

Large-Scale Computational Modeling of Fluid Flow in the Lung

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Cilium
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Cilia FSI
Metachronal
Airway flow
Aerosols
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- Applied Mathematics: Camassa, Forest, McLaughlin, Mitran

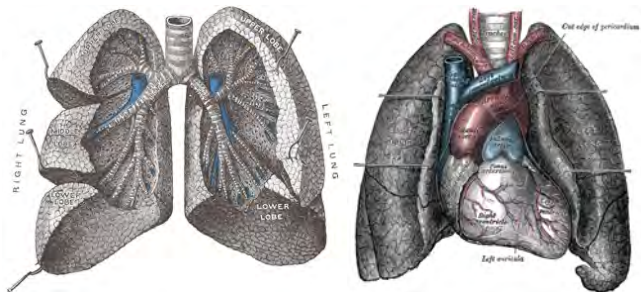
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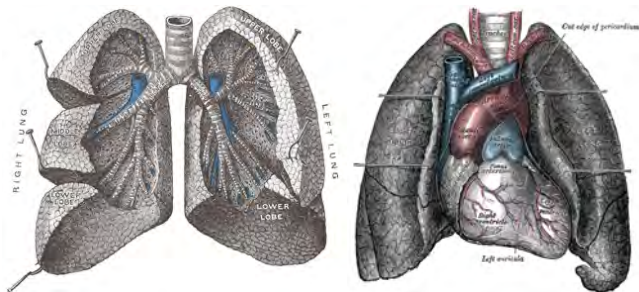
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- Physics: Superfine, Washburn

- Opened sections

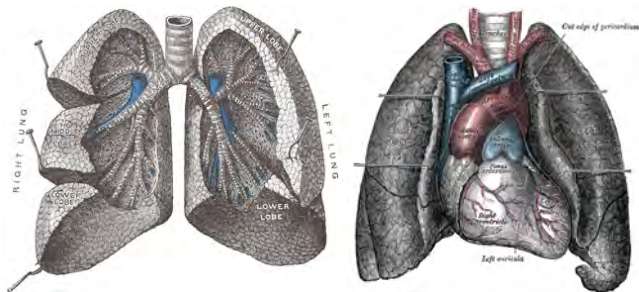


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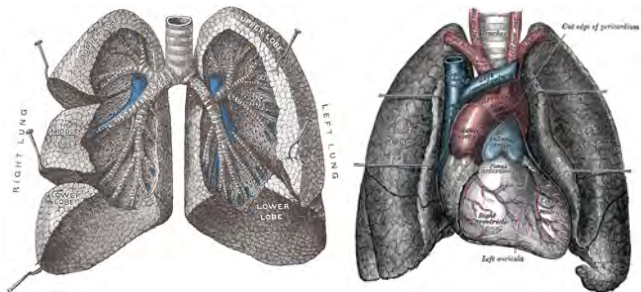
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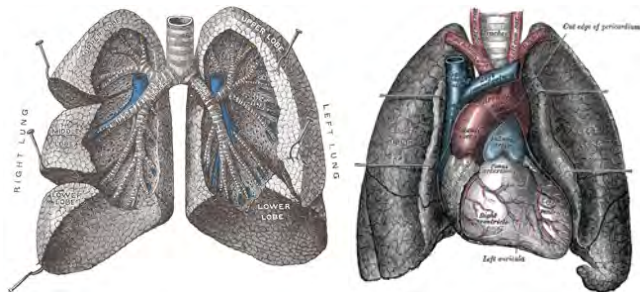
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- Daily indoor bacteria intake: 10⁷

- Airway cast



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- 20 generations, diameters $0.5 \leq D \leq 25$ (mm)

- Airway cast



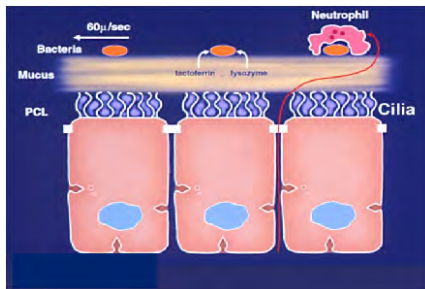
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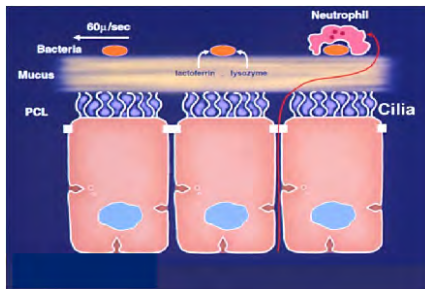


- 20 generations, diameters $0.5 \leq D \leq 25$ (mm)
- Reynolds numbers $1 \leq Re \leq 3000$, cough: 40,000
- Flow rate 200 ml/sec, speeds: $0.1 \leq V \leq 0.5$ m/s

- Epithelial region

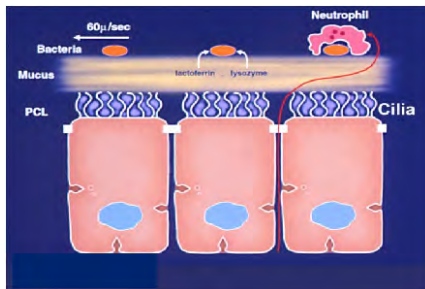


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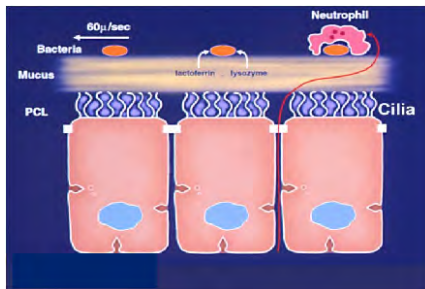
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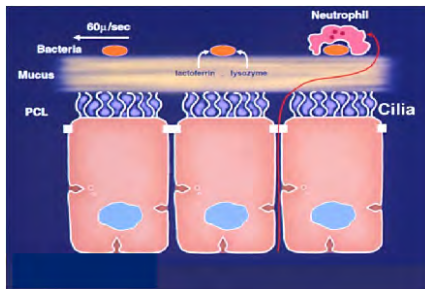
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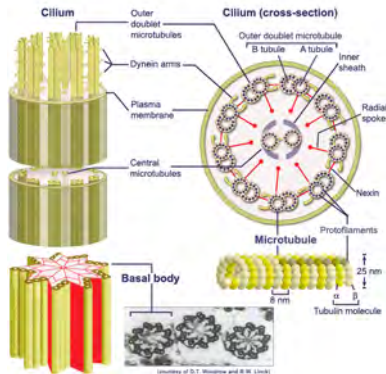
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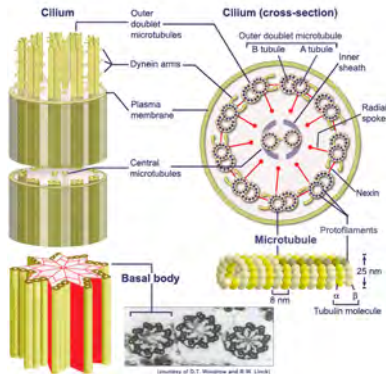


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- Mucus forms above PCL, viscoelastic, $Re < 10^{-3}$, $1 < We < 10$

- Cilium structure

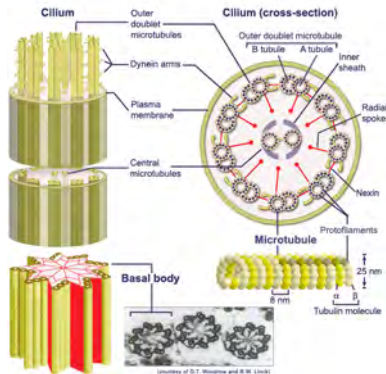


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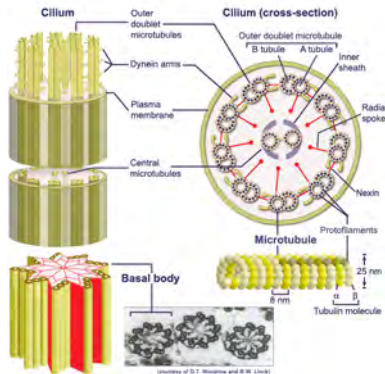
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- Dynein molecular motors induce bending, exert 6 pN per dynein

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- Coordination of 4000 dyneins stepping on microtubule tubulin dimer spiral

- Cystic fibrosis effectively treated by saline solution

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- At what critical viscoelastic properties does mucociliary flow start?

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- Control of various mucin types (mucosal agents)

- Aerosol trajectories in airway

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- Pathogen evacuation by mucociliary clearance, cough

- Viscoelastic computation algorithms

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- Complex airflow in branching airway network

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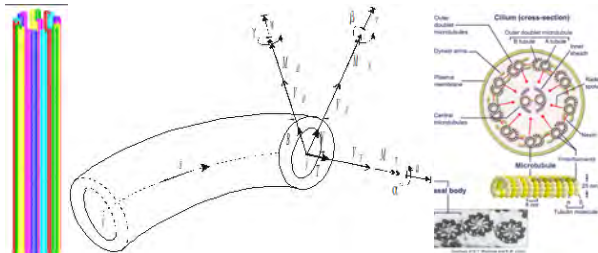
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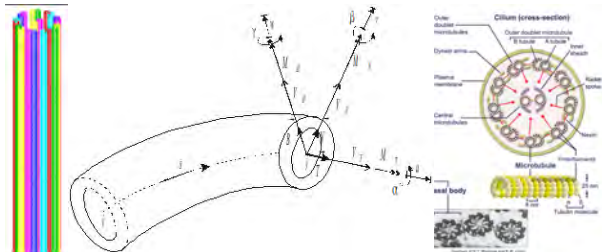
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- Elastic membrane, springs, beams

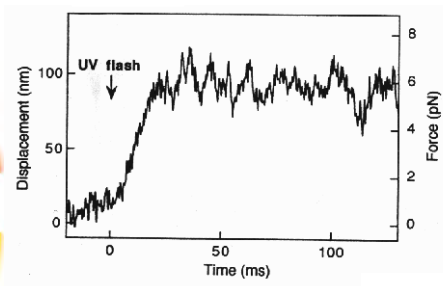
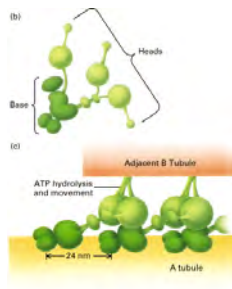


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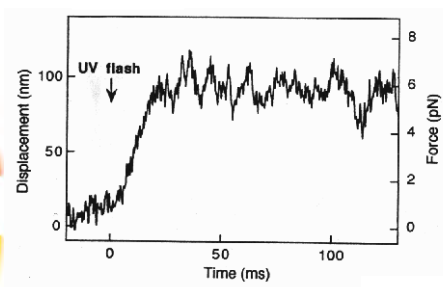
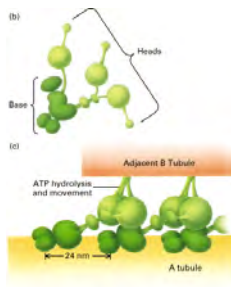


- Large deflection beams: total Lagrangean Timoshenko beam elements

- Biased random walk model for dyneins



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- Alternative model: force interpolation

$$F^{(m)}(s, t) = p^{(m)}(s) \cos(k^{(m)}s - \omega t + \varphi^{(m)})$$

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- Inhomogeneous viscoelastic

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- Inhomogeneous viscoelastic
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$$\nabla \cdot v = 0$$

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- Momentum equation

$$\mathbf{v}_t + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\nabla p + \nu \nabla^2 \mathbf{v} + \nabla \cdot \boldsymbol{\tau}$$

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- Viscoelastic stress reflects microscopic configuration

$$\tau(x, t) = \int_M k(x, t, p) f(x, t, p) d\mu(p)$$

- Typical constitutive law (Oldroyd-B)

$$\tau_t + (v \cdot \nabla)\tau - \nabla v^T \tau - \tau \nabla v = \mu_p (\nabla v + \nabla v^T) - \tau / \lambda$$

- Mostly incompressible (though in cough Mach can reach 0.4)

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- Particulate-laden, here a one-way interaction approach is used

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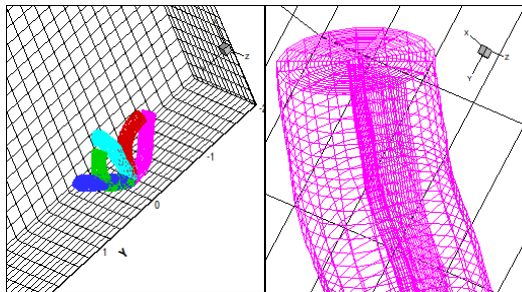
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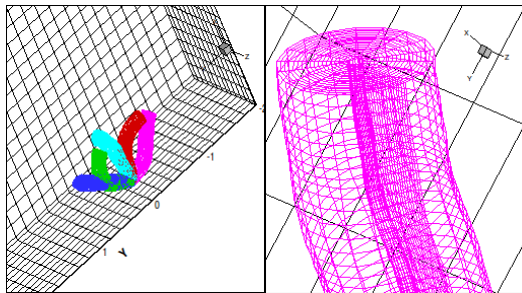
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- Overlapping grids, background Cartesian, moving body-fitted

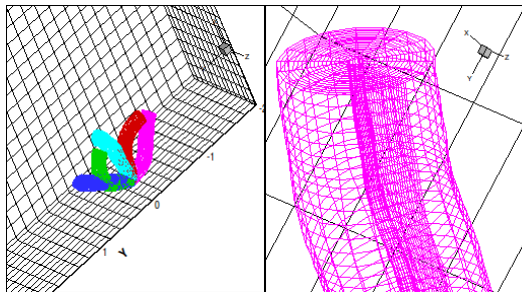


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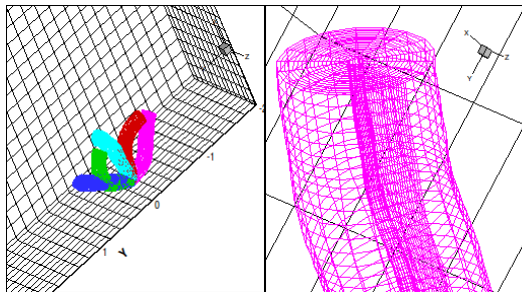
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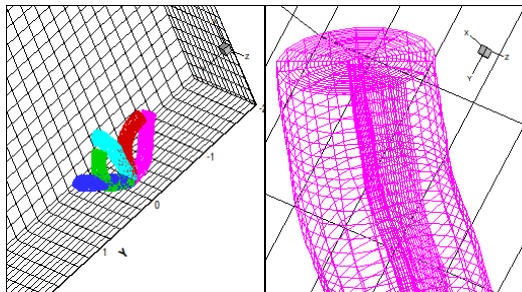
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- Solve for overall flow with forces from cilia

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- Solve for flow around cilia with b.c. on edge of body-fitted grid from obackground flow

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- 2-direction orthogonal body-fitted coordinates

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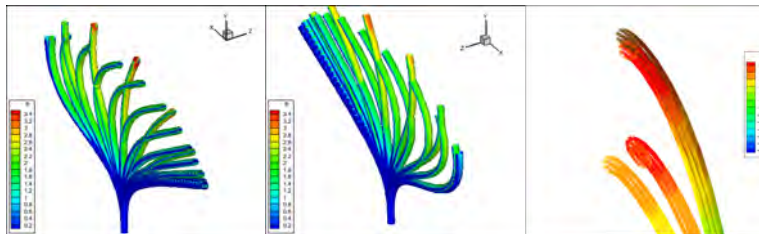
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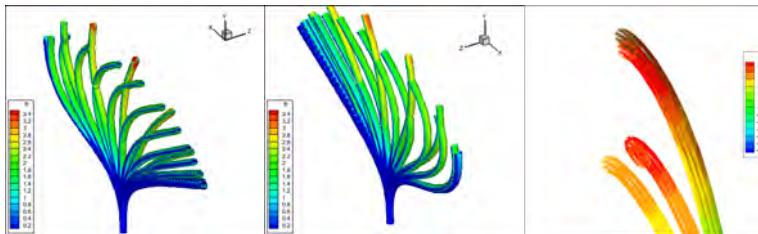
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- Orthogonal coordinates allow FFT's
- FFT's implemented on GPU's for sustained 40-60 GFLOPs

- Normal stresses and bending moment

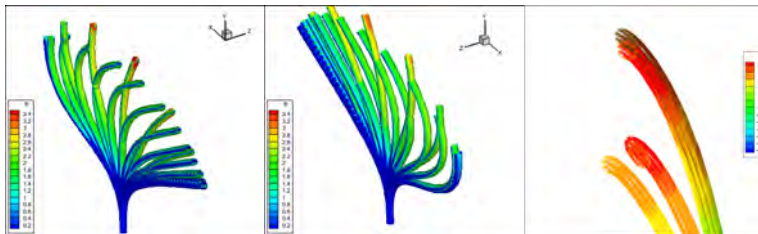


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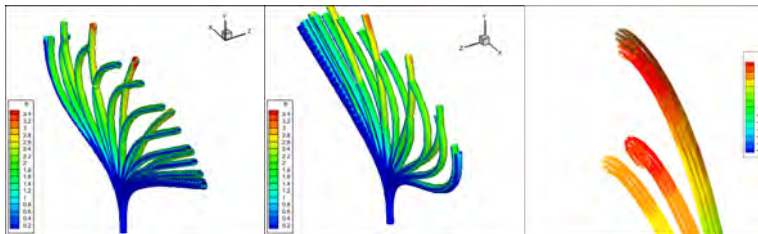
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- Propulsion achieved by decrease in frontal area
- Cilium is stiff in power stroke, limp in recovery stroke

- Enhanced transport achieved by a 'conveyor belt', metachronal wave

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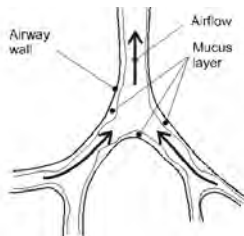
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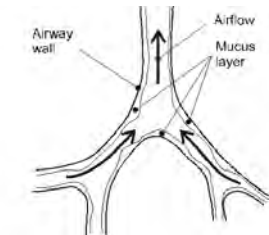
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- Verified also from dynein random walker model
- Coordination animations

- Mucus flows, slip boundary condition

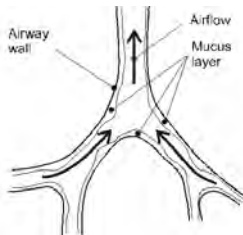


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- Database of boundary conditions w.r.t. ASL thickness, air velocity

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- Database of boundary conditions w.r.t. ASL thickness, air velocity
- Impose tangential stress boundary condition at ASL thickness for airflow

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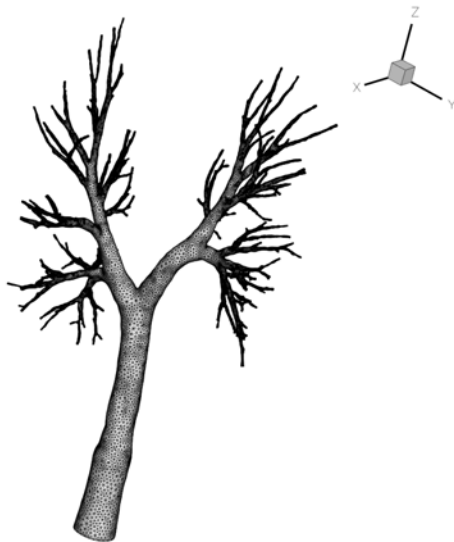
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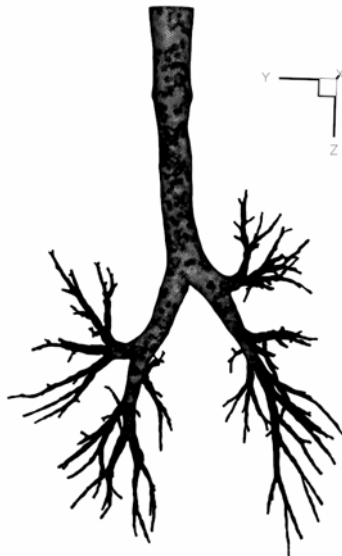
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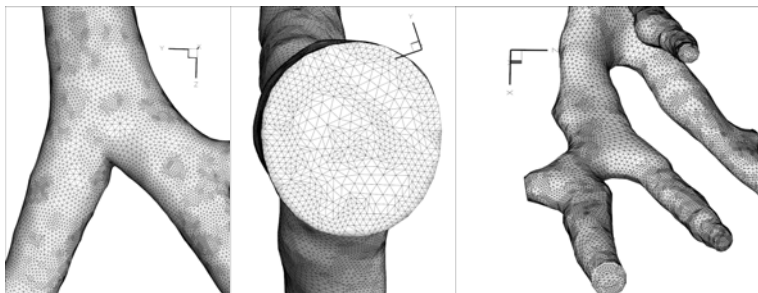
- Surface triangulation from MRI



- Build adapted tetrahedral grid from surface triangulation



- Grid regions



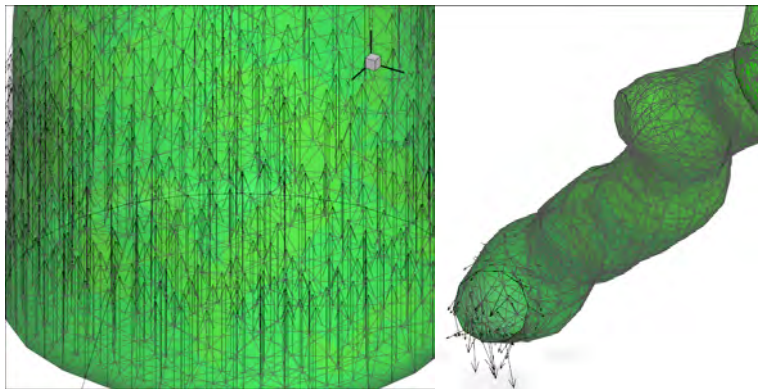
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- Adaptive, cell-based, octal tree algorithm

- Velocity vectors, pressure contours



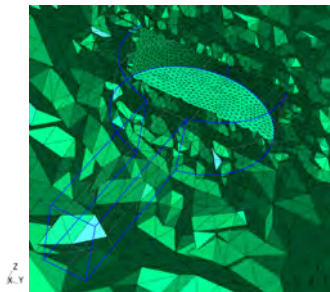
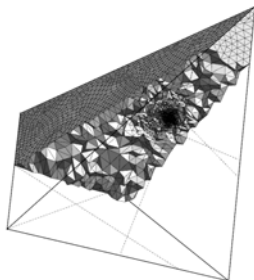
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- Direct numerical simulation

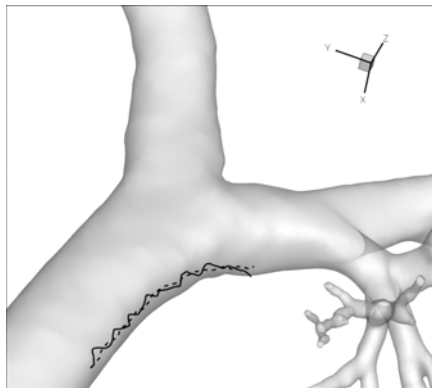
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- Evaluate influence of aerosol shape, compare to spheres

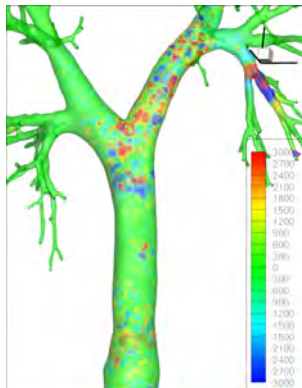
- Refine one airway grid tetrahedron until DNS resolution is achieved



- Spherical vs non-spherical trajectories



- 1 week 64 CPU core study of difference in spherical/non-spherical deposition patterns



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