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Best Practices for Introducing Undergraduate Students to Computational and Interdisciplinary Research
SIAM Annual Meeting
July 13, 2012
UG Students as change agents
University & K-12 STEM Collaboration

Sarah M. Venuti (Undergraduate Student)
Avis Foster (Undergraduate Student)
Kris Kappmeyer (K-12 Teacher)
Alicia Hamar (High School Student)
Stephanie Alley (Undergraduate Student)
Andrew Samuelson (Graduate Student)

Transforming Practice Through Undergraduate Researchers, P. Seshaiyer, Council on undergraduate research Quarterly, Fall 2012.
REU: COMPUTATIONAL MATHEMATICS AND NONLINEAR DYNAMICS OF BIOLOGICAL, BIO-INSPIRED AND ENGINEERING SYSTEMS

- Stipend $3375; Free on-campus housing and meals; Travel allowance up to $550 and more!
- Supports 12 students and 2 K-12 teachers each year
- http://math.gmu.edu/reu

Sample Research Topics

- Modeling using deterministic and stochastic differential equations
- Computational biology, biomechanics and neuroscience
- Mathematics of Materials
- Nonlinear dynamics and Micro Air Vehicles

 NSF
 GEORGE MASON UNIVERSITY
Selected Quotes from participants

- "It has inspired me to push the limits, to keep asking questions and keep believing we can solve any problem."
- "I have been exposed to many applications that I did not know existed before."
- "I used to think doing research in math was purely proof based. Now I see that research in math has endless possibilities."
- "The research program has greatly helped me to answer the question that my students always seem to have...when am I ever going to use this?"
Nature of Student Activities

- Lecture Series
- Mentoring Club
- Guest Colloquium
- REU Participant Seminars
- Computational Laboratory
- Scientific and Social Tours
- Lesson Study
Sample Computational Mathematics Projects

A Computational Model for Batten Behavior in Micro Air Vehicles
Syeda Khadija F. Zaidi (University of Maryland, College Park)

Applying Numerical Methods to Fluid Structure Interactions in Biological Systems
Courtney Chancellor (Southern Methodist University)

Ordinary Differential Equations in Green Oxidation Processes
Angela Dapolite (Clarkson University)

Viscoelastic Modeling of Biological Tissue in an Idealized Cerebral Aneurysm
Kris Kappmeyer (H-B Woodlawn Highschool)

Modeling Evaporation from the pre-lens tear film over a contact lens
Amber Xu (Carnegie Mellon University)

Optimization of an Antenna Structure for a Photovoltaic Device
Emily Forney (Clemson University)

Analysis of Spherical Inflation Models for Intracranial Saccular Aneurysm Elasto-dynamics
James Halsall (Farmingdale State College, New York)
Multidisciplinary Research in Mathematics

• As concluded by the National Research Council: Undergraduate education will not change in a permanent way through the efforts of “Lone Rangers.” Change requires ongoing interaction among communities of people and institutions that will reinforce and drive reform.

• Research that happens across traditional mathematics and at the edges of traditional disciplines.

• Here is the problem, find the mathematics to solve it!
Saccular Aneurysms: Rupture
Identification of **Rupture Potential**

- Characterization of material properties
- Contact constraints
- Elasto-dynamics
- **Coupled flow-structure interaction**
Bifurcating Artery-Aneurysm Model
MAV: Membrane Wing Deflection

Padmanabhan Seshaiyer
George Mason University
Experimental Challenges in MAV Design

- Small size
- High surface-to-volume ratio
- Constrained weight and volume limitations
- Low Reynolds number regime
- Low aspect ratio fixed to rotary to flapping wings
- Longer flight time
- Better range-payload performance
Computational Challenges in MAV Design

- Structural Dynamics
- Fluid Dynamics
- Guidance & Control
- Propulsion & Power

FSI
Beam-Fluid Interaction
What makes these problems interesting?

- Fully three-dimensional
- Heterogeneous/Homogeneous
- Anisotropic/Isotropic
- Compressible/Incompressible
- Non-linearity/Linear
- Large/Small Deformations
- Dynamic/Static
- And more ........
Key Steps in Mechanics

- Kinematics
- Forces
- Balance Relations
- Constitutive Formulation
- Boundary/Initial Conditions

Boundary/Initial Value Problem
Solution Methodology

Physical System

Mathematical Model
Predator-Prey Problem

\[
\frac{dY}{dt} = \alpha_1 Y - \alpha_2 XY
\]

\[
\frac{dX}{dt} = -\alpha_3 X + \alpha_4 XY
\]

\[
Y(0) = Y_0
\]

\[
X(0) = X_0
\]
Displacement of a Linear Elastic Bar

\[ \sigma \propto \frac{du}{dx} \quad \Rightarrow \quad \sigma = K \frac{du}{dx} \]

\[ d\sigma = -f(x) \]

\[ -\frac{d}{dx} \left( K \frac{du}{dx} \right) = f(x) \]

\[ u(a) = 0 \]

\[ u(b) = 0 \]
Solution Methodology

- Physical System
- Mathematical Model
- Analytical Solution

Compare
Finding an Analytical Solution

**BVP**

\[- \frac{d}{dx} \left( K \frac{du}{dx} \right) = f(x)\]

\[u(a) = 0\]

\[u(b) = 0\]

**IVP**

\[\frac{dY}{dt} = \alpha_1 Y - \alpha_2 XY\]

\[\frac{dX}{dt} = -\alpha_3 X + \alpha_4 XY\]

\[Y(0) = Y_0\]

\[X(0) = X_0\]
Solution Methodology

Physical System

Mathematical Model

Analytical Solution

Numerical Solution

Experimental Data

Compare

Compare

Compare
Experimental Data \rightarrow BVP or IVP

- Finite Element Methods
- Finite Difference Methods
- Shooting Methods
- Runge Kutta Methods

Solution to a System of Equations

- Direct Methods
- Error Analysis
- Indirect Methods

Solution to BVP/IVP
Flow-structure interaction (FSI)

Fluid: \( \Omega_f \times (0,T) \)
\[
\rho_f \frac{\partial \vec{u}}{\partial t} - \nu \Delta \vec{u} + (\vec{u} \cdot \nabla) \vec{u} + \nabla p = f \\
\nabla \cdot \vec{u} = 0
\]

Solid: \( \Omega_s \times (0,T) \)
\[
\rho_s \frac{\partial^2 \vec{w}}{\partial t^2} - \nabla \cdot \vec{\sigma} = \vec{b} \\
\vec{\sigma} = \lambda \text{tr}(\tilde{\varepsilon}) + 2\mu \tilde{\varepsilon} \\
\tilde{\varepsilon} = 0.5 \left[ \nabla w + (\nabla w)^T \right]
\]
Modeling Arterial Wall-Flow Interaction

Mathematical Model

Modeling, Analysis and Computation of Fluid Structure Interaction Models for Biological Systems
S. Minerva Venuti and P. Seshaiyer (Mentor), SIAM Undergraduate Research Online (2010)
### One-dimensional Model

![Diagram](image)

- Inner wall
- Outer wall
- Arterial Wall
- Blood
- Spinal Fluid
- $X_b = X_0 \sin(\omega t)$

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$</td>
<td>1000 kg/m$^3$</td>
<td>density of spinal fluid</td>
</tr>
<tr>
<td>$\mu$</td>
<td>0 Stokes</td>
<td>viscosity of spinal fluid</td>
</tr>
<tr>
<td>$c$</td>
<td>1500 m/s</td>
<td>velocity of spinal fluid</td>
</tr>
<tr>
<td>$m$</td>
<td>1.0 kg</td>
<td>mass of the arterial wall</td>
</tr>
<tr>
<td>$a$</td>
<td>0.01 m$^2$</td>
<td>area of the outer arterial wall</td>
</tr>
<tr>
<td>$k$</td>
<td>8000 N/m</td>
<td>spring constant</td>
</tr>
<tr>
<td>$\omega$</td>
<td>1 rad/s</td>
<td>frequency of heart beat</td>
</tr>
<tr>
<td>$X_0$</td>
<td>0.01</td>
<td>amplitude of heart beat</td>
</tr>
<tr>
<td>$X_b$</td>
<td>0.01</td>
<td>displacement imposed by the pressure exerted against the arterial wall by the blood</td>
</tr>
</tbody>
</table>
Coupled FSI System

\[
\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \quad 0 < x < L
\]

\[-\rho c^2 \frac{\partial u}{\partial x} a + m \dot{u}(0, t) + k \ddot{u}(0, t) - kX_0 \sin(\omega t) = 0 \quad \text{for } x = 0\]

\[u(L, t) = -c \frac{\partial u}{\partial x}(L, t) \quad \text{for } x = L\]

\[u(x, 0) = \dot{u}(x, 0) = 0\]
Analytical Solution

\[ u(0, t) = Ae^{r_1 t} + Be^{r_2 t} + C \cos t + D \sin t \]

\[ r_1 = -\frac{\rho ac/m - \sqrt{(\rho ac/m)^2 - 4(k/m)}}{2} \]

\[ r_2 = -\frac{\rho ac/m + \sqrt{(\rho ac/m)^2 - 4(k/m)}}{2} \]

\[ A = \frac{(k/m)X_0\omega}{(r_1 - r_2)(r_1^2 + \omega^2)} \]

\[ B = \frac{(k/m)X_0\omega}{(r_2 - r_1)(r_2^2 + \omega^2)} \]

\[ C = -\frac{(k/m)X_0\omega\rho ac m}{\rho^2 a^2 c^2 \omega^2 + m^2 \omega^4 - 2m^2 \omega^2 (k/m) + k^2} \]

\[ D = -\frac{(k/m)X_0\omega m(m\omega^2 - k)}{\rho^2 a^2 c^2 \omega^2 + m^2 \omega^4 - 2m^2 \omega^2 (k/m) + k^2} \]
Displacement at x=0
Variations on parameter $k$ - stiffness

$K=4000$  

$K=16000$  

$K=8000$  

$K=32000$
Variations of rho - density

Rho = 500

Rho = 2000

Rho = 1000

Rho = 4000
How does new research problems evolve?

\[
F_{\text{blood}} = kX_0 \cos \omega t
\]

\[
\rho \frac{\partial v}{\partial t} + \rho v \frac{\partial v}{\partial x} + \frac{\partial P}{\partial x} + \mu \frac{\partial^2 v}{\partial x^2} = F
\]
What type of transformative research and training can one do?

- Modify Key Assumptions
- Build Realistic Geometry
- Optimize Mathematical Techniques
- Enhance Mathematical Software
- Match Experimental Data
- Refine Mathematical Model
- Perform Parameter Estimation Studies
My Contacts!

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Thank You