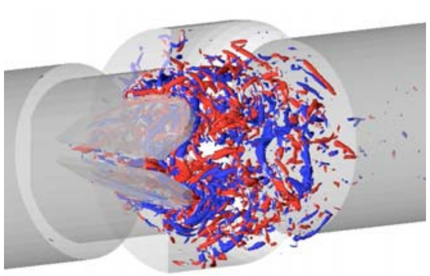
UNIVERSITY OF MARYLAND

Tackling Turbulence Biological Flows



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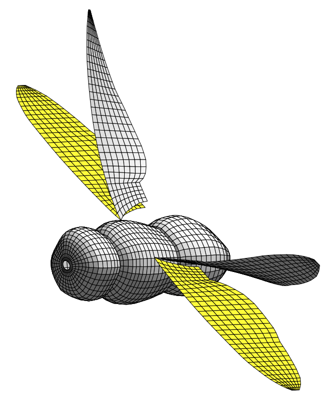


Supported by NSF (Grant CTS-0347011)
AFOSR (Grant 050421-7793) ONR (Grant 072789-8812)

Outline

- Introduction
- Simulating biological flows
  - Fluid-structure interactions
  - Embedded Boundary Method
- Applications
  - Treatment of aortic valve stenosis
- Summary and Future Research

Introduction

What are biological flows?

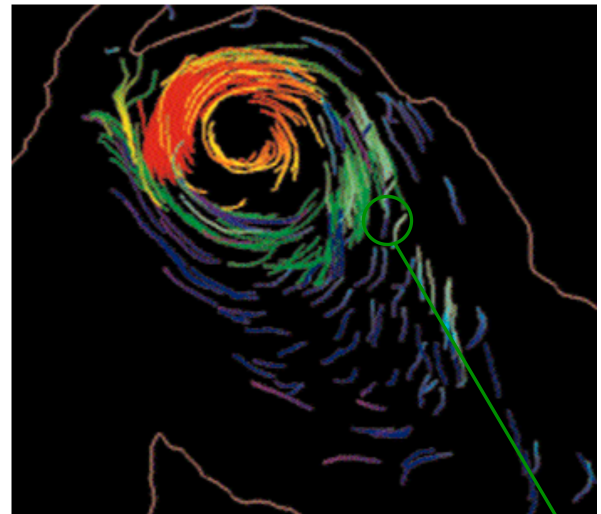
Internal flows: The human body, where fluids *play a critical role, i.e.*

- Respiratory system
- Circulatory system
- ……….

A variety of flow phenomena at multiple scales:

- Organ level (Re<8000)
- Cellular level
- Molecular level

cm

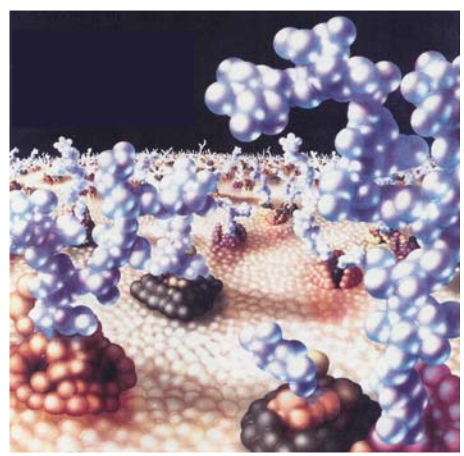


Flow patterns in the human aorta

μm

Blood elements

nm



Molecules on the cell surface

Introduction

What are biological flows?

External flows: Other organisms that move and feed in the water and air, i.e.

- Micro organisms
- Birds, insects, …
- Fish
- ………

Wide Re number range: $0.01<Re<10^6$

mayfly

dragonfly

Yellow fin tuna

Introduction

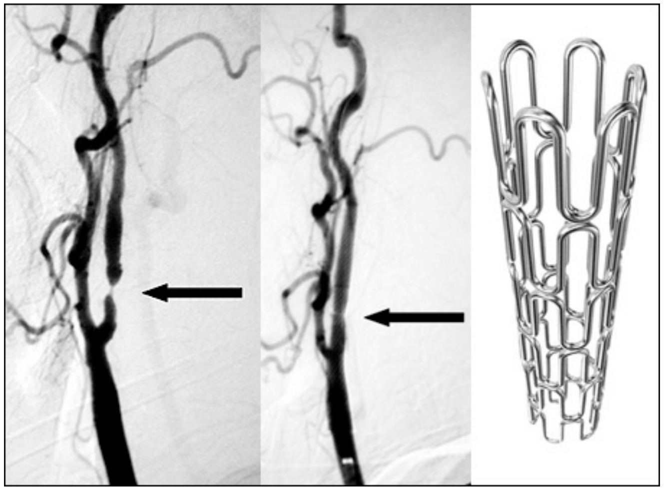
Is turbulence important in biological flows?

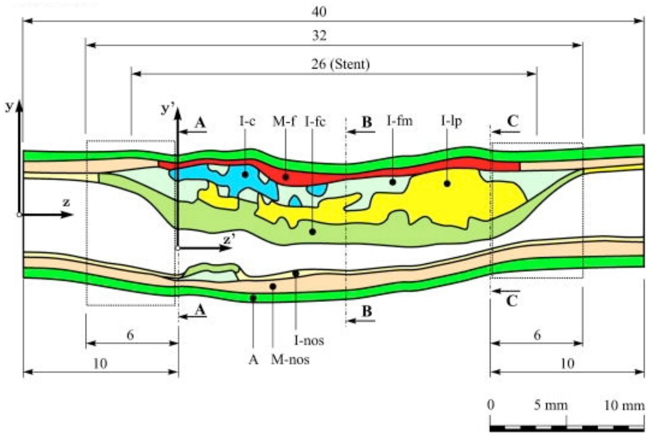
Example 1: Turbulence is the exception in the circulation. It appears in pathologic situations and triggers some unique biological responses:

- Atherosclerosis
- Medical implants can trigger turbulence
- Medical devices

Turbulence is NOT desirable in blood circulation and there is a need to better understand and control (avoid) it:

- Disease research
- Surgical Planning
- Devise Design





Blocked artery treated with stent

Introduction

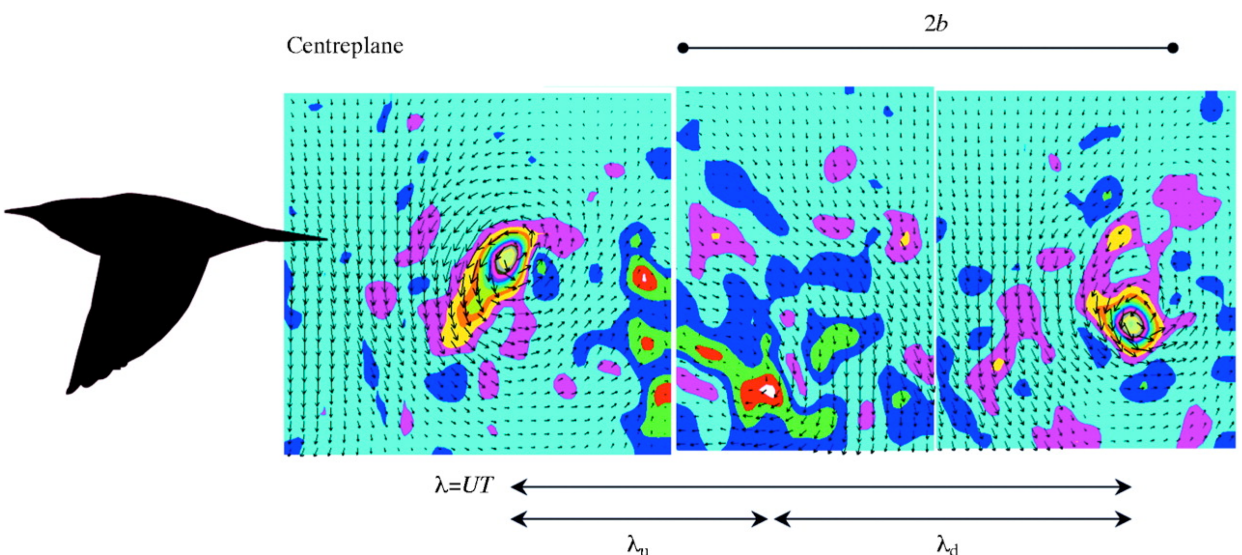
Is turbulence important in biological flows?

Example 2: In external flows Re number can be higher. Turbulent wakes can be observed in:

- Insect and bird flight
- Fish swimming
- Man-made devices (μAVs, UAVs, etc.)

Impact on:

- Unsteady aerodynamics
- Devise Design



Wake of a thrush nightingale in free flight (G. Spedding)

Introduction

Simulations of biological flows?

Basic characteristics:

- Unsteady fully three-dimensional flows
- Transitional, non-equilibrium flows
- RANS closures not appropriate

Eddy resolving approaches like Direct Numerical Simulations (DNS) or Large-Eddy Simulations (LES) are ideal

Feasible: low and moderate Re numbers

What are the challenges in LES/DNS?

- Geometric complexity
- Fluid Structure Interactions
- Complex Fluids
- Unsteady boundary conditions
- …………

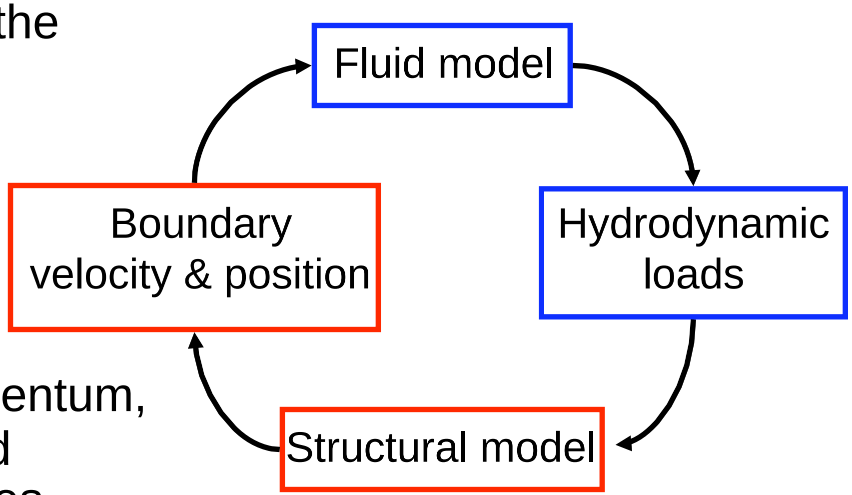
- Very little work has been done on FSI in LES
- Priority in order to cover a wide area of applications

Methodologies

Fluid-Structure interactions

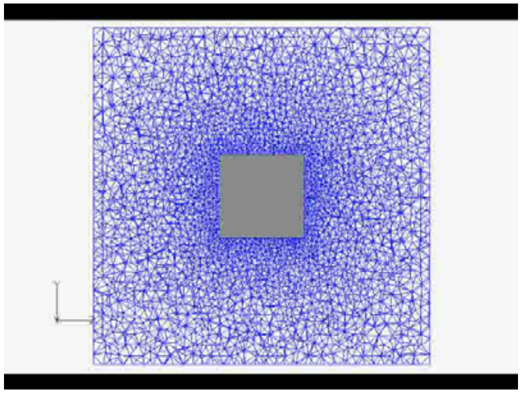
- Fluid-Structure interaction simulations are among the most challenging problems in computational mechanics. In grid based methods two are the main challenges:
  - Boundary motion
  - Coupling scheme

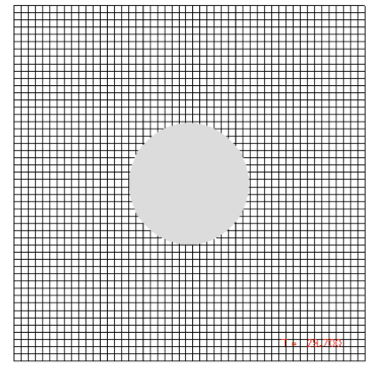
- DNS/LES also requires optimal mass, momentum, and energy conservation properties to avoid contamination of the smallest resolved scales



Methodologies

Fluid-Structure interactions





Boundary conforming methods (BCM)

- Grid deformation is required to satisfy the conformation constrain
- Equations need to be modified to account for relative motion to the grid
- Boundary conditions are imposed as with stationary bodies
- Flexible in clustering grid points
- For large deformations grid quality is an issue for stability and efficiency

Non-Boundary conforming methods (nBCM)

- A fixed Eulerian grid is used at all times
- Equations of motion remain unchanged
- Imposition of boundary conditions is not trivial
- Inflexible in clustering grid points
- Quality of the solution does not depend on how large deformations are

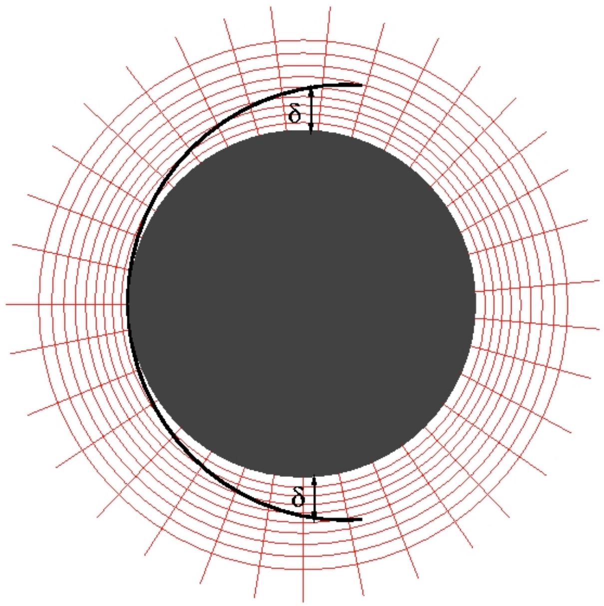
NBCM can be cost/efficient for DNS/LES at moderate Re

- Imposition of B.C. on a grid not aligned to body
- Coupling with structural model
- Adaptive mesh refinement

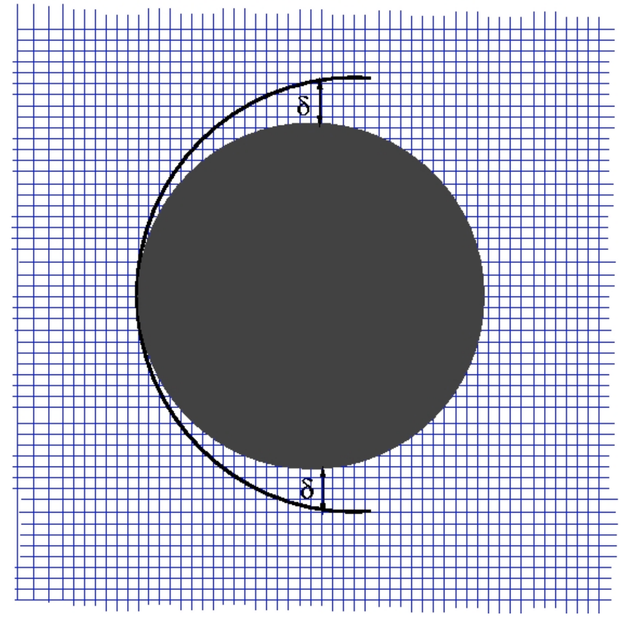
Methodologies

resolution requirements

Boundary-Conforming Methods (BCM)



Non-Boundary-Conforming Methods (NBCM)



- **As Re ↑, total number of grid points grows faster for NBCM than BCM**
- **For laminar boundary layers, number of points of NBCM / BCM ∝ Re^n**

Methodologies

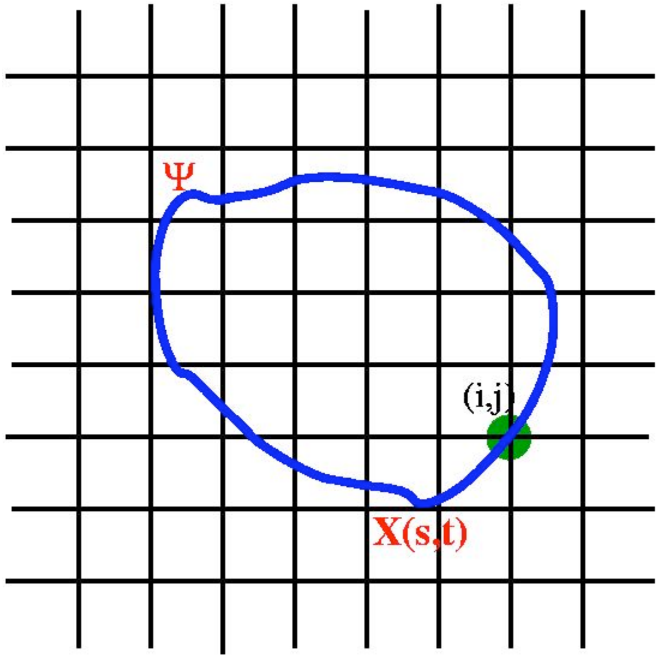
The embedded boundary approach

Assume that the Dirichlet boundary condition, u_Ψ, needs to be enforced at point (i,j) and u_{ij} is an approximation to the solution of the N-S equations:

$$\frac{(u_{ij}^{n+1} - u_{ij}^{n})}{\Delta t} = RHS + f_{ij}, \qquad (1)$$

To compute f_{ij} replace u_{ij}^{n+1} with u_Ψ in equation (1) and solve for the forcing:

$$f_{ij} = \frac{(u_\Psi - u_{ij}^{n})}{\Delta t} - RHS. \qquad (2)$$



- Practically the solution is reconstructed locally to satisfy boundary conditions (*Fadlun et. al. 2000*)
- This is equivalent to the use of a forcing function

Methodologies

Embedded boundary method: implementation

- Step 1: Establishment of the grid/interface relation
- Step 2: Reconstruction of the solution near the immersed boundary
- Step 4: Treatment of points that change phase

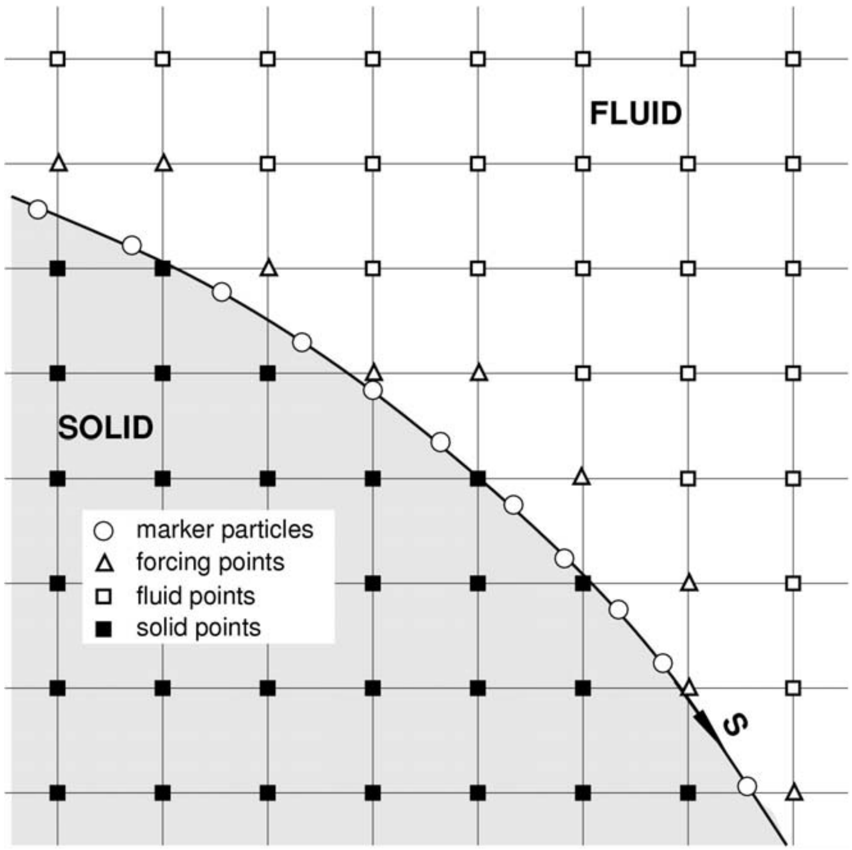
Methodologies
(Basic Fluid Solver)

- Cartesian/Cylindrical coordinates
- Semi-implicit Crank-Nicolson/Adams Bashforth fractional step method
- Second order central difference on a staggered grid
- The Lagrangian dynamic eddy viscosity model is used for the parameterization of the SGS
- Solver is parallelized using domain a decomposition approach

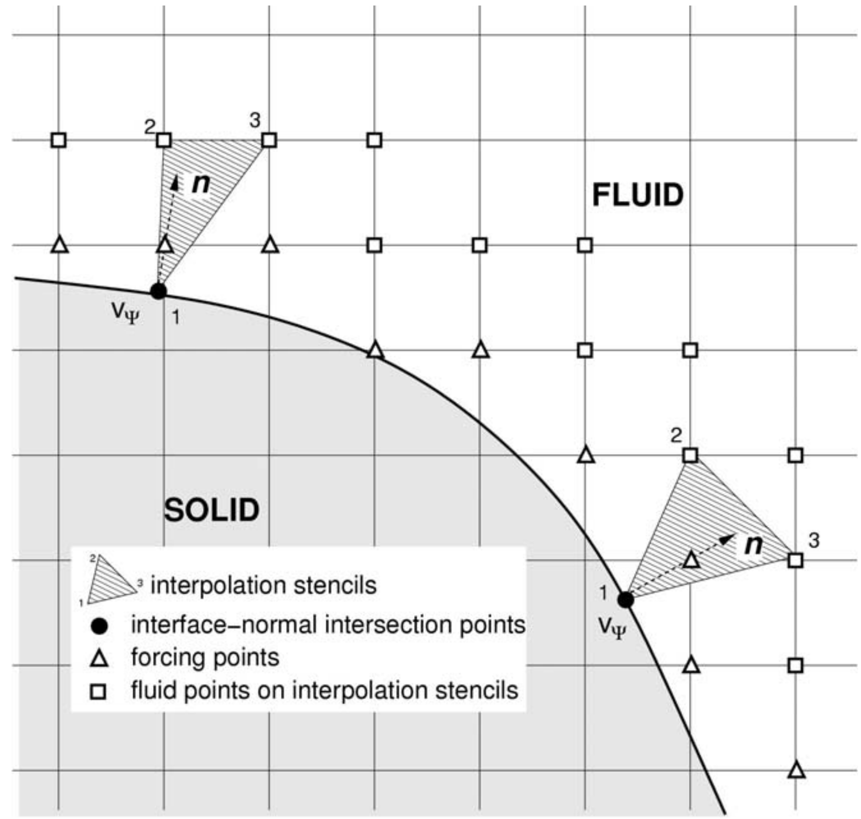
Methodologies

Embedded boundary method: Steps 1-3

Tagging



Local Reconstruction



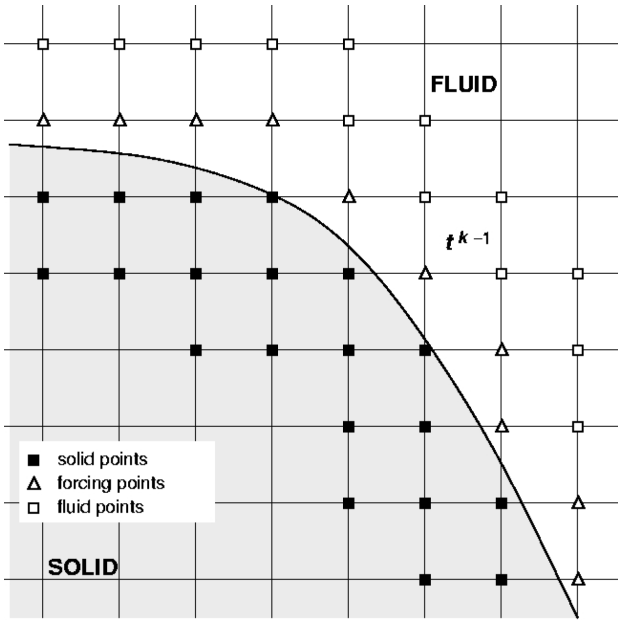
△ Boundary Points; ■ Solid Points; □ Fluid Points

B.C. for interface applied on boundary points

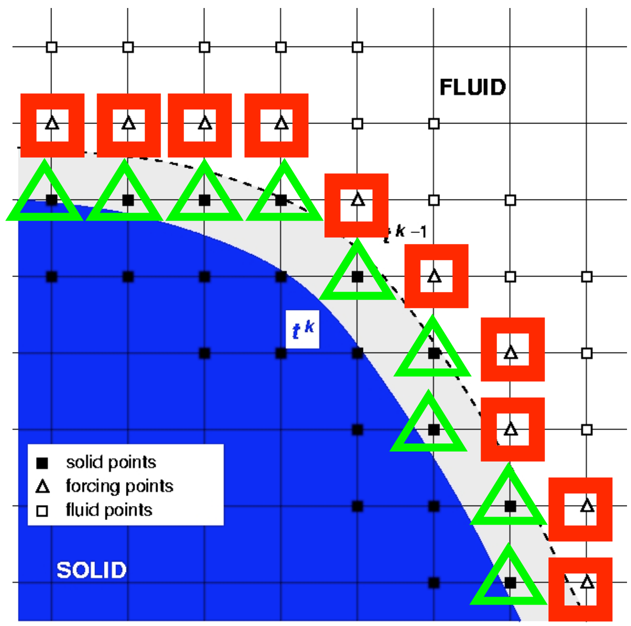
Methodologies

Embedded boundary method: Step 4

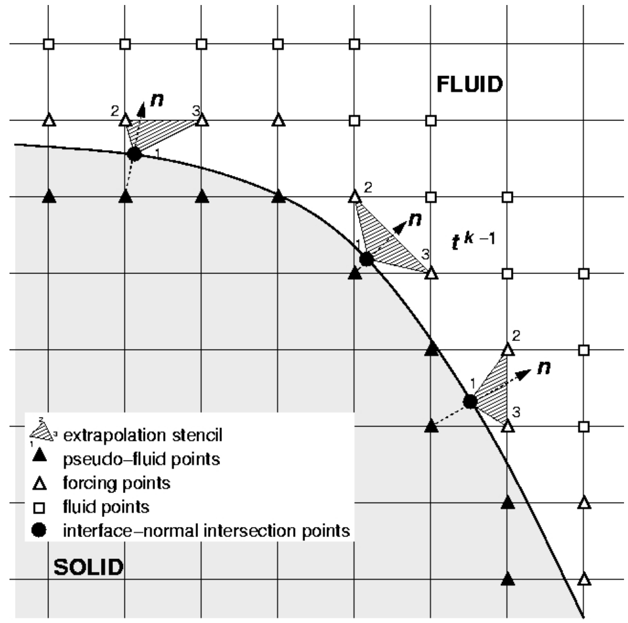
Time Step *k* -1



Time Step *k*



Time Step *k* -1



: Old Boundary Points → New Fluid Points
Physical Solution at Time Step *k* -1
Non-physical Derivatives at Time Step *k* -1

Field Extension at Time Step *k* -1:
Extrapolate Solution near the Interface
Both Solution and Its derivatives are orrect

Balaras *Comput. & Fluids* 2004 Yang & Balaras *J. Comput. Phys*. 2006

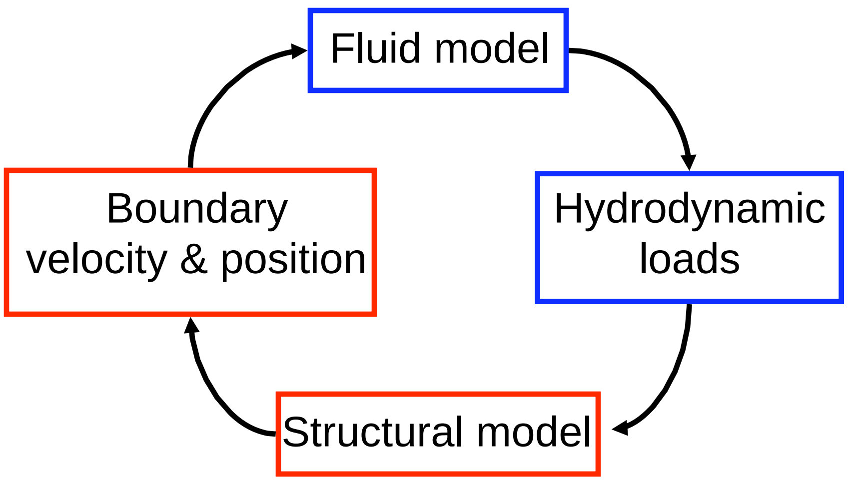
Methodologies

Coupling scheme

Two general categories of coupling schemes:

- Weak coupling: Equations for fluid and structure are advanced sequentially using the latest info available.

- Strong coupling: Equations for fluid and structure are advanced simultaneously



Which one?

- Weak coupling schemes are unstable for low density ratios

- Strong coupling computationally expensive

Methodologies

Strong Coupling scheme

$$ {}^{p}\mathbf{y}^{j} = \mathbf{y}^{j-4} + \frac{4}{3}\Delta t \left(2\ \mathbf{F}^{j-1} - \mathbf{F}^{j-2} + 2\ \mathbf{F}^{j-3}\right) $$

$$ \mathbf{y}^{j} = {}^{k+1}\mathbf{y}^{j} - \mathbf{e}^{j} $$

$$ \begin{aligned} \frac{\hat{u}_i^k - u_i^{k-1}}{\Delta t} &= RHS_i^k + f_i^k \\ \frac{\partial \phi^k}{\partial x_i \partial x_i} &= \frac{1}{\alpha_k \Delta t}\frac{\partial \hat{u}_i^k}{\partial x_i}, \\ u_i^k &= \hat{u}_i^k - \alpha_k \Delta t \frac{\partial \phi^k}{\partial x_i}, \\ p^k &= p^{k-1} + \phi^k \end{aligned} $$

$$ e^{j} = \left\| {}^{k+1}\mathbf{y}^{j} - {}^{k}\mathbf{y}^{j} \right\|_{\infty} $$

$$ {}^{k+1}\mathbf{y}^{j} = \frac{1}{8}\left[9\ \mathbf{y}^{j-1} - \mathbf{y}^{j-3} + 3\Delta t \left({}^{k}\mathbf{F}^{j} + 2\ \mathbf{F}^{j-1} - \mathbf{F}^{j-2}\right)\right] $$

Methodologies

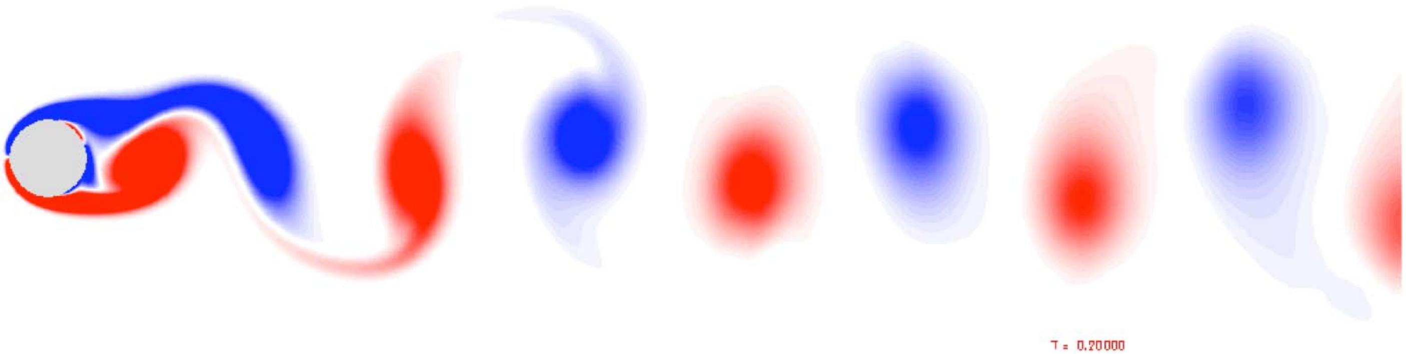
Coupling scheme: stability

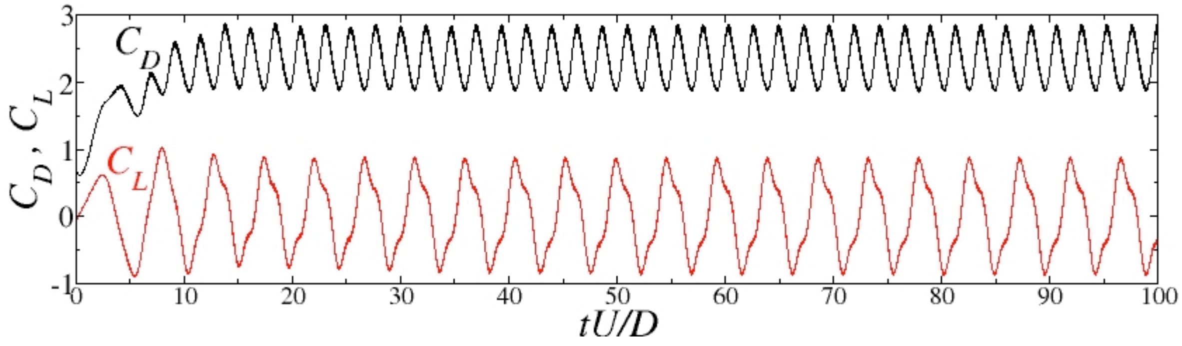
Re = UD/ν = 200

Damping Ratio ζ=0.004

Mass Ratio n = 0.89

Reduced Velocity U_{red} = 4

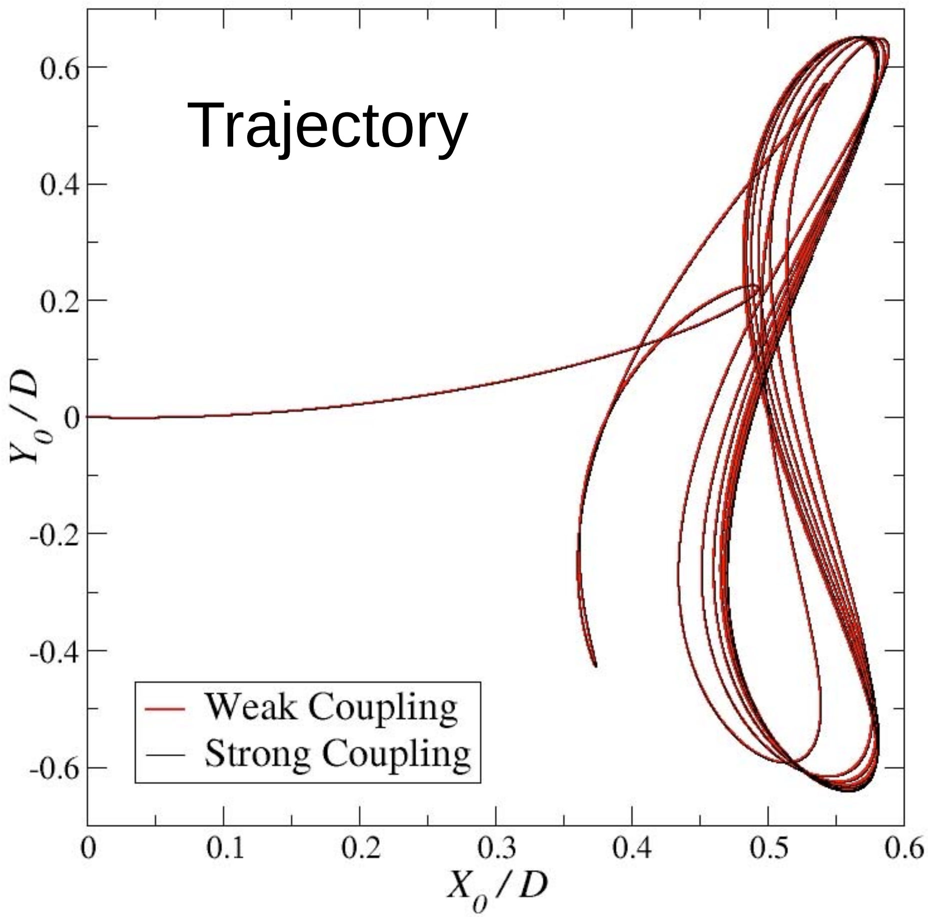




Methodologies

Coupling scheme: stability

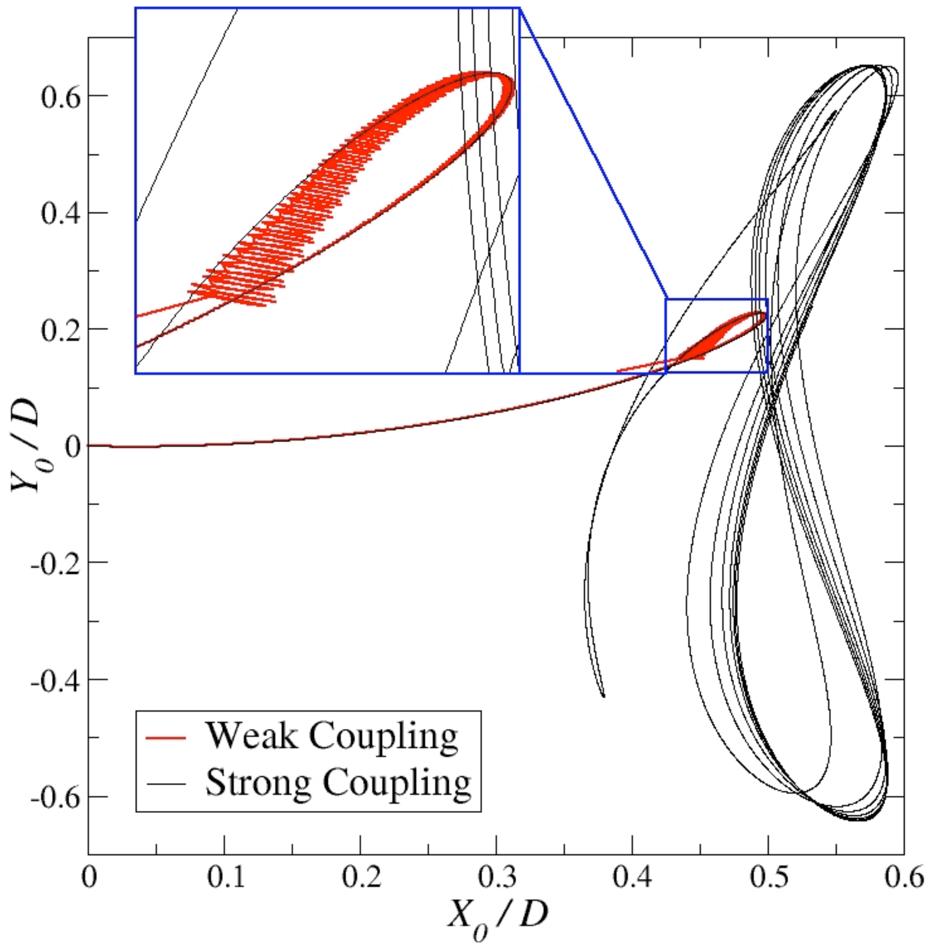
Mass Ratio n = 0.89



Ignorable Differences

Strong Coupling: $N_{iter} \approx 4$

Mass Ratio n = 0.88



Weak Coupling: Diverges

Strong Coupling: Stable

Methodologies

Coupling scheme: robustness

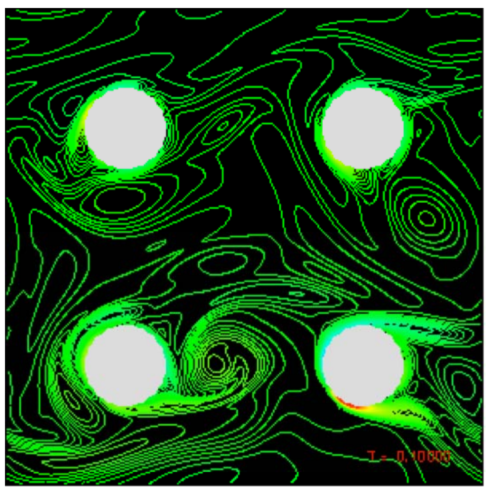
- Re = $U_{bulk}D/\nu$ = 200
- Mass Ratio n = 10
- Damping Ratio ζ=0.03
- Reduced Velocity U_{red} = 5

Yang et. al. *J. Fluids & Structures* 2007

2 x 1 DoFs

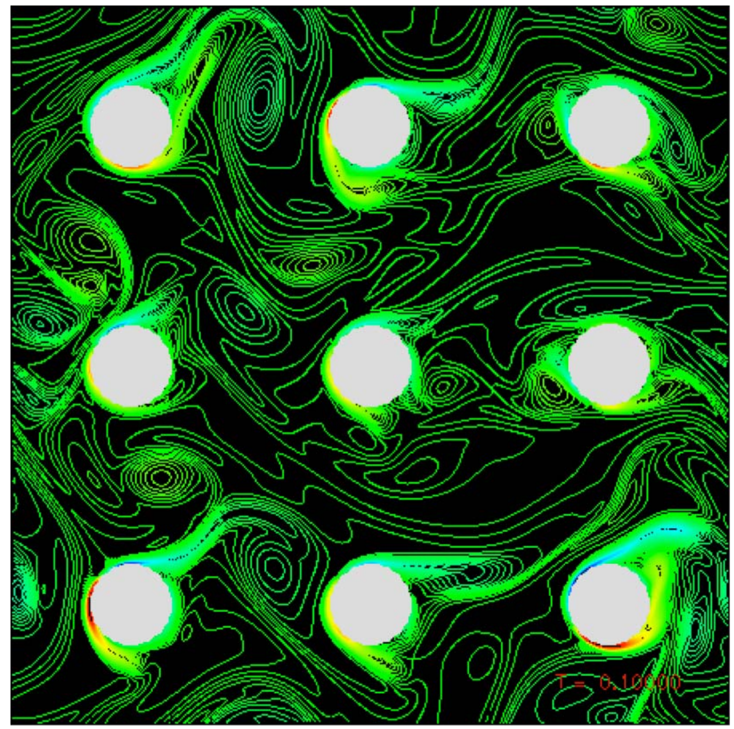
N_{iter}/timestep≈1.7

2 x 4 DoFs



N_{iter}/timestep ≈ 2

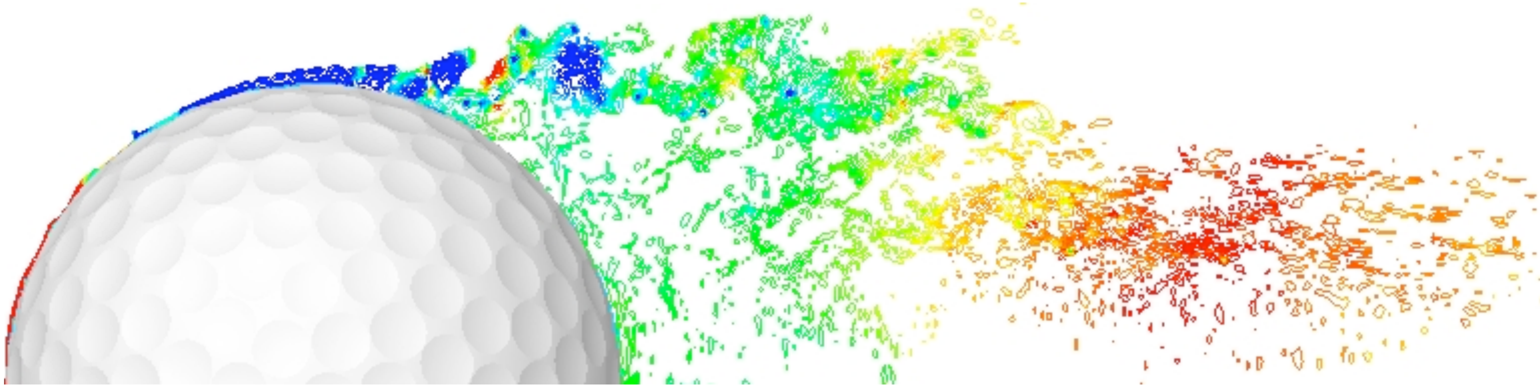
2 x 9 DoFs



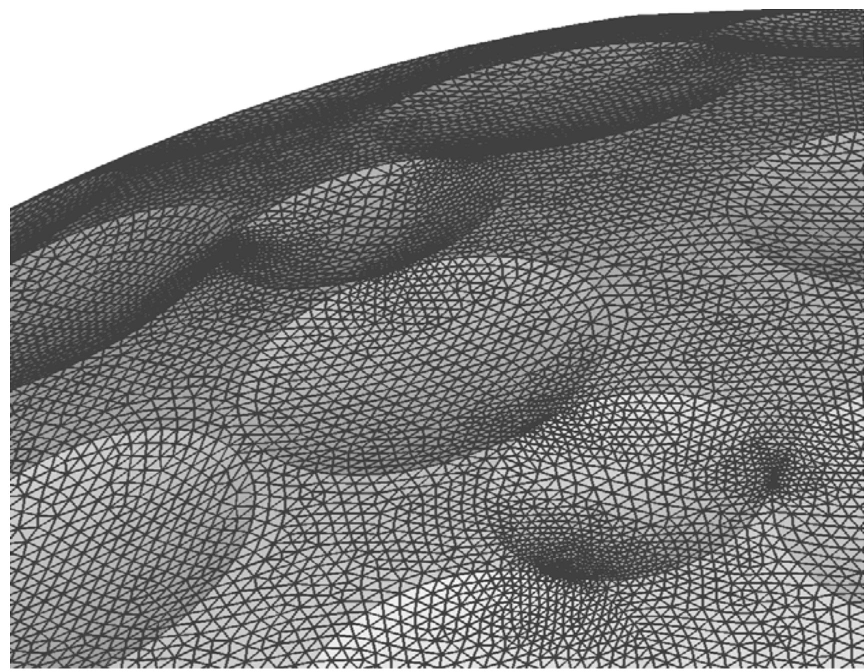
N_{iter}/timestep ≈ 2

Methodologies

code performance: flow around a golf ball



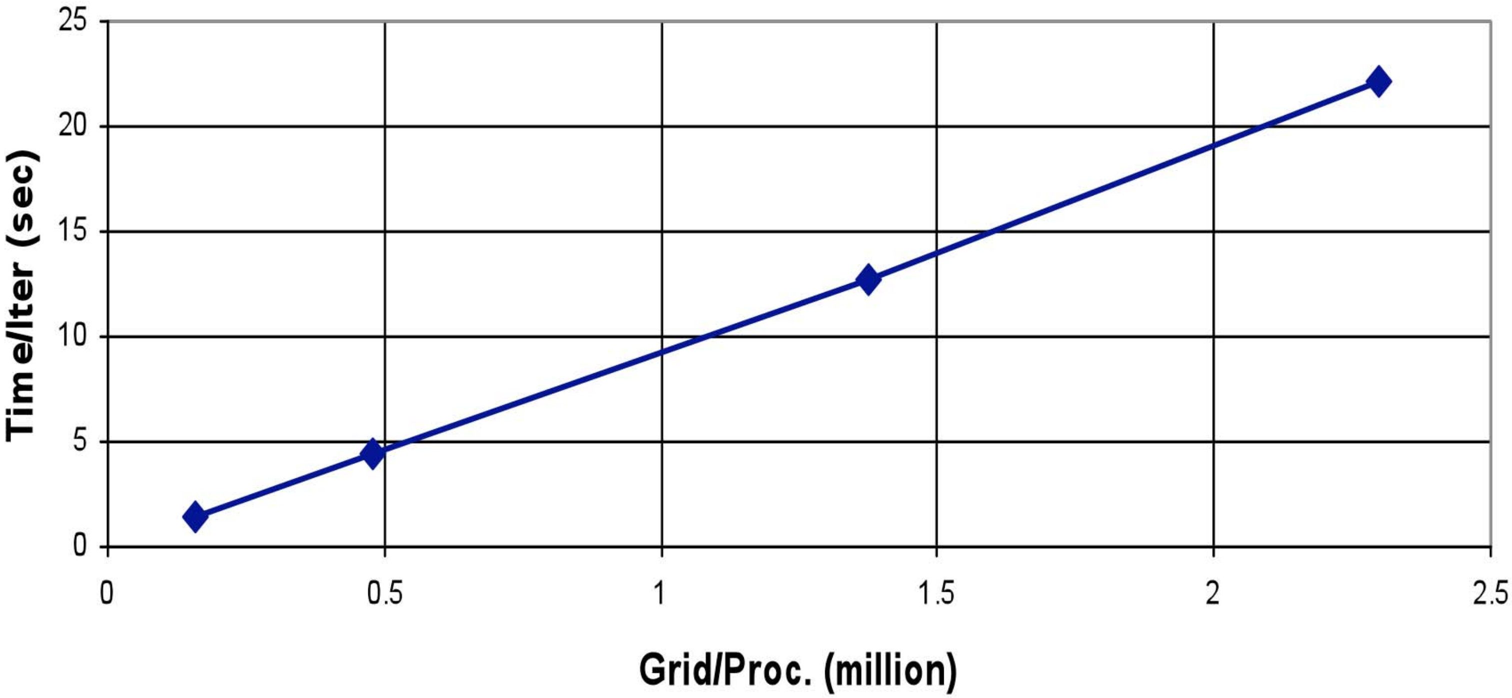
- Grid resolution:
  - Marginal grid: **61 million** points
    - 316 x 127 x 1502 (64 proc)
  - Coarse grid: **172 million** points
    - 536 x 127 x 2502 (125 proc)
  - Intermediate grid: **575 million** points
    - 760 x 252 x 3002 (250 proc)
  - Fine grid: **1.14 billion** points
    - 760 x 502 x 3002 (500 proc)



surface mesh

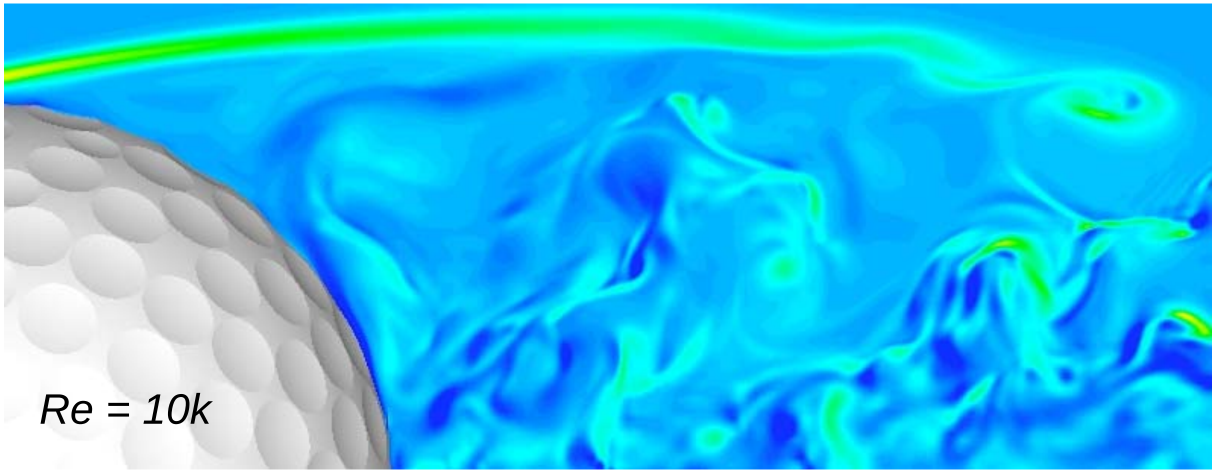
Methodologies

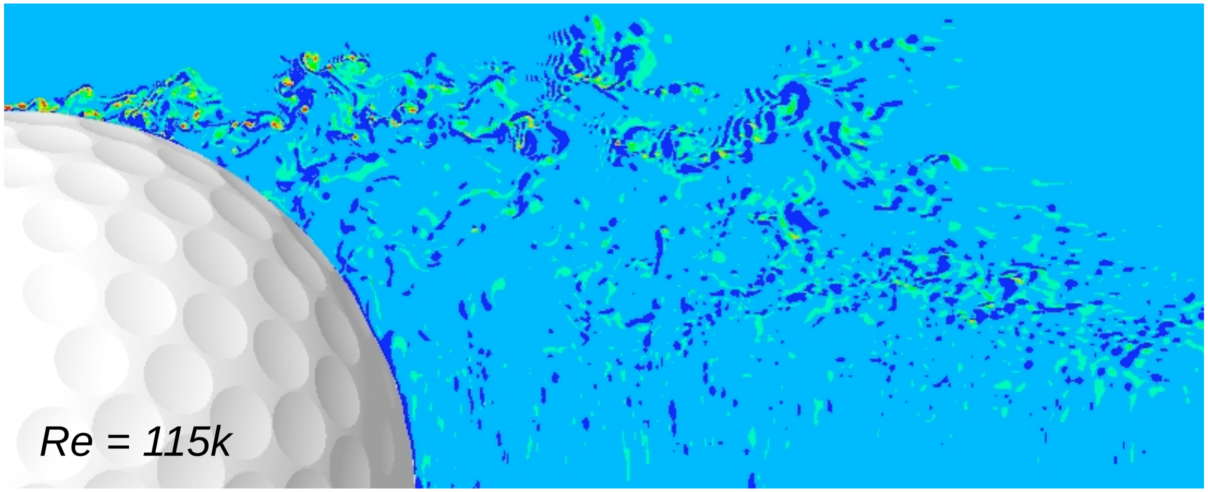
code performance: flow around a golf ball



Methodologies

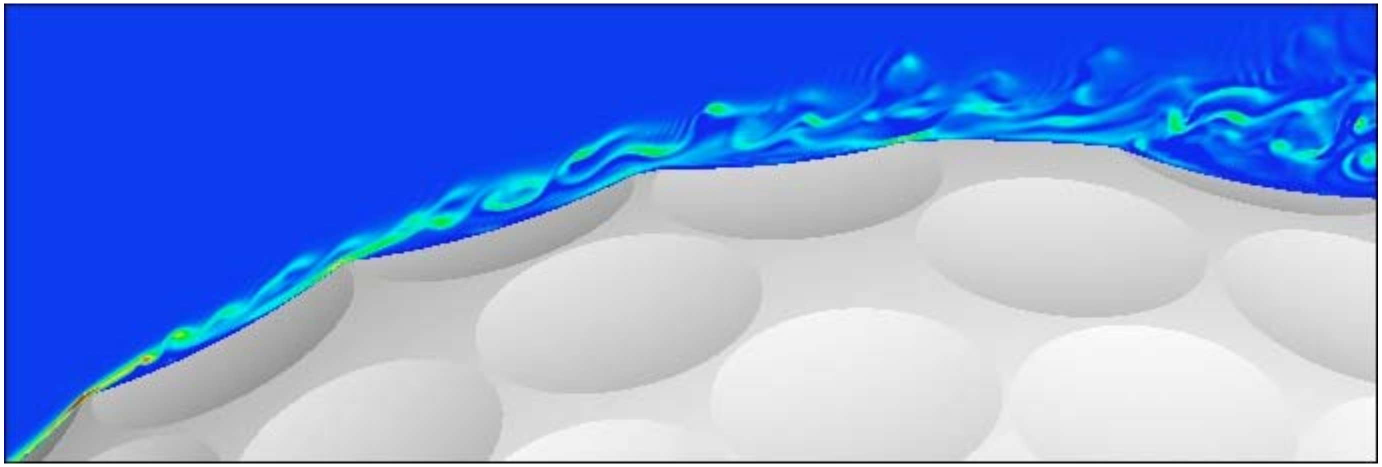
code performance: flow around a golf ball

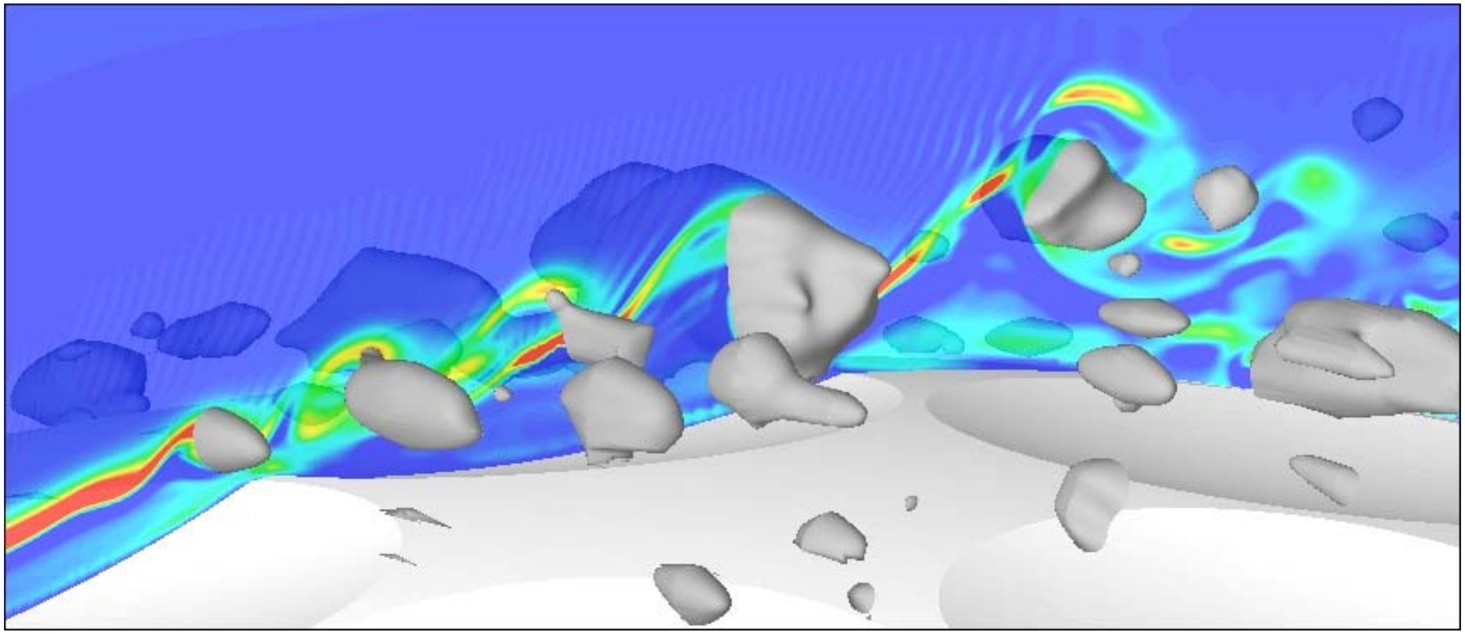




Methodologies

code performance: flow around a golf ball





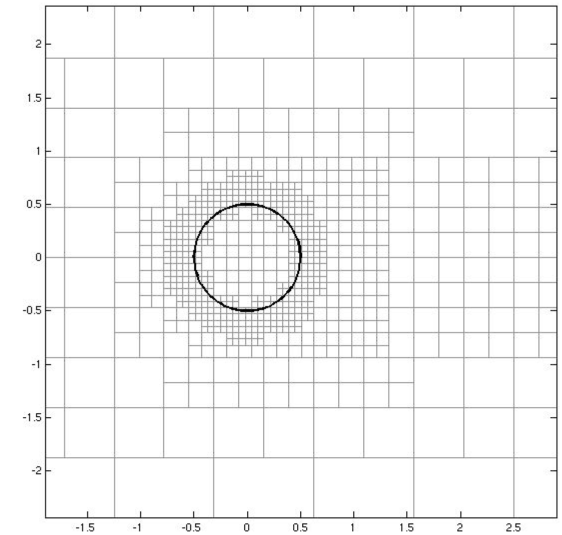
Methodologies

Adaptive mesh refinement

- Flexibility in distributing grid nodes is important in moving boundary problems

- Local refinement of a sub-grid block is performed by bisection in each coordinate direction.

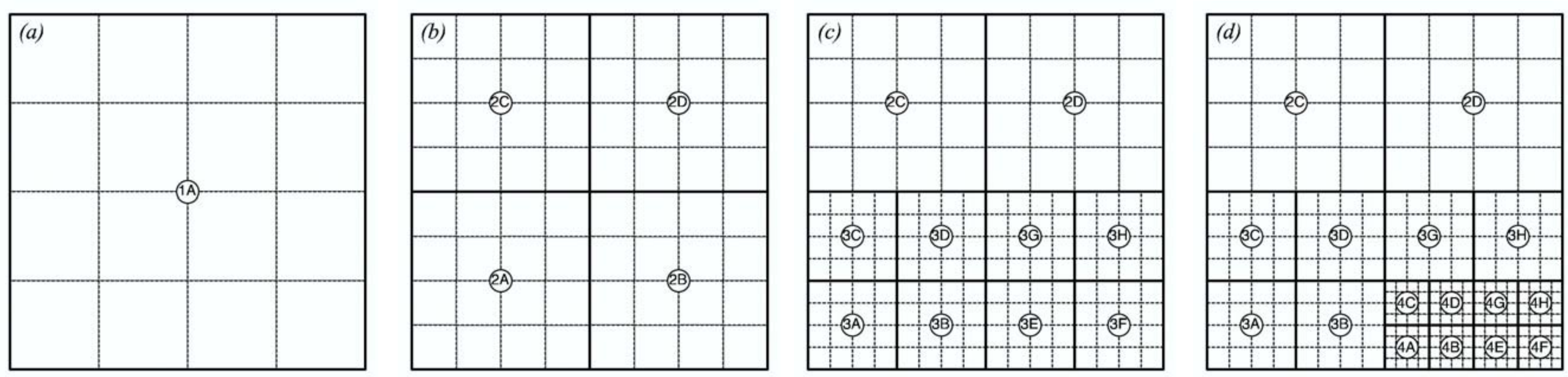
- Each sub-grid block has a structured Cartesian topology and utilizes the single block solver described before



Cross-section of locally refined grid around a sphere

Adaptive Mesh Refinement

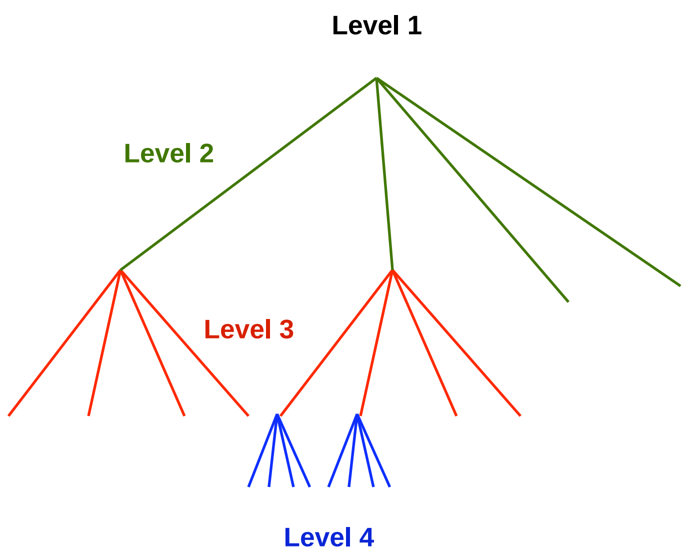
topology



Divide the domain in sub-blocks. Each sub-grid block has a structured Cartesian topology, and is part of a tree data structure that covers the entire computational domain.

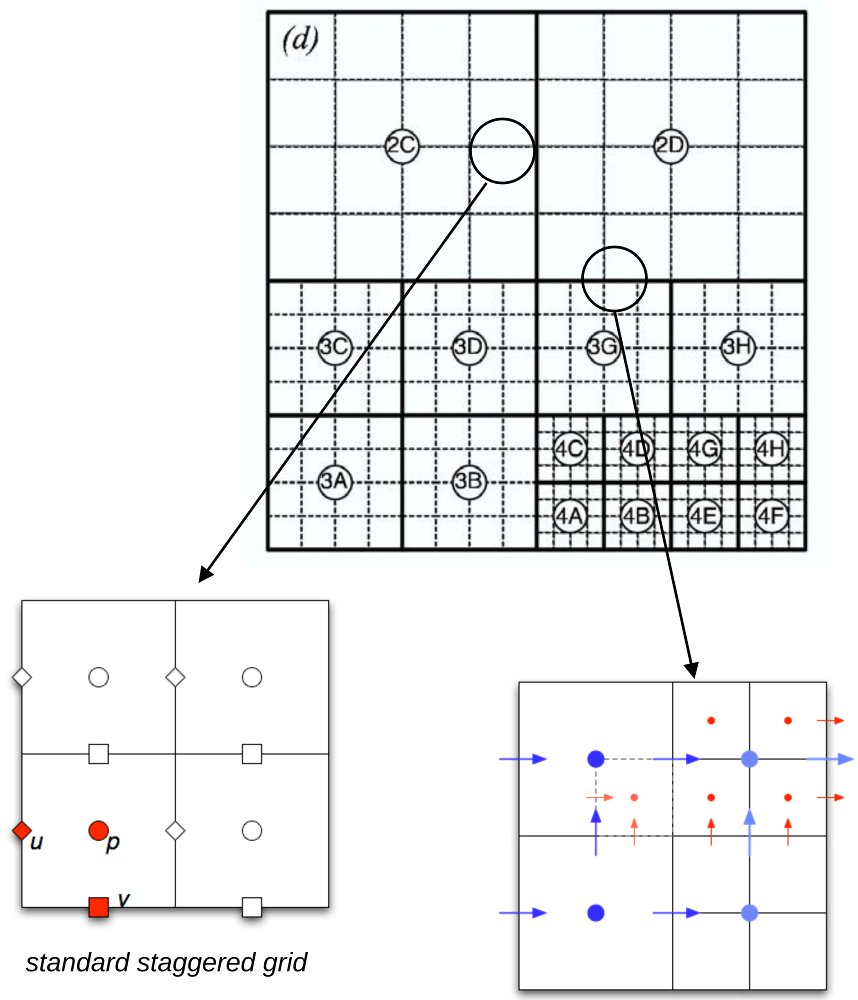
Local refinement of a sub-grid block is performed by bisection in each coordinate direction.

Number of nodes in each sub-block remains constant



Adaptive mesh refinement: overview

- We use a **projection method**, where advective and diffusive terms are advanced explicitly
- We use the **Paramesh toolkit** (developed by MacNeice and Olson) for the implementation of the AMR process. The package creates and maintains the hierarchy of sub-grid blocks, with each block containing a fixed number of grid points.
- A **single-block Cartesian** grid solver is employed in each sub-grid block:
    - standard staggered grid in each sub-block
    - second-order central finite-differences
- A **multigrid** solver is used for the **Poisson** equation (adapted from **FLASH**)
- **Guard cells** are used to discretize equations at the interior coarse-fine interfaces



standard staggered grid

coarse-fine interface

Adaptive mesh refinement: accuracy

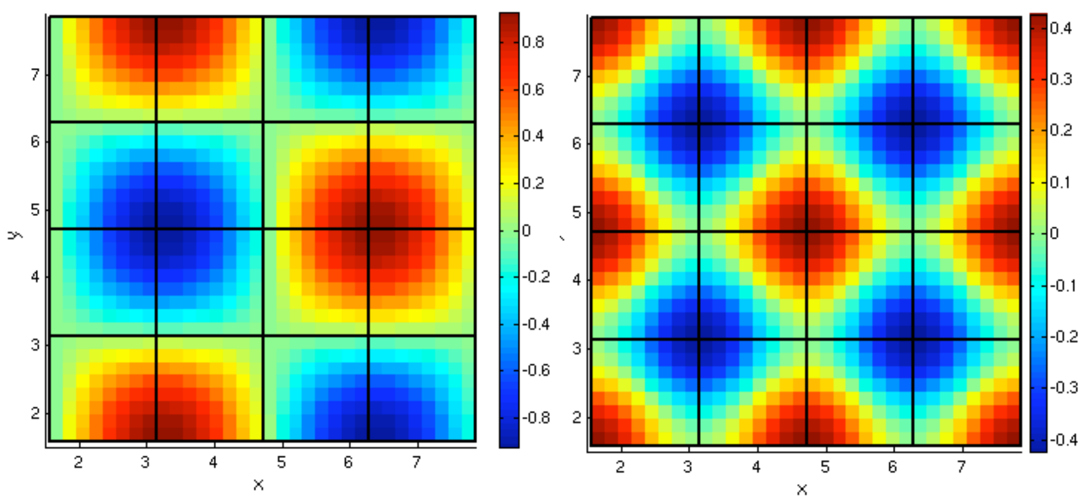
Validation: Taylor Green Vortex

- Compare numerical solution to analytical solution of 2D Navier-Stokes equations
- Domain:
  [π/2, 5π/2]x [π/2, 5π/2]
- Homogeneous Dirichlet/Neumann velocity boundary conditions and Neumann pressure boundary condition

$$u = -e^{-2t}\cos x \sin y$$

$$v = e^{-2t}\sin x \cos y$$

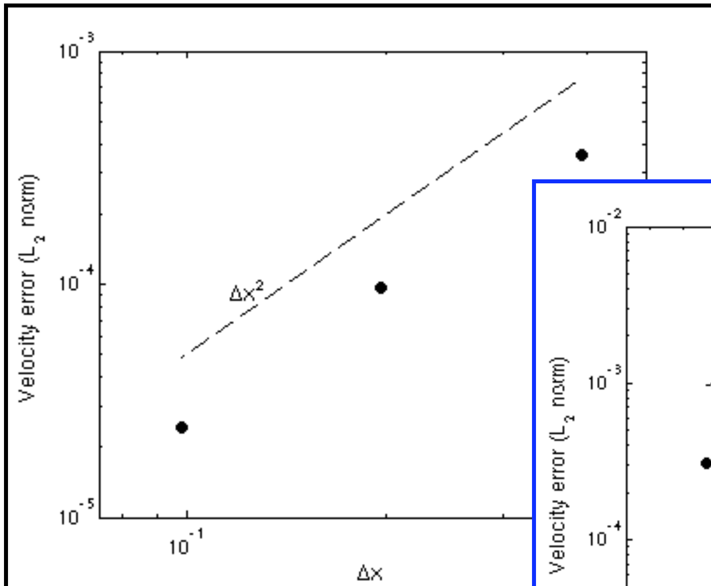
$$p = -\frac{e^{-4t}}{4}\left(\cos 2x + \cos 2y\right)$$



u *p*

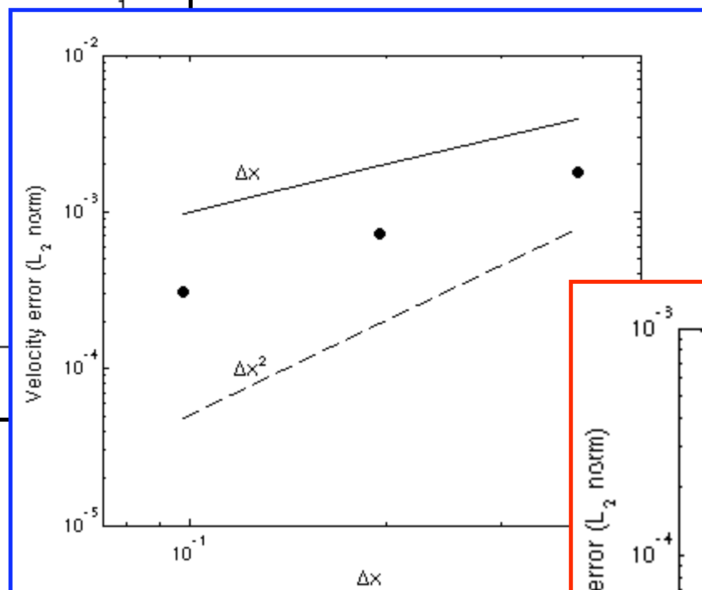
Adaptive mesh refinement: accuracy

Validation: Taylor Green Vortex

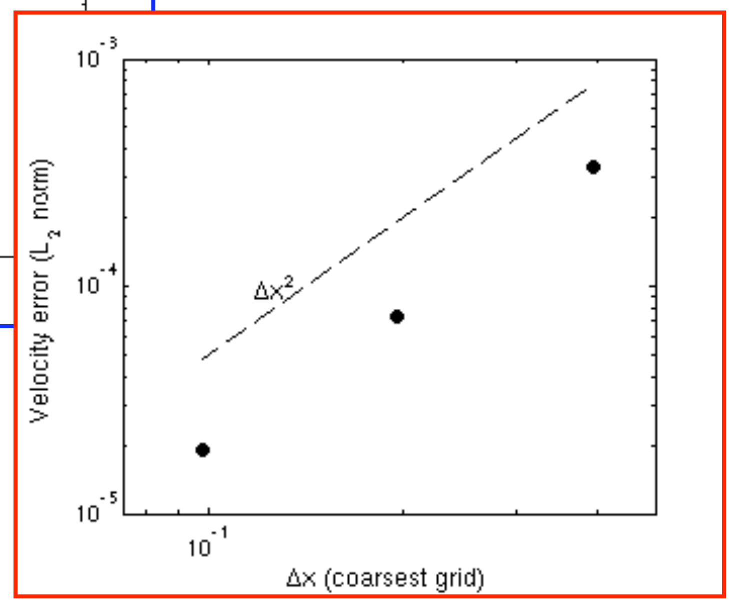


Uniform domain

Domain with 2 refinement levels linear interpolation



Domain with 2 refinement levels quadratic interpolation

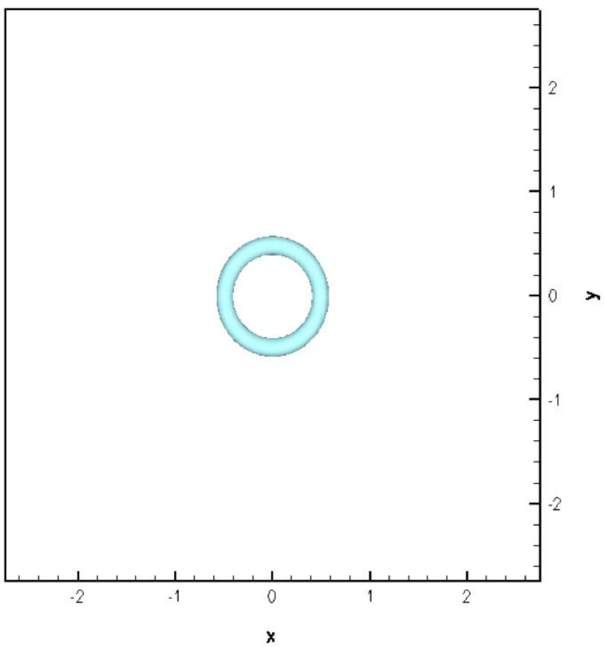


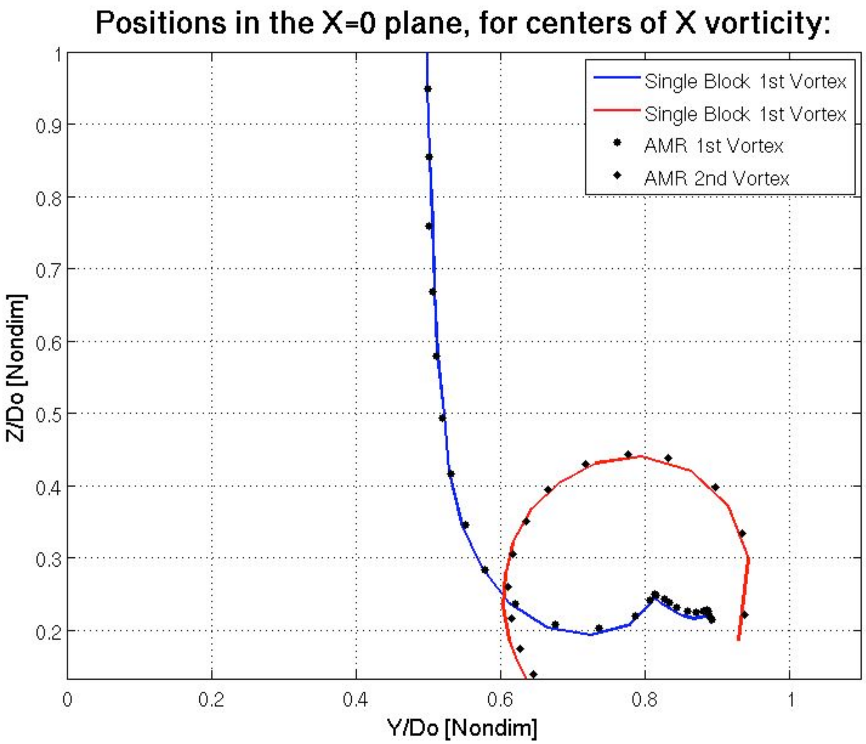
- interpolation strategy is critical in maintaining the 2nd order accuracy of numerical scheme

Adaptive mesh refinement: validation

Vortex Ring impinging on a wall, Re ≈ 570

- Compare AMR solution to numerical solution using a Single Block, Cartesian solver.
- Velocity Dirichlet BCs in top and Bottom Boundaries, periodic on side walls. Pressure Neumann BCs.





Q contour for vortex impinging normal to a wall, Re ≈ 570 (top view)

Adaptive mesh refinement: validation

Vortex Ring impinging on a wall, Re ≈ 570

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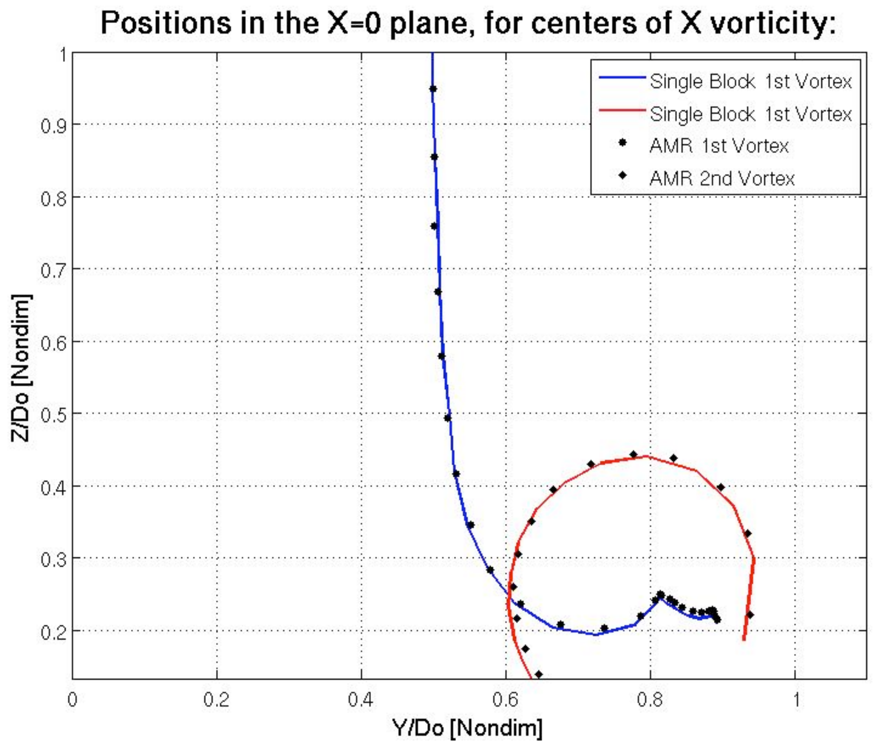
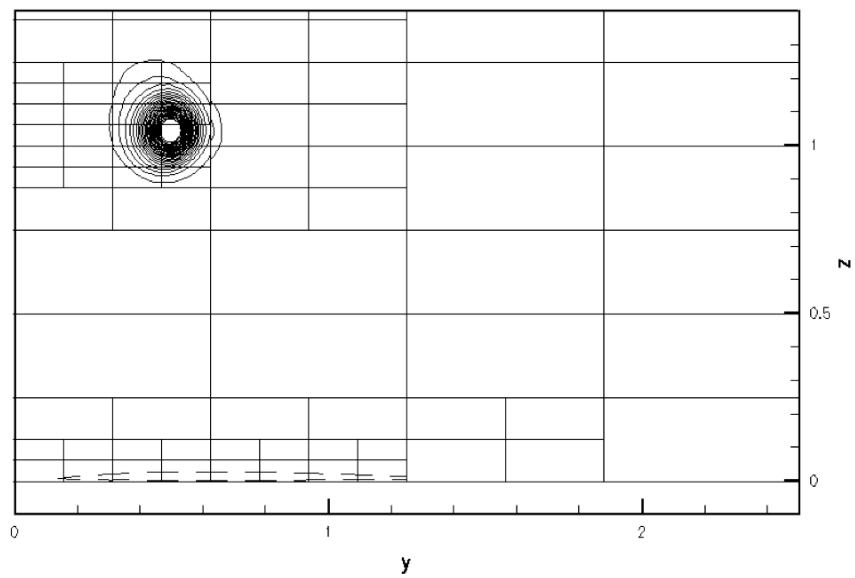
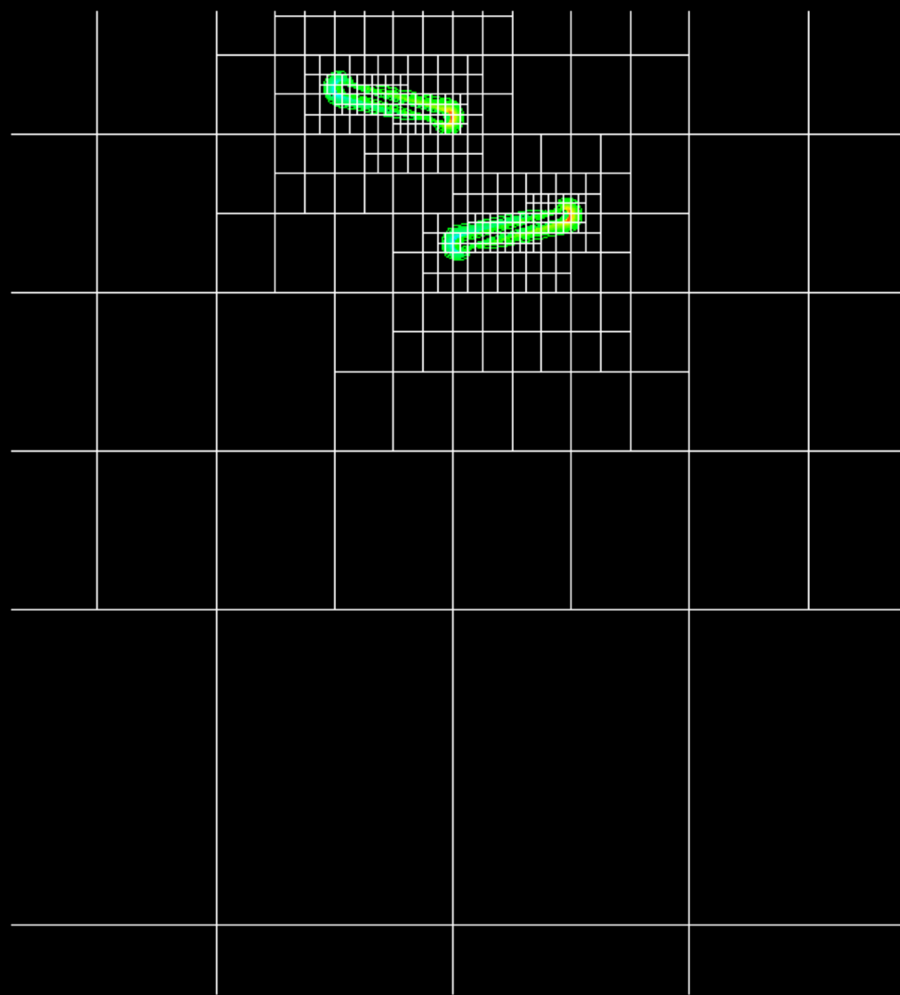




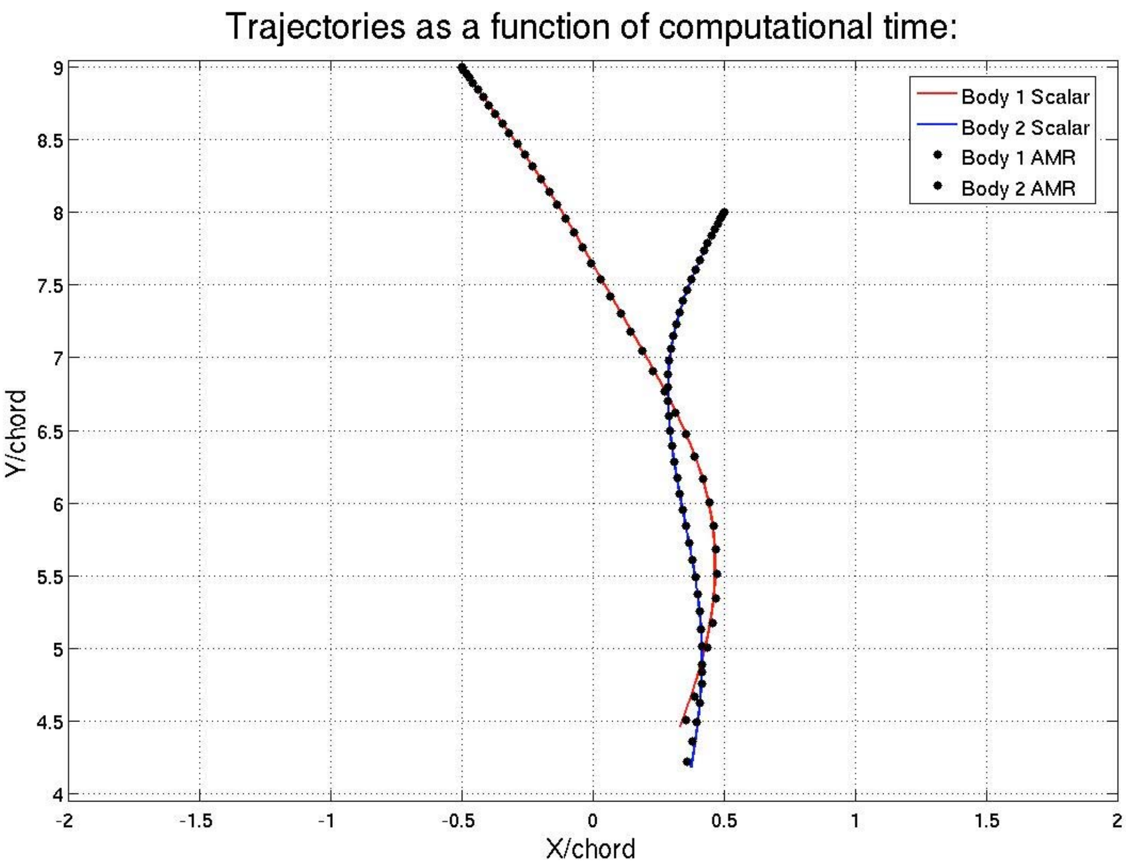
vorticity isolines at a cross section, Re ≈ 570

Falling plates: results



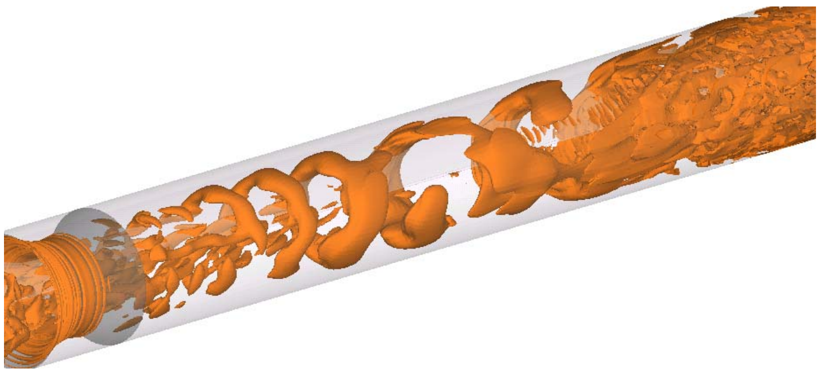
Vorticity contours and Block boundaries for AMR calculation.

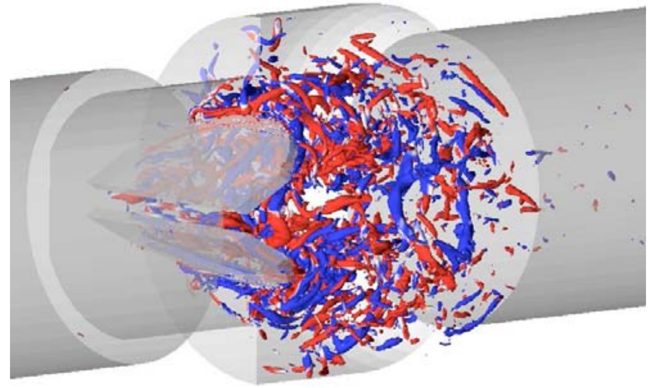
Falling plates: results

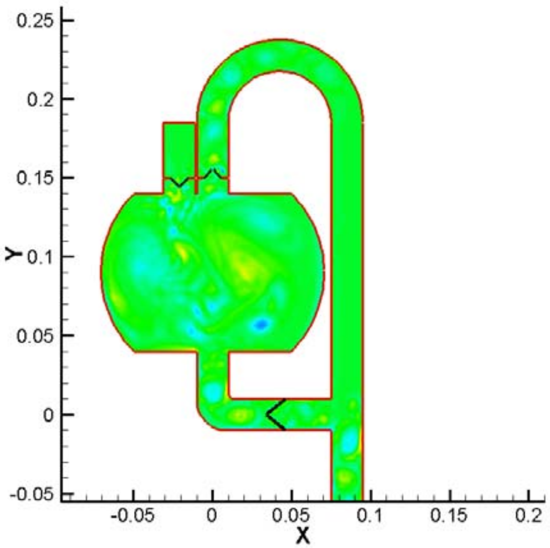


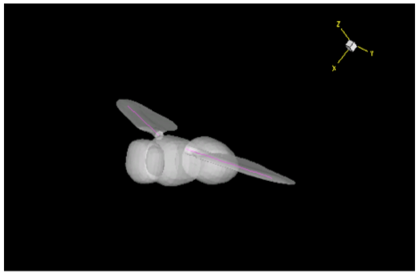
Vanella, Rabenold & Balaras, *J. Comp. Phys. 2008* (under review)

Applications

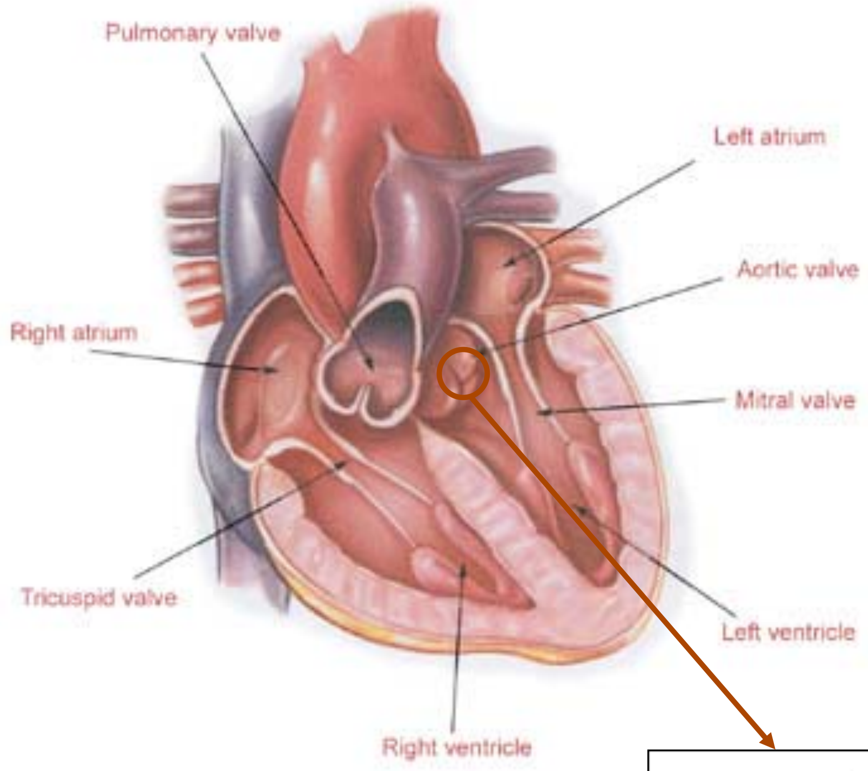


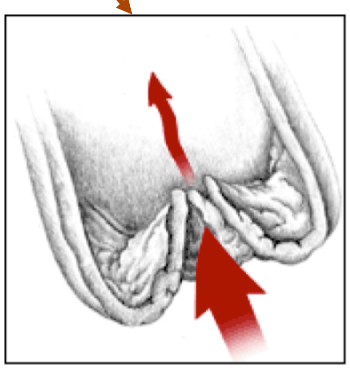






Heart valve disease





CALCIFIED AORTIC VALVE

- 4 chambers
  - 2 atriums
  - 2 ventricles
- 4 valves
  - 2 atrioventricular
  - 2 semilunar
- Left side; high pressure
- Right side: low pressure
- Mitrial and Aortic valves are the most commonly affected valves

Heart valve disease

- Replacement of defective heart valves with artificial prostheses is a 'safe' and routine surgical procedure worldwide (180,000/year)
- Several different types of prosthetic valves:
  - Mechanical HV
    - high durability, excellent biocompatibility, low level of transvalvular pressure drop
    - Hemolysis and thrombus formation are major complications
  - Bioprosthetic (tissue) HV
    - (better hemodynamics, long-term anticoagulants not required)

Mechanical bi-leaflet

Bio-prosthetic

Heart valve disease

- Valvular Heart Disease:
  - Not regarded as major public health problem
  - Common and Underdiagnosed?

Burden of valvular heart diseases: a population-based study

Vuyisile T Nkomo, Julius M Gardin, Thomas N Skelton, John S Gottdiener, Christopher G Scott, Maurice Enriquez-Sarano

Background Valvular heart diseases are not usually regarded as a major public-health problem. Our aim was to assess their prevalence and effect on overall survival in the general population.

Methods We pooled population-based studies to obtain data for 11 911 randomly selected adults from the general population who had been assessed prospectively with echocardiography. We also analysed data from a community study of 16 501 adults who had been assessed by clinically indicated echocardiography.

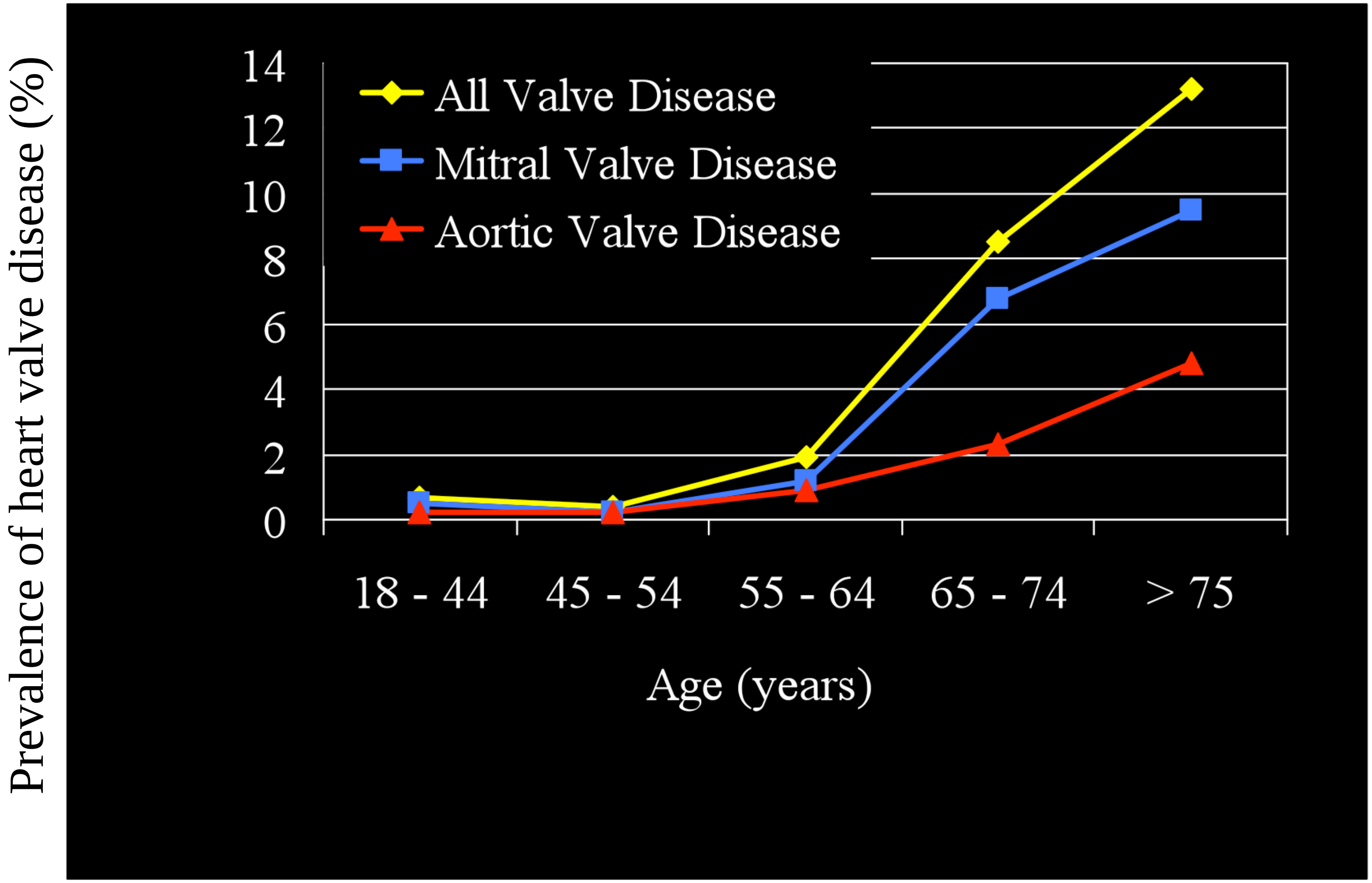
Lancet 2006; 368: 1005–11

Published Online August 18, 2006 DOI:10.1016/S0140-6736(06)69208-8

See Comment page 969

Mayo Clinic, Rochester, MN,

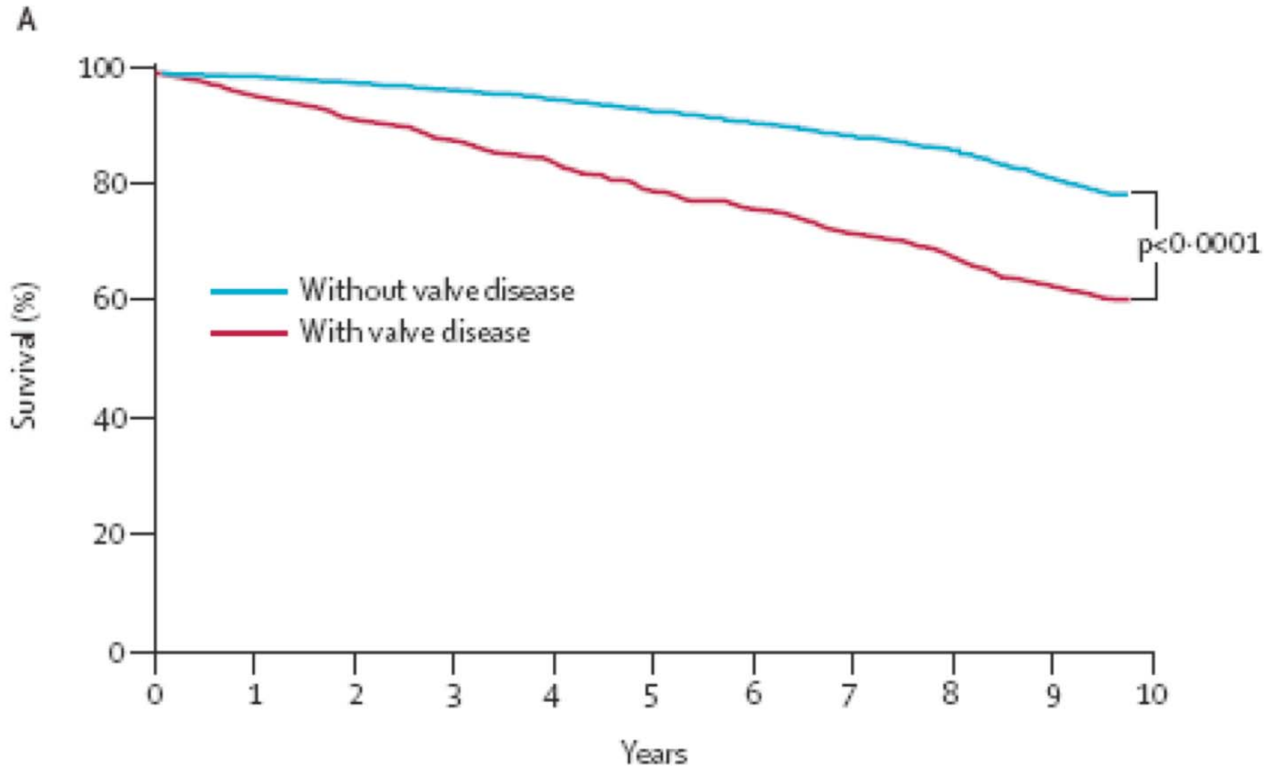
Heart valve disease



Nkomo VT et al. Burden of valvular heart diseases: a population-based study
Lancet 2006; 368:1005-11

Heart valve disease

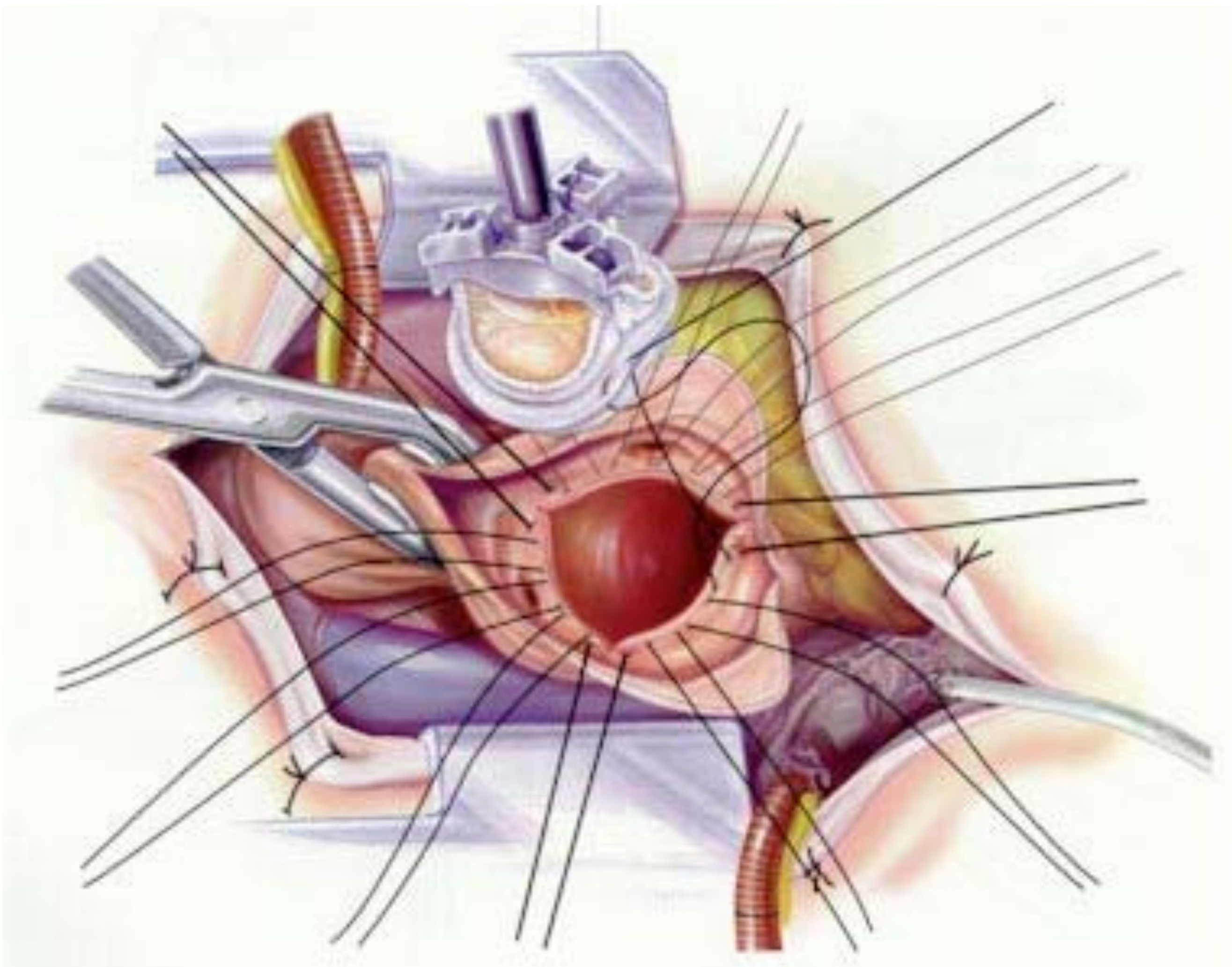
Survival after detection of moderate or severe valvular heart disease



Number at risk										
Valve disease	615	591	566	541	503	456	438	413	376	331
No valve disease	11296	11207	11050	10785	9507	8215	8001	7735	5054	3233

Nkomo VT et al. Burden of valvular heart diseases: a population-based study *Lancet* 2006; 368:1005-11

Treatment: Conventional AVR



Treatment: Conventional AVR

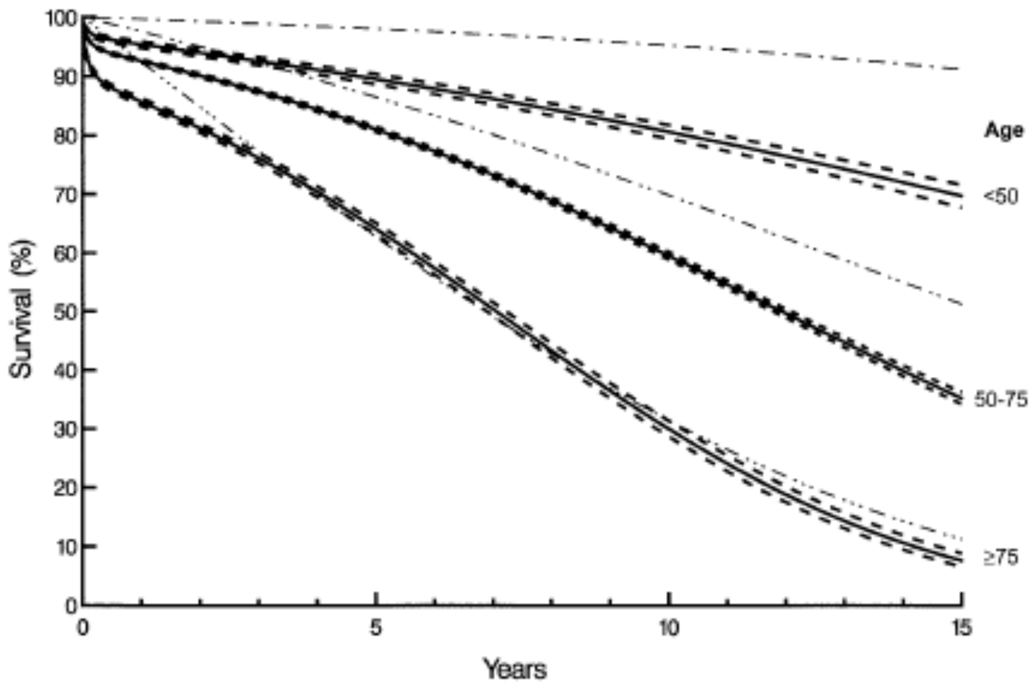
Current Status

Mean Age:	**66 years**
Prior Operation:	**17 %**
Cross-clamp time:	**80 minutes**
Perfusion time:	**110 minutes**
Operative Mortality:	**4 %**
Major Complications:	**18 %**
CVA:	**2 %**
Renal Failure	**5 %**

Source: Society of Thoracic Surgeons Database

Treatment: Conventional AVR

Perioperative mortality



Survival after aortic valve replacement by age. From Blackstone et al. 2003

Treatment: Conventional AVR

Long-term results with conventional AVR: Bad for the Brain

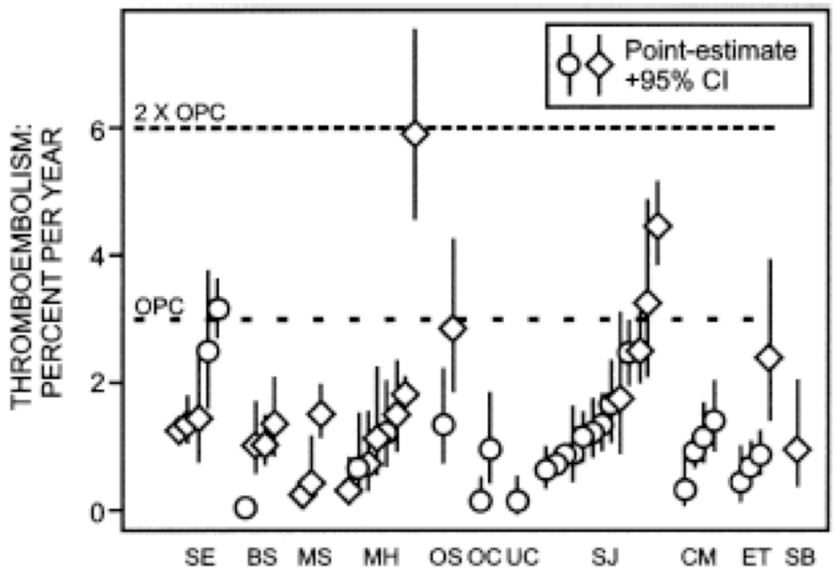


Figure 3. Thromboembolism rates for mechanical aortic valves. The vertical axis is the linearized rate in percentage per year. Each symbol represents one series. Circles indicate that only late events were used to calculate the rates; diamonds indicate that both early and late events were used. BS = Bjork Shiley; CM = Carbomedics; ET = Edwards Tekna or Duromedics; MH = Medtronic Hall; MS = Monostrut; OC = Omnicarbon; OPC = FDA's Objective Performance Criteria (from reference 29); OS = Omniscience; SB = Sorbin Bicarbon; SE = Starr Edwards; SJ = St. Jude; UC = Ultracor. From reference 29.

Treatment: Conventional AVR

Long-term results:

Causes of Death (% of all Deaths)*

	Mechanical	Bioprosthetic
Prosthesis related	37%	41%
Cardiac –not prosthesis related	17%	21 %
Noncardiac	36%	26%
Undetermined	10%	12%

At 15 years, **20 percent** had suffered a stroke: **Bad for the Brain**

* (Hammermeister, Sethi et al. 2000)
From The VA prospective valve replacement study – follow-up = ***15 years***.

Treatment: Conventional AVR

What is the role of LES/DNS?

1. Need to better correlate hemodynamic performance of current prosthetic valves to thromboembolic complications

2. Design better implants

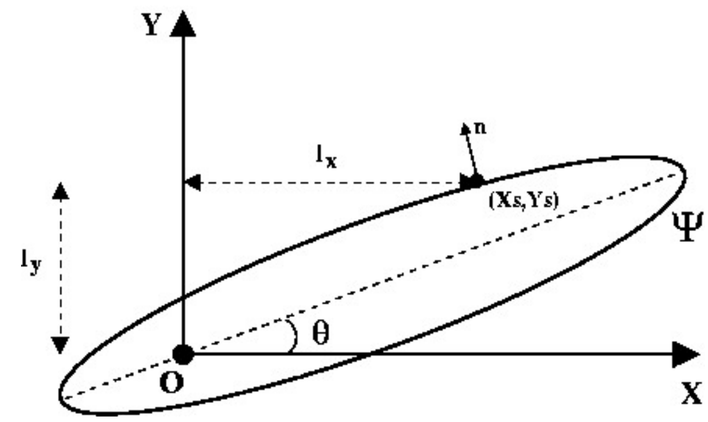
Flow around prosthetic heart valves

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} + \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_j \partial x_j} + f_i,$$

$$\frac{\partial u_i}{\partial x_i} = 0,$$

$$\mathbf{I}\,\ddot{\theta} + c\,\dot{\theta} = \mathbf{M_o},$$

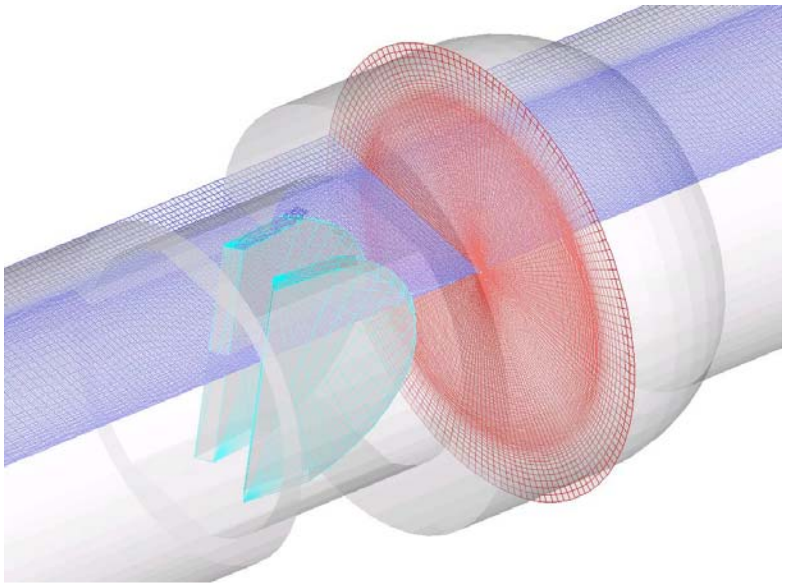
$$\mathbf{M_o} = \int_{\Psi} \{-l_y(\sigma_{xj} n_j) + l_x(\sigma_{yj} n_j)\} d\psi,$$



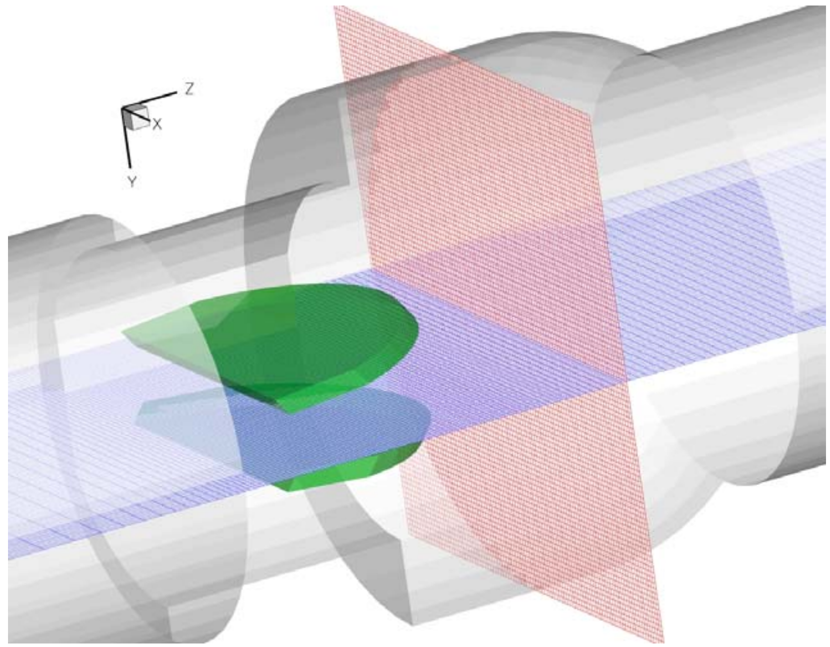
The incompressible Navier-Stokes equations governing fluid motion are solved as a coupled system with the ODE governing the motion the leaflet

Flow around prosthetic heart valves

Used different grid types and sizes:



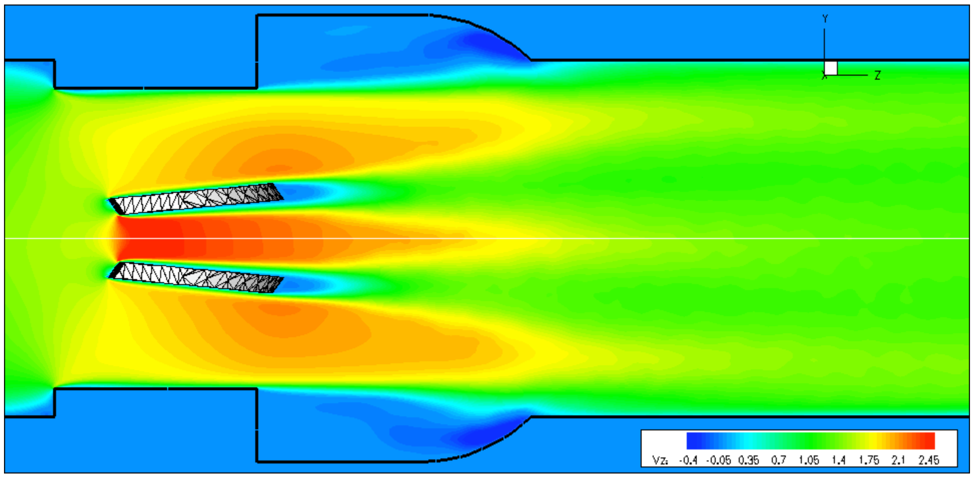
Cylindrical coordinates
CY2: 329 × 141 × 246



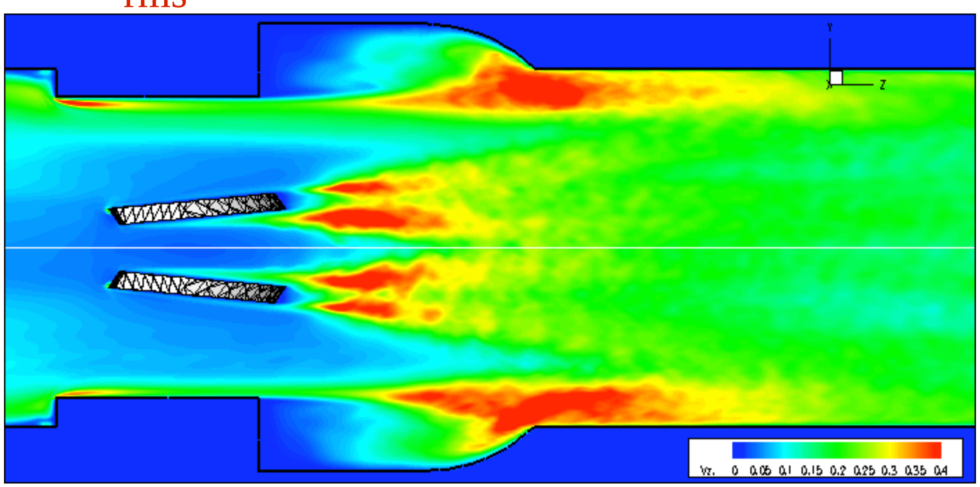
Cartesian coordinates
CT2: 640 × 200 × 200

Steady flow, Re=4000

<u>

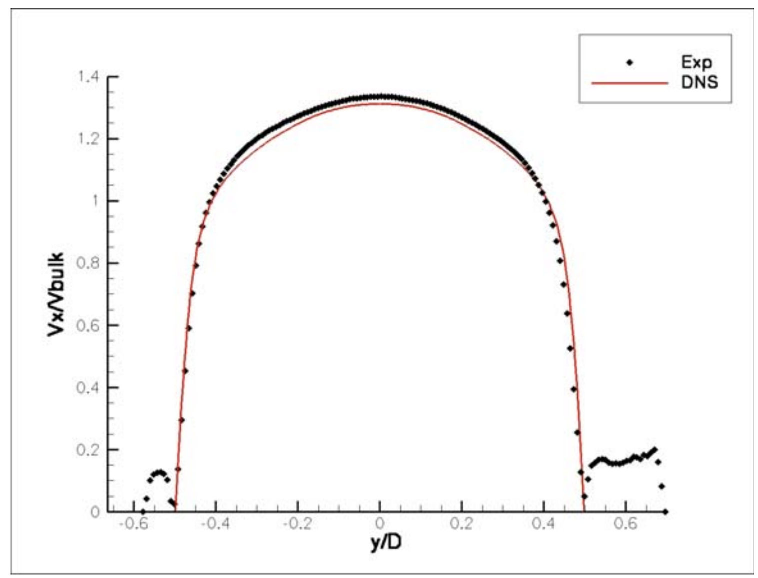


<u_{rms}>

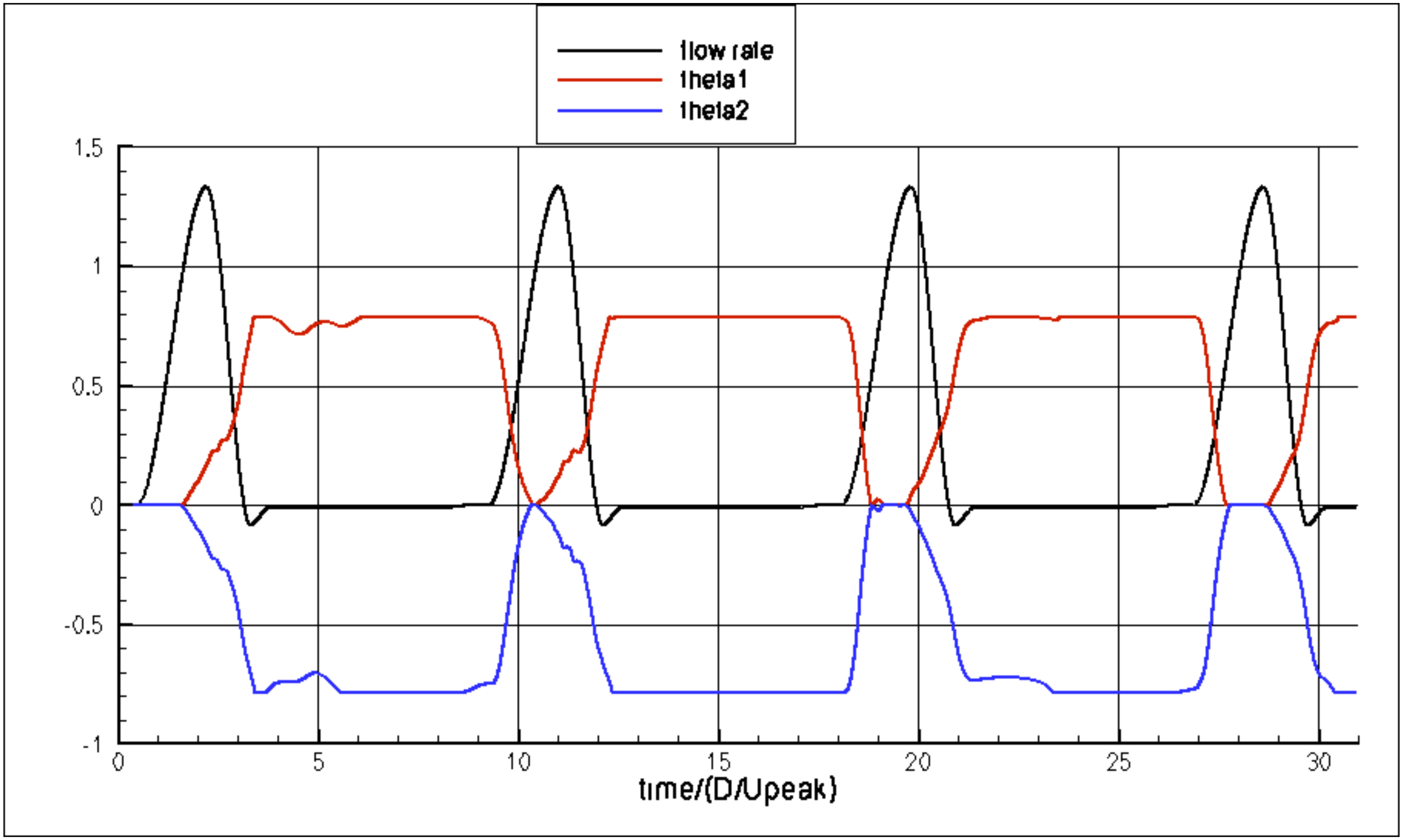


- Re = $U_b D/\nu$ = 4000

<u> at the inflow plane



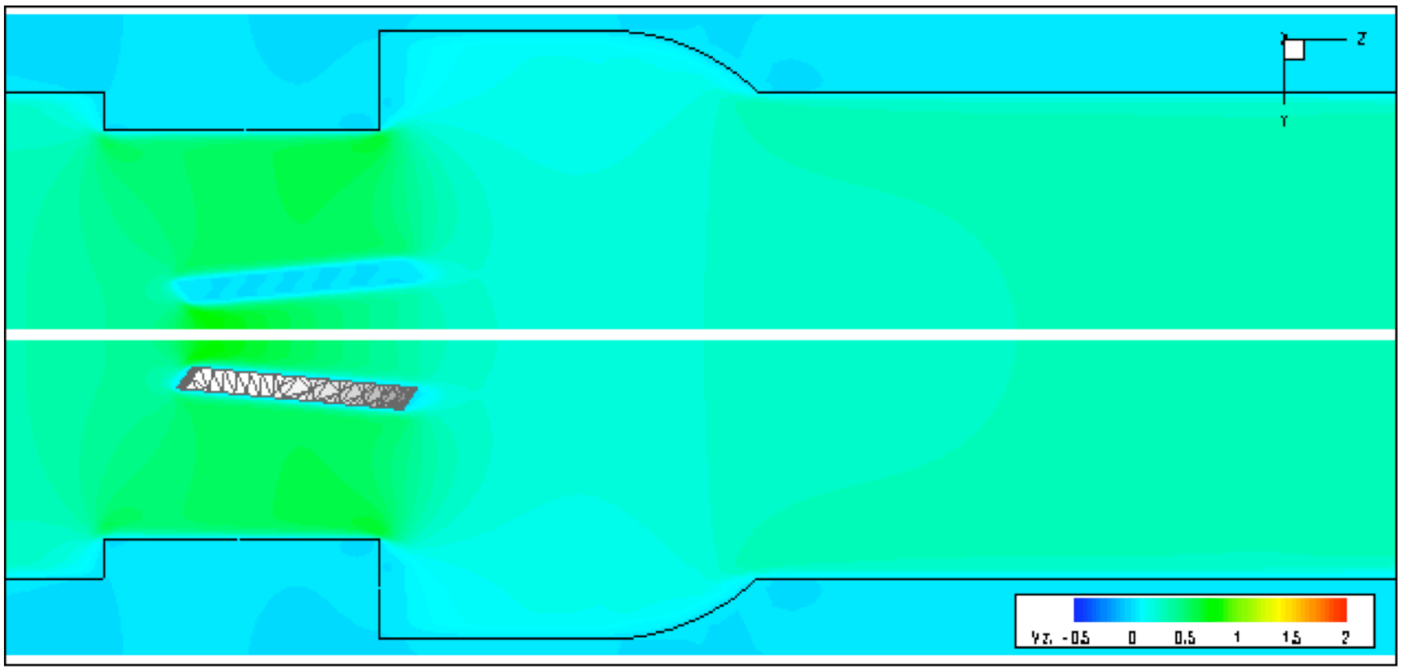
FSI: Pulsatile flow, Re_{peak}=6000



Variation of the flow rate and opening angles during the cycle

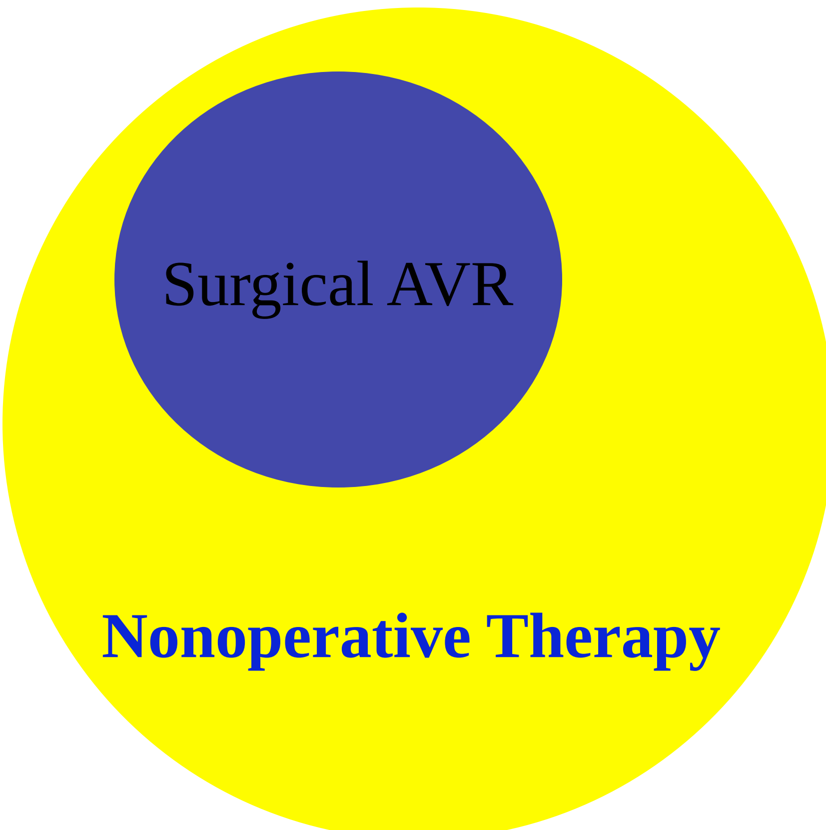
FSI: Pulsatile flow, Re_{peak}=6000

Variation of the instantaneous streamwise velocity at y-z palne



Treatment: Conventional AVR

AVR Surgery: Denied to Many Patients ?



"Not a surgical candidate…"

- -Too old
- -Too sick
- -Won't tolerate operation

Treatment: Conventional AVR

AVR Surgery: Denied to Many Patients ?

124 patients > 60 years*

- Symptomatic AS
- 39 % Aortic valve replacement

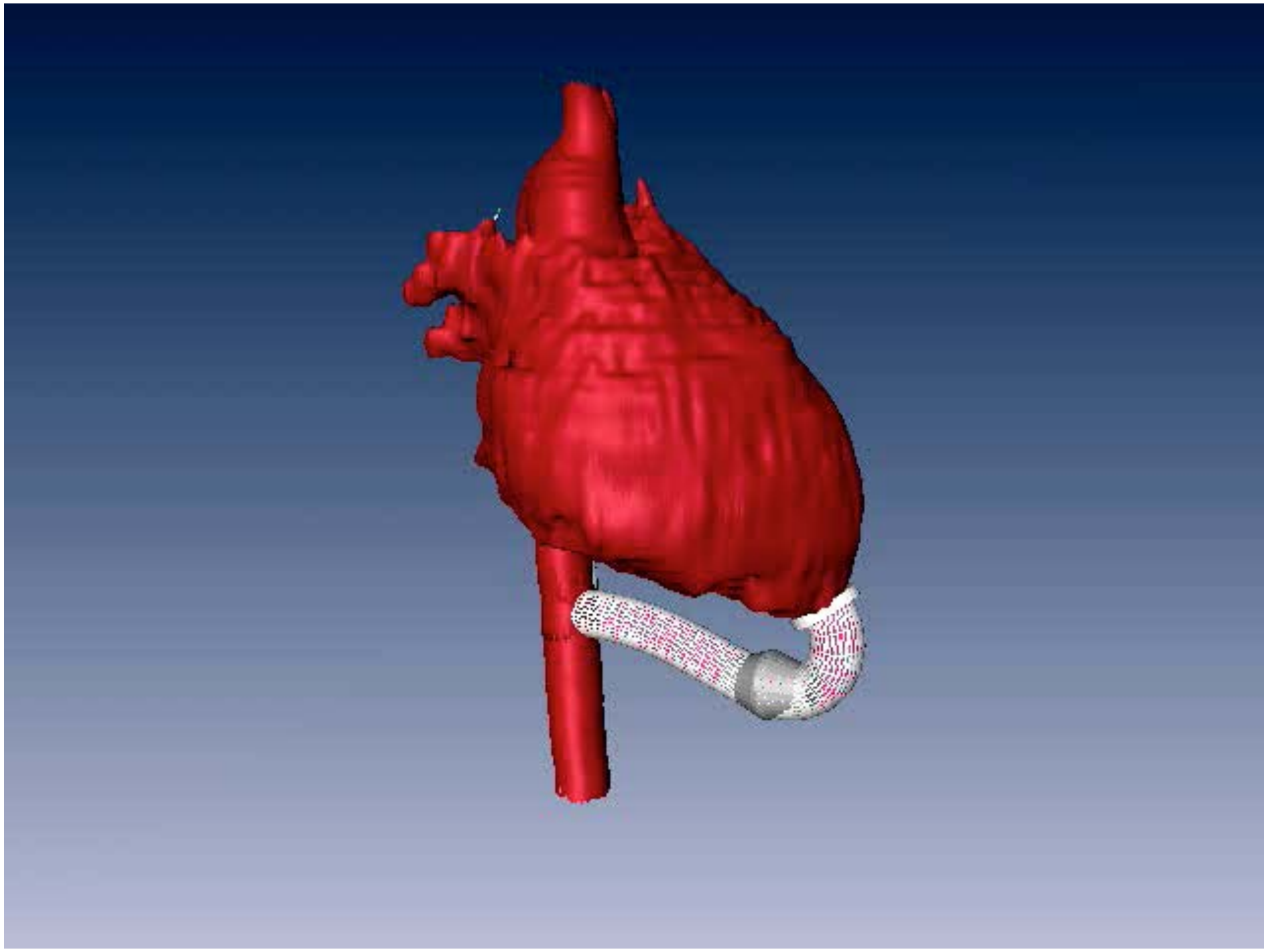
Age	Surgery
60 – 69	77 %
70 – 79	60 %
> 80	22 %

* *Charlson E, et al.* Decision-making and outcomes in severe symptomatic aortic stenosis *J Heart Valve Dis 2006;15(3):312-21.*

The Alternative: Aortic Valve Bypass

- Aortic Valve Bypass (or Apicoaortic Conduit)
  - Creates a new outflow from the apex of the left ventricle to descending aorta.
    - Conceived by Carrel in 1910
    - Performed experimentally by Sarnoff in 1955
    - Clinically by Templeton in 1962
    - First in man reported by J.W.Brown in 1974
    - More than 100 operations U. Maryland recently

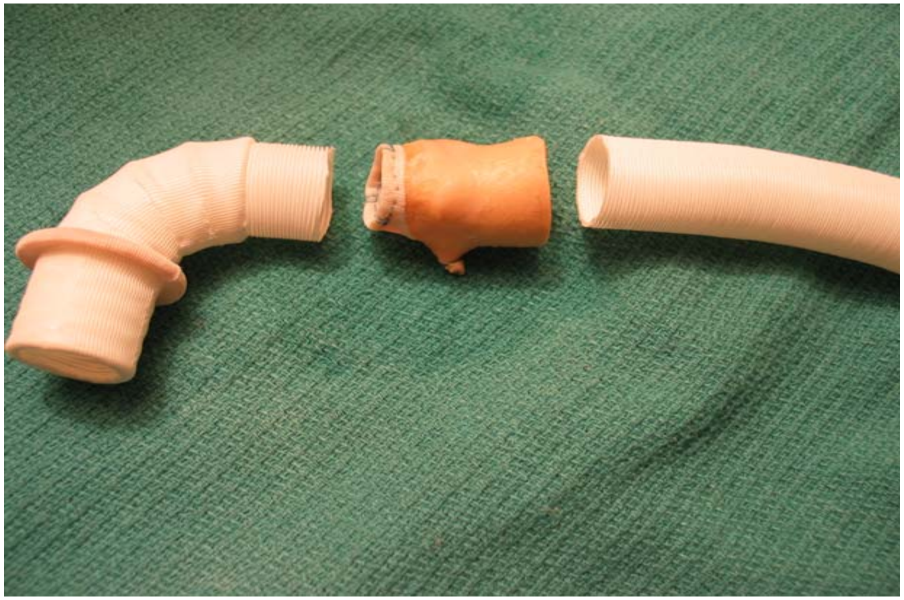
The Alternative: Aortic Valve Bypass



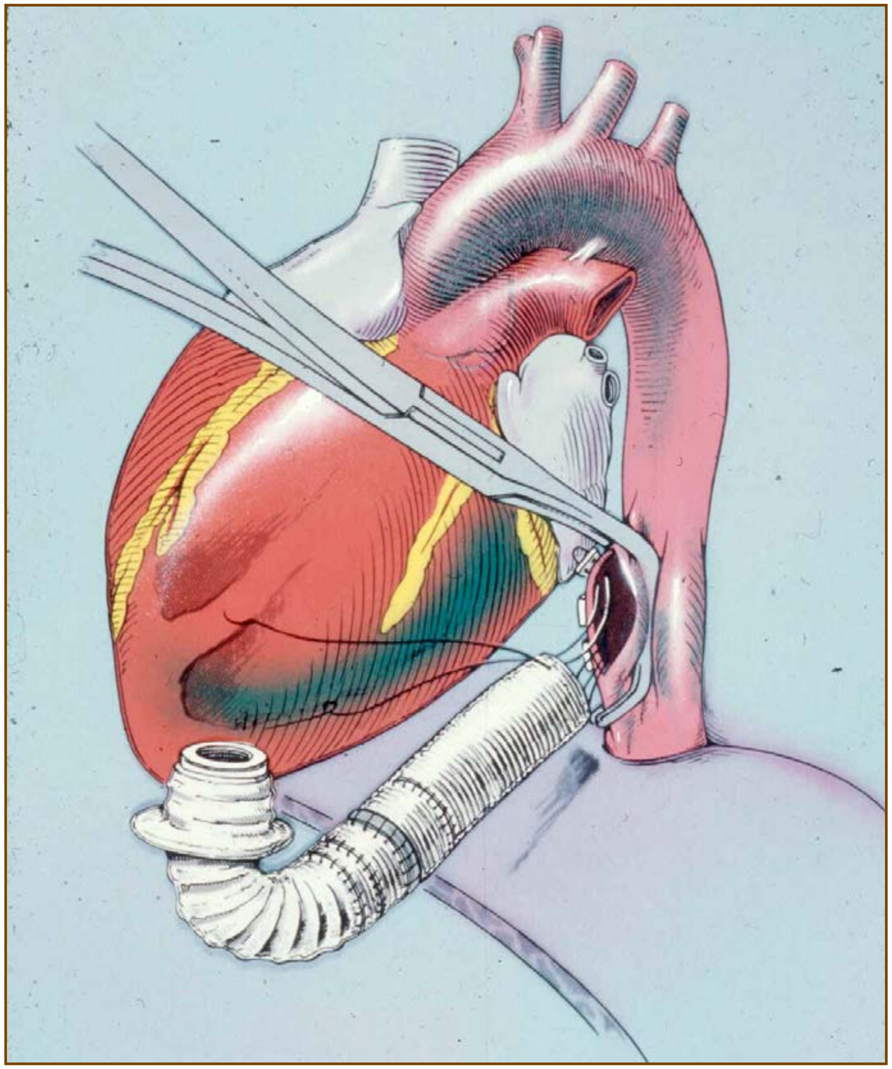
The Alternative: Aortic Valve Bypass

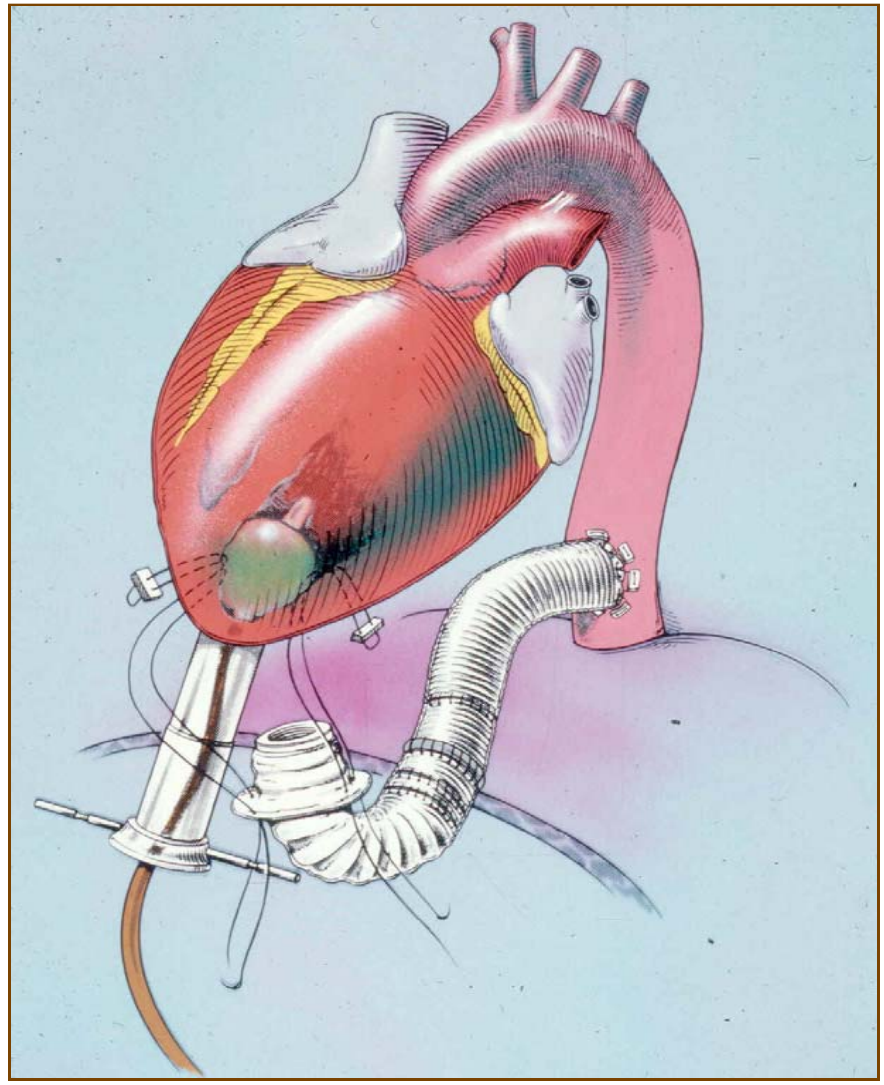
AVB Components

- Left Ventricle Connector (LV connector)
- Prosthetic Valve
- Vascular Graft (if not part of valve)



The Alternative: Aortic Valve Bypass





The Alternative: Aortic Valve Bypass

Advantages of Aortic Valve Bypass

- Avoid sternotomy (patent grafts)
- No aortic cross-clamping
- No (or minimal) cardiopulmonary bypass (*BEATING HEART operation!*)
- Patient-prosthesis mismatch impossible
- Brain Protective

Current application: Very High-Risk Patients

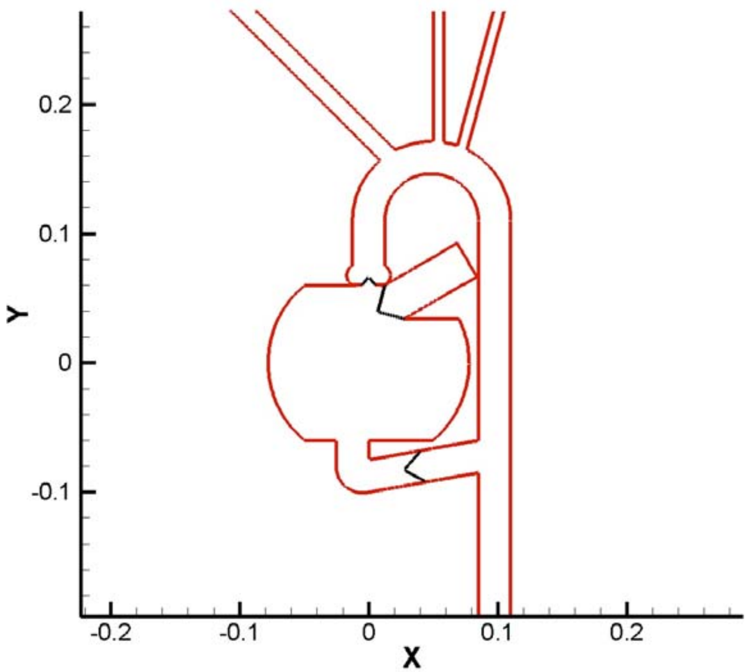
The Alternative: Aortic Valve Bypass

Open Questions:

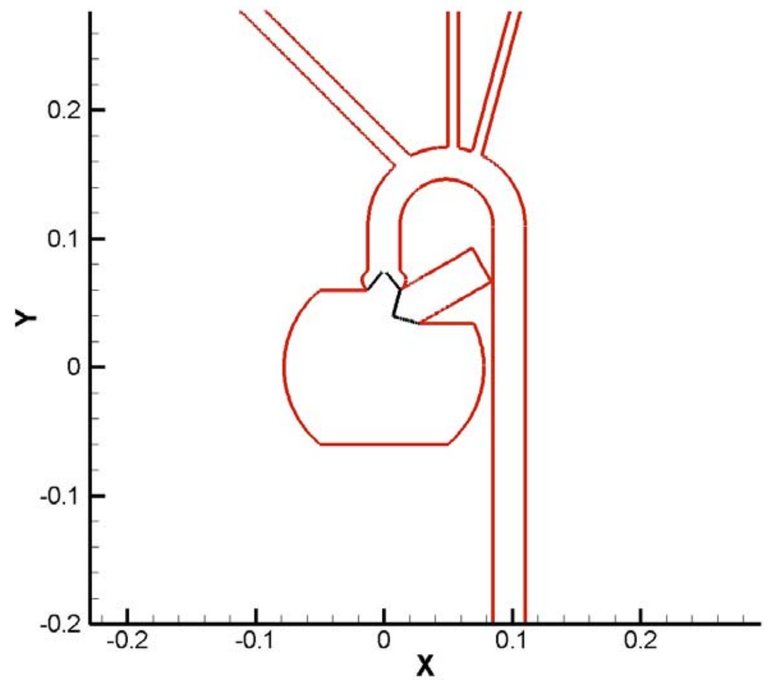
- What is the relative blood flow through the conduit and the native aortic valve?
- How much retrograde flow is there? How much stasis is there in the descending aorta? Is there a known "threshold" where thrombosis might occur?
- Is blood flow to brain and coronaries unchanged compared to normal anatomy?
- Can we predict the final left ventricular outflow gradient and the size of the conduit
- What would be the SMALLEST conduit we could use to achieve adequate relief?

The Alternative: Aortic Valve Bypass

Set-up of preliminary computations

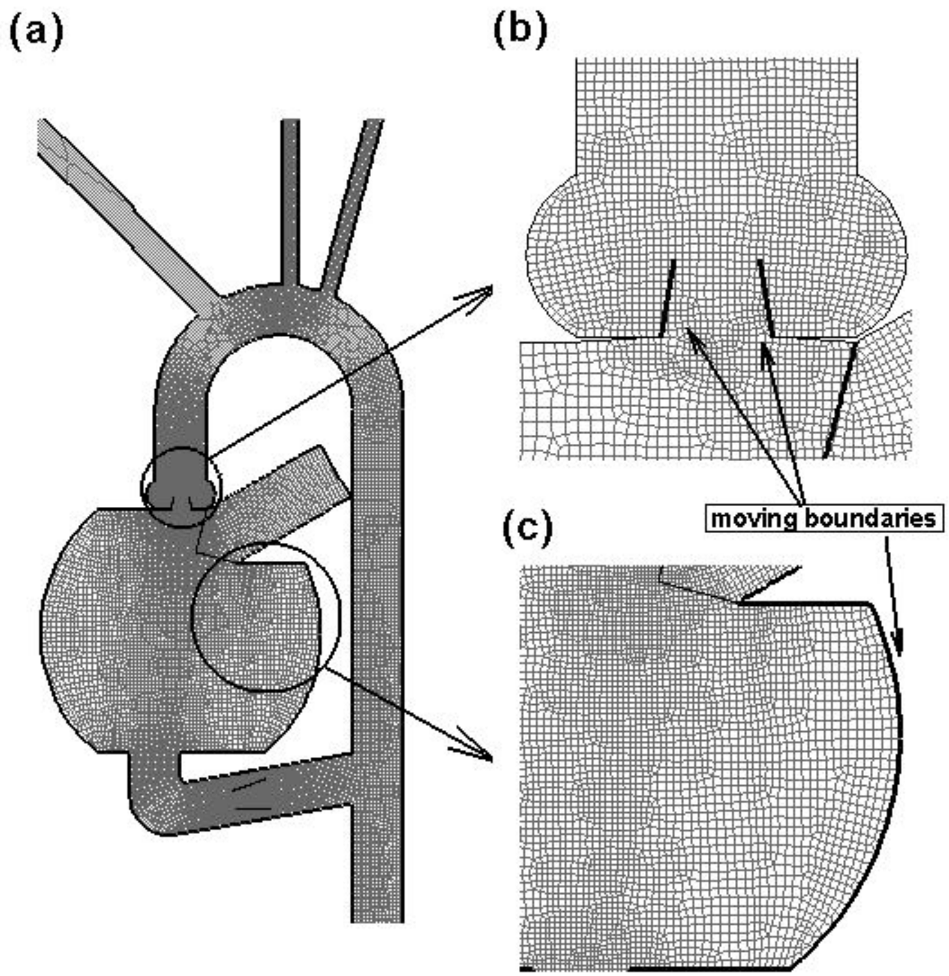


AVB geometry

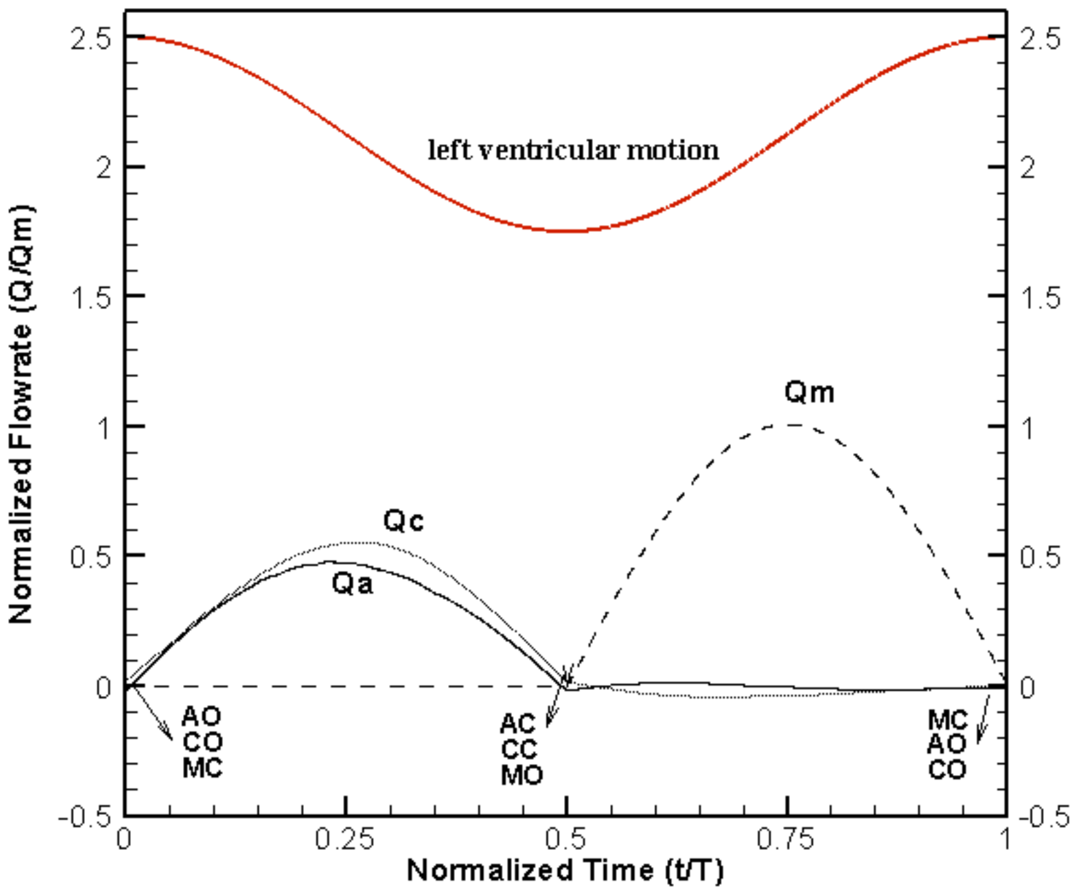


Normal geometry

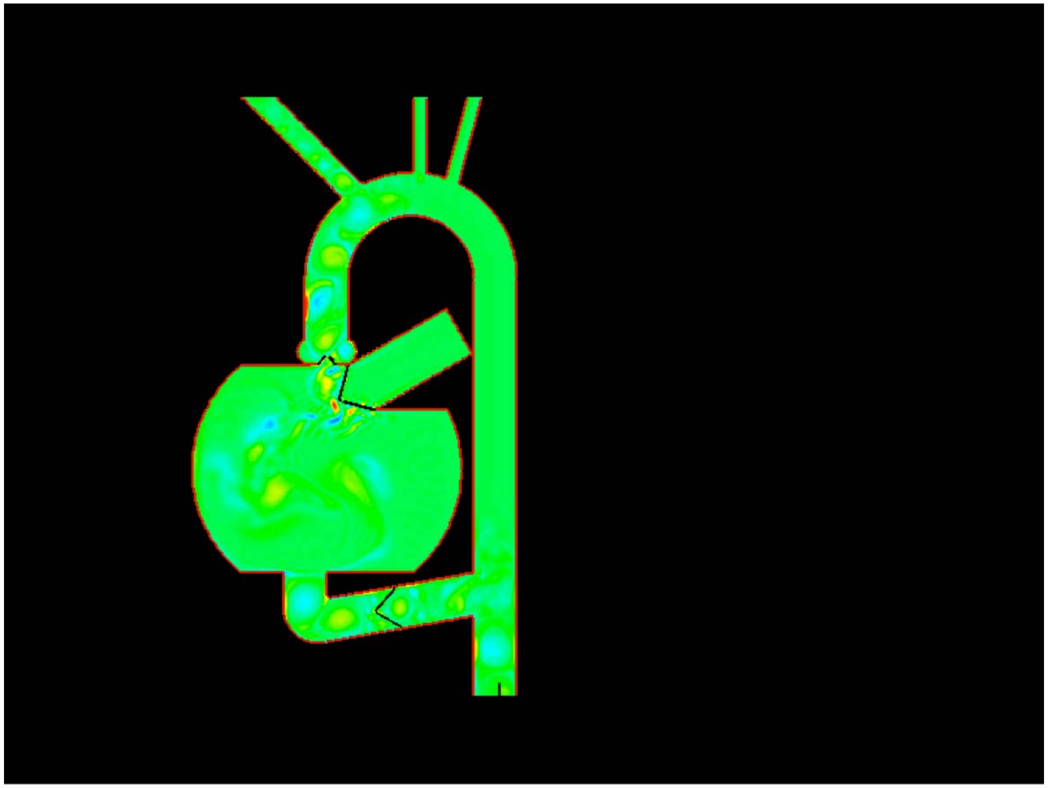
The Alternative: Aortic Valve Bypass



The Alternative: Aortic Valve Bypass



The Alternative: Aortic Valve Bypass



The Alternative: Aortic Valve Bypass

Table 1: Summary of the computations

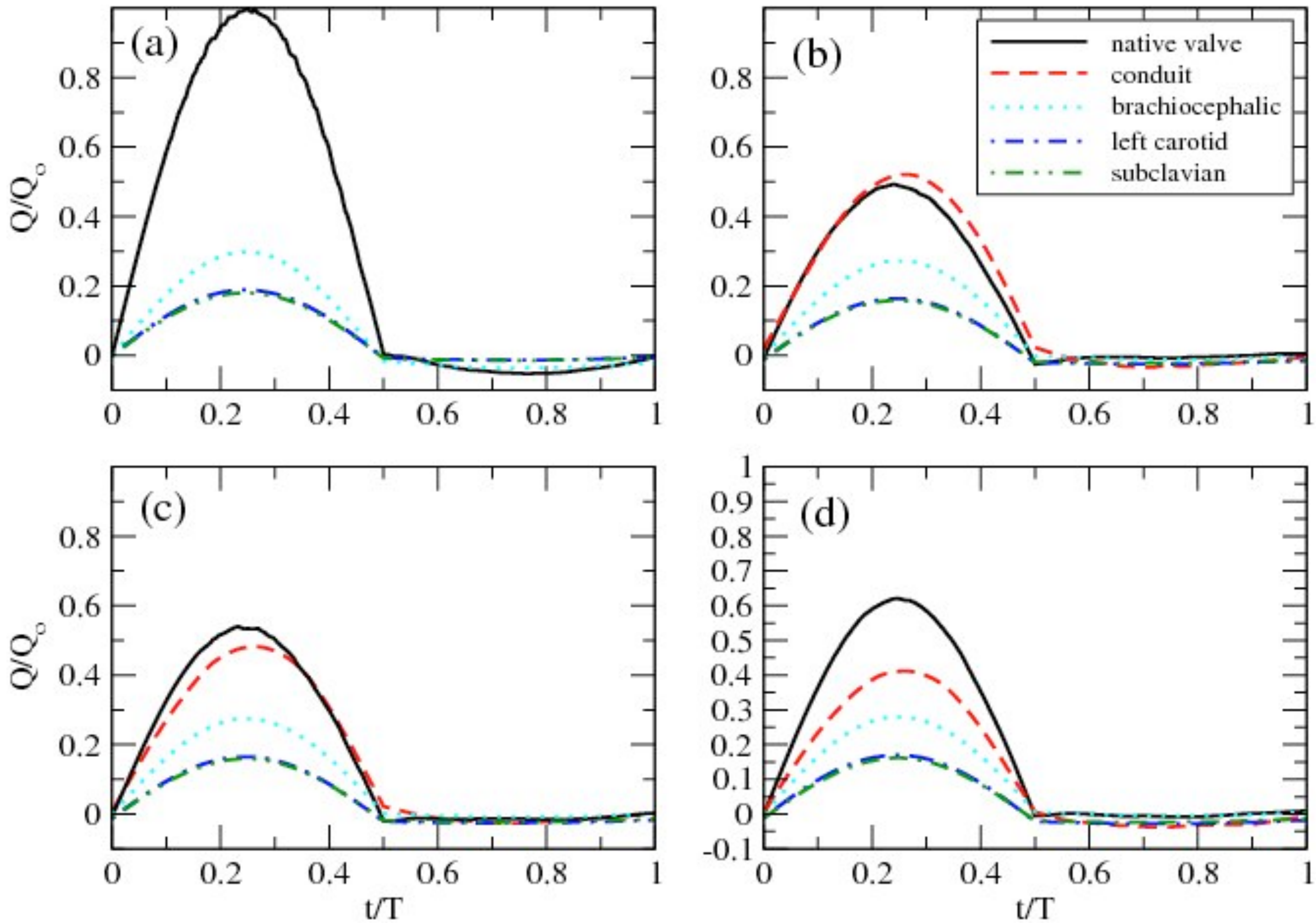
Case	Native Aortic Valve Stenosis *(%)*	Diameter of AVB Conduit *D(mm)*
I – Normal	0	No conduit
II –AS	80	No conduit
III – AS + 20 mm AVB	80	20
IV – AS + 16 mm AVB	80	16
V – AS + 10 mm AVB	80	10

Table 2: Native Aortic valve gradients.

	Clinical data		Numerical data (2-D)	
	Mean (mmHg)	Mean Normalized	Mean (mmHg)**	Mean Normalized
Case II (80% stenosis)	43.0±7.0*	1	43.0	1
Case III (AVB, D=20mm)	8.8±3.3*	0.21	12.5	0.29
Case IV (AVB, D=16mm)	-	-	13.8	0.32
Case V (AVB, D=10mm)	-	-	17.6	0.41

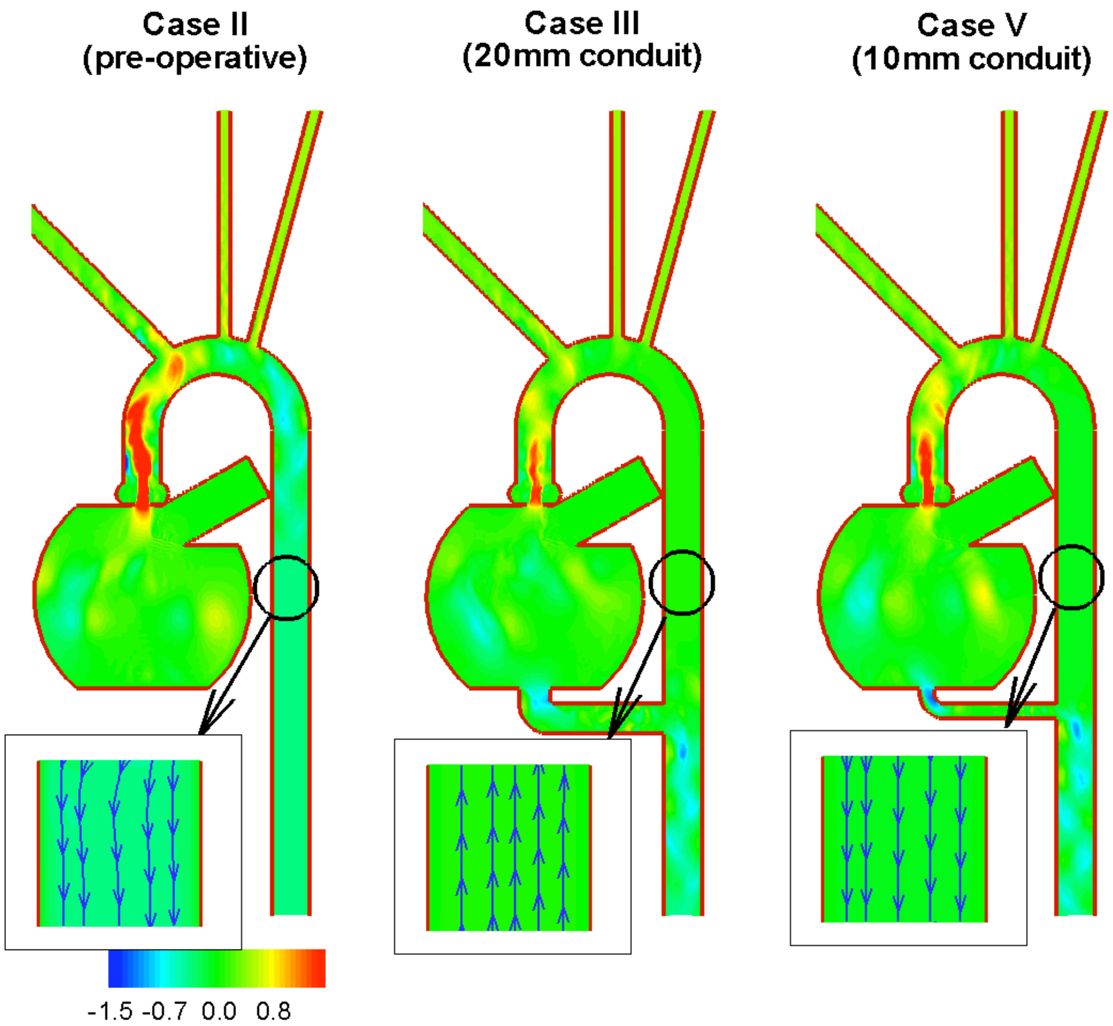
The Alternative: Aortic Valve Bypass

Flowrate distribution



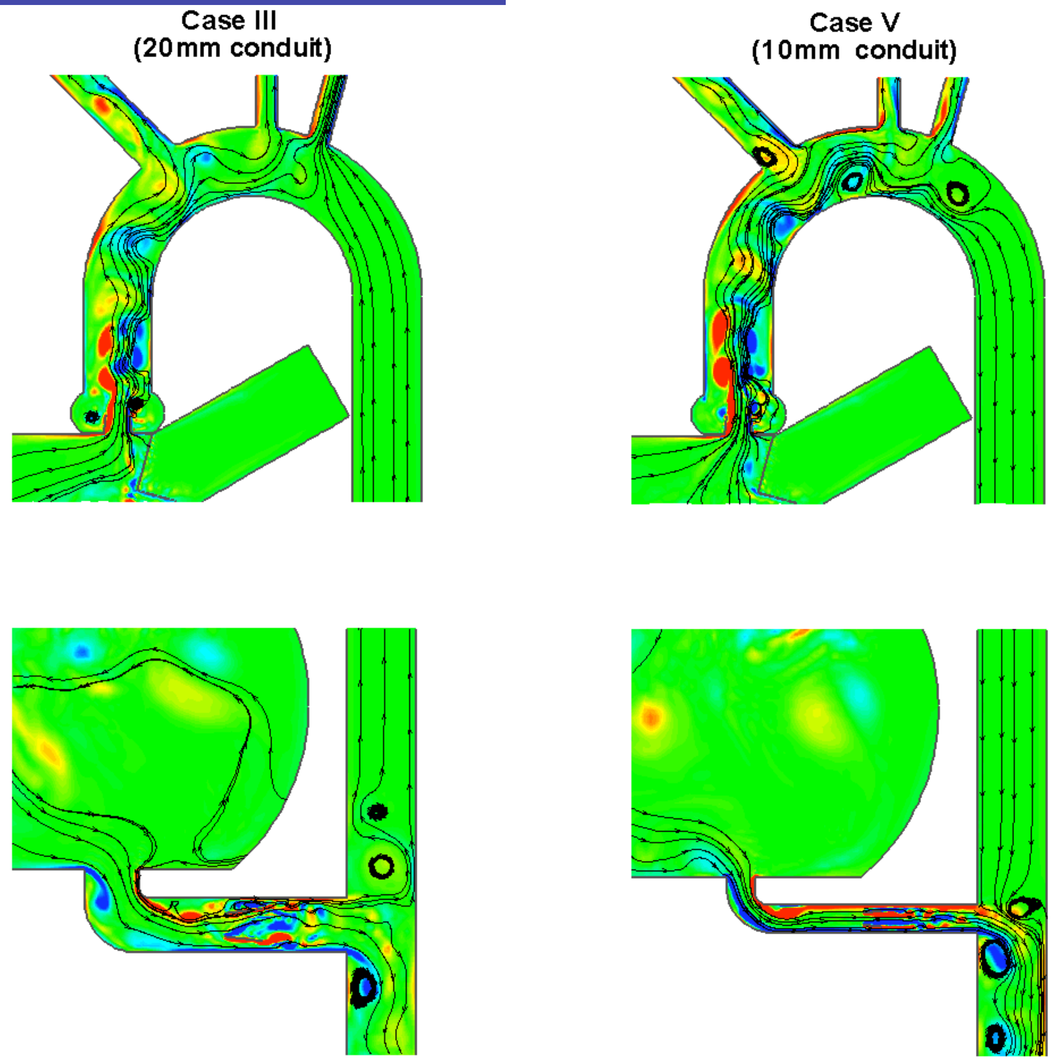
The Alternative: Aortic Valve Bypass

Velocity isolines at peak systole



The Alternative: Aortic Valve Bypass

Vorticity isolines at peak systole



"Let's just start cutting and see what happens."

Acknowledgements

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  - Antonio Cristallo