National Science Foundation workshop on:

March 29-30, 2004
Arlington, VA

Control and System Integration of Micro- and Nano-Scale Systems

Benjamin Shapiro, University of Maryland

Organizing Committee:

Gregory Chirikjian, Johns Hopkins University

Liwei Lin, University of California at Berkeley

Costas Maranas, Pennsylvania State University

Marvin White, Lehigh University

Minami Yoda, Georgia Institute of Technology

NSF Support:

Kishan Baheti, ECS

Maria Burka, CTS

Delcie Durham, DMII

Masayoshi Tomizuka, CMS

How this started …

My group is aimed at design and control of micro-fluidic systems and we are generally frustrated by the low degree of collaboration and communication between modelers, fabrication people, control theorists, mathematicians, organic chemists, …

We keep having to recreate on the micro scale what researchers have been doing for years on the macro scale (e.g. "control ready" modeling) …

And we aren't the only ones with this problem …

So through Maria Burka and Kishan Baheti, I went to NSF and proposed …

*A workshop that will bring together the **control and systems design** community with the **micro- and nano-system** fabrication and device design communities. It would identify high-payoff interdisciplinary research directions, and it would provide input to NSF for future basic science research needs …*

This talk gives a summary of the discussions and recommendations from that workshop.

Micro/Nano Systems are Characterized by …

•Extremely small length scales (down to molecular scales for nano systems)

→Can pack lots of actuators and sensors into a tiny space = amazing capabilities.

•The interaction of many different physical phenomena across many different length and time scales.

→ Extremely complex phenomena, hard to understand and to quantify.

•Large manufacturing variability, sensitive dependence on trace quantities of chemicals

→ Lots of system uncertainty.

•Need dedicated, delicate, ***expensive*** equipment to measure even basic quantities

→Measurements are limited and can be noisy. Is hard to debug system errors.

Control & System Integration Design Tools are Characterized by …

•Distributed control and sensing techniques (J. Burns, B. Bamieh, R. D'Andrea, ..)

→Optimal placing of actuators/sensors, coordinated control, data extraction, …

•System analysis/design tools built to capture coupling across temporal and spatial scales

→ These tools may aid understanding the physics (but their application will not be simple – no "silver bullet")

•Control theory tools have been built to address robustness (J. Doyle + many others)

→ Quantify and design for uncertainty.

•System identification tools, design of experiments, data mining, other?

→Some of these mathematical tools may help. Need research collaboration.

These two groups should talk

Benjamin Shapiro
UNIVERSITY OF MARYLAND

Sequence of events and response from the research community …

- *October 2003:* Proposed workshop topic to NSF.
- *Nov/Dec 2003*: Selected and finalized organizing committee.

Chose 6 theme areas based on input from NSF and committee.

- *January 2004*: Formally announced the workshop.
- *Jan – March 3, 2004*: Received 407 applications.
- *March 3-5, 2004*: Organizing committee selected 90 people.
- *March 8, 2004*: Sent out invitations.

- *March 29,30*: The workshop.

- *June 30:* Present recommendations at ACC
- *(very soon):* Report finalized and made public.

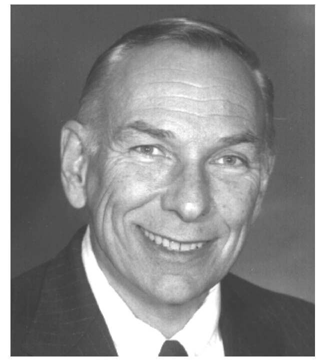
Thanks to:

Organizing Committee:

Gregory
Chirikjian

Liwei
Lin

Costas
Maranas



Marvin
White

Minami
Yoda

National Science Foundation:

Kishan Baheti, Maria Burka, Delcie Durham, and Masayoshi Tomizuka

Logistical Support:

Becky Copeland, Jeff Coriale, Dale Morey, Lisa Press, and Susan Warren at the University of Maryland. Cheryl Muza at NSF.

Workshop was organized according to six theme areas chosen by NSF and the organizing committee …

- MEMS Design/Fabrication, Devices, and Systems.
- Nano Fabrication
- Biological (or Biomolecular/Biochemical) and Chemical Systems on Micro/Nano- Scales.
- BioMEMS and/or Nanobiotechnological Systems
- Control Systems with a MEMS and/or Nano Perspective
- Measurement, Modeling, and Model Validation at the Micro- and Nanoscale.

Workshop organization:

DAY ONE:
- Seminars in the morning: one overview + one per theme.
- Theme discussions by area of expertise.
- Theme representatives report back to the main audience with initial recommended research areas.

DAY TWO:
- Two overview seminars.
- Theme discussions with audience randomly reorganized.
- Theme representatives report back to main audience with finalized list of research recommendations per theme.
- Discussion in main audience.

AFTER WORKSHOP: Draft of report sent out for comment.

All participants at the workshop submitted quad charts on their research goals, research approach, and bottlenecks.

These quad charts are a very succinct summary of some really fascinating research efforts. They are all available at:

http://www.engr.umd.edu/nsf/

It is amazing how the same research themes repeat across very different research areas …

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Implantable, Intelligent, Wireless Biological Microsystem

Darrin J. Young
Case Western Reserve University

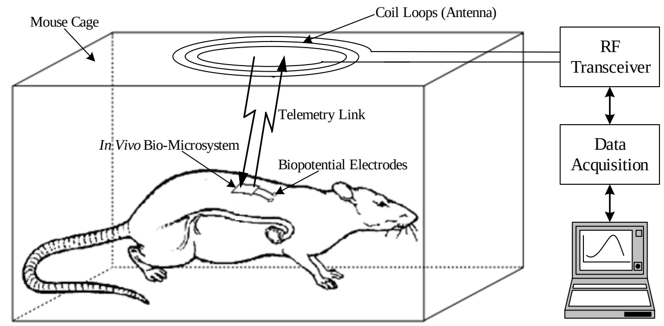
Goals and Potential Impact if Successful

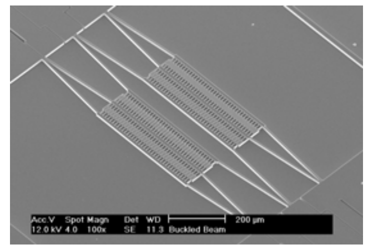
Goal:

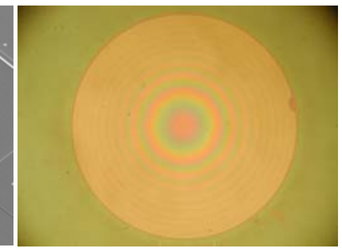
(1) To develop implantable, intelligent, wireless biological µ-sensing system
(2) To develop advanced biological signal processing for identifying new genetic functions
(3) To develop interdisciplinary research and education

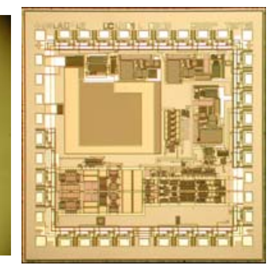
Potential Impact:

(1) Innovative biological research methods to gain better understanding of systems biology and new genetic functions discovery
(2) Revolutionizing health care system and innovative treatment for diseases
(3) Future interdisciplinary (Engineering/Bio) researchers









Approach and/or Accomplishments

Approach:

- Optimal micro-implant-system architecture
- Miniature micromachined sensors array
- Innovative bio-sensing-packaging technologies
- Advanced bio-signal processing techniques

Accomplishments

- Innovative minimally-invasive long-term blood pressure monitoring system
- Micromachined strain, pressure, and activity sensors
- Low power CMOS IC for sensor array interface & telemetry

Bottlenecks and Open Research Questions

(1) Incompatible micro/nano fabrication technology of sensors (physical, biological, and chemical) and electronics, making it very difficult for system integration and assembly
(2) In-vivo energy/power sources are limited. Implant-rechargeable battery with RF coils is the only current option, limiting the overall system miniaturization.
(3) Communication gap between engineering (design and fabrication) and bio/medical people
(4) How micro/nano fabrication with micro/nano system design can be effectively applied to address critical biological scientific questions?

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Self-assembled Nanostructures in Thin Films

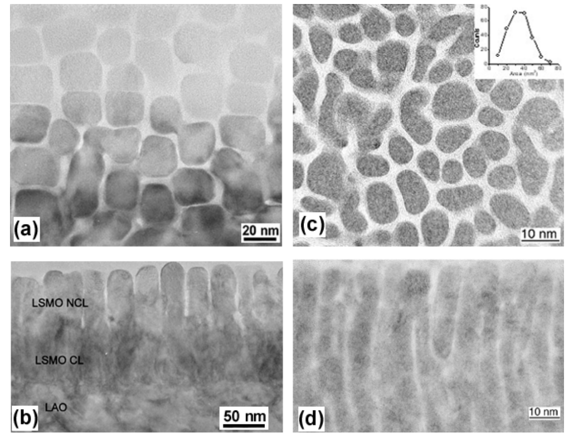
Efstathios Meletis
Louisiana State University

Goals and Potential Impact if Successful

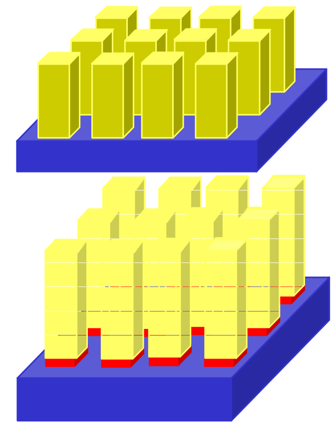
Control self-assembly of oxide and metallic nanostructures through fundamental understanding for:
-nanofabrication and nano-imprinting
-nanopatterning and templating
-nanoelectronic devices, nanosensors, memory devices, etc.

Development of a novel 'bottom-up' method to design and manufacture nanodevices.

Require fundamental understanding of the self-assembling mechanism through innovating experimentation coupled with atomistic modeling and simulation to capture the nanoscale physical phenomena involved.
Integrating nanostructures in devices.



(a), (c) Plan-view TEM and (b), (d) XTEM of $La_{0.8}Sr_{0.2}MnO_3$/ LAO and Co/DLC **nanostructured film**.



Ordered nanorods formed by (a) direct deposition on a substrate or (b) nano seed fabrication.

Approach and/or Accomplishments

EXPERIMENTAL:
Device and design appropriate experiments to explore and understand the the role of processing and material parameters on the resulting self-assembled nanostructures.

MODELING:
Use combined atomistic (molecular dynamics and kinetic Monte Carlo) and mesoscale simulations to model nanostructure growth and extend the model to design future systems of interest.

ACCOMPLISHMENTS:
Self-assembled nanorods have been achieved in Co/DLC nanocomposite and $La_{0.8}Sr_{0.2}MnO_3$/ $LaAlO_3$ epitaxial films.

Beniamin Shapiro
UNIVERSITY OF MARYLAND

Bottlenecks and Open Research Questions

– **Appropriate processing techniques** that can capture and control range of parameters dominating the self-assembling process are needed. This applies to both, ceramic and metallic nanostructures.

– **Better coordination between experimental and theoretical studies.**

– **Multiscale modeling and simulation methods** are needed to better handle the time and length scales involved.

– **Lack of appropriate methods** for integrating the self-assembled nanostructures into nano/micro devices.

Nanofabrication of materials by self-assembly

Brad Paden
UC Santa Barbara

Goals

- Coat surfaces with dense uniform self assembled monolayer using two synthetic routes: **organic solvent & supercritical CO_2**
- Observable macroscopic properties due to monolayer

We are creating inorganic/organic materials with a nano-interface and functionality.

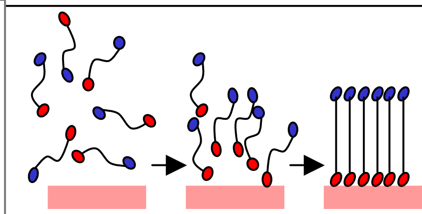
Applications

I. Composite Materials
Enhancement of strength, toughness
Adhesion, release

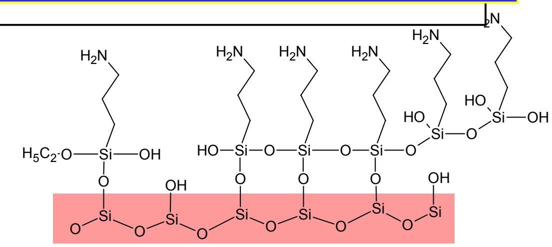
II. Antimicrobials
Medical devices (catheters, implants, etc.)
Medical sensors

III. Chemical Sensors
Medical Diagnostics
Molecular detectors

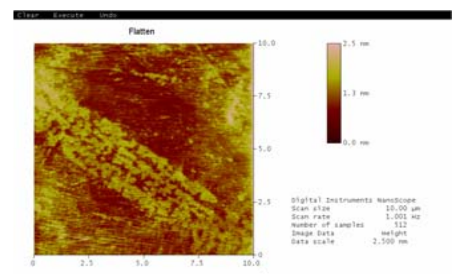
IV. Filter media



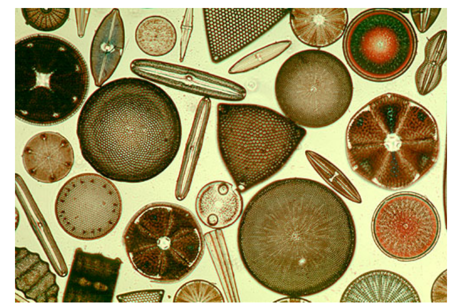
Thermodynamic self assembly on surface



Covalent bonds
Surface-silane, silane-silane



AFM coated Si Wafer



Diatoms (100's nm each)

Approach

Control
Temperature and pressure in the $SCCO_2$ system will affect solubility, reaction dynamics and material losses
Material hydration for surface reaction
Silane concentration
Fluid mixing for diffusion of reactants

Modeling
Equilibrium phase behavior of reactants to maximize solubility
Reaction kinetics of silanization (T, P, conc.)

Problems and future concerns

- Obtaining uniform coverage and maximum cross-linking between surface silanes
- Characterization methods: AFM and solid-state NMR
- Coating materials which are inert (carbon fiber) without degrading the materials properties.
- Characterizing macroscopic improvements resulting from nanometer sized additions
- We are far from what nature can already do - diatoms form spontaneously at room temperature and are very strong and porous.

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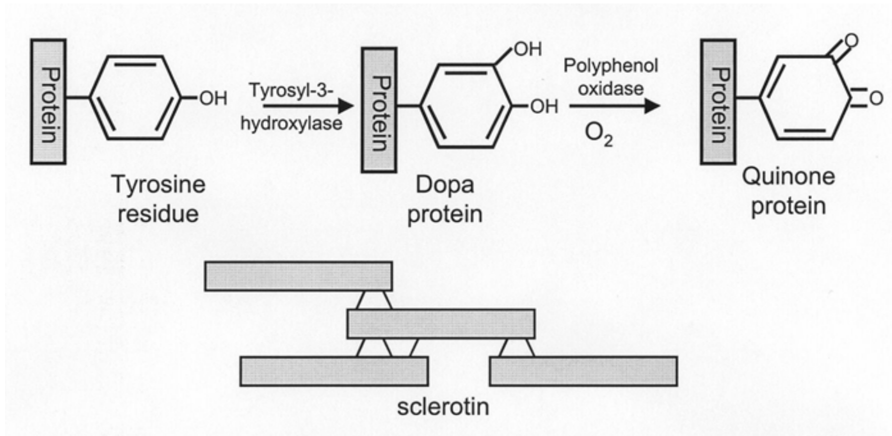
Director, Center for Microencapsulation and Drug Delivery

Allison C. Rice-Ficht
Texas A&M HSC

Goals and Potential Impact if Successful

Goals:
To implement, through emulsion and microfluidic technology, the use of novel proteins and peptides for 1) the production of micro and nanoscale release vehicles and 2) adhesives for an aqueous environment.
To use self-assembling proteins as scaffolds for controlled release vehicles.
Impact: Provide completely new and innovative solutions to controlled release at the micro and nanoscale level. Provide new adhesives for aqueous environments and self-healing applications for materials.

Chemical basis for glues and sealants



Approach and/or Accomplishments

Using emulsion technologies, we have employed novel proteins and peptides for the production of controlled release systems. Taking advantage of quinone chemistry we have used protein derivatives as adhesives, mimicking natural processes and using the recombinant form of natural protein glue composites. Collaboration with engineers is opening new doors for assessment of materials properties and applications of these protein based glues and sealants.

Bottlenecks and Open Research Questions

How to interface biological and engineering systems at a practical level. To carry proof of concept into practice.

Benjamin Shapiro
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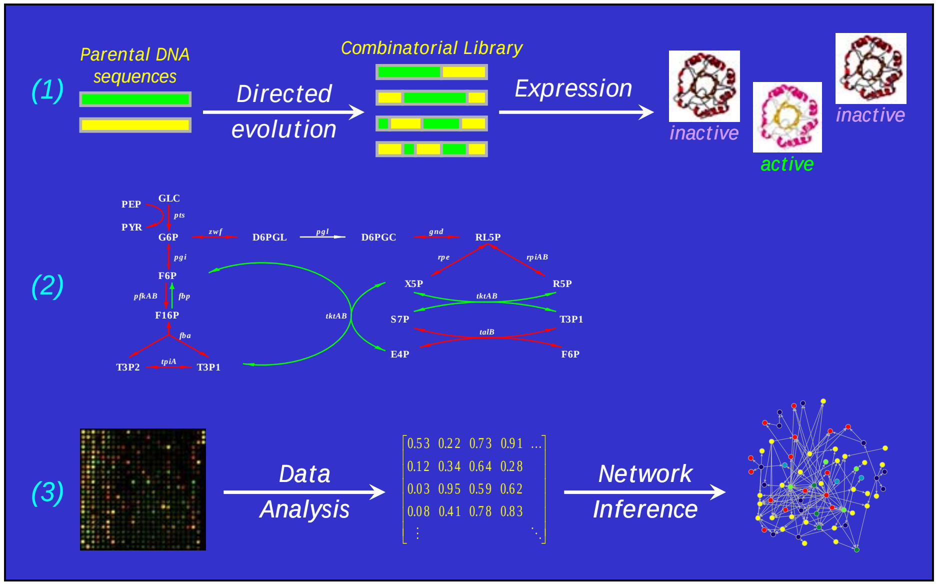
Analysis and Design of Biological Systems and Networks

Costas D. Maranas
Penn State

Goals and Potential Impact if Successful

-Computational design of combinatorial protein librairies
-Design of “sensing” molecules
-Metabolic pathway analysis and optimization
-Topological analysis of structural features of biological networks
-Microbial strain optimization
-Elucidation and verification of regulatory networks
-Real options based planning approaches for R&D portfolio optimization



Approach and/or Accomplishments

-Use of combinatorial optimization techniques (i.e., MILP and stochastic) to search through molecular and network alternatives.
-Use of potential energy models of molecular interactions (i.e., CHARMM) and scoring functions to evaluate the strength of binding events.
-Use of stoichiometry, regulatory informations and kinetic representations to describe interactions in metabolic and regulatory networks

Moore, G.L. and C.D. Maranas (2004), “Computational Challenges in Combinatorial Library Design for Protein Engineering,” *AIChE J.*, 50, 252-262.
Saraf, M.C., A.R. Horswill, S.J. Benkovic, and C.D. Maranass (2004), "FamClash: A Method for Ranking the Activity of Engineered Enzymes," *Proc. Natl. Acad. Sci. USA*, in press
Burgard, A.P., E.V. Nikolaev, C.H. Schilling, and C.D. Maranas (2004), "Flux Coupling Analysis of Genome-scale Metabolic Reconstructions," *Genome Research*, 14(2), 301-312
Burgard, A.P., P. Pharkya, and C.D. Maranas (2003), "OptKnock: A Bilevel Programming Framework for Identifying Gene Knockout Strategies for Microbial Strain Optimization,“ *Biotechnology and Bioengineering*, 84, 647-657.

Bottlenecks and Open Research Questions

How do we design customized molecular sensors with customized affinities for desired target molecules ?

How can we elucidate the complex web of interactions in living systems ?

How can we redesign living cells to be more attuned to engineering objectives such as overproduction or sensing?

Modeling Conformational Transitions in Macromolecules

Gregory Chirikjian
Johns Hopkins Univ.

Goals and Potential Impact if Successful

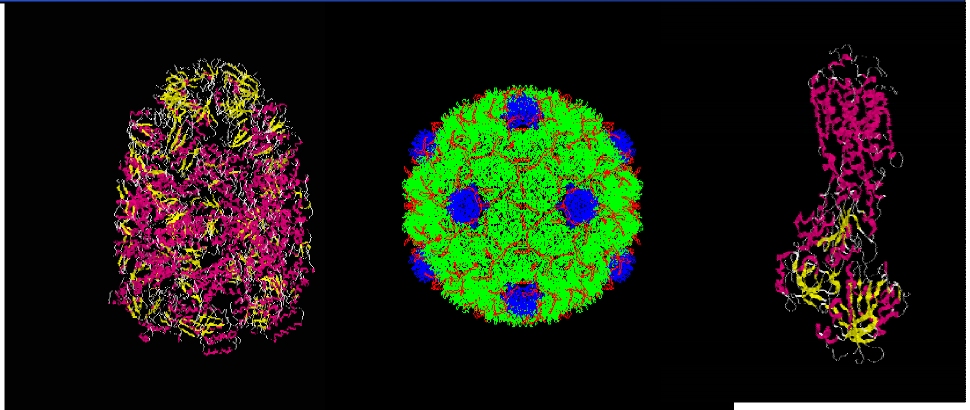
Model the kinematics and mechanics of biological macromolecules in order to:

-Understand better the mechanisms by which naturally occurring molecular machines function;

-Establish design principles for man-made molecular machines

-Develop plant models for such systems for use in control algorithms.

Perform statistical (structural-bioinformatics) analysis of data in the protein data bank using theory of Lie groups and other mathematics developed in geometric control theory literature



Examples of Molecular Machines: (left) GroEL/GroES, HK97 Capsid, (right) Ion Channel

Approach and/or Accomplishments

We have developed mechanical models of macromolecular motions and performed analyses such as those reported in:

- Lee, S., Chirikjian, G.S., ``Inter-Helical Angle and Distance Preferences in Globular Proteins," Biophysical Journal, Vol. 86, pp. 1105-1117, Feb 2004.
- Kim, M.K., Jernigan, R.L., Chirikjian, G.S., ``An elastic network model of HK97 capsid maturation," Journal of Structural Biology, 143 (2): 107-117 AUG 2003.
- Chirikjian, G.S., ``A Methodology for Determining Mechanical Properties of Macromolecules from Ensemble Motion Data," Trends in Analytical Chemistry, Vol. 22, No. 9, pp. 549-553, Sept. 2003.

Bottlenecks and Open Research Questions

-Can we develop simplified models for extremely complex macromolecular systems, or must one use very detailed quantum-mechanical or all-atom classical chemical physics descriptions ?

- How do we bridge the gap between experimental and theoretical/computational research in this area ?
- Are there any natural boundaries between nanotechnology, structural biology, bioinformatics, and the computational modeling of biomolecular machines ?
- As with any cross-disciplinary effort, how do we establish appropriate metrics for evaluation of research quality?

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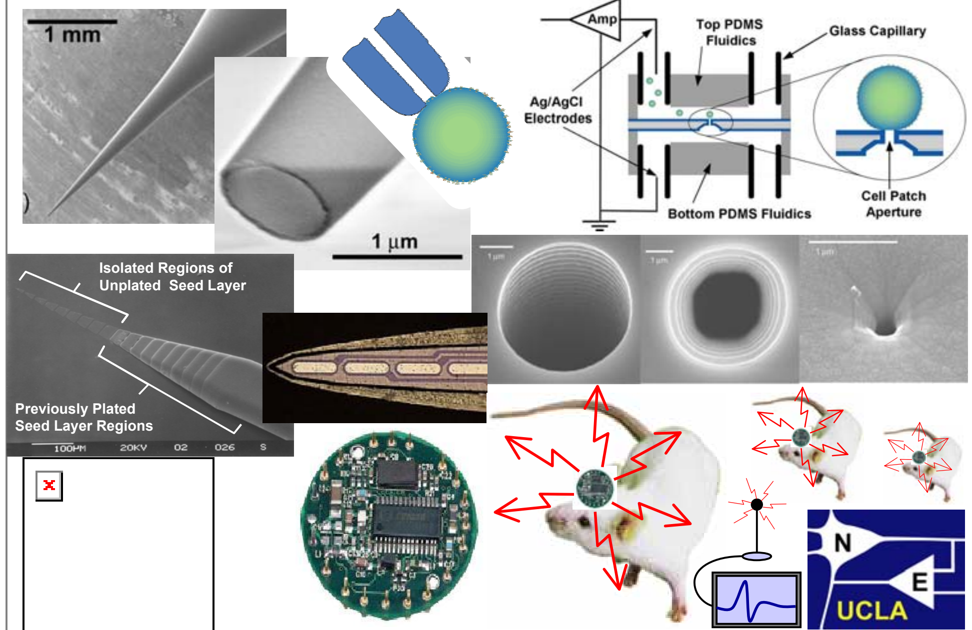
NeuroMEMS – using Micro/Nano Technology for Neuroscience

Jack W. Judy
UCLA

Goals and Potential Impact if Successful

- **Use Micro/Nano fabrication to produce MEMS/NEMS that enable new neuroscience or improve productivity**
- **Brain research is frequently <u>technologically limited</u>**
  - existing techniques are effective but *slow / inefficient*
  - most neuroscientists cannot advance techniques much
    - unaware of alternatives, lack training, and resources
- **MEMS/NEMS technology can make significant impact**
  - micro/nano-scale sensors, actuators, and systems
    - directly monitor and control at all levels of scale:
      - molecular, organelle, cellular, and systems of cells
  - combine with *closed-loop control* for more impact
- **Understanding the brain is the next *"<u>Grand Challenge</u>"***
  - long-term and multidisciplinary research area
  - NSF is the agency to enable this area of technology



Approaches and Accomplishments

- **Micro/Nano Systems for Intracellular Interface**
  - integrated nanomachined structures with a microfluidic system to monitor real-time cellular physiology
- **Microtechnologies for Interfacing with Deep Brain Regions**
  - deep brain regions provide regulation and control
    - fine motor control, metabolism regulation, emotions, …
  - existing technologies (cortical probes) not sufficient
    - longer, more accurate, less damage, multielectrode, ICs
- **Integrate Bi-Directional Wireless Telemetry Technology**
  - studies with direct-wired connections have limitations:
    - restricts movement, limits behavior, limits experimental duration, prevents socialization → *changes outcomes?*
  - wireless sensor technology has advanced considerably
    - TinyOS-based animal-mounted platform developed with COTS technology for low-bandwidth applications
    - high-bandwidth platform being studied – *<u>high demand</u>*

Bottlenecks and Open Research Questions

- **Unreliable Cellular Connection (so-called *gigaohm seal*)**
  - conventional pipettes work but are <u>not understood</u>
  - complex materials, surface-chemistry, biology issue
    - *collaborations are required to break up this "log jam"*
- **Batch-Fabricated 3-D Microelectrode Probe Arrays**
  - current methods yield 2-D microelectrode array or require complex assembly to obtain full 3-D array
  - integration of microfluidics would be very beneficial
  - probe material should be stiff during implantation and flexible after implantation (reduce artifacts & damage)
    - *new fabrication concepts and resources are needed*
- **Chip-Scale, High-Speed, Low-Power, Wireless Platforms**
  - current focus is on large networks of inexpensive low-bandwidth sensor motes that are *not* small enough
    - *NeuroMEMS needs a smaller, faster, smarter platform*

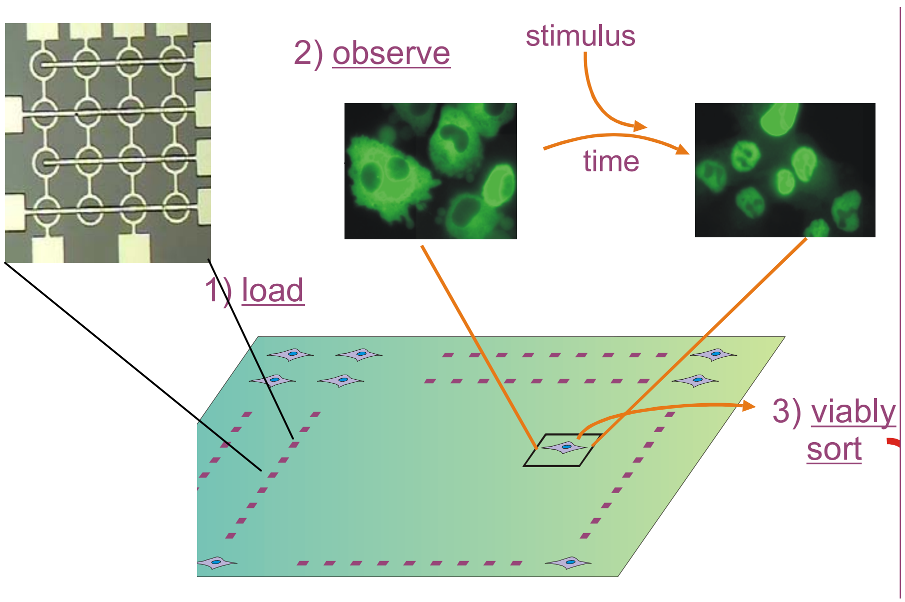
Microtechnology for cellular measurements

Joel Voldman
MIT

Goals and Potential Impact if Successful

• Goal: to create microtechnology that can acquire novel information from cells
    • to build models of cell function

•The potential impact is to aid in understanding biological systems
    •Drug discovery
    •Human health
    •Basic biological science



Approach and/or Accomplishments

•Our approach is to use extensive modeling to predict performance *before* fabrication

•This is what enables design of non-intuitive structures that can meet complex system needs

•One example in figure
    •A cytometer that can image and then sort cells
    •Uses electric fields—dielectrophoresis—to manipulate cells
    •Combines functionalities of microscopy and flow cytometry
    •Enables new analyses of spatial/temporal cell processes

Bottlenecks and Open Research Questions

-System-level approaches to working with cells
    -Reliable operation with many cells is *the* biggest challenge
    -Need protocols, surface treatments, design approaches that are tolerant to the immense biological variability
-Interactions of cells and microsystems
    -Genome-wide and molecular analysis of artifacts
Modeling tools
    -That are fast enough to be able to *design* devices involving liquids, electric fields, and particles
-Materials
    -Non-fluorescent photopatternable polymers

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Dynamics and Control of Bio-nanorobots

T. J. Tarn
Washington University in St. Louis

Goals and Potential Impact if Successful

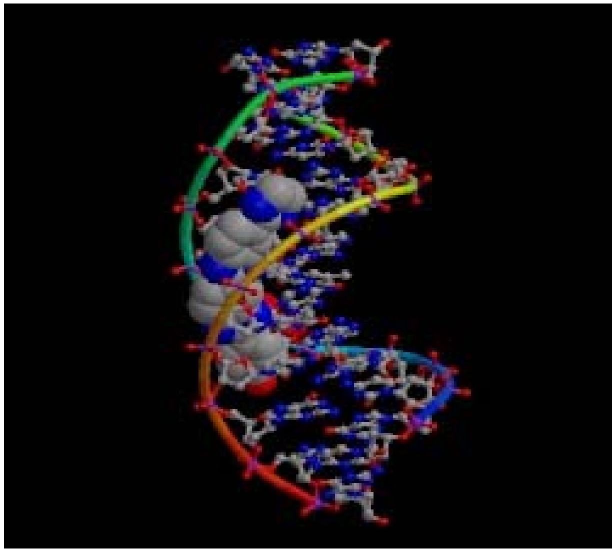
- Find a way to build and control bio-nanorobots.
- Understand nano-scale dynamics: how does a bio-nanorobot handle system dynamics?
- Understand nano-scale control: how is the information being transferred and used for bio-nanorobots?

Direct impact: nano-medicine and nano-fabrication.

- Medicine: better drug design and disease treatment. Man-made bio-nanorobots can be used as vaccines or antibodies against disease.
- Manufacturing: nano-fabrication for nanotechnology. Bio-nanorobots may be assembled and form multi-degree of freedom nanodevices for nanoworld manipulations.

Right figure:

Conformation of B-DNA containing O6-ethyl-G-C base pairs stabilized by minor groove binding drugs



http://www.rcsb.org/pdb/

Approach and/or Accomplishments

- Mathematical modeling: a correct modeling of bio-nanorobtos is the key for understand dynamics and control of bio-nanorobots. Start with ODE model to extend to PDE's.
- Control: extended application of distributed and decentralized control methods from advanced control theories.
- Bottom-up fabrication based on quantum mechanical control.

The author has accumulated many years of excellent research experience in dynamics and control. Solid background and achievements for mathematical modeling and control of dynamic systems including Robotic Systems and Quantum Mechanical Control Systems

Bottlenecks and Open Research Questions

- The key is to construct dynamic models at nano-scale.
- **Verification.** Right tools or methods to check accuracy and correctness of the modeling and control. This is a very challenging topic in nano-scale.
- **Implementation.** The difficulty is that it is not known how a bio-nanorobot is controlled, specifically, how to organize bio-molecules to have some kinds of intelligent properties.
- **New physical laws.** Is there any new physical law at nano-scale that can be used for understanding system dynamics and control of bio-nanorobots?

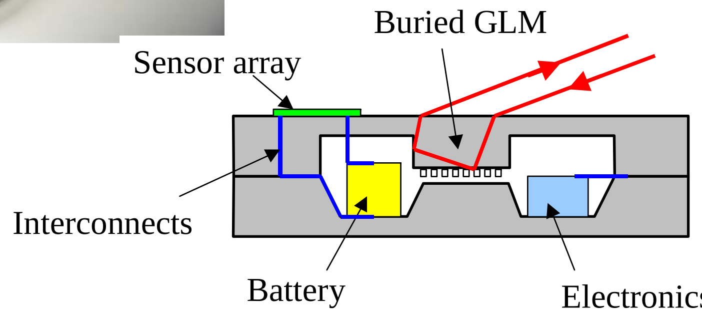
Metrology, Modeling, and Control in Nano-scale Manufacture??

Kameshwar Poolla
UC Berkeley

Goals and Potential Impact if Successful

Our research has focused on process control and metrology solutions for semiconductor manufacturing. The issues here might well be different than those in nano-scale manufacturing. For example, we believe that tomogrpahic methods at the interconnect level can be used to isolate defects in simple repetitive nano-structures. In the context of this workshop, our goals are to determine the roles of metrology, modeling and control in the manufacture of nano-scale structures and devices.

Sensor arrays for IC manufacture



Approach and/or Accomplishments

Our approach has been to

- First, build autonomous arrays of sensors using MEMS, standard CMOS, or even thick film techniques
- Second, to use these sensors to build process models that relate recipe settings to product parameters such as gate CD
- Third, to use control methods to optimize the processes.

We have successfully built arrays of sensors to monitor a variety of process variables such as temperature, etch rate, ion density. We have used these sensors to control litho and plasma processes. Our efforts have had commercial success and have been implemented in high-volume production facilities yielding a reduction of across wafer CD non-uniformity by 30% in sub 150nm pattern transfer.

Bottlenecks and Open Research Questions

•It is very impressive to see that simple repetitive structures of various materials can be made at the nano-scale using self-assembly or other approaches. Interconnecting such structures to form functionally addressable or (better still) programmable devices seems to me a major bottleneck. Reliability, self diagnostics or nano-scale assemblies are other key issue. Can biologically inspired mechanisms be developed to address these challenges? Are there process control challenges? Is it simply too early to examine manufacturing issues for nano-scale devices? Is there a role for tomography or other metrology methods in fault detection and isolation for nano structures?

Benjamin Shapiro
UNIVERSITY OF MARYLAND

Micro- and Nano-Scale Assembly

Jason J. Gorman
NIST

Goals and Potential Impact if Successful

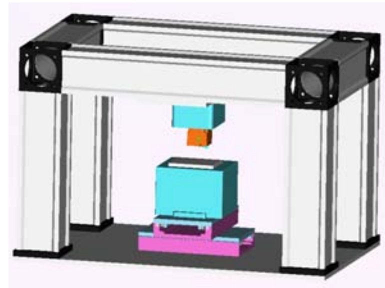
One goal of the Integrated Nano-to-Millimeter Manufacturing Program is to develop methods and systems which support an integrated approach to control, modify, manipulate and assemble across mm and nm scales. Two manipulation and assembly systems are currently being explored:

Microassembly using Mechanical Manipulation

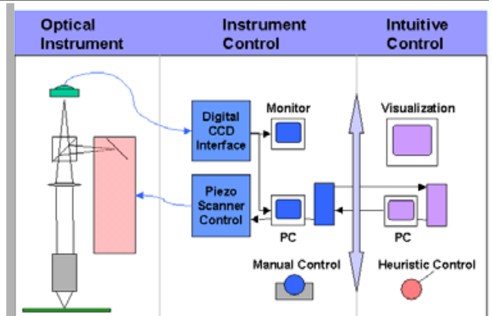
- Automated dexterous assembly of hybrid MEMS and opto-electronic devices
- Achieve flexibility and reliability suitable for real world production

Micro- and Nano-Scale Assembly using Optical Tweezers

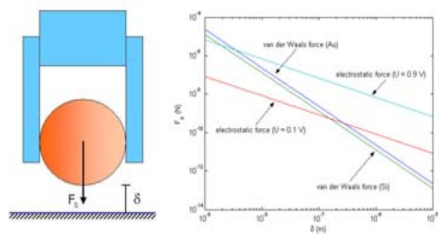
- Multi-dimensional assembly of components with complex geometries and varying optical properties
- Applications include nano-scale optical devices and high-bandwidth automated DNA sequencing



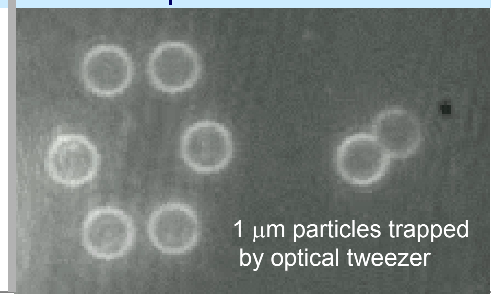
microassembly



optical tweezers



surface forces during assembly



Approach and/or Accomplishments

Models

- Integrate macro-scale (robot dynamics), micro-scale (MEMS dynamics, friction), and nano-scale (surface forces) models
- Develop approaches for modeling optical trapping of non-spherical, non-refractive components

Control Systems

- Utilize combinations of robust and adaptive control to address inherent nonlinearities and incomplete models at the micro- and nano-scales
- Estimation-based controllers due to inferred sensing of processes

Virtual Interfaces

- Provide model-based feedback of assembly forces and heuristic rules to constrain motions during telemanipulation

Bottlenecks and Open Research Questions

Sensors and Sensing Techniques

- There is a need for suitable small robust position and force sensors
- Image processing has severe bandwidth and resolution limitations in tracking the motion of nanoparticles

Modeling

- Most modeling efforts at the micro and nano-scales concentrate on simple geometries
- 6 DOF models for complex geometries are required, along with model reduction techniques for real-time implementation

Driving Applications in Nanotechnology

- Applications in nanotechnology will determine which assumptions for assembly are acceptable. However, these applications are not mature enough to provide the necessary feedback.

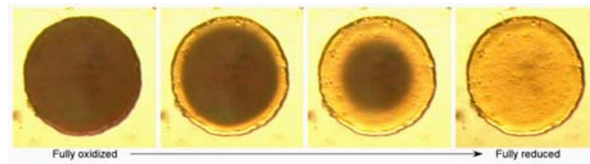
Modeling and Control of Micro Fluidic Systems

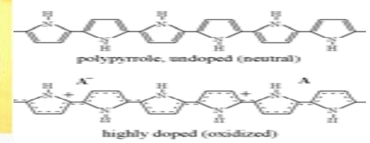
Benjamin Shapiro
University of Maryland

Goals and Potential Impact if Successful

(Feedback) control of micro-fluidic systems such as:
-Lab-on-a-chip systems
-Conjugated polymer “conducting plastic” in bio-fluids micro actuators
-Steering of bio-particles/chemicals in micro-fluidic devices for biological screening, micro drug delivery, etc.
Create integrated systems that work in messy enviroments.

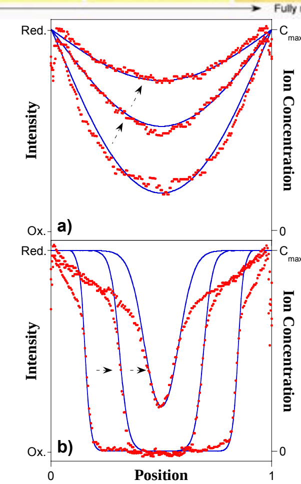
Require feedback on the micro/nano scale for the same reason that it is required on the macro scale: allows systems to function with large degrees of noise and uncertainty, create robust performance, accomplish complex coordinated tasks, integrated sensing/actuation.



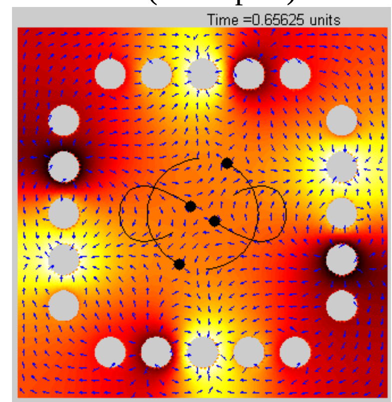


Oxidation fronts in conjugated polymer films.

Experiments (E.Smela) versus Theory (B.Shapiro)



Flow Control Micro Fluidic Tweezers (B.Shapiro)



Approach and/or Accomplishments

MODELING:
-Identify dominant physical effects by intuition, theory, back-of-the-envelope analysis, experimentation, …
-Create PDE models of dominant effects. Quantify unknown parameters by careful experiments, system identification, ..

CONTROL:
-Pose practical tasks (such as split drops precisely using electrically actuated surface tension forces) as tractable mathematical problems (updated least squares control of pinch points).
-Extend/develop PDE control theory to: PDE control on changing topology, non-smooth behavior (interface control) ..

Bottlenecks and Open Research Questions

-Modeling, analysis, and design tools appropriate for control of micro/nano systems are largely unavailable. My lab spends the majority of its time creating control ready models and recreating tools available on the macro scale for the micro scale (such as model reduction tools).
-Communication gaps: Controls people don’t speak the same language as the fabrication people who don’t speak the same language as the organic chemistry people who ..
-What are the dominant physics? Given a complex bio/chemical system, how do we decide what physical phenomena really matter? Combine knowledge bases?
-System integration: Design tools. Coupling. Robust nonlinear system ID. Appropriate sensing/actuation. …

Workshop was organized according to six theme areas chosen by NSF and the organizing committee …

- MEMS Design/Fabrication, Devices, and Systems.
- Nano Fabrication
- Biological (or Biomolecular/Biochemical) and Chemical Systems on Micro/Nano- Scales.
- BioMEMS and/or Nanobiotechnological Systems
- Control Systems with a MEMS and/or Nano Perspective
- Measurement, Modeling, and Model Validation at the Micro- and Nanoscale.

Bio-Particle Manipulations in Microfluidic Systems

Ali Beskok
Texas A&M University

Goals and Potential Impact if Successful

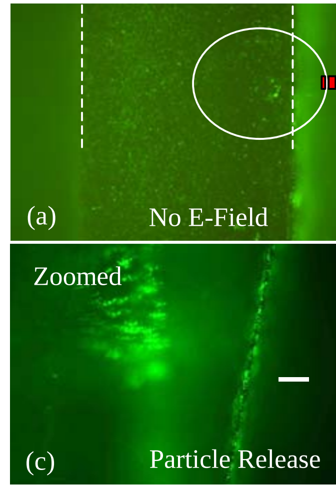
I. Design of microfluidic systems for

a) Concentration, capture and release of microbial contaminants from drinking and recycled water.
b) Drug delivery using micro-encapsulated protein micro-spheres.
c) Fluid and species flow control and mixing using electrokinetics and chaotic advection.

II. Colloidal particle aggregation during electrophoretic deposition on patterned electrodes, and dielectrophoresis.

a) Particle aggregation in cracks (defects) and constrained geometries — Self healing materials.
b) Colloidal self assembly and crystallization.

III. Microfluidic device control and integration.



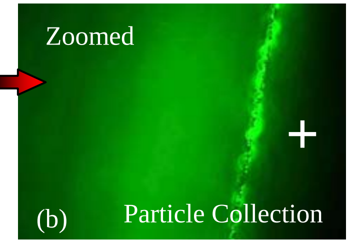
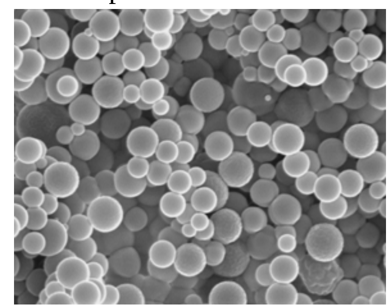


Figure 1: Snapshots of fluorescent particle capture (b) and release (c) on electrode surfaces.

Figure 2: SEM pictures of 2μm BSA micro-spheres.



Approach and Accomplishments

I. Experiments:

a) Proof of concept of bio-particle capture on electrode surfaces is shown in Figure 1. Careful experimentation is planned to investigate capture and particle release.
b) BSA & BSA+vpB based micro-spheres prepared using water in oil emulsification. Theoretical correlation to predict average size is developed (Figure 2).
c) Experiments to study particle aggregation on patterned electrodes during electrophoretic deposition is underway.

II. Theory and Modeling:

a) Numerical simulation of electrokinetic flows and mixing.
b) Particle tracking, chaotic mixing & mixing quantification.
c) Theoretical modeling of electrophoretic deposition:
Determination of dominant physical effects from experiments.

Benjamin Shapiro
UNIVERSITY OF MARYLAND

Bottlenecks and Open Research Questions

I. Development of theory and numerical models, and validation with experiments

a) Identify important parameters that contribute to flow physics from intuition and experiments.
b) Electrokinetic transport models involving moving boundaries, realistic particle shapes, particle-particle and particle-wall interactions.
c) Model particle erosion and particle diffusion (for drug delivery).

II. Scale homogenization

Bridging the gap between the nano and micro-scales and processes, and relate these to macroscopic device/system behavior.

Control of Atomic-Scale Process Dynamics

Martha Gallivan
Georgia Tech

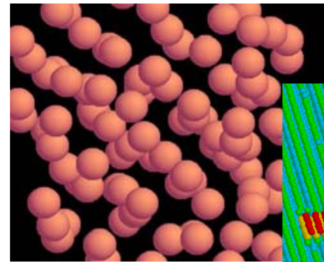
Goals and Potential Impact if Successful

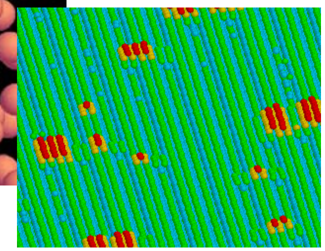
Goal: to design new materials and devices using predictive models and formal optimization
- particularly challenging when the process must be described at the molecular level

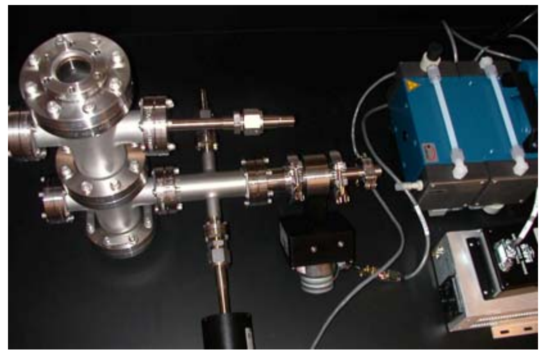
Examples
- fabrication of integrated circuits
- polymer architecture control in processing

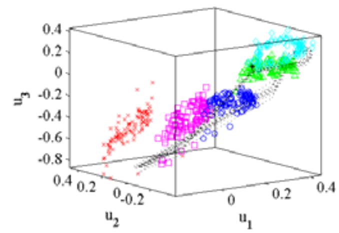
Impact: development of better electronic devices for computing and communications, rational design of advanced materials

- Detailed models
- Reduced dynamics
- Experimental implementation









Approach and/or Accomplishments

- Identify and focus on industrially relevant problems
- Develop detailed physical models via our own experiments, through collaboration, and through literature models.
- Use standard model reduction algorithms *and* physical understanding to develop more compact process models
- Apply systems tools like optimization and feedback control

Example: ultra-high vacuum thin film deposition of Ge
- estimated activation energies in experiment
- developed Monte Carlo and reduced models of morphology evolution
- computed optimal temperature history in the presence of equipment constraints

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UNIVERSITY OF MARYLAND

Bottlenecks and Open Research Questions

1. How predictive are the models developed by computational chemistry and materials science? How predictive will they be in the future?
2. How will nanoscale devices be manufactured in the future? What will the balance be among lithography, stereolithography, nanopositioning, and self-assembly?
3. What will the computer of the future look like? CMOS, molecular switches, quantum computing? What should we be focusing on?

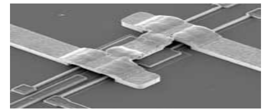
Numerical Macromodeling for MEMS/NEMS

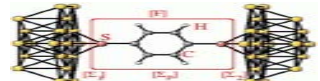
Jacob White
MIT EECS/RLE

Goal: Develop CAD tools which support MEMS/NEMS use in systems to reduce Design Time from Years to Months

- Must Optimize New Technology in System
  - **Do MEMS filters improve RF systems?**
- Must Address Nonlinear Model Reduction
  - **Trajectory and Statistical methods**
- New efforts on design parameterized MOR
  - **Enables automatic optimization**

Numerical Model Reduction





Lundstrom et al.

Automatic

$$\frac{dx_r(t)}{dt} = F(x_r(t)) + b_r u(t)$$

$$y(t) = c_r^T x_r(t)$$

- For Linear Problems – Many techniques
  - **Krylov-subspace, truncated balance realization, etc**
- For Nonlinear Problems
  - **Trajectory and Statistical methods**
- New efforts on design parameterized ROM

<u>Approach and/or Accomplishments</u>

- Fast Integral Equation Solvers
  - Faststokes, FastImp, Precorrected-FFT
- Parameterized MOR
  - Extraction of Geometrically parameterized inductors from 3-D E-M solvers
  - Multidimensional Krylov Methods
- Nonlinear MOR
  - Trajectory Piecewise-linear approaches
  - Perturbation TBR analysis

<u>Bottlenecks and Open Research Questions</u>

- Flexible Fast Coupled Domain Solvers
  - Need to plug-and-play new physics
  - Must handle very complicated 3-D
- Numerical Model Reduction Essential
  - Nonlinear MOR still unreliable
  - Must also include parameterization
  - Massively coupled problems!
- Co-Optimization
  - Parameterized MOR offers new opportunites

Workshop recommendations are grouped according to three subjects …

- System integration
- System control
- Education and infrastructure needs

Micro/Nano System Integration Research Recommendations

What are the tools required for integration?
(Focus on needs that required cross-theme collaborations.)

System integration goals:
-Integration across disparate length and time scales
-Integration between hard and soft fabrication techniques
-Integration of inorganic, organic, and living systems.
-Integration of in-situ sensors and actuators for real time control

Workshop participants identified two major needs …
- Systems level measurement: diagnostics and micro/nano sensors
- Parsimonious (keep essentials only) models for design & control

Systems level measurement: diagnostics and micro/nano sensors

Needed to: clarify physical phenomena, and provide input and validation for models of micro/nano systems.

- Improve diagnostics = benchtop micro/nano measurement methods
- Integrated sensors = miniaturize diagnostics for real time control

Parsimonious (keep essentials only) models for design & control

Need models for system design, optimization, and control.

- Models must be carefully chosen: must contain enough physics to be predictive, but must remain computationally tractable
- Create by physical insight (crucial) and model reduction (helpful)
- Available FEM/CFD modeling tools not appropriate for design: controls researchers must have a hand in creating new modeling tools
- Need to bridge gap between molecular and continuum scale models
- Methods needed to determine point at which model is good enough

System Control Research Recommendations

Micro/nano systems have lots of uncertainty, ability to sense/actuate in a distributed way on tiny length scales, plus desire high performance
→ many opportunities for feedback control.

Fabrication Process Control

Difficult to achieve reproducible results at the nano scale. Nanotubes: "Repeat the same procedure, get different results each time" Jun Jiao

-Control: real time process monitoring to improve reproducibility
-Consider sensor/actuator placement early in the plant design.

-"Micro + Control = Nano", e.g. Resistive heating + microbridge = nanowires.

Control for Nano Assembly and Object Manipulation

Metin Sitti will talk about that next …

'On-Chip' Control inside Micro/Nano Systems

For self-contained miniaturized systems, sensors, actuators, and control hardware/software must be included inside a micro system.

- Modeling for control design
- Sensors, actuators, and control logic circuits must be optimally distributed inside a small volume
- Software and Digital Signal Processing (DSP) too slow/big: will need to go back to analog control logic in some instances
- Need high degree of robustness, noise rejection, and fault tolerance

Robust control, distributed control, system identification and state estimation, and optimization tools could be used to address issues.

Control of Heterogeneous Systems

Interactions between continuous and discrete dynamics, interfacial and bulk effects, organic/inorganic interactions, …

- Need modeling and control tools for heterogeneous systems: a challenging area that is already being addressed by controls researchers, but need closer link between control and micro/nano research.

Control of Systems that Combine Biology and Engineering

Aiming at implantable medical sensors and systems.

- Control devices to conform to cells/living organisms.
- Improve measurement and data extraction methods.
- Develop algorithms to control behavior of implanted devices: algorithms must adapt to feedback mechanisms inside the body.
- There is an opportunity to learn control from biological systems.

Education, Collaboration, and Infrastructure Rec'd

Education next generation of cross-disciplinary students *and faculty*

- Cross-disciplinary student exchange programs. Co-advise students.
- Gordon conference type summer workshops in AFM, micro-fluidics, ..
- Cross-disciplinary curricula for undergrad and grad level.
- Tenure process: should encourage, not penalize, collaboration.

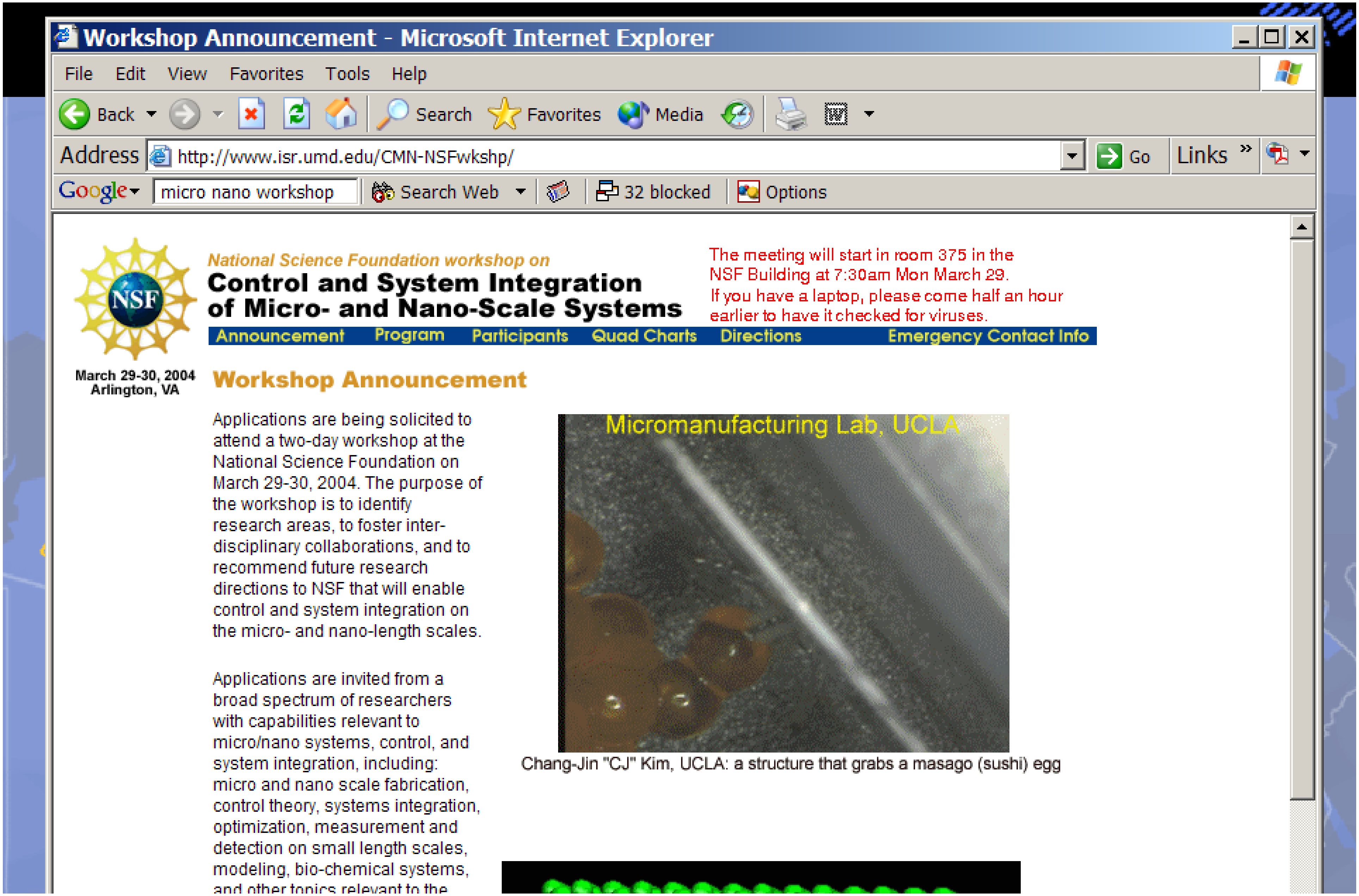
Modeling infrastructure for system integration and control

- Commercial and academic modeling tools must be "control ready".
- Peer reviewed database of models for sub-classes of systems.

Develop widely available fabrication infrastructure

- MOSIS for bio-chemistry and bio-medical applications.
- Publicly funded/available nano fab facilities.

Report + workshop info: http://www.isr.umd.edu/CMN-NSFwkshp/


Workshop Announcement - Microsoft Internet Explorer

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Address http://www.isr.umd.edu/CMN-NSFwkshp/ Go Links

Google micro nano workshop Search Web 32 blocked Options

March 29-30, 2004
Arlington, VA

National Science Foundation workshop on

Control and System Integration of Micro- and Nano-Scale Systems

The meeting will start in room 375 in the NSF Building at 7:30am Mon March 29.
If you have a laptop, please come half an hour earlier to have it checked for viruses.

Announcement Program Participants Quad Charts Directions Emergency Contact Info

Workshop Announcement

Applications are being solicited to attend a two-day workshop at the National Science Foundation on March 29-30, 2004. The purpose of the workshop is to identify research areas, to foster inter-disciplinary collaborations, and to recommend future research directions to NSF that will enable control and system integration on the micro- and nano-length scales.

Applications are invited from a broad spectrum of researchers with capabilities relevant to micro/nano systems, control, and system integration, including: micro and nano scale fabrication, control theory, systems integration, optimization, measurement and detection on small length scales, modeling, bio-chemical systems, and other topics relevant to the

Micromanufacturing Lab, UCLA

Chang-Jin "CJ" Kim, UCLA: a structure that grabs a masago (sushi) egg