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

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CRUNCH group:

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Kelsi Hirai - Undergraduate Student (1D flow modeling)

Nabeel Gillani - Undergraduate Student (arterial geometry reconstruction)

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

Team Members

Brown University: CRUNCH GROUP
  - S. J. Sherwin

Imperial College, UK: A. Yakhot

Ben-Gurion University, Israel: N.T. Karonis

Northern Illinois University: J. Insley, M. Papka

ANL:

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.
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,…
Arterial Flow Simulations: Multi-step Process

1. MRI
2. Simulation
3. Data analysis
4. Simulation
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 ....
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**.

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**Grinberg & Karniadakis, Outflow Boundary Conditions for Arterial Networks with Multiple Outlets, ABME, 2008.

Flow Simulations in Arterial Networks: Boundary Conditions

**Inflow** boundary conditions are obtained from PC-MRI measurements (provided by T. Anor, Children’s Hospital)

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


1. Define \( f(t) = \frac{Q_1(t)}{Q_2(t)} \)

2. Set \( R_1 = 100 \)

3. Compute \( R_2(t) = R_1 f(t) \)

\[
P_j + R_j C_j \frac{dP_j}{dt} = R_j Q_j \\
\frac{Q_j(t)}{Q_1(t)} = \frac{R_i(t)}{R_j(t)} + \epsilon
\]

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

\[ R_1 Q_1 \approx R_2 Q_2 \approx R_3 Q_3 \approx R_j Q_j \]

**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

(a) Low velocity flows in the posterior temporal region
(b) Backflow in the anterior cerebral area
(c) High velocity flows in the anterior commissure
(d) ICA and posterior temporal areas
Multi-Domain Decomposition: for High Resolution 3D Flow Simulations in Arterial Networks

Ranger – 0.5PFLOPS computer at TACC
3D Unsteady Flow in Cranial Arteries of a Healthy Subject

Anterior Cerebral

Anterior Comm.

Middle Cerebral

Post. Cerebral

Basilar

L. ICA

L. Vertebral

Posterior Temporal

Unsteady Flow

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)

\[ E \quad 4.5 \text{ Mpa} \]
\[ \Delta P \quad 150 \text{ mmHg} \]

Flow Rate 150 mL/min

Num of mode (4, 4)
Num of Elements (58929, 5628)
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 need to develop a methodology for validation of the mathematical models employed.

The success of the FSI modeling depends on accurate estimates on the arterial wall properties. It also requires modeling of the interactions between the arteries and the surrounding tissues.
1D Flow Modeling

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

- Does not model 3D effects
1D Flow Modeling

\[
\frac{\partial A}{\partial t} + \frac{\partial A U}{\partial x} = 0
\]

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

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

dash-dot – 1D, $\beta_0=8$

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

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, $\beta_0=8$

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

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 – $\beta_0$

$\beta_0 = 1 \pm 25\%$
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

**gOREK** – 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 carotid artery from MR images

Reconstruction of brain arteries from MR images

Use of “Spherigon” – surface smoothing technique developed for visualization*