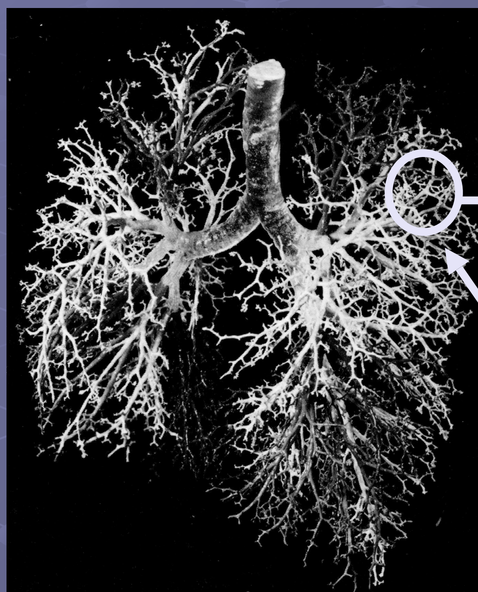
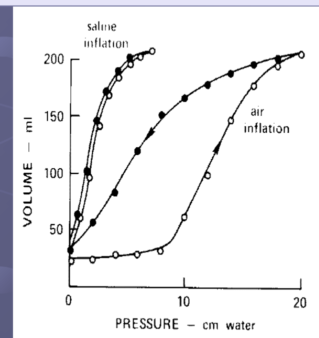
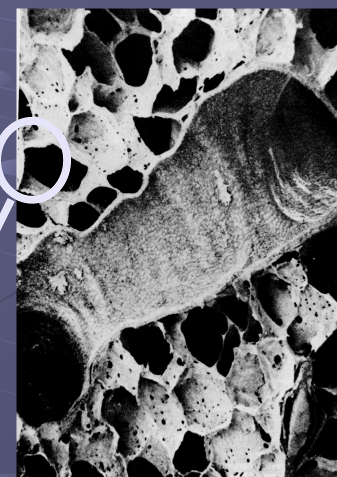
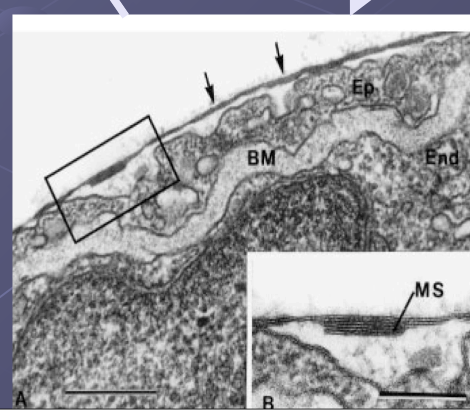
Computational fluid dynamics investigations of pulmonary airway









Respiratory Distress Syndrome

Lung Immaturity

↓

Surfactant Insufficiency

↓

Atelectasis

↓

Epithelial Injury

↓

Alveolar Leakage

↓

Hyaline membranes

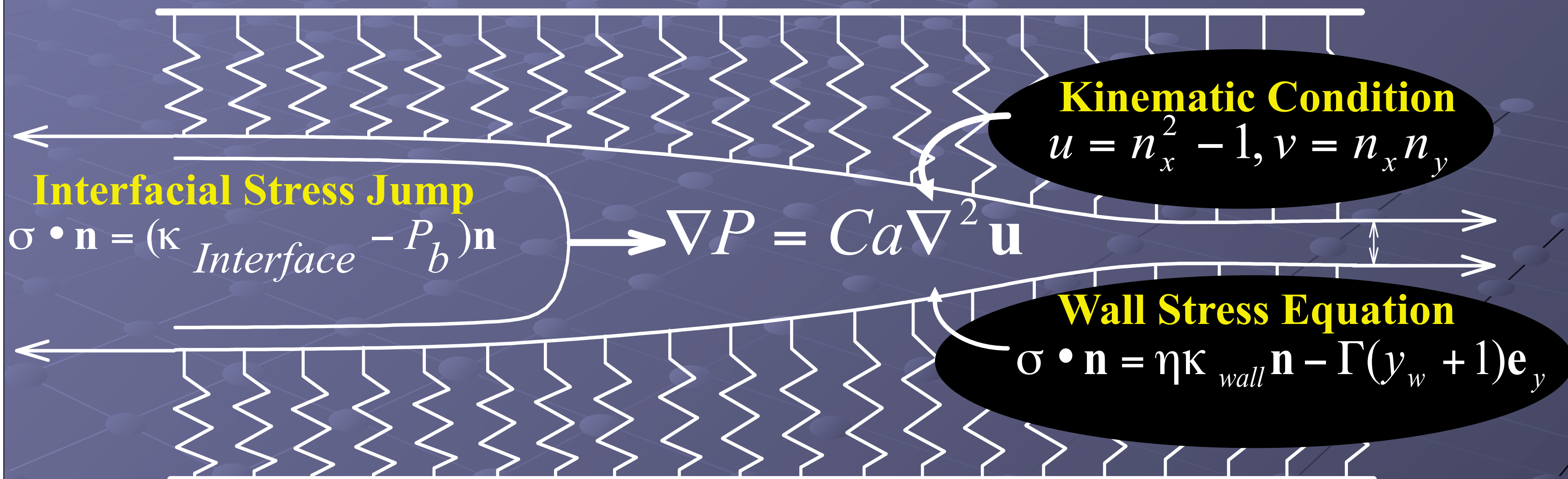
↓

Fibrosis

Motivation

To determine the mechanical stimulus associated with airway damage from the reopening of a pulmonary airway.

Mathematical Model Formulation



Dimensionless Parameters

Ca = ❍U/♑ = Dimensionless Velocity

♒ = T/♑ = Dimensionless Wall Tension

☝ = KH²/♑ = Dimensionless Wall Stiffness

The Computational Model

Evolution Eqn

$$\frac{\partial h^*}{\partial t^*} = -\frac{\partial q^*}{\partial x^*}$$

Kinematic Condition

$$\frac{d\underline{\mathrm{Y}}^*}{dt^*} \times \hat{\mathrm{n}} = \underline{\mathrm{u}}^* \times \hat{\mathrm{n}}$$

Stokes Flow

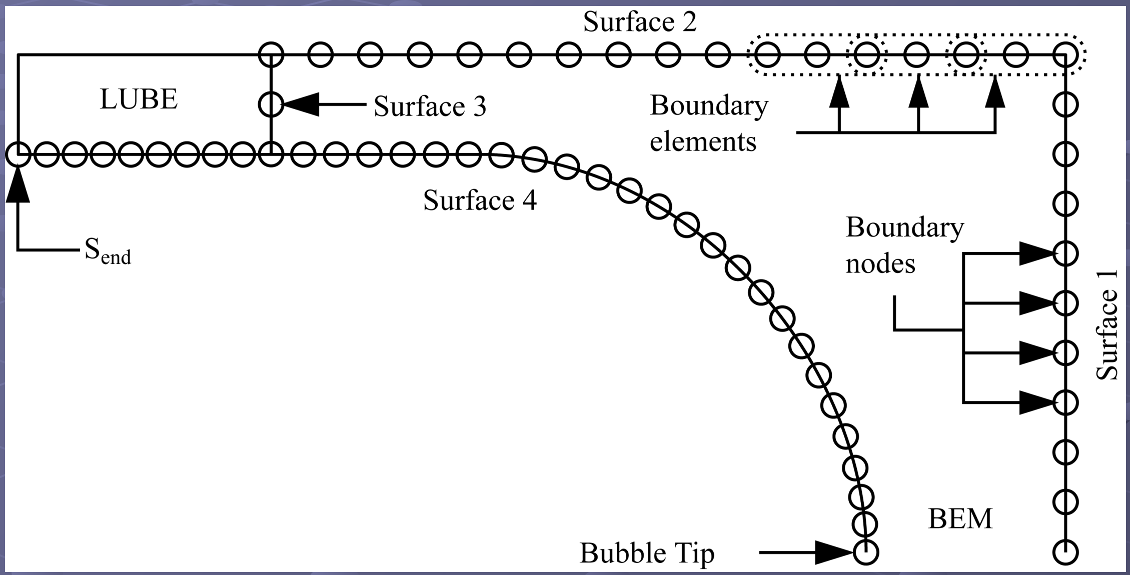
$$\underline{\nabla} P^* = \mu \nabla^{*2} \underline{\mathrm{u}}^*$$

Stress Balance

$$\underline{\tau}^*_{eq} = \gamma^*(s)\kappa^* \hat{\mathrm{n}} + \frac{d\gamma^*}{ds^*}\hat{t}$$

LUBRICATION THEORY | **BOUNDARY ELEMENT**

Boundary Element Formulation



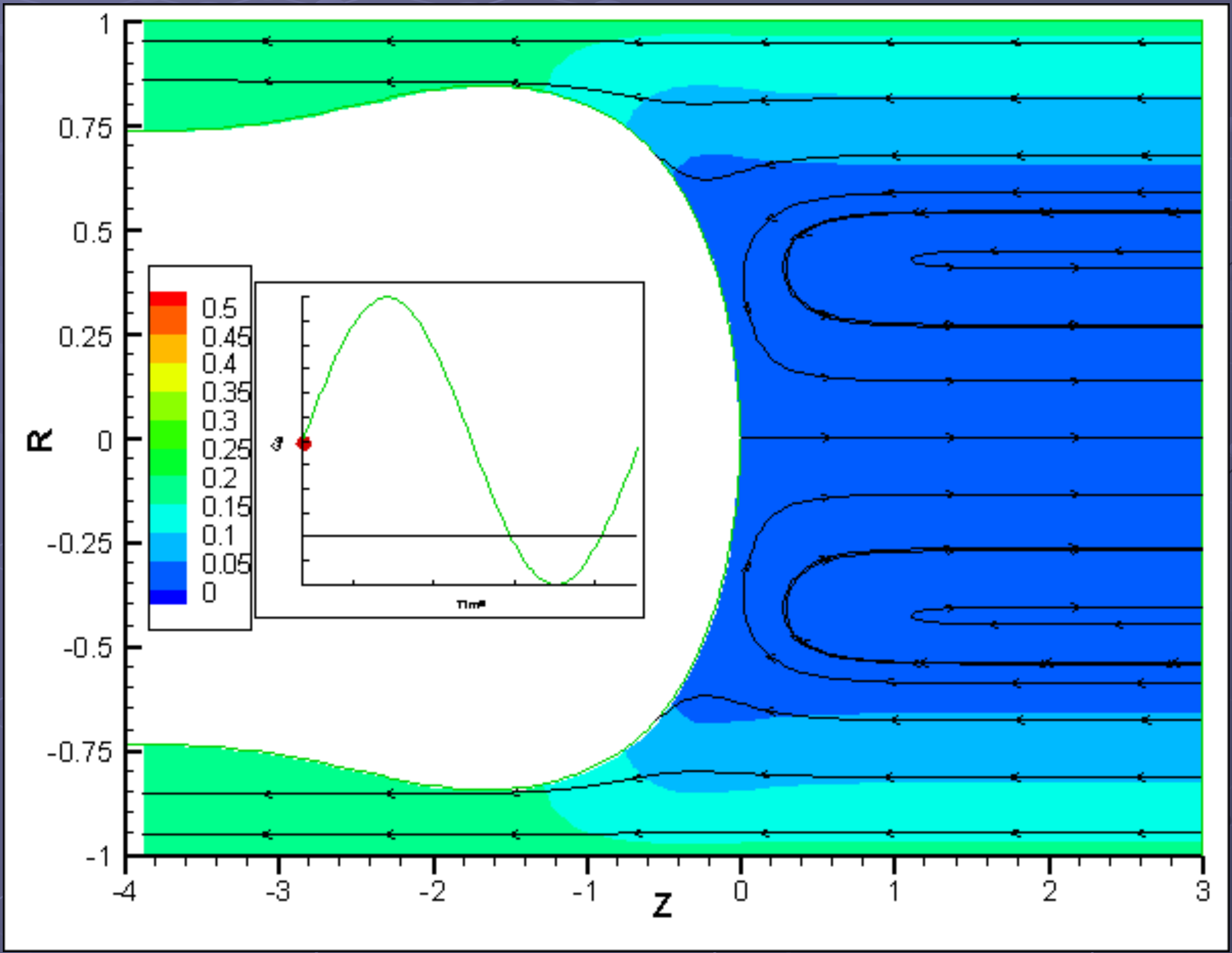
$$C_{ki}u_i(\mathbf{x}) + \int_S T_{ik}(\mathbf{x},\mathbf{y})dS(\mathbf{y}) = \int_S U_{ik}(\mathbf{x},\mathbf{y})\pi_i(\mathbf{y})dS(\mathbf{y})$$

$$U_{ik} = -\frac{1}{4\pi}\left(\delta_{ik}\log|\mathbf{x}-\mathbf{y}| - \frac{(x_i - y_i)(x_k - y_k)}{|\mathbf{x}-\mathbf{y}|^2}\right),$$

$$T_{ik} = -\frac{1}{\pi}\frac{(x_i - y_i)(x_j - y_j)(x_k - y_k)n_j(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^4}.$$

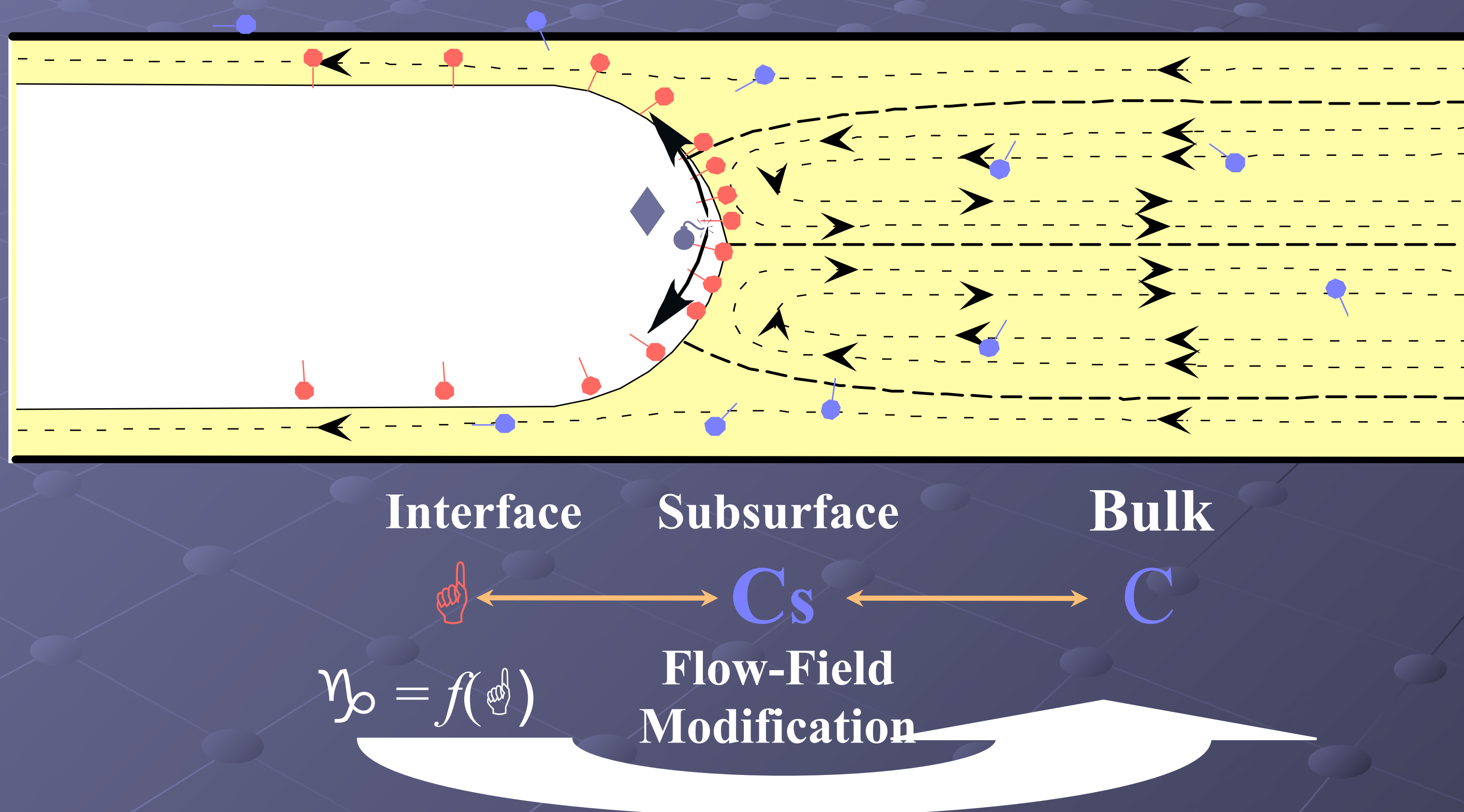
Pulsatile Flow Animation

A=5, Ca_m=0.1, Ω=0.06



General Concepts

- **Surfactant physicochemical interactions result from three interacting relationships.**



Marangoni Stress on Interface Retards Bubble Motion.

Interfacial Transport (Monolayer)

$$\frac{d\Gamma_0}{dt} + \frac{\partial}{\partial s}\left(\Gamma_0 u_s\right) + \Gamma_0 \kappa u_n = St_0^a C_s\left(1 - \Gamma_0\right) - St_0^d\left(\Gamma_0\right) - j_0^{coll}$$

surface stretching

adsorption

desorption

collapse

Transport Parameters

$$St_0^a = \frac{ak_0^a C}{U} = \frac{ak_0^a C\mu}{\gamma_{eq}}; \quad St_0^d = \frac{ak_0^d}{U} = \frac{ak_0^d \mu}{\gamma_{eq}}$$

Adsorption **Desorption**

Assume: C=10 mg/ml, γ_{eq}=22 dyn/cm

$10^{-4} < St_0^a < 10^{-3}$ $10^{-7} < St_0^d < 10^{-6}$

To retain the correct balance between sorption and velocities (since Ca ~ 0.1, not 10^{-3}), we investigate

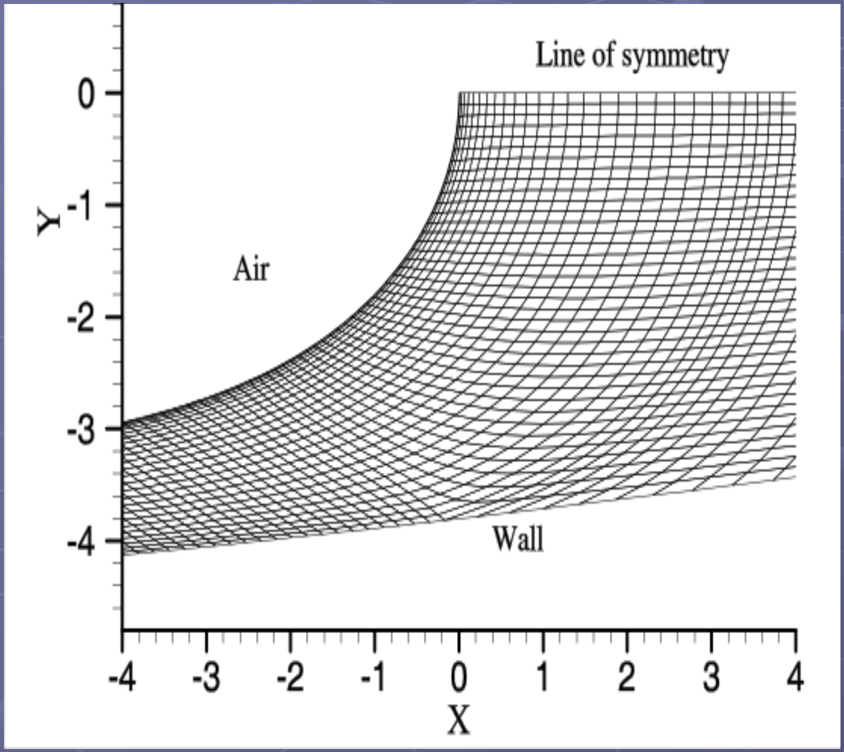
$St_0^a = 10^{-2}$ $St_0^d = 10^{-4}$ ☝$_{max}$ = 1.3

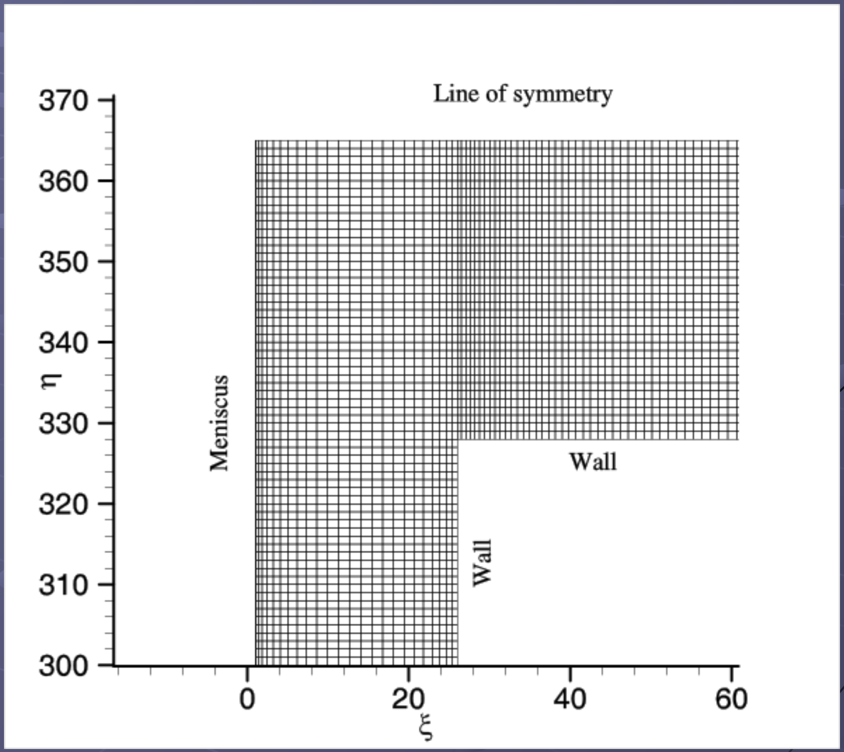
Solution Process: Fluid-Structure Interactions with Surfactant Physicochemical Interactions

Initialize: Assume equilibrium (constant surface tension) conditions: BEM to estimate interfacial and wall shapes given estimates of stress condition at interface and velocity estimate for the wall.

- Using a Newton's method, the domain is updated until the kinematic boundary condition at the air-liquid interface and the wall stress condition are simultaneously satisfied.
- Use BEM to compute the velocity field in the domain.
- Use finite-volume method to determine the interfacial and bulk surfactant distribution on a staggered grid for a given surfactant flux at the bubble surface. The interfacial and bulk concentrations are recomputed iteratively until the flux condition is satisfied.
- Given the new concentration field, the interfaces are updated
- Steady state is reached only when the shapes and the fluxes have converged.

Finite-Volume Mesh

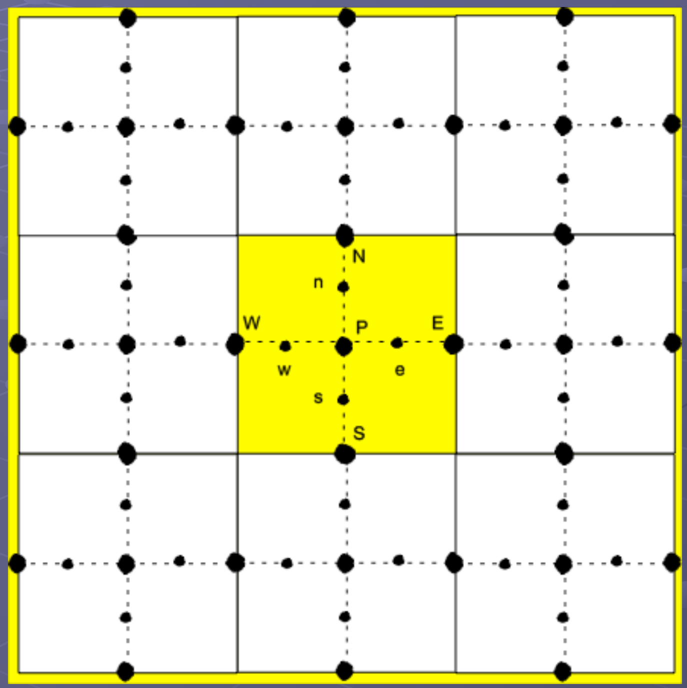




Boundary-fitted coordinates are used to describe the grid of our domain since its boundaries do not easily line up with the usual Cartesian coordinate system. The transformations between the physical and computational domains are obtained by solving a system of Poisson equations (See, for example Thompson and Fletcher).

Transport Stencil

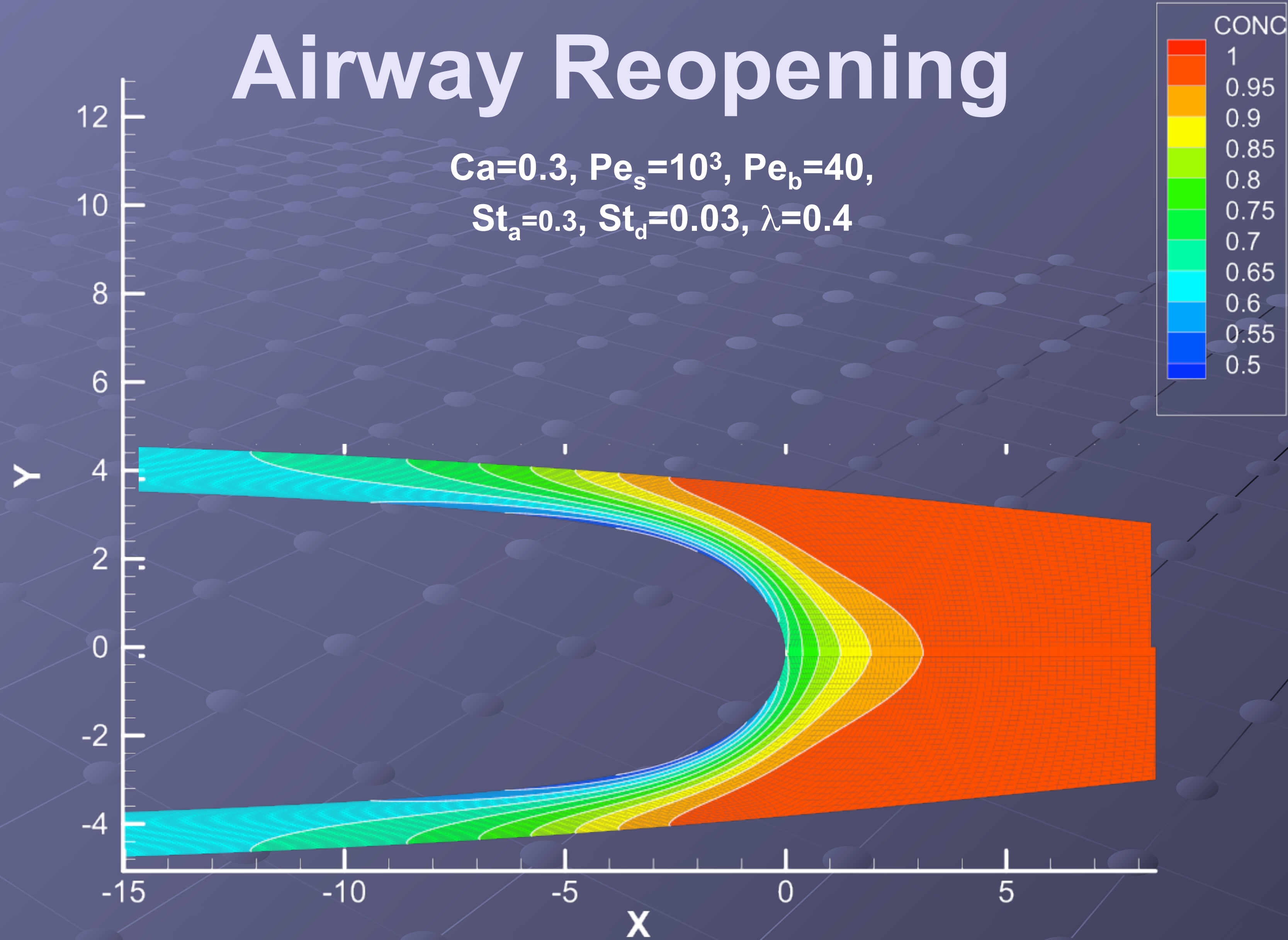
Finite Volume Method



$$(CJ)_t + \left[\left(F^{\xi} - G^{\xi} \right) C - \frac{1}{Pe_b} \frac{B_{11}}{J} C_{\xi} \right]_{\xi} + \left[\left(F^{\eta} - G^{\eta} \right) C - \frac{1}{Pe_b} \frac{B_{22}}{J} C_{\eta} \right]_{\eta} =$$

$$\frac{1}{Pe_b} \left[\left(\frac{B_{12}}{J} C_{\eta} \right)_{\xi} + \left(\frac{B_{12}}{J} C_{\xi} \right)_{\eta} \right]$$

Concentration Field in Airway Reopening



D. Halpern, 2008

Computational Requirements of Numerical Method

- Approximately 400 nodes on the BEM domain -> 800 unknowns. Linear system is solved using a Gaussian elimination routine from LAPACK.
- The interfaces are determined using a Newton's method (MINPACK). This is not parallelized. There is room for improvement here.
- The internal grid consists of approximately 30,000 nodes. The linear system is sparse and banded. Solved using SUPERLU (serial version).

Computational Requirements

- Storage: 100Mb/simulation.
- CPU: ~300 CPU hours/simulation

Funding: NIH R01 HL-81266, P20 EB001432