Introduction:
Image-Mesh-Simulation Pipeline

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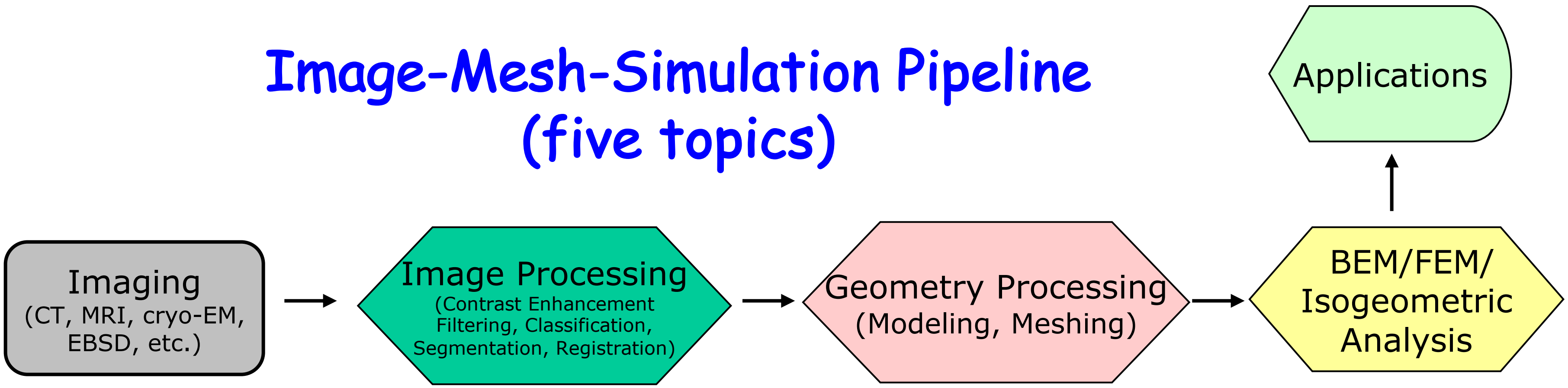
Image-Mesh-Simulation Pipeline (five topics)



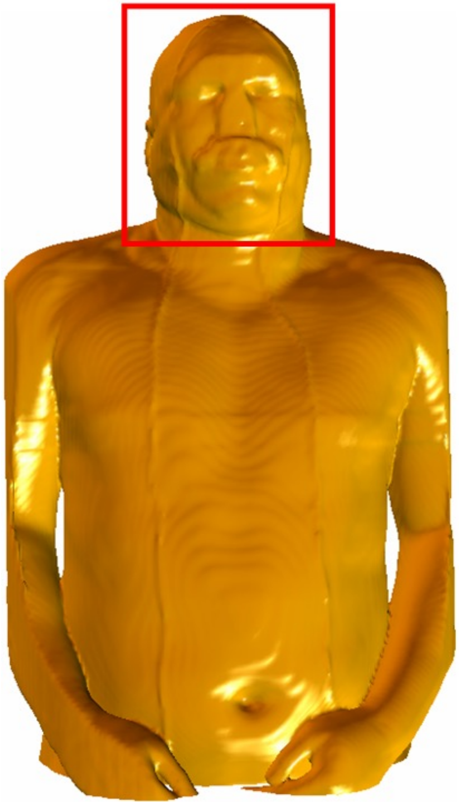
1. Imaging techniques: CT, MRI, cryo-EM, fluoroscopy, etc.
2. Image processing: contrast enhancement, filtering, segmentation, registration
3. Geometry processing: geometric modeling, mesh generation, quality improvement
4. Computational mechanics: finite element method and its extension
5. Applications: computational biomedicine/material sciences/engineering

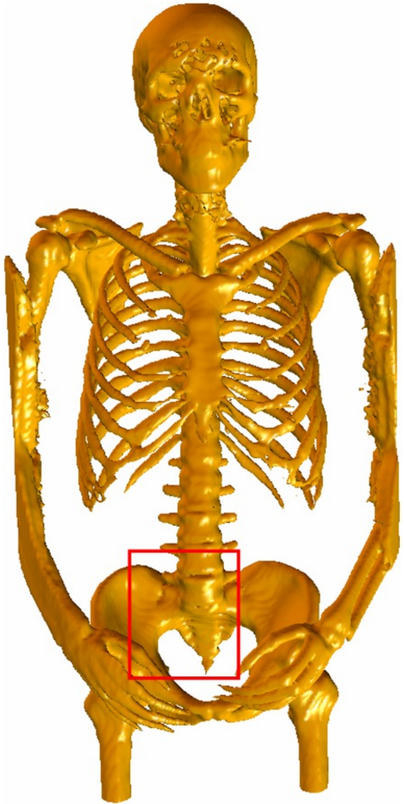
Biomedical Imaging Data

- The imaging data is a scalar field over a 2D/3D rectilinear grid.

$V = \{F(i, j, k) \mid i, j, k$ are indices of x, y, z coordinates in a rectilinear grid.$\}$

Isocontour: $F(i, j, k) = \text{constant}$





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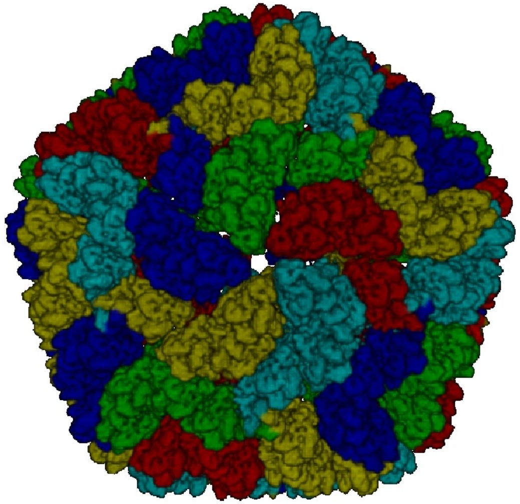
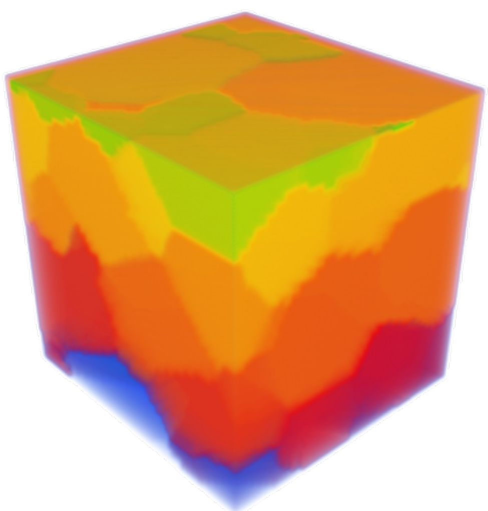
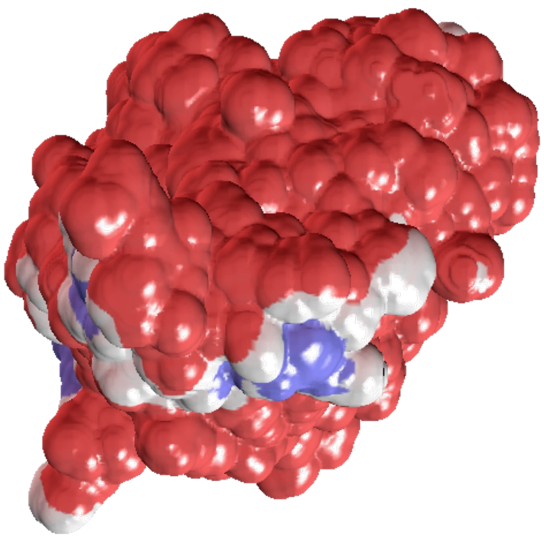
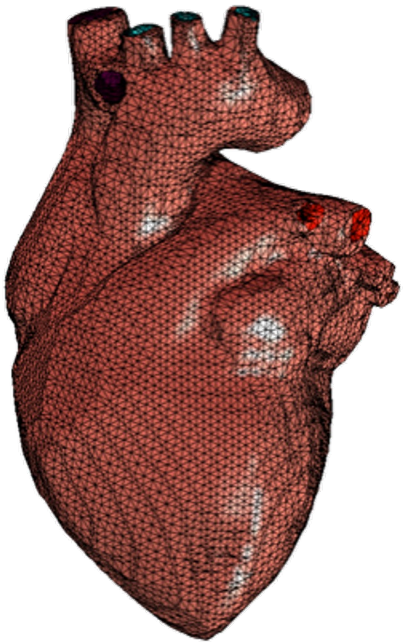
Motivation

- Finite element simulations need meshes.
- Geometric model exists as a level set in volumetric data.
  - Scanned data:
    - CT/MRI/Ultra Sound
    - Cryo-EM
    - EBSD
  - Constructed from a function:
    - Signed distance function
    - Electron density map
    - Electron static potential









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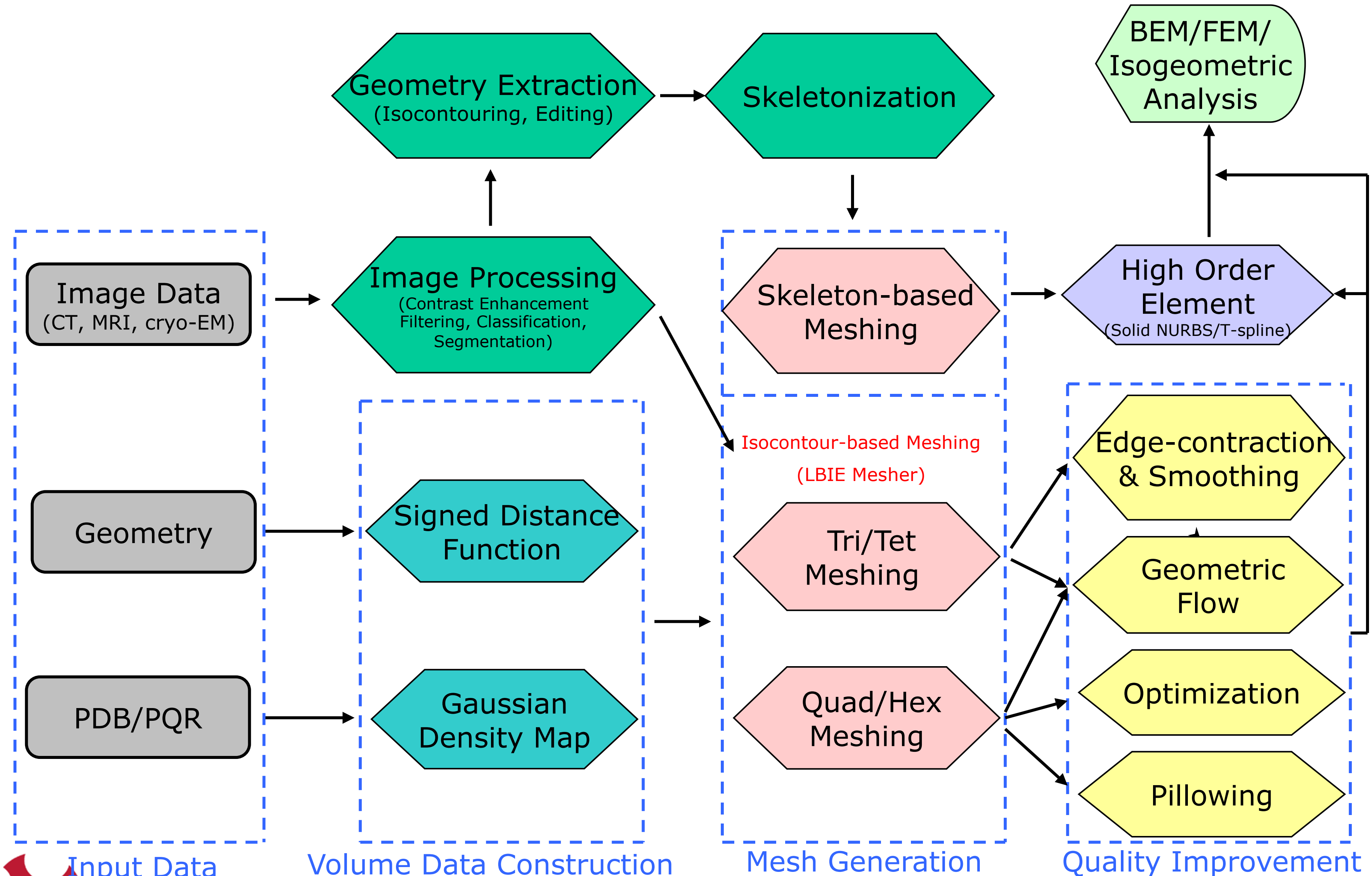
Meshing Pipelines



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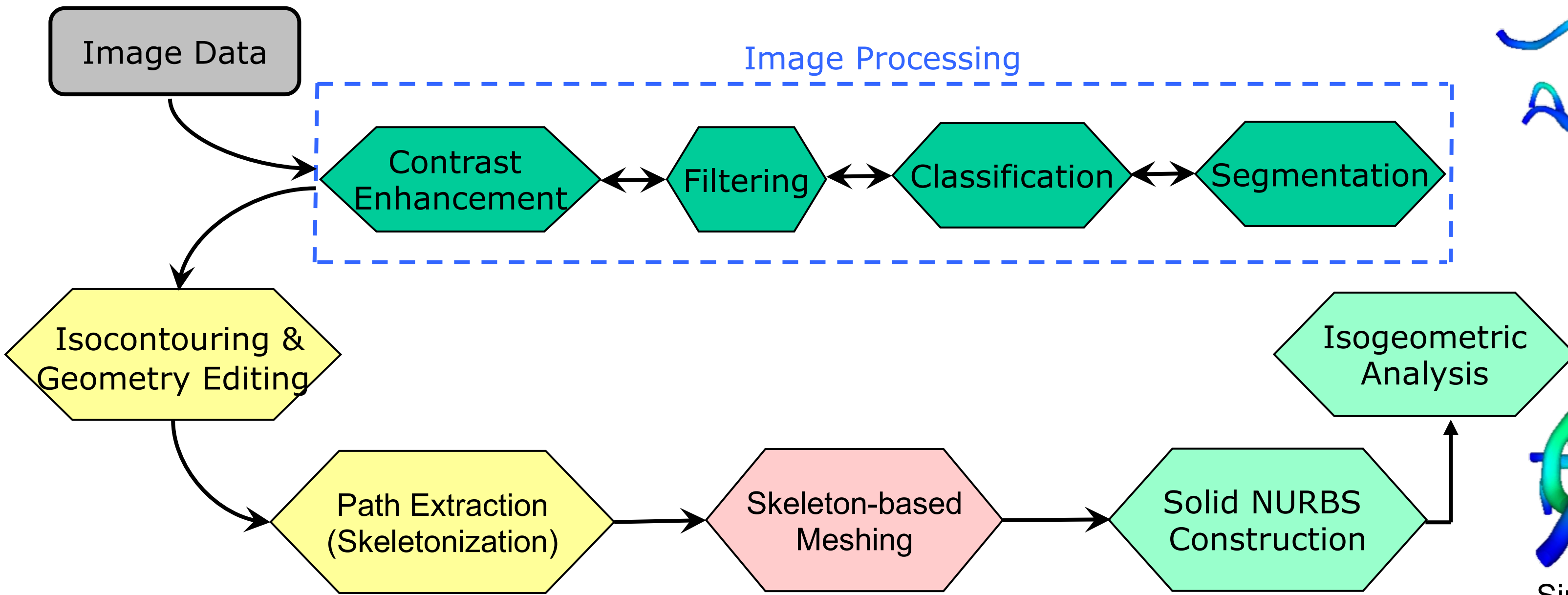
Application Examples in Computational Biomedicine

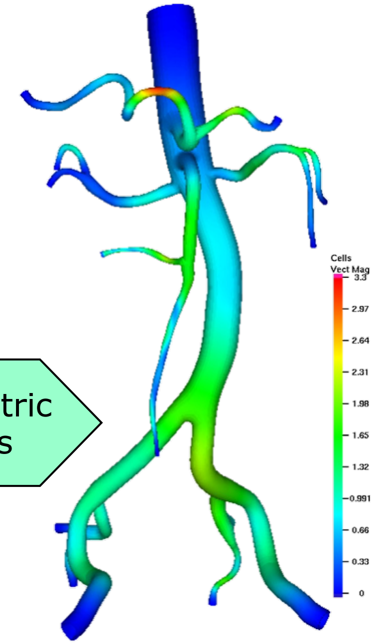
- Cardiovascular blood flow simulation
- Brain biomechanics
- Laser therapy for prostate cancer treatment

Cardiovascular Blood Flow Simulation

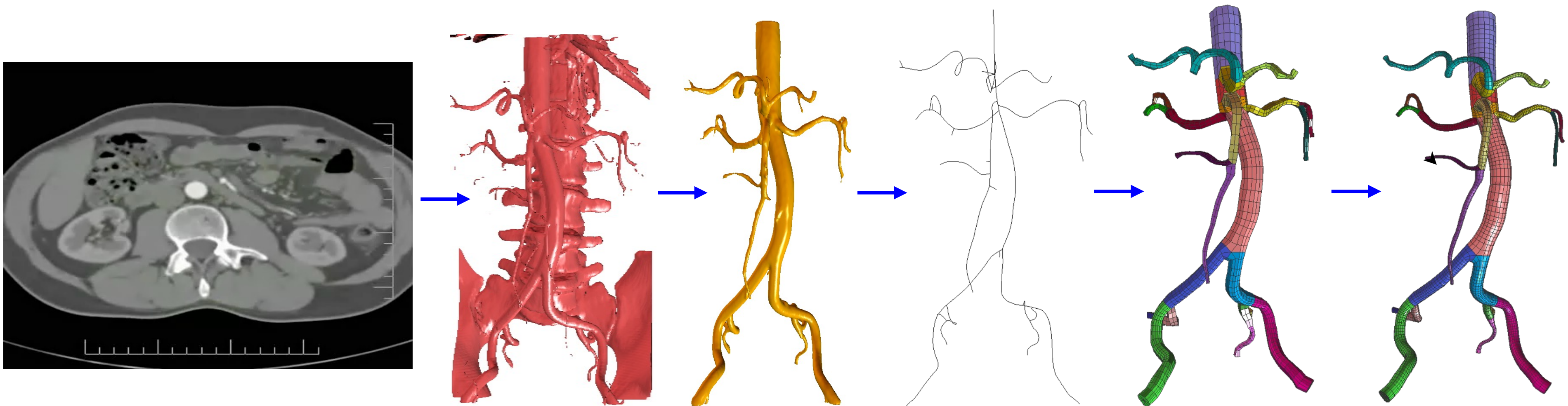
- Computational Fluid Dynamics (CFD) has been used in cardiovascular blood flow simulations.
- Simulation results can be used to analyze the blood flow pattern and provide prediction on diagnosis and treatment planning.
- Simulation results can also be used in medical device design and optimization.

Cardiovascular Blood Flow Simulation



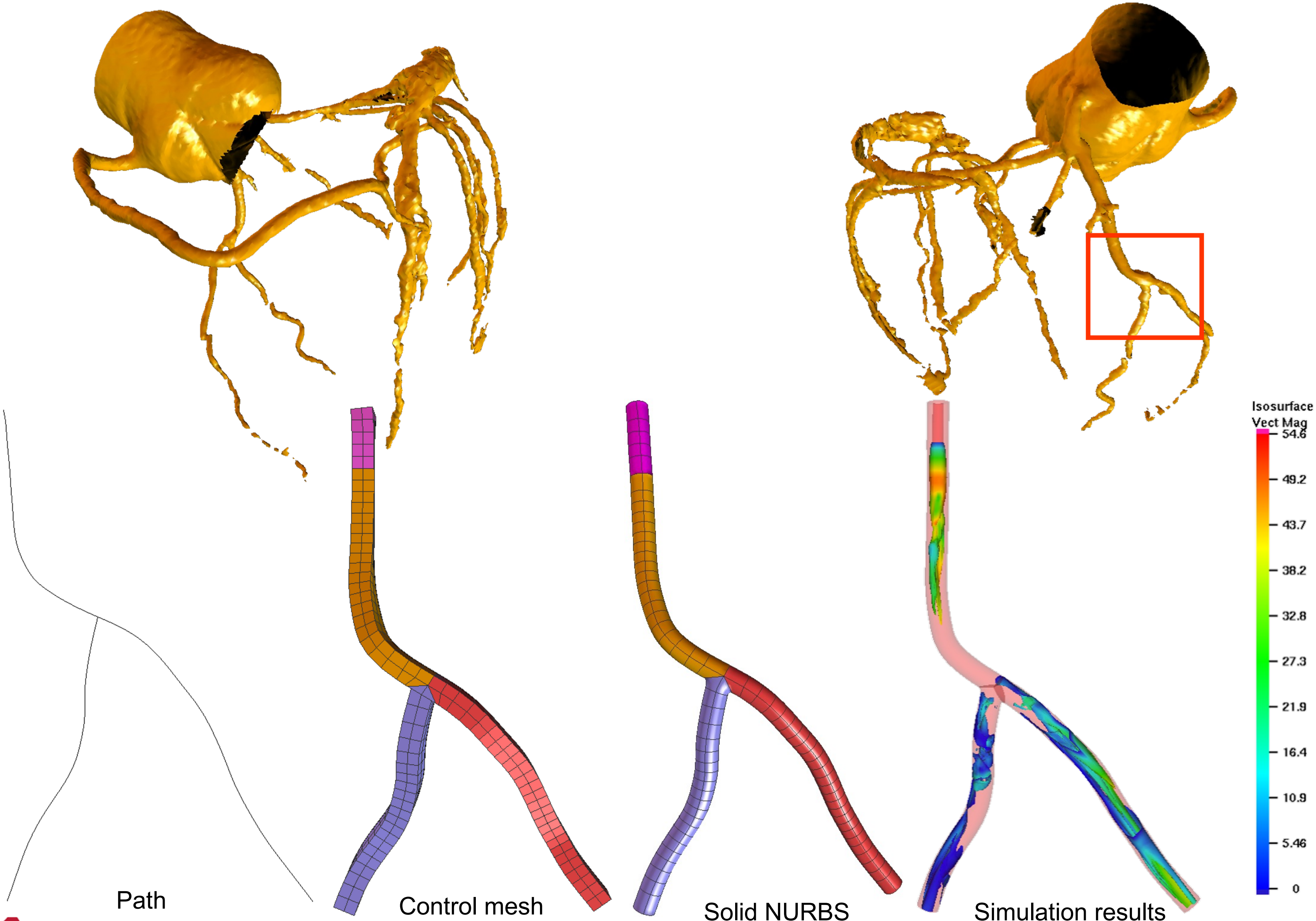


Simulation results

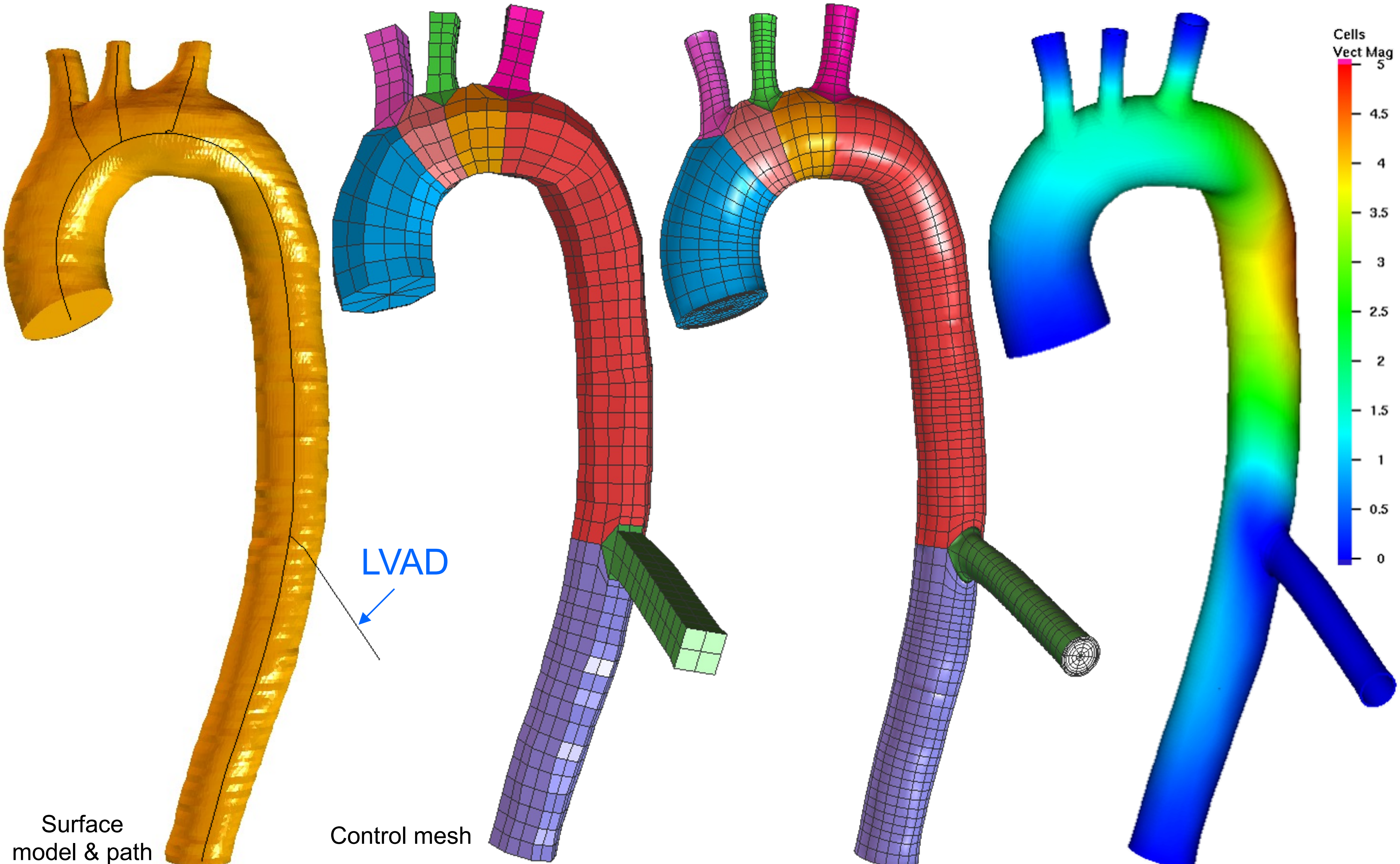


CT64 data   Contouring   Surface model   Path   Control mesh   Hex Solid NURBS

Coronary Arteries – Drug Delivery Analysis



Thoracic Aorta – Computer-Aided Surgical Device Design
(Left ventricle assistant device)



Surface model & path

Control mesh

Solid NURBS

Simulation results

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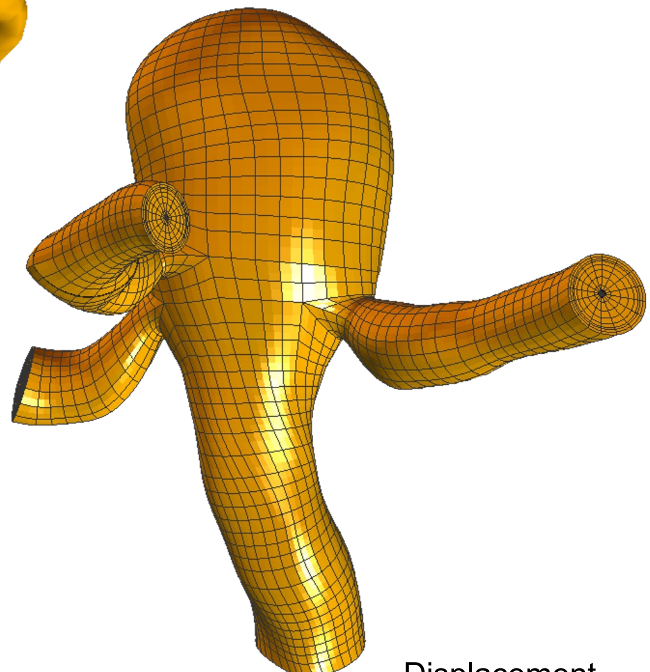
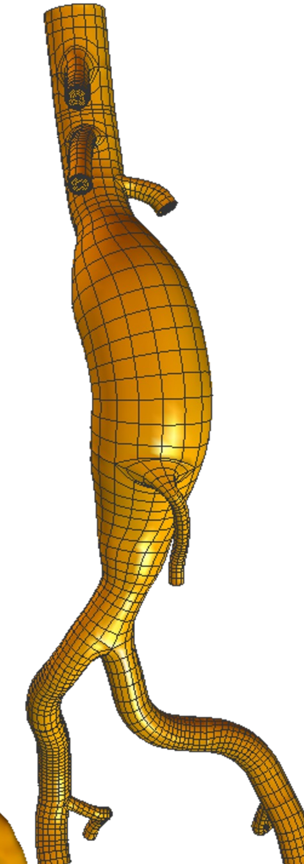
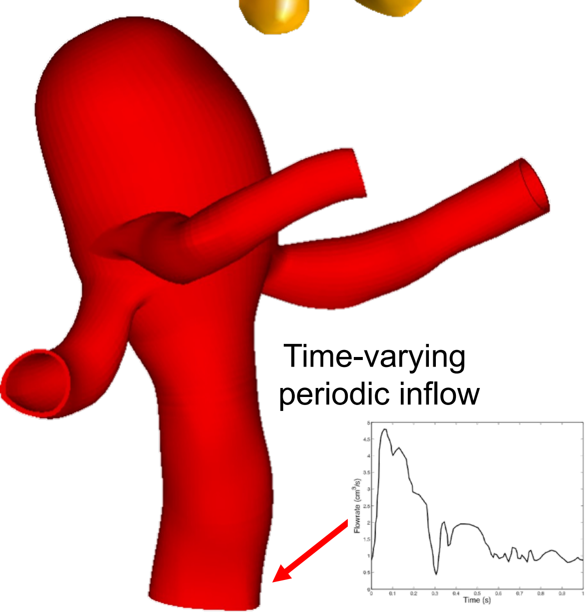
Collaborators: T. Kvamsdal at SINTEF and Y. Bazilevs at UCSD

Aneurysms

(Analysis Suitable Models)

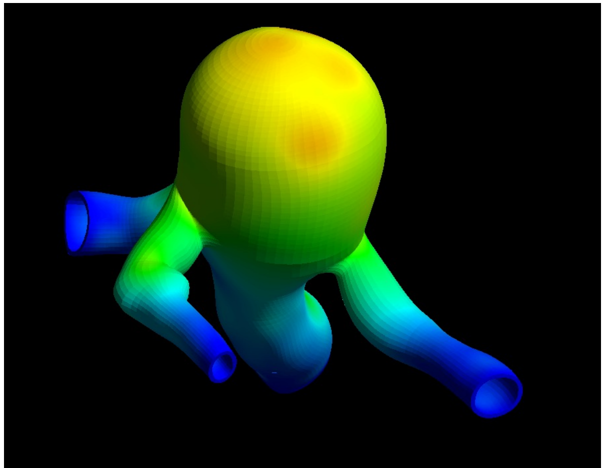




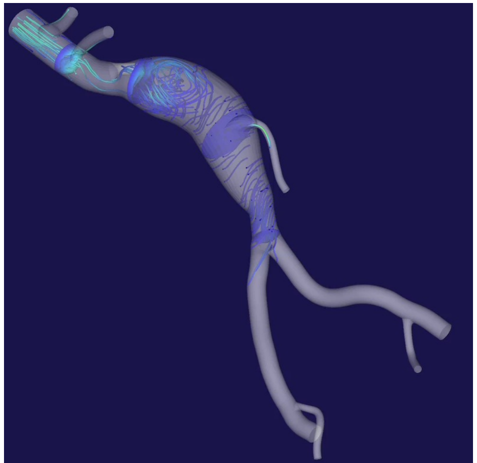


Time-varying periodic inflow

Displacement

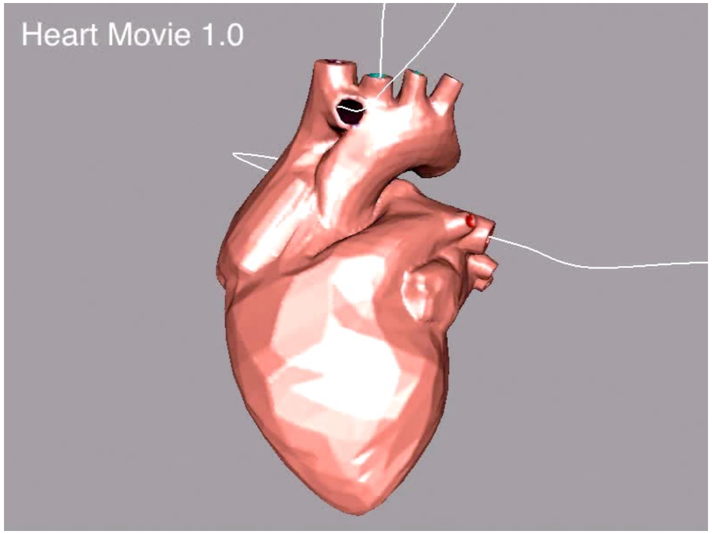


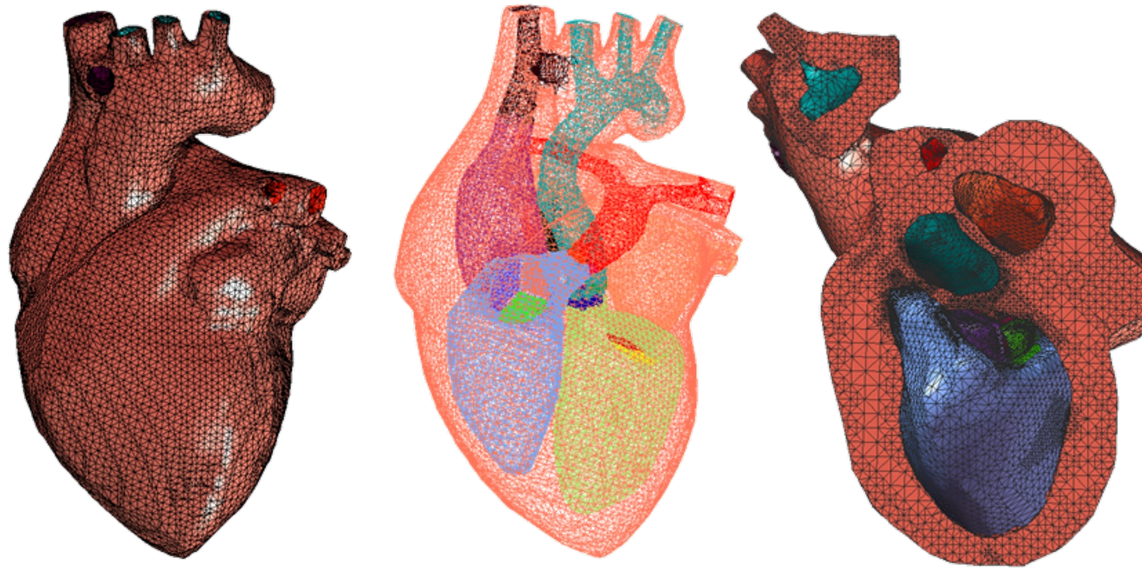
Stream lines

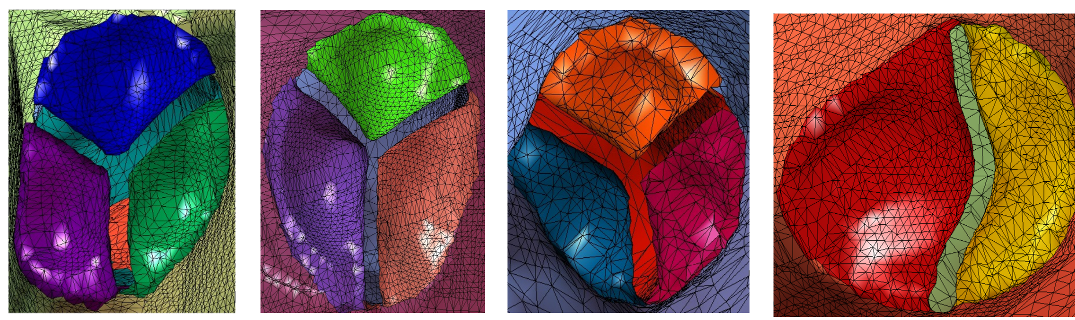


Collaborators: Prof. Wing-Kam Liu (NWU), Prof. Xiaodong Wang (NJIT)

Heart: Multiple Materials detection







aortic valve | tricuspid valve | pulmonary valve | mitral valve

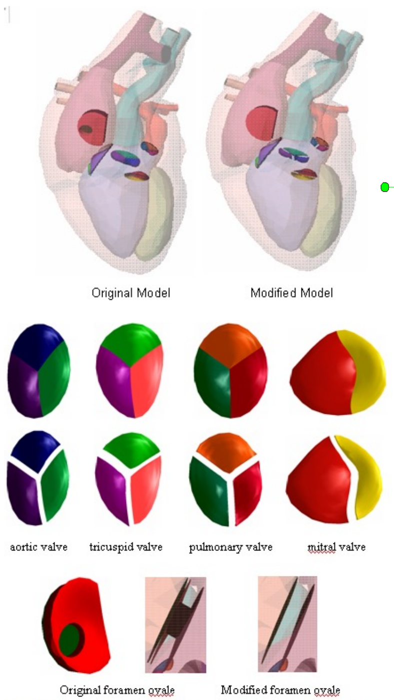
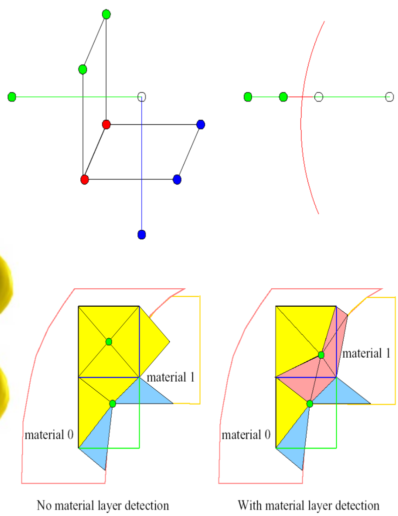


Fig. 2. The original model from NYU* and the modified model. Note*: With permission of New York University, Copyright 1994-2004.

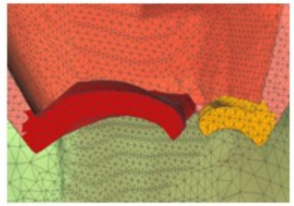


Reference: Y. Zhang, C. Bajaj. **Finite Element Meshing for Cardiac Analysis**. *ICES Technical Report 04-26, UT-Austin*, 2004.

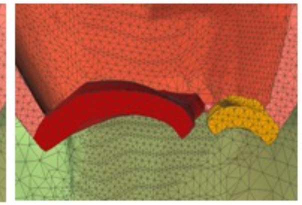
Collaborators: Prof. Wing-Kam Liu (NWU), Prof. Xiaodong Wang (NJIT)

Blood Flow Simulation inside Educational Heart Model

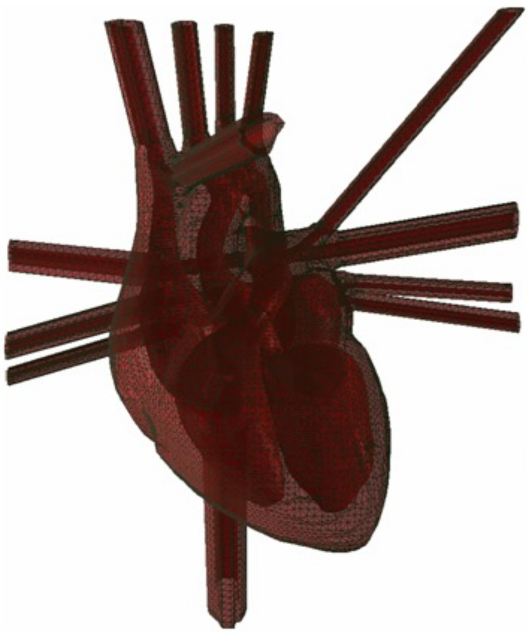
Application: The heart model is put inside a cubic container, and all the blood vessels are extended to the container boundary. The constructed meshes are being used in the simulation of blood flow using immersed continuum method, the distribution of velocity, shear stress, pressure and locations of flow recirculation are analyzed. It is useful for the heart valve design and the understanding of blood circulation disease.



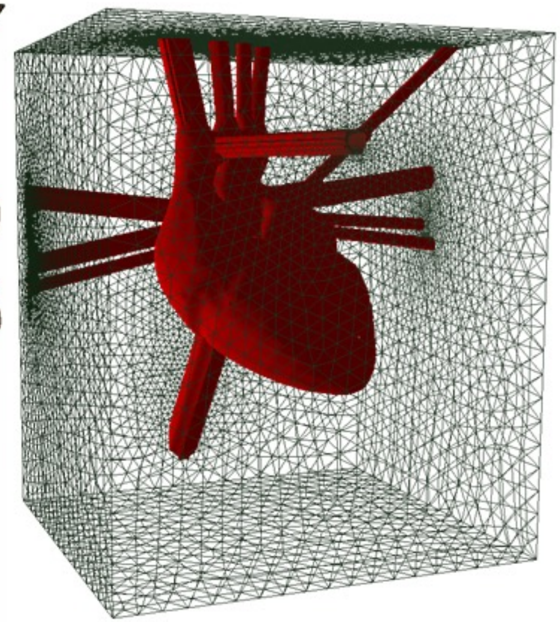
Before material layer detection



After material layer detection

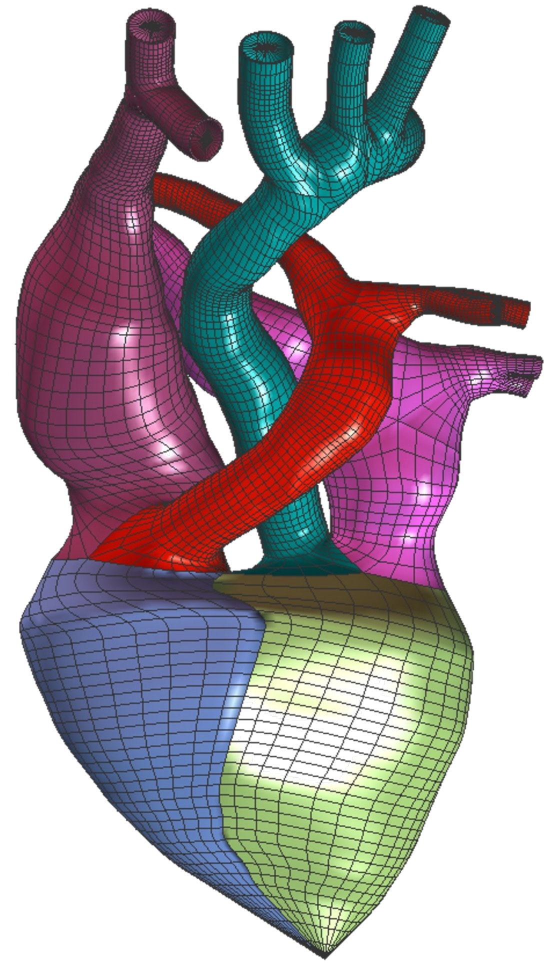


The heart model with extensions



The heart model immersed in the fluid mesh

Fig. 5. The resulting adaptive and quality tetrahedral mesh for the cardiac model and the heart model used in the simulation of blood flow.



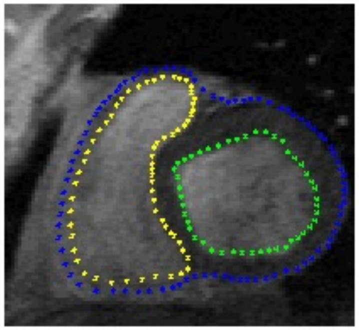
Solid NURBS (fluid + muscle)

- W. K. Liu, G. Chen, X. Wang, Y. Zhang, C. Bajaj, T. Hughes. **A Study of a Three-Dimensional Heart Model Using Immersed Continuum Method**. *Manuscript*, 2004.
- W. K. Liu, Y. Liu, D. Farrell, L. Zhang, X. Wang, Y. Fukui, N. Patankar, Y. Zhang, C. L. Bajaj, J. Lee, J. Hong, X. Chen, H. Hsu. **Immersed Finite Element Method and Its Applications to Biological Systems**. CMAME, 195(13-16):1722-1749, 2006.

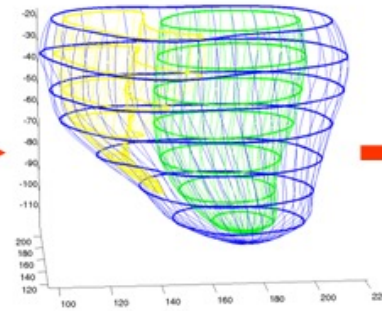
Application: Heart-Lung-Torso

Collaborator:
Simula Research Lab, Norway

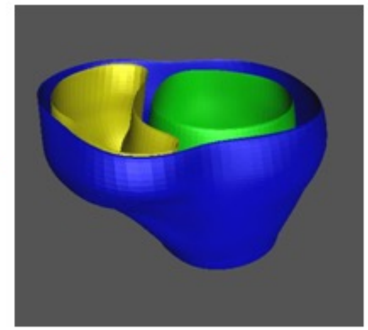
* To simulate the electronic activity of the heart.



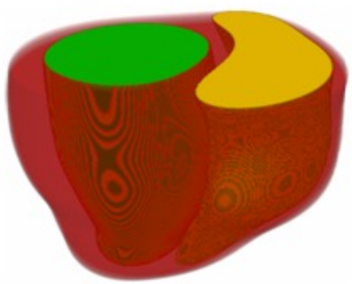
Raw MRI data



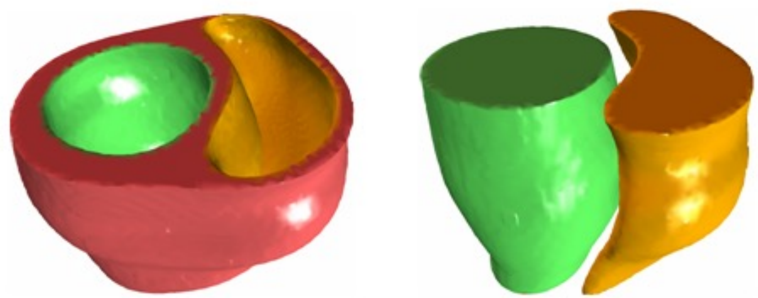
Manually digitized slices



Continuous model

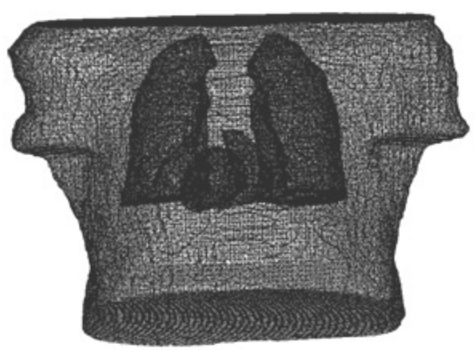


Volume rendering

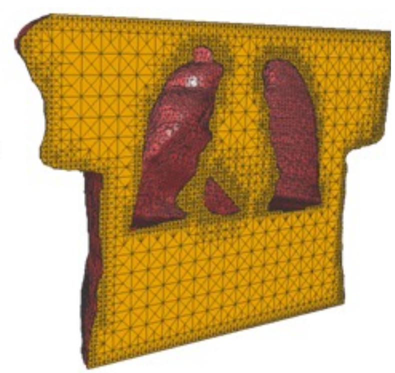


Smooth shading

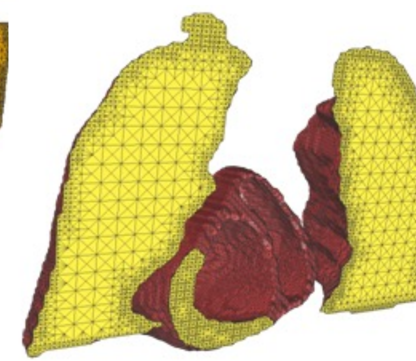
Volume rendering



Wireframe

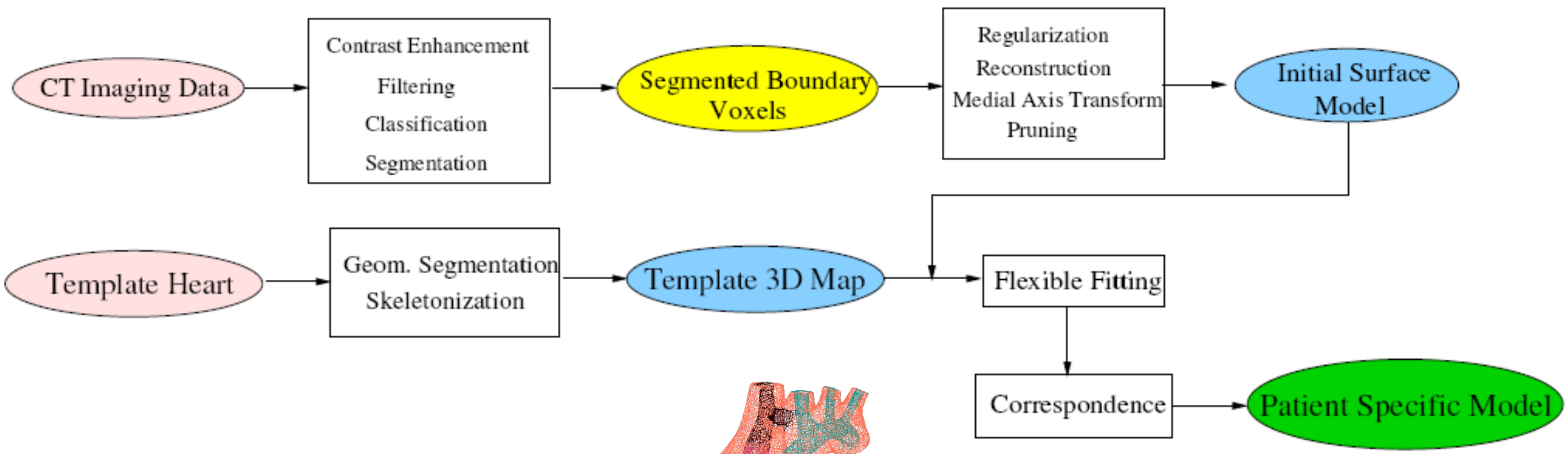


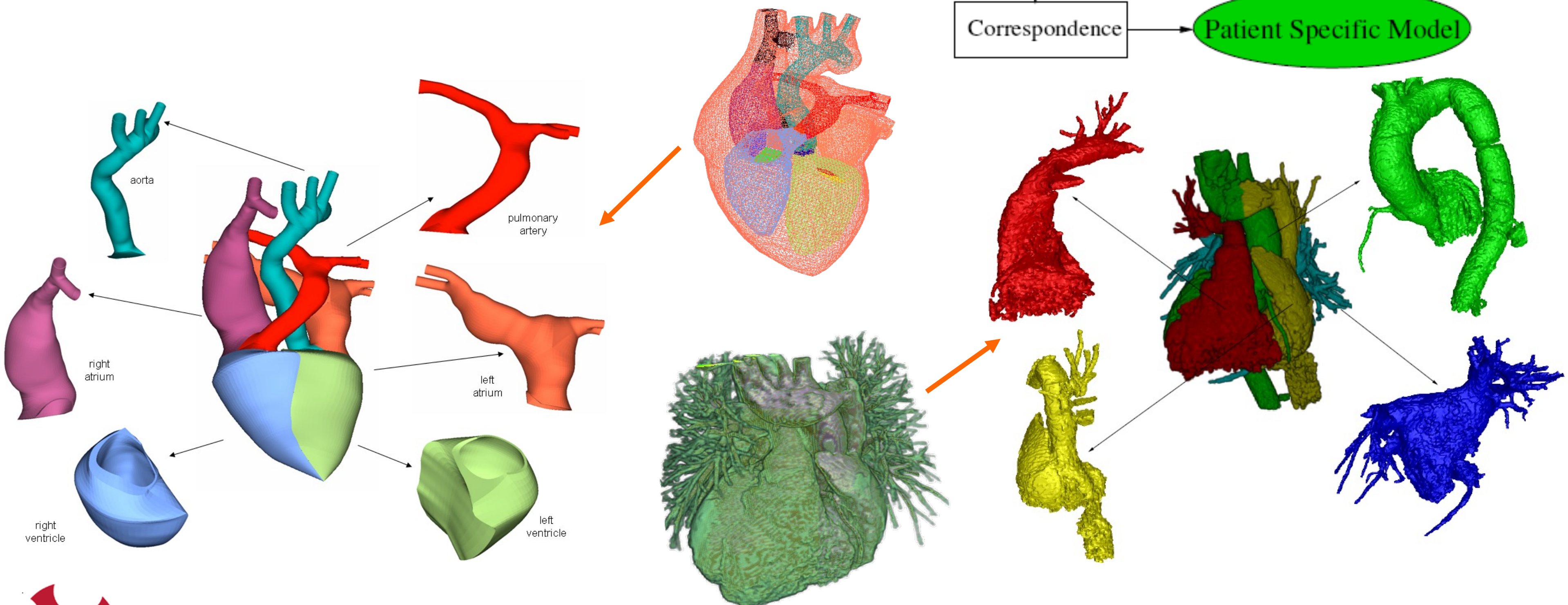
Exterior (124716 verts, 615370 tets)



Interior (160739 verts, 782821 tets)

Patient Specific Models of the Human Heart



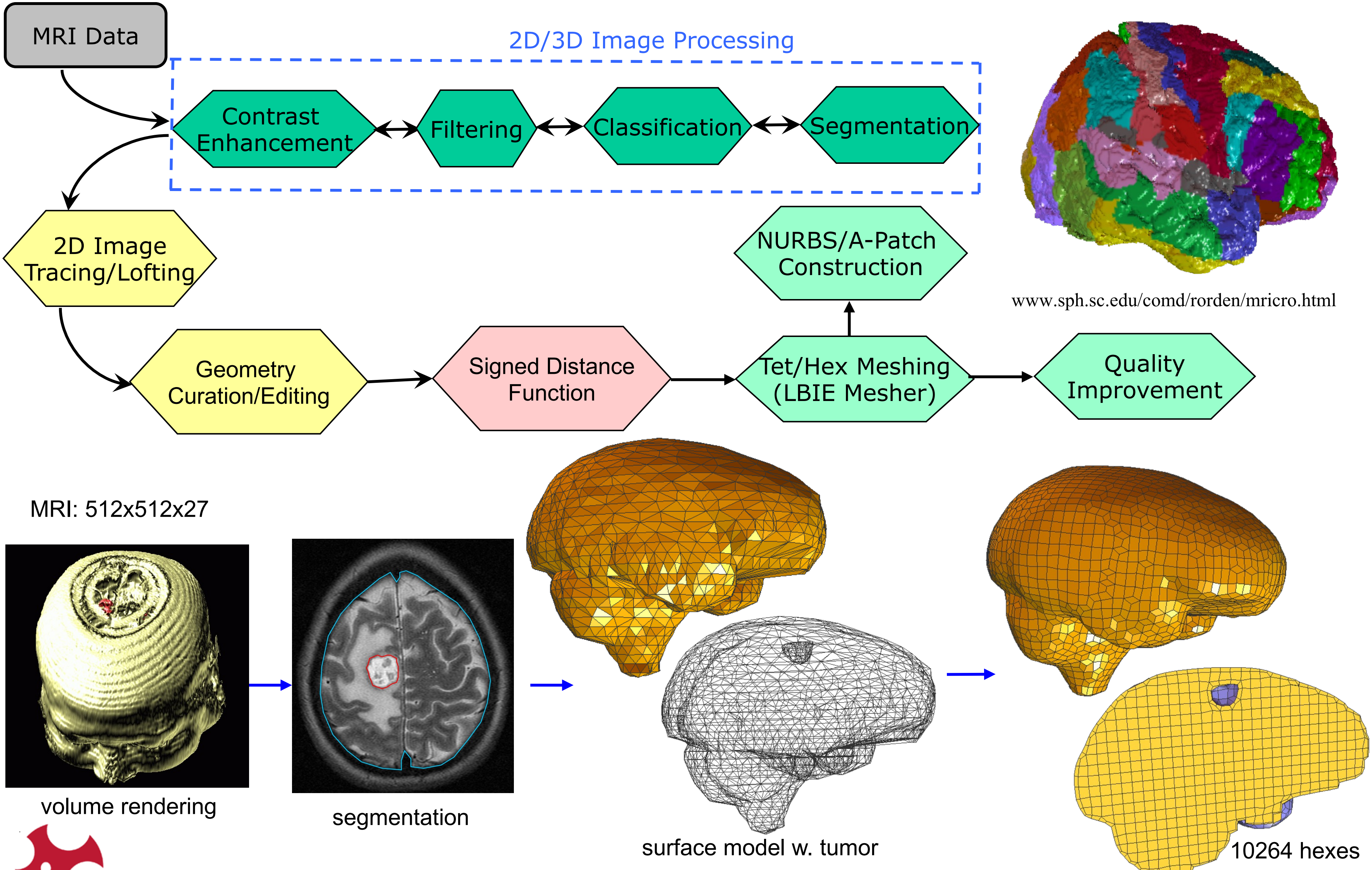


Brain Bio-Mechanics

- Brain biomechanics is very useful for computer-aided surgery.
- When the brain has a tumor in the brain, and the physician has to conduct surgery on it, the skull needs to be opened. Since the brain is a fluid-like structure, the brain shifts after the skull is open.
- Brain biomechanics can predict how much the brain shifts, and predict the new position of the tumor.
- Brain biomechanics can also calculate the reactive forces on the surgical tools, which is useful for the design of medical devices.

Application: Brain Bio-Mechanics

* To analyze brain shift and the reaction force of surgical tools.



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Laser Therapy of Prostate Cancer Treatment Planning

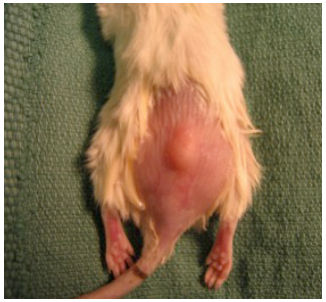
- Prostate cancer is the 2^{nd} leading cause of cancer-related deaths in the United States.
- There are two kinds of method to kill cancer cells: increase the local temperature (laser therapy) or decrease the local temperature (cryo-surgery).
- When we use laser therapy for treatment, it is important to design the laser power, pulse duration (dose), shooting angle, number of laser probes, etc.
- Biomechanics can predict the laser therapy results after a certain period (e.g., one month) by solving a bio-heat equation.
- The simulation results can also be validated by comparing with MRTI data (Magnetic Resonance Temperature Imaging)

Dynamic Data-Driven System for Laser Treatment of Cancer

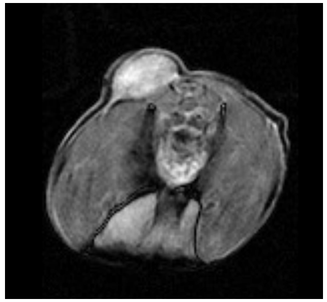
* To estimate radiation dosage and make treatment plan

Collaborators:

- Prof. J. Tinsley Oden (UT-Austin)
- Prof. Kenneth Diller (UT-Austin)
- Prof. James C. Browne (UT-Austin)
- Prof. John Hazle (M.D. Anderson, Houston)
- Prof. Nicole Rylander (VT)

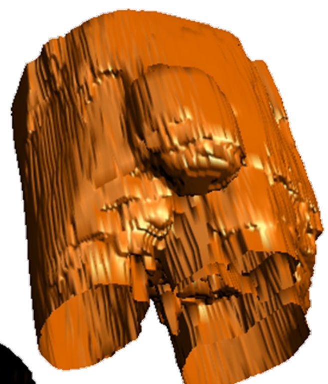


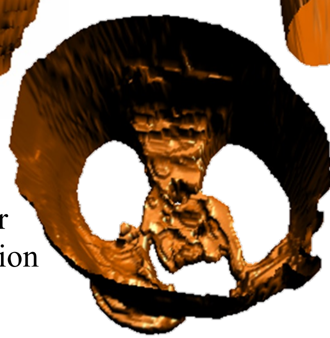
Mouse + Tumor

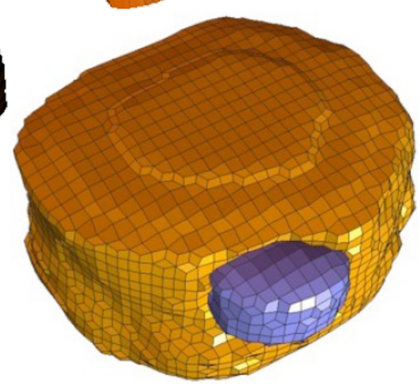


A slice of MRI data

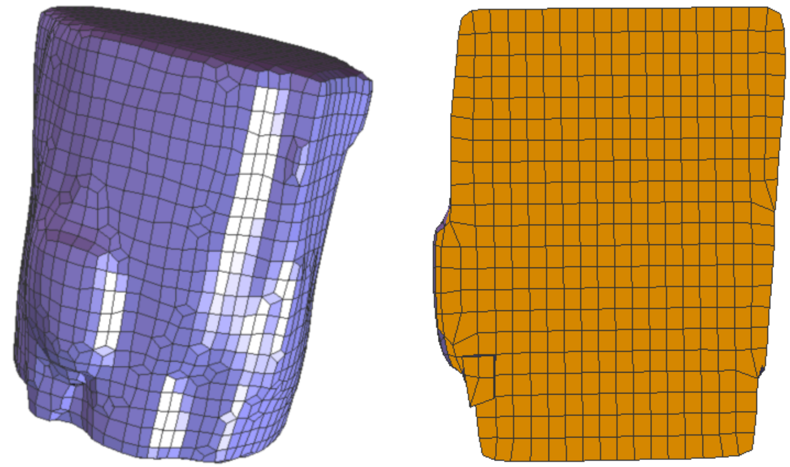
Segmented result



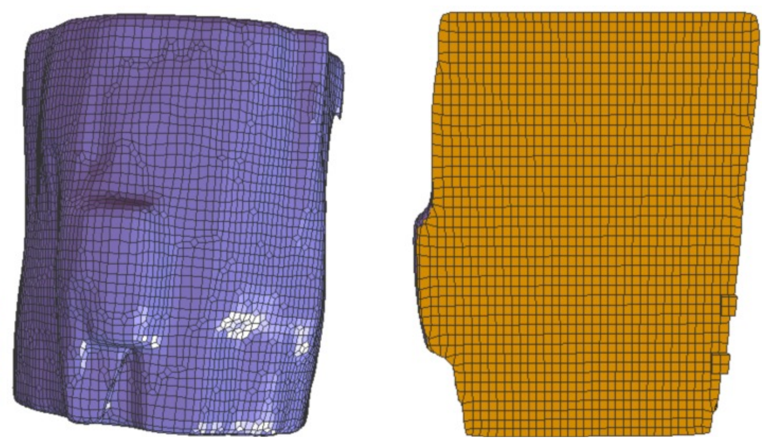




Isocontouring after automatic segmentation



One coarse mesh (7754 vertices, 6486 hexes)



One fine mesh (58211 vertices, 53128 hexes)

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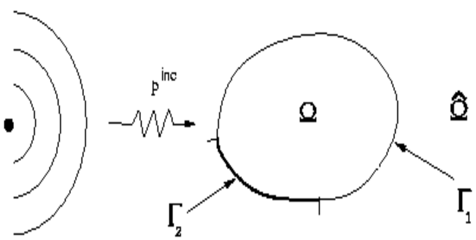
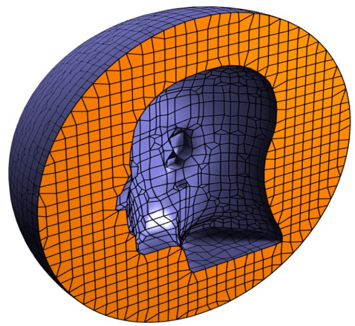
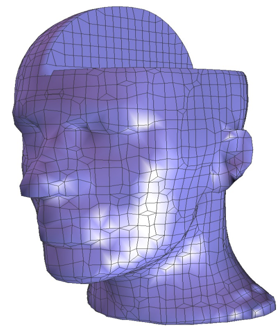
Collaborators: L. Demkowicz, T. Walsh

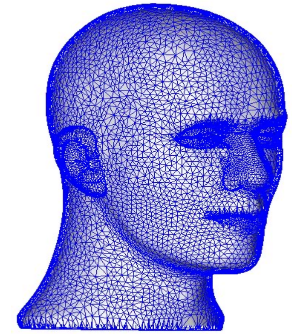
Patient Specific Computational Prototyping of Sound Localization

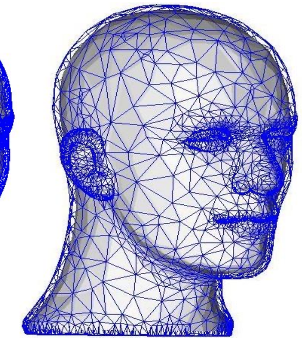
- CT/MRI Imaging → Boundary Element Meshes → Acoustics Pressure Scattering/Absorption (Helmholtz) → Visualization

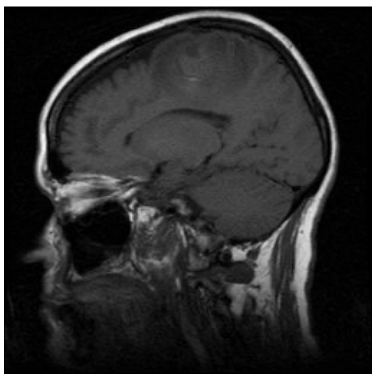


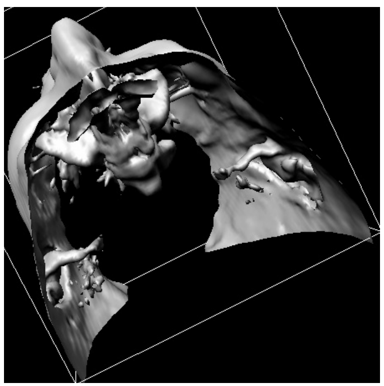


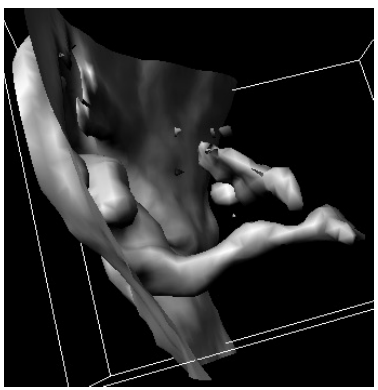


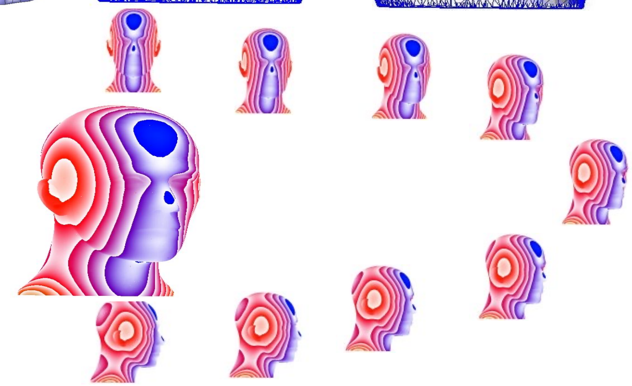




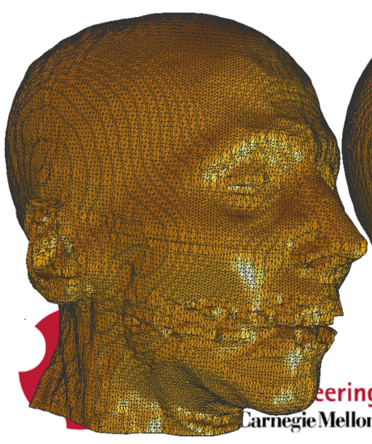


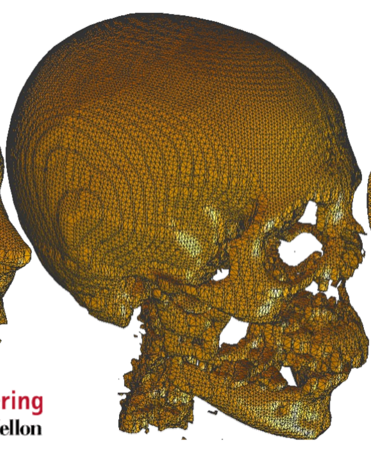


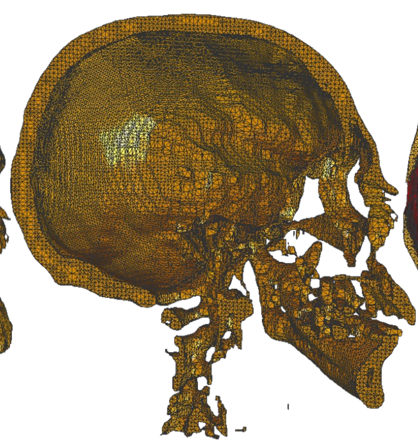


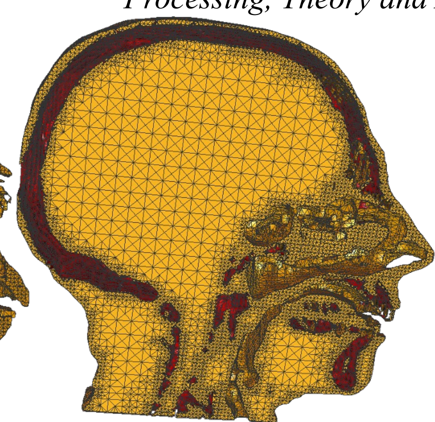


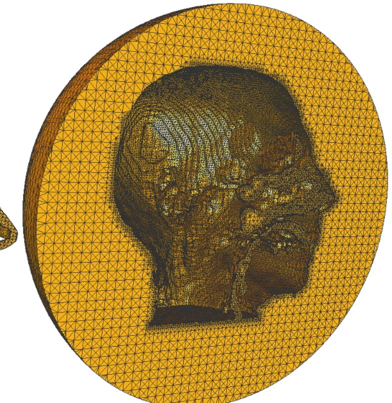
• C. Bajaj, G. Xu, J. Warren, *Geometric Modeling and Processing, Theory and Application 2002, 73-82.*







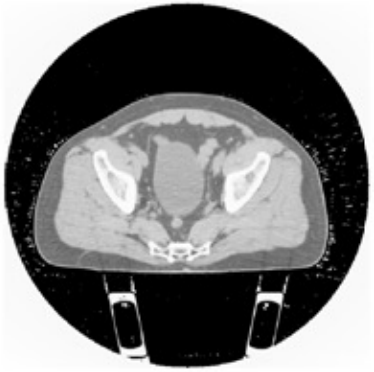


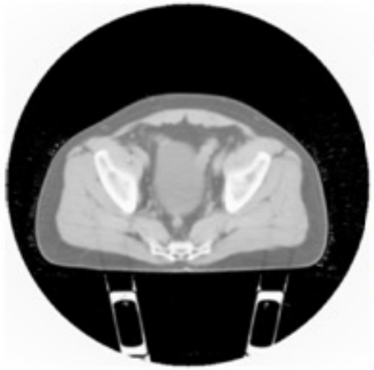


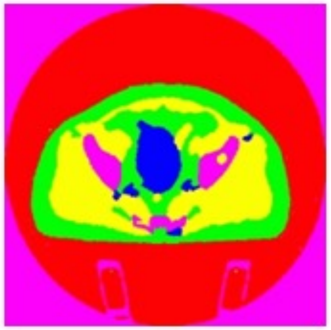
Application – 4D Radiation Treatment Planning

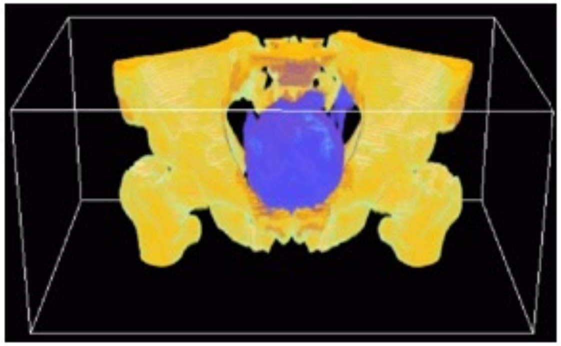
* To estimate radiation dosage and make treatment plan.

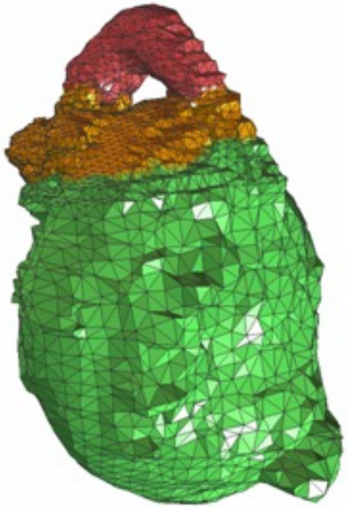
Approach: Filtering → Classification & Segmentation → Meshing → Quality Improvement

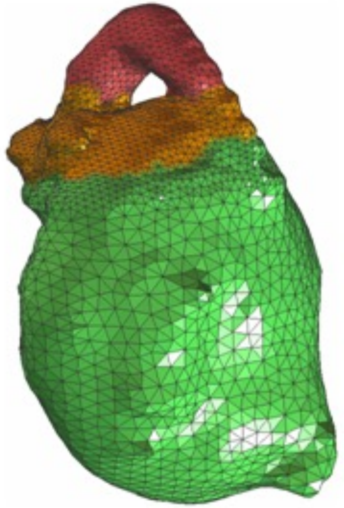

An Original Slice

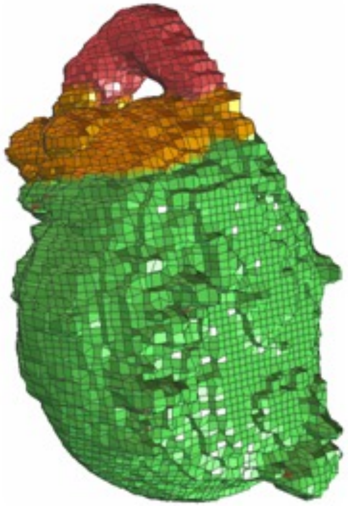

After Filtering

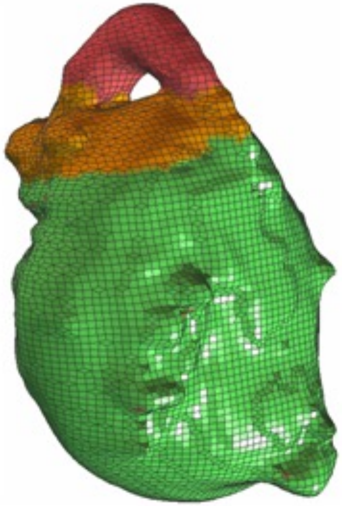

After Classification


Segmented Bladder (blue)


Original (4465 verts, 8962 tris)


After Quality Improvement


Original (9595 verts, 9644 quads)

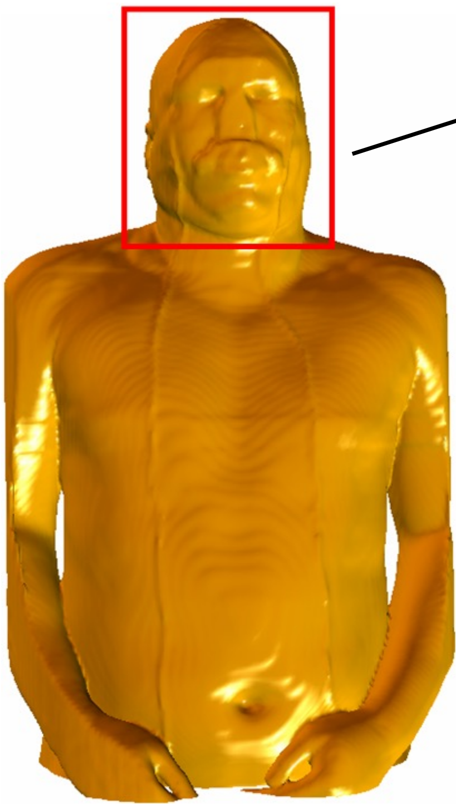

After Quality Improvement

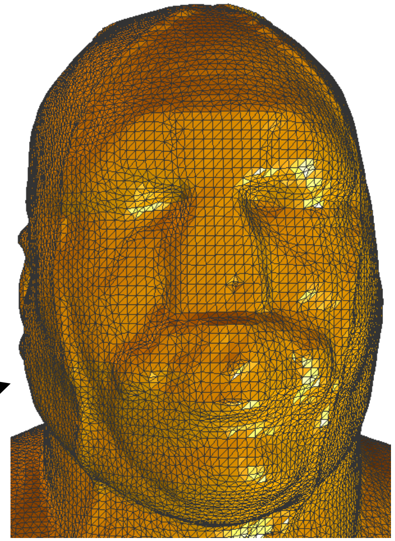
Collaborators: Dr. Radhe Mohan, Dr. Lei Dong
(MD Anderson Cancer Center)

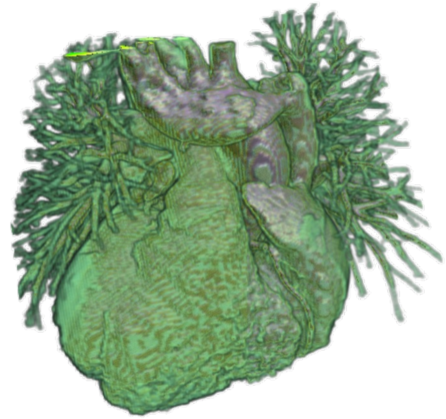
Mechanical Engineering
Carnegie Mellon

Application: Visual Human

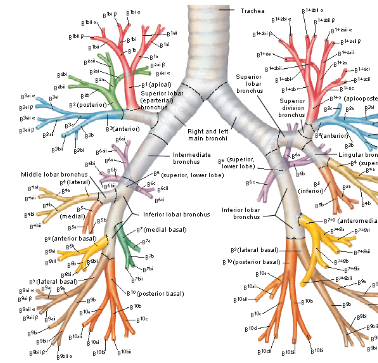
Collaborator: Dr. Gladish, MD-Anderson

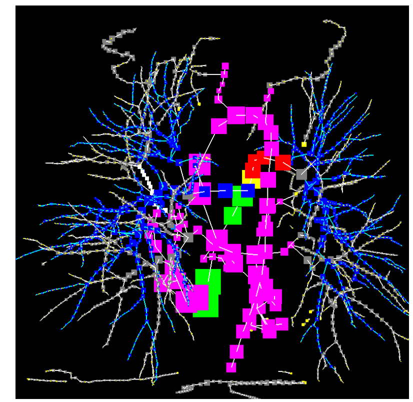


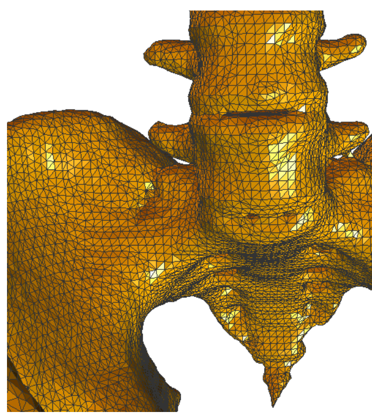


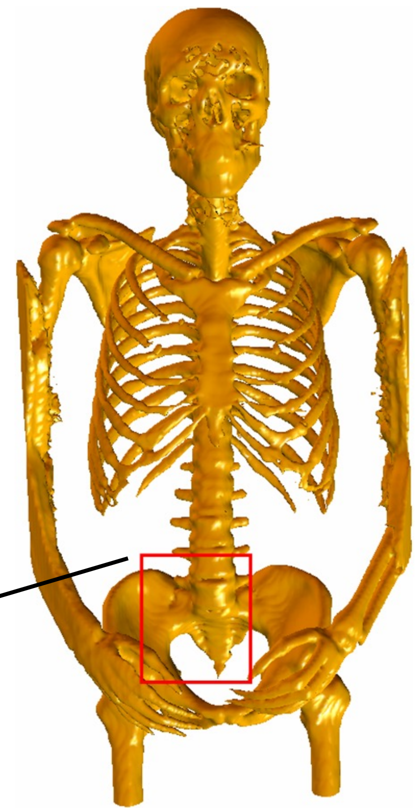


Pulmonary Embolism (PE) Detection









Mechanical Engineering
Carnegie Mellon

Application Examples in Computational Biology

- Implicit solvation modeling for biomolecules
- Diffusion rate calculation for mAChE
- Neuromuscular junction system
- Rice dwarf virus structure reconstruction

Implicit Solvation Models for Biomolecules

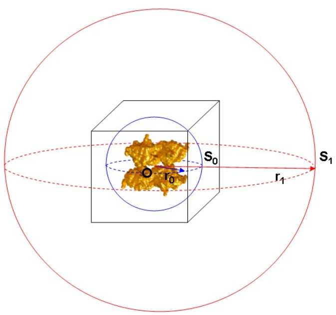
- Gaussian kernel function $G(x) = \sum_{i=1}^{N} e^{B_i\left(\frac{\|x-x_i\|^2}{r_i^2}-1\right)}$ $\longrightarrow$ $G(x, C) = \sum_{i=1}^{N} e^{C(\|x-x_i\|^2 - r_i^2)}$ where $C = B_i/r_i^2$

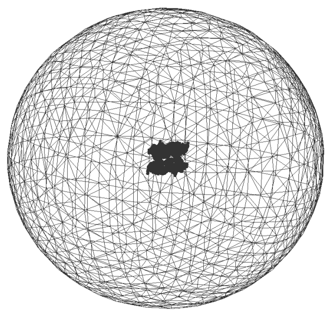
  where (x_i, r_i) are the center and radius of the ith atom in the biomolecule, and $B_i < 0$ is called 'blobbiness'

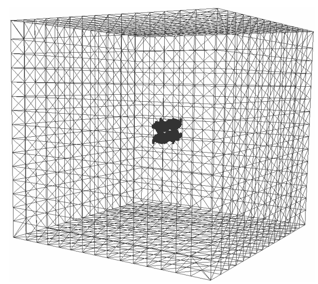
- There are four steps in our biomolecular meshing process:
  - Data acquisition – construct electron density map from atomic data (PDB/PQR)
  - Primary mesh extraction
  - Mesh extension – generate the exterior mesh
  - Quality improvement – use geometric flows

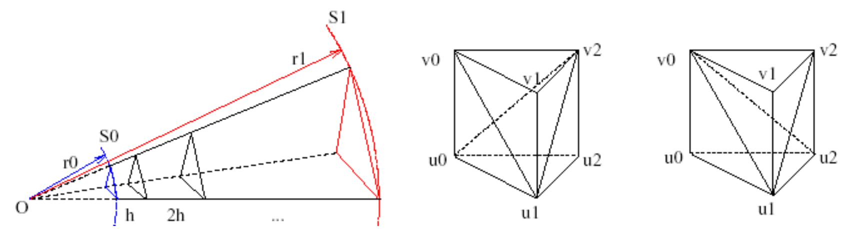
References:

- Y. Zhang, G. Xu, C. Bajaj. **Quality Meshing of Implicit Solvation Models of Biomolecular Structures**. *CAGD*, 23(6):510-530, 2006.

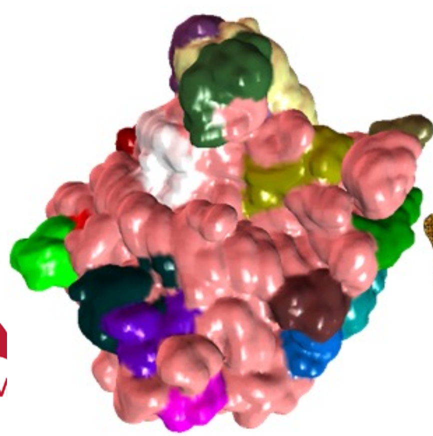


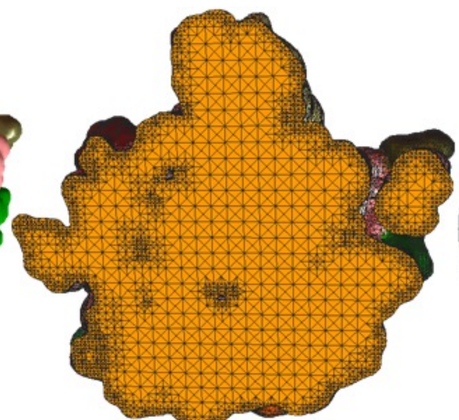


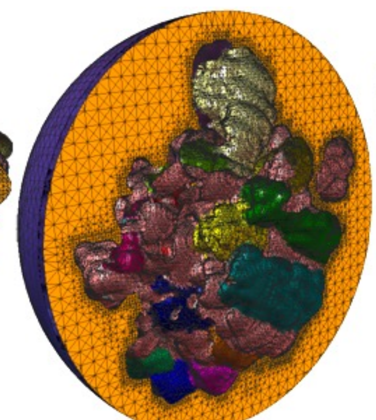


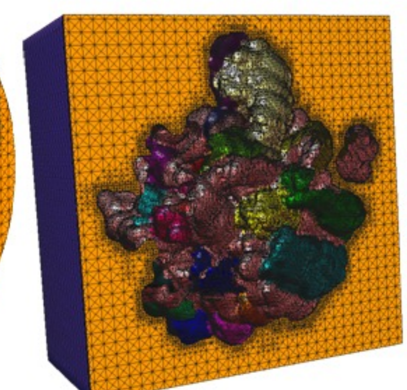


$$r_0 + h + 2h + \cdots + nh = r_1 \implies h = \frac{2(r_1 - r_0)}{n(n+1)}$$







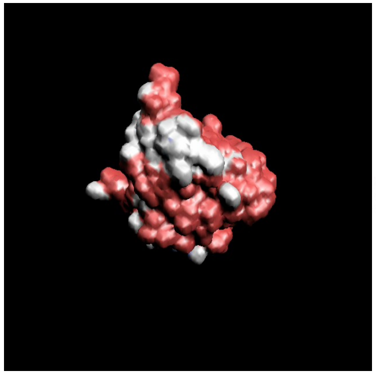


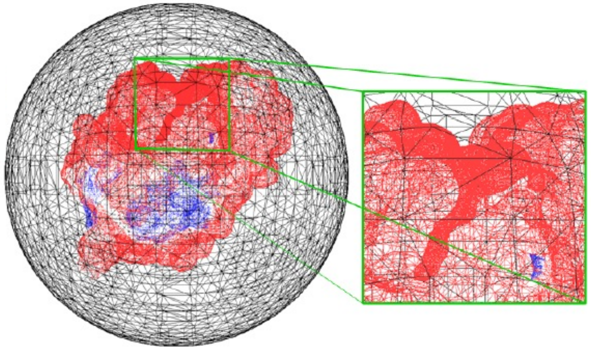
Collaborators:

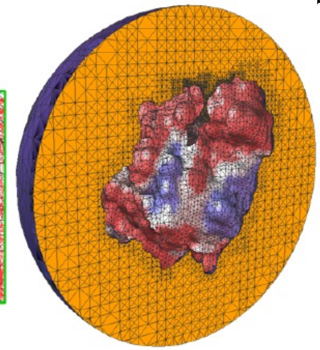
•Prof. Nathan A. Baker (WUSTL)

•Prof. J. Andrew McCammon (UCSD)

Diffusion Simulation of Biomolecules



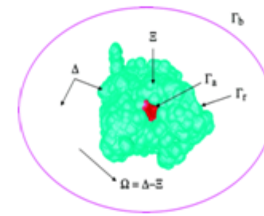




* Smoluchowski Equation:

$$\frac{\partial p(\vec{r},t)}{\partial t} = \nabla \cdot D(\vec{r})[\nabla p(\vec{r}) + \beta p(\vec{r}) \nabla U(\vec{r})] = 0$$

Or in flux operator J: $\nabla \cdot \vec{J}p(\vec{r}) = 0$ $\quad \vec{J}p(\vec{r}) = D(\vec{r})[\nabla p(\vec{r}) + \beta p(\vec{r}) \nabla U(\vec{r})]$



Schematic of problem domain [3]

- Δ -- whole domain
- Ξ -- biomolecule domain
- Ω -- free space in Δ
- Γ_a – reactive region
- Γ_r – reflective region
- Γ_b – boundary for Δ

(1) $p(\vec{r}) = p_{bulk}$ for $\vec{r} \in \Gamma_b$

(2) $p(\vec{r}) = 0$ (Dirichlet BC) for $\vec{r} \in \Gamma_a$

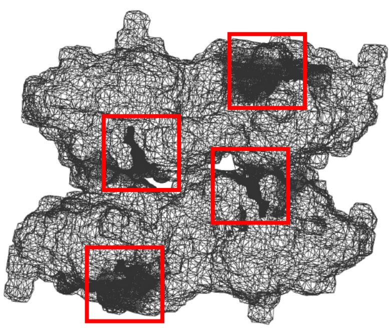
or $\vec{n} \cdot \vec{J}p(\vec{r}) = \alpha(\vec{r})\, p(\vec{r})$ (Robin BC)

(3) $\vec{n} \cdot \vec{J}p(\vec{r}) = 0$ for $x \in \Gamma_r$

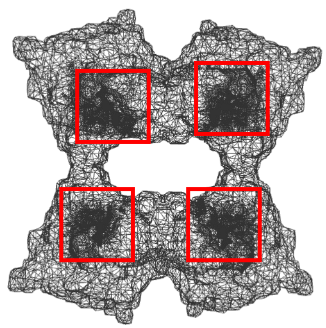
Diffusion rate:

$$k = \frac{\int_{\Gamma_a} \vec{n} \cdot \vec{J}p(\vec{r})\, dS}{p_{bulk}}$$

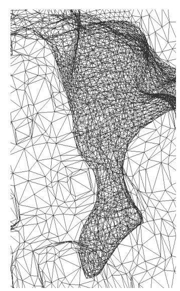
- Tetrameric mAChE



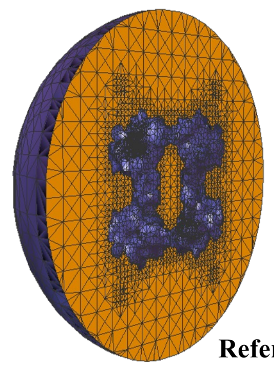
1C2O



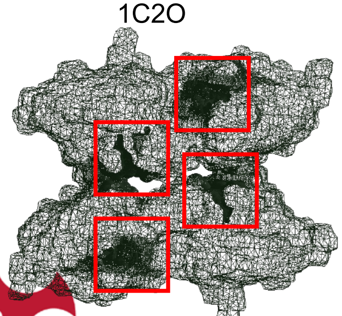
1C2B



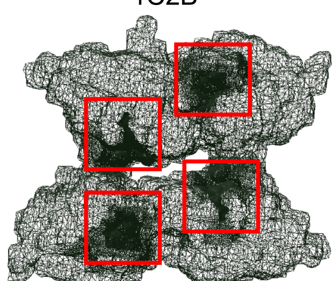
cavity



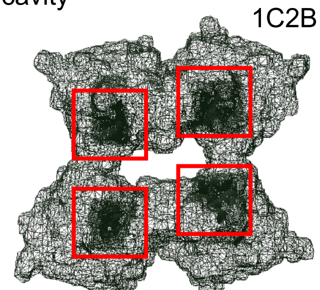
1C2B



Int4



Int3

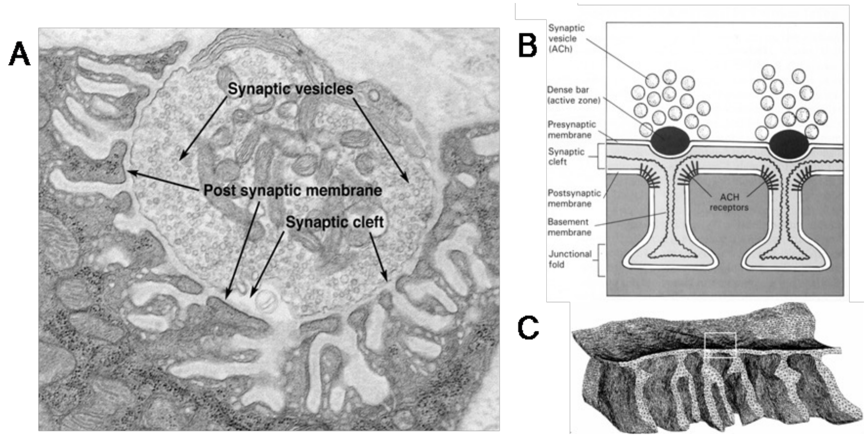


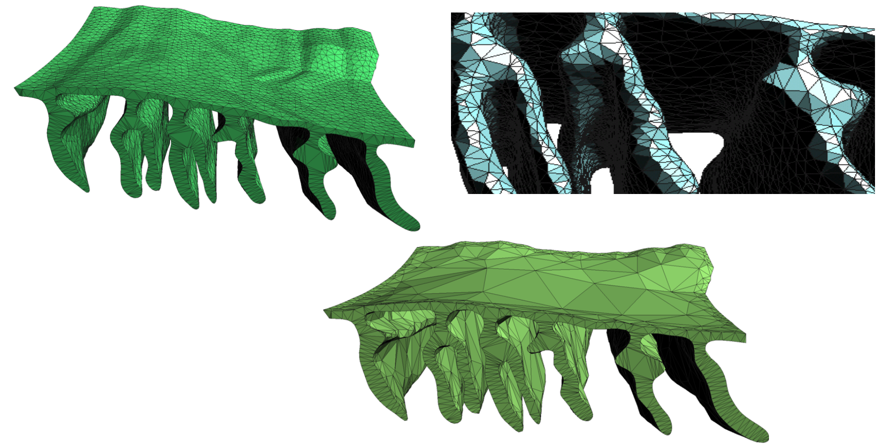
Int2

References:

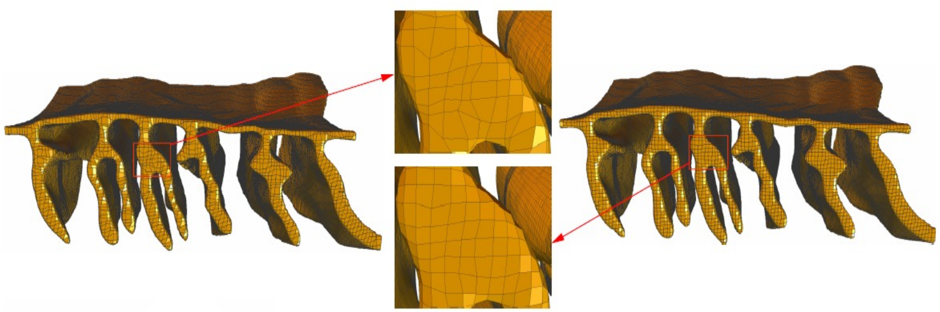
1. D. Zhang, J. Suen, Y. Zhang, Y. Song, Z. Radic, P. Taylor, M. J. Holst, C. Bajaj, N. A. Baker, J. A. McCammon. **Tetrameric Mouse Acetylcholinesterase: Continuum Diffusion Rate Calculations by Solving the Steady-State Smoluchowski Equation Using Finite Element Methods**. *Biophysical J.* 88(3):1659-1665, 2005.
2. Y. Song, Y. Zhang, C. Bajaj, N. Baker. **Continuum Diffusion Reaction Rate Calculations of Wild Type and Mutant Mouse Acetylcholinesterase: Adaptive Finite Element Analysis**. *Biophysical J.* 87(3):1558-1566, 2004.
3. Y. Song, Y. Zhang, T. Shen, C. Bajaj, J. McCammon, N. Baker. **Finite Element Solution of the Steady-state Smoluchowski Equation for Rate Constant Calculations**. *Biophysical J.*, 86(4):2017-2029, 2004.

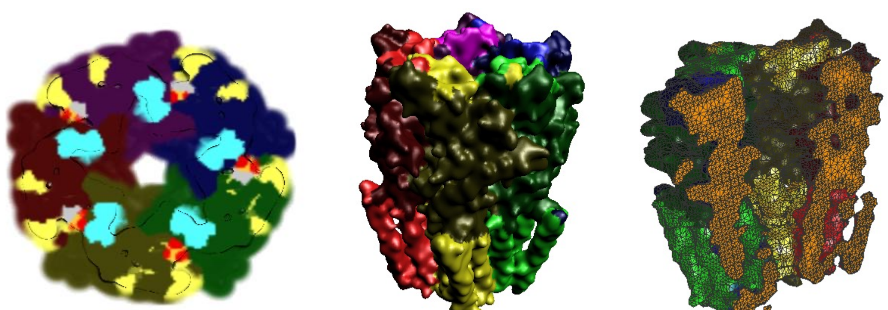
Application: Neuro-Muscular Junction at Molecular and Cellular Scales

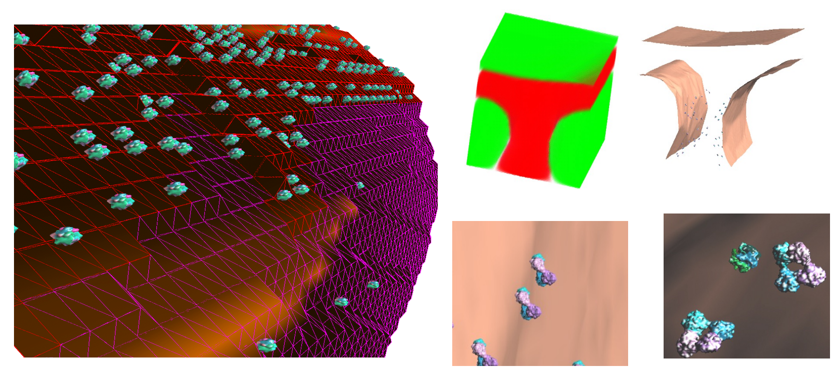




Decimated Tet Meshes





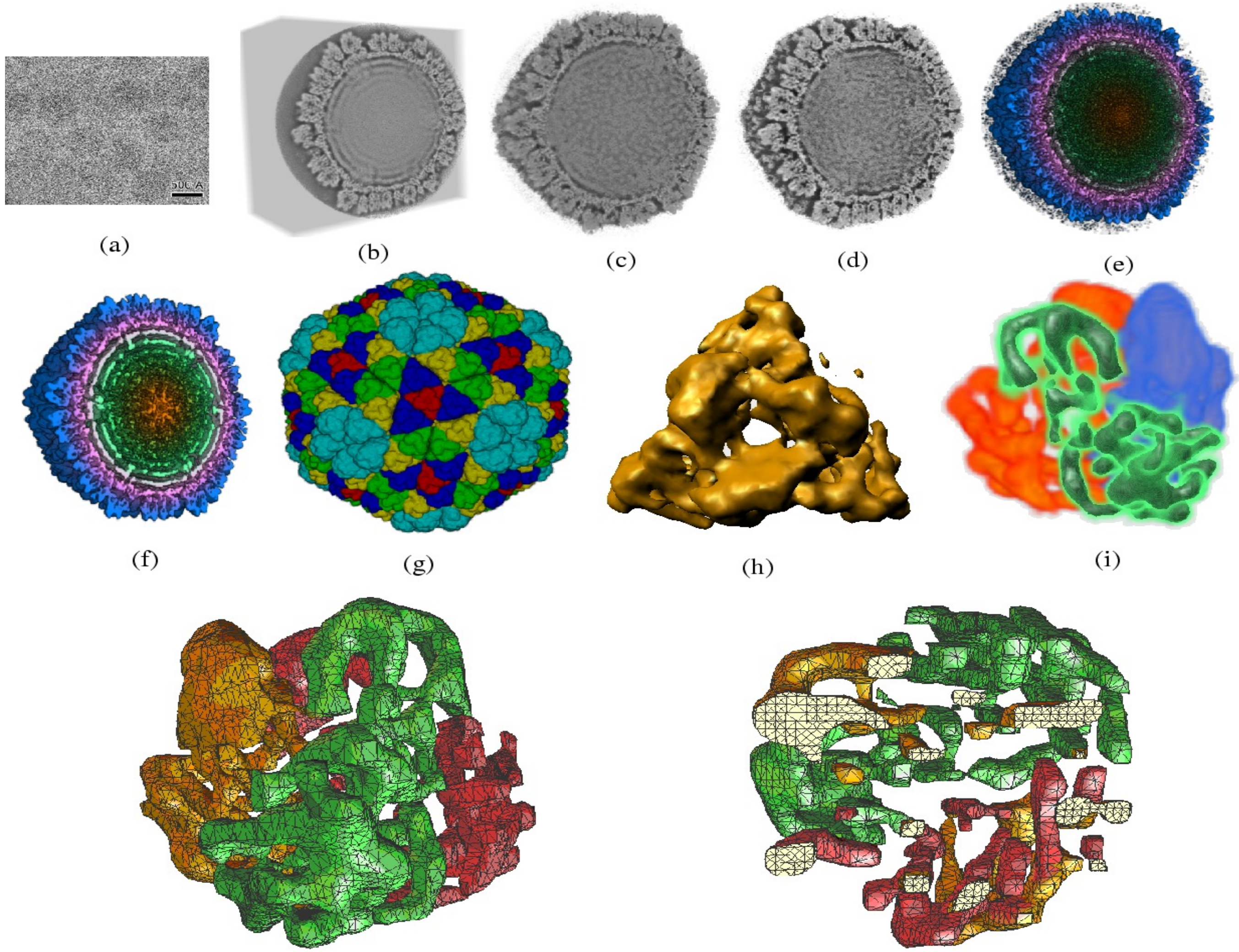


Collaborators: Nathan Baker (Wash. U), Andy McCammon, Mike Holst, Mark Ellisman (UCSD)

Rice Dwarf Virus Structure Reconstruction

Collaborators:
- Dr. Wah Chiu (NCMI, Baylor College of Medicine)
- Dr. A. Sali (UCSF)

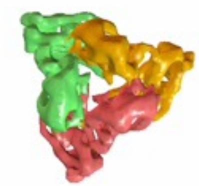
Approach: Contrast Enhancement → Filtering → Segmentation → Meshing



(a) (b) (c) (d) (e)

(f) (g) (h) (i)

(j) (k)

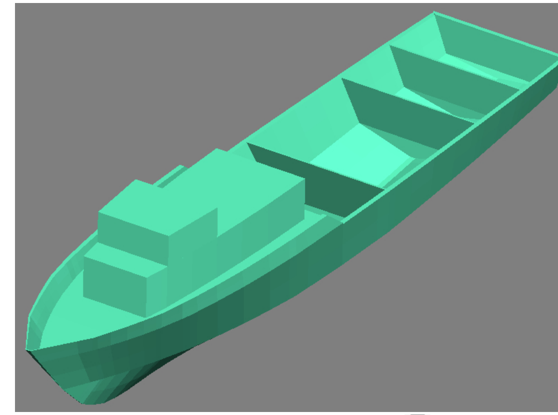


Application Examples in Other Engineering Fields

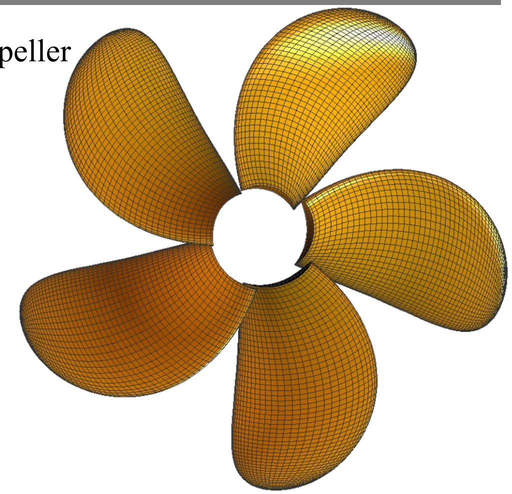
Applications:

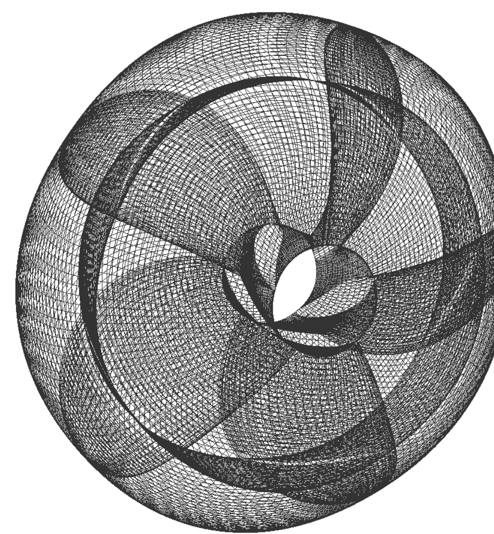
- Boat & Propeller – Navy projects
- Trabecular Bone Mechanics - Osteoporosis
- Nano-Composite Material
- Oil Reservoir Modeling (Petroleum Eng.)
- Bubble Simulation (Emulsion)

Boat

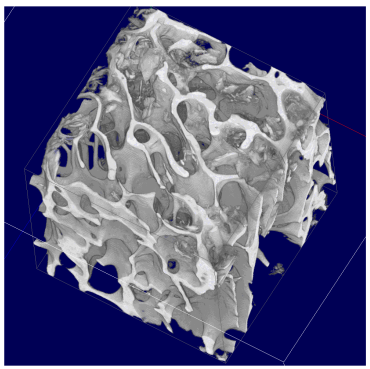


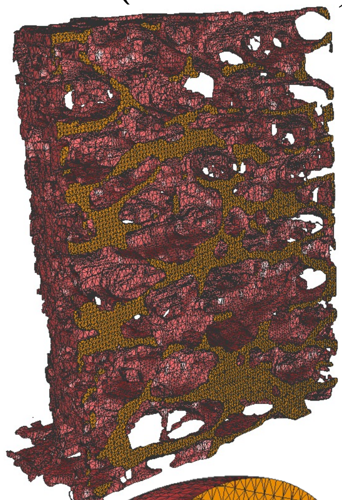
Propeller

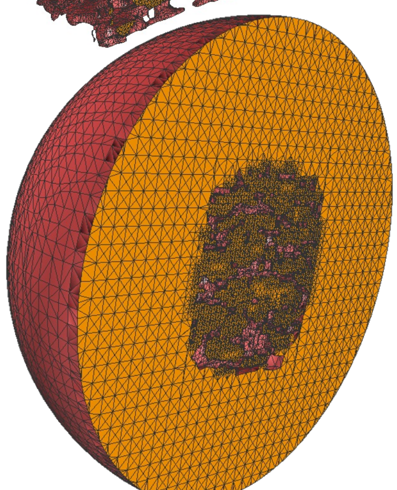




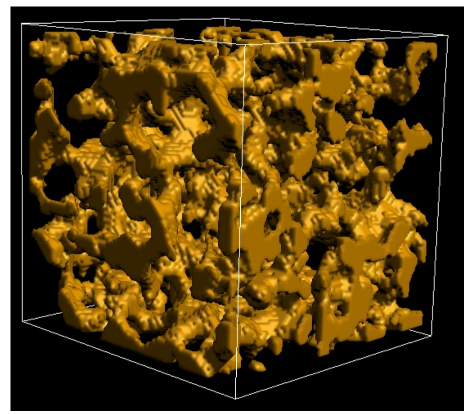
Bone

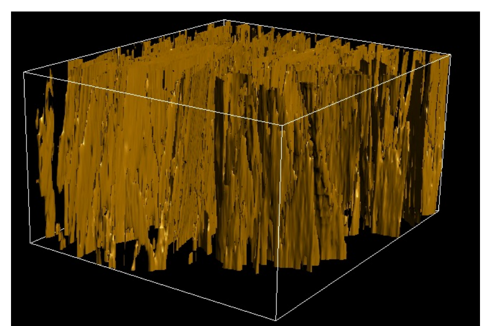






Foam





Nano-Composite Material

Summary: Five Topics

- Computational modeling is a relatively new interdisciplinary research field, and it has a lot of applications. All the required knowledge can be organized into the following five basic topics:

    1. Scanning/Imaging Techniques
    2. Image Processing
    3. Geometry Processing
        - Computational Geometry
        - Mesh Generation
        - Visualization
    4. Computational Mechanics (Finite Element Method)
    5. Applications