UNC-CH Comp/Phys/APSc 715

Custom Applications for
nanoScale Science
Medicine
High-Energy Physics

Administrative

- Presentations next week
  - ***Brief*** data and goal intro
  - Describe ideal design
    - What perceptual characteristics help user do task?
    - Why parameters chosen (color map, viewpoint)?
    - Consider second-best approach
  - Describe implementation if any (and demo)
  - Evaluation plan or report

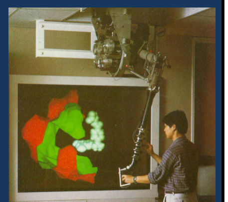
Overview

- Three Custom microscope control & molecular manipulation applications
- Advanced Model Fitting and Analysis
- Coupling visualization and control (beyond toolkits)
- Scientist & computer scientist collaboration

- A Crazy Idea

Docker

- Ming Ouh-Young's dissertation project
  - Showed NTE factor-of-2 speedup with haptics
  - 6-DOF positioning task
  - "Lock and Key" problem
  - Hard surface + electrostatic



Rendering SPM Data has always been a problem

VOLUME 50, NUMBER 2 PHYSICAL REVIEW LETTERS 10 JANUARY

7 × 7 Reconstruction on Si(111) Resolved in Real Space

G. Binnig, H. Rohrer, Ch. Gerber, and E. Weibel
IBM Zurich Research Laboratory, 8803 Rüschlikon-ZH, Switzerland

(Received 17 November 1982)

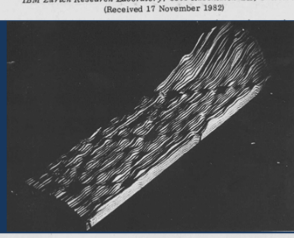
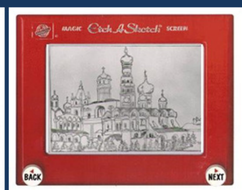


FIG. 6. 7×7 reconstruction of Si(111). (a) Relief assembled from the original recorder traces, from Binnig *et al.* (1983b), © 1983 The American Physical Society, and (b) processed image of the 7×7 reconstruction of Si(111). Characteristic of the rhombohedral surface unit cell are the corner hole and the 12 maxima, the adatoms. In the processed image, the six adatoms in the right half of the rhombi appear higher. This is an electronic inequivalence on the surface owing to a structural left-right inequivalence in the underlying layers. The reconstruction extends undisturbed to the immediate vicinity of the large "atom hill" on the right.

What this rendering seems like to me

What they've done with it

- Simply Incredible!



- Imagine what they could do with ink!

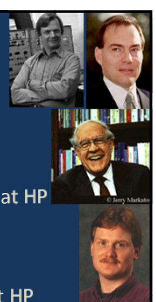
nanoManipulator

A virtual environment interface to SPM

The Goal:
- Remove boundaries between user and sample
- Can we make experiments on the molecular scale as easy as rolling a pencil or pushing a golf ball?

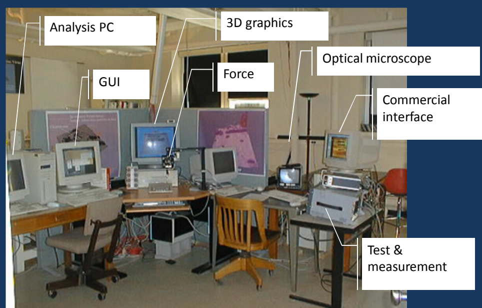

© 1997 UNC-CH
Todd Gaul, Photographer

Conception

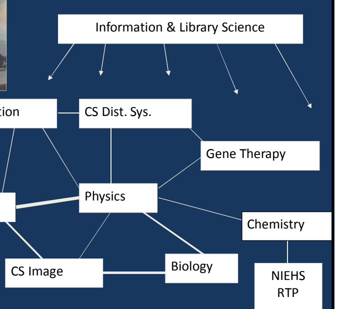


- R. Stanley Williams
  - Then professor of Chemistry at UCLA
  - Now head of nanocomputing research at HP
- Warren Robinett
  - Then director of HMD research at UNC
  - Later doing nanocomputing research at HP
- My dissertation topic in Computer Science
  - Under direction of Frederick P. Brooks, Jr.

Interoperability

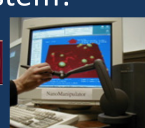


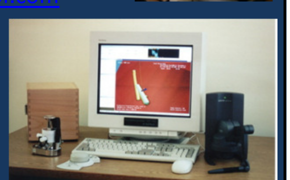
nanoManipulator Collaborators



Now a Commercial System!

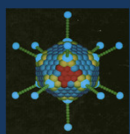
- nanoManipulator DP-100
- 2001 R&D 100 Award Winner
- www.nanomanipulator.com

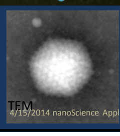




Adenovirus: Imaging icosahedral shape with advanced rendering

Adenovirus
85 nm
Icosahedral

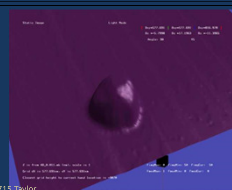




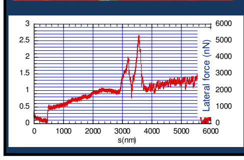
AFM Images

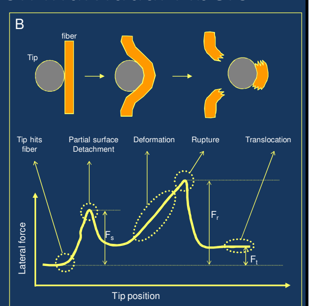
Color by slope:
Flat=dark
Steep=bright

Specular highlights through Directional illumination

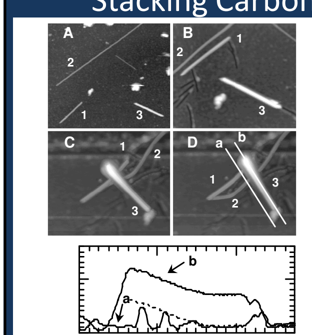


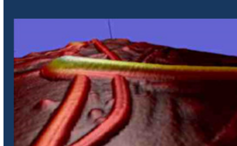
Measurements on Individual Fibers

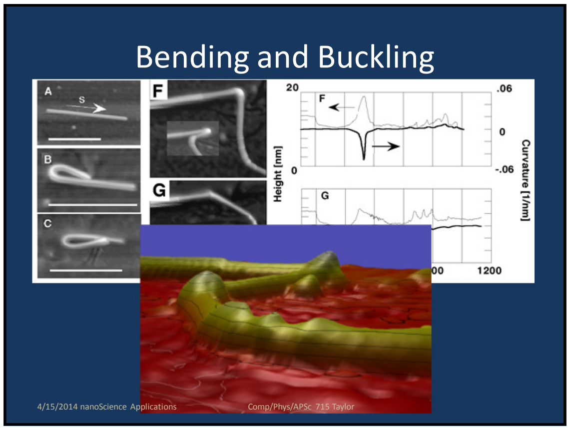




Stacking Carbon Nanotubes






Bending and Buckling
A
S
B
C
F
G
20
0
.06
0
-.06
Height [nm]
Curvature [1/nm]
1200
4/15/2014 nanoScience Applications
Comp/Phys/APSc 715 Taylor


Question: Which Interface is *Best*?
5
1
2
3
4
4/15/2014 nanoScience Applications
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4/15/2014 nanoScience Applications
Comp/Phys/APSc 715 Taylor
18

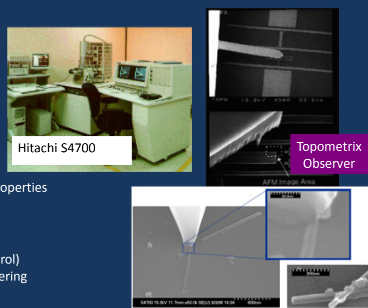
NIMS: SEM + AFM

Combine the best of:

SEM:
- Imaging
- elemental analysis
- ebeam lithography

AFM:
- topography
- local (mech., elect,..) properties
- manipulation

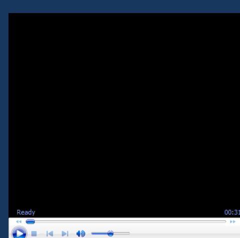
nM:
- Manipulation (XYZ control)
- Multiple Data Set Rendering
- Registration



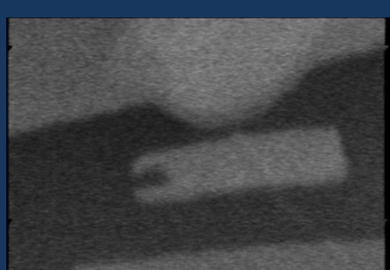
SEM/AFM in action

- Hand-controlled AFM
- Zooms in on nanotube
- “Twangs” nanotube

- Play movie

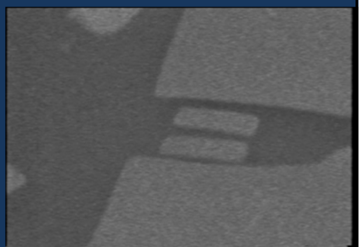


SEM/AFM in action

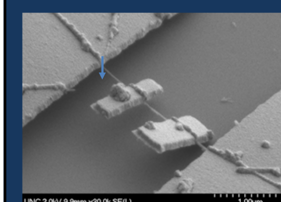


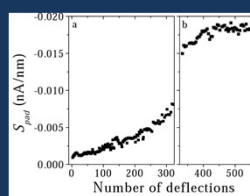
SEM/AFM in action

- Two paddles
  - Suspended on tube
- Tip comes down
- Paddle sticks
- Tries to pry off
- Game over



Measuring Torsion



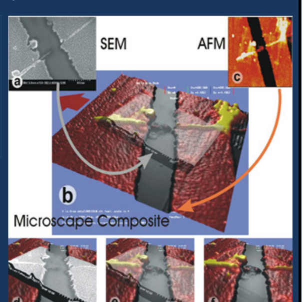


Force curves all at single point (+/-50nm)on single paddle

Force gets 20x larger after repeats!

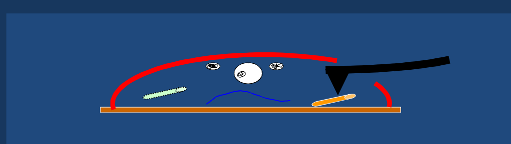
SEM/AFM

Challenges:
- Real-Time overlay/registration
- E Beam Lith Integration
- Optimized Integration of Data Sets
- 3D manipulation-where is the tip?



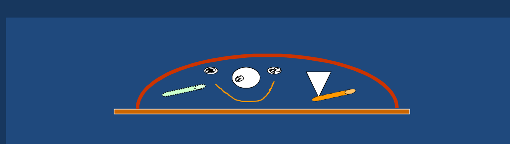
3DFM: The Next Step in Biological Force Microscopy

- How to do force microscopy inside a cell?



* Puncture the cell membrane to image inside the cell?

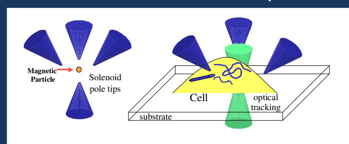
One Solution: Put the Probe Inside the Cell



- Problems:
  - How to measure the probe's position?
  - How to apply forces?

Our Solution

3-D Force Microscope



- Magnetic fields apply forces to magnetic particle
- Particle position is monitored using optical tracking
  1. Very specific forces
  2. Little localized optical heating
  3. Relatively high forces

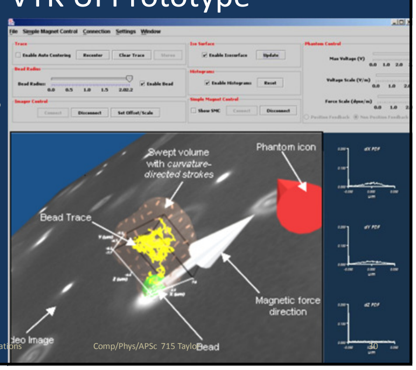
3DFM: Concept Video

- Link to video

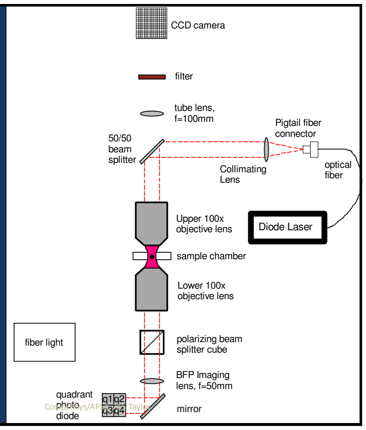
VTK UI Prototype

2D Video
More controls

Slivered surf
Wireframe
bead

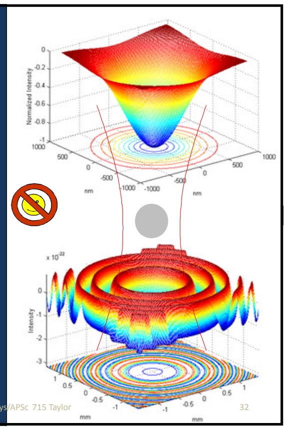


Optical Layout: Laser tracking



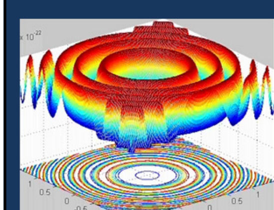
Optical Tracking

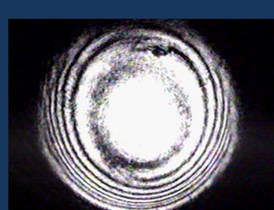
- Incident beam (maximum in center)
- Bead Scattering
- Resulting pattern (maximum in center)
- Terrible Visualization
  - Rainbow scale
  - No shading on surfaces
  - Down/blue is more



Z Tracking, QPD Image

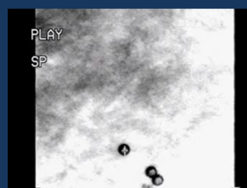
Theoretical Image Measured Image



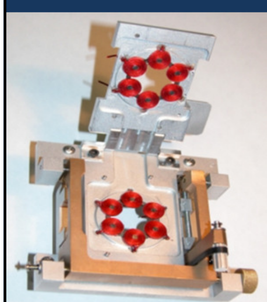


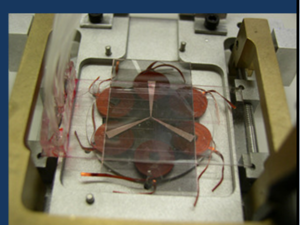
3D Tracking: Bead Capture

- Bead 2.8 microns in diameter attached to cilium
  - Two beats uncaptured
  - Several captured
  - Note background (XY)
  - Note focus (Z)
  - Video link

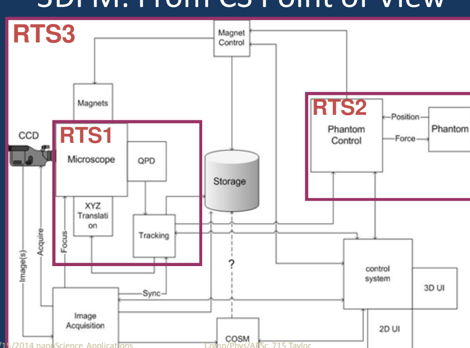


3dFM: Magnetic Drive

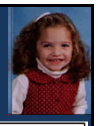




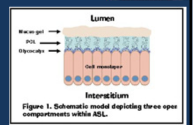
3DFM: From CS Point of View



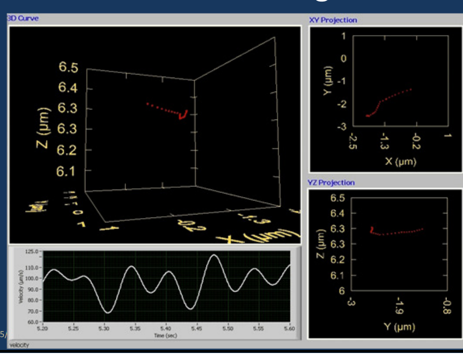
Initial Experiment Target: CF



- CF gene controls Cl^- and Na^+ transport through cells
- Affects airway secretions (mucin)
- Mucociliary clearance is the first line of defense against inhaled particulates, aerosols, etc.
- Particulate-laden mucus transported by cilia
  - beating in a mucus-free periciliary liquid (PCL)
  - to the glottis where it is expelled and swallowed

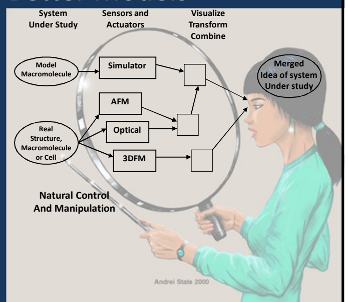


Tracked cilium beating at 15 Hz



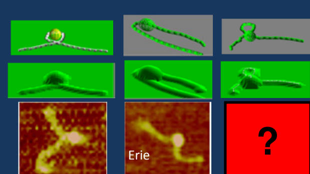
Tools to help Scientists Build Better Models

- Extract Model
- Display Model with Experiment
- Simulate scan of model with microscope
- Enable direct visual comparisons



Rapid Microscope Simulation

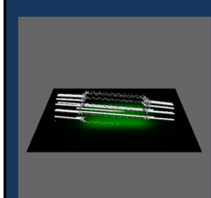
"What Should I See?"
Dilation and Erosion using Arbitrary Tip

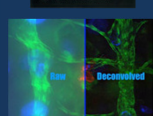


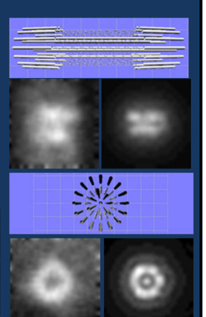
Location of Mitotic Spindle: Cory Quammen

Problem: What is the geometry of the mitotic spindle?
Investigator: Kerry Bloom, Biology

Optimization of a Structural Model





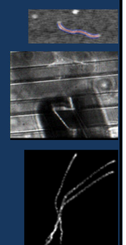


Real image Simulated

"Model-based deconvolution"

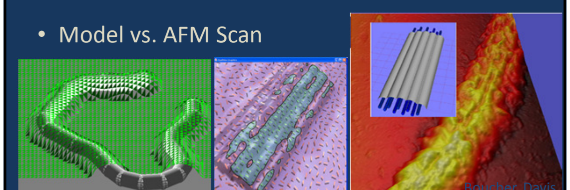
Putting it Together: Fibrin (Conceptual)

- Extract
  - Fibrin model from optical (Tube Tracer)
  - Estimate fluorophore locations (FSM-like)
- Track
  - Motion of fluorophores (FSM-like)
- Optimize
  - Find expected motion (Lin NSF grant)
  - Find expected image (Fluoro-sim)
  - Adjust model parameters for best fit (MIBO)
- Compare
  - Actual and simulated images (nM, ScalarStack)
  - Quantitative: Simulated and measured displacements

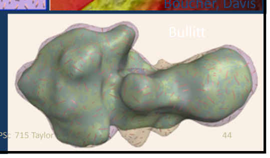


Comparing Two Surfaces: Chris Weigle

- Model vs. AFM Scan



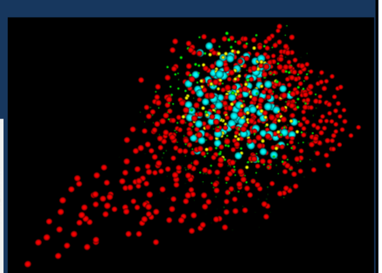
- Manual vs. Automatic:
- Tumor vs. Isodose



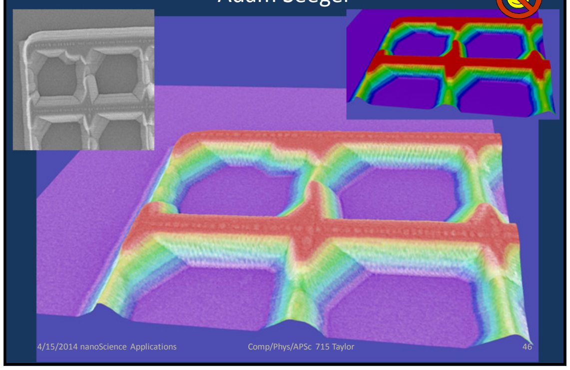
Viz: Multivariate 3D Display David Feng

- Virtual Cell
  - Loew
  - P41 Collab

National Resource for Cell Analysis and Modeling



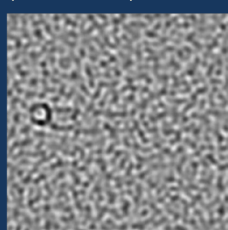
AFM + Simulate BSE from SEM: Adam Seeger



GPU-Accelerated TEM Simulation: David Borland

Multislice

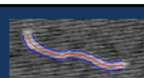
(20 minutes)



Kinematic

(Let's see…)

AMF&A: Summary



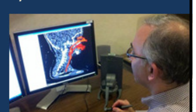
- Scientist or image analysis estimates model of object(s) scanned by a microscope
- Computer produces detailed result of applying a specified transfer function (model of instrument behavior) to this model to produce *"what should I see in the image if my model is correct?"*
- Scientist or image analysis compares the detailed simulation with experiment image, *"does my model predict this?"*
- Scientist or optimization code adjusts model trying to make simulated image better fit experiment image, *"is this better?"*

Insight into Instrument Behavior

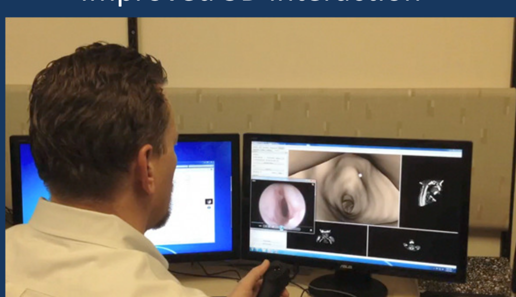
Insight into Model Correctness

Virtual Pediatric Airways Workbench

- Virtual Bronchoscopy + Flow
  - Stereo 3D graphics display
  - Automatic front-surface removal
  - Add flow-simulation data
- Virtual Surgery
  - Force-feedback pen can edit geometry
- Workflow Integration System
- Inter-Technique Comparison Tool
  - Geometry vs. geometry
  - Flow vs. flow

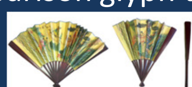


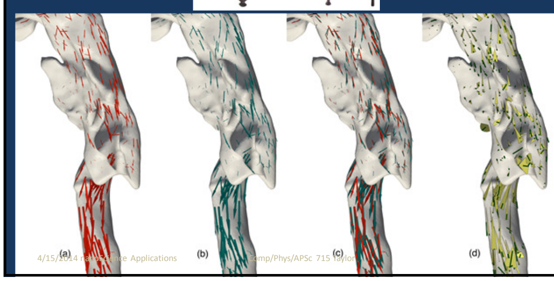
Improved 3D interaction



Surface textures for improved shape perception

Vector comparison glyph technique

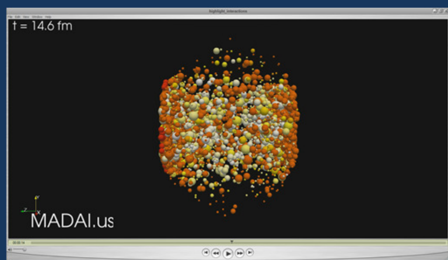




Modeling and Data Analysis Initiative

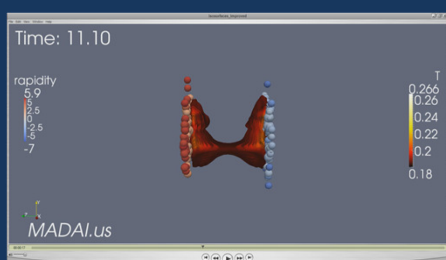
- NSF-sponsored project
- Statistics + Visualization
- Scientific domains
  - Particle collisions
  - Weather
  - Galaxy Formation, Universe formation
  - Supernovae

MADAI Workbench: ParaView++



Radius = sqrt(mass); color is time since creation (brightest = newest)

MADAI Workbench: ParaView++

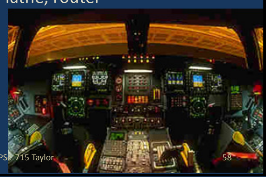


Radius = sqrt(mass); color is rapidity (signed speed in X)

The Right Tool for the Job…

- All-in-one, not optimal for any
  - Sears ShopSmith
  - *Computer (WIMP) interface*

- Finely-tuned for the task
  - Specific power tools: table saw, lathe, router
  - Automobile, airplane cockpit
  - Bill Buxton: Bow for violin
  - *What computers should be*



CS Through the Science Lens

- Changing relationships between scientists and computers
  - Taking numbers to computer priesthood
  - Entering numbers on office computer
  - Connecting data collection computer to instrument
  - The computer interface *is* the instrument interface
- Bad news: The knobs and poking around and tools each designed for their function are replaced by keyboard and mouse
- Good news: Enables arbitrary mappings (in particular, we are looking for the natural and effective ones) and *new* knobs, poking, tools
  - Requires careful crafting in Visualization and UI design

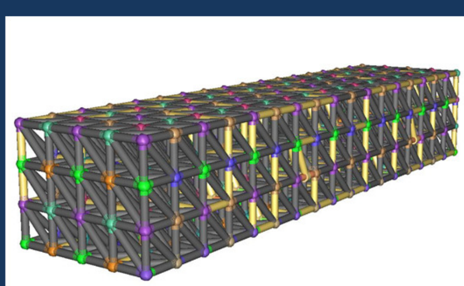
Science seen through CS Lens

- Scientists are a source of many problems
  - Some are solvable with pedestrian CS (Undergraduate use as learning tool, visualization course may do)
  - Some are stretches or require new application (Visualization Case Study, Masters Thesis)
  - Some are really hard (CS dissertations, whole new project directions)
- Our main goal is cool new research, in CS and PS

How does it go?

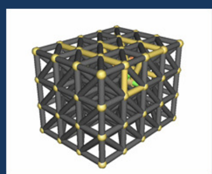
- Team Building
  - Goodwill forms as each feels heard, and valued
  - Trust and increased engagement comes as results arrive
- Arms Race
  - Scientists ask for capabilities "yesterday"
  - CS looking for features for "3 months from now"
  - With the AIMS system, CS is ahead!
  - Need to start the software at least as soon as HW
- Iterative design: Having a new tool for a task changes the task

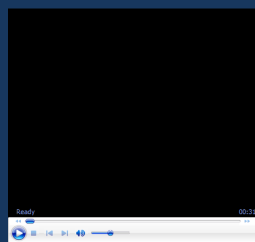
Crazy Idea: DNA + Nanotube Comp 1 Bit Full Adder: Chris Dwyer



Crazy Idea: DNA + Nanotube Comp: Assembly of NAND gate

- Link to movie

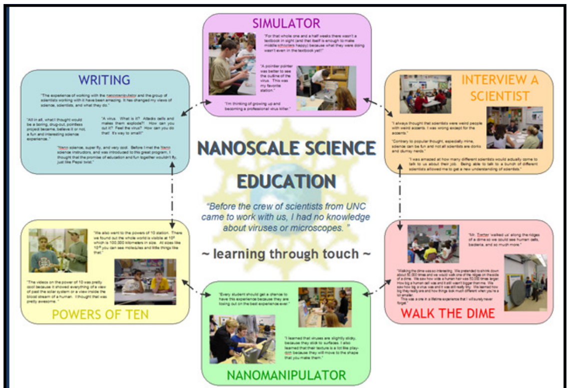




Credits

- UNC-CH nanoScale Science Research Group
  - www.cismm.org
- Modeling & Data Analysis Initiative
  - madai.us

Extra slides



SIMULATOR

"For that whole one and a half weeks there wasn't a textbook in sight (and that itself is enough to make middle schoolers happy) because what they were doing wasn't even in the textbook yet!!"

"A pointier pointer was better to see the outline of the virus. This was my favorite station."

"I'm thinking of growing up and becoming a professional virus killer."


INTERVIEW A SCIENTIST
"I always thought that scientists were weird people with weird accents. I was wrong except for the accents."
"Contrary to popular thought, especially mine, science can be fun and not all scientists are dorks and clumsy nerds."
"I was amazed at how many different scientists would actually come to talk to us about their job. Being able to talk to a bunch of different scientists allowed me to get a new understanding of scientists."
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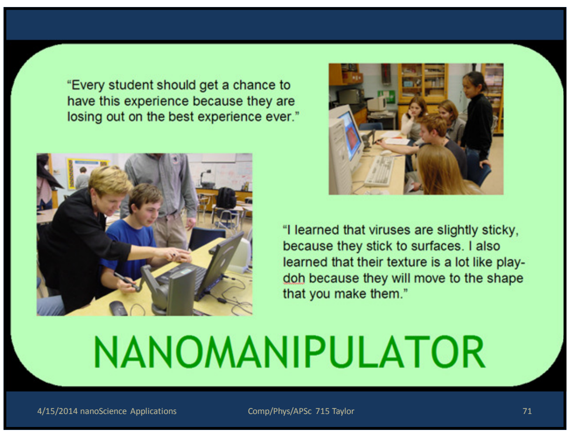
"Every student should get a chance to have this experience because they are losing out on the best experience ever."
"I learned that viruses are slightly sticky, because they stick to surfaces. I also learned that their texture is a lot like play-doh because they will move to the shape that you make them."
NANOMANIPULATOR
4/15/2014 nanoScience Applications
Comp/Phys/APSc 715 Taylor
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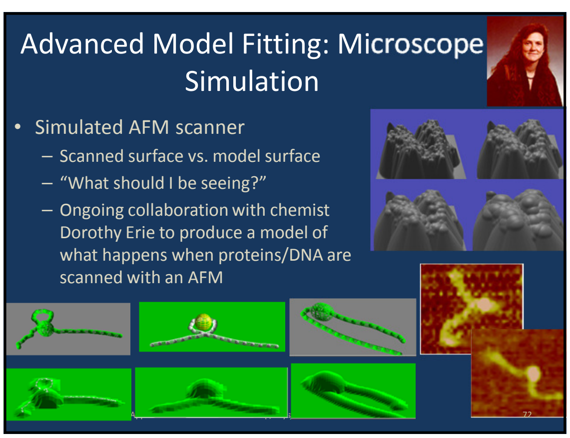
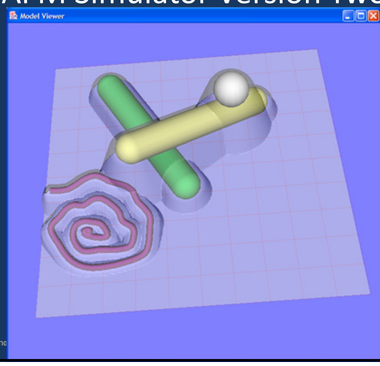
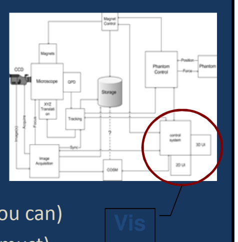

Advanced Model Fitting: Microscope Simulation
• Simulated AFM scanner
– Scanned surface vs. model surface
– "What should I be seeing?"
– Ongoing collaboration with chemist Dorothy Erie to produce a model of what happens when proteins/DNA are scanned with an AFM

AFM Simulator Version Two



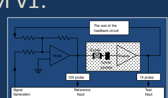
Beyond the Toolkits

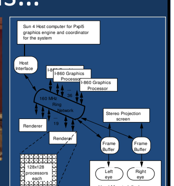
- Why/When?
  - Extreme performance
  - Tightly-coupled systems
- How?
  - Extend the toolkits! (when you can)
  - Any way you can (when you must)
  - "A tale of two Systems…"



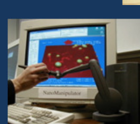
"A Tale of 2+ Systems…"

nM v1:

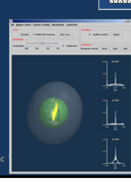




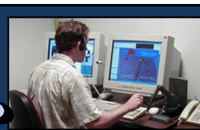
nM v3:

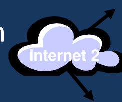


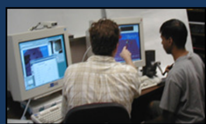
3DFM v1:

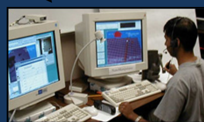


Tele-nM for Collaboration







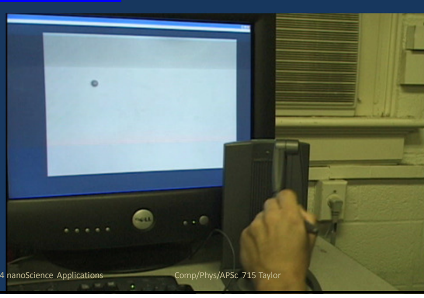


Face-to-face:
- social interactions is natural
- cooperative physical activities are natural
- teams share a single user scientific instrument.

Distributed:
- social interaction is *mediated by technology*
- shared physical activities are difficult
- the instrument must support access by multiple users over the network.

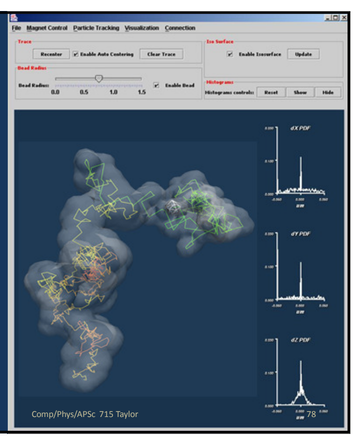
Bead Pulled in Circle

- [Link to movie]



VTK UI Prototype

- Parameter menus
- Bead Histogram
- Yellow trace
- Green estimate
- Translucent volume swept by bead
- Complicated path from Brownian motion simulator



3DFM: CS Challenges

- Data Visualization
  - Overlaying volume, surface, line-trace data: both visually and haptically
  - Displaying surfaces with uncertain borders
- Computation and Rendering
  - Real-time volume convolution and display (COSM)
  - Incremental updates of a subset of the volume
- Measurement and Control Theory
  - Tracking the bead, estimation of forces, viscosity and other system state parameters

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What does it take?

- Sustained hard work across disciplines
  - CS: Russ Taylor, Mary Whitton, Leandra Vicci, Gary Bishop, Greg Welch, Steve Pizer, Prasun Dewan, Paul Morris, David Marshburn, Kurtis Keller, Aron Helser, Tom Hudson, Adam Seeger, David Borland, Yoni Fridman, Alexandra Bokinsky, Alvin Richardson, Chris Dwyer, Chris Weigle, Haris Fretzagias, Jonathan Robbins, Jameson Miller, Tatsuhiro Segi, Ben Wilde, Rajeev Dassani
  - P&A/MS: Rich Superfine, Sean Washburn, Mike Falvo, Lu-Chang Qin, Stefan Seelecke, Stergios Papadakis, Garrett Matthews, Kalpit Desai, Jay Fisher, Jeremy Cribb, Sreeja Panmanabhan, Andrea Hilchey, Lloyd Carol, Michael Stadermann, Adam Hall, Aarish Patel, Rohit Prakash, Debbie Sill
  - SILS/EDU: Diane Sonnenwald, Gail Jones, Dennis Kubasko, Michele Kloda, Tom Trettor, Atsuko Negishi, Kelly Maglaughlin
- Sustained funding
  - $1M+: NIH/NCRR (12+ yr), NSF/HPCC (5+ yr), NSF/ROLE (3 yr), ONR/MURI (5 yr), ARO/DURIP (2 yr), Keck Foundation (1 time)

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