OKLAHOMA STATE UNIVERSITY

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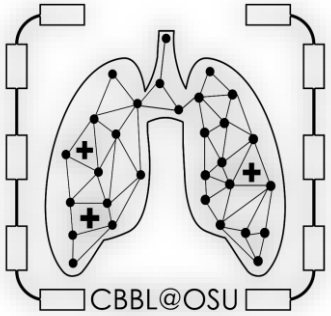
Computational Modeling Work in Targeted Pulmonary Drug Delivery

Yu FENG, Ph.D.



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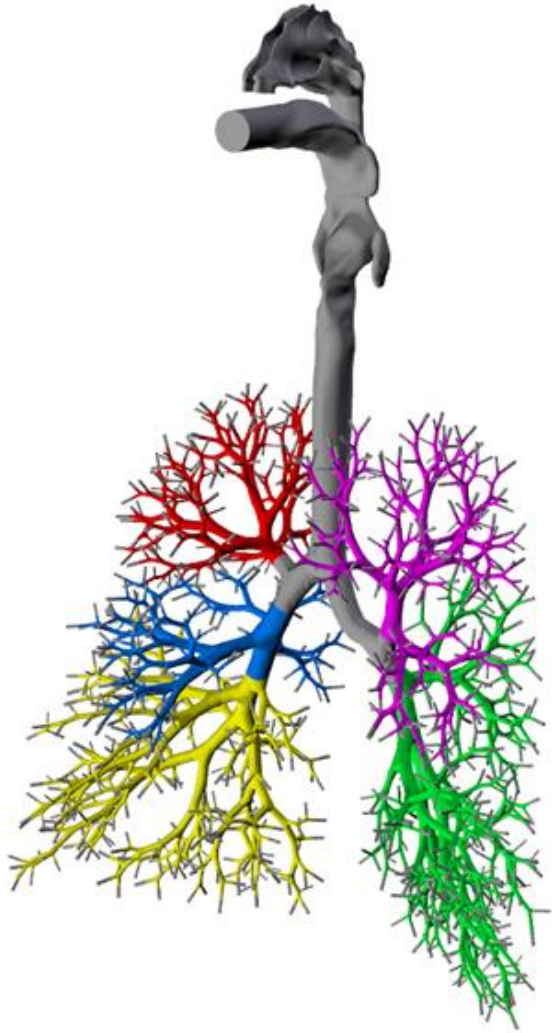
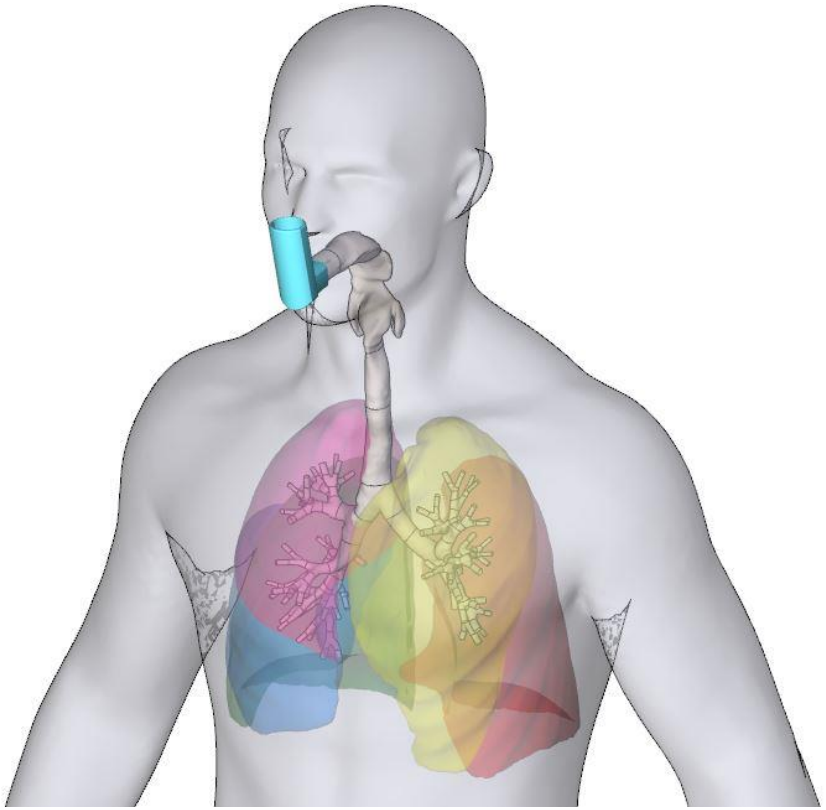
Motivations

- **Animal Studies and Clinical Studies**
  - Invasive
  - Expensive
  - Long Research Cycle
  - Imaging Resolution Limitations
- **Alternative Methods**
  - *In-Silico* Studies based on the Natural Laws of Physics



Targeted Pulmonary Drug Delivery

- **Background**
  - Pulmonary Drug Delivery Advantages
  - Low Efficiency Induced Side-effects
- **Goal**
  - Higher regional deposition efficiency
  - Reduced side-effects
- **Preliminary Study Implications**
  - Low inhalation flow rate
  - Refined release position



Governing Equations (Euler-Lagrange)

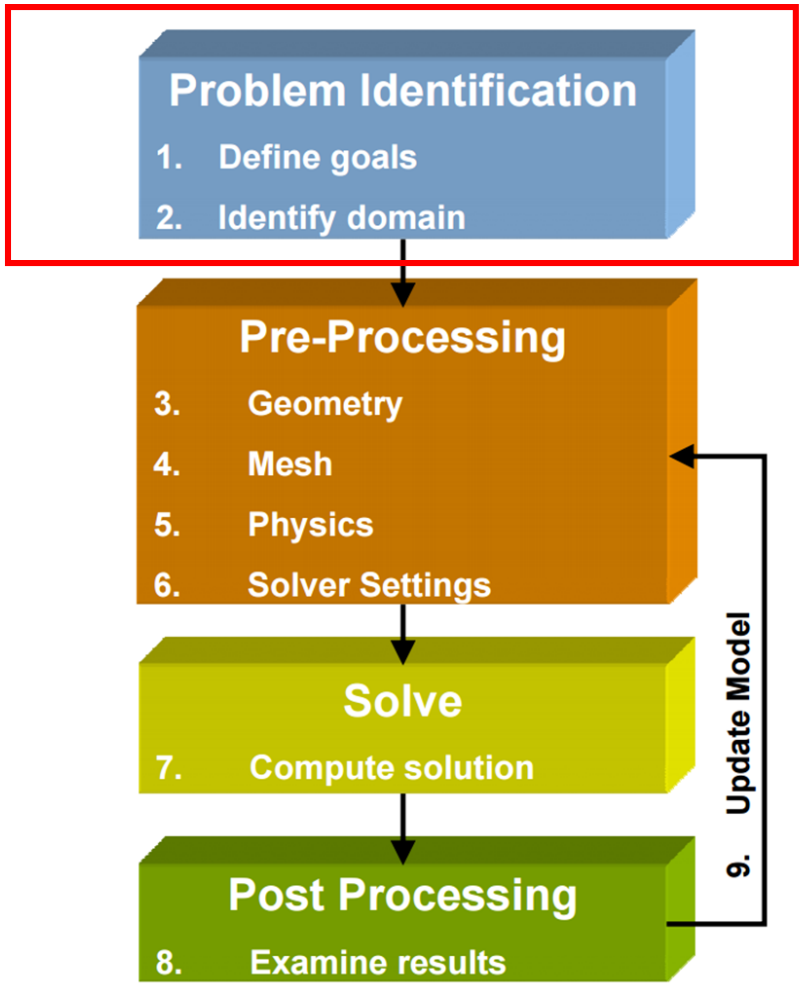
- **Primary Phase (Airflow)**

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} = 0$$

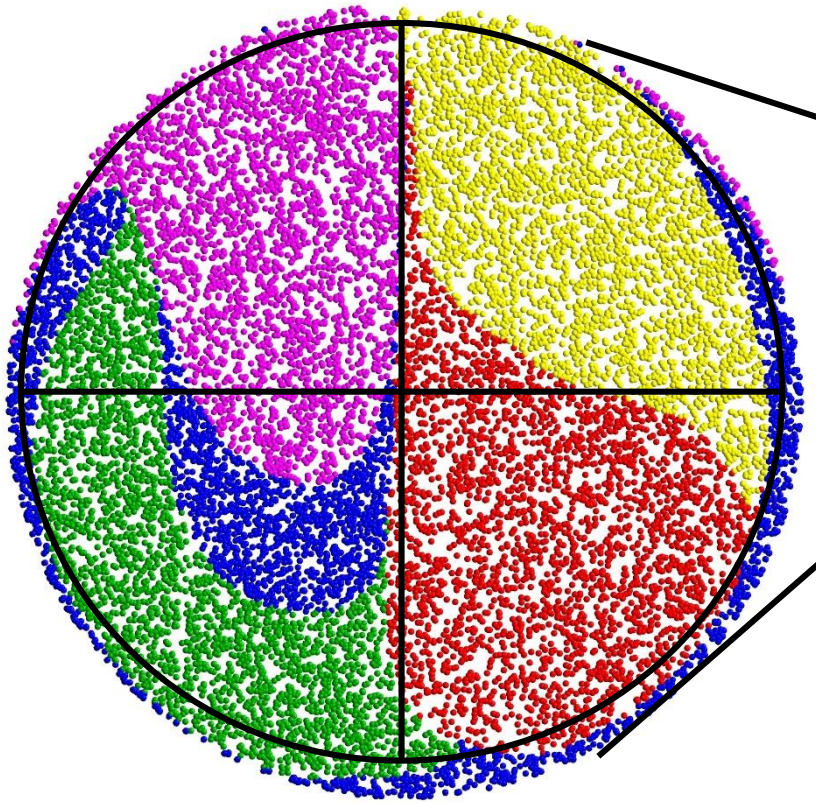
$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + g_i$$

- **Secondary Phase (Pulmonary Drug Particles)**

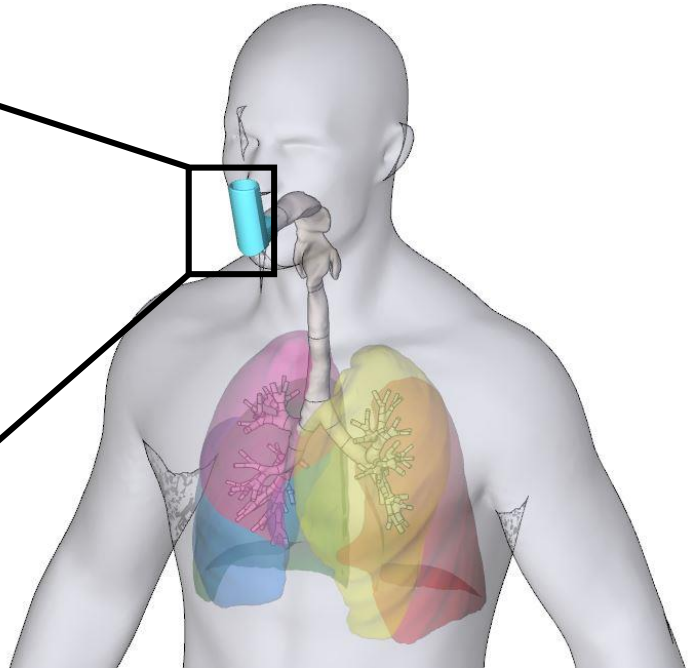
$$\frac{d}{dt}(m_p u_i^p) == F_i^D + F_i^L + F_i^{BM} + F_i^G$$



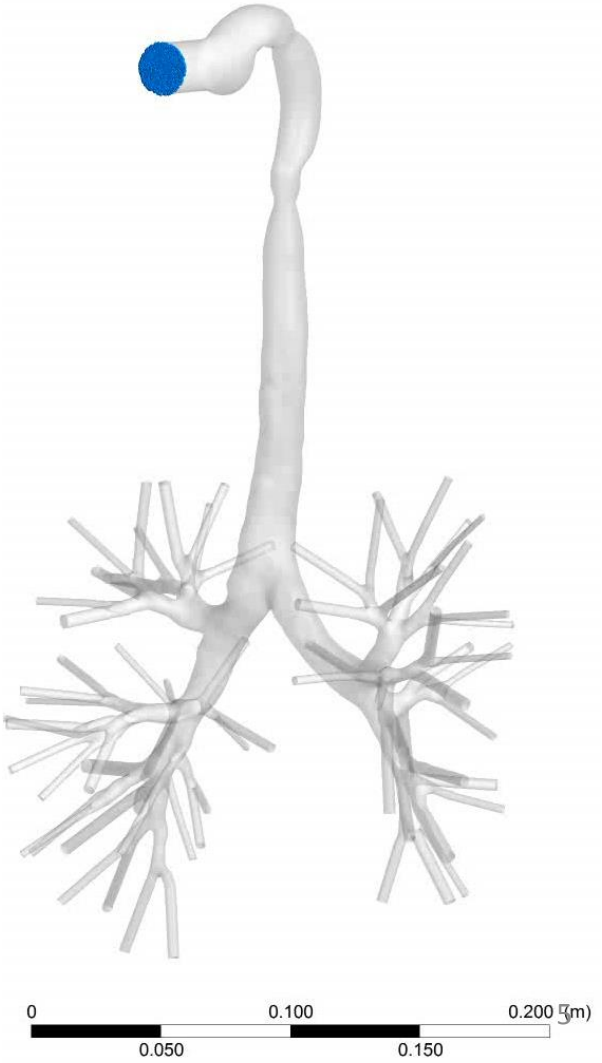
Conventional Pulmonary Drug Delivery



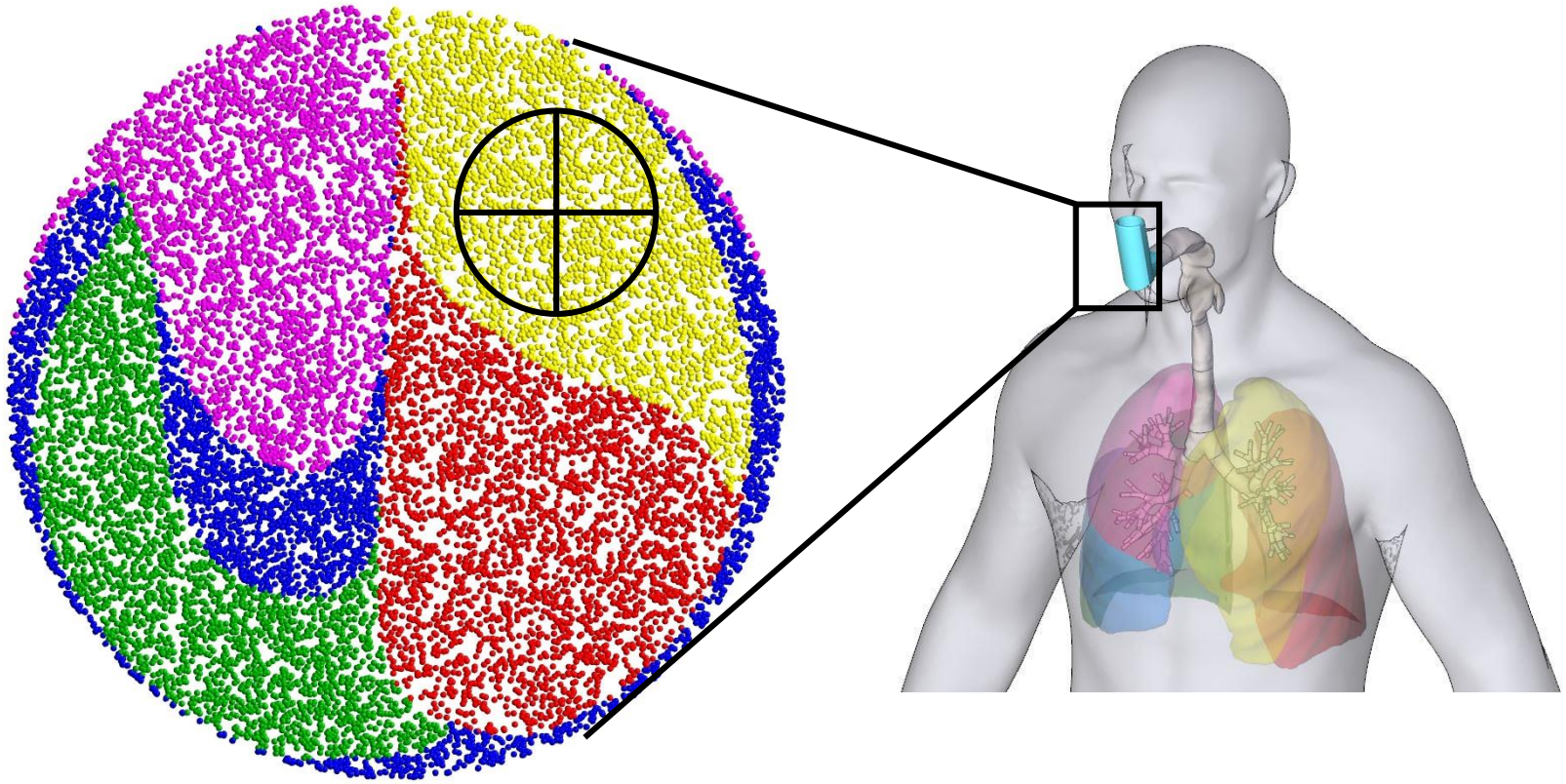
Drug Particle Release Map
Q_{in}=1 L/min d_p= 1 micron



⊕ Drug Release Position

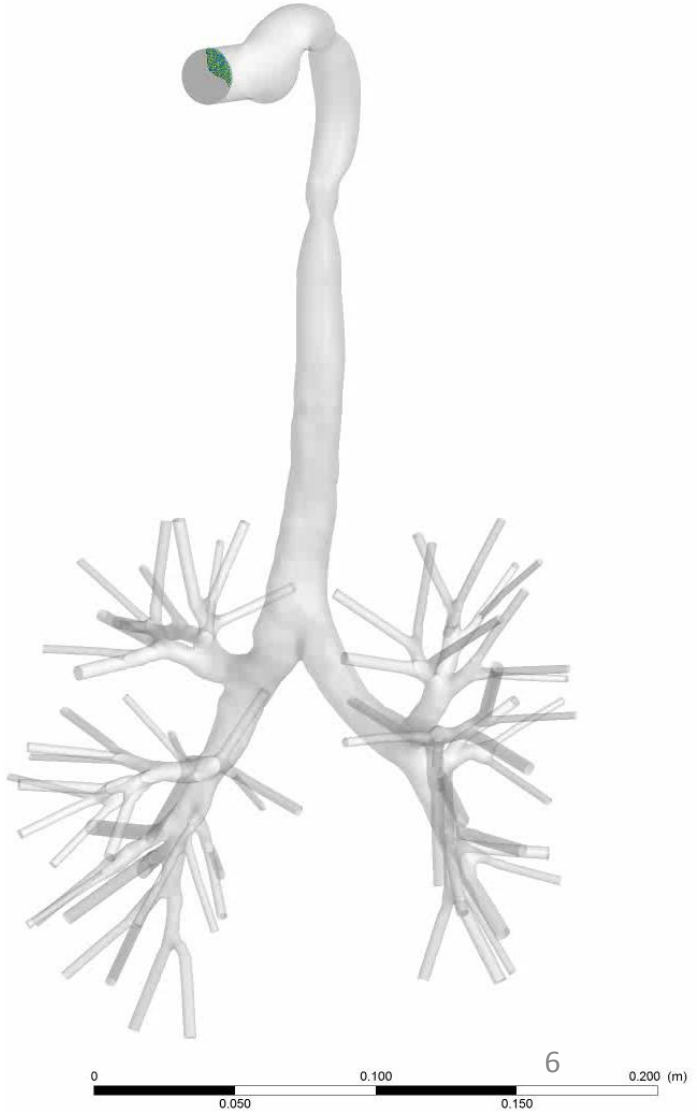


Targeted Pulmonary Drug Delivery (Left Upper Lobe)

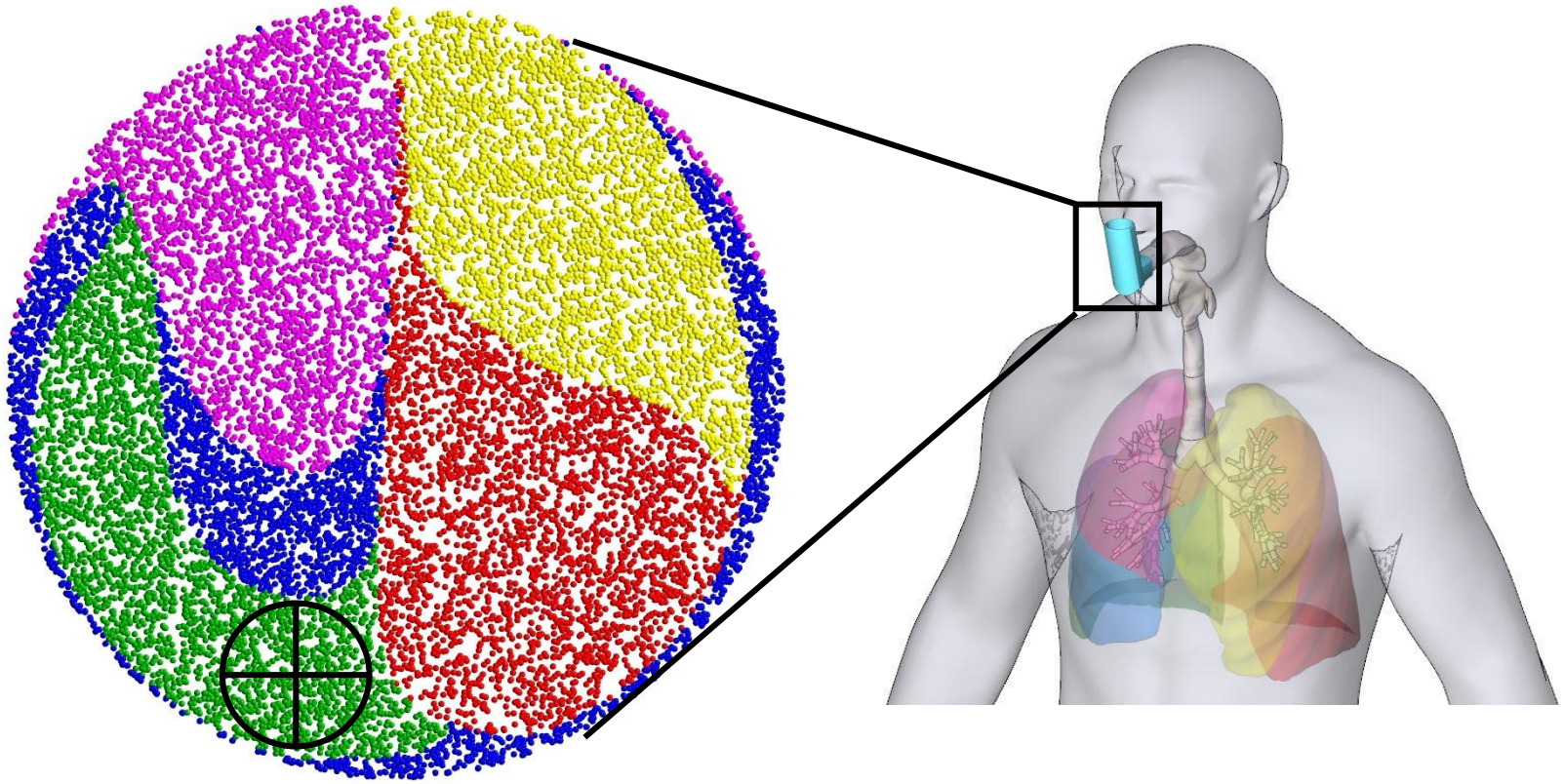


Drug Particle Release Map
Q_{in}=1 L/min d_p= 1 micron

⊕ Drug Release Position

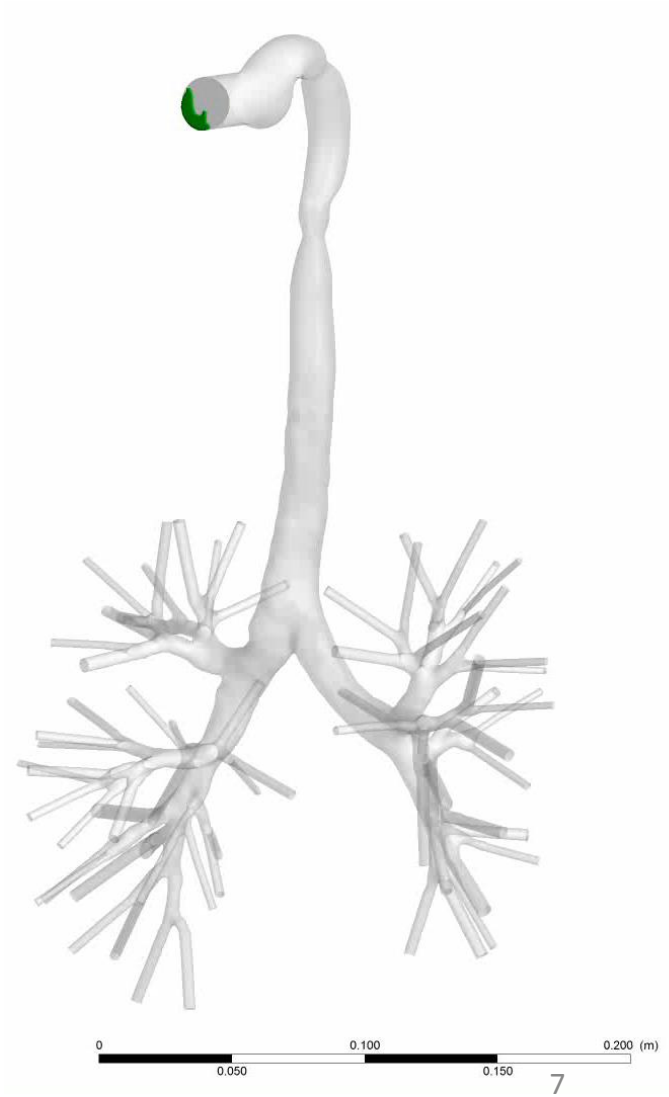


Targeted Pulmonary Drug Delivery (Right Lower Lobe)



Drug Particle Release Map
Q_{in}=1 L/min d_p= 1 micron

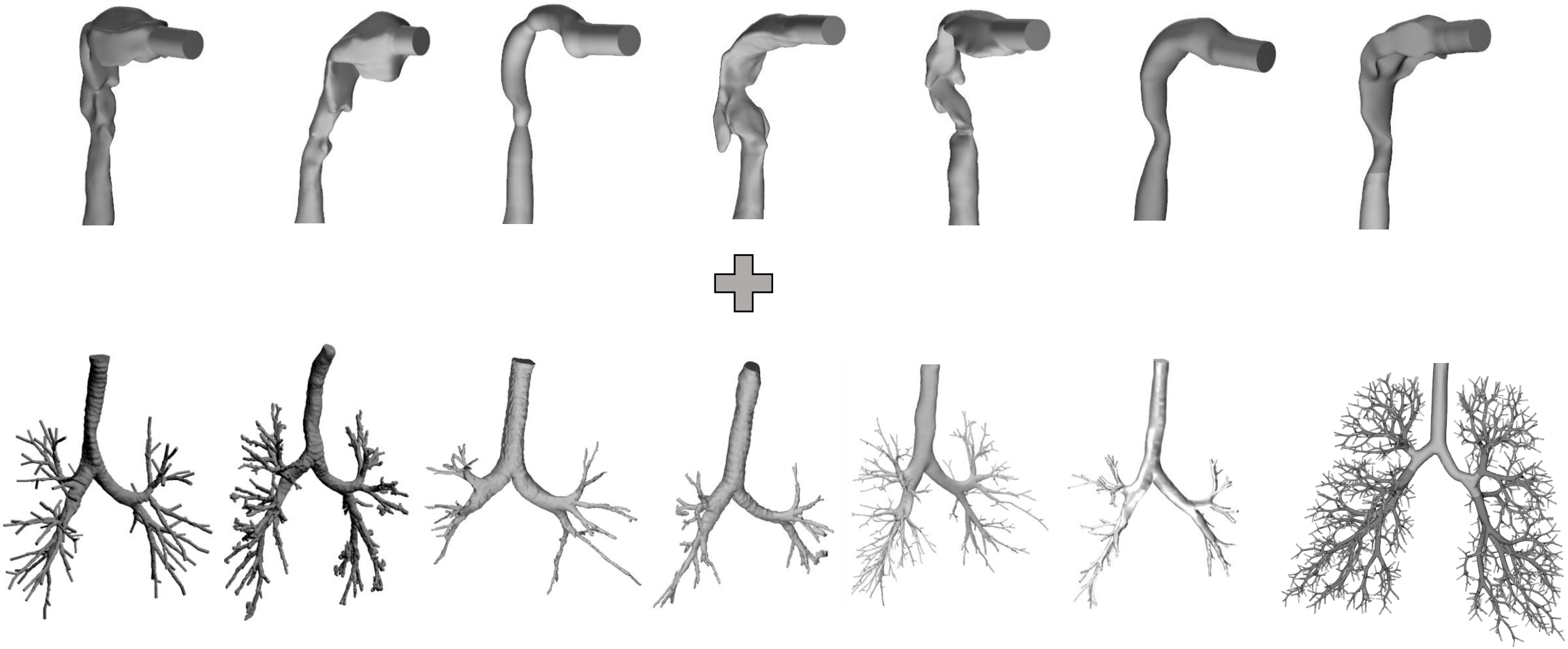
⊕ Drug Release Position



Challenges and Future Directions

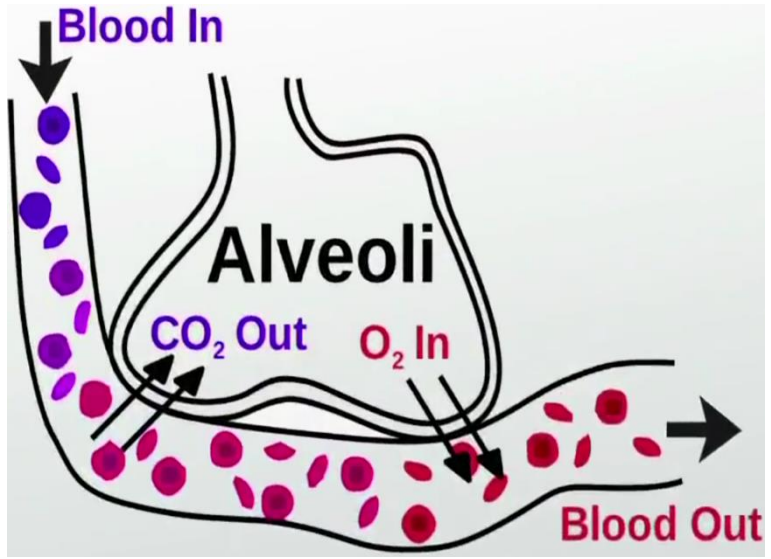
- **Intersubject Variability Study**
  - CFPD Simulation Results with Error Bars
- **Next-Generation Inhaler Design**
  - Low Actuation Flow Rate
- **Precise Treatment Plan**
  - Fast and Accurate
  - Big Data and Machine Learning

Intersubject Variability Study

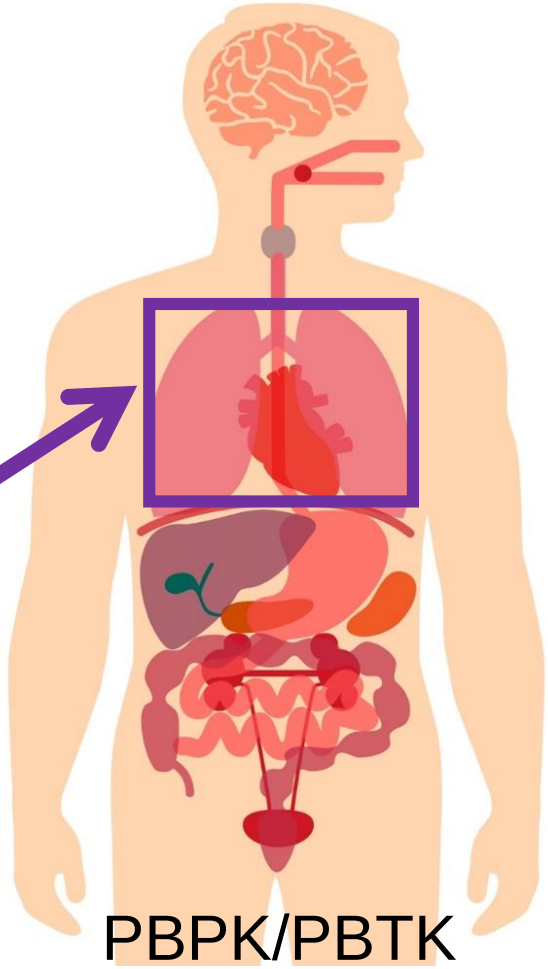


Bring the Simulation to Health Endpoints

CFPD



Drug Translocation



PBPK/PBTK

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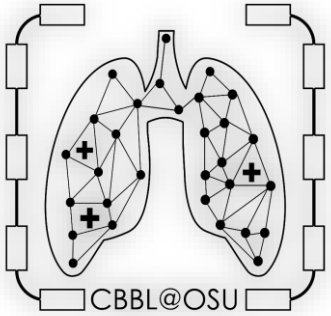
Thank you for your attention!

PI: Yu FENG, Ph.D.



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