Workshops on Computational Modeling of Complex Systems

Flavio Fenton and Nancy Griffeth
March 28, 2011
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
Outline

- Recruiting and Admission: Nancy
- 2011 Workshop on Atrial Fibrillation
  - Week 1: Flavio
  - Weeks 2-3 and Evaluation: Nancy
- Student Results and Paper: Flavio
- 2012 Workshop on Cellular Signaling Pathways
2011 Workshop: Recruiting and Admission

- Target Colleges: Lehman, Hunter, Brooklyn, Queens, CCNY
- Applicants:

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### 2011 Workshop: Student Characteristics

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Workshop Outline

- Biology background: Week 1 (Flavio Fenton, Rupinder Singh)
- Mathematical and Programming background: Week 2
- Student Project: Week 3
Week 2

- Mathematical preliminaries
  - Modeling exercise and differential equations – Terri Grosso
  - Numerical Integration – Kai Zhao
  - Introduction to CUDA – Joshua Rogers
  - The 4V Model and Code – Ezio Bartocci
Week 3

- Students worked in 5 groups (same as week 2)
- Flavio assigned parameters to each group
- Using Ezio’s code on various CUDA machines*, students generated data
- Flavio reviewed the work via Skype

*Thanks to Brian Murphy and NVIDIA
Week 1

- Complex Systems and Biological Background
  - CMACS and its goals
  - Chaos and complex systems
  - Experimental exercises with oscillators
  - Relation between oscillators and cardiac cells
  - Mathematical modeling of cardiac cells
  - Cardiac arrhythmias and its study by computer simulations
Week 1

- Saline Oscillator
Week 1

- Saline Oscillator
Week 1

- Saline Oscillator
Week 1

- Saline Oscillator
Week 1

Chemical Oscillators

Briggs-Rauscher and Belousov-Zhabotinsky
Week 1

- Chemical Oscillators
  Briggs-Rauscher and Belousov-Zhabotinsky
Students Results
Teaching cardiac electrophysiology modeling to undergraduate students: Lab exercises and GPU programming for the study of arrhythmias and spiral wave dynamics

Ezio Bartocci\(^1\), Rupinder Singh\(^2\), Frederick B. von Stein\(^3\), Avessie Amedome\(^4\), Alan Joseph J. Caceres\(^4\), Juan Castillo\(^4\), Evan Closser\(^4\), Gabriel Deards\(^4\), Andriy Goltsev\(^4\), Roumwelle Sta. Ines\(^4\), Cem Isbilir\(^4\), Joan K. Marc\(^4\), Diquan Moore\(^4\), Dana Pardi\(^4\), Sandeep Sadhu\(^4\), Samuel Sanchez\(^4\), Pooja Sharma\(^4\), Anoopa Singh\(^4\), Joshua Rogers\(^4\), Aron Wolinetz\(^4\), Terri Grosso-Applewhite\(^4\), Kai Zhao\(^4\), Andrew B. Filipski\(^5\), Robert F. Gilmour Jr\(^3\), Radu Grosu\(^5\), James Glimm\(^1\), Scott A Smolka\(^5\), Elizabeth M. Cherry\(^3,7\), Edmund M. Clarke\(^8\), Nancy Griffeth\(^4\), Flavio H. Fenton\(^3\)

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Student Evaluations – Specific Learning Objectives

- Analyze models
- Biological processes
- Build models
- Verify properties
- Scientific Hypotheses
- How research works
Best things about workshop...

- **Learning experience**
  - A ground-up exposure to the process of formulating a model
  - Running the Simulations of the Spiral waves on the cuda GPU
  - Learning how heart fibrillation works
  - Learning about the resources and technology … necessary for … research
  - Applications of parallel computation to simulate the human heart

- **Collaboration**
  - The opportunity to collaborate with other peers in different disciplines.
  - Seeing how every area of science (Biology, Math) work together to solve the real world problems from very distinguished professors

- **Future plans**
  - This workshop inspired me to pursue information outside of my own discipline.
  - Getting a sense that I am capable of doing similar research
Suggested improvements

- More of the biological background relevant to our models. I really enjoyed Robert Gilmore’s presentation … it would have been more helpful to begin with [it].
- [Topics], whether biology, math, or programming, [were] first presented in a complex manner and then more simply.
- More time to working on projects and presentations
- I would do the Math first.
- [More on] how to construct a basic differential equation that describes some simple behavior
- **Week one**: general introductions of the concept to students of all majors.
  **Week two**: separate students by majors and provide more intense learning in the field related to each group
  **Week three**: final project
Planned 2012 Workshop

- Challenge problem: Pancreatic Cancer
- Collaborators: Jim Faeder, Ed Clarke, ...