

Agenda for the Retreat

- 9-9:30 Welcome and Goals
- 9:30-9:45 Proposed SAB members
- 9:45 -11 Home Runs
- 11-11:30 Break
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- 3:30 Refreshments and/or faculty meeting



Simbios Retreat 2005

Goals for Simbios

Scott L. Delp
Russ B. Altman

Stanford University

NIH National Centers

1999: Smarr/Botstein report recommended increased NIH support of biomedical computation, including national centers

2001: planning grants awarded

2004: broad competition for "National Centers for Biomedical Computing"

Four awards made in 2004

Three more awards in 2005

NIH vision: National Centers

“National Centers for Biomedical Computing (NCBC) will develop and implement the core of a universal computing infrastructure that is urgently needed to speed progress in biomedical research. The centers will create innovative software programs and other tools that enable the biomedical community to integrate, analyze, model, simulate, and share data on human health and disease.”

Components of a center

- Biomedical computation research
- Driving biological problems, from funded NIH research
- Education
- Dissemination/Outreach
- Infrastructure
- Administration

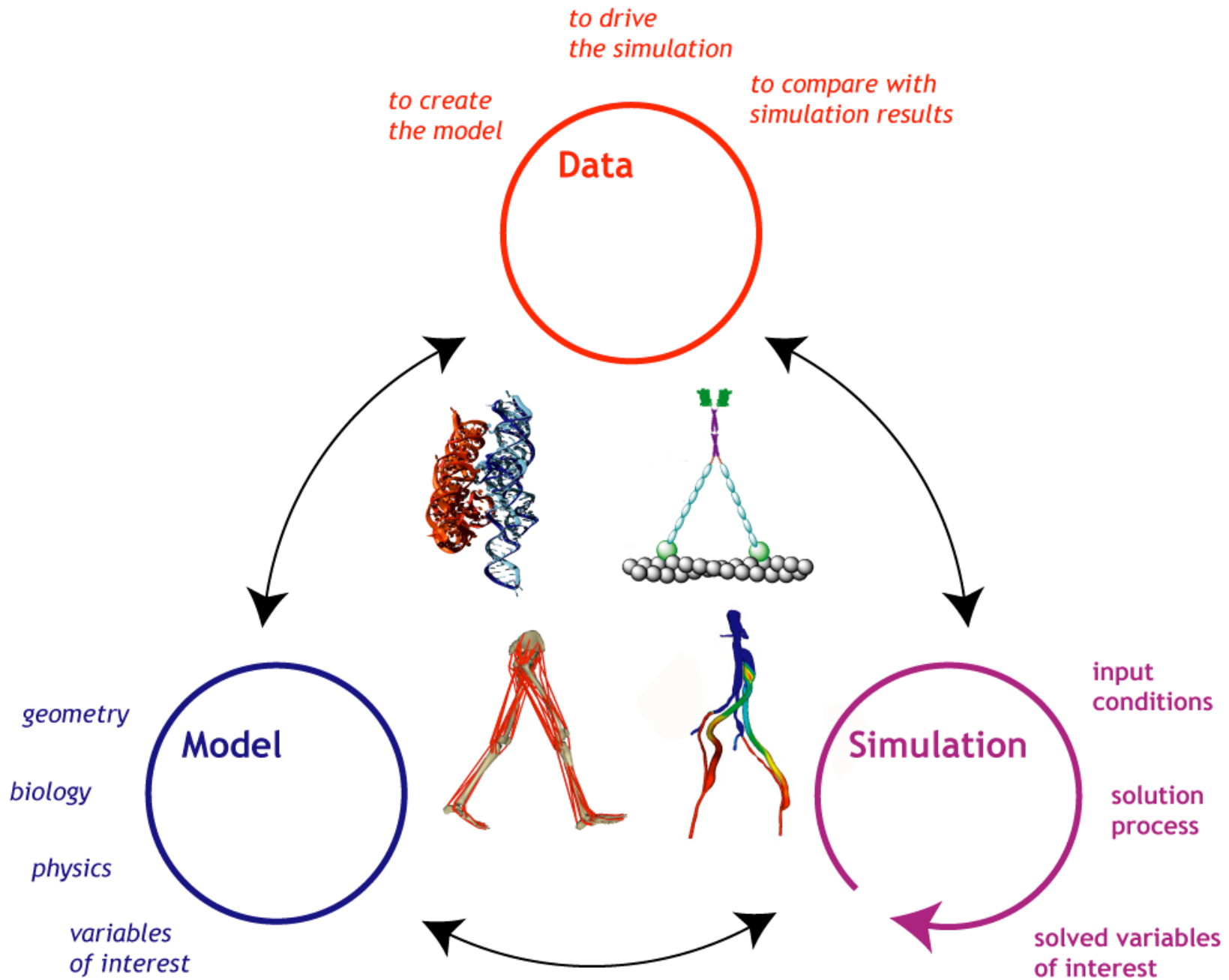
Why physics-based simulation in biology?

- Simulation provides structure-function relationship
- Simulation of biological can be used to plan individualized therapy
- Multiple fragmented scientific communities do simulation (e.g. molecular dynamics, biomechanics) based on $F = m a$
- No common software platform to facilitate sharing, transfer of innovation, linking of scales
- No easy method to disseminate tools to biomedical researchers without simulation expertise.

Simbios: National Center for **SIM**ulation of **BIO**logical **S**tructure

MISSION: Enable biomedical scientists to develop and share accurate simulations of biological structures—from molecules to organisms.

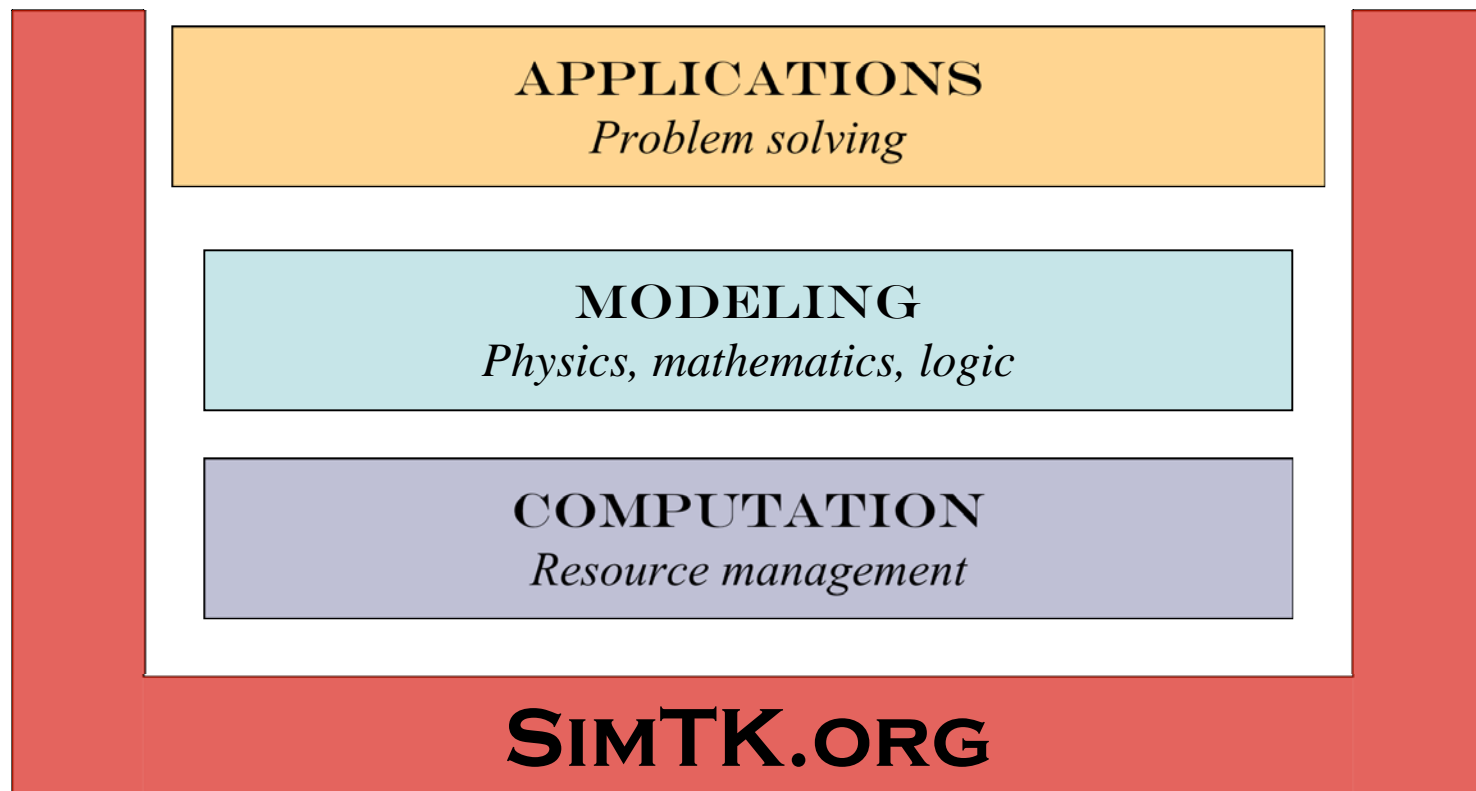
1. Perform innovative research in methods for biological structure dynamic simulation (from molecules to organisms)
2. Disseminate these (and other) methods to the biomedical research community through a **Simulation toolkit = SimTK**



Measures of Success

- Quality of biomedical **research**
(measured by impact of publications)
- Quality of **methods**
- Quality of **software** (measured by
number of users)

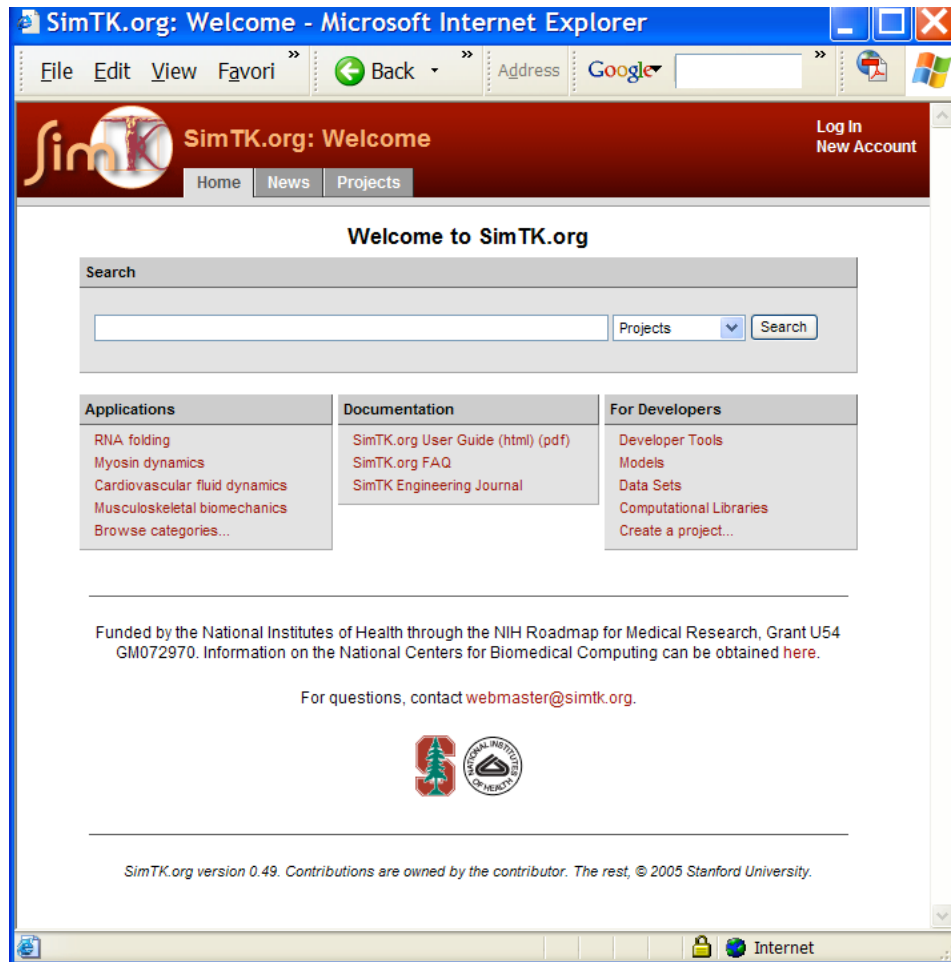
SimTK organization



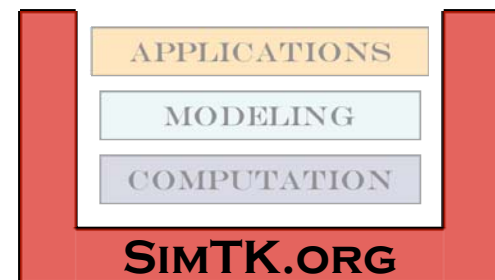
“Buy-in” possible at several levels

Milestones from year 1

- Established SimTK.org (\approx 60 projects)

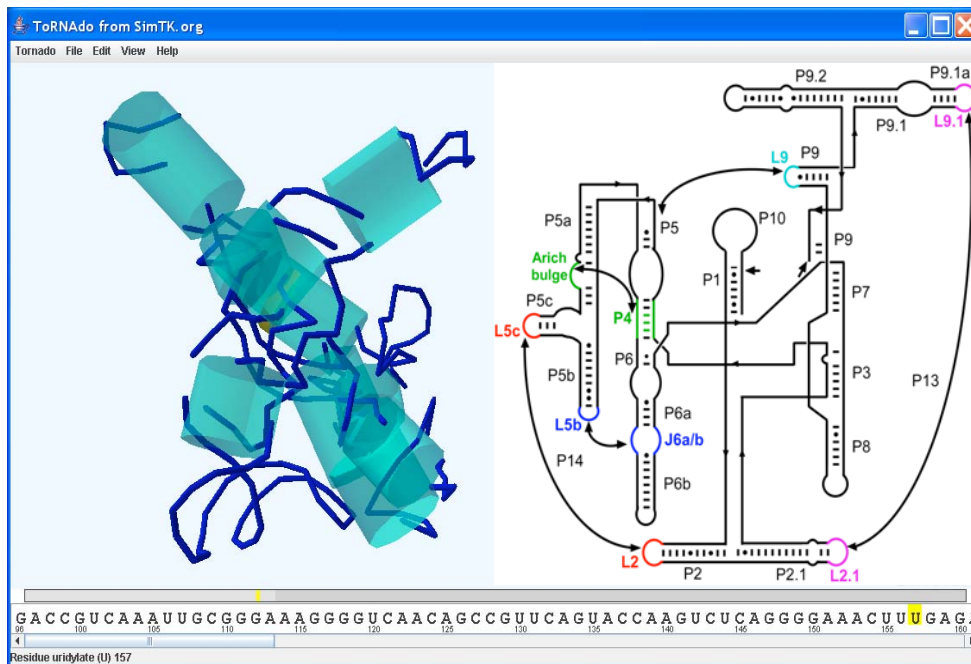


SourceForge-like
"federated"
model



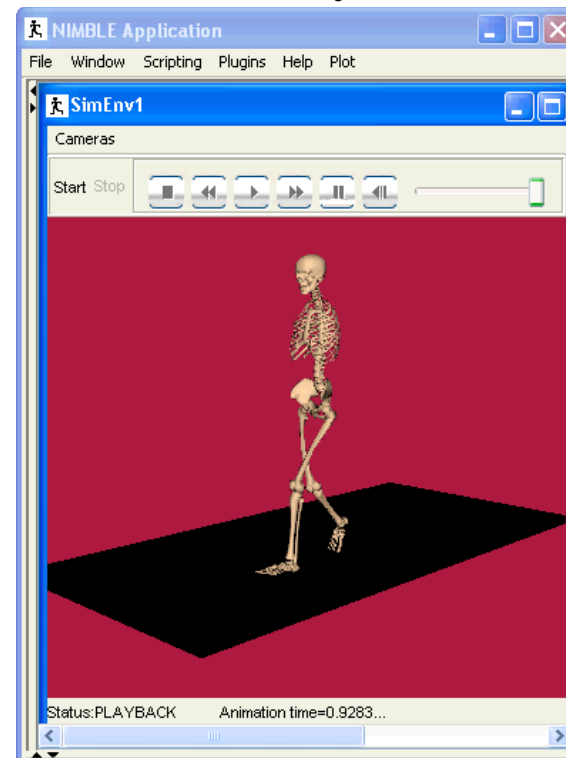
Milestone from year 1

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Biomedical Computation Review

<http://BiomedicalComputationReview.org/>



- Dissemination effort of Simbios but very broad in scope
- A magazine (not a journal) to help foster a wide community of those interested in various aspects of biomedical computation

David Paik, Kathy Miller



DIVERSE DISCIPLINES, ONE COMMUNITY

Biomedical Computation REVIEW

Packing It All In

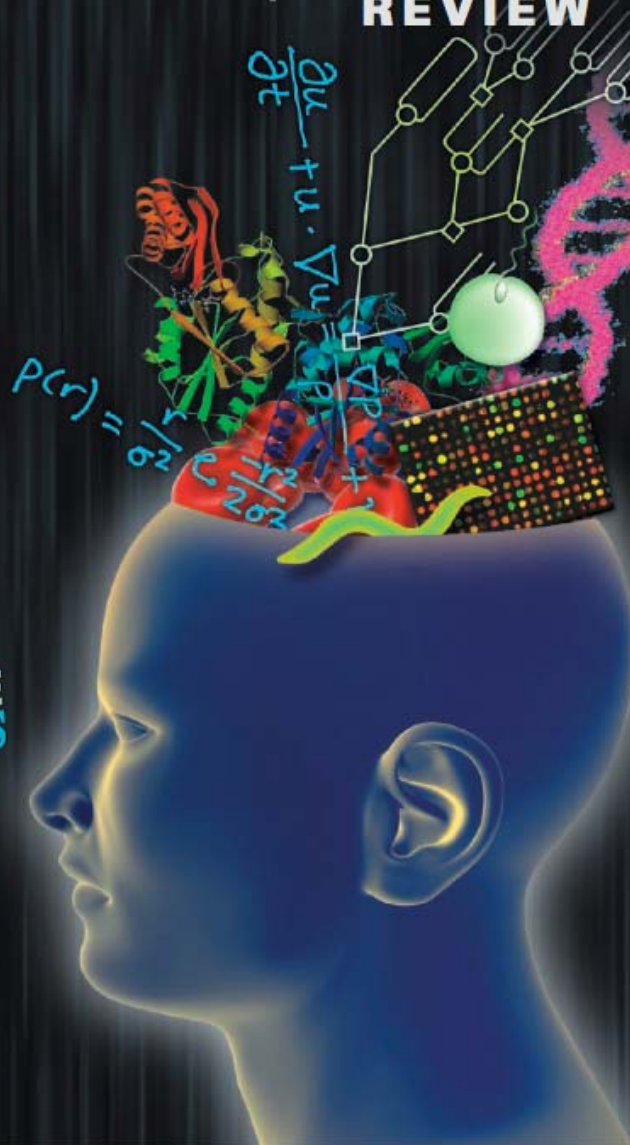
Curricula for
biomedical
computation

PLUS:

The dawn of **BRAIN-MACHINE INTERFACES**

Brain implants are
giving hope to the
disabled and
revolutionizing
neuroscience

Fall 2005

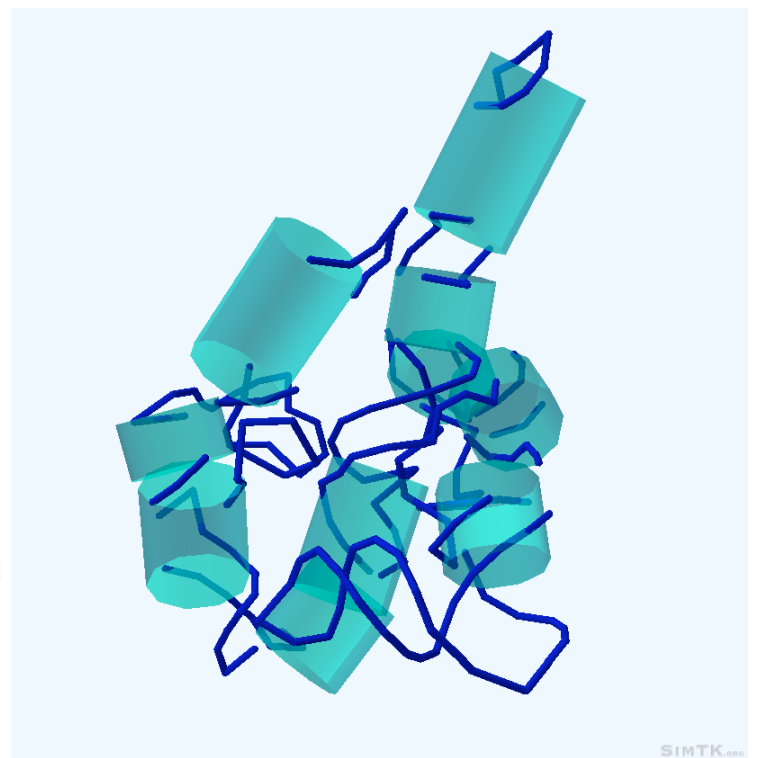
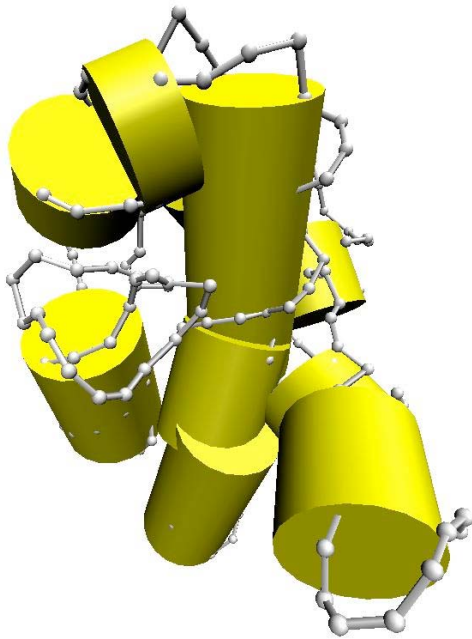
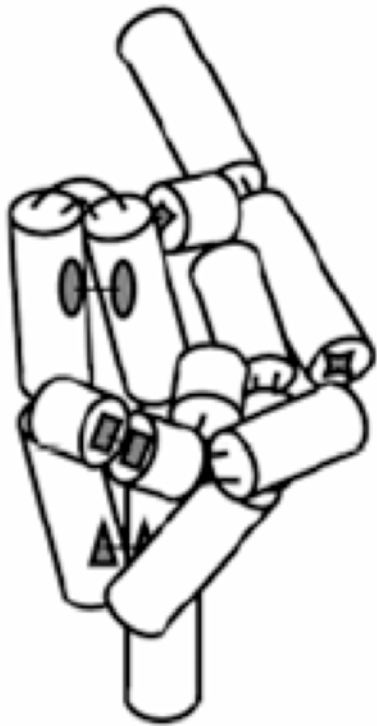


Fall
2005,
Issue #2

Milestone from year 1

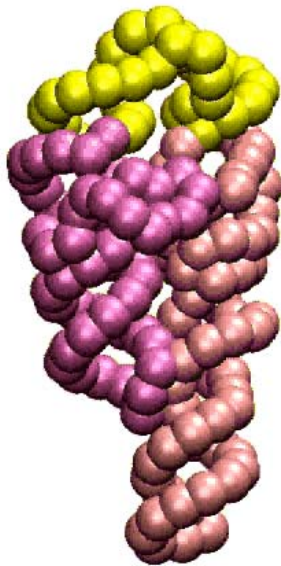
- Established SimTK.org
- Initiated development of three applications (ISIM, toRNAdo, openSim)
- Biomedical Computation Review
- Fantastic array of research in physics-based simulation in biology and medicine

Methods for automatically "segmenting" a molecule into bigger units.

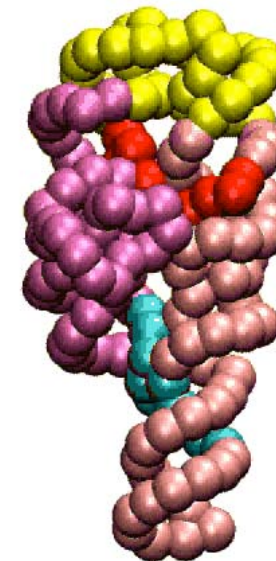


SIMTK.com

Segment RNA into 1 sphere/base



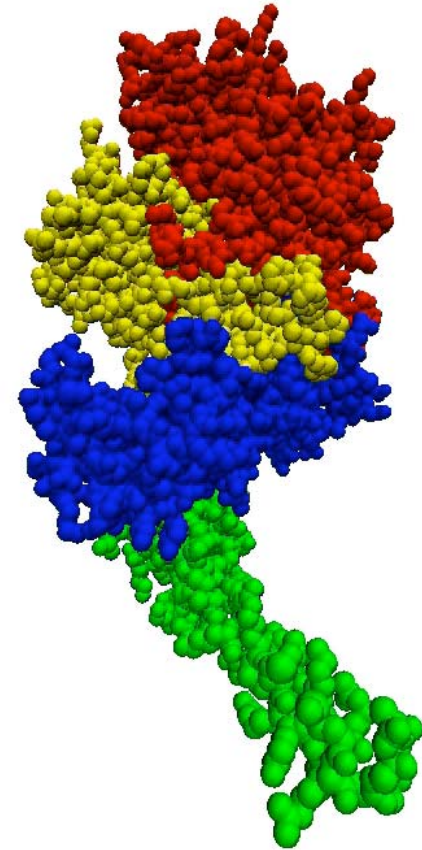
Only forces for secondary structure



Forces to keep molecule Intact turned on

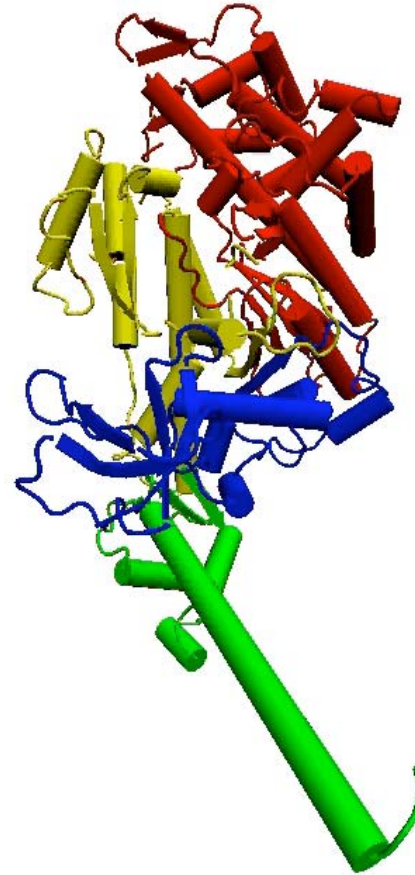
Segmenting larger ensembles: Myosin

Simulating the
interconversion of two
myosin conformations



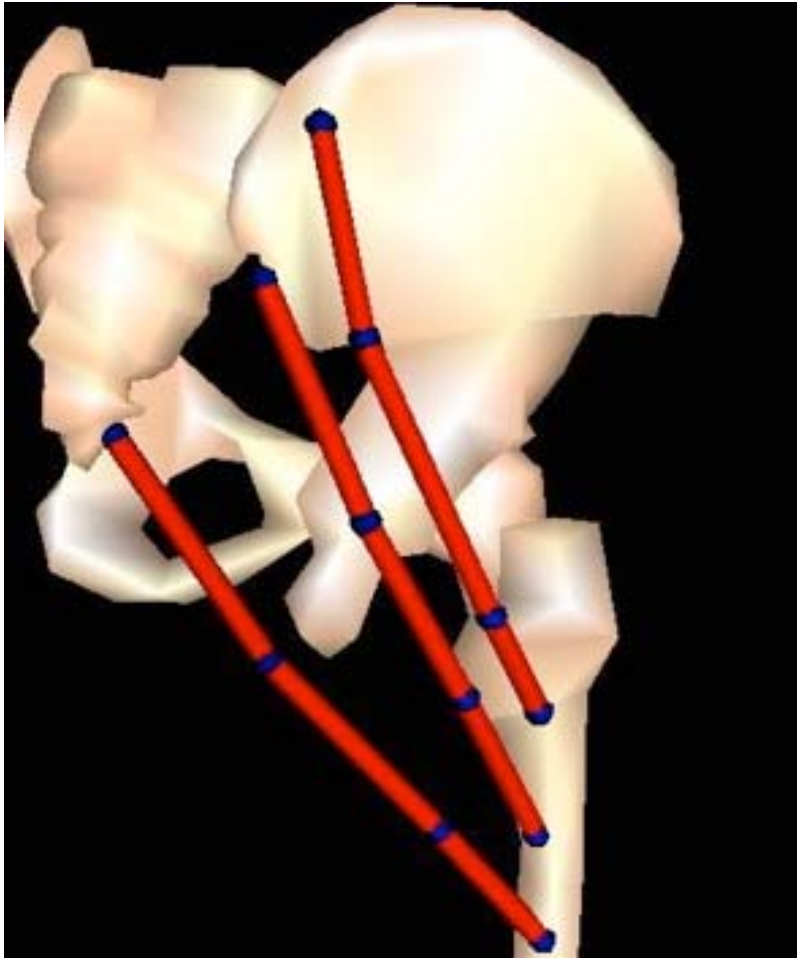
Segmented Myosin

Reduce complexity
Of simulation with
4 rigid bodies.

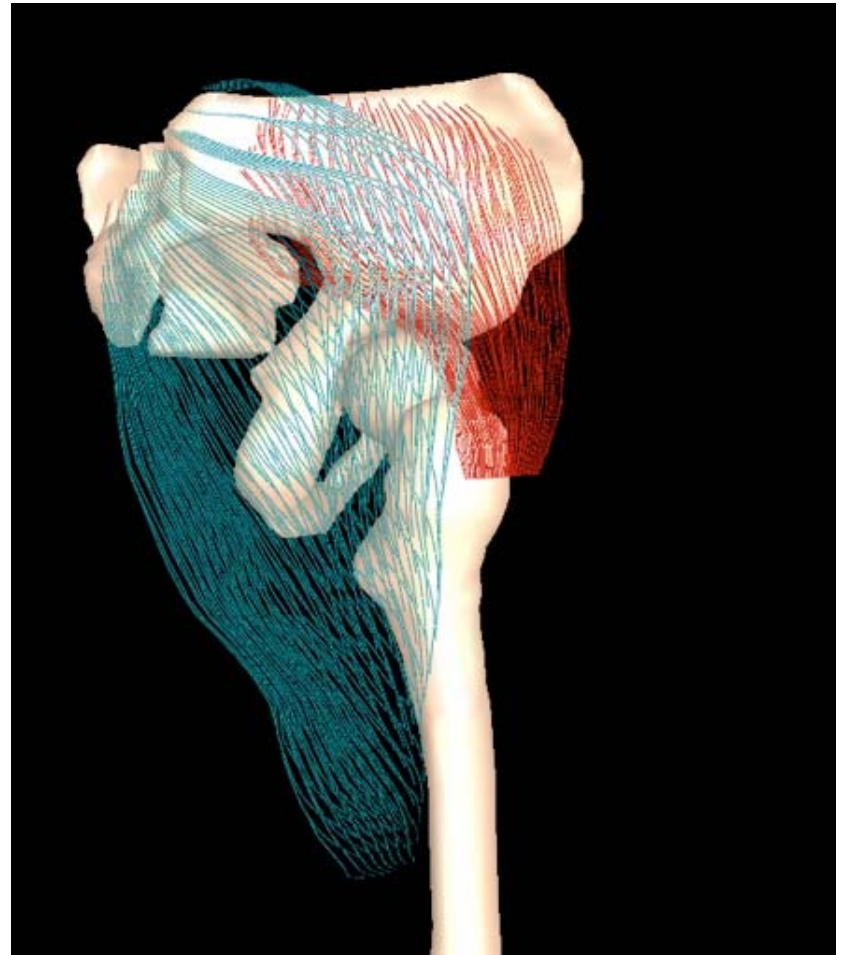


Two models of muscle

1. Vector model of muscle force

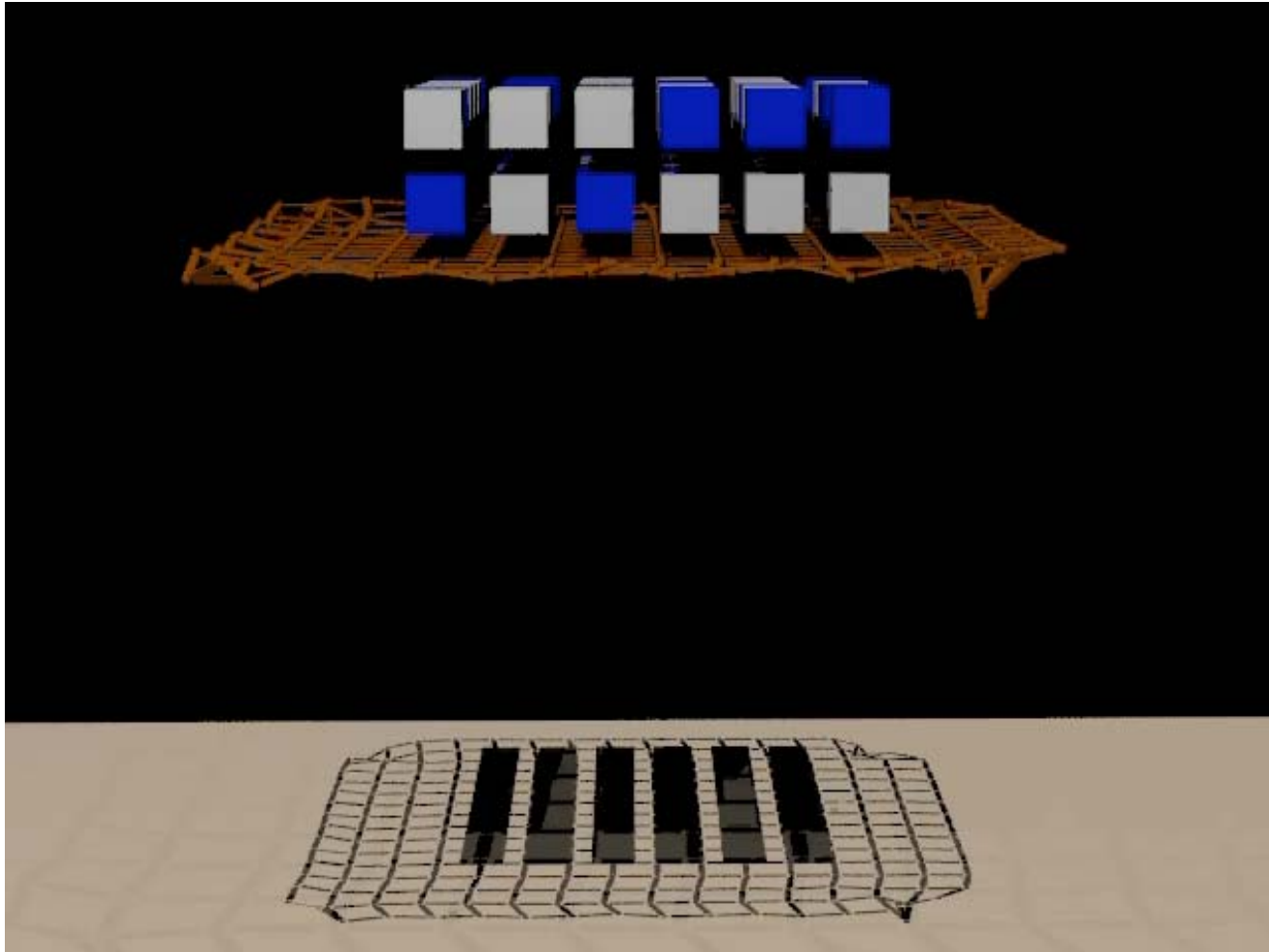


2. More accurate 3D model of muscle



Simulating articulated rigid bodies

Blocks and net collide



Rachel Weinstein, Ron Fedkiw, and others



Eftychios Sifakis, Igor Neverov, Ron Fedkiw





James Spudich



David Paik



Leonidas
Guibas



Pat Hanrahan



Chris Bruns



Osussama
Khatib



Jean-Claude
Latombe



Jung-Chi Liao



Adrian Lew



Allison Arnold



Jeanette Schmidt



Rachel
Weinstein



Kathy Miller



Charles Taylor



Christopher
Zari



Eftychios
Sifakis



David Parker



Paula Petrone



Russ Altman



Scott Delp



Padma
Sundaram



Peter Pinsky



Michael
Levitt



Alex Labute



Alain Laederach



Clay Anderson



Silvia Blemker



Blanca Pineda



Ron Fedkiw



Peter
Feenstra



Bryan Keller

James Warren



Jack Middleton



Vijay Pande



Sandy Napel



Ayman Habib



Randy Radmer



Daniel
Herschlag



Michael Sherman

Goals for Year 2

- Continued scientific productivity
- Cardiovascular DBP kick-off
- Collaborating R01s begin
- Release SimTK 1.0 with first apps
- Engage SIMBIOS team in using SimTK
- Expand user base for SimTK nationally+
- First dissemination events for each DBP
- Design new biosimulation class (grad)
- Three issues of BCR

Goals for Retreat

- Identify goals for the future
- Design a course to teach physics-based simulation and use SimTK
- Identify valuable external software
- Prioritize internal development
- Engage the team and get your input

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