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)
- Super Computing 2004
- 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 Canterbury 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
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

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CFD Contribution to Commercial Aircraft Design

- NASA Tech
  - PANAIR
  - A411
  - A502
  - FL022 Cartesian HSR
  - TLNS3D
  - TLNS3D-MB
  - OVERFLOW

- Boeing Tools
  - Tranair
  - TLNS3D IWD
  - Unstructured

- Boeing Products
  - A502 A488
  - A502 A488
  - A502 A488
  - A502 A488
  - A502 A488
  - A502 A488

- 1980 state of the art
  - 1980 state of the art
  - 1980 state of the art
  - 1980 state of the art
  - 1980 state of the art
  - 1980 state of the art

- Modern close coupled nacelle installation, 0.02 Mach faster than 737-200
  - Modern close coupled nacelle installation, 0.02 Mach faster than 737-200

- 21% thicker faster wing than 757-757 technology
  - 21% thicker faster wing than 757-757 technology

- Highly constrained wing design Faster wing than 737-300
  - Highly constrained wing design Faster wing than 737-300

- Successful multipoint optimization design
  - Successful multipoint optimization design

- CFD for Loads and Stability and Control
  - CFD for Loads and Stability and Control

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
Historical Note

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

1. CFD solution of HGM (c. 1983)
2. Propulsion CFD, Pump technology in the early 90s
3. New flight Engine in 1995

Integrated Simulation Environment

- Grand Challenges
- Next Generation Codes & Algorithms
  - OVERFLOW: NASA Software of the Year (Honorable Mention) STS107/RTF
  - INS10: NASA Software of the Year Pump/Flowliner
  - CART3D: NASA Software of the Year STS 107/RTF
- And more....

- Modeling Environment Comp Sci TOOLS
  - Compilers
  - Scaling and Porting
  - Parallelization Tools

- Analysis & Visualization

- Data & Computation Management
  - AeroDB
  - ILAB
  - KGA

- Storage
- CPUs
- Network
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: inducer, 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

- Launch Tower
- Multiple Bodies
- Thermal Stress
- Acoustics

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

\[ M_{\infty} = 2.46 \]
\[ \alpha = 2.08^\circ \]

4 million grid points
16 hours on 64 SQI
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
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.

Turbopump Design Problems

Can lead to cost growth, engine failure or vehicle loss

- Cavitation induced environments
- Interaction between pump and feedline leads to flow-liner cracks
- Impeller unsteady loads
- Loads and interaction with preburner
- Turbine unsteady loads

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: Kins. 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
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 countermeasure development

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

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

<table>
<thead>
<tr>
<th>Vessel</th>
<th>Radius (cm)</th>
<th>Number</th>
<th>Area (cm²)</th>
<th>Wall Thickness (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aorta</td>
<td>1.2</td>
<td>1</td>
<td>4.5</td>
<td>0.2</td>
</tr>
<tr>
<td>Arteries</td>
<td>0.2</td>
<td>159</td>
<td>2.0</td>
<td>0.1</td>
</tr>
<tr>
<td>Arterioles</td>
<td>1.5x10⁻³</td>
<td>5.7x10⁻⁷</td>
<td>400</td>
<td>2x10⁻³</td>
</tr>
<tr>
<td>Capillaries</td>
<td>3x10⁻⁷</td>
<td>1.6x10⁻¹⁰</td>
<td>4500</td>
<td>1x10⁻⁴</td>
</tr>
<tr>
<td>Venules</td>
<td>1x10⁻¹</td>
<td>1.3x10⁻⁹</td>
<td>4000</td>
<td>2x10⁻⁴</td>
</tr>
<tr>
<td>Veins</td>
<td>0.25</td>
<td>200</td>
<td>40</td>
<td>0.05</td>
</tr>
<tr>
<td>Vena cava</td>
<td>1.5</td>
<td>1</td>
<td>18</td>
<td>0.15</td>
</tr>
</tbody>
</table>

- 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 unconsciousness
  - Red-out: -3G makes retina engorged with blood

Optimal blood supply to the brain is crucial for astronauts performance

Brain Schematic
- 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

Source: http://www.strokecenter.org
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

Normal Circle of Willis

Anatomical Variations

Fetal circulation - variation Circle of Willis
Anatomical Variations

Simple geometric definition

MRA
(superposition over 3 planes)
Code Validation: Carotid bifurcation

- CCA Diameter, $2r = 8$ mm
- Flow ratio, $Q_\text{e}/Q_\text{c} = 0.45$
- Mean velocity, $U = 7$ cm/s
- KSCN Density, $\rho = 1410$ kg/m$^3$
- KSCN Viscosity, $\nu = 2.9$ 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

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)

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
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, $\nu = 3.5$ 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)
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)

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

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

Digital Astronaut Central Integrating System
(Circulatory Dynamics-Based Modified Guyton Model)

Non-muscle Ox Delivery
Kidney Dynamic
Pulmonary Dynamics...etc

Digital Astronaut 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

IMAG
Liver and intestine for drug/nutrient absorption evaluation

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 in 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)
Biomedical Challenges

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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