Slides for proposed talk at
Hanyang University, Seoul, Korea
March 31, 2005 (tentative)

"High-Fidelity Simulation in Biomedical and Aerospace Engineering"
By Dochan Kwak

Export Control Information

All the material in this presentation are in public domain and have been disseminated previously in the following publications and meeting presentations

- 3rd International Conference in CFD, Toronto, Canada, July 2004
  (plenary talk by Ron Bailey, also written version in the proceedings)
- D. Kwak and C. Kiris, "Successes and Challenges of Incompressible Flow Simulation" presented at the 16th AIAA Computational Fluid dynamics Conference, Orlando, FL, June 23-26, 2003
- Super Computing 2004
- Kim, C. S., Kiris, C. and Kwak, D., 'Numerical Models of Human Circulatory System under Altered Gravity,' *AIAA Paper 2004-1092*, AIAA 42nd Aerospace Sciences Meeting, Reno, Nevada, Jan. 5-8, 2004.
- Kwak, D., Kiris, C. and Kim, C.S., 'Computational Challenges of Viscous Incompressible Flows,' *Computers & Fluids* **34,** pp283-299, 2005.
- Biomedical and Digital Human related slides are generated using available info in public domain, such as in Journals and university colleagues (Prof. Tim David of Canterbuty University, NZ and, Prof. Stan Berger of UC Berkeley)

Outline of Talk

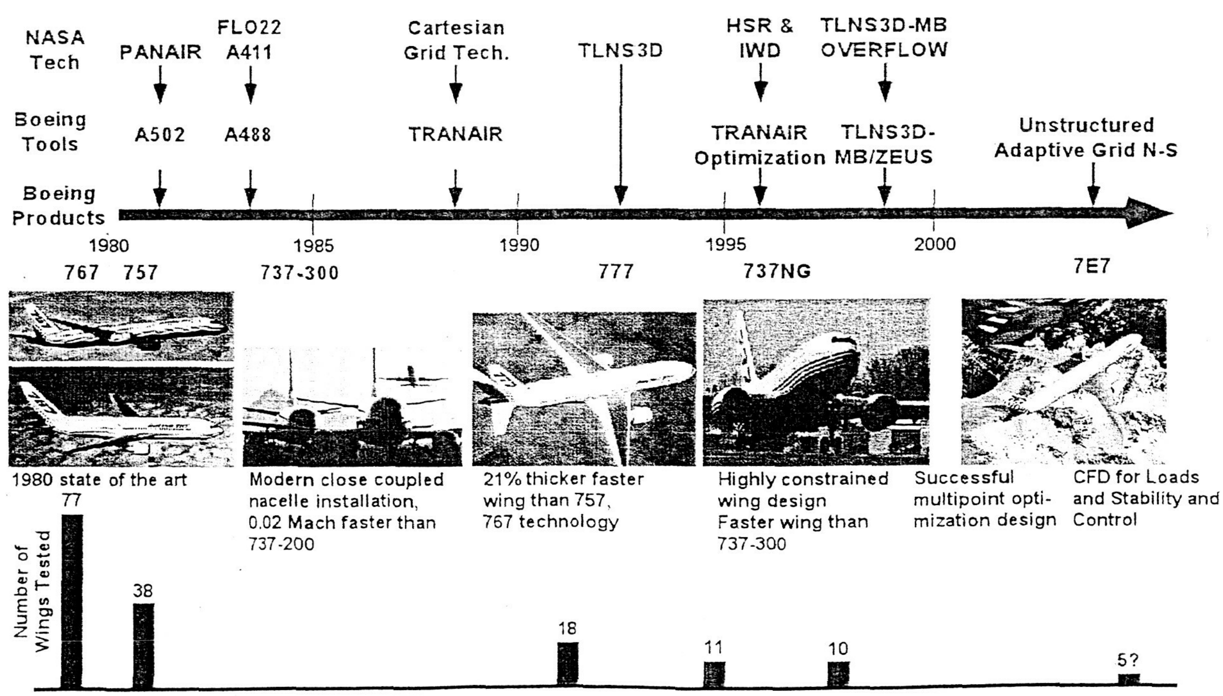
- **Introduction / Background**
- **Modeling and Simulation Challenges in Aerospace Engineering**
- **Modeling and Simulation Challenges in Biomedical Engineering**
  - Digital Astronaut
- **Project Columbia**
- **Summary and Discussion**

Status of CFD

- **Pioneered the field of flow simulation** for
  - Obtaining engineering solutions for complex configurations (One of major goals of 80s)
  - Understanding flow physics (critical to mission)
- **Functionality** was the most important features primarily concerned about "performance" prediction (of aerospace vehicles), and then reduce design cycle time
  - CFD is routinely used in aerodynamic design of aircraft
    ⇒ There are a few remaining challenges, e.g. high-lift, aeroacoustics
  - Design of aircraft engine components is validated by CFD
    ⇒ CFD-based engine design is yet to be realized
  - CFD can provide detailed analysis of rocket engine components
    ⇒ Analysis/design of entire engine / entire sub-systems are yet to be accomplished
- There are **many success stories**
  - Commercial aircraft design
  - SSME HGM redesign
  - Mechanical heart assist device

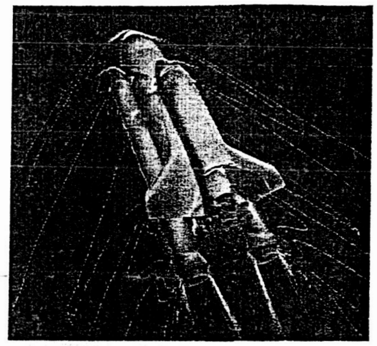
  ...list goes on
- **New advances are often driven by problems or mishaps**

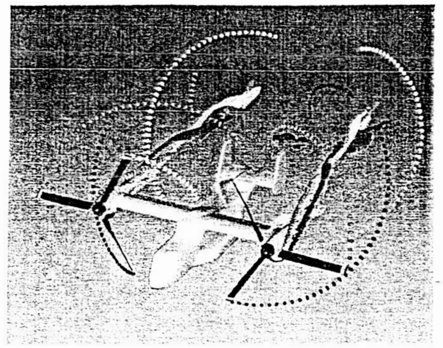
CFD Contribution to Commercial Aircraft Design

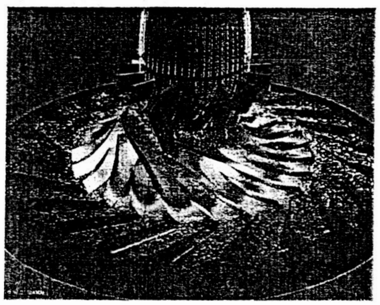


BOEING

Examples of Current Simulation Capabilities for Complex Flow



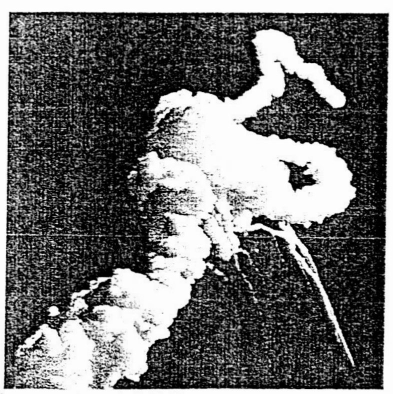




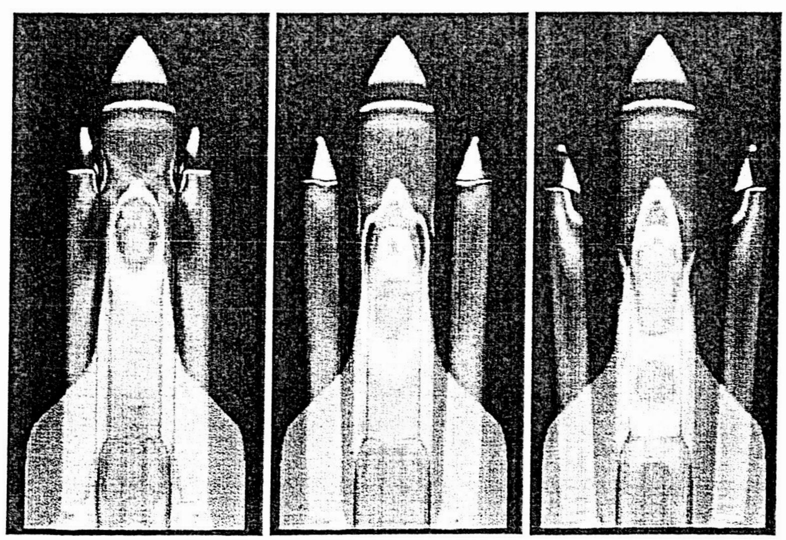
- Steady and unsteady flows over complex configurations
- Bodies in relative motion
- Multiple scale problems
- CFD very good at:
  - Flow analysis
  - Sorting through preliminary designs
- Still lacks
  - Prediction capability
  - Automation

Historical Note

- Space Shuttle Challenger Disaster has lead to key technological advances that facilitate computational aerodynamic forensics



Jan 28, 1986

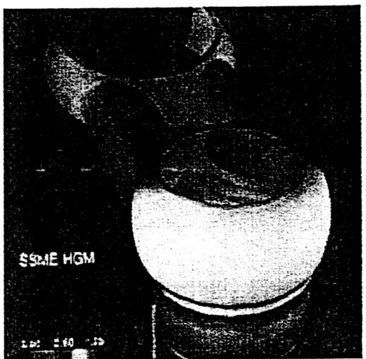


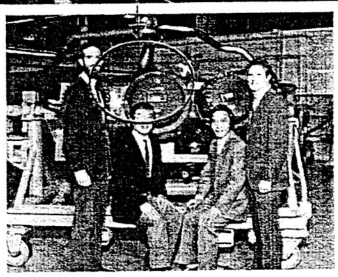
Dec 1988

Historical Note

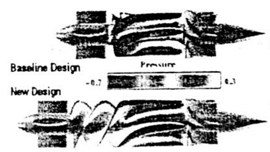
- Space Shuttle Main Engine Phase II+ redesign work in the early 80s accelerated CFD applications to rocket propulsion systems development

CFD solution of HGM (c 1983)

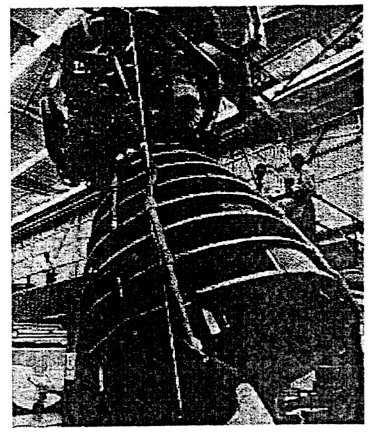




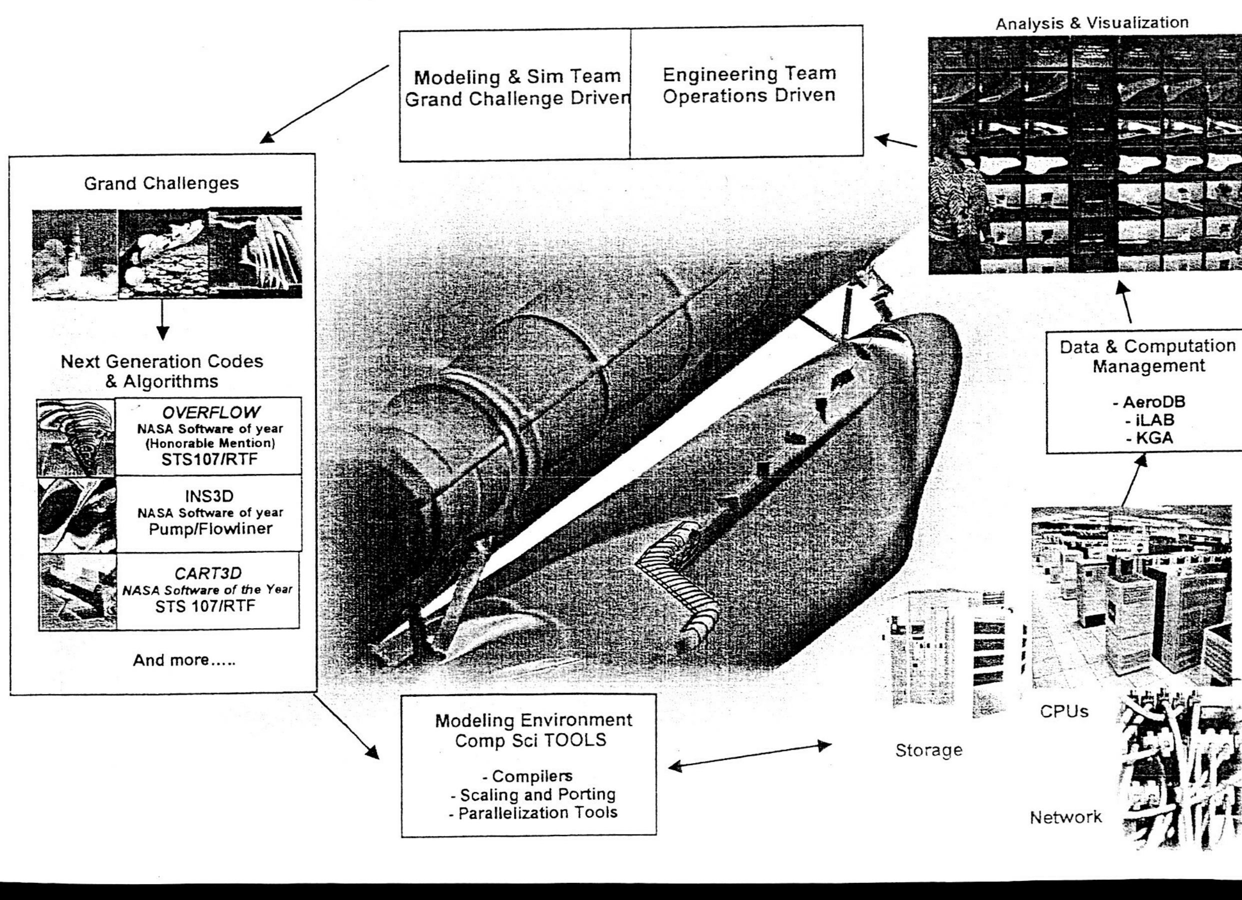
Propulsion CFD, Pump technology in the early 90s



New flight Engine in 1995



Integrated Simulation Environment



HEC Challenges in Aerospace Engineering

Primary focus of "Modeling and Simulation" has been changed from performance prediction to mission impact

- Expand flight envelope, reduce design cycle time, and enhance safety
  - Digital Flight
    6-DOF, S&C database generation, Grid quality issues etc.
- Mission simulation
  - Integrated Launch/Ascent Simulation
    e.g. Shuttle's Return To Flight
  - Descent / Entry / Landing
  - Mixed Fidelity Systems Simulation for Risk Evaluation
- High-fidelity simulation of complex system
  - Liquid Rocket Subsystem Simulation
    e.g. turbopump systems: induce, impeller, diffuser etc.
- Bioastronautics
  - Digital Astronaut

⇒ Requires increased processor speed, larger memory, data analysis and management, faster network: CFD, CS and Facility

Integrated Launch/Ascend Simulation

Goal:
To provide automated high-fidelity simulation capability for vehicle in launch/ascent environment.

Objectives:

•Mission design & analysis

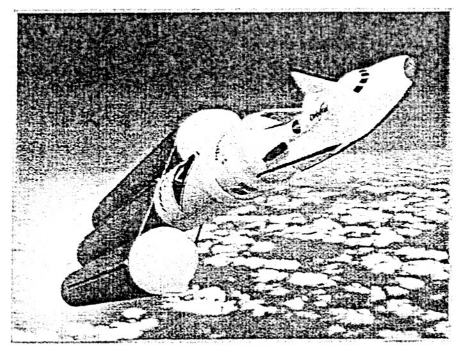
•Plan & evaluate readiness to launch

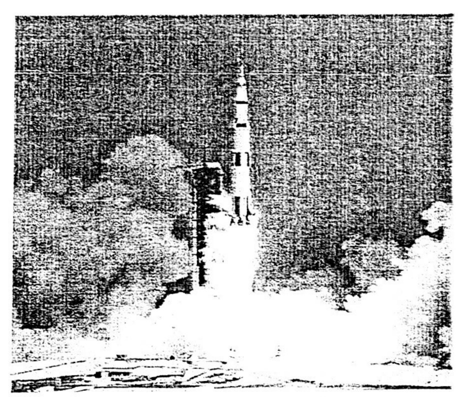
•Trajectory optimization

•Risk and safety evaluation

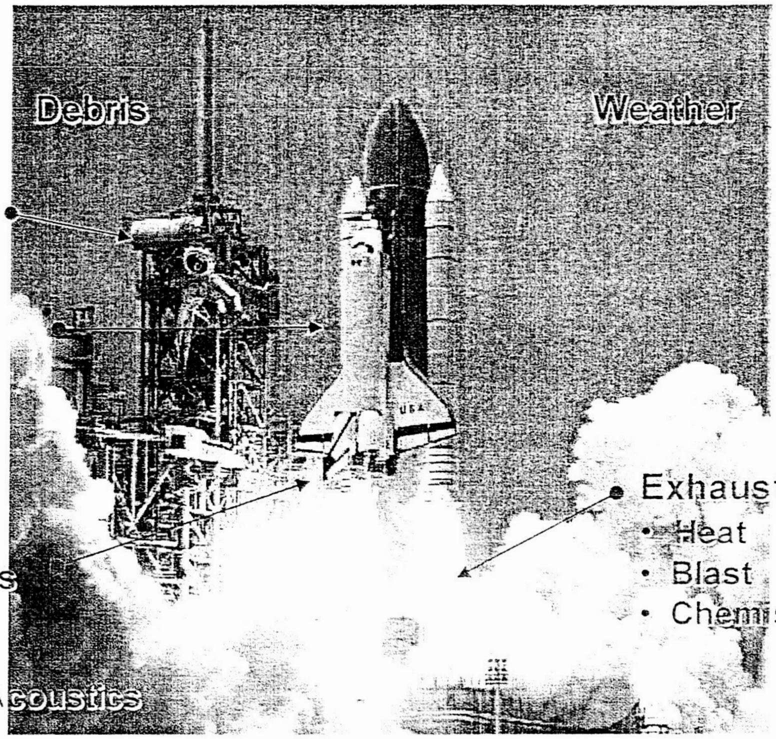
•Failure/abort recovery analysis

•Rapid response to critical events



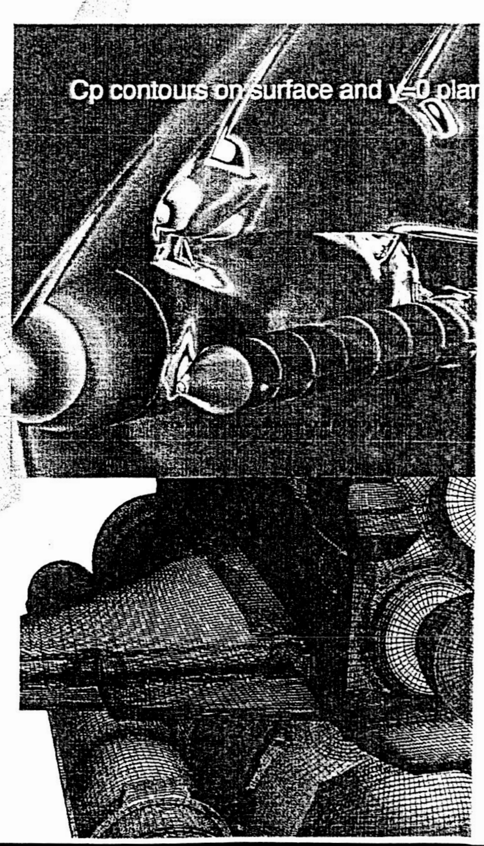


High-Fidelity Launch/Ascent Simulation Features



Example of Overset Grid System and Solution

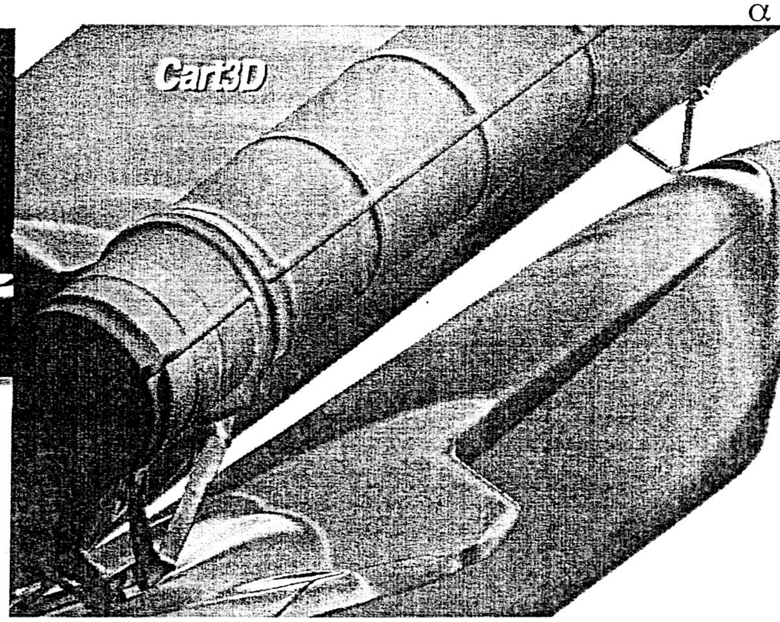
- Rapidly generate grid systems for different control-surface deflections, and different combinations of components
  - 1 hour to change control-surface deflections
- Overset grid generation utilizes Chimera Grid Tools and Pegasus5 software
- Rapid turn around
  - 24 hours of wallclock time
  - 32 SGI Altix CPUs (Itanium-2 CPUs)



Example of Current Moving Body Capability

- Multiple-exposure of moving-body simulation of debris event
- Dozens of other examples in literature

$M_\infty = 2.46$
$\alpha = 2.08°$



4 million grid points
16 hours on 64 SGI
Origin(600MHz) CPU's

Isobars
multiple exposure

High-Fidelity Launch/Ascent Simulation - "Digital Launch"

Modeling and Simulation Challenges
- Complexity
- 6-DOF multiple-body flight
- Debris impact scenarios
- Integrate vibration data and fuel exhaust data from propulsion simulation
- Integrate acoustic environment and fuel accumulation from engine exhaust
- Thermal stress analysis on structure

Computation
- Simulation until vehicle has passed tower (e.g. 3 sec.)
- Time step determined by exhaust blast waves
- Length scale assumed 1 foot
- Time accurate Euler simulation for most of ascent
- 100 million grid points
- Current Solution Time: less than one day on 12TF Platform
- Real Design & Engineering Model for Ascent/Abort Scenario:
    - Weather
    - Viscous effects
    - Exhaust Chemistry
    - Acoustics environment (ignition overpressure)

HEC Requirement for High-Fidelity Design
- 1 day & 60-120 TF Platform

Liquid Rocket Subsystem Simulation

Goal:

To provide a high-fidelity computational framework for design and analysis of the fuel/oxidizer supply subsystem for liquid rocket propulsion systems.

Objective:

- Decrease design cost
- Improve performance and reliability

  Critical path for:

  - Retrofitting (i.e. determining fuel-line crack issue for Space Shuttle Program)

  - Investigating new designs for future engines.

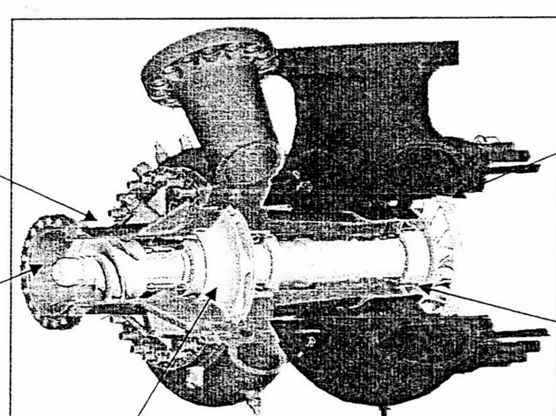
EXAMPLE OF A ROCKET ENGINE PUMP

UNSTEADY AND TRANSIENT FLOW IN LH2/LOX FEEDLINE

High Pressure Fuel Turbopump

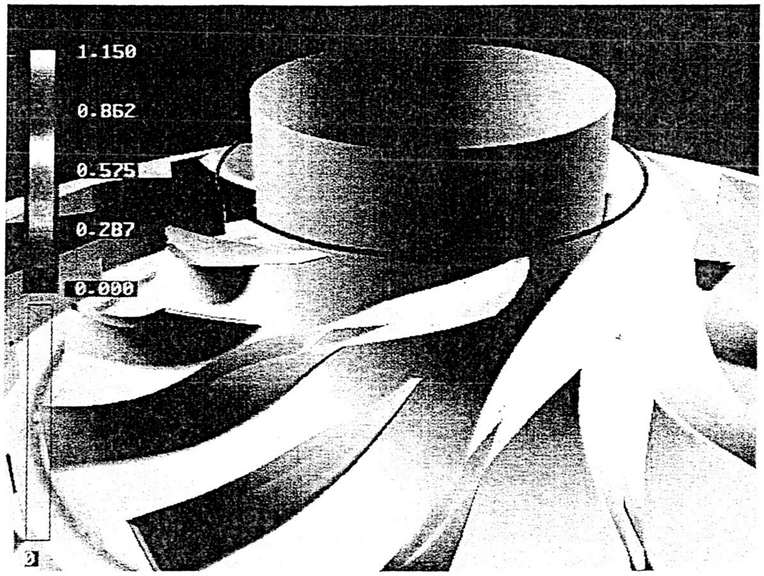
Turbopump Design Problems

Can lead to cost growth, engine failure or vehicle loss



Liquid Rocket Fuel System Cause of Most Failures

Wide-Range Flow Impeller-Diffuser



Code INS3D
34.3 Million Grid Points, 114 Zones
One Rotation takes 3.5 days on 128 SGI Origin (600 MHz) CPU's [.015 TF]

Source: Kiris, et. al., NASA ARC

Liquid Rocket Subsystem Simulation

Modeling and Simulation Challenges:

•Complex geometry: CAD-to-solution scripting capability.
•Boundary layer transition and separation
•Transient flow phenomena.
•Tip Vortices
•Cavitation
•Parallel, scalable computational procedure.
•Systems analysis capability for trade study in designing components
•Accurate prediction of flow-induced vibration

Computation

•Simplified Model

– upstream and downstream manifolds/ducting, and coupled shroud and hub cavities, ignores cavitation,
– 150 million grid points
– 10 revolutions
– Extrapolate INS3D
– Requires four days on 12 TF Platform

HEC Requirement for High-Fidelity Design

– Fuel system with piping and four turbopumps
– 2 day solution & 240-600 TF Platform

Human Modeling and Simulation

Potential Applications

Biomedical Research:
- To interpret large quantities of data, guide experiments
- Drug-design, development and testing

Medical Practice:
- Diagnosis- Identify irregularities
- Treatment- Plan treatment procedures
- Monitoring- during space flight

Education and training:
- Cell-level computation, organ modeling, gross anatomy etc. for K-12 to practitioners

Modeling human factors, disease control etc...

There are many players
- NIH and their Affiliates
- DoD
- NASA - Bioastronautics (Digital Astronaut is an element in this)
- Universities - Bioengineering Centers and Medical Schools
- Industry

Digital Astronaut

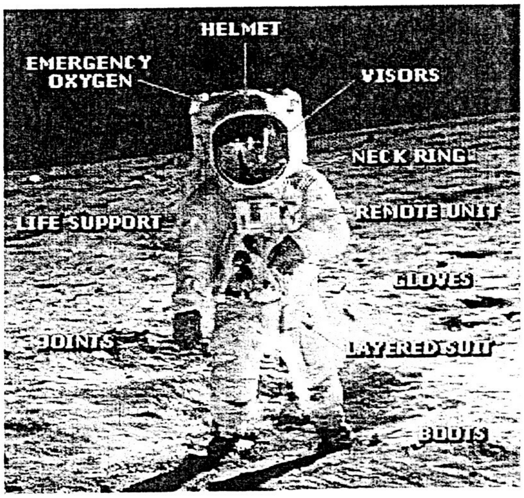
Goal:
To provide high-fidelity simulation for predicting human performance in space flight and develop countermeasures

Objectives:
- Assess impact of altered gravity on crew during mission and post-mission recovery
- Guide counter measure development

Approach:
- Develop integrated DA system
  - Circulatory dynamics-based performance model

This work is being performed in collaboration with other biomedical research organizations

INTEGRATED IMPACT ON ASTRONAUT'S PERFORMANCE



RADIATION SHIELDS

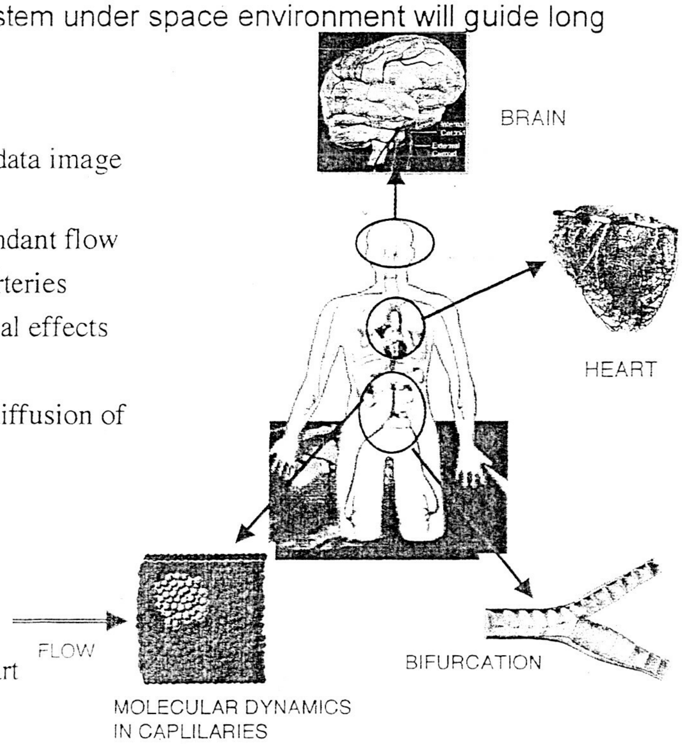
MICROGRAVITY CIRCULATORY SYSTEM

Circulatory System Simulation for Human Space Flights

Scenario: Blood circulation will have major impacts on crew during and post mission. Simulation of entire human circulatory system under space environment will guide long duration human space flights.

Modeling and Simulation Challenges:

- Digitize anatomical data - Mapping MRA data image processing
- Computational hemodynamics - time dependant flow
- Blood flow simulation in large and small arteries
  - Non-Newtonian modeling and gravitational effects
- Biologically complex (cell chemistry)
- Structural computation of vessel wall and diffusion of molecules through the wall
- Auto-regulation and control model
  - Boundary conditions for truncated model
- Difficult to validate, but possible
- Multi-disciplinary team
  - Collaborators often geographically far apart



Circulation-Based Performance Model

- Arterial sizes and numbers

Vessel	Radius (cm)	Number	Area (cm^2)	Wall Thickness (cm)
Aorta	1.25	1	4.5	0.2
Arteries	0.2	159	20	0.1
Arterioles	1.5×10^{-3}	5.7×10^{7}	400	2x10-3
Capillaries	3×10^{-4}	1.6×10^{10}	4500	1x10-4
Venules	1×10^{-3}	1.3×10^{9}	4000	2x10-4
Veins	0.25	200	40	0.05
Vena cava	1.5	1	18	0.15

- Modeling the network is necessary

- High-fidelity model for selected area - Brain

Why brain/blood flow first?

Biomedical Study

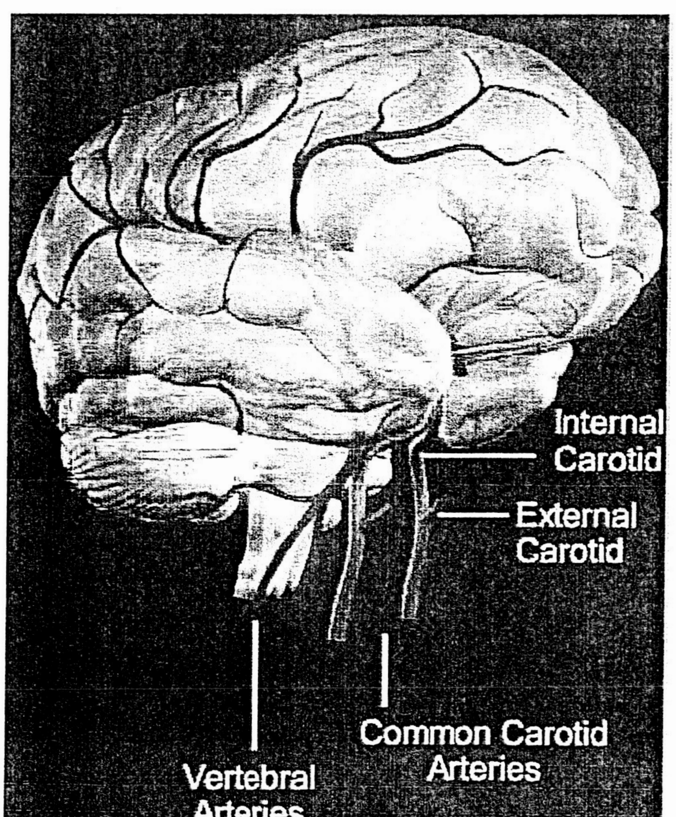
- Stroke is the third largest cause of death
- Stroke is the leading cause of long term disability
- Incidence of stroke is projected to triple in the next 30 years

Bioastronautics / Digital Astronaut

- High G manoeuvres induce significant blood flow variations with ischaemic consequences.
  - Black-out: +8G causes unconciousness
  - Red-out: -3G makes retina engorged with blood

Optimal blood supply to the brain is crucial for astronauts performance

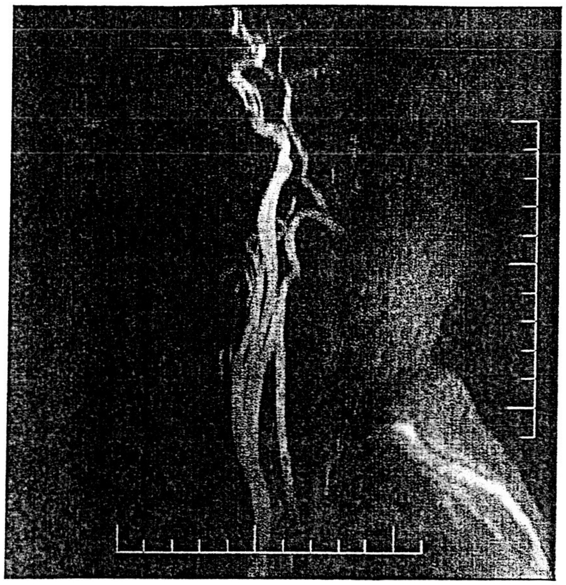
Brain Schematic



Source- http://www.strokecenter.org

- CCA (Common Carotid Arteries)
  - ECA (External Carotid Arteries) : Supply blood to face and scalp area
  - ICA (Internal Carotid Arteries):
  - Supply blood to the front 3/5 of the cerebrum
- Vertebrobasilar Artery
  - Supply back 2/5 of the cerebrum, part of the cerebellum, and the brain stem

Cerebro-vascular Geometry



The Circle of Willis (CoW)

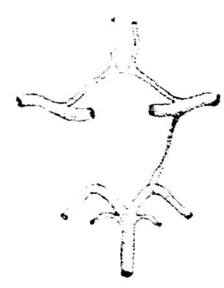
- Located at the Base of the Brain, beneath the hypothalamus
- Responsible for collateral distributing blood to the major regions of the brain.

The Anatomical Dilemma

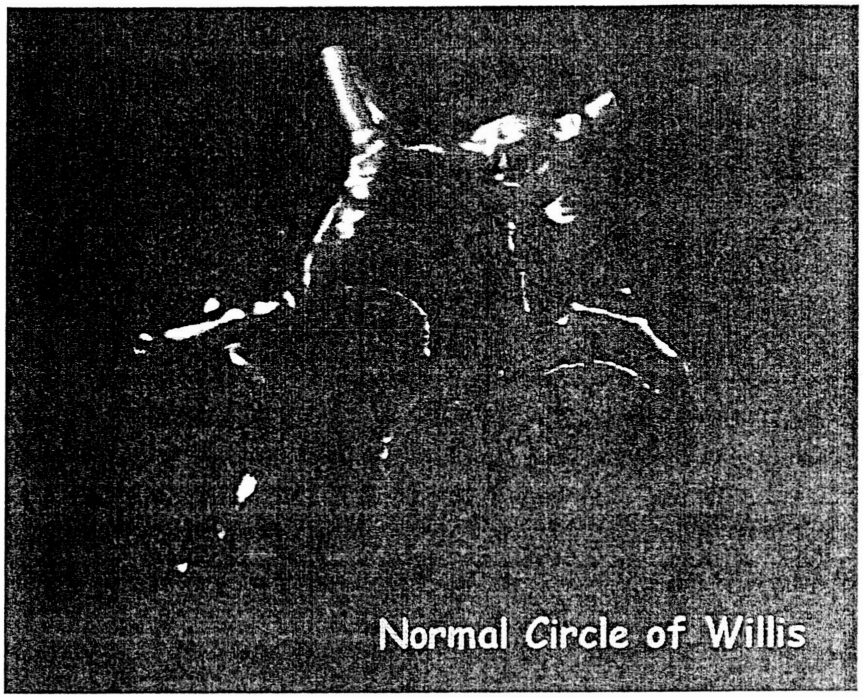
•Approximately 50% of the population has a complete CoW

•Variation in the communicating arteries is common.

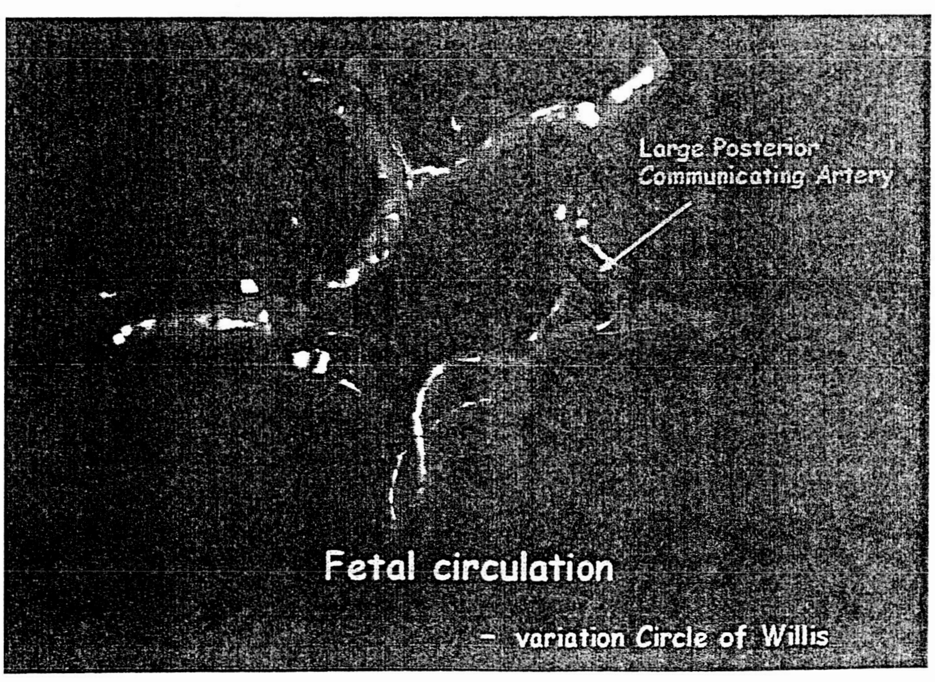
•Combined with the effects of hydrostatic pressure variation can cause cerebral dysfunction



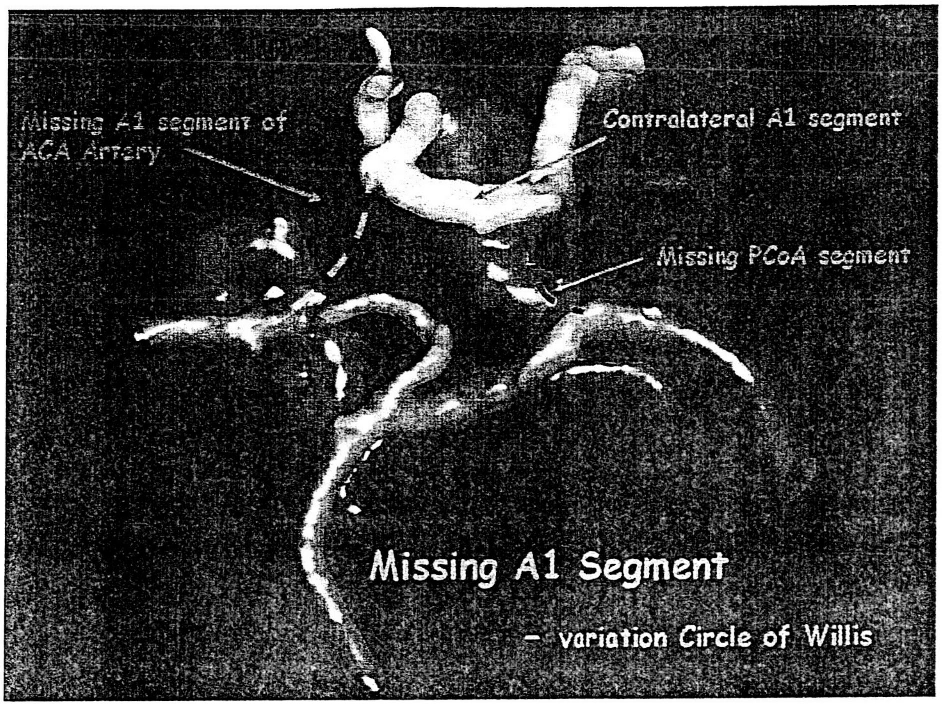
Anatomical Variations



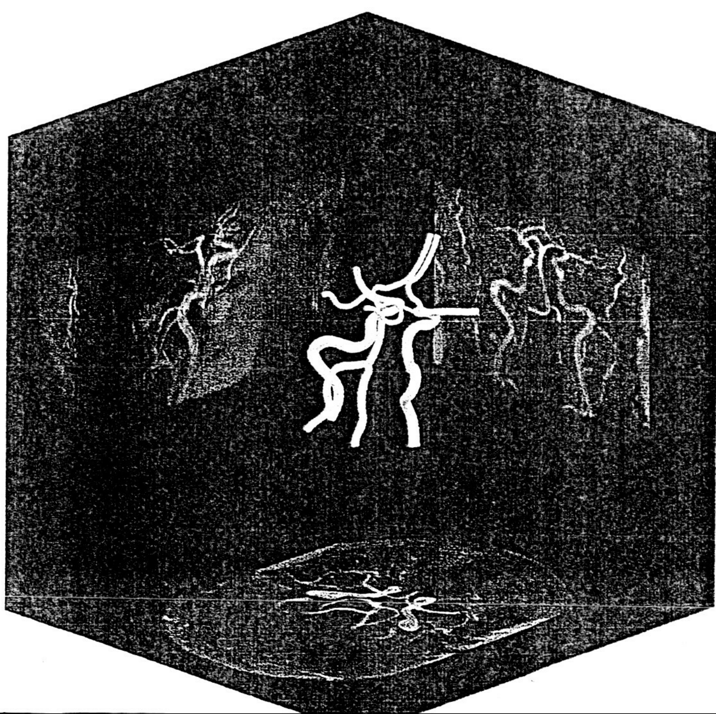
Anatomical Variations



Anatomical Variations

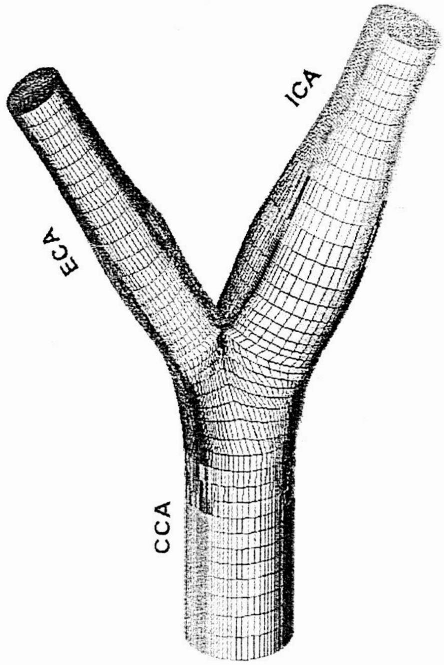


Simple geometric definition



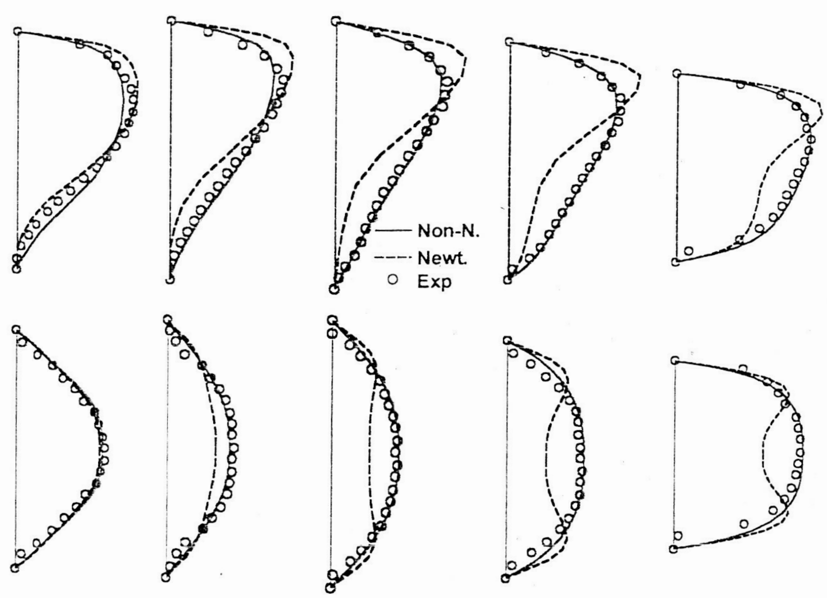
MRA
(superposition over 3 planes)

Code Validation: Carotid bifurcation

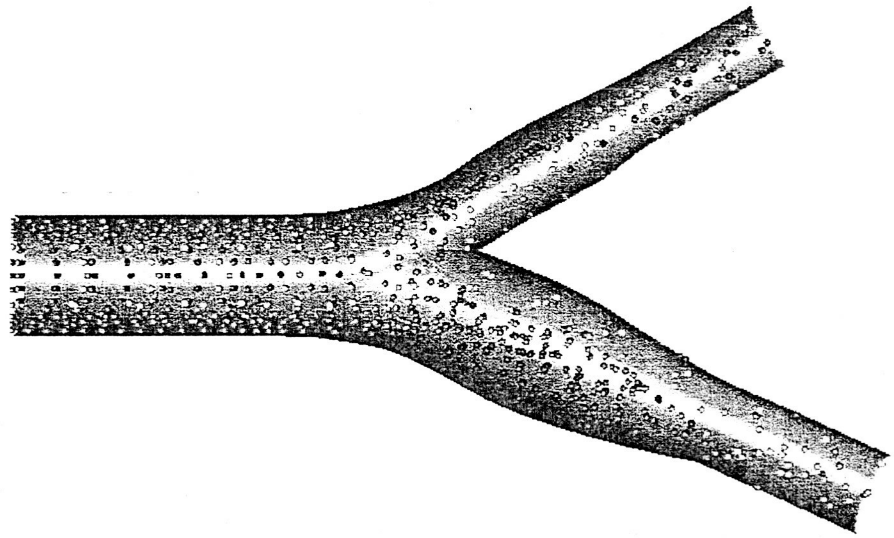


- CCA Diameter, 2r = 8 mm
- Flow ratio, Qe/Qc = 0.45
- Mean velocity, U = 7 cm/s
- KSCN Density, rho = 1410 kg/m^3
- KSCN Viscosity, v = 2.9 cPoise = 0.0029 Pa s
- Reynolds number, Re = 270.0
  - (Exp data from Gijsen, et al. 1999a)
- Chimera overset grid w/ 8 blocks
- Grid size: 41x21x25=21,525

Code Validation: Carotid bifurcation

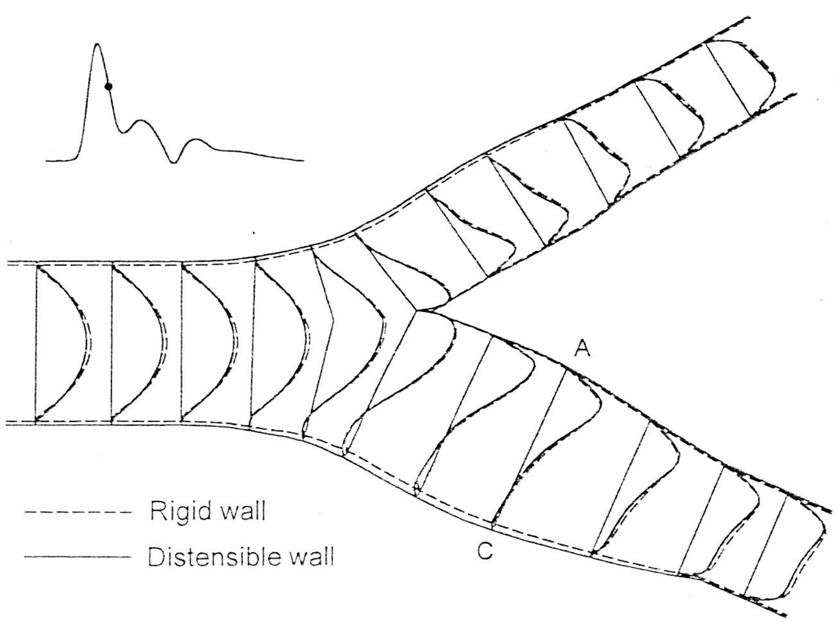


Axial velocity profiles in the internal carotid (Re=270)



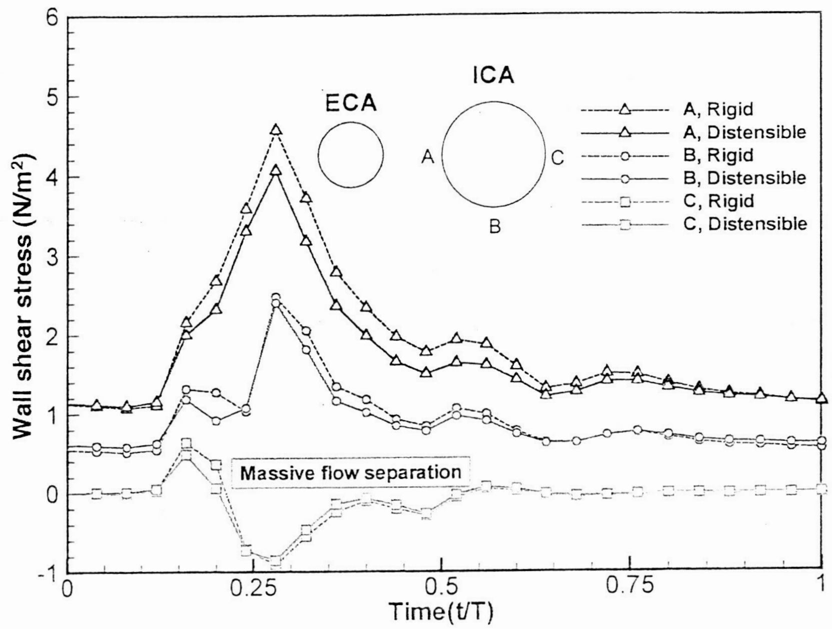
Particle tracing through a carotid arterial bifurcation (Re=388)

Effects of Wall Distensibility



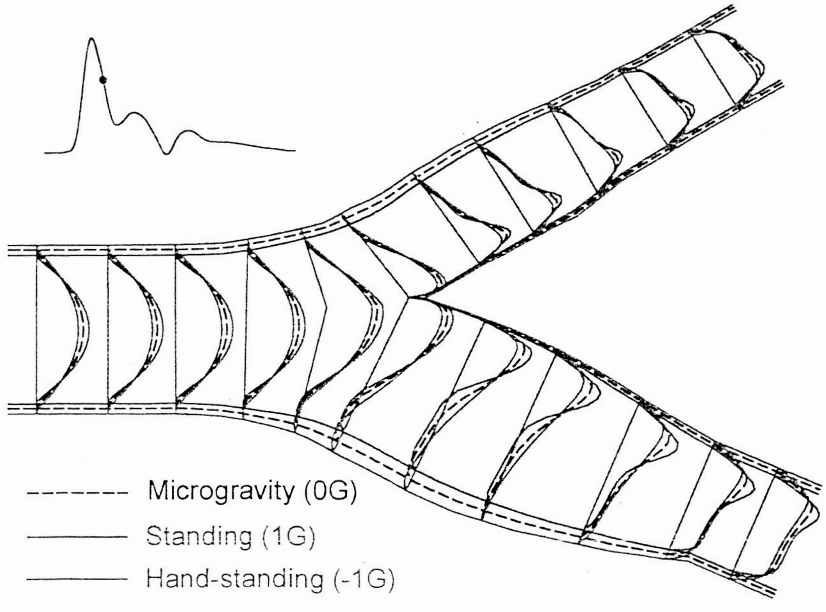
Axial velocity profiles at systolic deceleration (Re=388)

Effects of Wall Distensibility



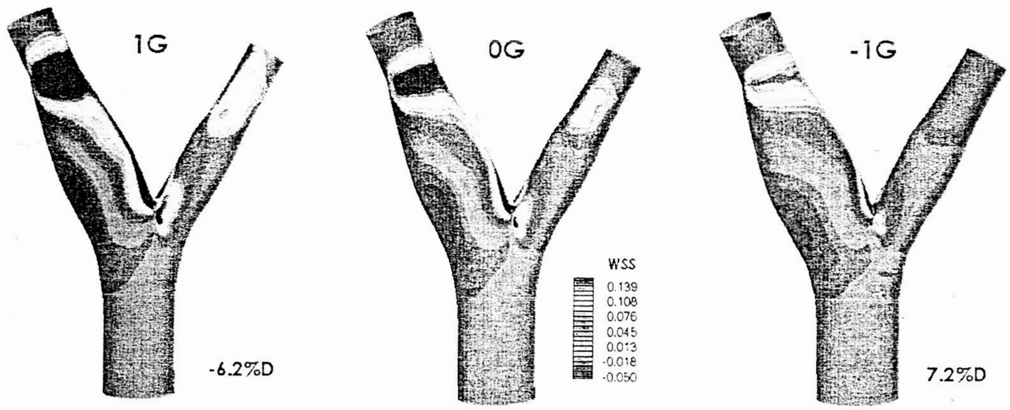
Temporal wall shear stress during a heart pulse (Re=388)

Effects of Wall Distensibility



Axial velocity profiles due to gravitational variation (Re=388)

Effects of Wall Distensibility

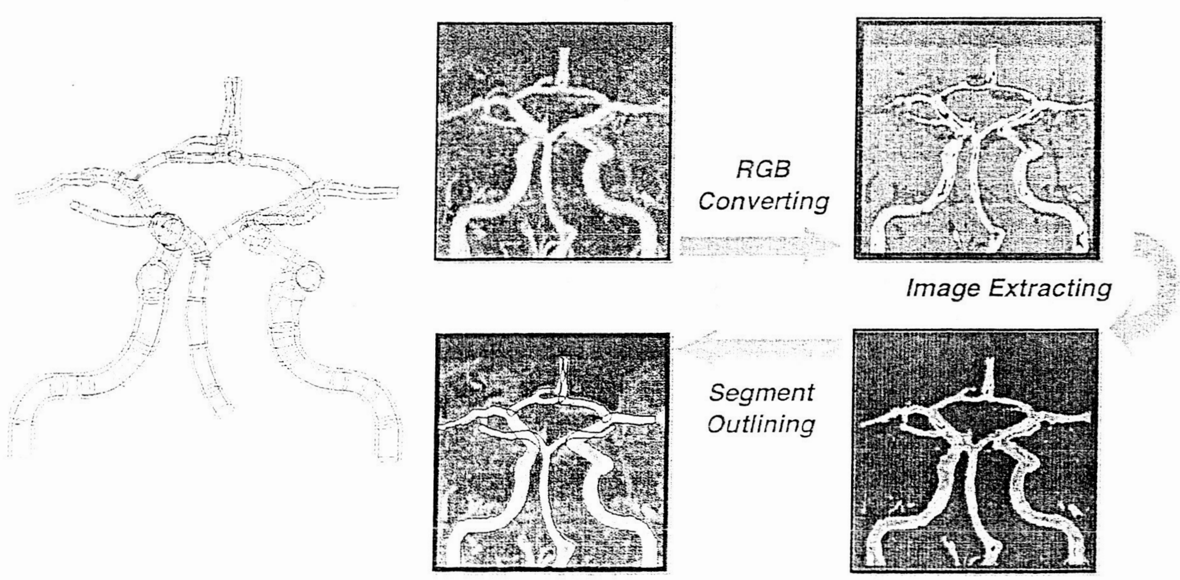


(a) Standing *(b) Supine* *(c) Hand-Standing*

Wall shear stress distribution due to gravity variation

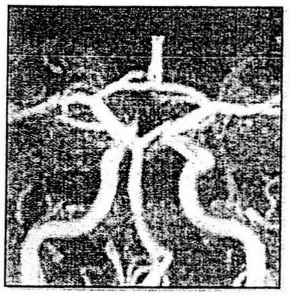
Geometry Definition

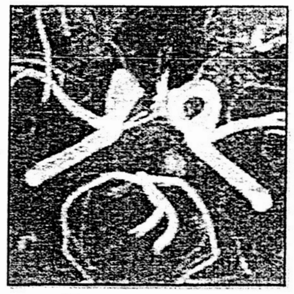
Image segmentation from MR Angiography : 3D Reconstruction



Geometry Definition

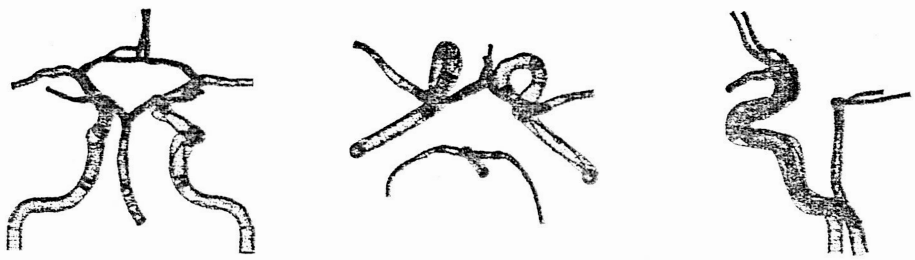
Magnetic Resonance Images (MRI) of human
Source: Professor Tim David, University of Canterbury, New Zealand


Coronal (Rear)

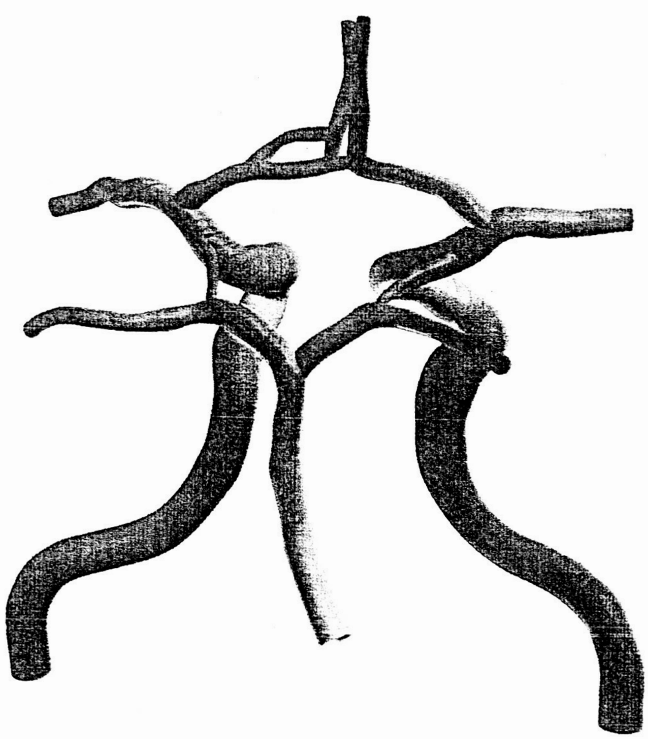

Transverse (Top)


Sagittal (Side)

Grid generated by digitized xyz data of the MRI above



Circle of Willis Simulation: Instantaneous Pressure

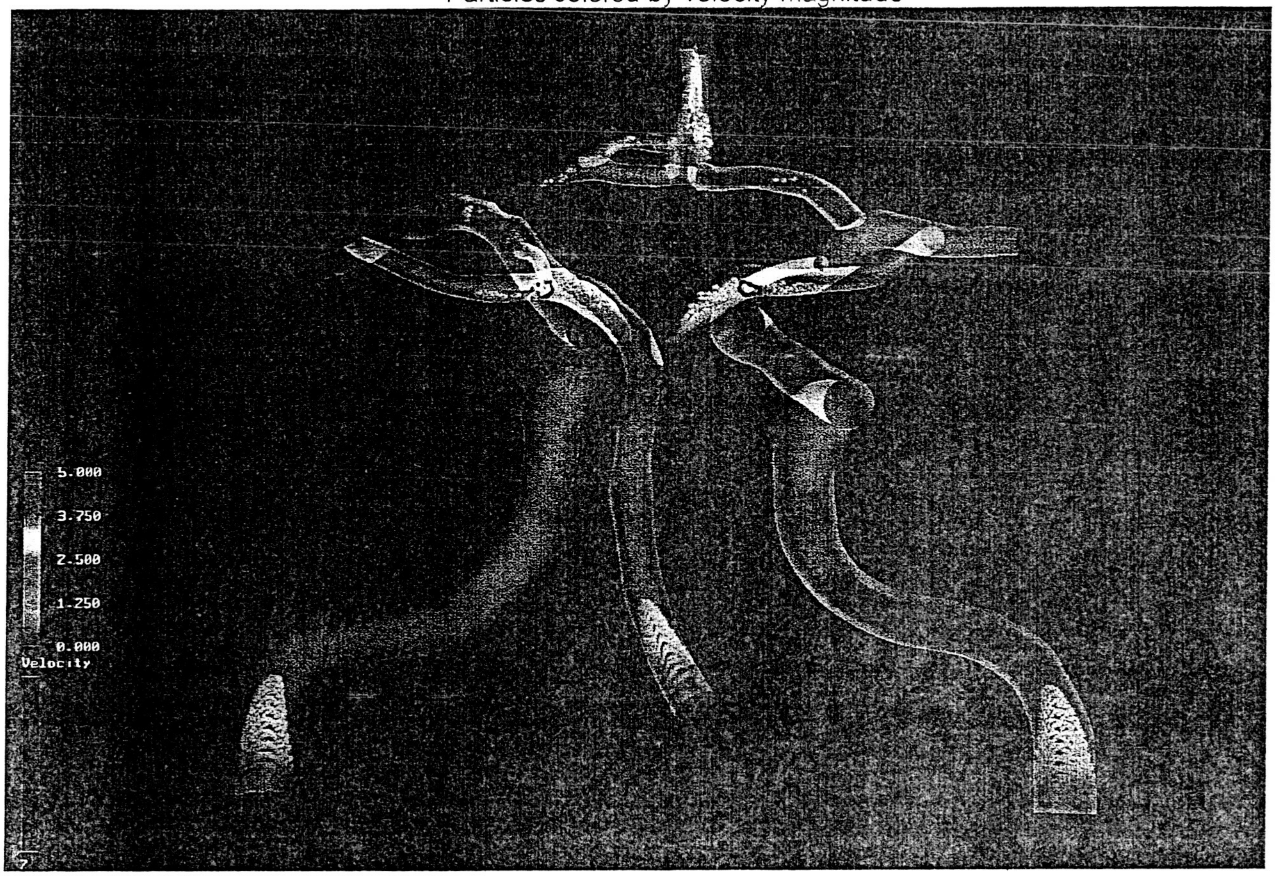


- Flow conditions:
- Left ICA diameter, 2r = 5.6 mm
- Mean velocity, U = 14 cm/s
- Blood density, rho = 1054 kg/m** 3
- Blood viscosity, v = 3.5 cPoise = 0.0035 Pa s
- Reynolds number, Re = 240.0

Code: INS3D
2 Million Grid Points
1 day to complete on 128 p.
SGI Origin 3000 (600Hz)

Circle of Willis Simulation

Particles colored by velocity magnitude



Biomedical Challenges

- How can we derive models which "replicate" human geometry and provide viable (i.e. believable to a physiologist) data in a reasonable timescale ?
- Investigate the coupling of complex cellular reaction mechanisms with mass transfer models and complex fluid dynamics (remember the geometry !)
- How to include hundreds of cell mechanisms that function in a healthy state (i.e. Ca2+)
- Fluid-structure interaction needs to be included
  - *Venous and lymph valves
  - *Artificial Heart Valves
    - –250,000 replacements in the US per year
    - –Mechanical –anticoagulant therapy
    - –Flexible – no drugs needed but NOT DURABLE

Some more math

- Try this arithmetic exercise:

  How many times does your heart beat every year ?
  37,000,000 (100,800 more in a leap year!)

  And every decade ?
  370,000,000 (obviously !)

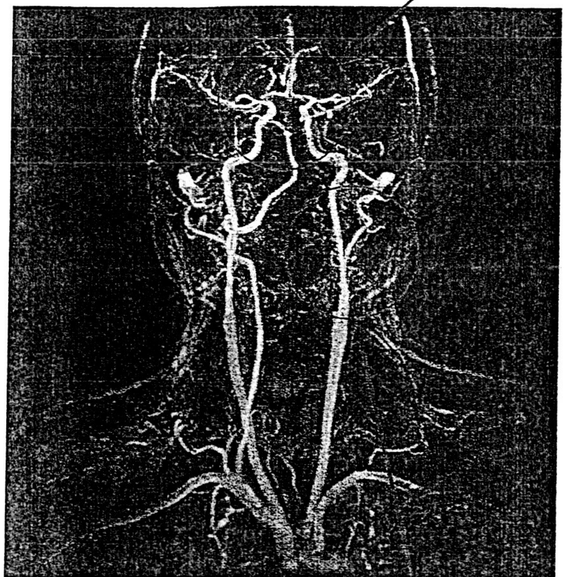
  In your life (Let's say 80 years !) ?
  30,000,000,000

More Challenges

- What are the fundamental parameters governing the proper, long-term functioning of heart valves, and how do we test for durability ?
- If we do accelerated testing are the dynamics different ?
- Does the valve operate differently in micro-gravity ?

Heart-Brain Circulation Dynamics

Circle of Willis



Carotid Bifurcation (Wall shear)

Why Heart-Brain circulation model first

- Further development of complex physiological models of auto-regulation in micro gravity, *heart-to-head*
- Pathways of large interacting particles, embolic stroke

High-Fidelity Biomedical Computing

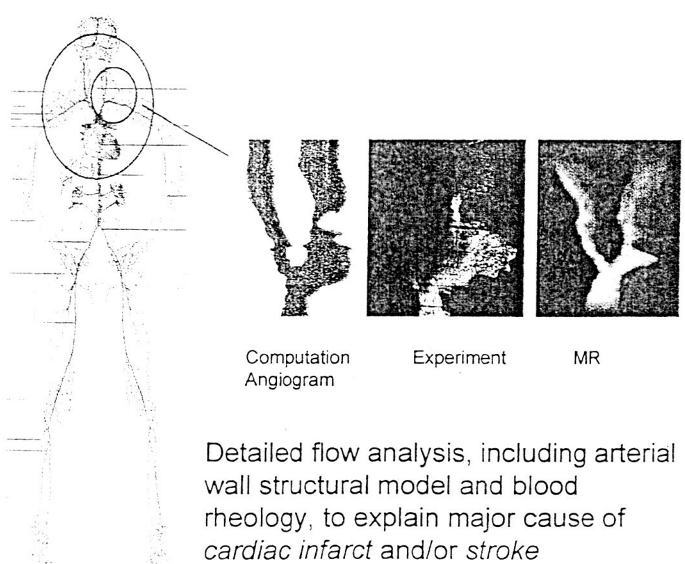
Flows in Atherosclerotic Stenotic Vessels

•Atherosclerosis causes gradual narrowing of arteries due to plaque growth

•Sufficient narrowing, or plaque rupture can lead to flow blockage and resulting tissue ischemia, leading in heart to *cardiac infarct*, in brain to *stroke.*

•Flow blockage and mechanical loading are important, for example, to determine tissue ischemia

•Local flow is neither fully turbulent nor laminar (*chaotic, disturbed transitional* etc.....)
⇒HEC will shed light on this local phenomena thru fine resolution computation (LES/DNS equivalent)



Computation Angiogram | Experiment | MR

Detailed flow analysis, including arterial wall structural model and blood rheology, to explain major cause of *cardiac infarct* and/or *stroke*

Integrated Digital Astronaut System

Digital Astronaut Performance Prediction

- To predict astronaut performance during short- and longer-duration space flight

Non-muscle Ox Delivery

Kidney Dynamics

Pulmonary Dynamics…etc

Non-muscle Local Blood Flow Control

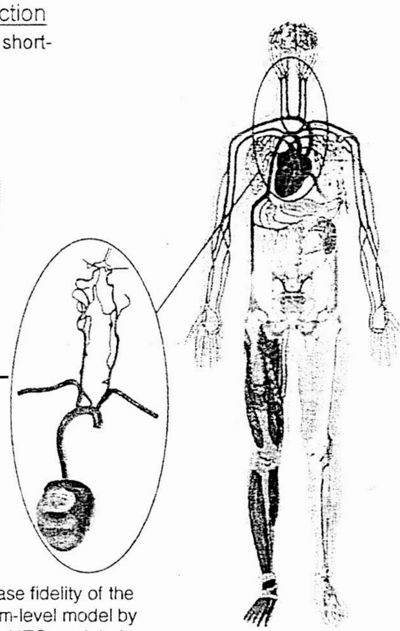
Heart Rate… Etc.

Digital Astronaut Central Integrating System

(Circulatory Dynamics-Based Modified Guyton Model)

IMAG Test-Bed and Other Existing Data

Skylab, ISS, Simulation Data



Increase fidelity of the system-level model by fusing HEC model of Heart-Aorta-Brain (CoW) and archived data

Image-Guided Monitoring

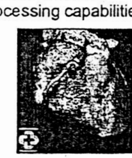
-High fidelity simulations of crew anatomy and physiology to monitor flight risks and to provide countermeasures to mitigate

- •Effects of Radiation
- •Effects due to gravitational and environmental factors

Liver and Intestine for drug/nutrient absorption evaluation

Kidney for monitoring renal function and fluid processing capabilities

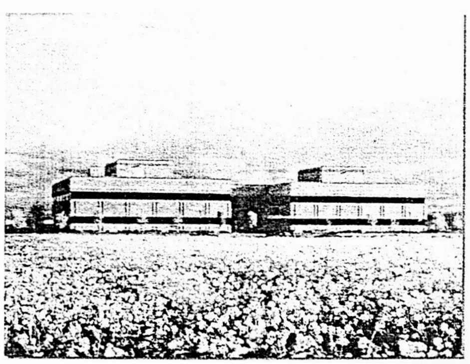
3D reconstruction of ascending vasculature from the aortic arch to the Circle of Willis for hemodynamic modeling

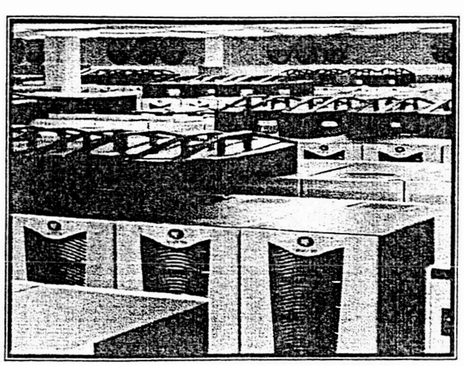


4D reconstruction of the heart for simulating changes to cardiac activity

"Columbia" Supercomputer, Storage, & Networks enables high-fidelity Digital Astronaut System

"Columbia": World Class Supercomputing

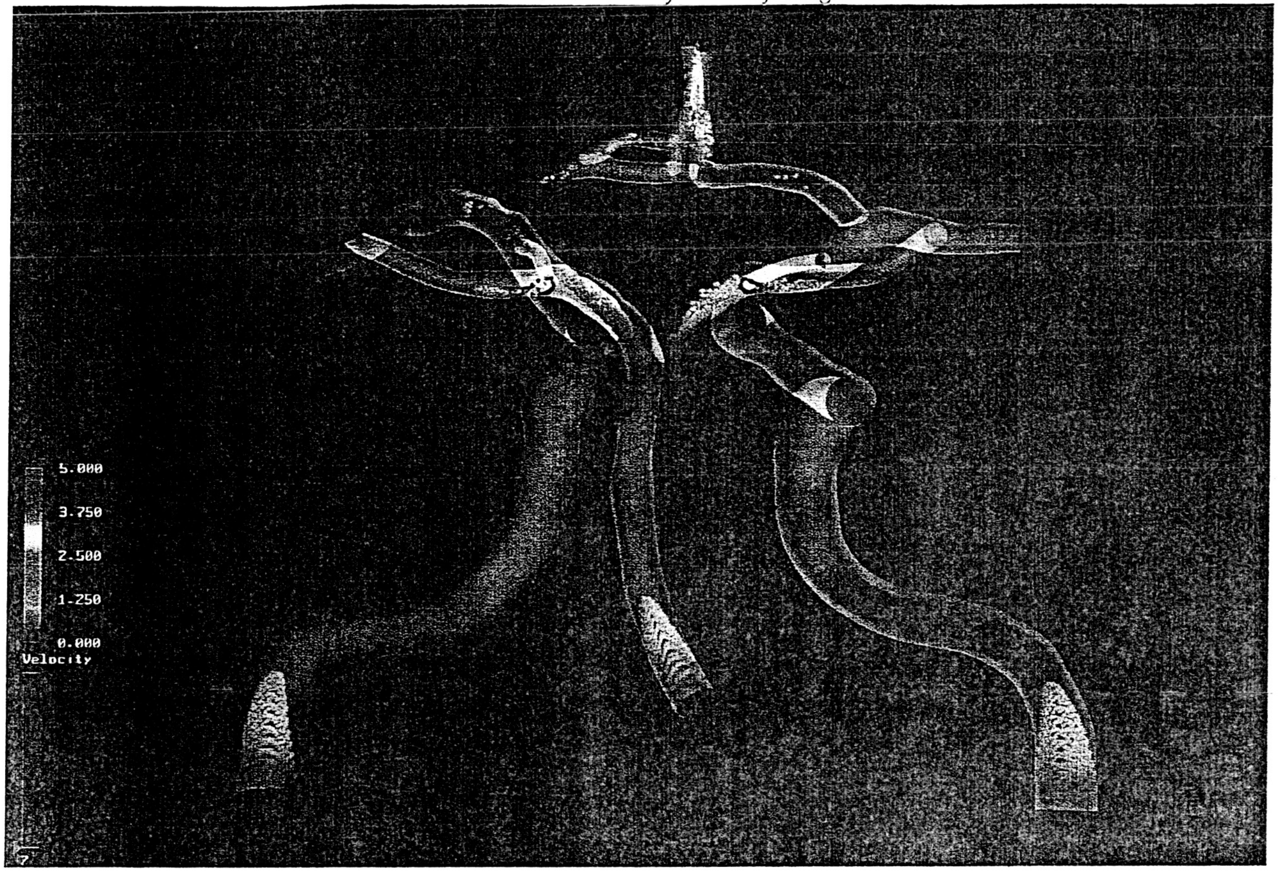




- The NAS houses the world's fastest operational supercomputer providing 61TF of compute capability to the NASA user community
- Columbia is a 20-node supercomputer built on proven 512-processor nodes
- Columbia is the largest SGI system in the world with over 10,000 Intel Itanium2 processors
- Columbia provides the largest node size incorporating commodity parts (512) and the largest shared memory environment (2048)

Circle of Willis Simulation

Particles colored by velocity magnitude



Biomedical Challenges

- How can we derive models which "replicate" human geometry and provide viable (i.e. believable to a physiologist) data in a reasonable timescale ?
- Investigate the coupling of complex cellular reaction mechanisms with mass transfer models and complex fluid dynamics (remember the geometry !)
- How to include hundreds of cell mechanisms that function in a healthy state (i.e. Ca2+)
- Fluid-structure interaction needs to be included
  - ∗Venous and lymph valves
  - ∗Artificial Heart Valves
    - –250,000 replacements in the US per year
    - –Mechanical –anticoagulant therapy
    - –Flexible – no drugs needed but NOT DURABLE

Some more math

- Try this arithmetic exercise:

  How many times does your heart beat every year ?
  37,000,000 (100,800 more in a leap year!)

  And every decade ?
  370,000,000 (obviously !)

  In your life (Let's say 80 years !) ?
  30,000,000,000

More Challenges

- What are the fundamental parameters governing the proper, long-term functioning of heart valves, and how do we test for durability ?
- If we do accelerated testing are the dynamics different ?
- Does the valve operate differently in micro-gravity ?

Summary

- **High Fidelity Modeling and Simulation**
  - More accurate : enhanced via more physics based simulation
  - Enabling : some mission characteristics not understood otherwise
  - Affordable and becoming more cost effective
    e.g. "Columbia" offers a quantum leap in HEC resources at NASA

- **Resources and time**
  - Will help sustain future mission
    (ground and flight testing are expensive and time consuming)

- **Use of best simulation tools can**
  - Increase reliability and reduce mission risk