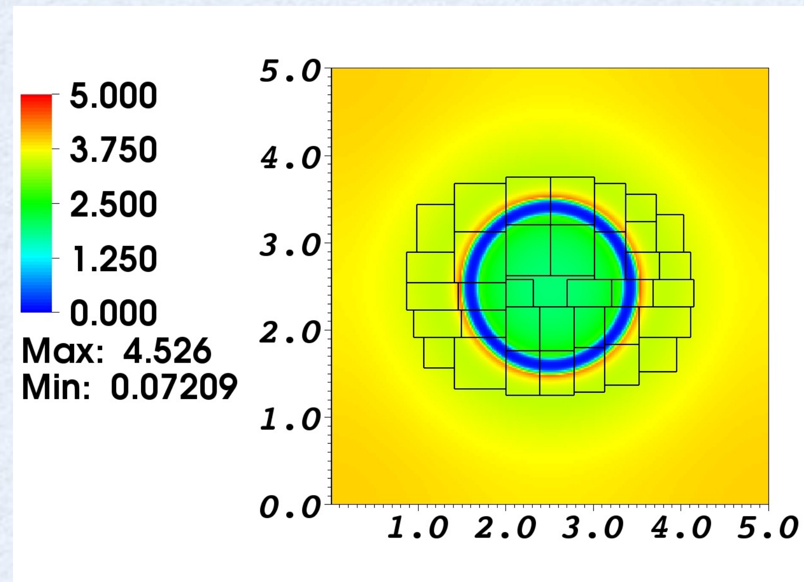
- Fast adaptive composite (FAC) method, preconditioner

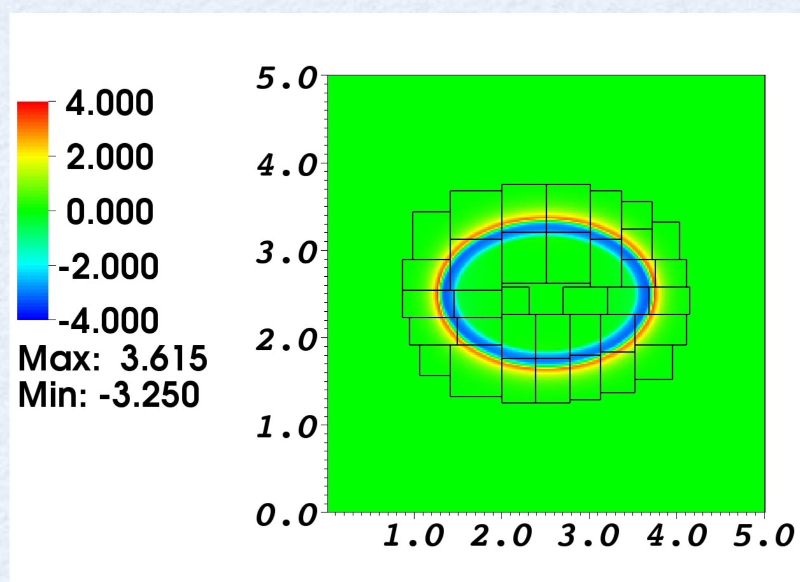
  two layers of ghost cells

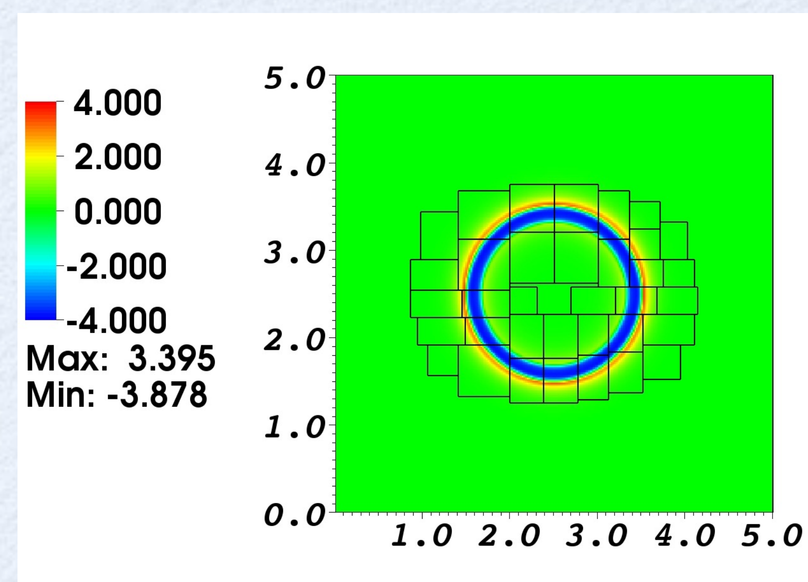
  bottom solver (PFMG), first order upwind
- GMRES, main solver

Advection-electrodiffusion with immersed boundary

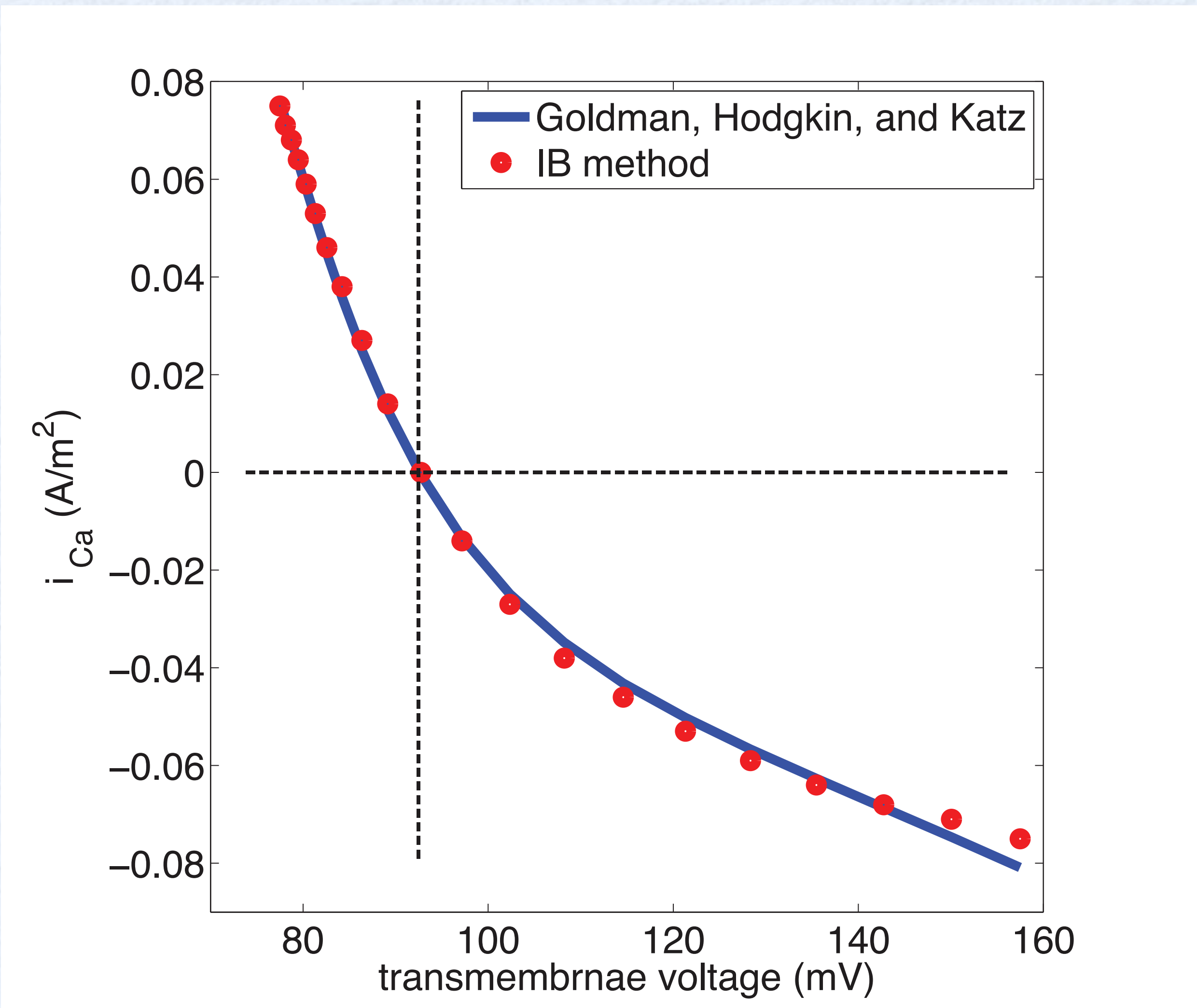


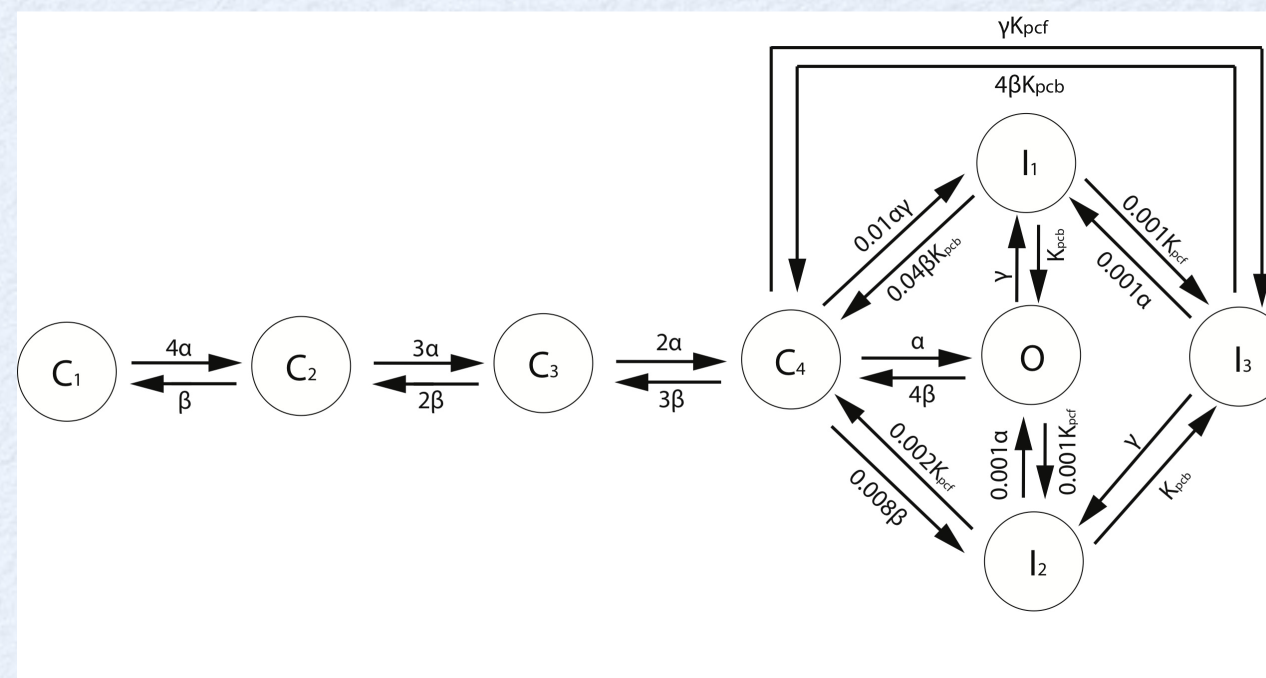






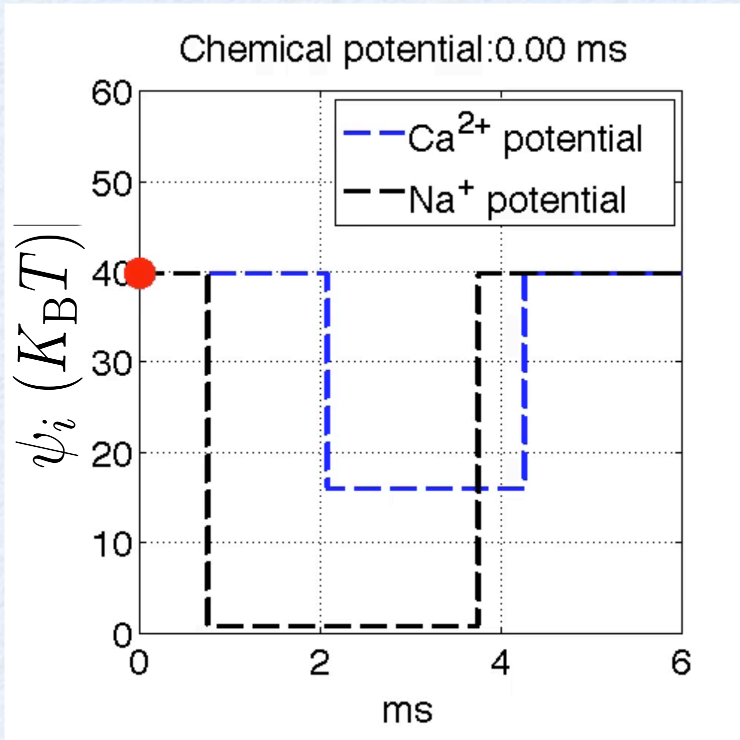
Voltage-sensitive calcium ion channels

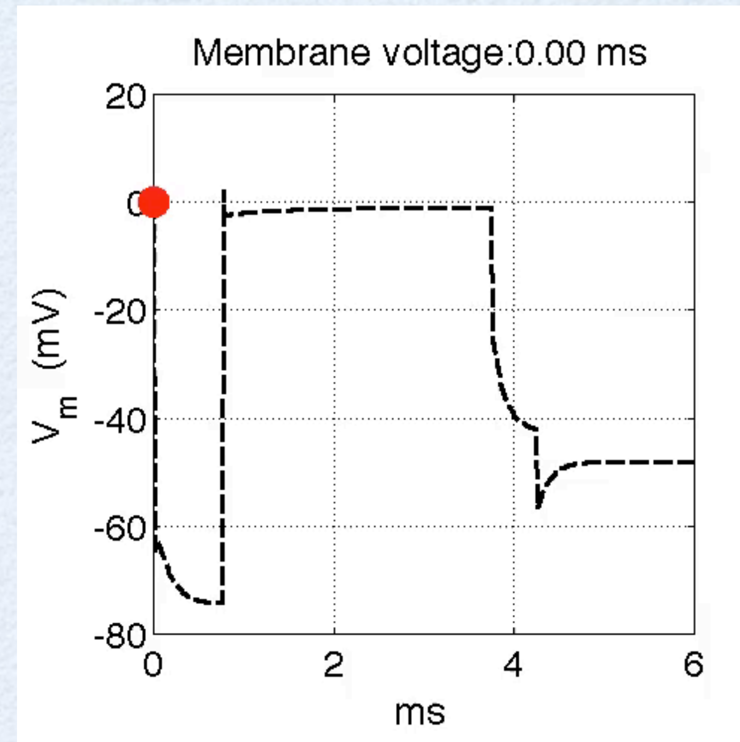


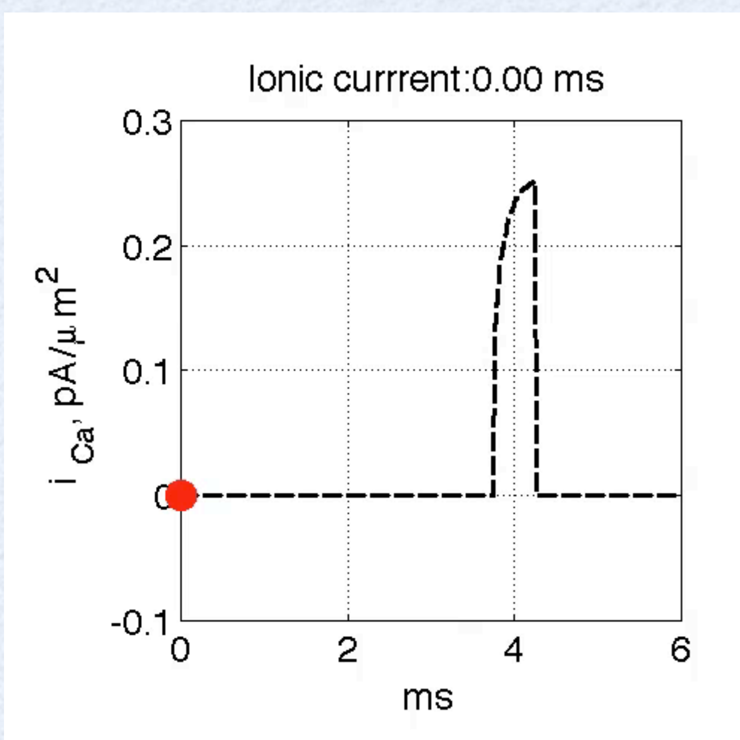


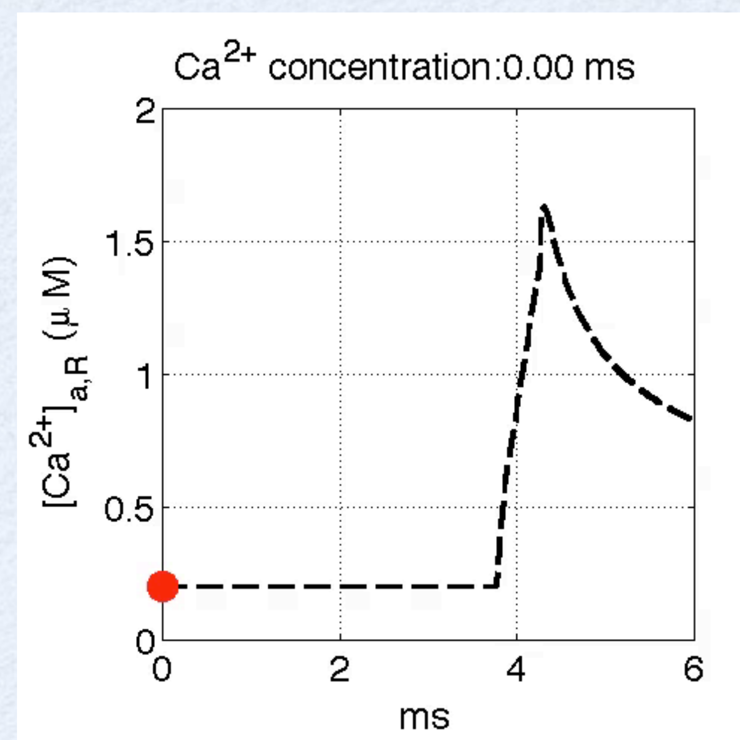
Rasmusson, et al. 2004

Voltage-sensitive calcium ion channels



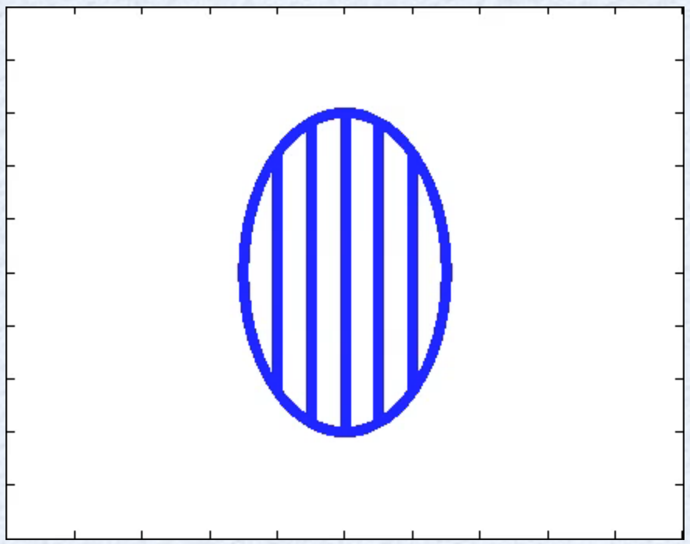




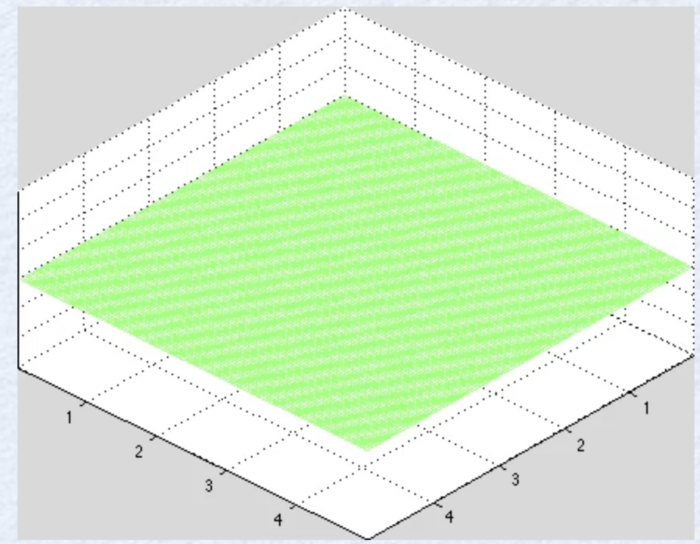


Concentration dependent contraction

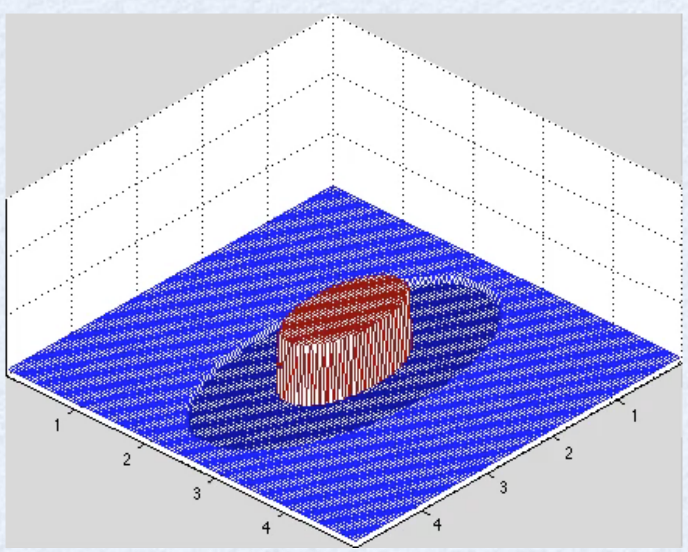
Fiber / membrane configuration



Electrical charge density

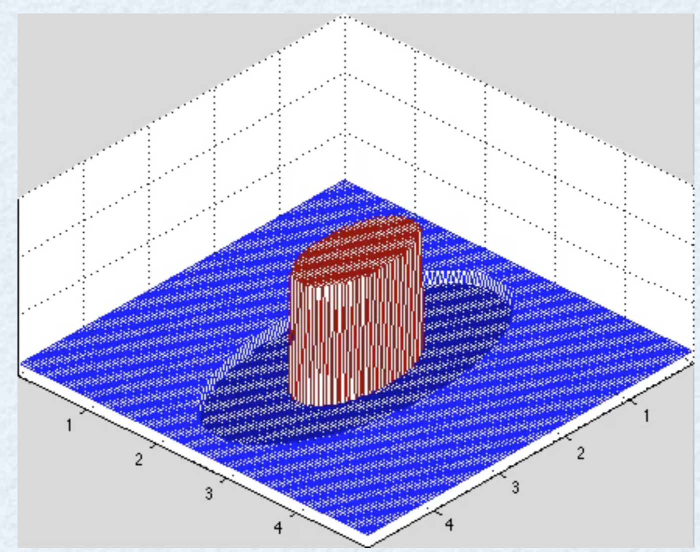


[Ca++]



membrane is mostly impermeable to Ca++

[Cl-]



membrane is freely permeable to Cl-

An immersed boundary method for two-phase fluids and gels

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

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

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

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

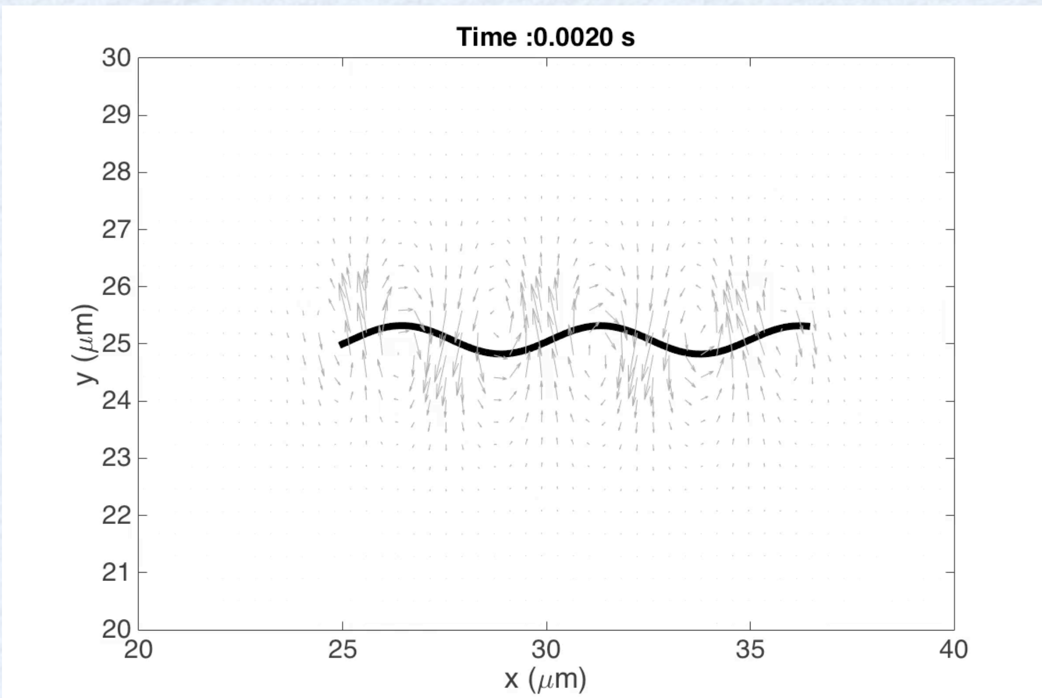
$$\nabla \cdot \{(1-\phi)\boldsymbol{v}_{\mathrm{f}} + \phi \boldsymbol{v}_{\mathrm{p}}\} = 0$$

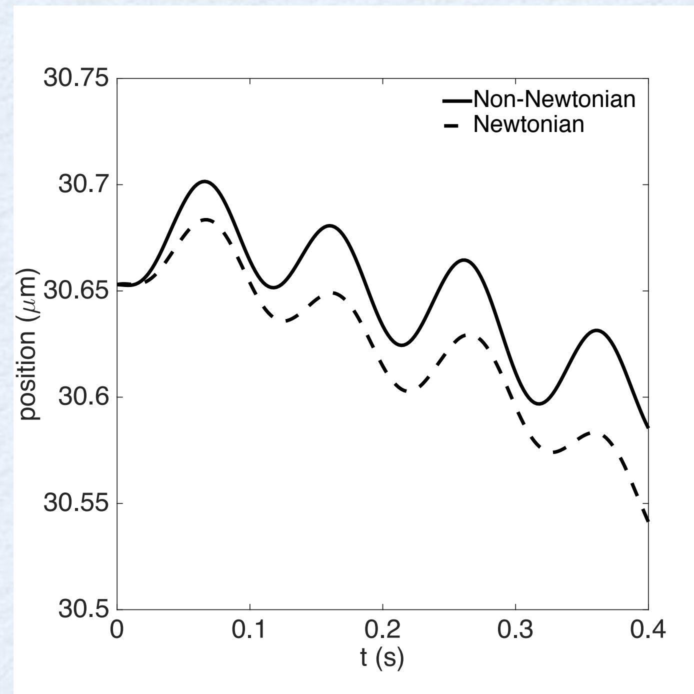
$$\boldsymbol{F}_{\mathrm{p}} \cdot \boldsymbol{T} = \Xi_{\mathrm{T}} S^*(\boldsymbol{v}_{\mathrm{f}} - \boldsymbol{v}_{\mathrm{p}}) \cdot \boldsymbol{T}$$

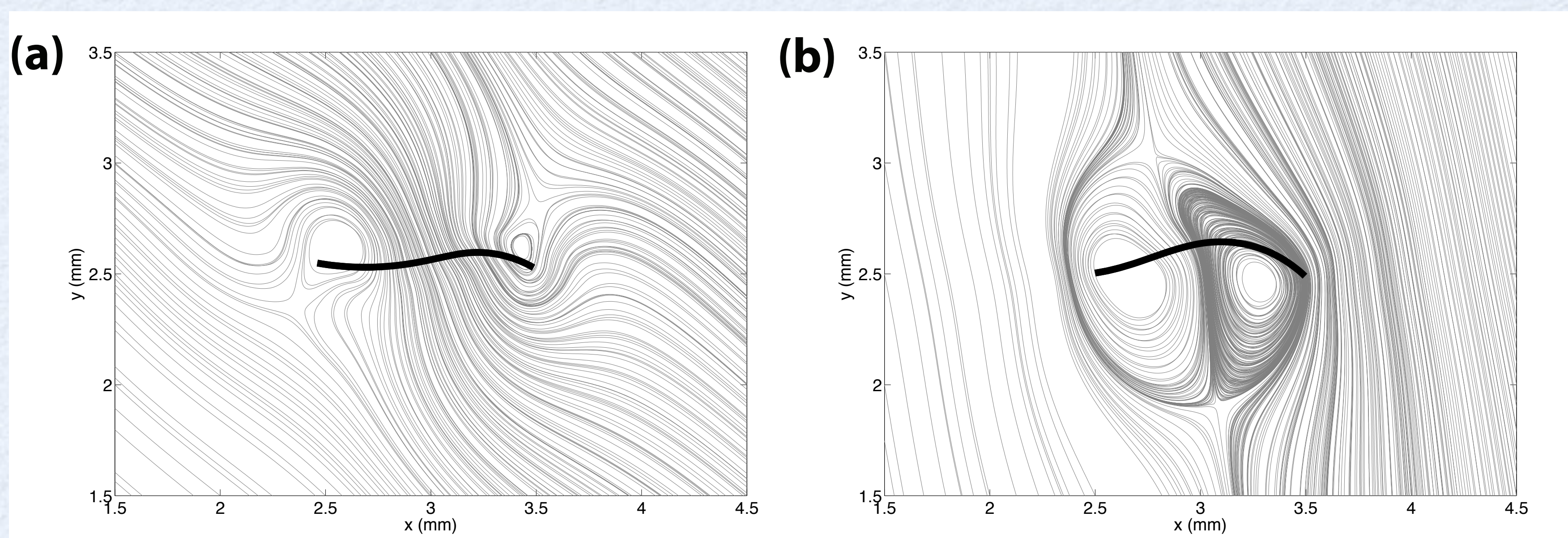
$$\boldsymbol{F}_{\mathrm{p}} \cdot \boldsymbol{N} = \Xi_{\mathrm{N}} S^*(\boldsymbol{v}_{\mathrm{f}} - \boldsymbol{v}_{\mathrm{p}}) \cdot \boldsymbol{N}$$

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

An immersed boundary method for two-phase fluids and gels

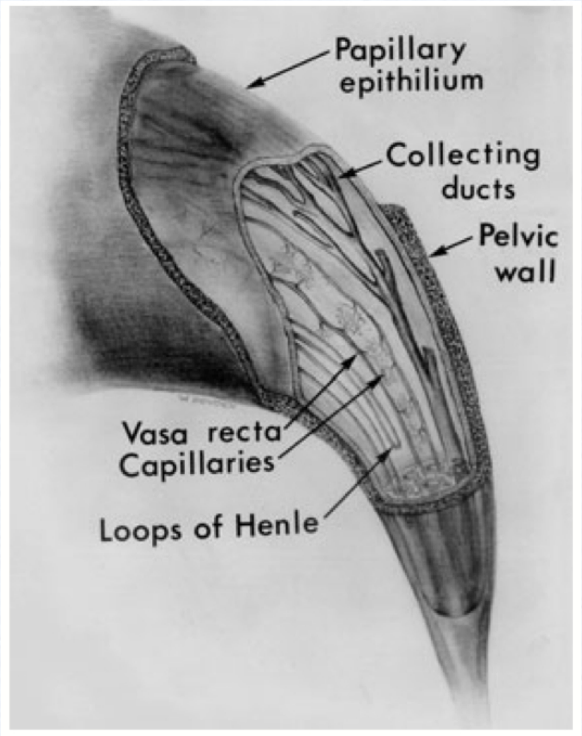


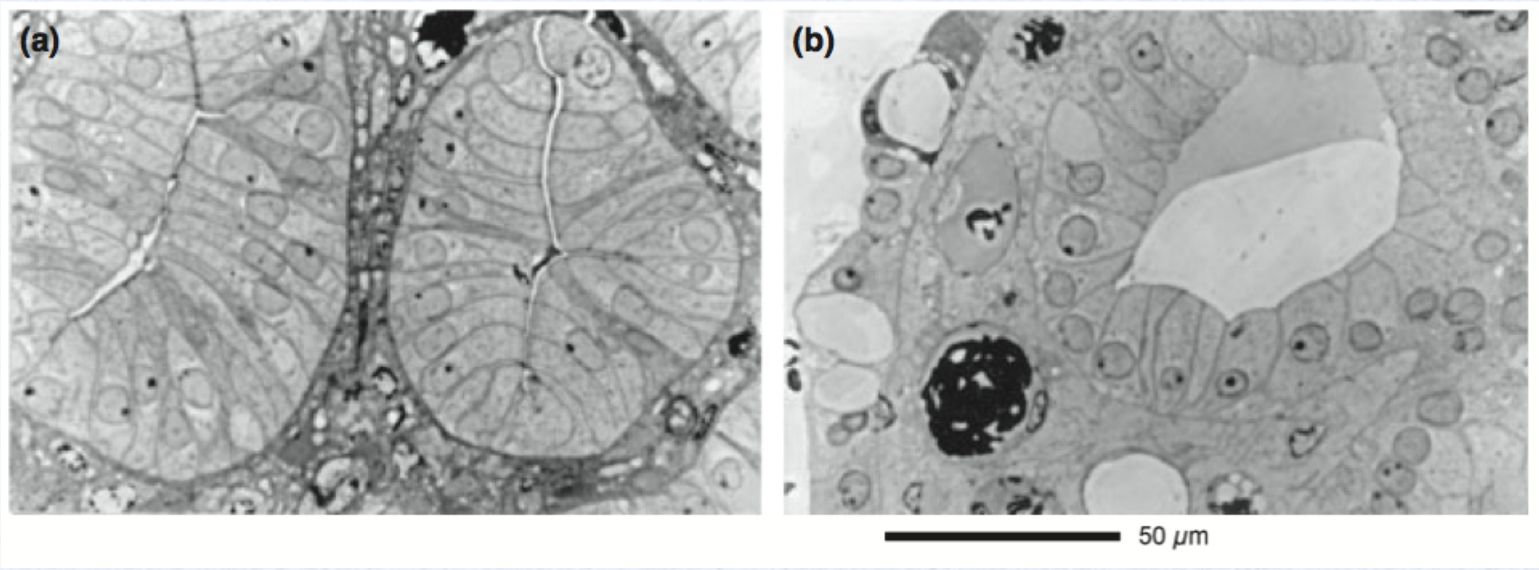




Lee and Wolgemuth, submitted

3D solute concentration of inner medulla in renal peristaltic contraction





Schmidt-Nielsen, et al. 2011

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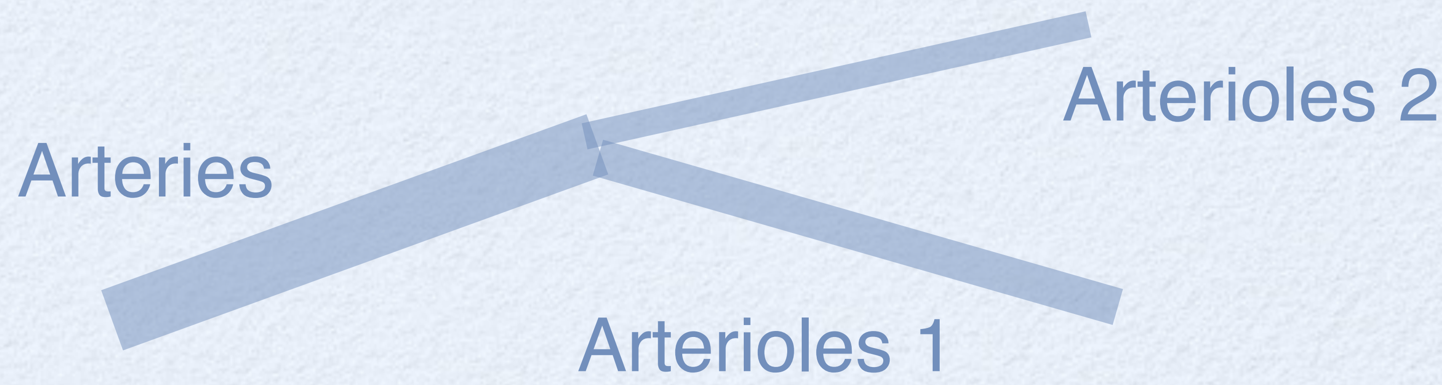
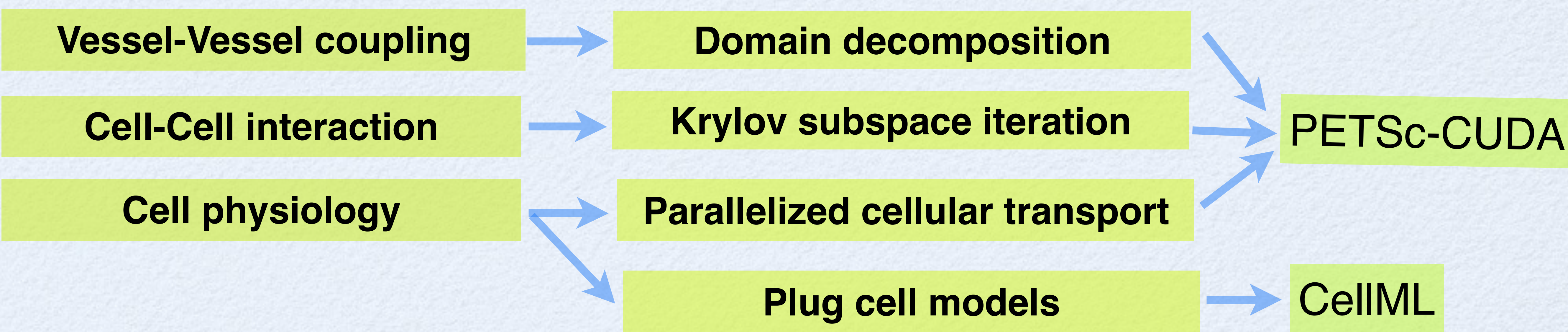
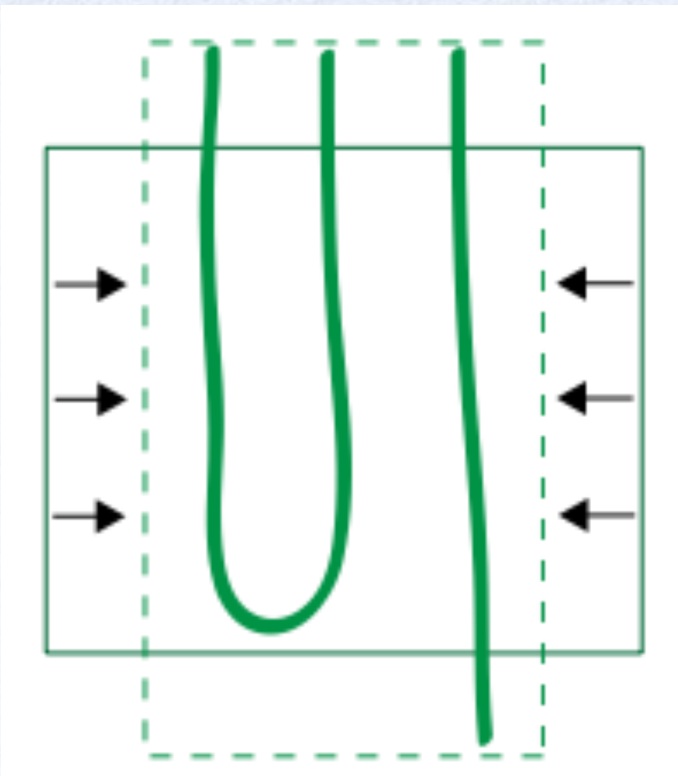
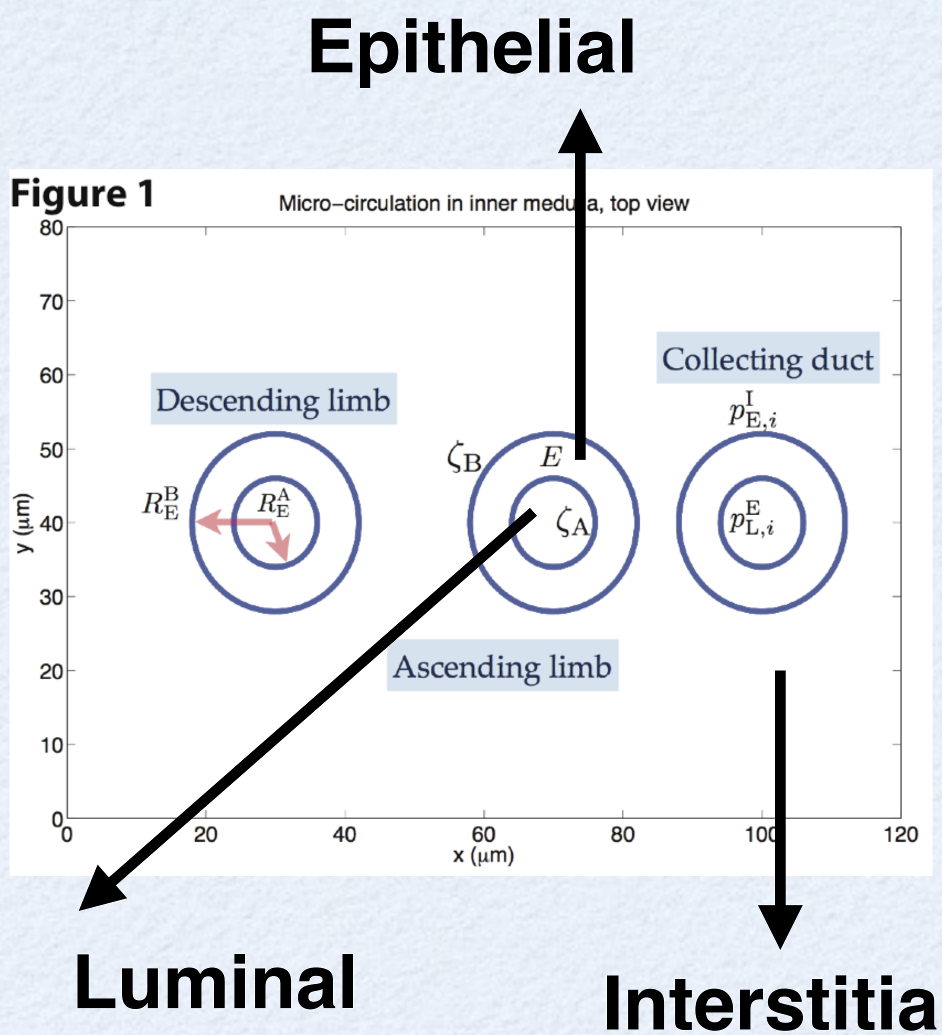
Multi-scale, large-scale computational framework

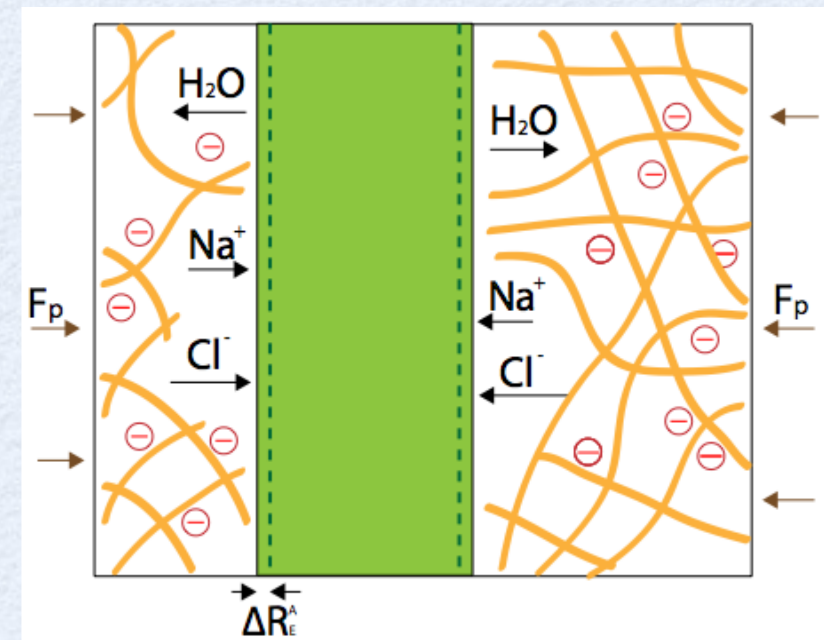




3D solute concentration of inner medulla in renal peristaltic contraction



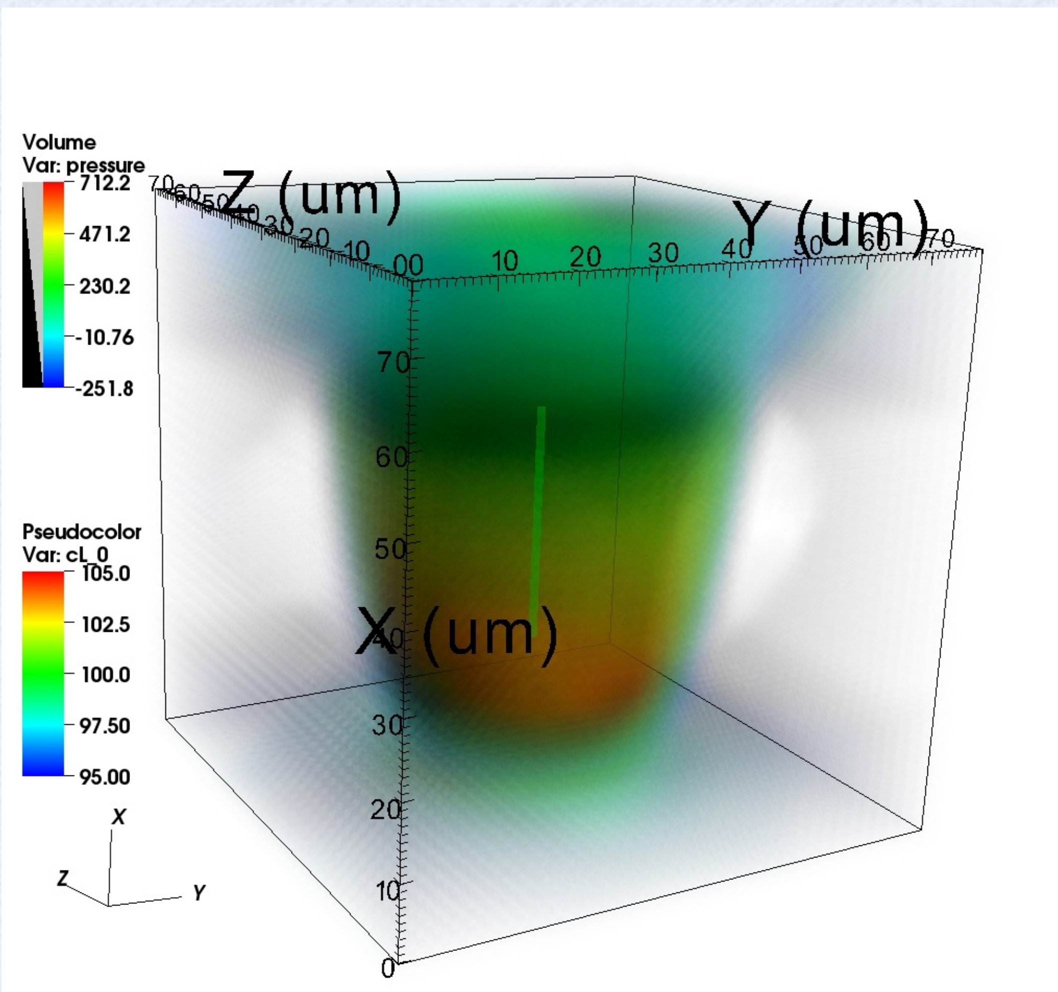




Hypothesis

1. Rectified epithelial transport with electrolytes in interstitial matrix
2. Rectified epithelial transport with viscoelasticity in interstitial matrix

3D peristaltic contraction



$$\zeta_{\mathrm{I}} u_{\mathrm{I}} = -\nabla p_{\mathrm{I}} + \int_{\Omega_{\mathrm{L}}^{\mathrm{P}}} \delta(\mathbf{x} - \mathbf{X}_{\mathrm{p}}(s))\mathbf{F}_{\mathrm{p}} ds$$

$$\nabla \cdot \mathbf{u}_{\mathrm{I}} = 0$$

$$F_{\mathrm{P}} = \sum_i \frac{\partial (F_{\mathrm{T}}^i \tau_i)}{\partial s_i}$$

$$F_{\mathrm{T}}^i = K_{s_i}(|\frac{\partial \mathbf{X}_{\mathrm{p}}}{\partial s_i}| - 1), \quad \tau_i = \frac{\partial \mathbf{X}_{\mathrm{p}}/\partial s_i}{|\partial \mathbf{X}_{\mathrm{p}}/\partial s_i|}$$

$$K_{s_1} = K_{s_1}^0 \sin(\omega t), \quad K_{s_2} = K_{s_2}^0$$

3D solute concentration

Luminal

$$\frac{\partial c_i^{\mathrm{L}}}{\partial t} + \frac{\partial J_i^{\mathrm{L}}}{\partial s} = -p_{\mathrm{L},i}^{\mathrm{E}}(c_i^{\mathrm{L}} - c_i^{\mathrm{E}})$$

$$J_i^{\mathrm{L}} = c_i^{\mathrm{L}} u_{\mathrm{L}}$$

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x}(\frac{q^2}{A}) + \frac{A}{\rho}\frac{\partial p_{\mathrm{L}}}{\partial x} = -2\frac{\pi \nu r}{\delta}\frac{q}{A}$$

$$p_{\mathrm{L}} = p_{\mathrm{I}}(\mathbf{X} + \mathbf{R}_{\mathrm{E}}^{\mathrm{B}}) + p_{\mathrm{E}}$$

Interstitial

$$\frac{\partial c_i^{\mathrm{I}}}{\partial t} + \nabla \cdot \mathbf{J}_i^{\mathrm{I}} = \int_{\Omega_{\mathrm{L}}} \delta(\mathbf{x} - \mathbf{X}(s) - \mathbf{R}_{\mathrm{E}}^{\mathrm{B}}(s,\theta)) p_{\mathrm{I},i}^{\mathrm{E}}(s)(c_i^{\mathrm{I}} - c_i^{\mathrm{E}}) ds d\theta$$

$$J_i^{\mathrm{I}} = -D_i^{\mathrm{I}} \nabla c_i^{\mathrm{I}}$$

$$-\frac{D_i^{\mathrm{I}}}{K_{\mathrm{B}}T}(\int_{\Omega_{\mathrm{L}}} \nabla \Psi_{\mathbf{R}_{\mathrm{E}}^{\mathrm{B}}}(\mathbf{x} - \mathbf{X}(s)) A(s) ds d\theta) c_i^I$$

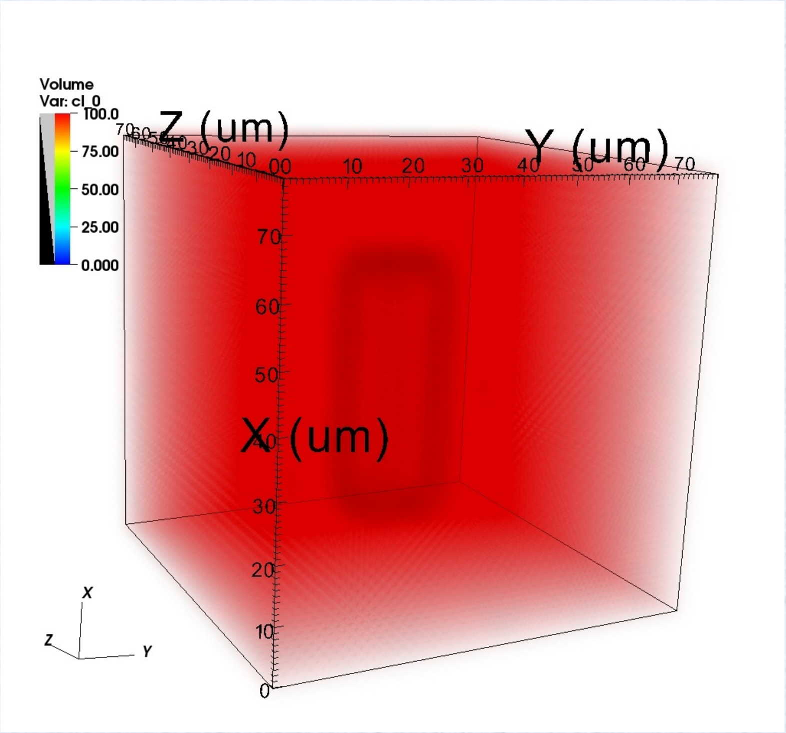
$$+u_{\mathrm{I}} c_i^{\mathrm{I}}$$

Epithelial

$$\frac{\partial c_i^{\mathrm{E}}}{\partial t} = -p_{\mathrm{E},i}^{\mathrm{I}}(c_i^{\mathrm{E}} - c_i^{\mathrm{I}}(\mathbf{X} + \mathbf{R}_{\mathrm{E}}^{\mathrm{B}})) - p_{\mathrm{E},i}^{\mathrm{L}}(c_i^{\mathrm{E}} - c_i^{\mathrm{L}})$$

$$\zeta_{\mathrm{A}} \frac{\partial R_{\mathrm{E}}^{\mathrm{A}}}{\partial t} = \Pi_{\mathrm{A}} RT \sum_i (c_i^{\mathrm{L}} - c_i^{\mathrm{E}})$$

$$\zeta_{\mathrm{B}} \frac{\partial R_{\mathrm{E}}^{\mathrm{B}}}{\partial t} = \Pi_{\mathrm{B}} RT \sum_i (c_i^{\mathrm{E}} - \tilde{c}_i^{\mathrm{I}}(\mathbf{X} + \mathbf{R}_{\mathrm{E}}^{\mathrm{B}}))$$



The Virtual Physiological Rat Project

Future work

Two-phase fluids and gels

Advection-electrodiffusion

3D IBAMR

Coupling with vasculature/tubular network

Acknowledgement

Courant Institute, New York University

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Boyce Griffith

Mount Sinai School of Medicine

Eric Sobie

University of Michigan

Daniel Beard, Brian Carlson

PETSc team, Barry Smith, Satish Balay

Hypre team, Robert Falgout

SAMRAI team

University of Pennsylvania

Dennis Discher

University of Arizona

Charles Wolgemuth

Medical College of Wisconsin

Allen Cowley

University of Wisconsin, Madison

Naomi Chesler

University College of London/ University of Auckland

Nicolas Smith, Taha Sochi

North Carolina State University

Mette Olufsen