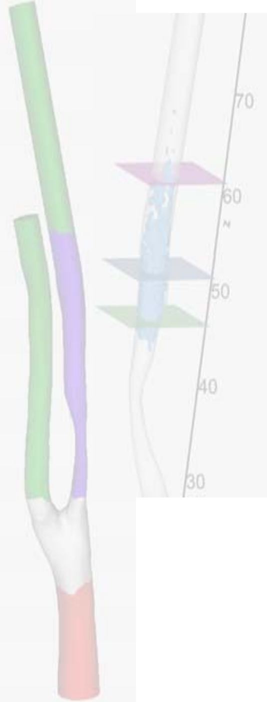
High Performance Scientific Computing - A New Physician Assistant (?)

Leopold Grinberg

Division of Applied Mathematics,

Brown University

CRUNCH group:



George Em Karniadakis – PI

Bruce Caswell – co-advisor (non-Newtonian and viscoelastic liquids)

Leopold Grinberg – Senior Research Associate

Hyoungsu Baek - PhD candidate (arterial flow modeling, aneurysms, fluid-structure interaction)

Yue Yu - PhD candidate (arterial flow modeling)

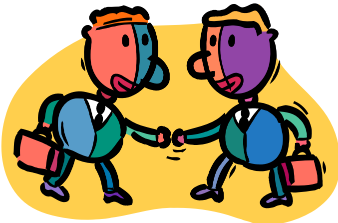
Huan Lei - PhD candidate (DPD, Red Blood Cells)

Wenxiao Pan - PhD candidate (DPD, rheology)

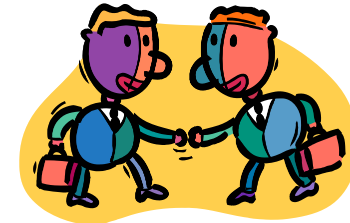
Kelsi Hirai - Undergraduate Student (1D fow modeling)

Nabeel Gillani - Undergraduate Student (arterial geometry reconstruction)

(we have more PhD students who work on other projects)



Grid of collaboration



Imperial College London

NORTHERN ILLINOIS UNIVERSITY

Ben Gurion University

academic collaboration

CRUNCH GROUP

computation visualization

TeraGrid

PITTSBURGH SUPERCOMPUTING CENTER

Argonne NATIONAL LABORATORY

TACC

NICS

NCSA

NSF

interdisciplinary collaboration

Children's Hospital Boston

The Hospital for Children

Rhode Island Hospital

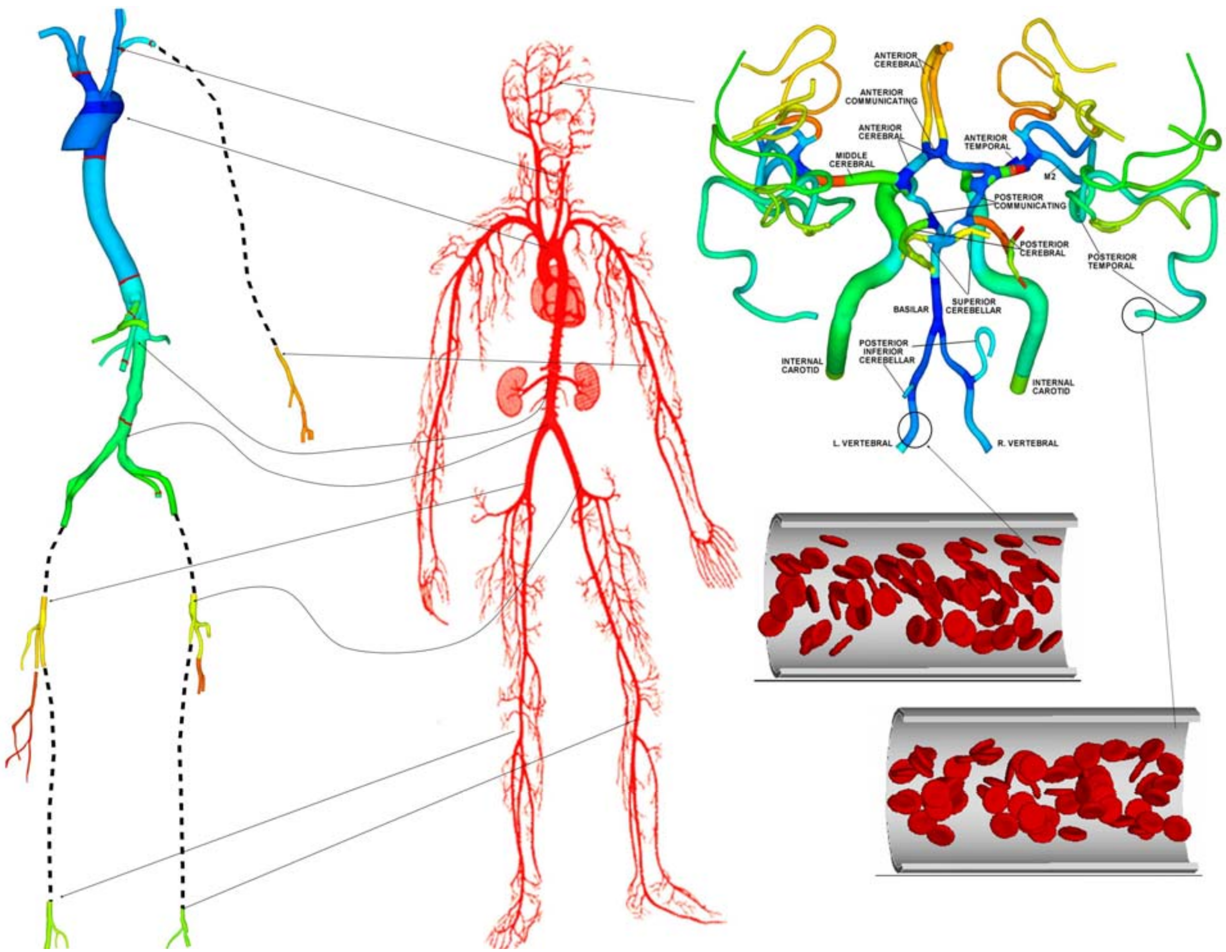
Team Members

Brown University:	**CRUNCH GROUP**
Imperial College, UK:	**S. J. Sherwin**
Ben-Gurion University, Israel:	**A. Yakhot**
Northern Illinois University:	**N.T. Karonis**
ANL:	**J. Insley, M. Papka**
Children's Hospital, MA:	**T. Anor, J. Madsen**
Rhode Island Hospital, RI:	**M. Jayaraman**
Hadassah Medical Center, Israel	

The **CRUNCH** group

A research group in the Division of Applied Mathematics. The thrust of its research is the development of numerical algorithms, visualization methods and parallel software for continuum and atomistic simulations in fluid mechanics and related applications.

Human Arterial-tree Simulations



Multi-scale simulations of the arterial flow will include Macro-, Meso- and Micro-vascular Networks (***MaN-MeN-MiN***)

Multi-physics simulations of the arterial flow will include: flow and structure interactions coupled simulations of vascular and neural systems,…

Grinberg *et al*. Clinical and Experimental Pharmacology and Physiology *36*(2), 2009

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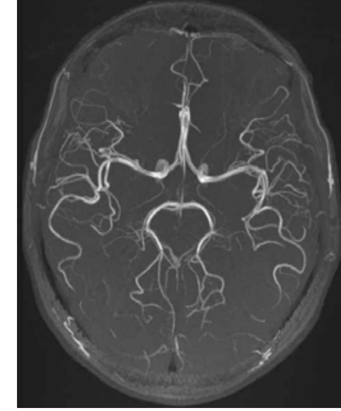
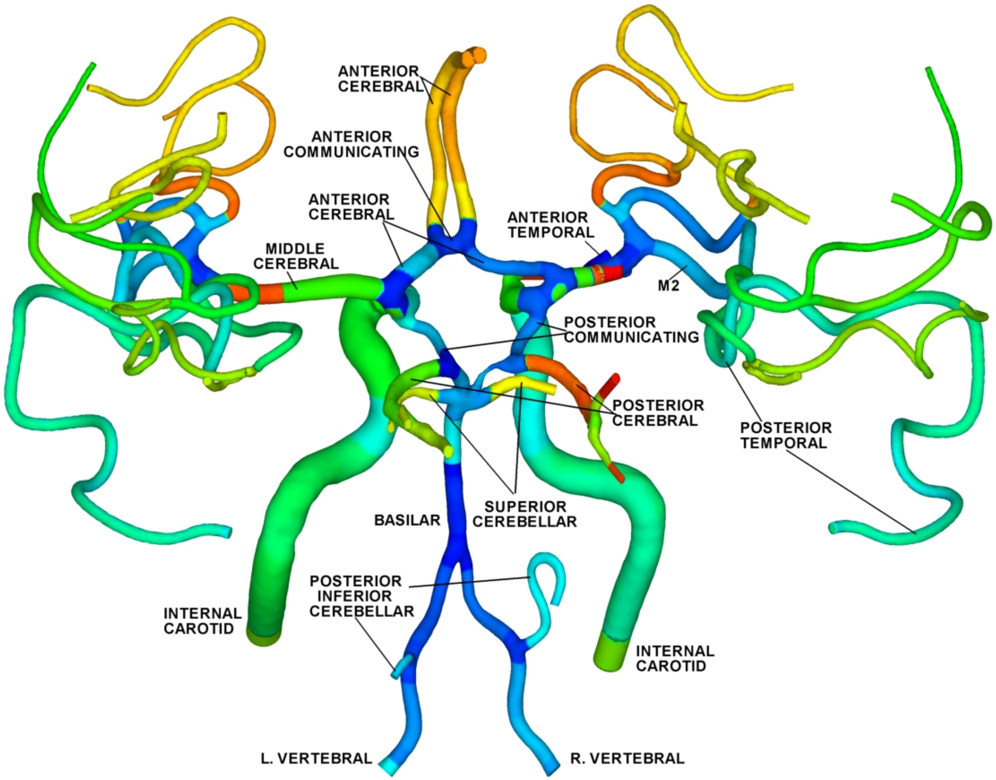
Arterial Flow Simulations: Multi-step Process



1



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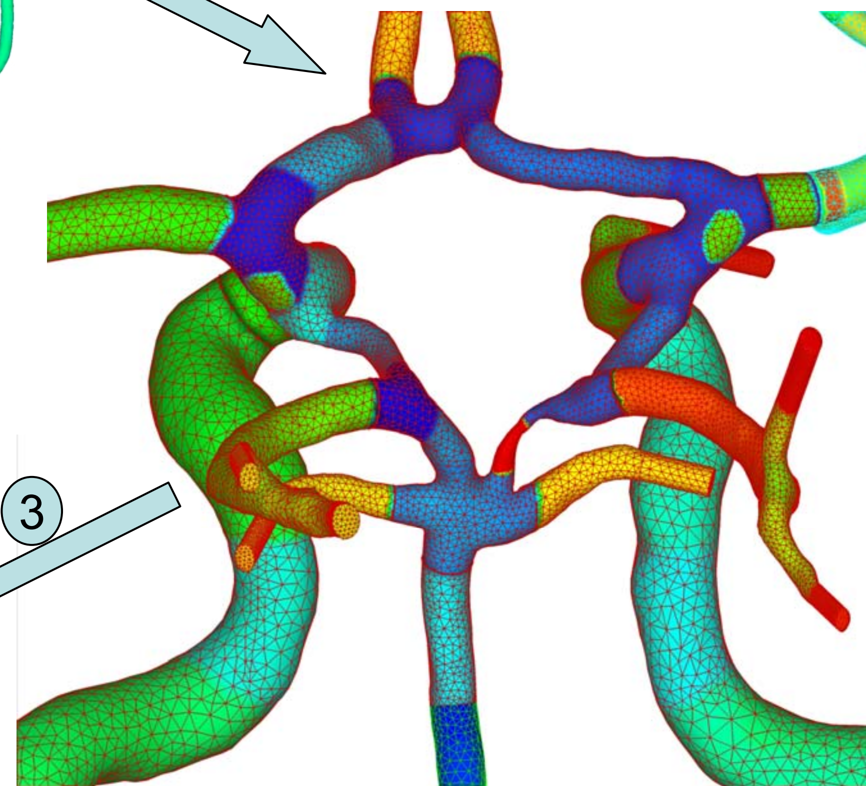


3

Simulation

4

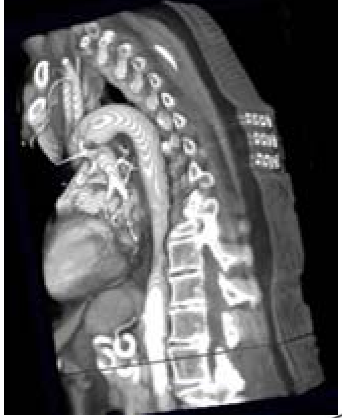
Data analysis

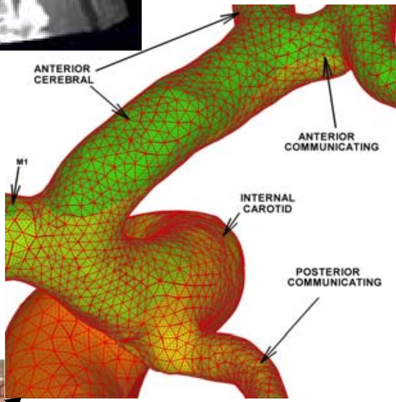
Challenges

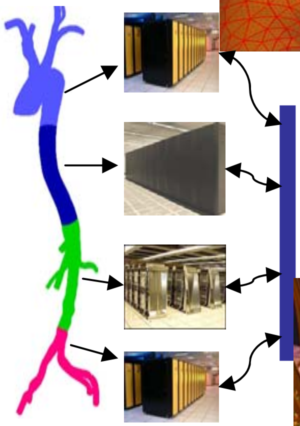
- Accurate reconstruction of arterial tree
- Numerical and parallel algorithms for solutions of PDEs with billions of unknowns
- Boundary conditions.

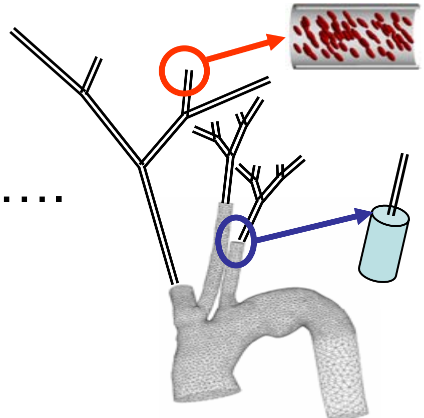
  Integration of in-vivo measurement into numerical simulation
- Data post-processing and analysis
- Validation and Verification
- Multi-scale modeling,

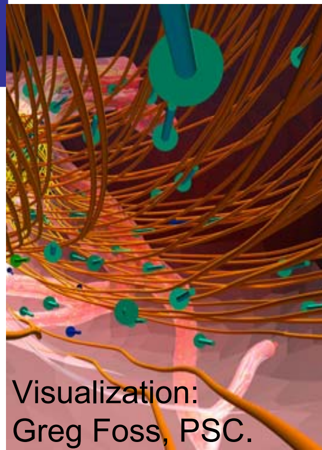
  interface boundary conditions ….










Visualization: Greg Foss, PSC.

Outline

- *Nektar*
- Boundary conditions
- High resolution 3D simulations
- 1D modeling of a flow in arterial networks
- Summary

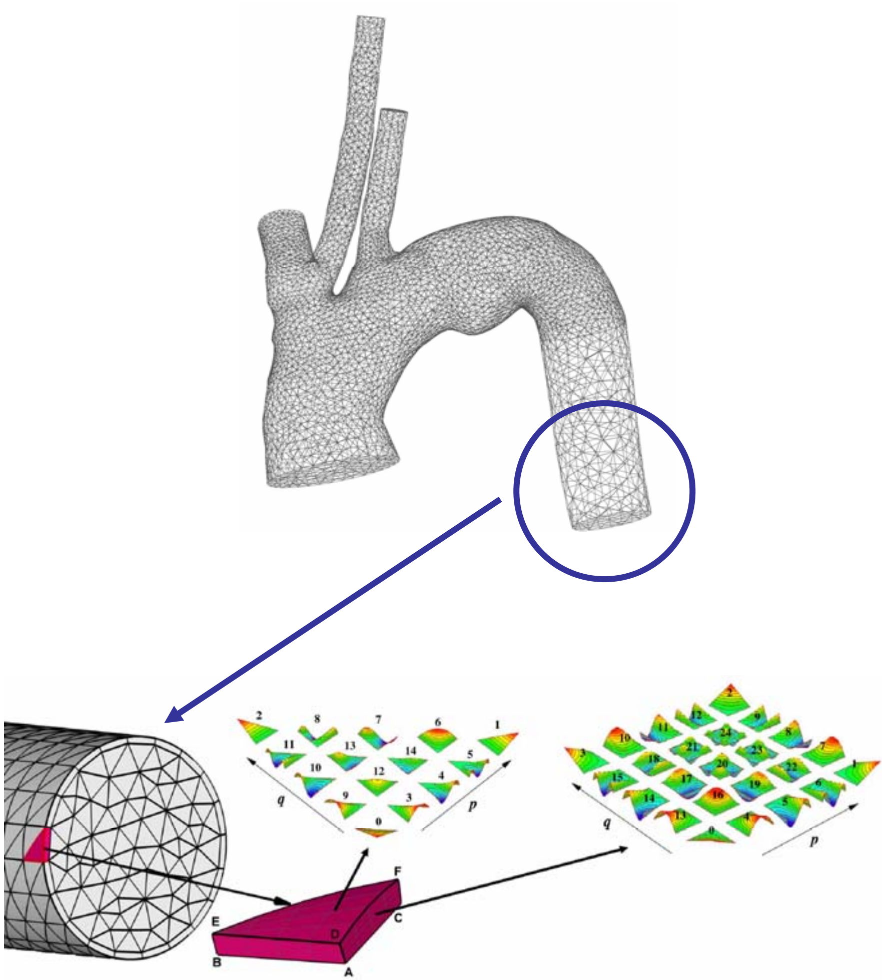
Flow Simulations: Software

- We employ the ***spectral/hp*** element code **NEKTAR*** developed in Brown University.

- The computational domain used by **NEKTAR** consists of structured or ***unstructured grids*** or a combination of both.

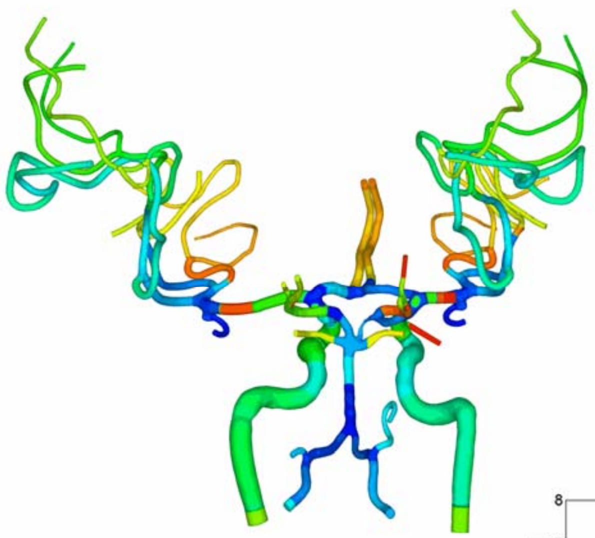
- A ***second-order splitting scheme*** was employed for temporal discretization***.

- Solution of extremely large problems is performed with ***two-level domain decomposition*** method, using ***hybrid*** continuous-discontinuous ***Galerkin projection***.



**Karniadakis & Sherwin, Spectral/hp Element Methods for CFD, 2005, 2nd edition, Oxford University Press*
***Grinberg & Karniadakis, Outflow Boundary Conditions for Arterial Networks with Multiple Outlets, ABME, 2008.*
****Karniadakis et al, High-order splitting methods for the incompressible Navier-Stokes equations, JCP, 1991.*

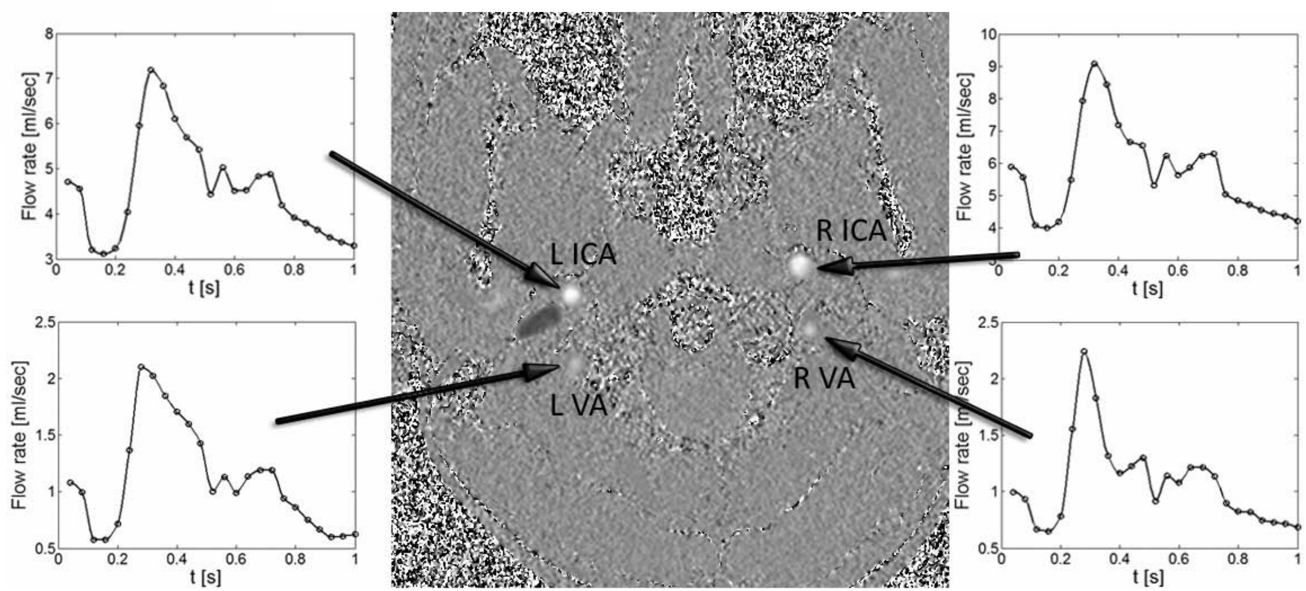
Flow Simulations in Arterial Networks: Boundary Conditions



Imposing patient-specific **outflow** boundary conditions is very challenging task

Inflow boundary conditions are obtained from PC-MRI measurements

(provided by T. Anor, Children's Hospital)



Outflow Boundary Conditions: Survey

- **Constant pressure boundary conditions**: reasonable for steady flow simulations, computationally efficient.
- **Resistance boundary condition**: based on the assumption of a linear dependence between the pressure and flow rate at each outlet. In rigid domains may lead to numerical instabilities since flow rate fluctuations at all frequencies are transferred to pressure oscillations. Computational complexity - integral of velocity at each outlet must be computed at each time step.
- **Windkassel model boundary conditions (RCR)**: flow rate fluctuations at all frequencies are transferred to the pressure, several parameters at each outlet that must be adjusted. Same computational complexity as resistance B.C.
- **Impedance boundary conditions:** The method is based on approximating the arterial network as 1D tree-like structure, where the linearized flow equations can be solved analytically. Accurate, from computational standpoint very expensive.

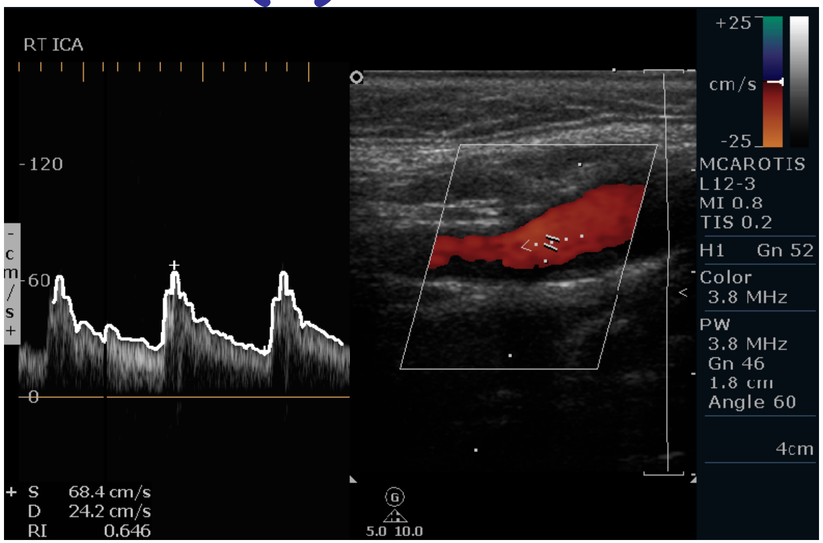
Our goal is to develop a new *scalable and efficient* type of pressure boundary condition applicable for *patient-specific* vascular flow simulations in domains with *multiple outlets*.

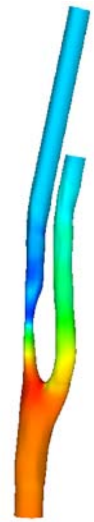
S. J. Sherwin et al., One-dimensional modeling of a vascular network in space-time variables, J. of Engineering Mathematics (2003).

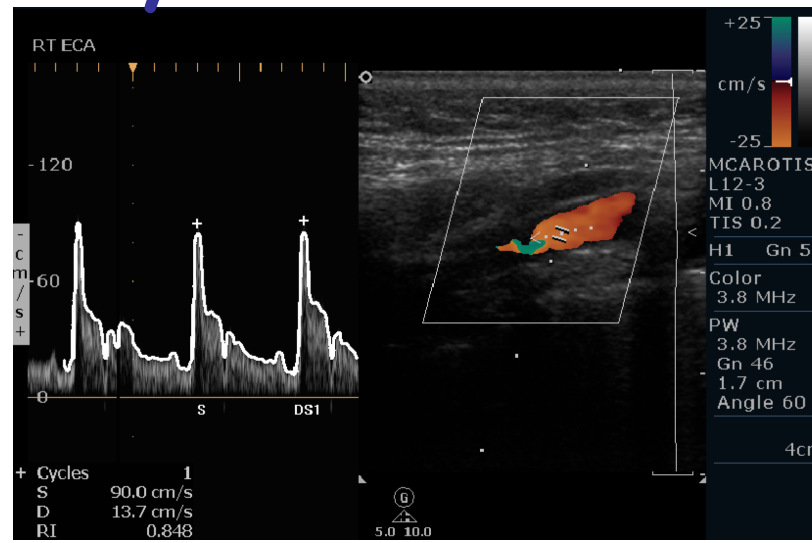
M. S. Olufsen, Structured tree outflow condition for blood flow in larger systemic arteries, Am. J. Physiol (1999).

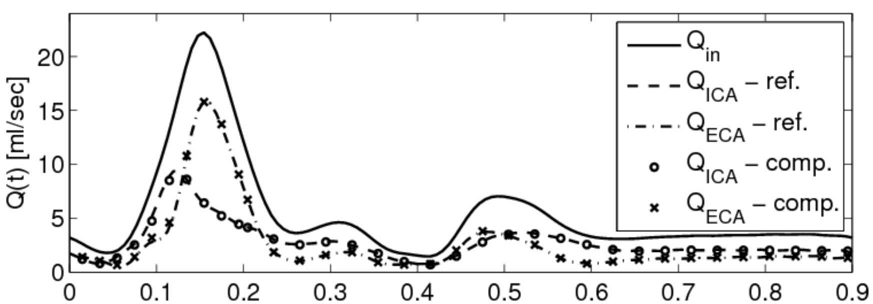
I. E. Vignon-Clementela et al., Outflow boundary conditions for three-dimensional finite element modeling of blood flow and pressure in arteries, Comp. Methods in Appl.Mech. and Eng. (2006)

Patient-specific Arterial Flow Simulations:
R(t)C Outflow Boundary Conditions



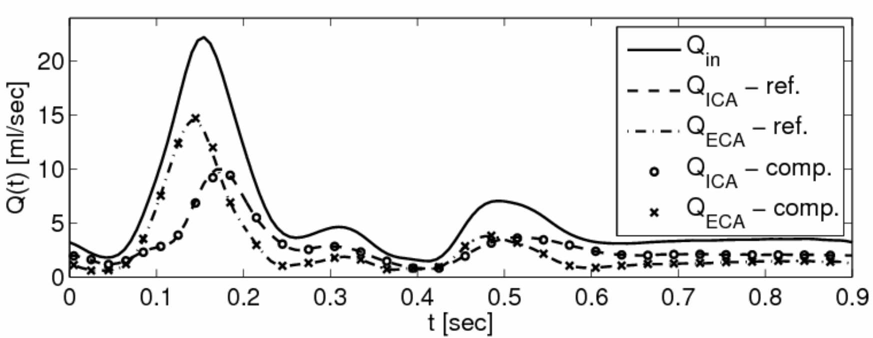






$$P_j + R_j C_j \frac{dP_j}{dt} = R_j Q_j$$

$$\frac{Q_j(t)}{Q_i(t)} = \frac{R_i(t)}{R_j(t)} + \varepsilon$$



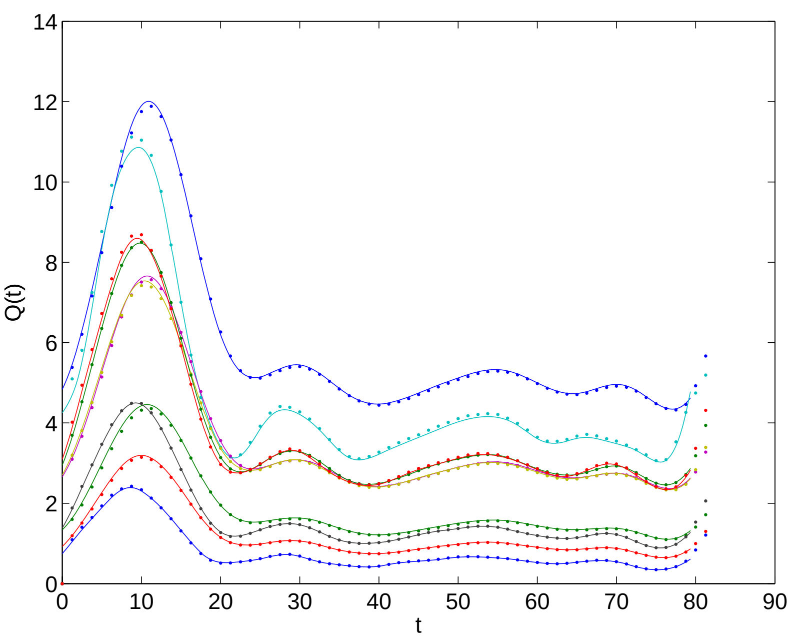
1. Define $f(t) = Q_1(t)/Q_2(t)$
2. Set $R_1=100$;
3. Compute $R_2(t) = R_1 f(t)$;

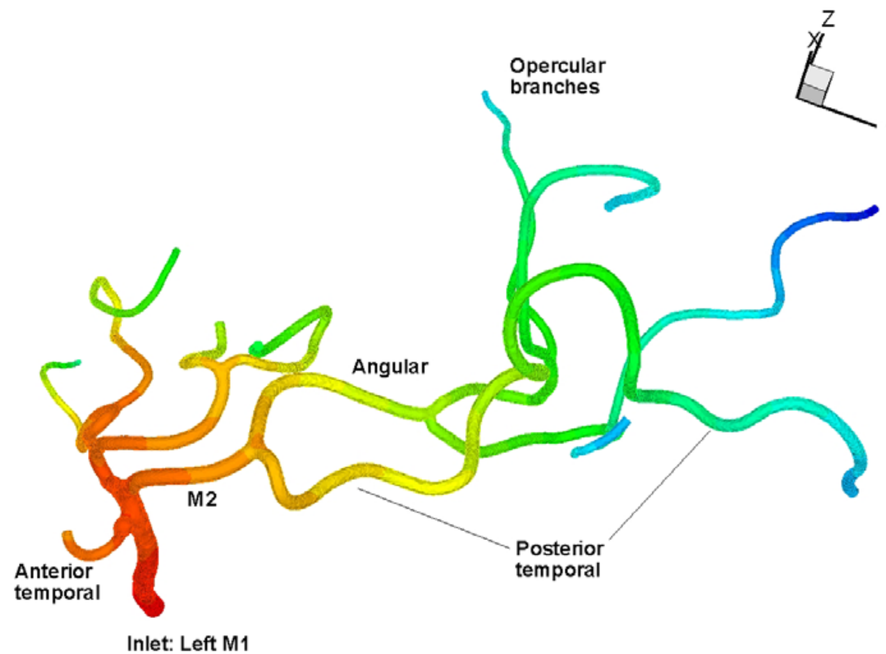
* L. Grinberg and G. E. Karniadakis, "Outflow Boundary Conditions for Arterial Networks with Multiple Outlets", *Annals of Biomed. Eng. 36(9), 2008.*

Simulation of Unsteady Flow in 20 Cranial Arteries with Impedance and R(t)C Boundary Conditions

The R(t)C boundary condition can be applied for arterial networks with an arbitrary number of segments, since

$$R_1Q_1 \cong R_2Q_2 \cong R_3Q_3 \cong R_jQ_j$$





solid line – reference solution (obtained in simulation with impedance boundary condition)
dots – simulation with R(t)C boundary condition

Boundary Conditions: Summary

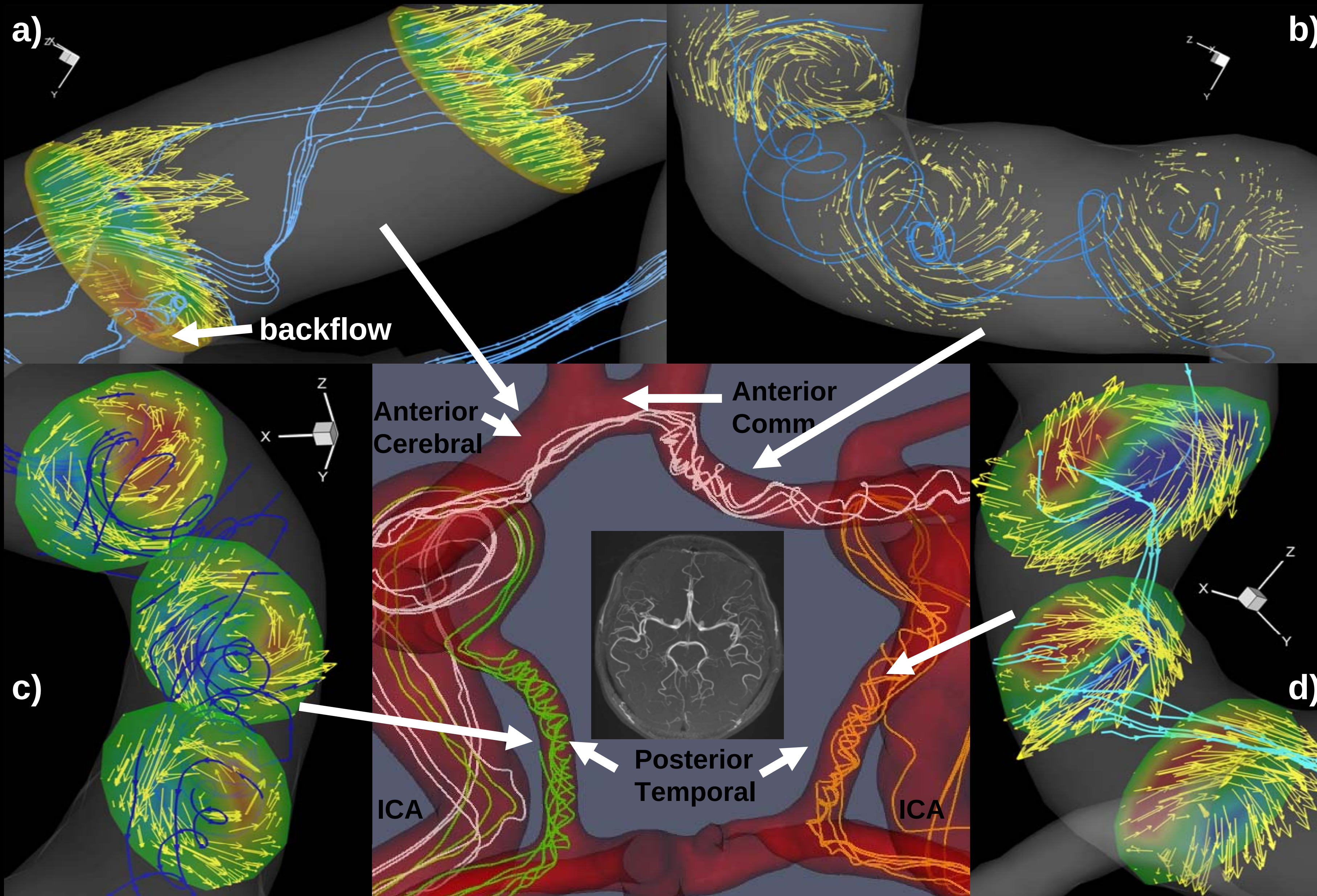
- Numerical simulations are performed in truncated domains, hence boundary conditions (B.C.) are essential.

- B.C. are used either to model or to impose the patient specific conditions.

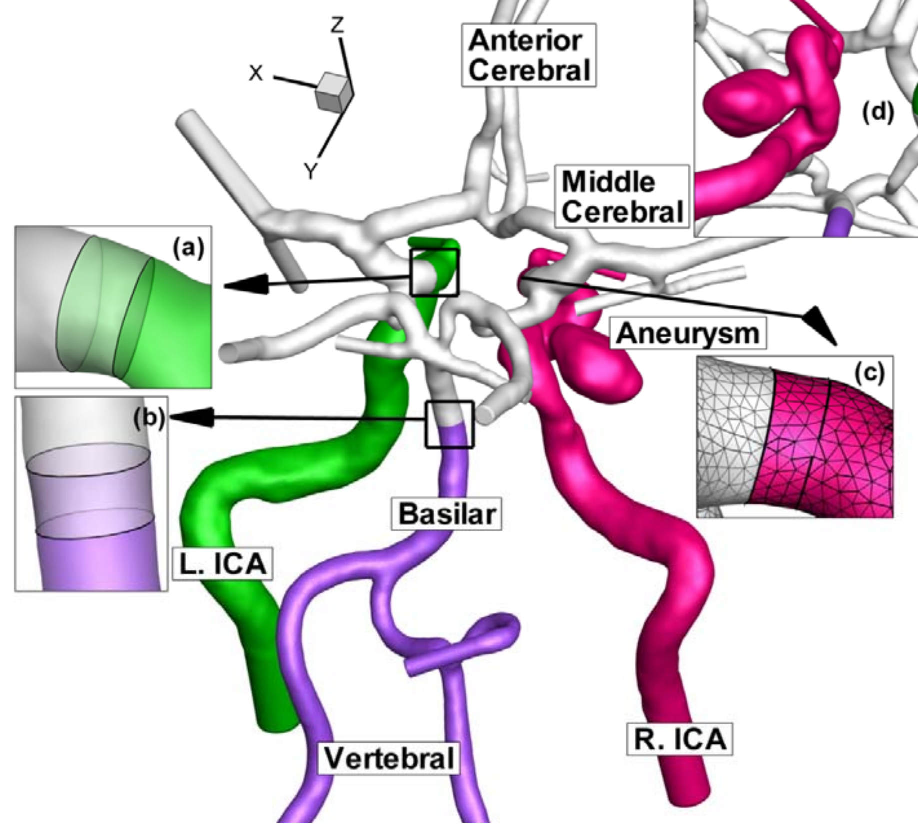
- R(t)C model allows seamless integration of clinically measured data into numerical simulation.

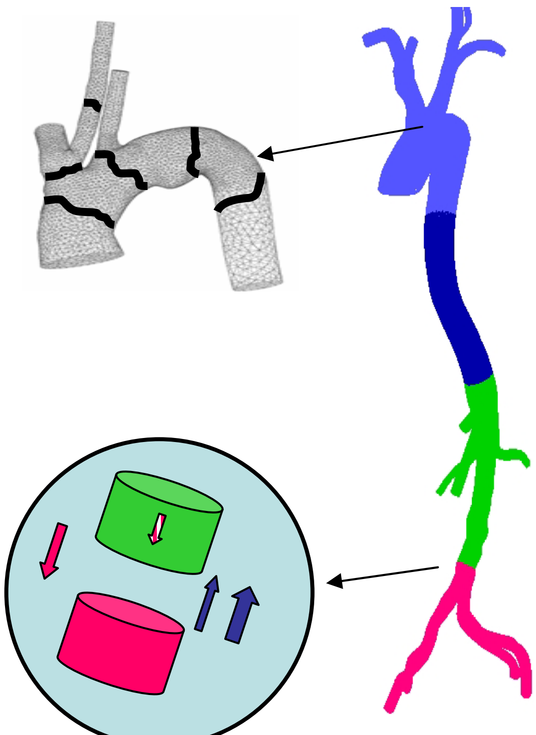
- It is crucial to have a *complete* data for the boundary conditions at both inlets and outlets. Such data should include at least the flow wave forms and correct phase shifts between the waveforms measured at different arteries.

High Resolution 3D Unsteady Flow Simulations in Arterial Networks



Multi-Domain Decomposition: for High Resolution 3D Flow Simulations in Arterial Networks





Ranger – 0.5PFLOPS computer at TACC

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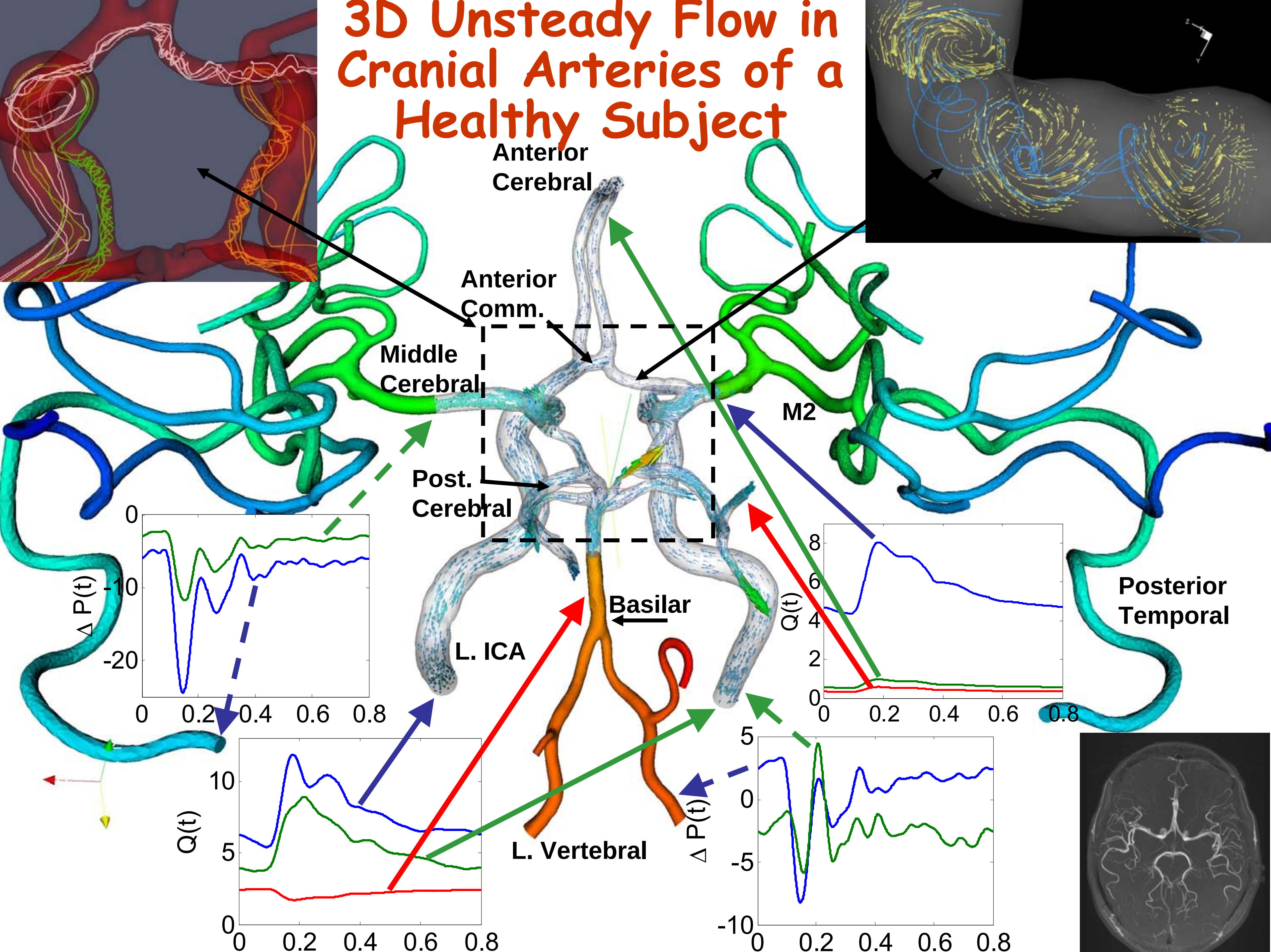
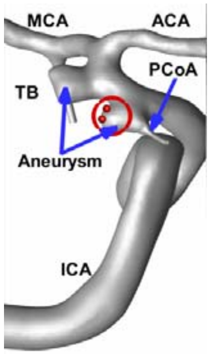
3D Unsteady Flow in Cranial Arteries of a Healthy Subject

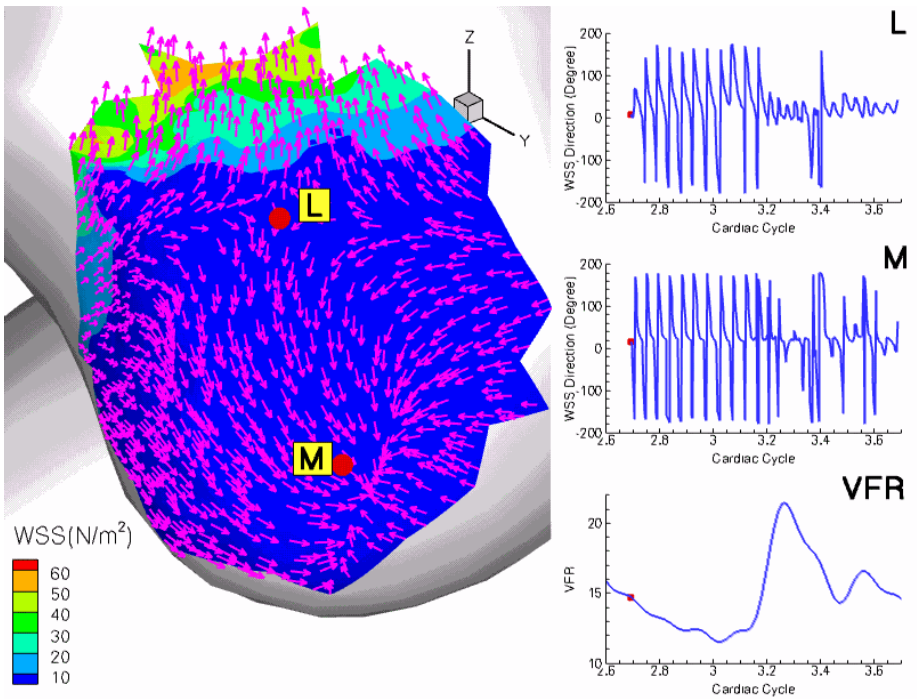


3D Unsteady Flow Simulations in the Intracranial Arterial Network: Wall Shear Stress

Patient-specific simulation of a flow in CoW. Arrows – normalized WSS; colors – pressure. Simulation has been performed on Ranger (TACC).

The stagnation points (lines) move around during the cardiac cycle. Due to this migration, WSS vectors rotate on the wall. (Courtesy of Hyoungsu Baek, Brown University).





FSI – Aneurysm in the ICA

(courtesy of H. Baek, Brown University)

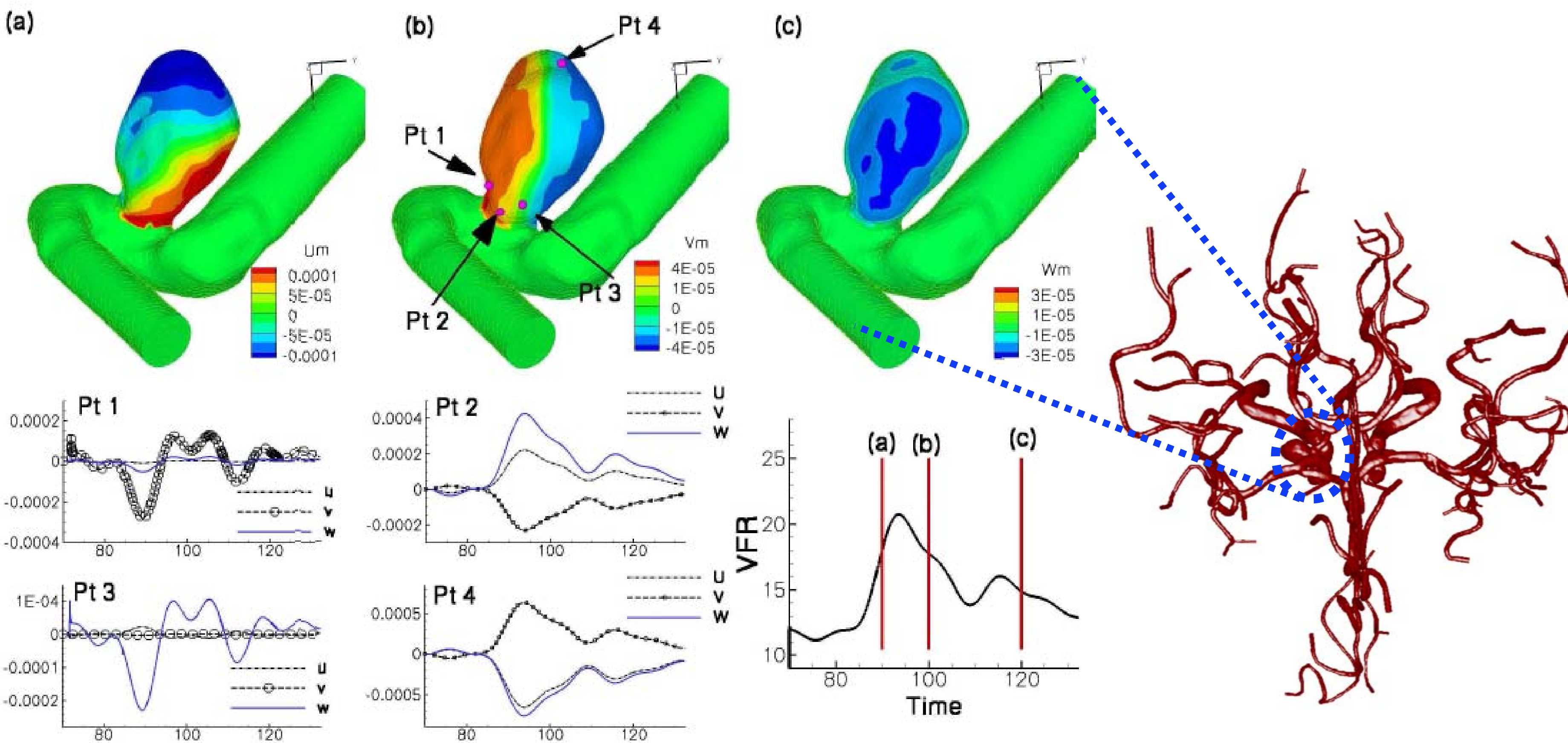
E 4.5 Mpa

ΔP 150 mmHg

Flow Rate 150 mL/min

Num of mode (4, 4)

Num of Elements (58929, 5628)



High Resolution 3D Unsteady Flow Simulations in Arterial Networks: Summary

• High resolution 3D simulations are feasible.

• Patient-specific simulations require patient-specific boundary conditions.

• More effort should be invested in the analysis of the results as well as careful planning of the new simulations.

• **There is a <u>need to develop a methodology for validation</u> of the mathematical models employed.**

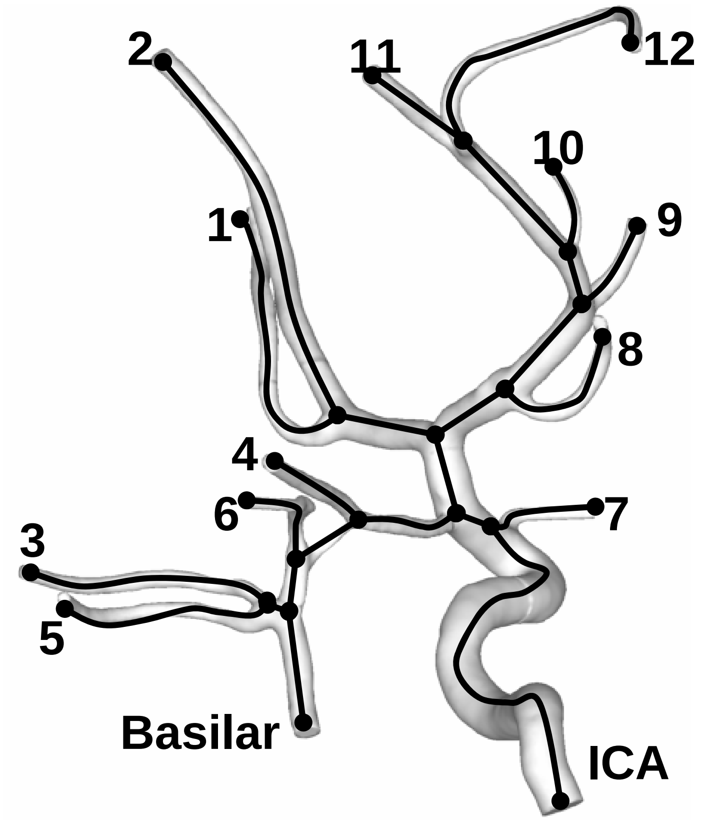
• **The success of the FSI modeling depends on accurate estimates on the <u>arterial wall properties</u>. It also requires modeling of the <u>interactions between the arteries and the surrounding tissues</u>.**

1D Flow Modeling

✓ Robust
✓ Easy to implement
✓ Good correlation with experimental results

- Does not model 3D effects

1D Flow Modeling

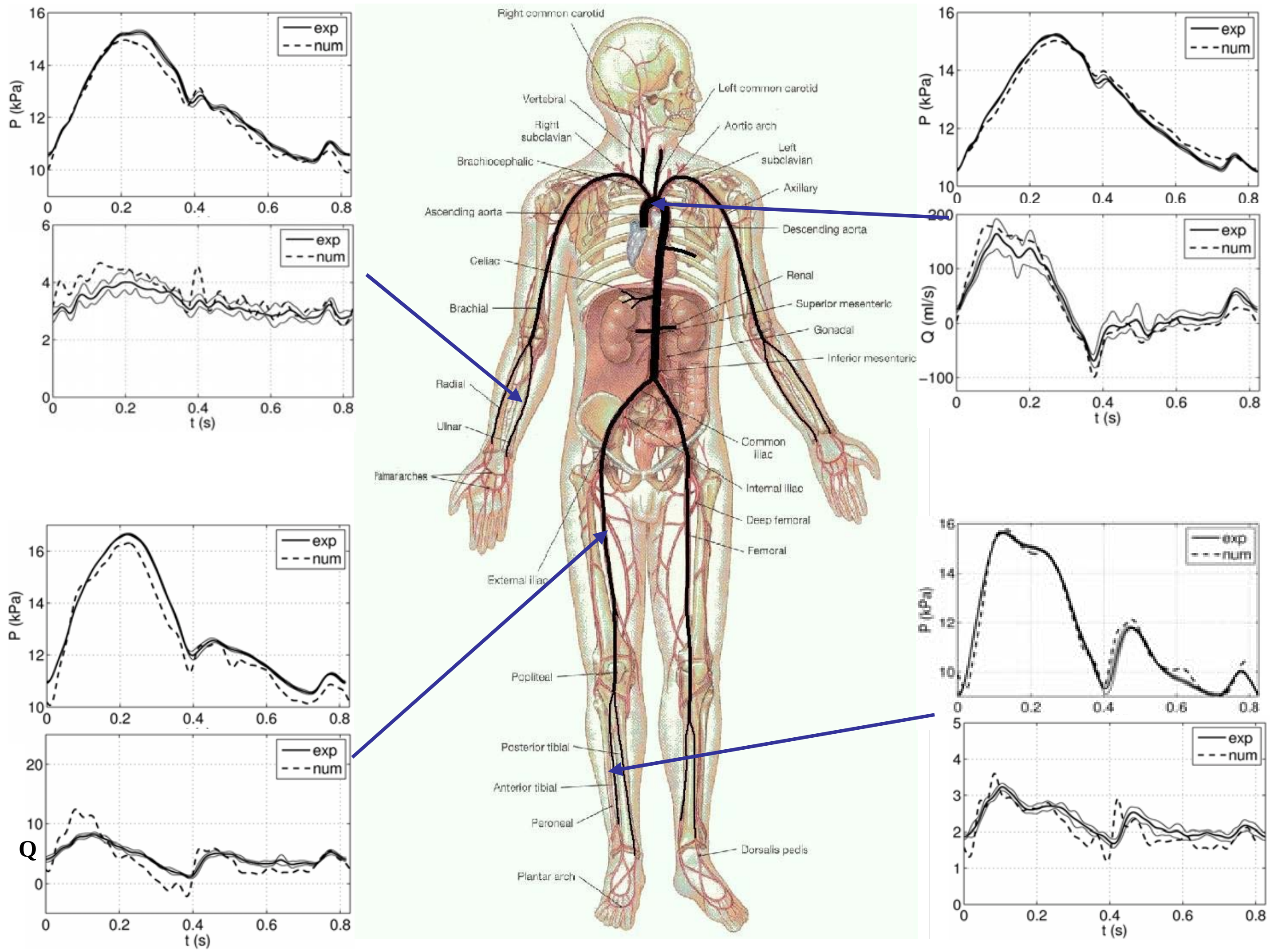


$$\frac{\partial A}{\partial t} + \frac{\partial AU}{\partial x} = 0$$

$$\frac{\partial U}{\partial t} + U\frac{\partial U}{\partial x} + \frac{1}{\rho}\frac{\partial P}{\partial x} = \frac{f}{\rho A}$$

$$p = \frac{\beta}{A_0}\left(\sqrt{A} - \sqrt{A_0}\right), \;\; \beta = \beta_0 \frac{\sqrt{\pi} hE}{1-\sigma^2}$$

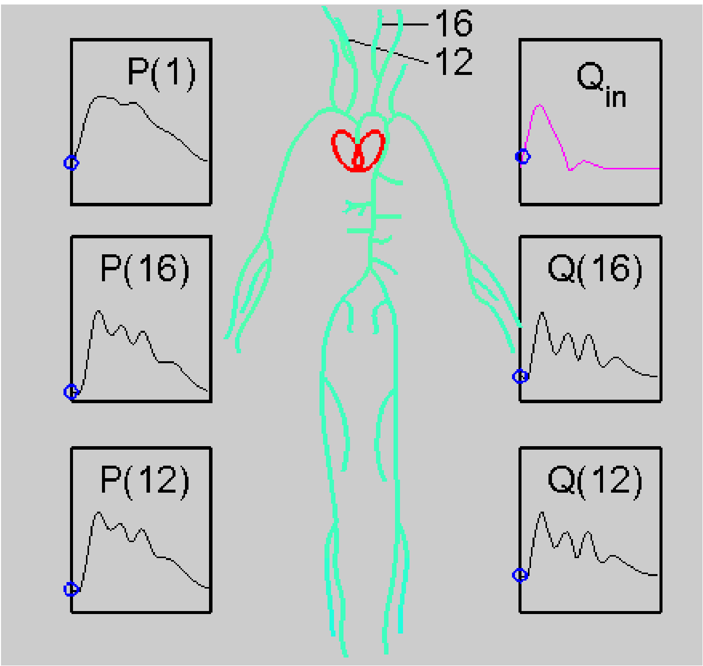
Experimental Validation: 1D Model
(Imperial College, UK and Ghent University, Belgium)



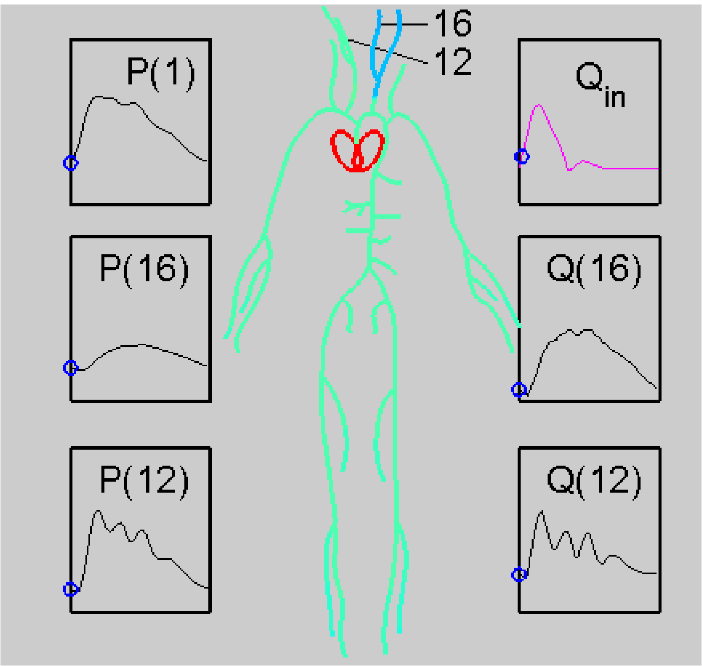
Three Generations of Bifurcations

1D Model for Arterial Tree

Pressure distribution in healthy arterial tree



Pressure distribution in arterial tree with stenosed artery

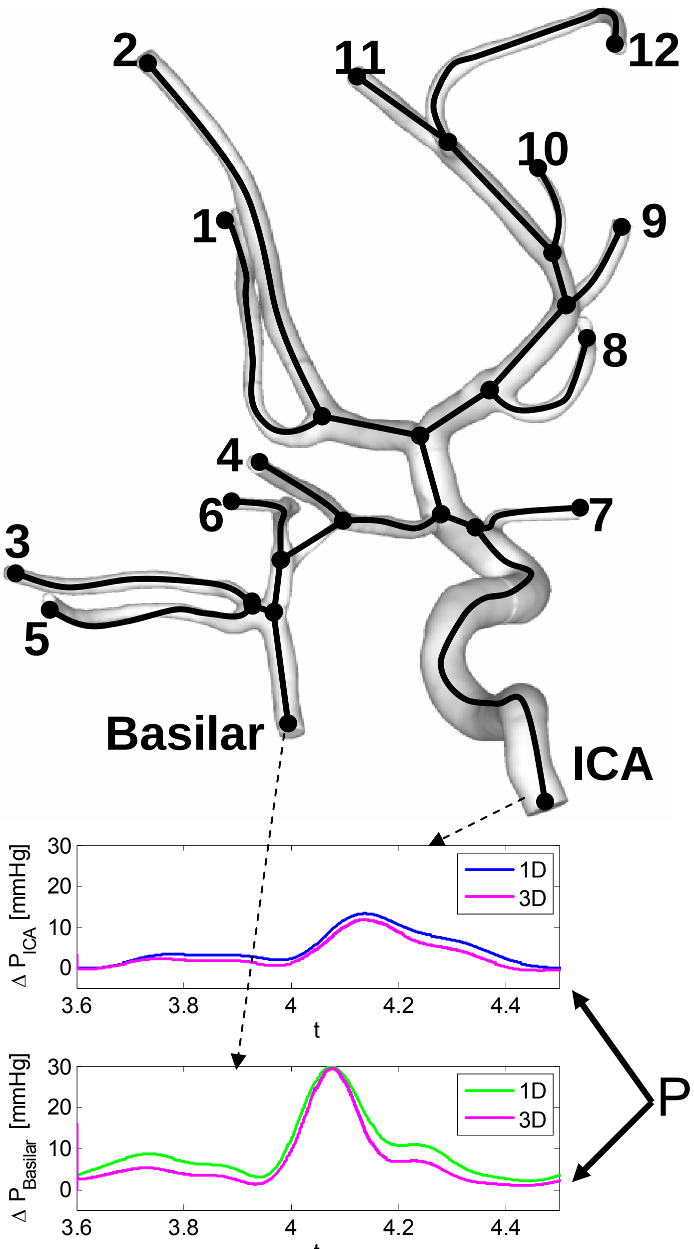


Q_{in}, P(1) – imposed flow rate and computed pressure at the inlet of aorta

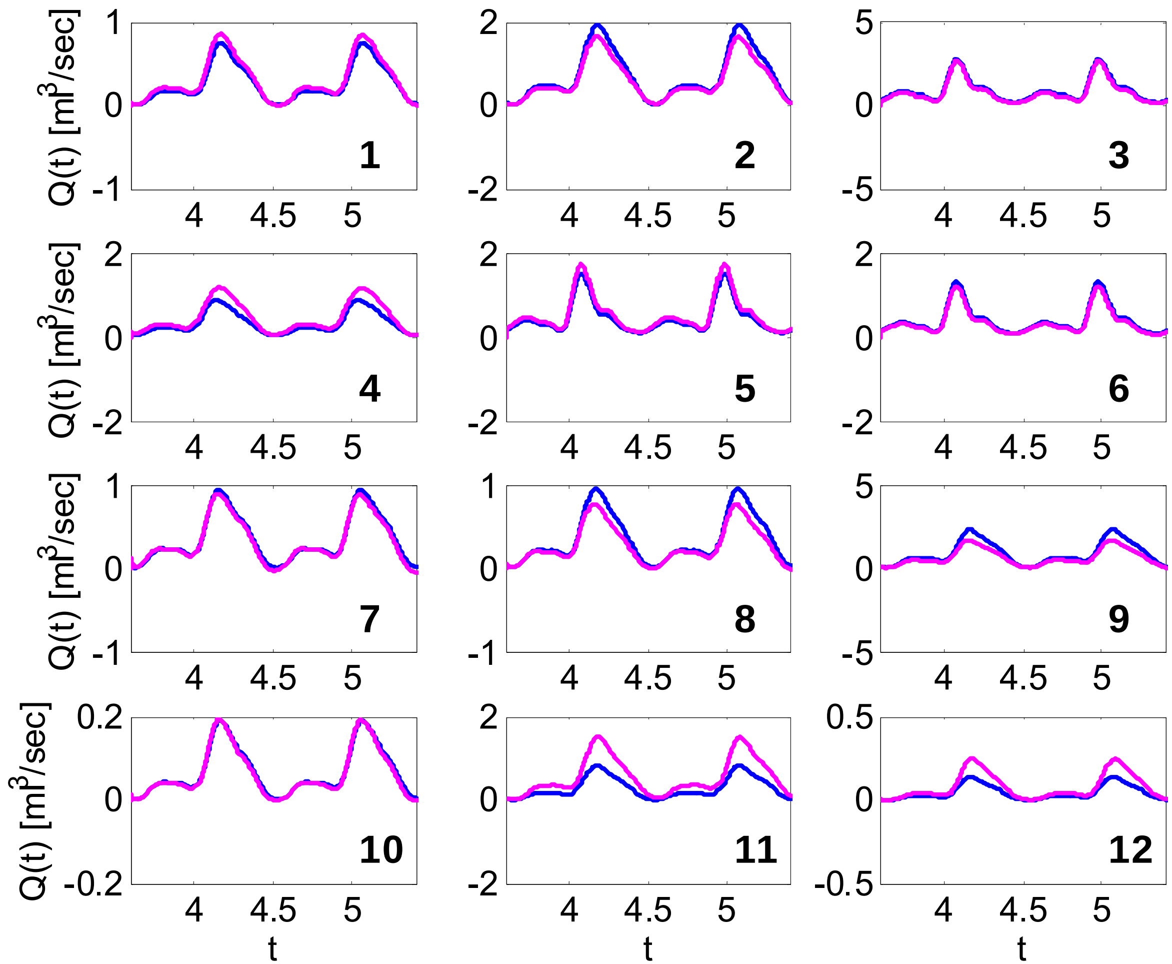
Q(12), P(12) – flow rate and pressure computed at the outlet of left internal carotid artery

Q(16), P(16) – flow rate and pressure computed at the outlet of right internal carotid artery

1D and 3D Modeling: Comparative Study



Flow rates predicted by 1D and 3D models



Pressure drop predicted by 1D and 3D models

B.C.: at inlet – waveform from PC-MRI
at outlets - constant pressure (P=0)

1D and 3D Modeling: Comparative Study

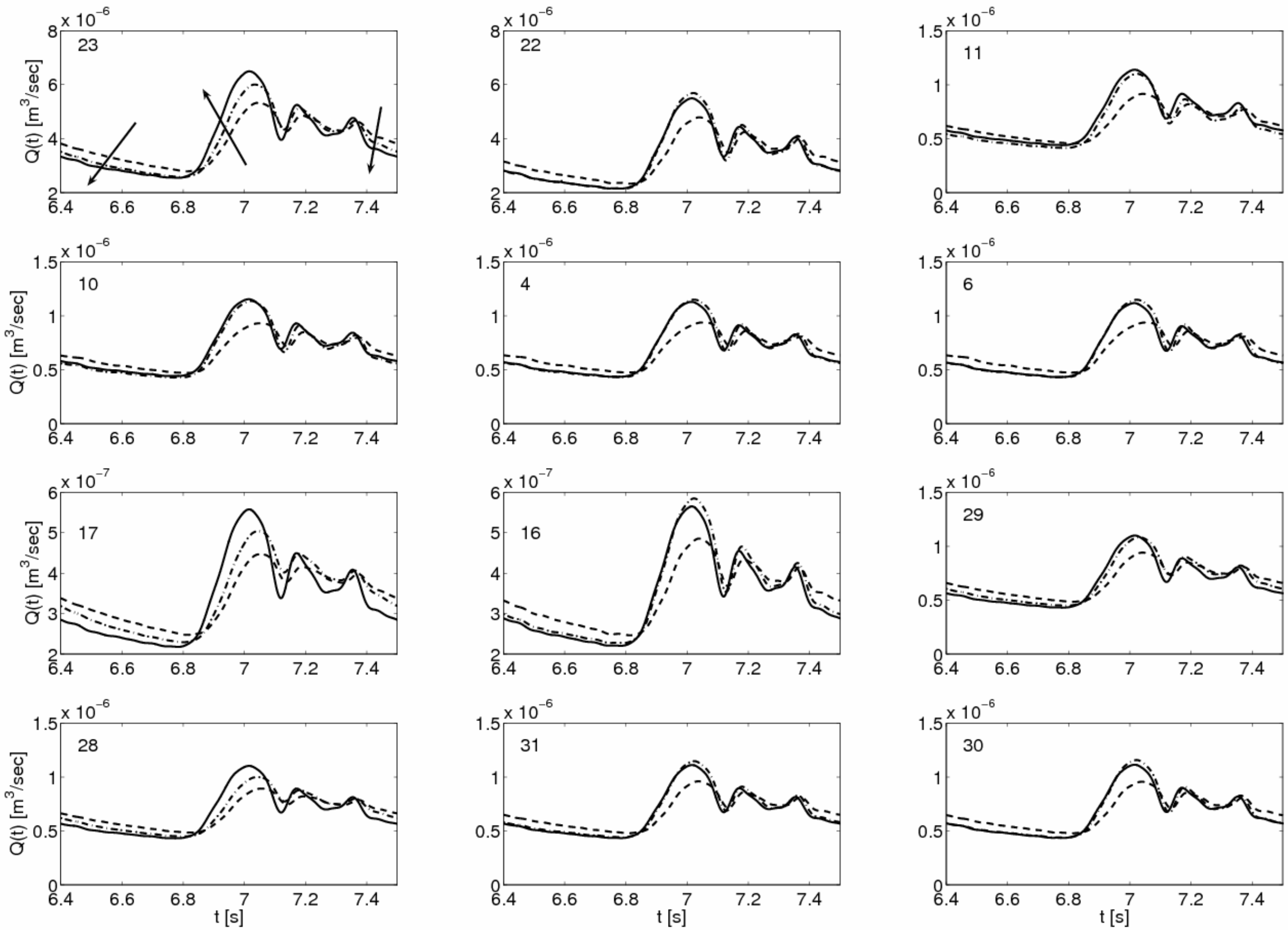
solid – 3D, rigid wall

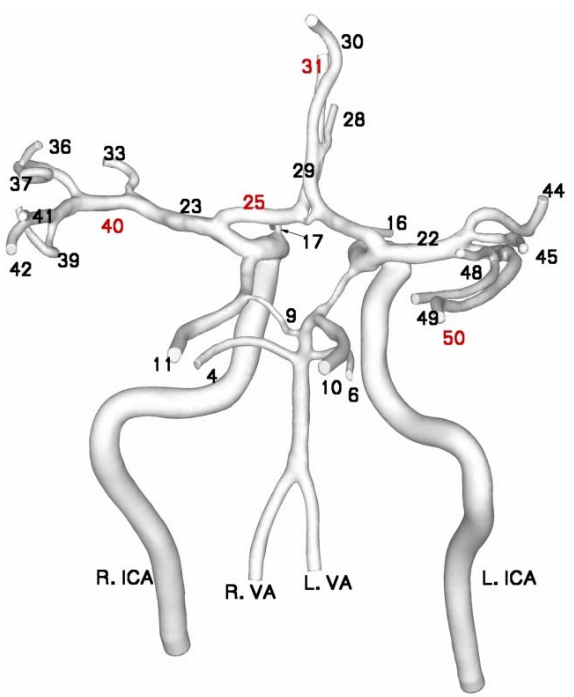
dash – 1D, β_0=1

dash-dot – 1D, β_0=8

$$\beta = \beta_0 \frac{\sqrt{\pi} hE}{1-\sigma^2}$$

flow rate waves Q(t)





B.C.: at inlet – waveform from PC-MRI
at outlets - RC model

(In collaboration with Elizabeth Cheever, Brown University)

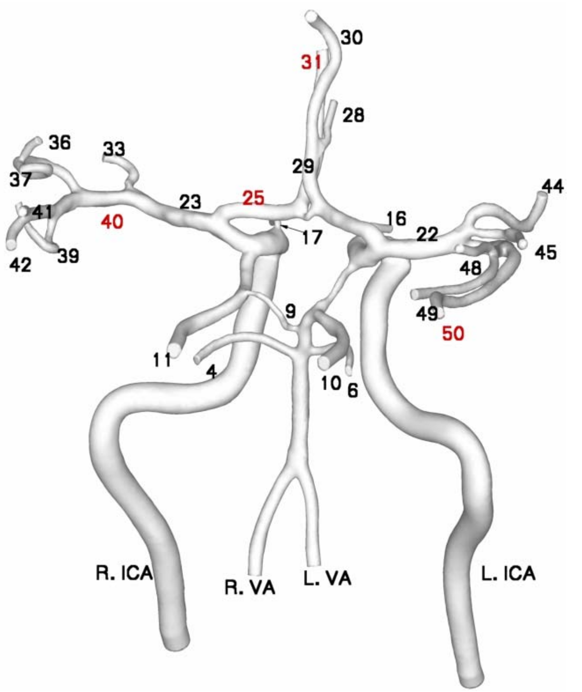
1D and 3D Modeling: Comparative Study

solid – 3D, rigid wall

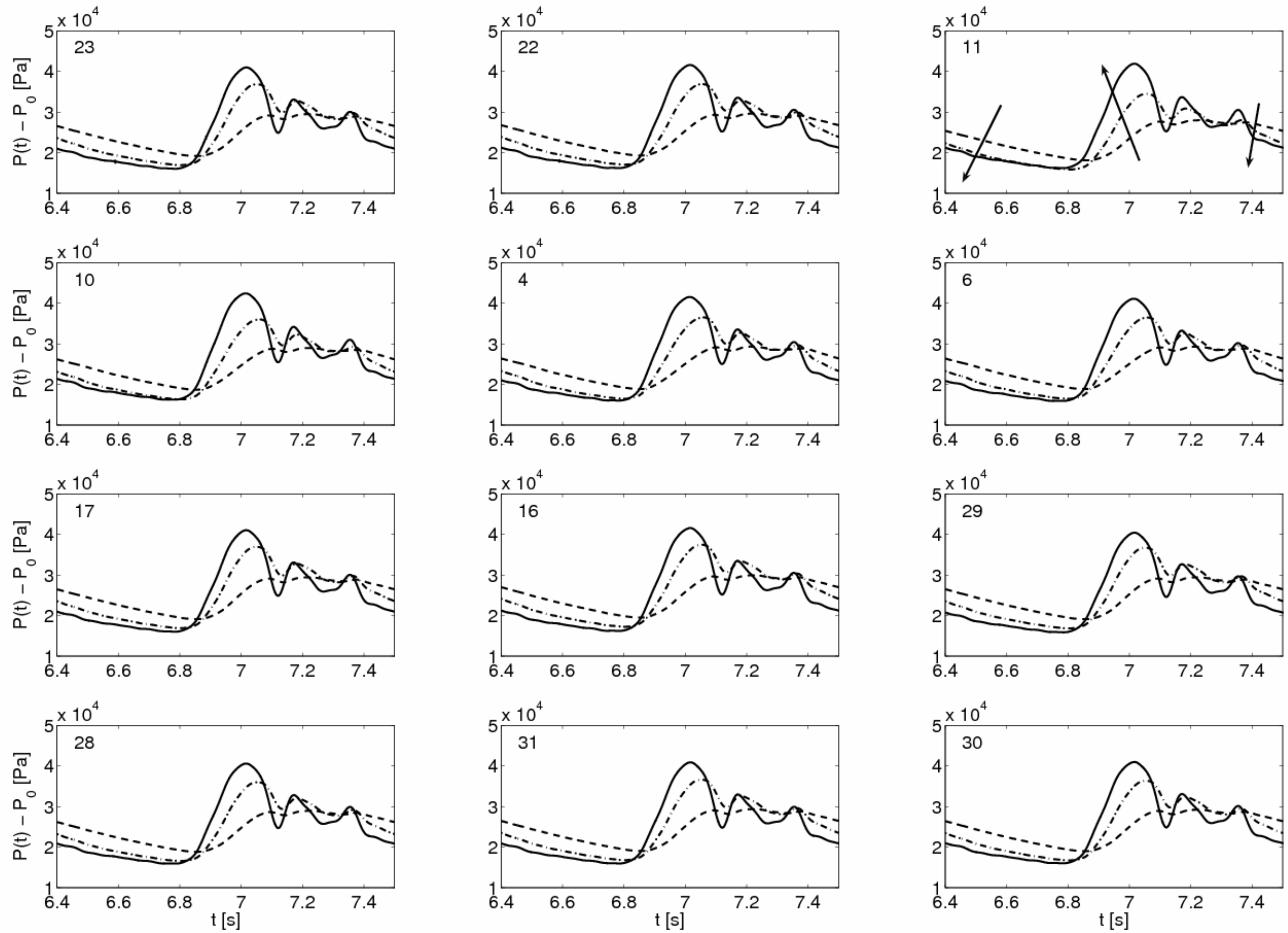
dash – 1D, $\beta_0=1$

dash-dot – 1D, $\beta_0=8$

$$\beta = \beta_0 \frac{\sqrt{\pi} h E}{1-\sigma^2}$$



pressure waves P(t)

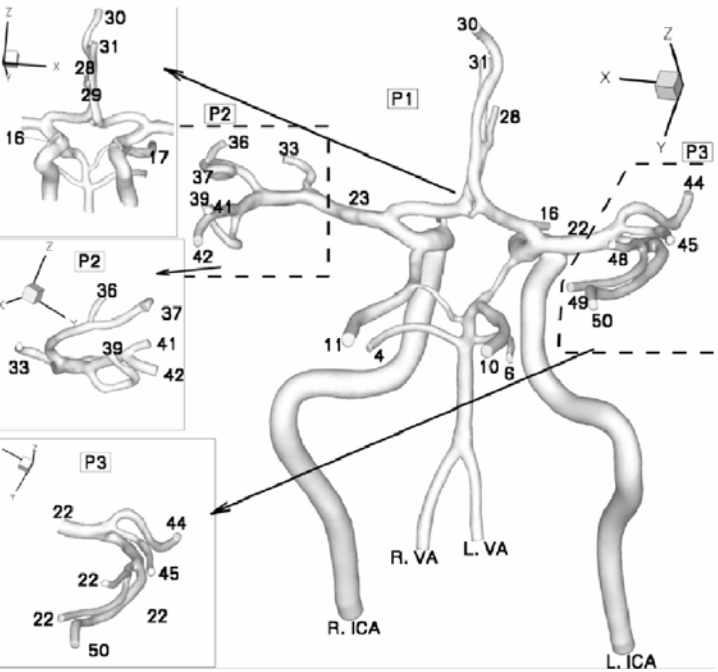


B.C.: at inlet – waveform from PC-MRI
at outlets - RC model

(In collaboration with Elizabeth Cheever, Brown University)

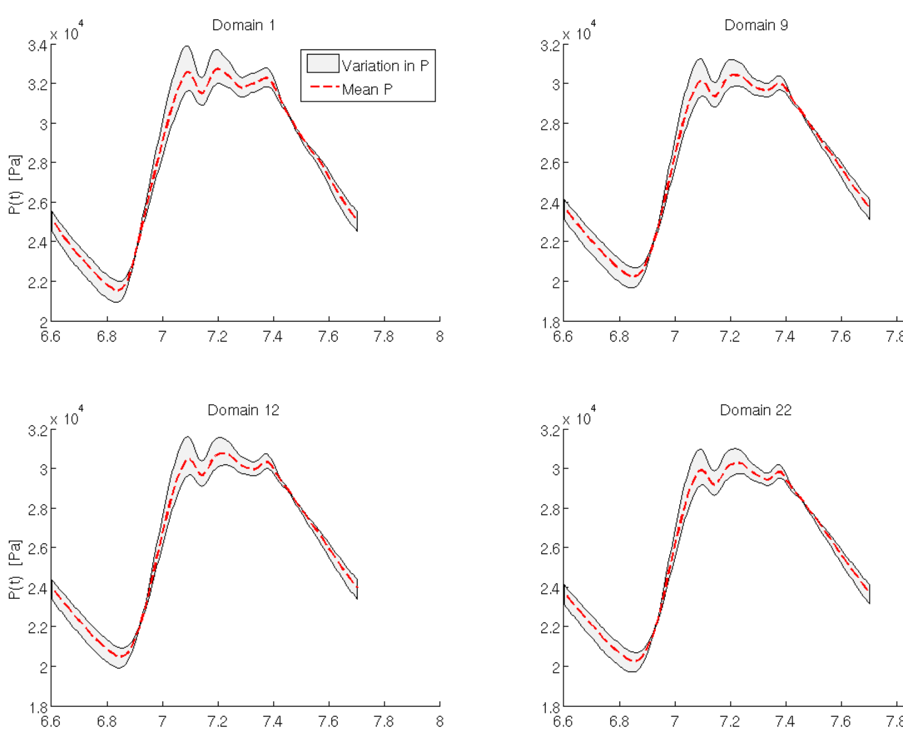
1D stochastic simulations: Hydrocephalus case

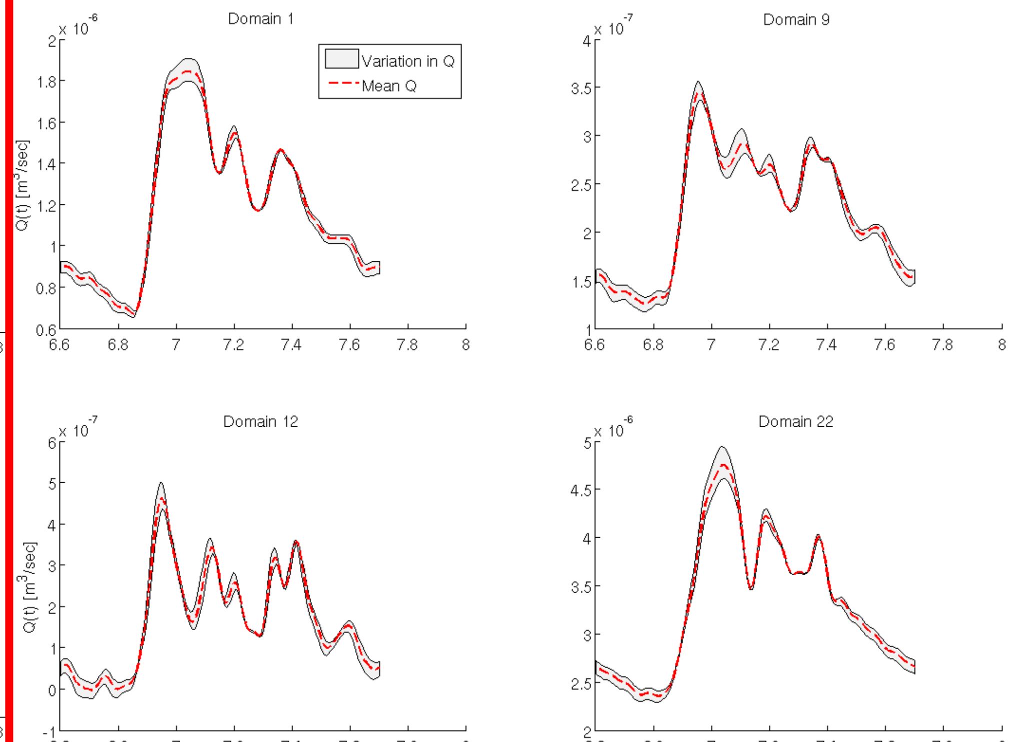
(In collaboration with Elizabeth Cheever, Brown University)



Stochastic parameter – β_0

$\beta_0 = 1 \pm 25\%$

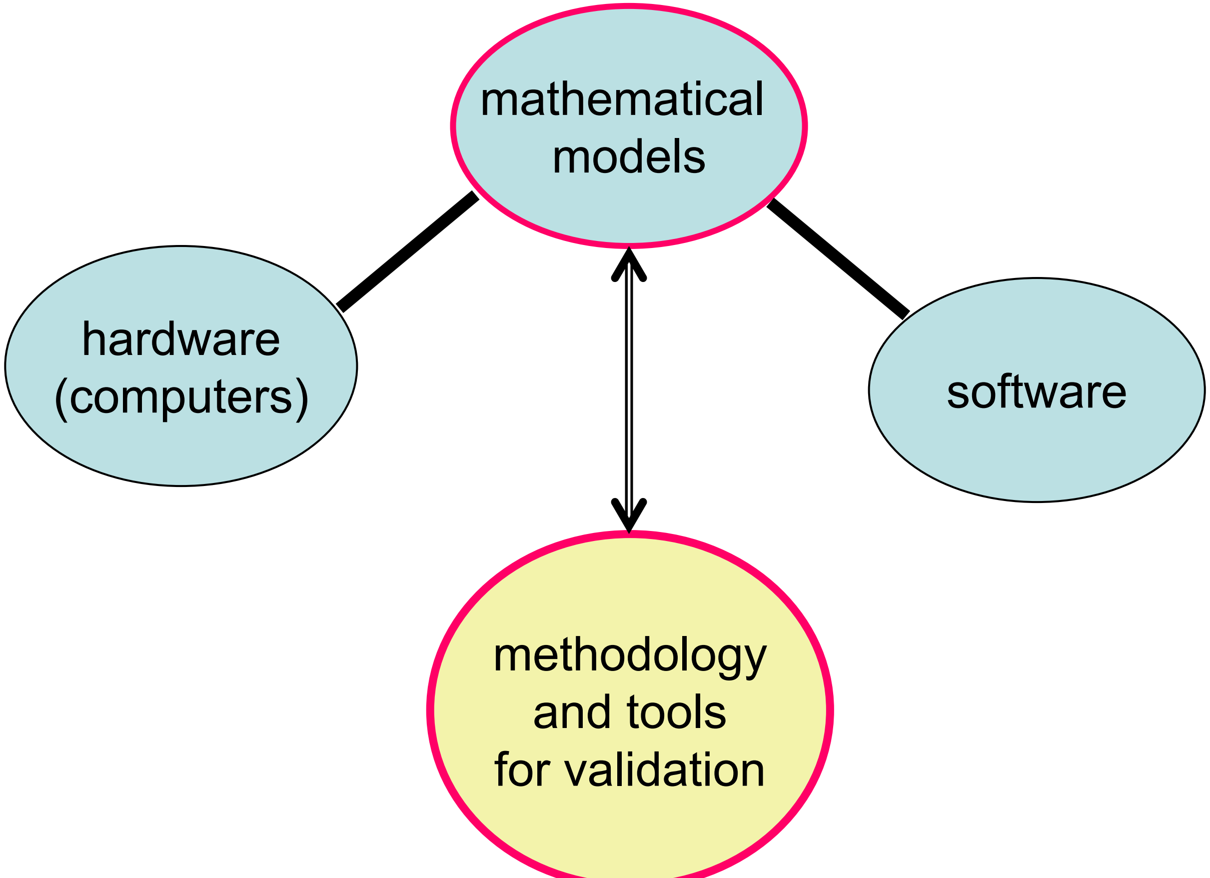




1D Modeling: Summary

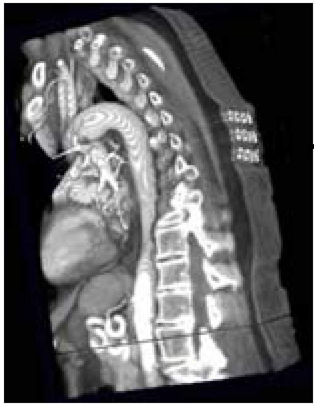
- 1D models is a powerful tool to obtain fast preliminary results of a flow simulation in complex arterial networks.
- 1D model (as well as the 3D model) requires boundary conditions and some estimates on elasticity parameters of the arterial wall properties.
- 1D model is computationally inexpensive and as such it is appropriate for sensitivity studies of a flow to some changes in the arterial network (missing vessels, stents, stenosed vessels, arterial wall stiffening, etc.)

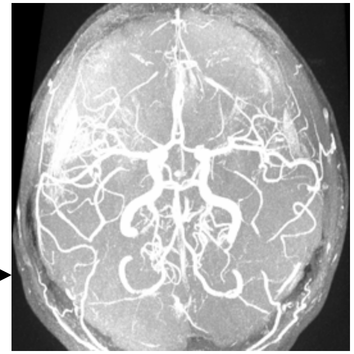
Summary


mathematical models
hardware (computers)
software
methodology and tools for validation

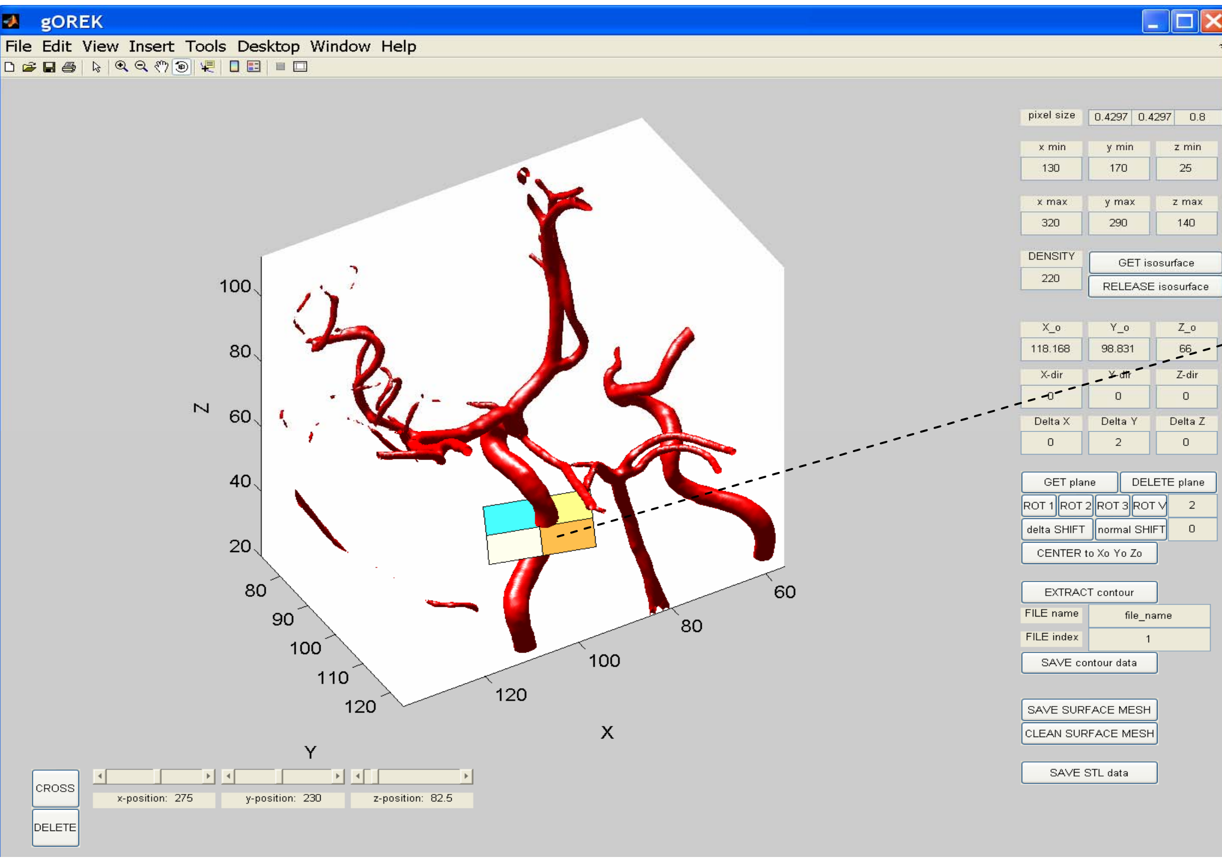
Thanks!

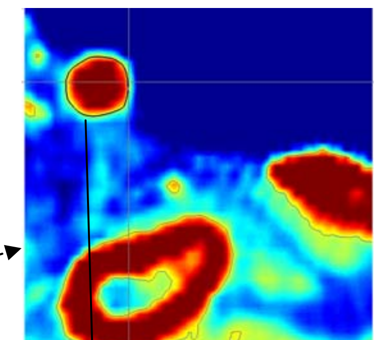
Patient-specific Arterial Flow Simulations: Geometry Reconstruction

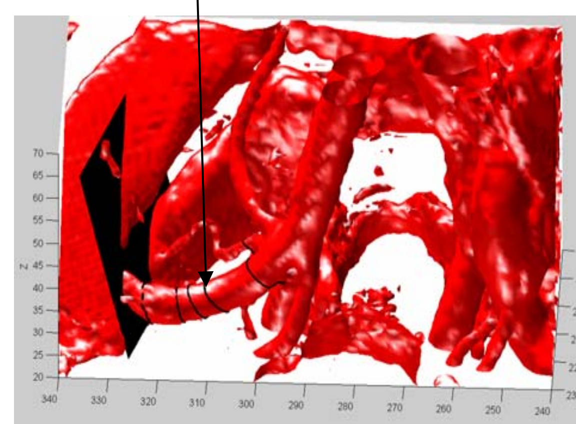




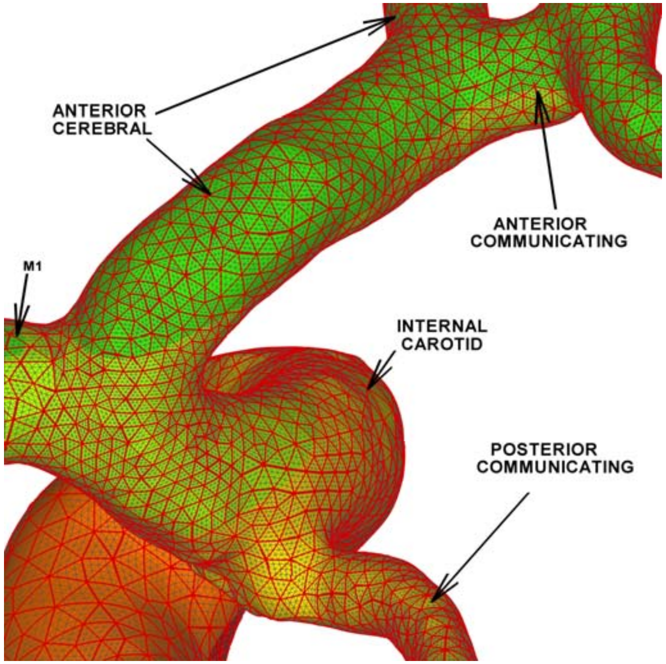
g*OREK* – GUI developed at Brown to reconstruct arterial wall.
Input: DICOM images
Output: patches of arterial wall geometry in STL or PLOT3D format.







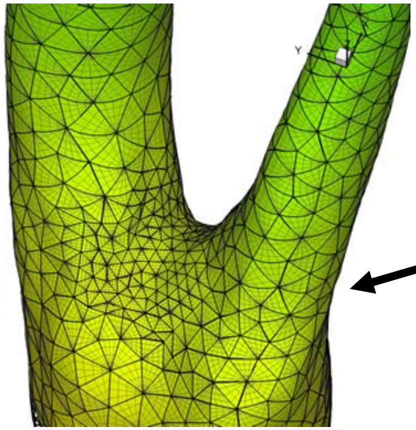
Surface mesh for high-order spectral/*hp* element simulation



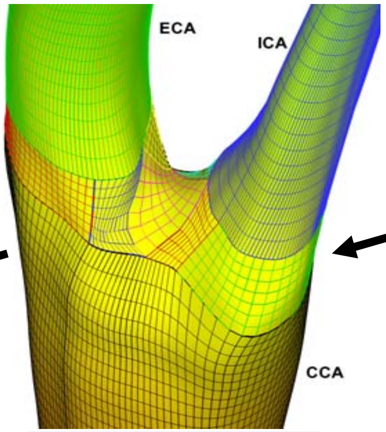
Reconstruction of brain arteries from MR images

Use of "Spherigon" – surface smoothing technique developed for visualization*

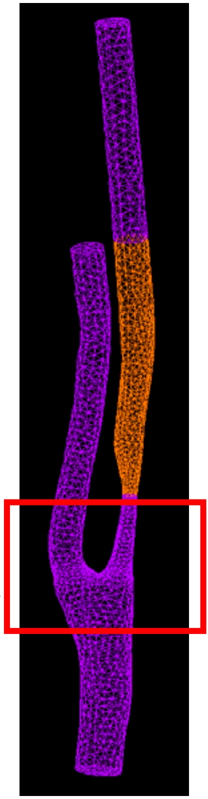
Reconstruction of carotid artery from MR images



Spectral/*hp* element grid



Parametric surface



*P. Volino et al. Proceedings of the Computer Animation (1998).