\Workshops on Computational Modeling of Complex Systems

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Workshop Objectives

- Disseminate project work among promising students
- Encourage enthusiasm for research and modeling complex systems
- Find good prospects for REU and graduate programs
- Encourage under-represented minorities to enter STEM fields
- Encourage inter-disciplinary work
- Develop course materials

Additional Workshop Benefits

- Collaboration in preparing workshop
- Dissemination of CMACS research
  - At Lehman
  - At other CUNY institutions (Hunter and Brooklyn)
- Preparation of students
  - For grad school and for research in related areas
  - To use the methods and tools developed under CMACS
- Feedback on tools

Outline

- Workshop series (2010-2014)
- 2010 Workshop on Modeling Signaling Pathways in the Cell
  - Syllabus
  - Students
  - Student Work
  - Outcomes
- Planned 2011 Workshop

Workshop Series

- Three weeks (most of January) each year
- Rotate challenge problems:

Challenge Problem	Year
1. **Signaling Pathways in Pancreatic Cancer**	Winter 2010 Faeder, Langmead
2. **Fibrillation Onset in Cardiac Tissue**	Winter 2011 Fenton, Gilmour, Grosu, Smolka
3. **Distributed Automotive Control**	Winter 2012
4. **Aerospace Control Software**	Winter 2013

Signaling Pathways in the Cell

- Motivated by pancreatic cancer challenge problem

- Materials and exercises by Jim Faeder, Chris Langmead, and Nancy Griffeth

- Final student presentations showed impressive development of skills

- Final student evaluations showed delight with workshop

Workshop Syllabus – Week 1

- Introduction
  - The life cycle of a cell
  - Mac OS X and Unix
  - The role of signaling in the cell's life cycle
  - Modeling biochemical systems
  - Chemical kinetics
  - Student exercise: Toy model

http://www.lehman.edu/academics/cmacs

Workshop Syllabus – Week 2

- ## Using modeling

  - Visiting lecture by **Jim Faeder**:
    Using Modeling to Bridge Scales in Biology

  - Wiring Diagrams

 - Student Exercise: Modeling the signaling at the G2 checkpoint in frog cells

Workshop Syllabus – Week 3

- **Model checking and final exercises**
  - Temporal Logic
  - Visiting Lecture by **Chris Langmead**: *Model Checking*
  - Student exercise: Modeling the EGFR signaling pathway
  - Final lecture by **Bud Mishra** *Modeling and Cancer*

Student population

- 15 out of 25 applicants selected
  - 6 from Lehman College
  - 4 from Brooklyn College
  - 4 from Queens College
  - 1 from Stony Brook
- Under-represented minorities
  - 2 African-American
  - 6 women
  - 2 Hispanic

Student population

- Majors
  - 7 mathematics
  - 3 computer science
  - 5 biological or chemical sciences
- Group Approach
  - Five groups of three for each exercise
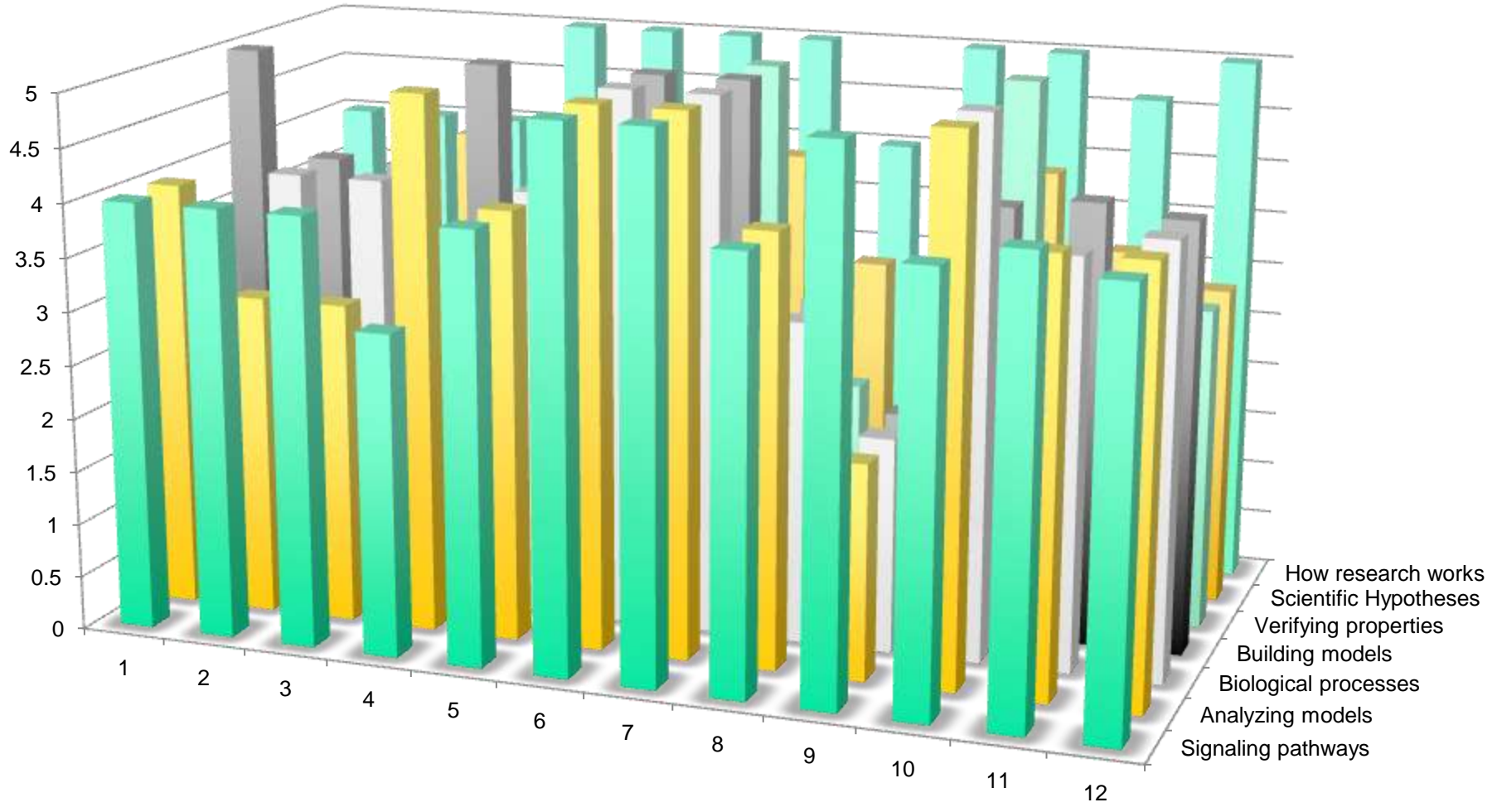 - One Bio, one CS, one Math
  - Re-arranged groups once

Student Evaluations – General Objectives
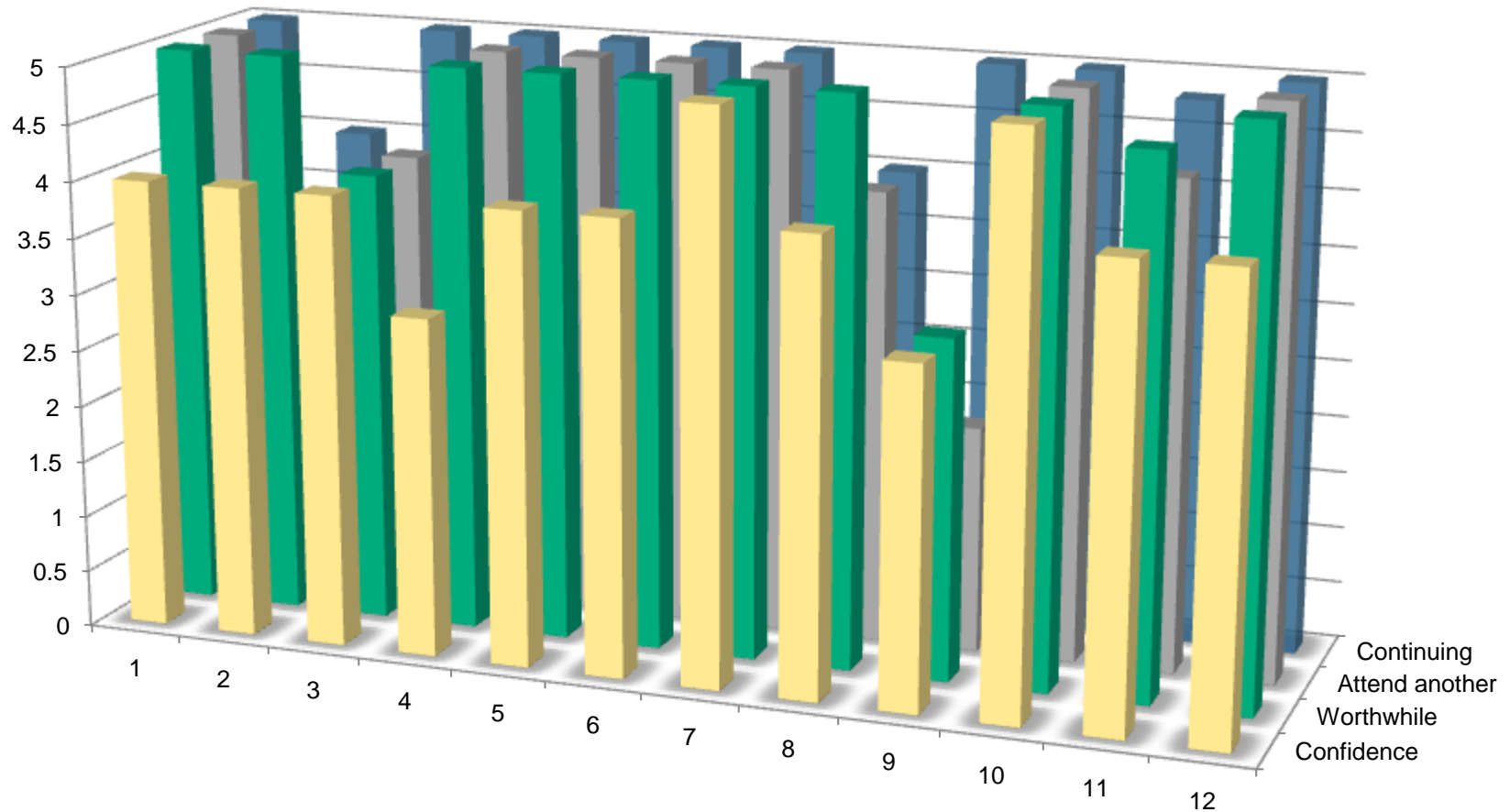
Student Evaluations – Specific Learning Objectives

Best things about workshop…

- "Working in groups to model was the most effective and fun way to spend time."
- "Working with others helped bring different perspectives and interpretations to questions and data."
- "Most interesting was model checking as a method to verify the models."
- "I really liked the speeches from the speakers that were invited to the workshop."

Best things about workshop…

- "It was amazing how people with different expertise backgrounds were able to come together and apply their knowledge and contribute in some way."

- "I liked how we examined the ways different scientific fields interact. I liked seeing how computer programming can aid in 'hard' science research."

- "Integrating multiple disciplines and methodologies and working in groups to build and analyze biological systems."

Best things about workshop…

- "Miss Griffeth is a very knowledgeable person and the right person to conduct a workshop like this."
- "Everything on this workshop was great"

Suggested improvements

- "Less time on cell biology at the outset and more time for modeling."

- "I would have the students work on their own models much sooner as that seemed to generate the most interest"

- "I would spend more time on reinforcing biological terms since there were many students who are majoring on other areas."

Suggested improvements

- "I would have put more emphasis on modeling the real biological models and tried to get through the basic biology and toy models faster."

- "If there was more emphasis on understanding the biological concepts maybe it would have been easier to build the models and use the computer programs."

Other outcomes

- Lehman advisory committee
  - New CS/Bio courses
  - Bioinformatics minor
- Potential Lehman collaborator (Stephen Redenti)
- Planned courses at Lehman
- New Bioinformatics minor for CS and Biology majors

Other outcomes

- **Relationships with other CUNY colleges**
    - Talks at other CUNY colleges
    - To develop: CUNY-wide advisory committee
- **Dissemination of CMACS ideas and tools to the grad assistants**
- **Several workshop attendees applying to REU programs**

Planned 2011 Workshop

- Challenge problem: Atrial Fibrillation

- Collaborators: Flavio Fenton, Robert Gilmour, Radu Grosu, Scott Smolka

Lessons learned from 2010

- Have a grad student from the project available for the first week
- Develop the material over the summer
  - More time to test and improve tools
- Add material on forming and testing hypotheses
- Break into groups by major subject for specialized tutorials
- Teaming exercises

Personal Research Interests

- Model Discovery (in computer networking)

- Modeling and model-checking biological systems (Faeder, Clarke, Redenti)

- Using Abstract Interpretation to Support Model Discovery (Cousot)