OpenFOAM as a Model Sharing Paradigm for Macro-Microscale Biomedical Simulation

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- **Model sharing at the macroscale: Requirements and Challenges**
- **OpenFOAM**
  - **Architecture**
  - **How it addresses macroscale modeling challenges**
  - **Biological and biomedical examples**

Model sharing at the macroscale

- ***Lots of progress*** **in model sharing in the micro-to-molecular scale biomedical research community → numerous successful model sharing frameworks:**
  - **SBML, CellML (and offspring)**
  - **CompuCell3D**
  - **CellX**
  - **FLAME**
  - **TRND**
- **Some macroscale approaches for animal/human motion, clinical data analysis, … outside the scope of what is discussed here**

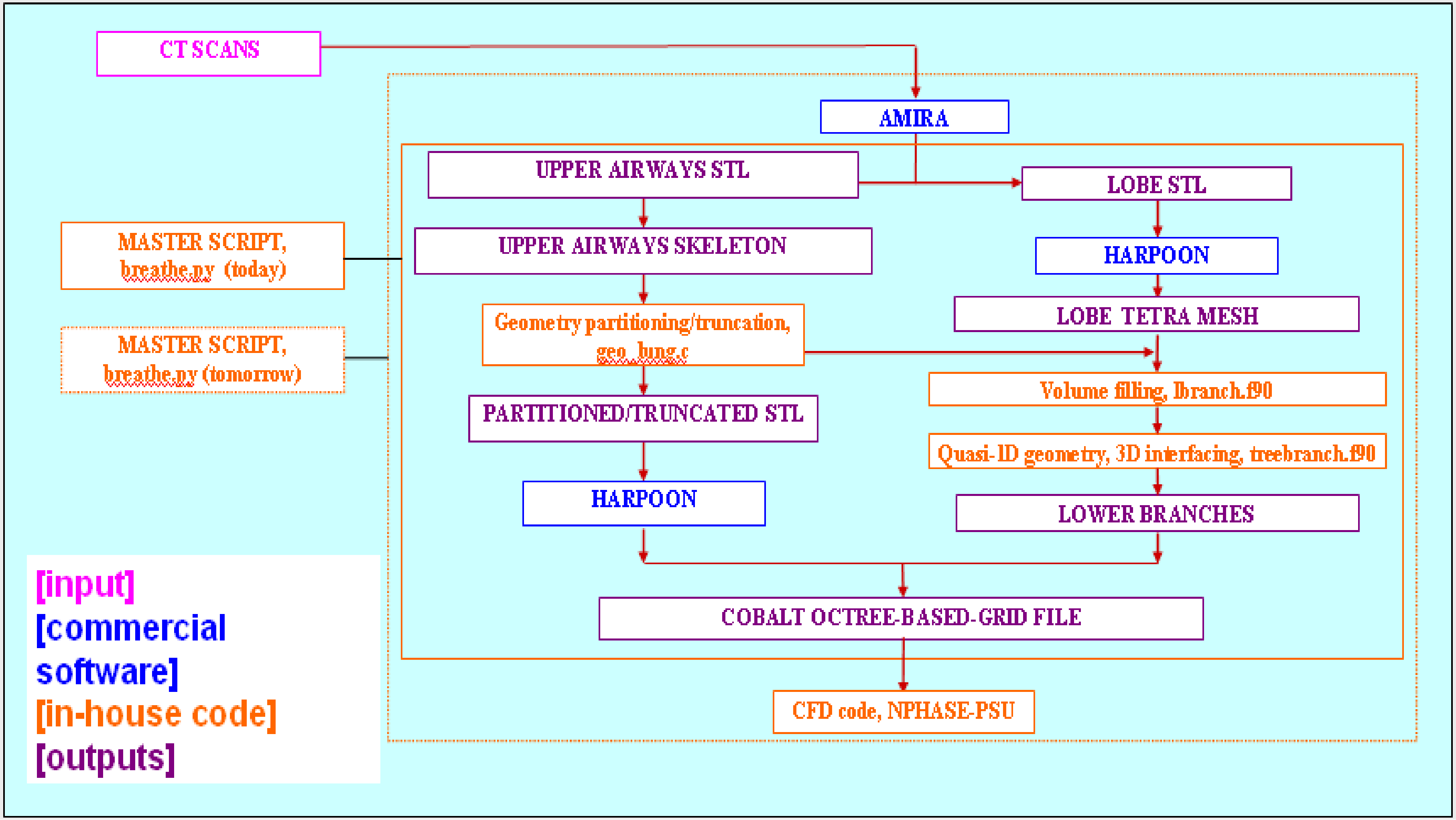
Model sharing at the macroscale

- Here we are concerned with space-time simulation of macroscale processes, i.e., those involving:
  - Medical image processing
  - Geometry processing
  - Computational Fluid Dynamics (CFD)
  - Computational Structural Mechanics (CSM)
  - Attendant meshing technology (motion, deformation, adaption)
  - Interfaces between these disciplines
  - Interfaces to microscales
- In this venue, we argue that ***comparatively little progress*** has been made in model sharing

Model sharing at the macroscale

- **"Model sharing" carries a significantly different set of implications at the micro/molecular scales than in 3D macro-scale bio-physics modeling**
- **Model sharing in this context can involve software components with *widely varying*:**
  - **Source code availability**
  - **Licensing and attendant costs (esp. for parallel)**
  - **I/O interfaces/GUIs**
  - **Data structures**
  - **Interfaces between flow-structure-mesh**
  - **Modularity (i.e., plug and play components)**
  - **Operating system requirements**
  - **Mesh topologies**
  - **Parallel execution frameworks (including domain decomposition)**
  - **Uncertain longevity**
  - **Required user training ➔ often significant (i.e., grid generation)**
  - **Other software engineering elements (e.g., scripting components)**
- **In short, they are hard to "share"**

How can I share this?



CT SCANS

AMIRA

UPPER AIRWAYS STL

UPPER AIRWAYS SKELETON

Geometry partitioning/truncation, geo_lung.c

PARTITIONED/TRUNCATED STL

HARPOON

LOBE STL

HARPOON

LOBE TETRA MESH

Volume filling, lbranch.f90

Quasi-1D geometry, 3D interfacing, treebranch.f90

LOWER BRANCHES

COBALT OCTREE-BASED-GRID FILE

CFD code, NPHASE-PSU

MASTER SCRIPT, breathe.py (today)

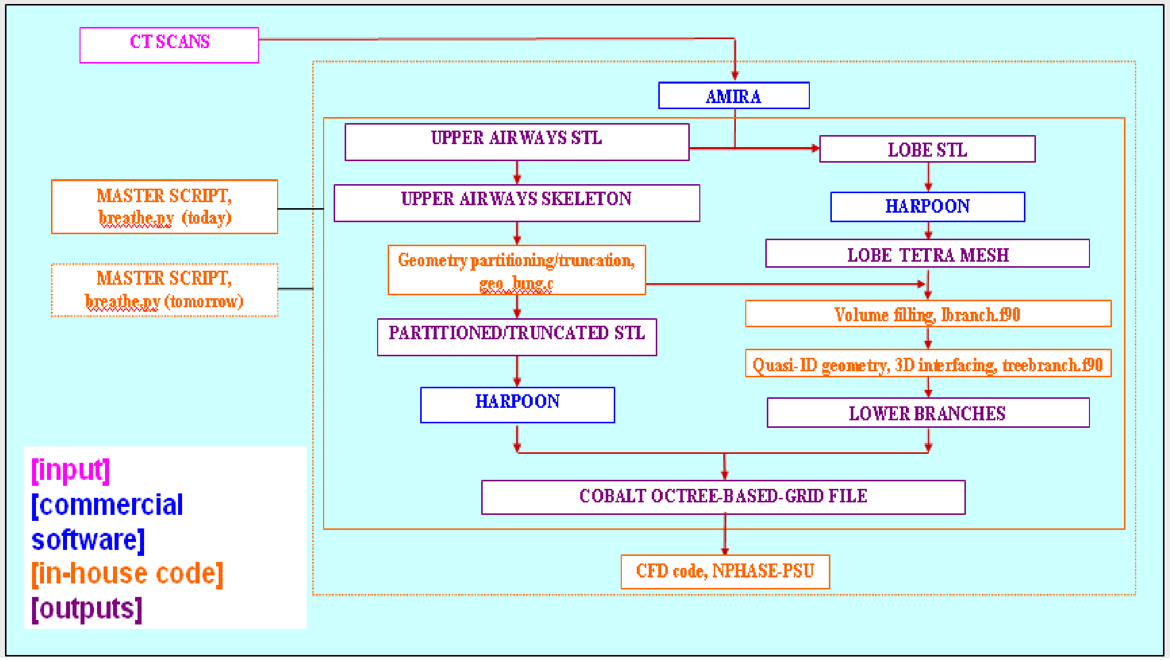
MASTER SCRIPT, breathe.py (tomorrow)

[input]
[commercial software]
[in-house code]
[outputs]

What can we share

- **In 2010, integration of the software components in complex multi-disciplinary computer modeling, is usually accomplished using scripts written in high-level languages such as PYTHON.**

  Such a master script (without its modeling components) could be usefully shared with others



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COBALT OCTREE-BASED-GRID FILE

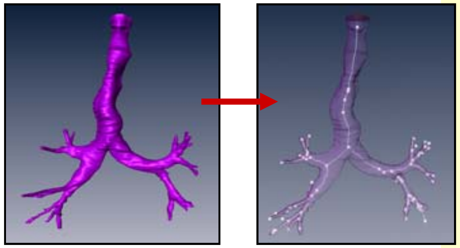
CFD code, NPHASE-PSU

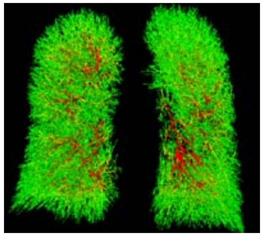
[input]
[commercial software]
[in-house code]
[outputs]

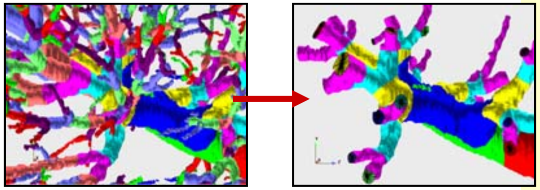
breathe.py

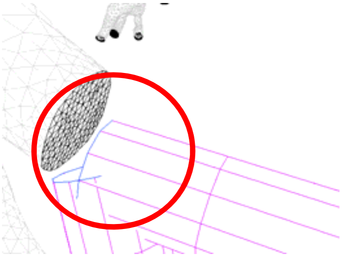
What can we share

- **Due to the complex geometries and multiple scales involved in biological systems, geometry and topology processing components are required, e.g.,**
  - **Volume filling**
  - **"thinning"**
  - **Truncation**
  - **Quasi-1D representations**
  - **Automatic attribute identification**
  - **.**
  - **.**
  - **.**









- **Often these components are small stand alone programs**

Such geometry and topology processing codes could be usefully shared with others

What is hard to share

- But for reasons discussed above the critical modeling components of CFD+CSM+meshing are hard to share.
- For example for me to "share" the respiration modeling toolkit developed under MSM would require:
  - breathe.py and several small C++ and Fortran geometry and topology processing codes (easily shared)
  - NPHASE-PSU – an open source general purpose unstructured CFD code (with limited CSM capability)
  - HARPOON – a commercial grid generation package
  - AMIRA – a commercial medical image processing tool
- So our approach was to design the toolkit such that these "hard to share" components could be swapped for other tools at the users' discretion.

What is hard to share

- **But even a very well software engineered scripting environment does not address *complexity* inherent in the analysis tools themselves. For example:**
  - **The CFD code has several respiration-simulation-specific components including:**
    - **Quasi-1D treatments for lower bronchioles**
    - **"Piston" boundary condition treatments**
    - **Data import of non-standard attributes including loss coefficients, generation number (and other topology), bronchiole length (and other geometric attributes), particle properties, mechanical properties of bronchioles**
    - **Application specific post-processing – various fluxes, pressure drops, deposition efficiency**
  - **For me to share these critical models requires that I either:**
    1) **Share the whole CFD code**
    2) **Resort to sharing only documentation of what/how these components are installed**

What is hard to share

1. **Sharing any CFD code has a subset of the issues brought forward on slide 5 (training/support, licensing, recompilation, parallel environment, attendant software [domain decomp, solver libraries, overset meshing], etc…)**

   Not a good option

2. **Sharing only documentation of what/how these components are installed requires each user to re-develop these software modules within the context of their chosen CFD platform. This • is contrary to model sharing philosophy, • requires reverification, and • may not even be possible.**

   Not a good option

What can’t we share

- The same types of issues come forward in the context of sharing CSM modeling.
- Also, very importantly, fluid-structure interaction approaches are hard to share. Specifically FSI schemes can be:
  - Loosely or strongly coupled
  - Involve single or multiple codes/modules
  - Have widely varying (and generally poor) parallel scaling
  - Have widely varying and application specific flow-structure interpolation schemes
  - Have widely varying and application specific mesh motion/adaption schemes and mesh topologies
- So again it is difficult or impossible to abstract the choices a model developer makes in the FSI context away from user-desired component codes.

Possible solutions

- **Commercial CFD-CSM-mesh motion/adaption**
  - **ANSYS multiphysics**
  - **Adina multiphysics**
  - **Other commercial solutions**
- ***In our view*, a commercial solution could only become an adequate model sharing vehicle if:**
  - **It was adopted as a community standard**
  - **Its cost was very low**
  - **It scaled well to many processors**
- ***In our view*, an open-source solution is more promising. One of these is OpenFOAM, which we discuss here. Others exist including Deal.II**

OpenFOAM

- **OpenFOAM (Open Field Operation and Manipulation) toolbox, http://www.opencfd.co.uk/openfoam/**
- **Open-source, open-development, freely extensible**
- **In our assessment, OpenFOAM has features that give it the potential for greatly expanding the ability of macro-scale biomedical modeling researchers to share their models directly.**
- **OpenFOAM is an object-oriented framework written in C++ , for customization and extension of numerical solvers for continuum mechanics problems including CFD, CSM, mesh motion/adaption and other disciplines.**

OpenFOAM

- **OpenFOAM permits the development of highly-customized solvers and utilities for numerical modeling and simulation of (among other things) coupled fluid-structural mechanics problems**
- **OpenFOAM approach: each *sub-model* (e.g., turbulence model, particle deposition model) or *high level component* (e.g., FSI solver, DNS solver, overset meshing) *can be developed and installed modularly alongside the standard and future OpenFOAM installations which are freely available.***

- **This is inherently amenable to model sharing since once users have adopted the richly capable baseline version of OpenFOAM (relevant here: CFD,CSM, mesh motion/adaption, arbitrary polyhedral unstructured, high order numerics, MPI parallel), they can easily integrate the sub-models or high level components of any other group in the community, and straightforwardly share their models with the community simply by downloading/posting the software from/to the OpenFOAM Wiki or one of numerous open forums (e.g., IMAG).**

OpenFOAM

- **This open, sharing-based, *free!* model development environment has led to OpenFOAM's explosive in growth recent years among macro-scale multi-physics simulation research communities (> 3,000 users worldwide.**
- **Beginning to build acceptance within the biomedical macro-scale physics modeling community where model sharing, dissemination and reuse could lead to more rapid research progress and efficient expenditures of sponsor support.**

OpenFOAM - Architecture

- **OpenFOAM architecture based upon Object Orientation and Generic Programming Techniques**
  - **Object-oriented approach handles complexity by splitting up the software into smaller and protected units, implemented and tested in isolation**
  - **This high-Level approach to programming critical for assuring interoperability of shared models**
  - **User developed code is outside of distribution source, libraries/applications ➔ shared to stand alongside current and future OpenFOAM distributions**
  - **Exploits standard powerful C++ contructs: classes, user defined typing, virtual functions and templates**
  - **You need to know/learn some C++!**

OpenFOAM – Baseline is richly capable

- **Parallelism:**
  - **Taken care of at a very low level: model developers don't have to worry about MPI details**
  - **Domain decomposition via multiple approaches (e.g., METIS)**
- **Multi-region modeling:**
  - **Interpolation/mapping between regions**
  - **Separate meshes for each region**
  - **Separate equations for each region; FSI, conjugate mass/heat transfer, etc.**
  - **Separate materials and properties for each region**
  - ***Ideal for macro-2-micro multi-scale modeling***

OpenFOAM – Baseline is richly capable

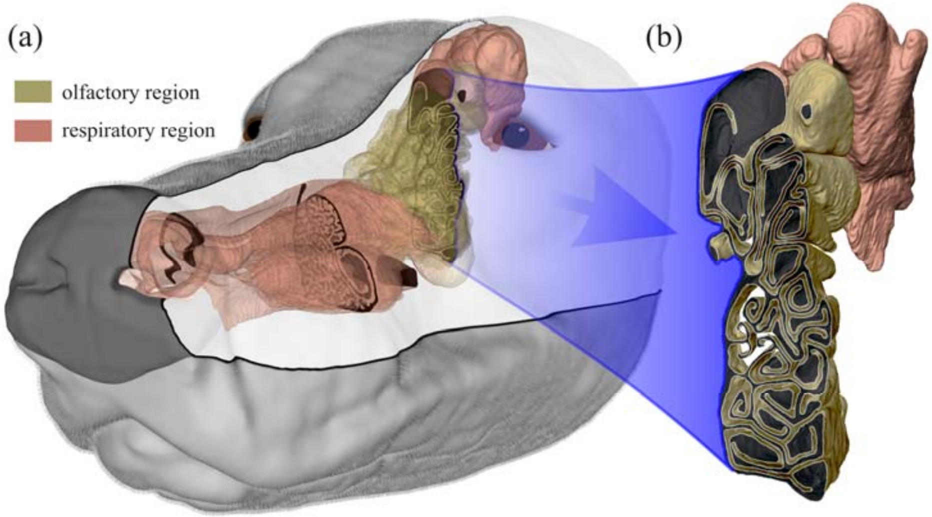
- Discretization for multi-region/multi-scale modeling
  - Finite volume method
  - Finite area method for thin layers on curved surfaces
  - Finite element method
  - Lagrangian particles/sprays/bubbles
- Arbitrary polyhedral support
  - Complex geometries
- Dynamic moving mesh
  - Prescribed and solution-dependent motions
  - Mesh motion: PDES, RBF, topology modification

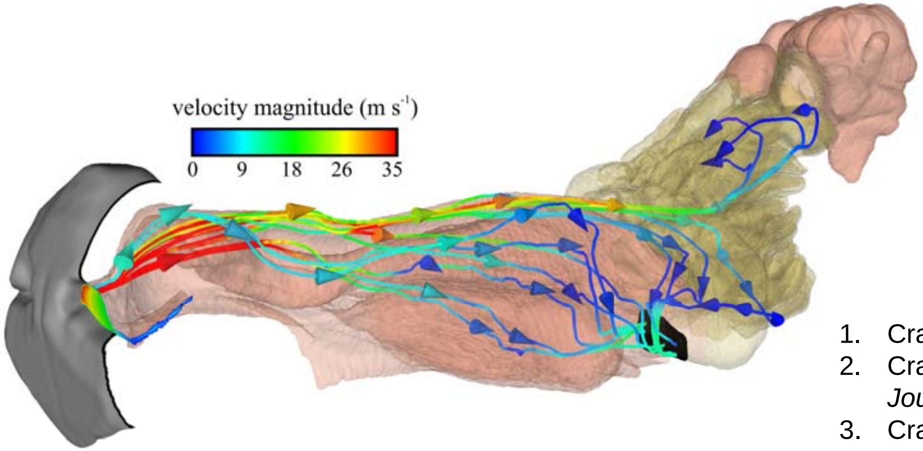
OpenFOAM – Baseline is richly capable

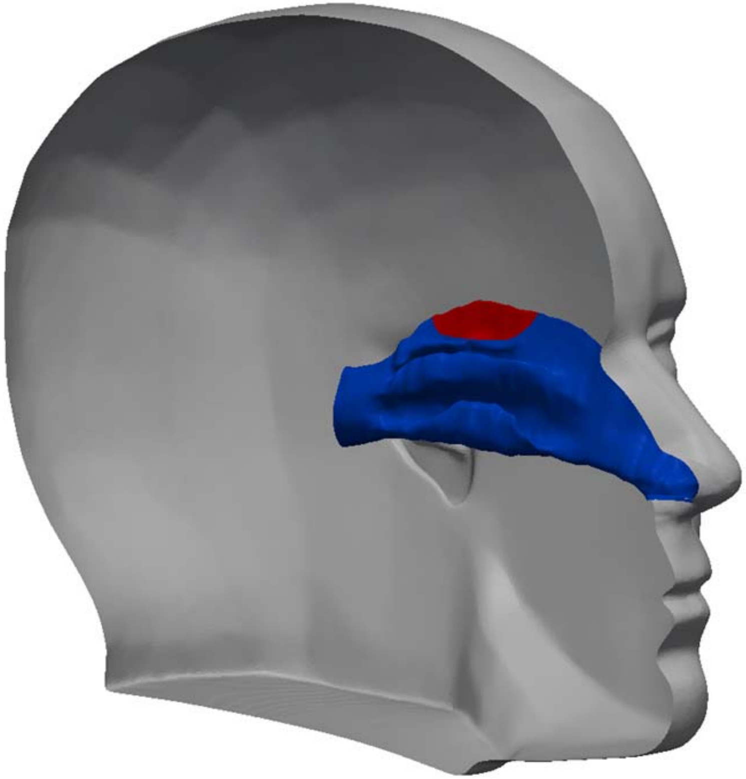
- Execution is much like any standard high-level scientific simulation package:
- Run-time selection of dynamically-loaded libraries
  - Finite-volume and other discretization schemes
  - Turbulence models: laminar, RANS, LES, DES
  - Dynamic meshing
  - Solution schemes for algebraic systems
  - Physical models: e.g., constitutive relations, equation of state, chemistry
  - Output choices
  - .
  - .
  - .

OpenFOAM - Biological and biomedical examples

Mammalian respiration and olfaction:



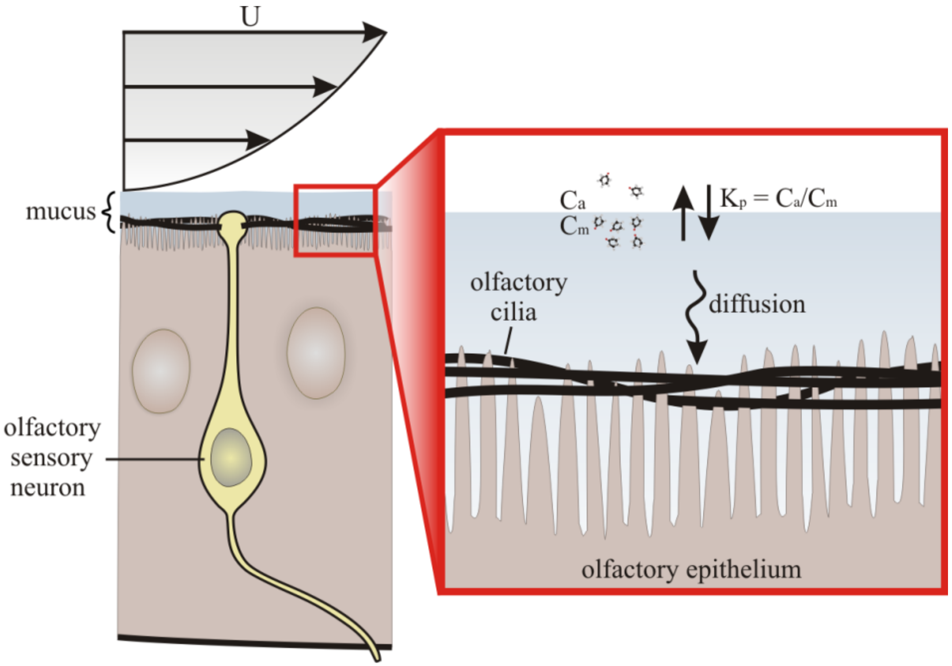


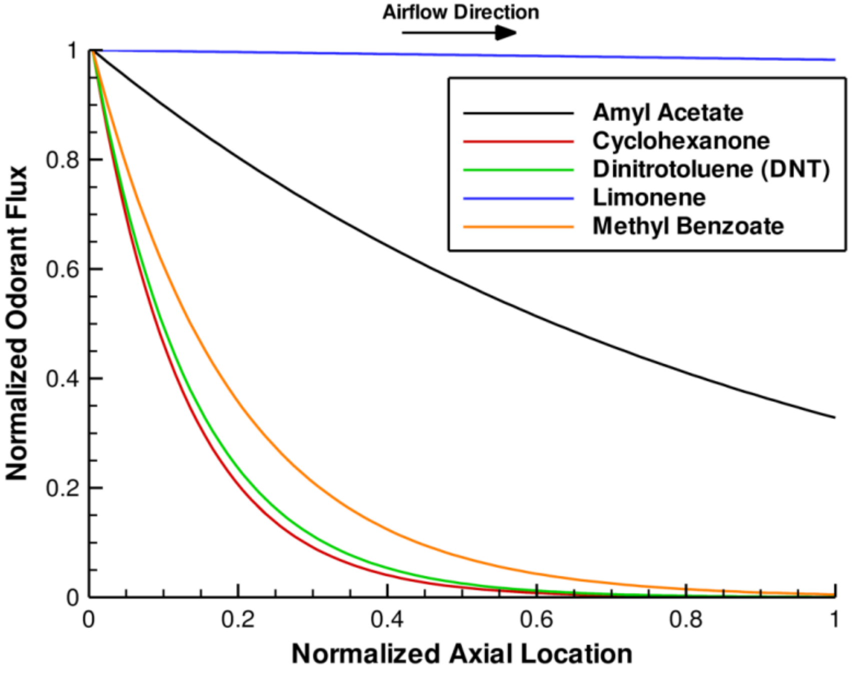


1. Craven, B. A., et al., 2007, *The Anatomical Record*, 290:1325-1340.
2. Craven, B. A., Paterson, E. G., Settles, G. S., and Lawson, M. J., 2009. *Journal of Biomechanical Engineering*, 131(091002):1-11.
3. Craven, B. A., Paterson, E. G., and Settles, G. S., 2009. *Journal of the Royal Society Interface* (published online before print Dec. 9, 2009).

OpenFOAM - Biological and biomedical examples

- **Multiphysics/multiregion modeling: vapor absorption/uptake (olfaction)**





1. Lawson, M. J., Craven, B. A., Paterson, E. G., and Settles, G. S., 2010, submitted to *Chemical Senses*.

OpenFOAM - Biological and biomedical examples

- **Fluid-structure interaction for heart pumps with polymeric deformable blades**

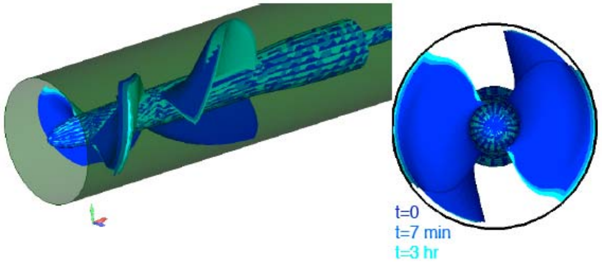


Figure 1: Notional impeller tip clearance dependency on time; obtained from a one-way fluid/solid coupling model with negative loads applied

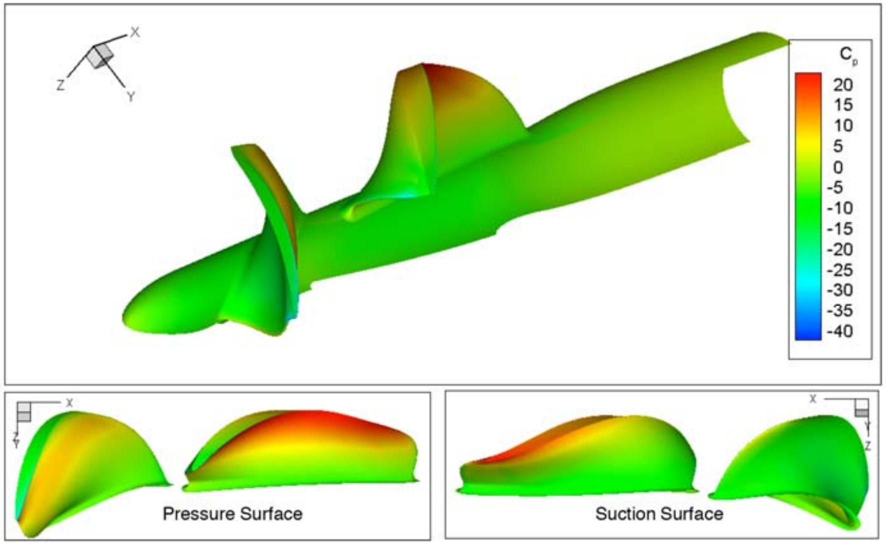


Figure 6: Impeller pressure contours from preliminary cyclic-symmetric CFD analysis

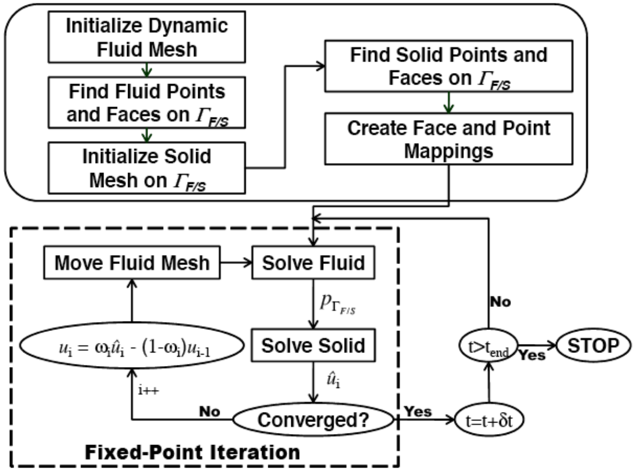


Figure 8: FSI solver implementation showing startup details and the fixed-point iteration of the partitioned approach

1. Campbell, Paterson, Reese, and Hambric, “Fluid–structure simulation of a viscoelastic hydrofoil subjected to quasi-steady flow, FSI 2009, Crete.
2. Campbell, PhD Thesis, Expected Dec. 2010.

OpenFOAM - Biological and biomedical examples

- **Fluid-structure interaction for heart pumps with polymeric deformable blades**

Validation Benchmark

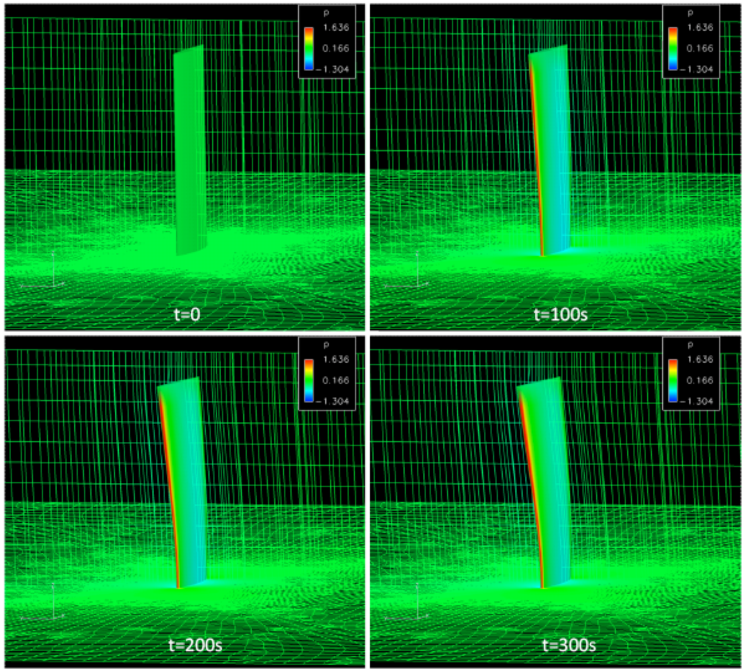


Figure 16: Mesh motion for single hydrofoil test case, front view; contours of pressure (kPa) shown on the foil surface and the cell edges; results shown for $t = 0$, 100, 200, and 300 s; images show a slice through the mesh near the mid-chord location in the y-z plane, flow is in the x-direction; the images show negligible cell deformation in the foil vicinity resulting from mesh motion with quadratic decay of the diffusion coefficient

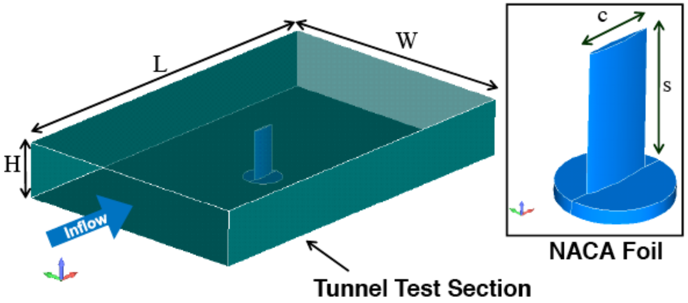
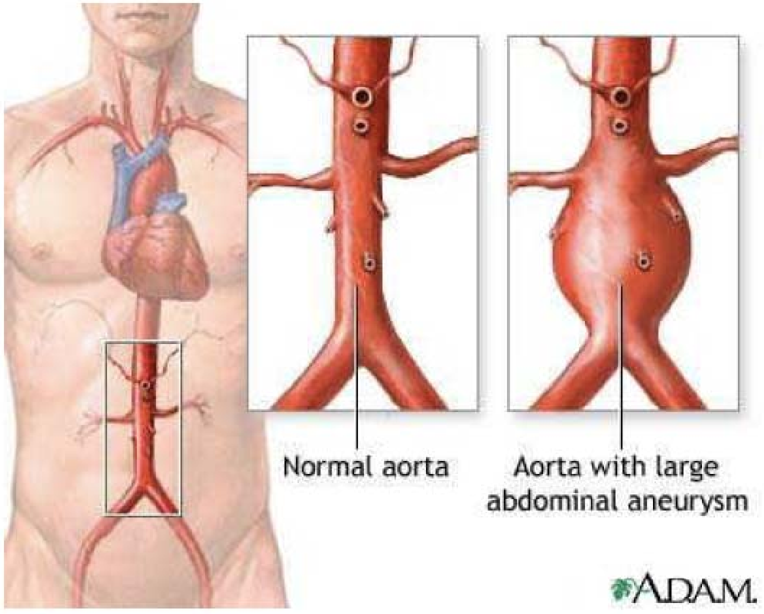


Figure 9: Flow over a cantilevered, modified NACA 66 hydrofoil with uniform inflow conditions situated in the rectangular test section of a 12-inch water tunnel; H is in the vertical direction

1. Campbell, Paterson, Reese, and Hambric, “Fluid–structure simulation of a viscoelastic hydrofoil subjected to quasi-steady flow, FSI 2009, Crete.
2. Campbell, PhD Thesis, Expected Dec. 2010.

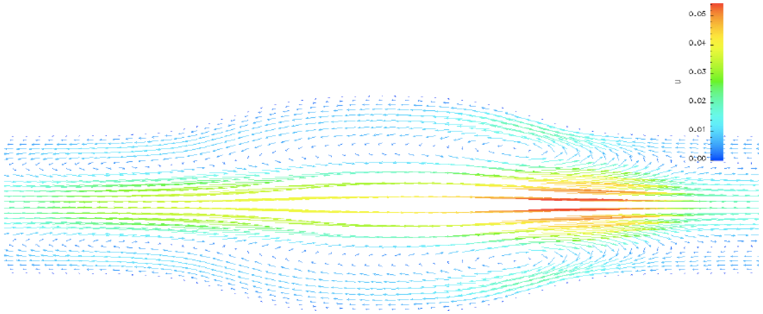
OpenFOAM - Biological and biomedical examples

- **FSI of Abdominal Aortic Aneurysms**

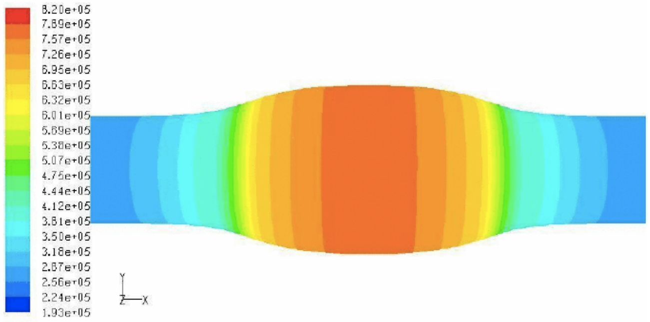


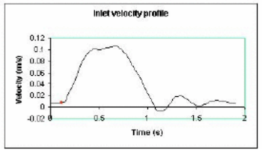
~90% mortality rate if rupture occurs

Fluid Flow



Stress – Model 2





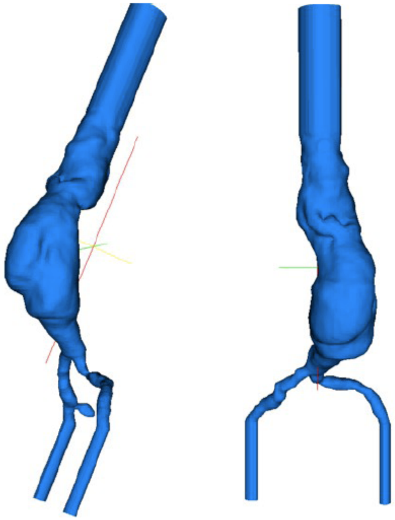
Kelly and O'Rourke, 2rd OpenFOAM Workshop, Zagreb, Croatia, 2007

OpenFOAM - Biological and biomedical examples

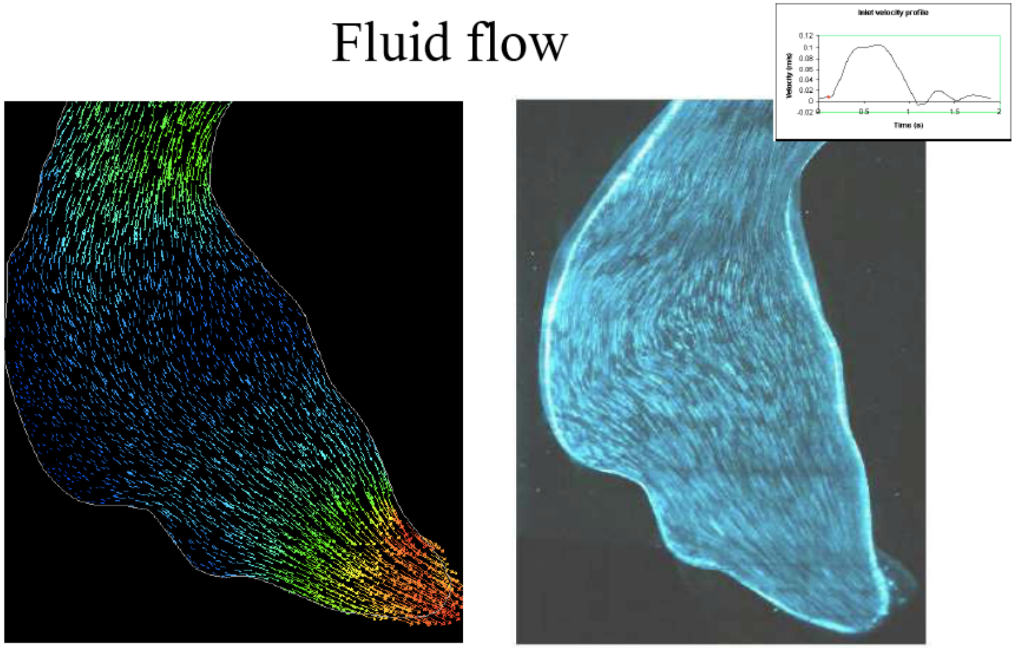
FSI of Abdominal Aortic Aneurysms

Patient based geometry

- Female patient
- 68 years old



Fluid flow



Flow visualisation results from "Haemodynamics of Abdominal Aortic Aneurysms: A Comparison between Idealised and Patient-Based Models", James McCullough, PhD thesis, UCD, 2006

Ivankovic, 2nd OpenFOAM Workshop, Zagreb, Croatia, 2007

OpenFOAM - Biological and biomedical examples

Cardiovascular fluid dynamics

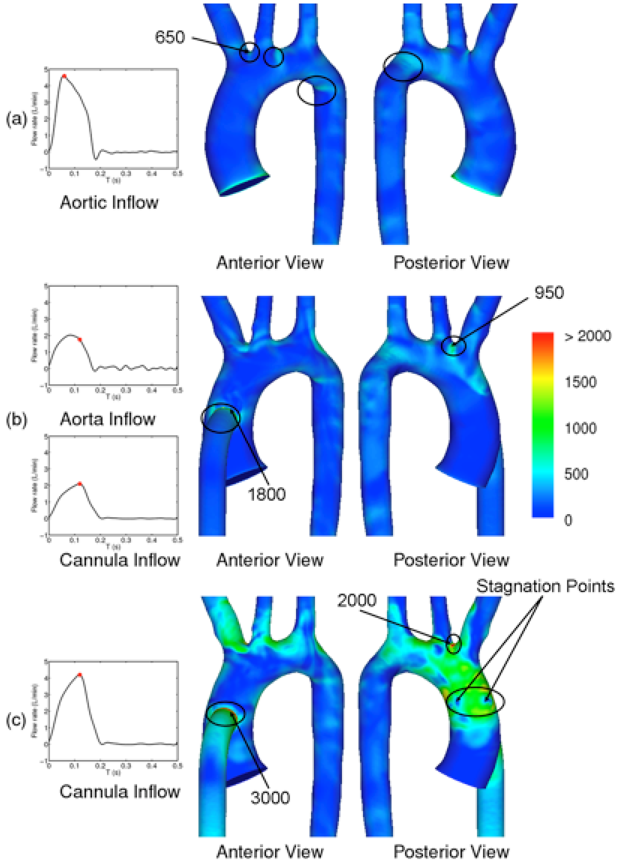


Figure 9. WSS magnitude (unit: dyn/cm2) contour at peak systole: (a) healthy pediatric aorta, (b) 50% bypass, (c) 100% bypass.

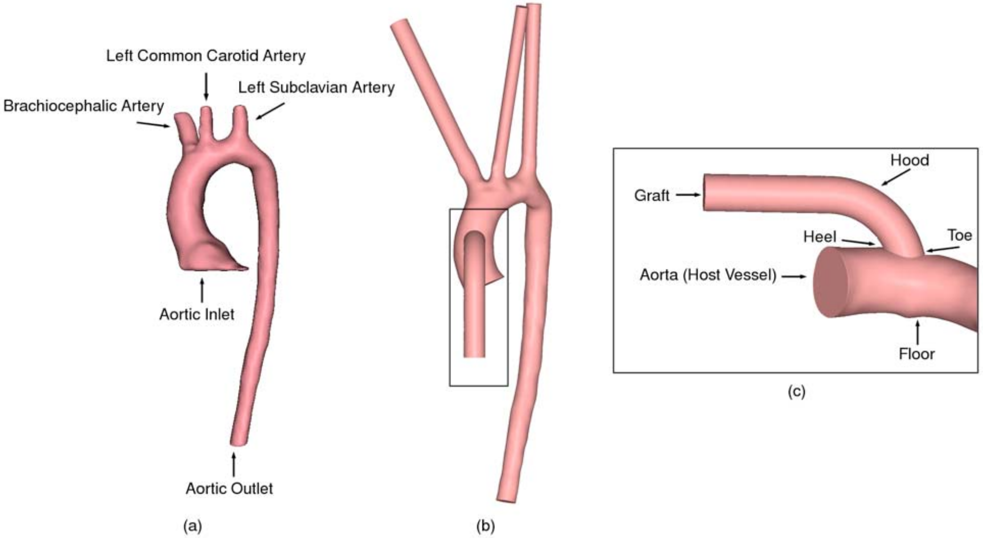
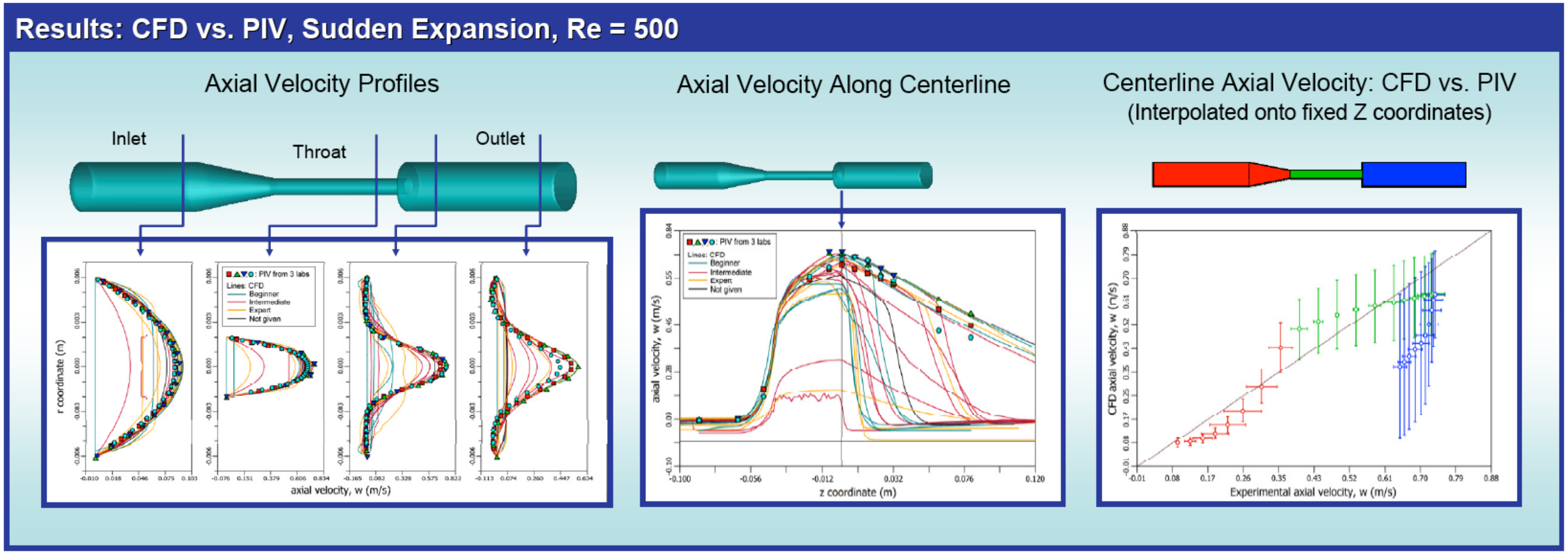


Figure 1. (a) Healthy pediatric patient specific aortic model; (b) Proximal anastomotic model; (c) Enlarged distal view of the graft junction indicated by the black square in Fig. 1 (b).

1. Yang, N., Deutsch, S., Paterson, E., and Manning, K., *Journal of Biomechanical Engineering, vol.* 131, No. 11, 9pp, Nov. 2009.
2. Yang, N., Deutsch, S., Paterson, E. and Manning, K., *Cardiovascular Engineering and Technology, 2009.*
3. Yang, N., Deutsch, S., Paterson, E. and Manning, K., *Journal of Biomechanical Engineering, 2009.*

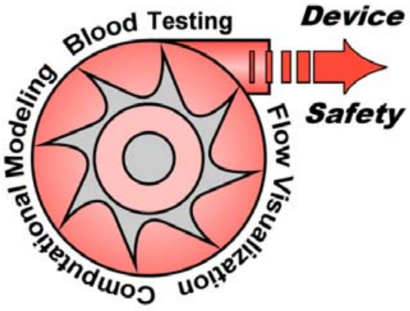
OpenFOAM - Biological and biomedical examples

Solver validation: FDA Critical Path Initiative



FDA

epi
Critical Path Initiative
Food & Drug Administration



1. Stewart, S.F.C., et al. "Preliminary Results of FDA's Interlaboratory Assessment of Computational Fluid Dynamics and Hemolysis in Medical Devices," FDA/NHLBI/NSF Workshop on Computer Methods for Cardiovascular Devices, June 1-2, 2009.
2. Stewart, S.F.C., et al. "Preliminary Results of FDA's "Critical Path" Project to Validate Computational Fluid Dynamic Methods Used in Medical Device Evaluation," 55th American Society for Artificial Organs Conference, Dallas, Texas, USA, May 28-30, 2009.

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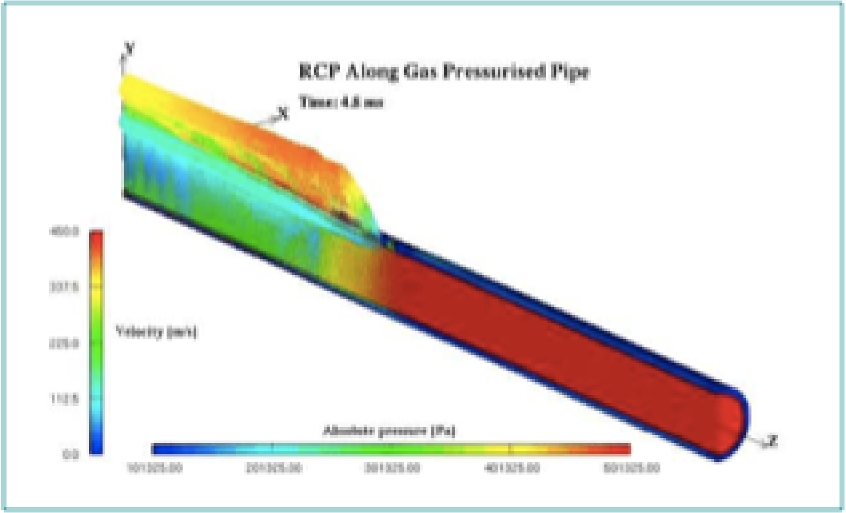
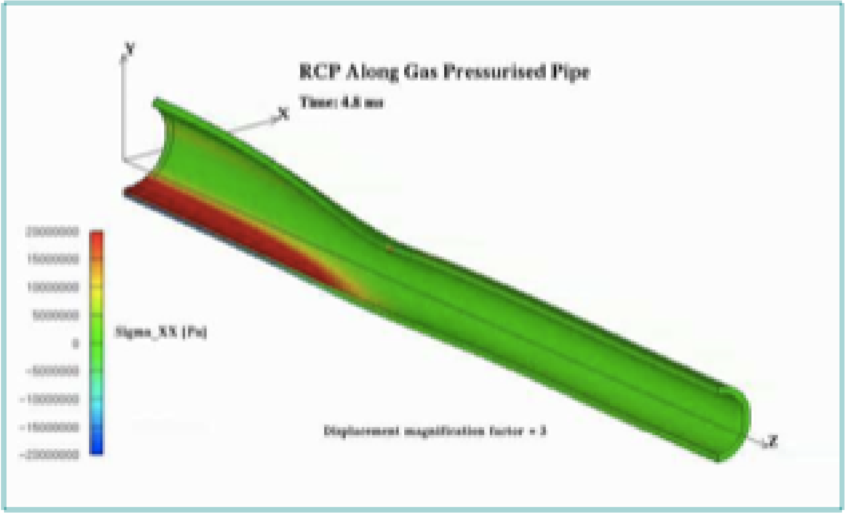
FSI of pipeline failure and crack propagation

Plastic Pipeline Failure: FSI With Crack Propagation

- Internal pressure drives crack propagation; crack opening depressurises the pipeline, dynamically interacting with the force driving crack propagation
- Custom coupled fluid and structures solver; patch-to-patch mapping tools for data transfer
- Crack model implemented as a derived boundary condition: damage model





Jasak, Personal Communication, 2009

Summary

- **OpenFOAM is a rapidly-emerging open-source computational continuum mechanics toolbox with the following advantages:**
  - **Open-source = free as in freedom (freedom to share with other biomedical researchers)**
  - **OpenFOAM architecture is inherently amenable to model sharing**
  - **Custom models, utilities, etc. (e.g., FSI solver, turbulence models, particle deposition models) are developed and installed modularly alongside the standard/baseline OpenFOAM installation**
  - **Ideal for CFD, CSM, and fully-coupled modeling of multiphysics problems (e.g., FSI)**

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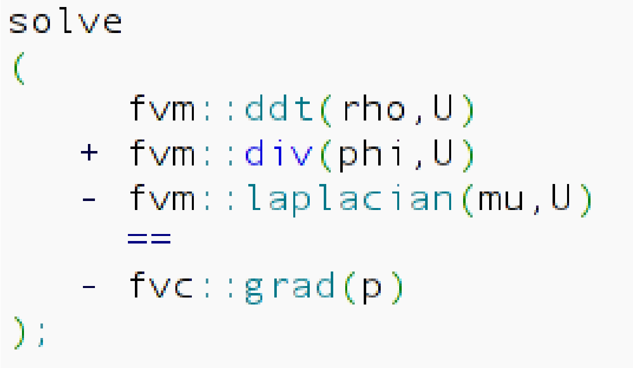
Summary

- **Because of its use of advanced object-oriented C++ programming concepts (e.g., operator overloading), OpenFOAM utilizes top-level mathematical descriptions of governing equations in human-readable form. Example:**

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \cdot \phi \mathbf{U} - \nabla \cdot \mu \nabla \mathbf{U} = -\nabla p \quad \longrightarrow$$



```
solve
(
      fvm::ddt(rho,U)
    + fvm::div(phi,U)
    - fvm::laplacian(mu,U)
      ==
    - fvc::grad(p)
);
```

- **OpenFOAM community (currently ~3000 members) is rapidly growing world-wide**
- **Community collaboration via wikis (e.g., http://openfoamwiki.net) and discussion forums (e.g., http://www.cfd-online.com/Forums/openfoam/)**
- **Fair documentation, plenty of tutorials and example cases for most solvers and utilities**