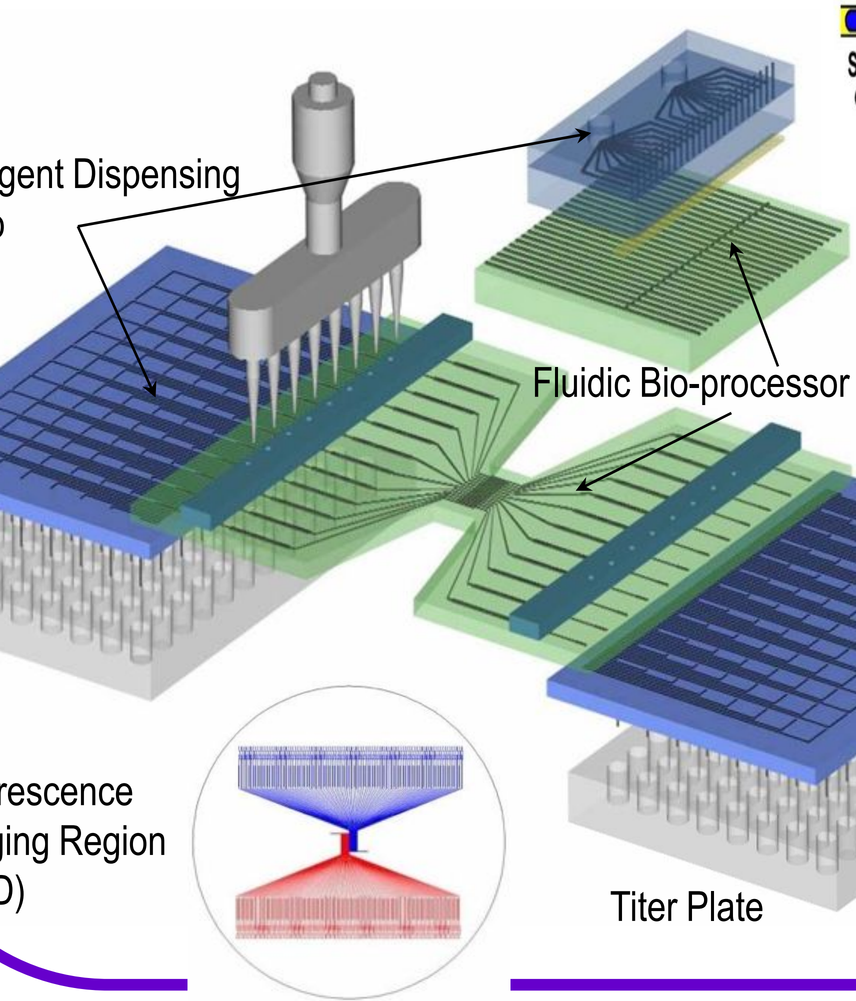
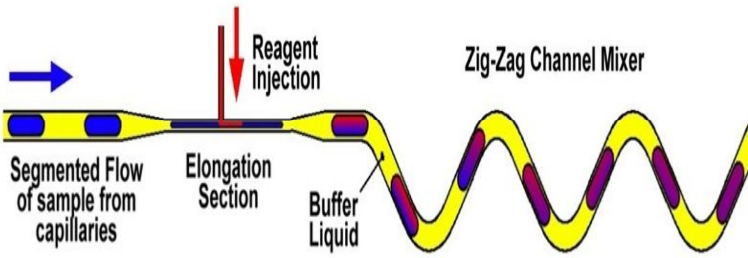
Posters by Okagbare, Kim, Rani, You, hrestha/Juneja, Walker

Small Molecule Sensor (Steve Soper, LSU)

en combinatorial library for inhibitors of L1-
- Genome instability





GACCGCTTTTTAAAAAGCATACA

CTGGCGAAAAATTTTTCGTATGT

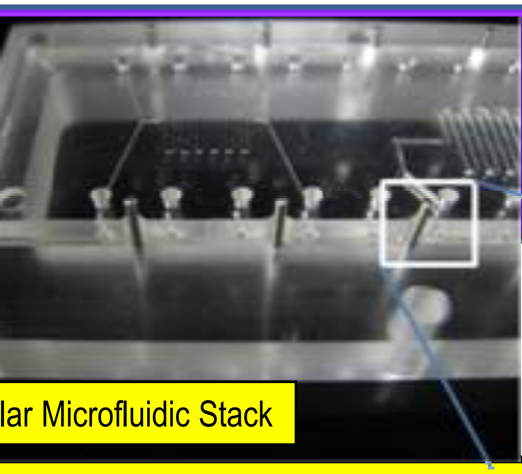
Substrate for L1-EN

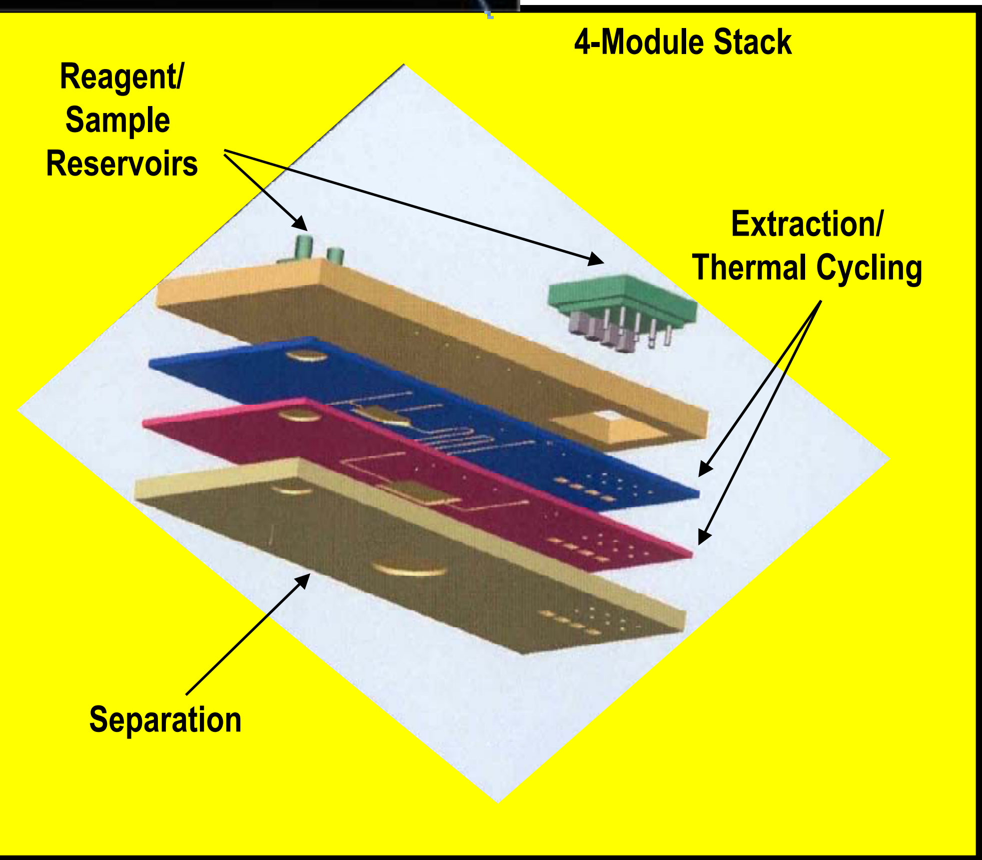
VALUE ADDED

- Current state-of-the-art instruments (Evotec);
  - process 140,000 samples day^{-1}
  - Robotic fluid handling
  - Uses 1-5 µL of reagents

Small Molecule Sensor System;
  - Process ~10^9 samples day^{-1}
  - Full automation affected by microfluidics
  - Imaging readout with high sensitivity
  - Uses 1-5 pL of reagents
- Interdisciplinary project (synthetic, analytical, material chemists; mechanical engineers; molecular biologists; pharmaceutical industry)
- Experimental chemists/engineers become familiar with HPC (WP3, WP4)
- CHALLENGE – How to mine and organize the data generated (WP1)

Genosensor System (Steve Soper, LSU)

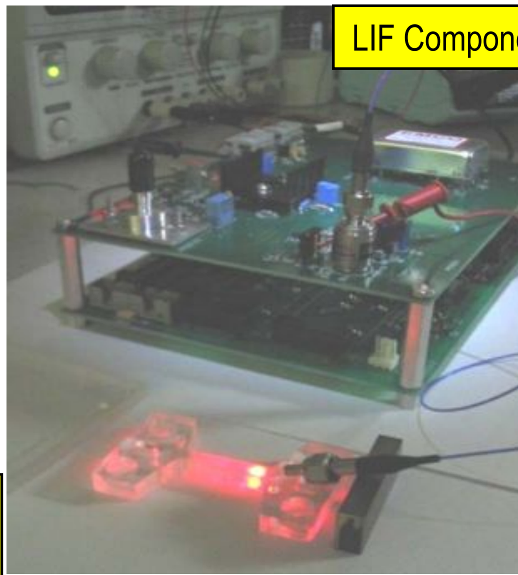


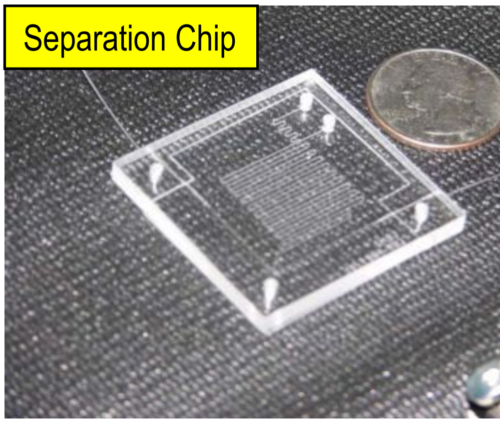


ation

20

Time (s)





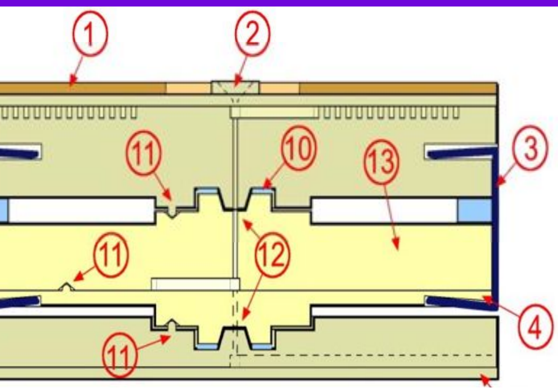
VALUE ADDED

- Current state-of-the-art instruments (ABI);
  - Multiple instruments for processing genetic samples
  - Large footprint and not field deployable
  - Requires specialized technicians to affect assay
  - Long assay turn-around time (6-8 h)

Genosensor System;
  - Full automation affected by microfluidics and process integration
  - Short assay turn-around-time (30 min)
  - Field deployable without sacrificing assay performance
- Interdisciplinary project (synthetic, analytical, material chemists; mechanical engineers; molecular biologists; computer scientists)
- Reduce design/development time using system-level modeling
- CHALLENGE – Fabricate integrated system with multiple processing steps (WP3; WP4)

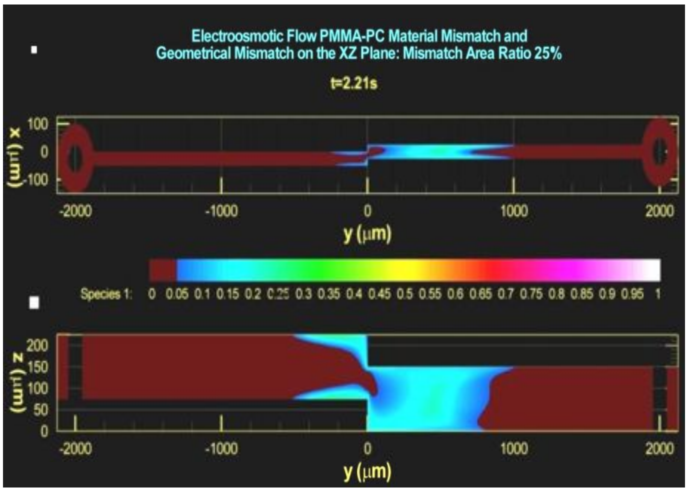
osters by Chen, You, Njoroge, Rani, Park, Kalghatgi

Genosensor System (Steve Soper, LSU)

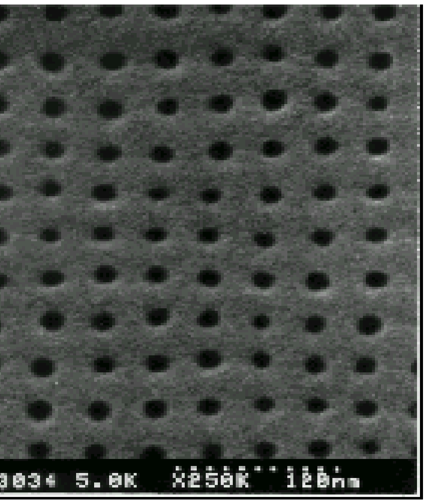


eptual drawing of super ophobic interconnect.

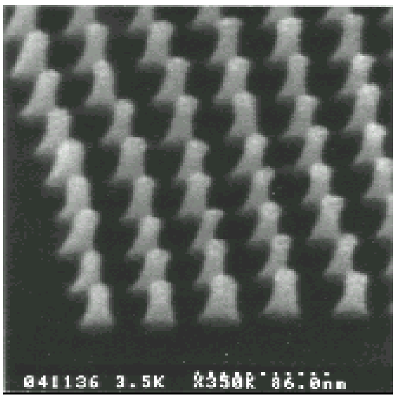
CFD simulation for module mis-alignment.



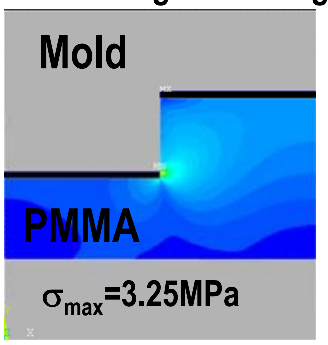
Interconnects:
Designing modu across different mate and sc
Computational Nee
CFD simulations Newtonian fluids ac mixed-scale mate (nano-to-microchann transport.

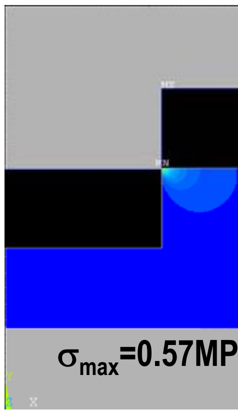


NIL



Stress during demolding



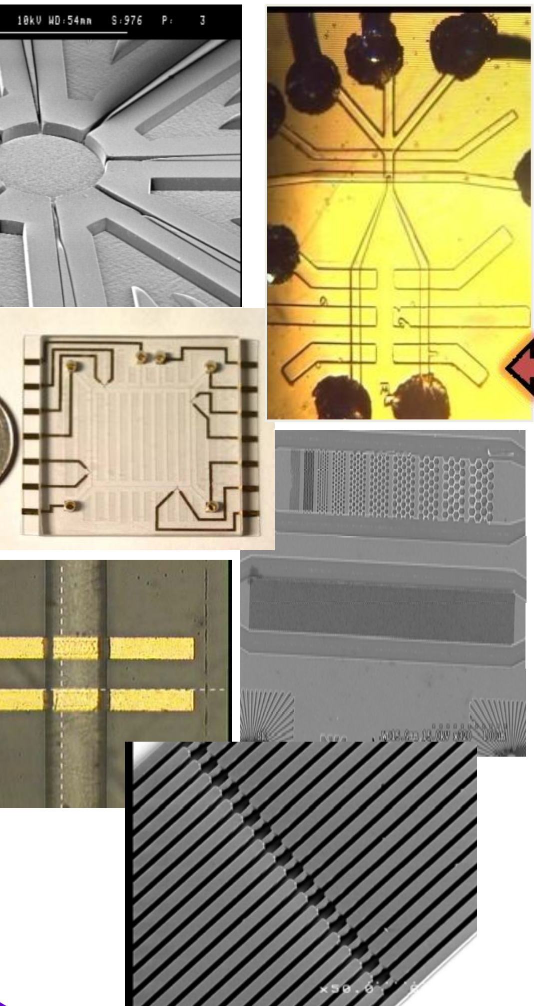


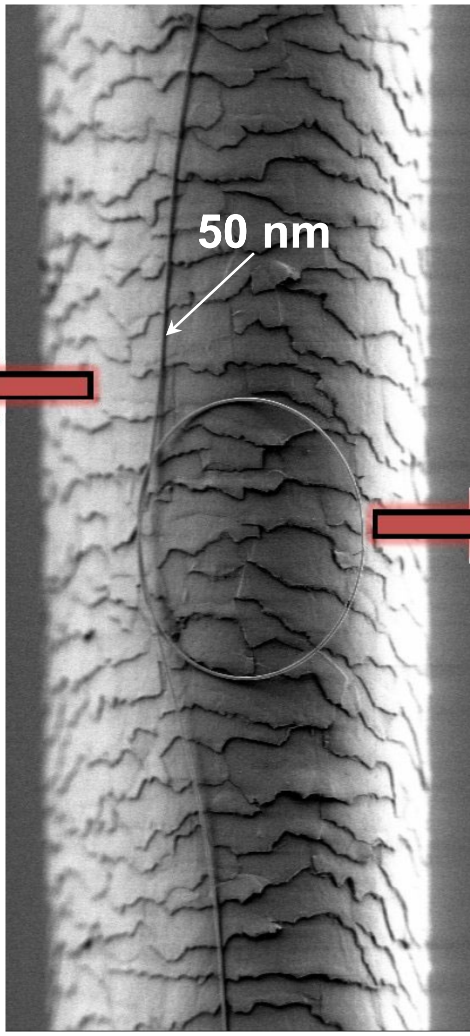
Nanofabrication : Nanoimprint lithography (NIL) to build nanostructure domains (extraction, extension)
Computational Needs – Modeling Non-Newtonian Fluids during mixed-scale replication.

Nanoscale Sensors: Rethinking the Molecular Processing Paradigm (Steve Soper, LSU)

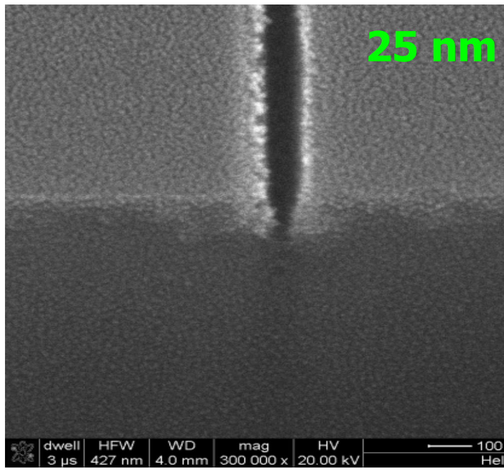
osters by Dufaud,
Lekpeli

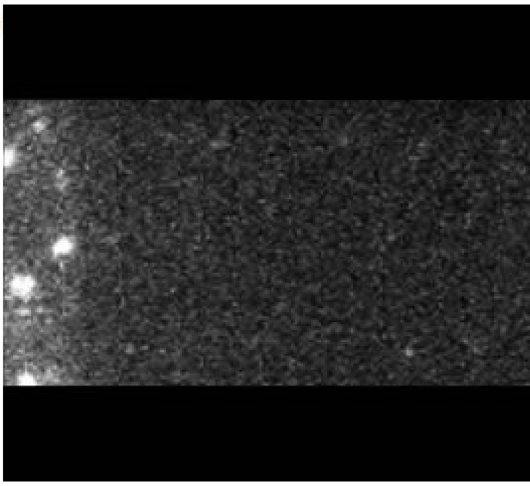
Microtechnology





Nanotechnology



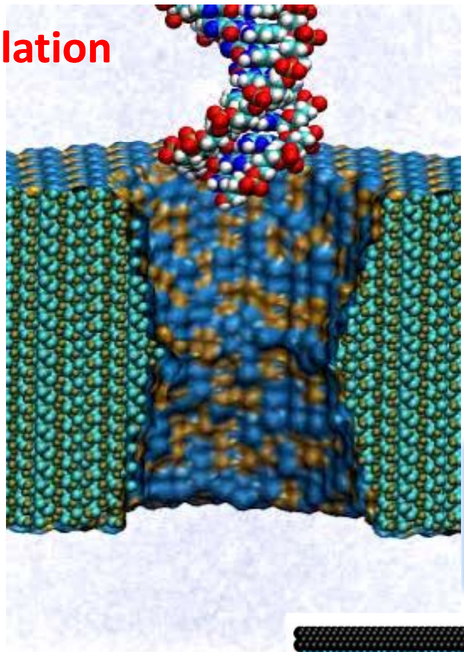


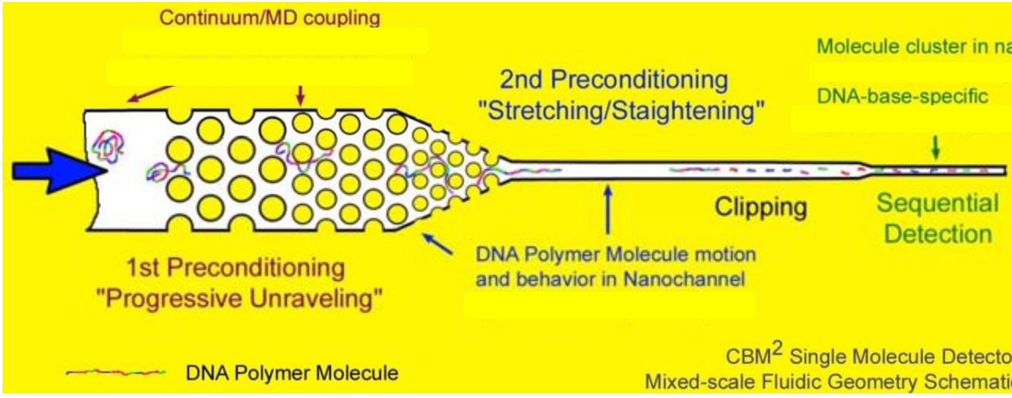
Menard and J. M. Ramsey, UNC

CyberTools Modeling of DNA Transport in Micro- / Nano-domains (Steve Soper, LSU)

Simulation

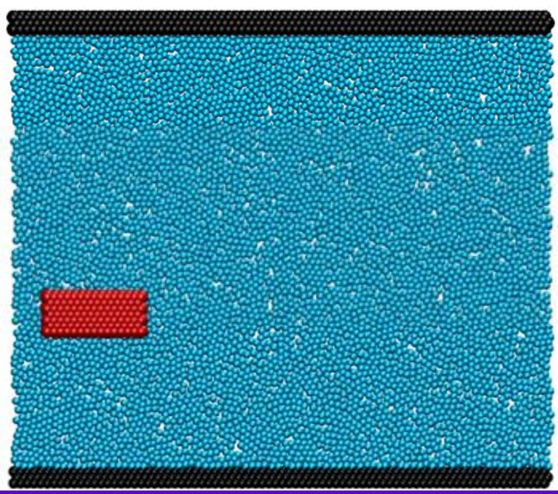
Schulten, *BioPhy. J.* 87 (2004) 2086.

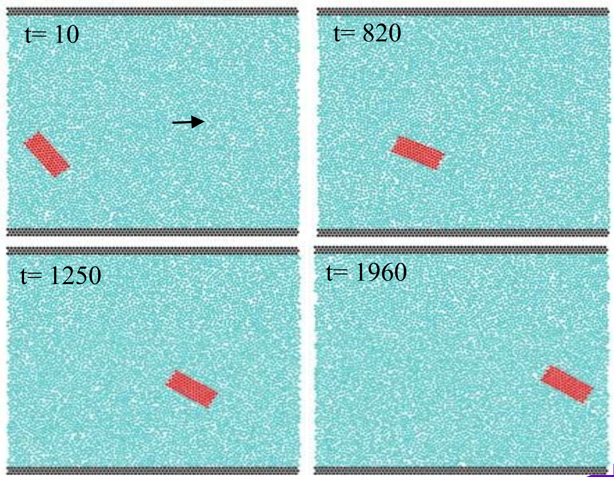




Problem – MD Simulations limited to ~100 ns; 'True' translocations are millisecond-scale events.

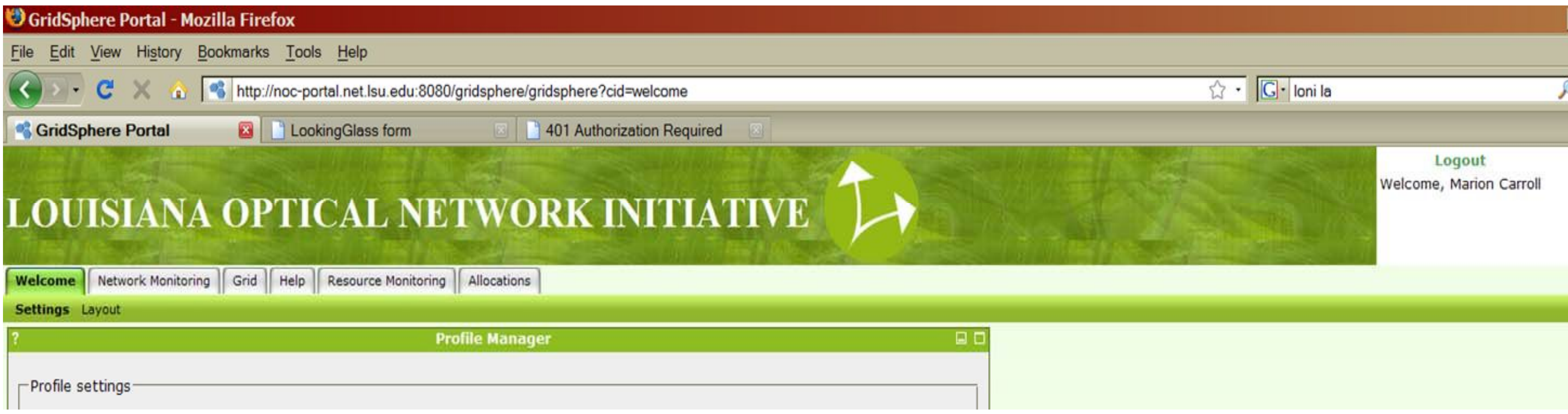
D Simulation using
nnard-Jones Fluid
M time steps, step
.16 ps; w ~ 25 nm; L
27 nm).





Discovery of new *Alu* Subfamilies using HPC (Marion Carroll, XU)

TREE_PUZZLE and Maximum Likelihood Analysis

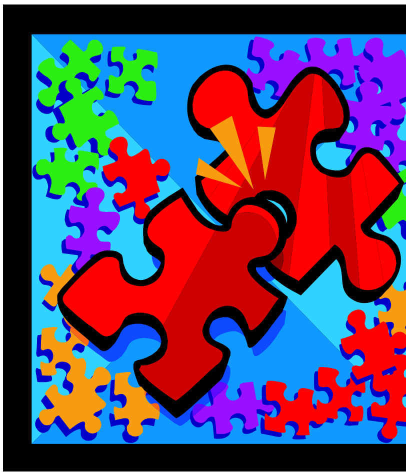


Queenbee HPC is employed to generate output files using TREE-PUZZLE that suggest divergence of uncharacterized Alu Y elements into subfamilies. Diagnostic mutations must then be described via sequence alignment in MEGA.

Tree-Puzzle Algorithm
(Marion Carroll, XU)

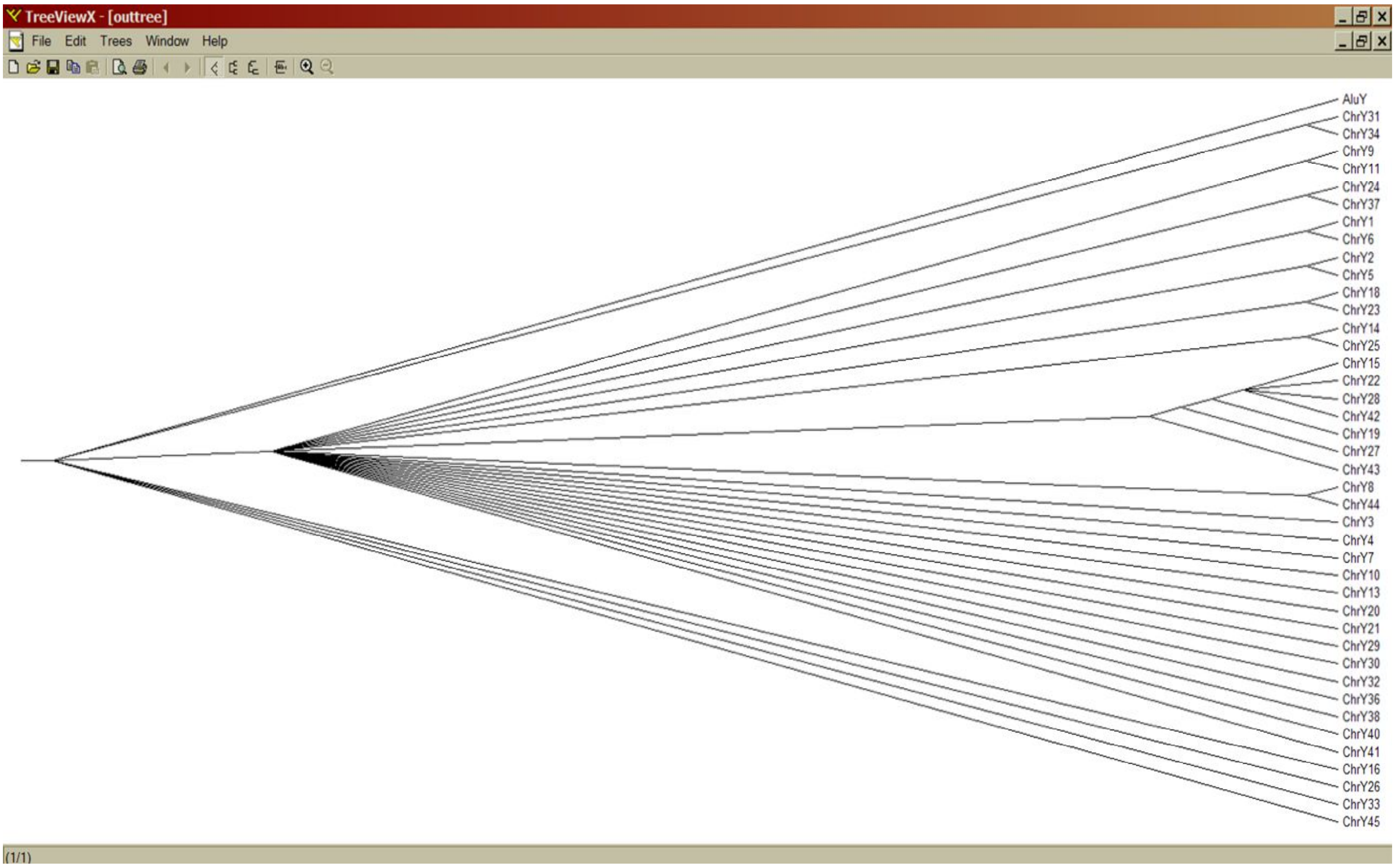
REE-PUZZLE is an application run on Queenbee
hat reconstructs phylogenetic trees from
ucleotide sequences by maximum likelihood.

REE-PUZZLE conducts a number
of statistical tests on the data set.
does a tree search algorithm or
uartet puzzling that allows analysis
f large data sets using MPI.



Output of Tree-Puzzle Analysis
(Marion Carroll, XU)

OUTTREE FILE



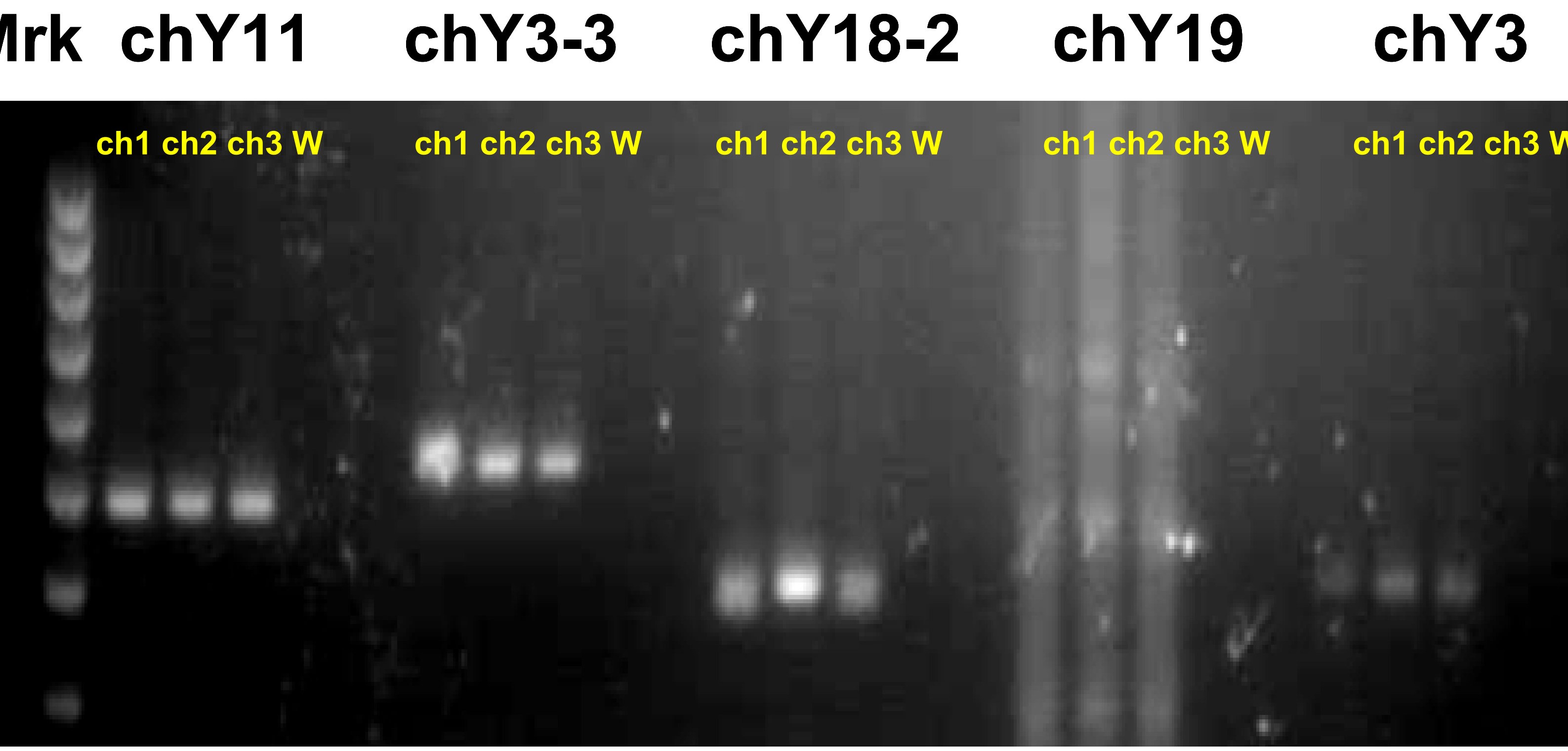
Tree-Puzzle Analysis Output
(Marion Carroll, XU)

Subfamily Diagnostic Mutations

```
                                                  7                              5
AluY Consensus   GGCCGGGCGCGGTGGCTCACGCCTGTAATCCCAGCACTTTGGGAGGCCGAGGCGGGCGG
  (6)AluYj5C     ..........................................................
(11)AluYj6C      ...............................................A.........
(49)AluYj7       ..............................T................A.........
                                                  4                               3

                                       2                              1
AluY Cons        AGAGGTCAGGAGATCGAGACCATCCTGGCTAACACGGTGAAACCCCGTCTCTACTAAAAA
AluYj5C          .......................T..........................T.............
AluYj6C          .......................T..........................T.............
AluYj7           .......................T..........................T.............
                                        2                              1

                                 3
AluY Cons        TACAAAAAATTAGCCGGGCGTGGTGGCGGGCGCCTGTAGTCCCAGCTACTCGGGAGGCTT
AluYj5C          ...........................T......................................
AluYj6C          ...........................T......................................
AluYj7           ...........................T......................................
                                  6

AluY Cons        GAGGCAGGAGAATGGCGTGAACCCGGGAGGCGGAGCTTGCAGTGAGCCGAGATCGCGCCA
AluYj5C          ..............................................................
AluYj6C          ..............................................................
AluYj7           ..............................................................

                          4                6
AluY Cons        CTGCACTCCAGCCTGGGCGACAGAGCGAGACTCCGTCTC
AluYj5C          ............A...............C....................
AluYj6C          ............A...............C....................
AluYj7           ............A...............C....................
                           5                7
```

Experimental Verification
(Marion Carroll, XU)

Chimp Alu Polymorphic Display



Microfabrication Infrastructure
(Pin-Chuan Chen, LSU)

ming Patterns
$^{-8}$m => 10^{-1}m

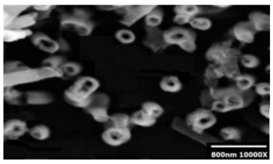
ray lithography

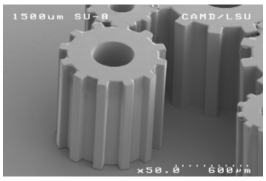
licro-milling

UV lithography

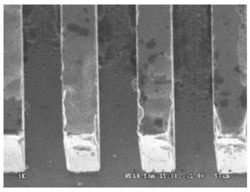
Excimer laser

Obducat
nano-imprinting

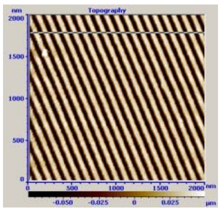




Filling Patterns (Metals)
10^{-8}m => 10^{-1}m



Replicating Patterns
10^{-8}m => 10^{-1}m

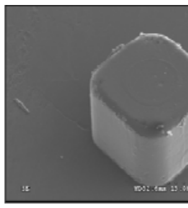


50 nm grating

Jenoptik HEX 02

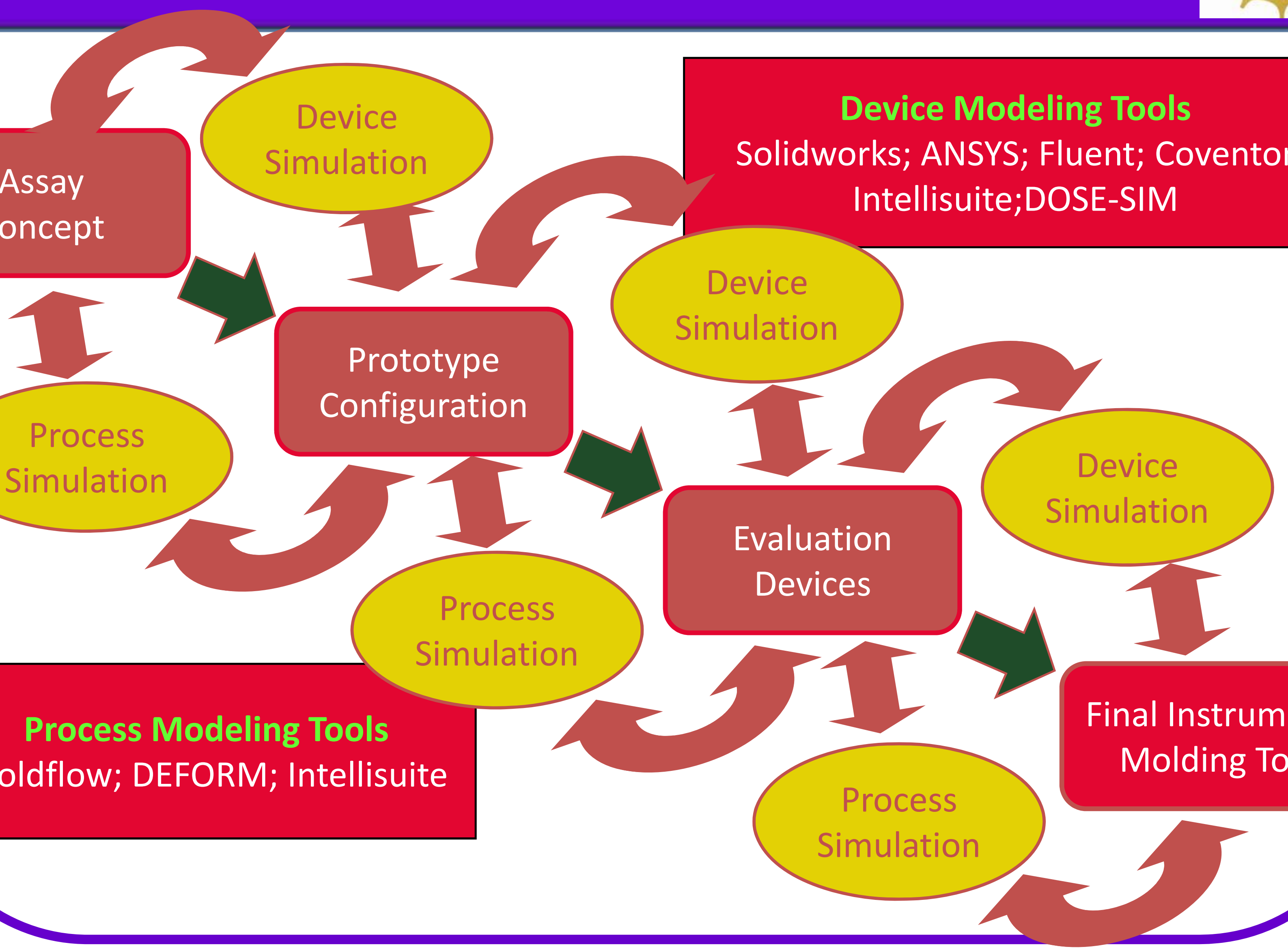
Battenfeld injection moldir

Double-sided
hot embossing



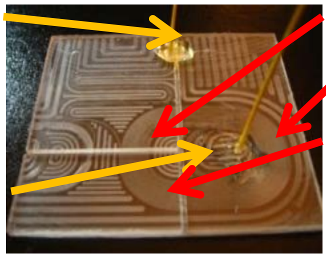
Injection m
cube

Design and Realization
(Pin-Chuan Chen, LSU)



In-Plane Thermal Management (Pin-Chuan Chen, LSU)

Original CFPCR (3 cm X 4 cm)

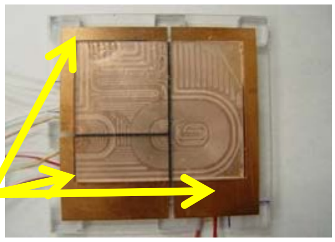


Denaturation (95°C)

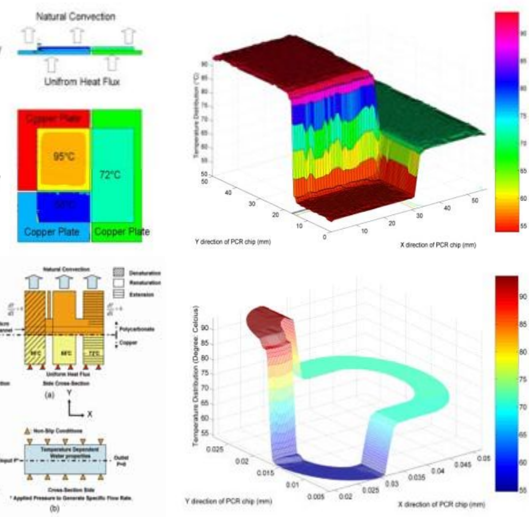
Extension (72°C)

Renaturation (55°C)

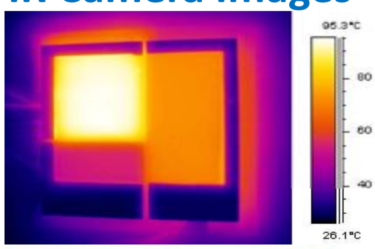
Copper Plates

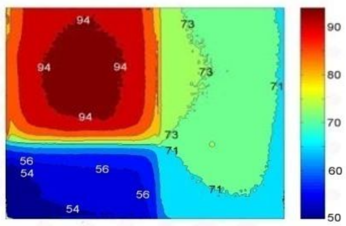


Finite Element Analysis

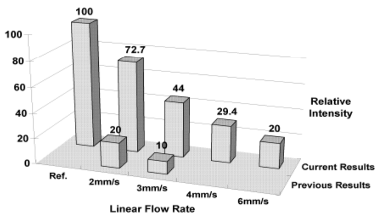


IR Camera Images

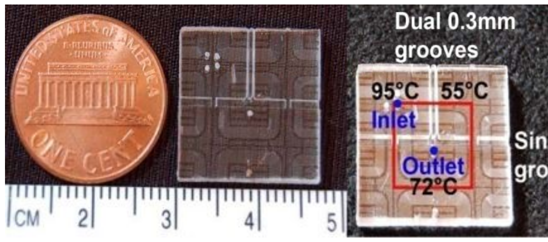




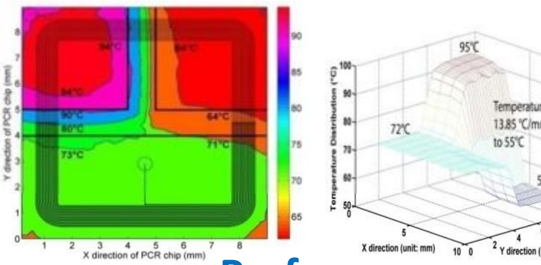
Improved Performance



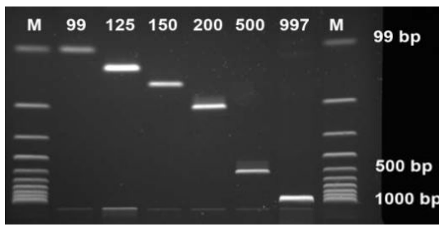
Small Area CFPCR (9 mm X 9

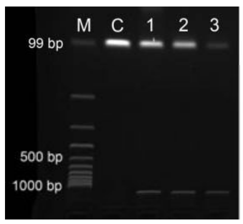


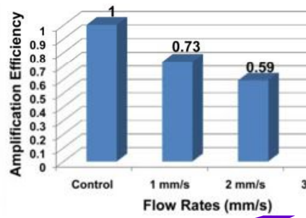
Finite Element Analys



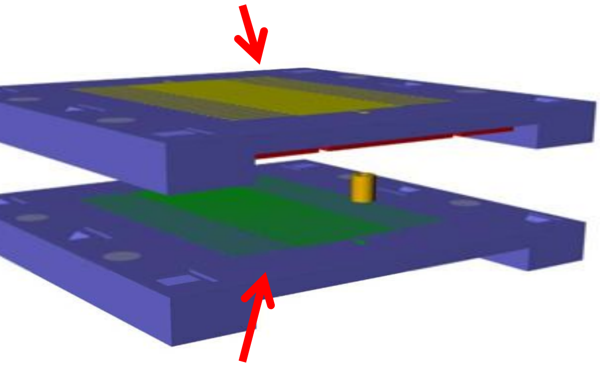
Performance

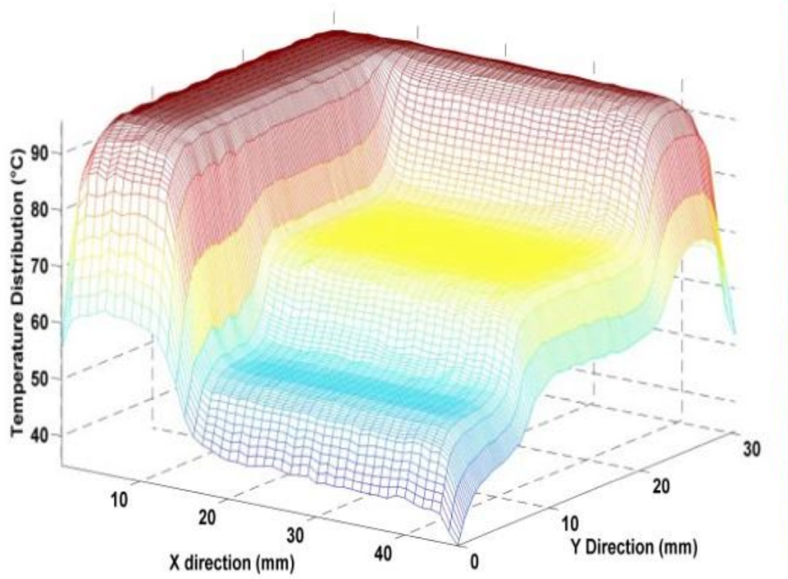


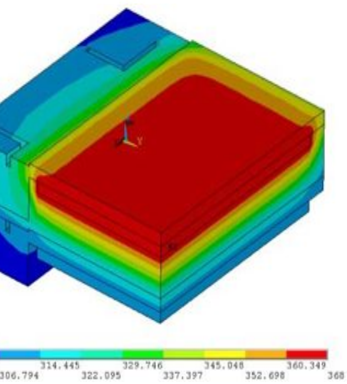


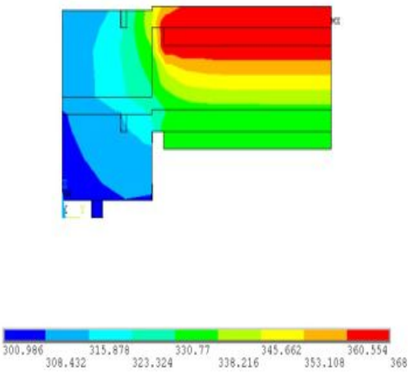


Stacked Thermal Management
(Pin-Chuan Chen, LSU)

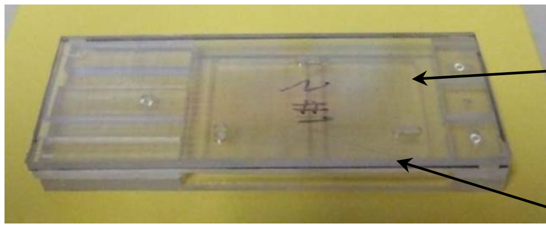


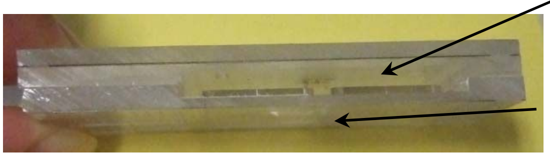




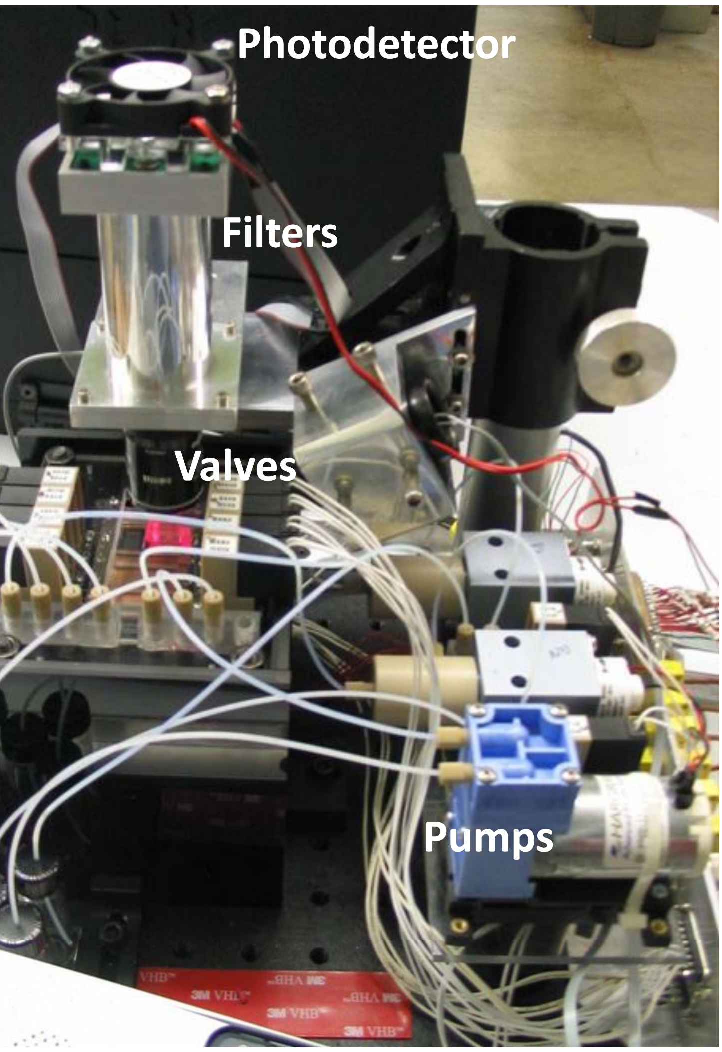


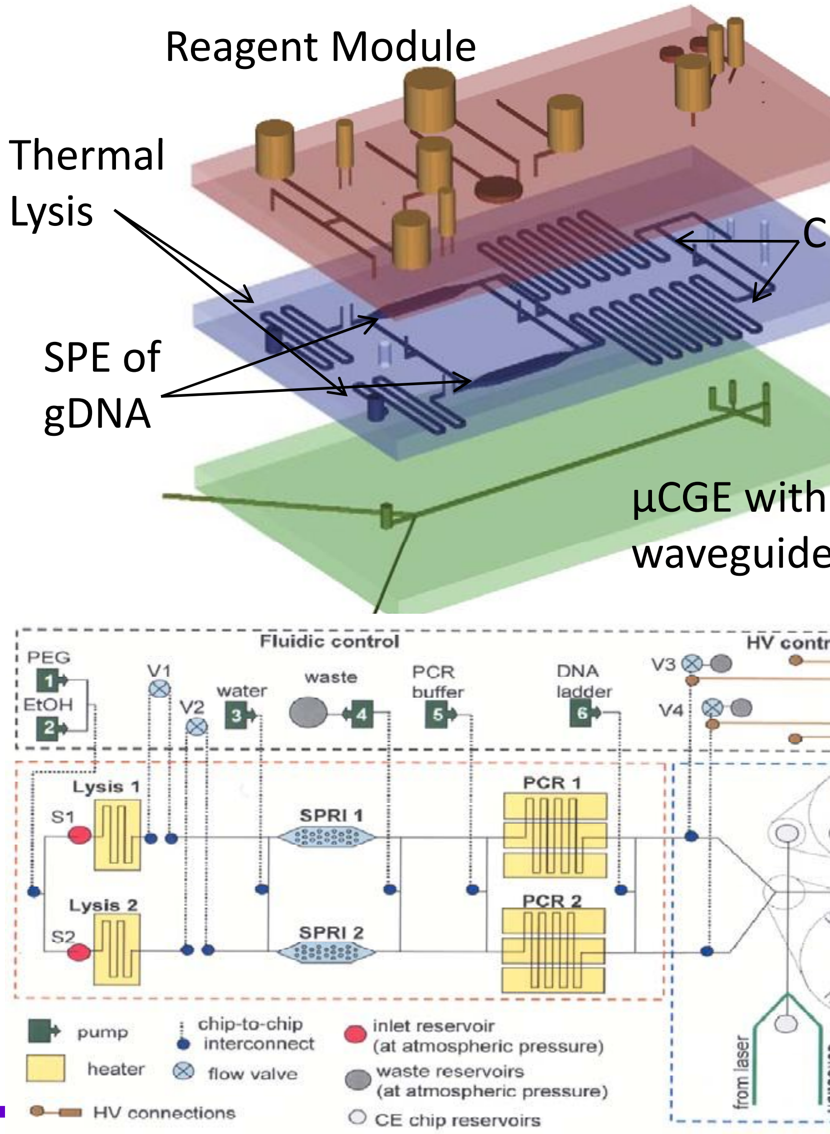
Finite Element Analysis to Understand Heat Transfer From Layer to Layer



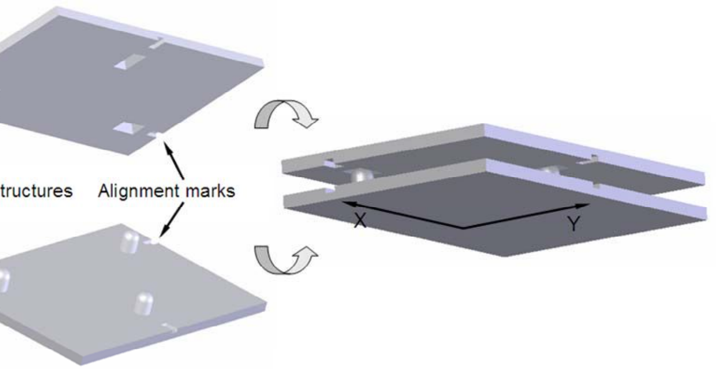


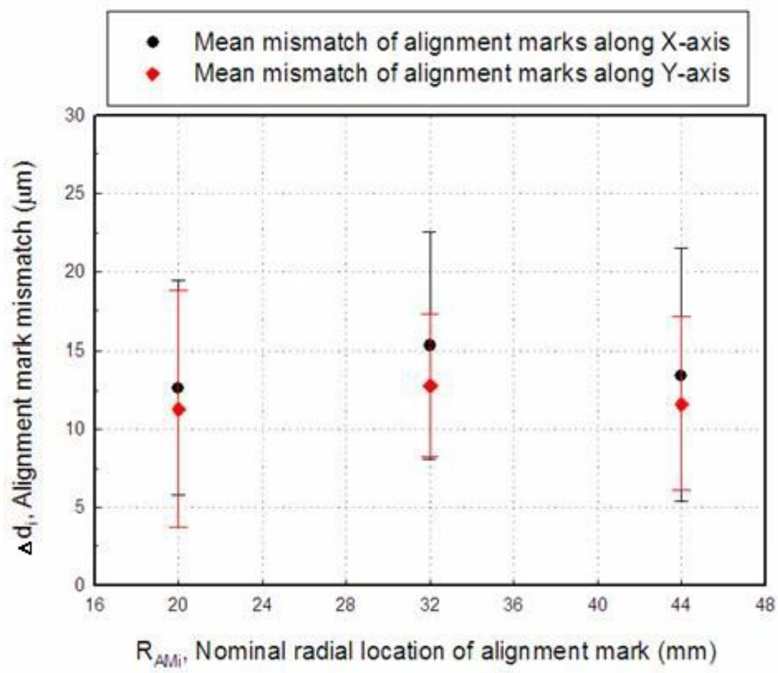
enosensor for Human Indentification
(Jason Emory, LSU)

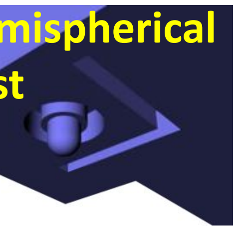


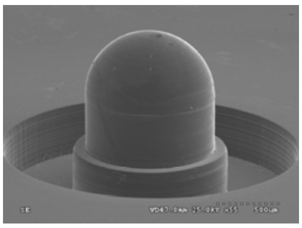


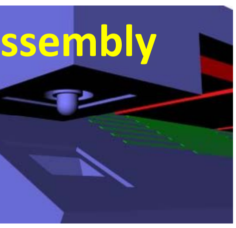
Passive Alignment Structures
(Jason Emory, LSU)

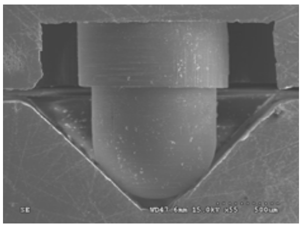


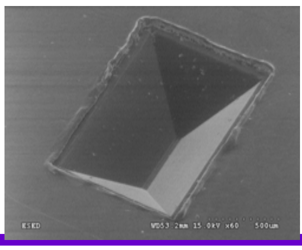






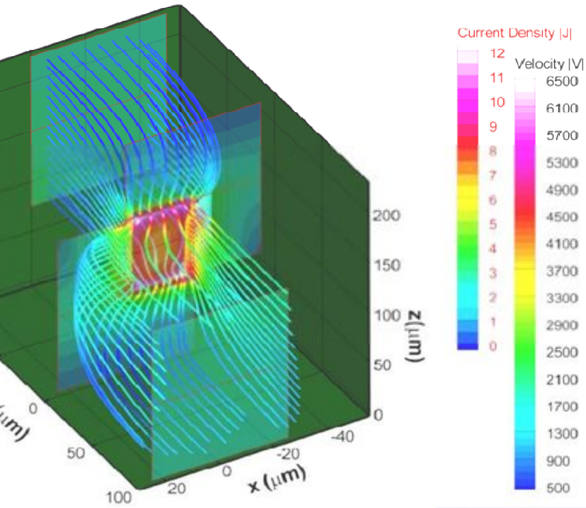


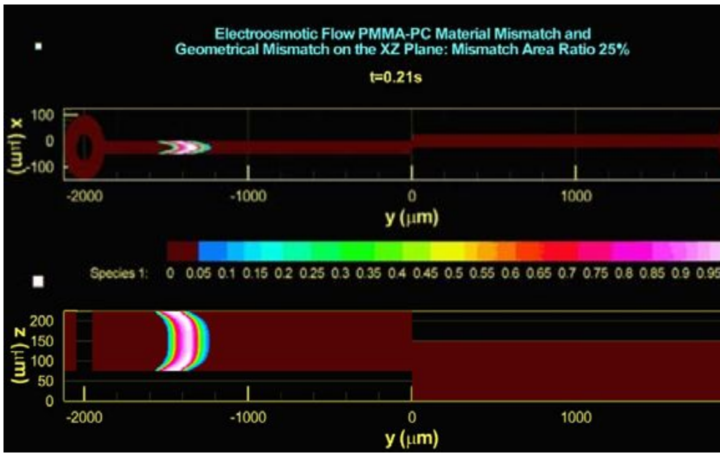




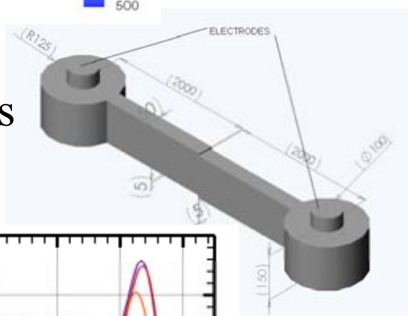
- **Mean lateral offset in X- and Y-axes 10-15 μms**
- **Not location dependent**
- **Nominal post height 925 μms**
- **Mean hot embossed post height 922 ± 2 μms**
- **Standard deviation < 6 μms**

Interconnects for Fluid Transfer between Modules (Jason Emory, LSU)

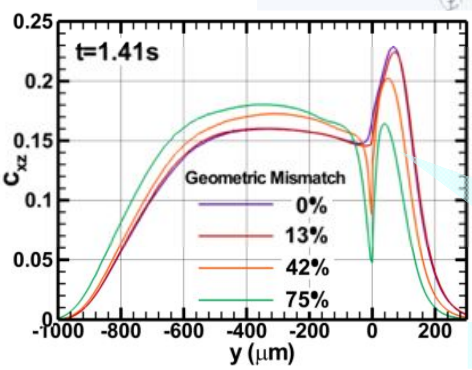


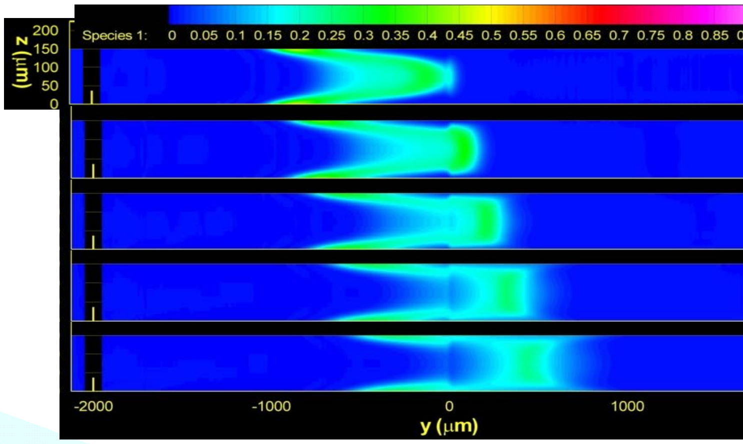


Q=7.03nL/s



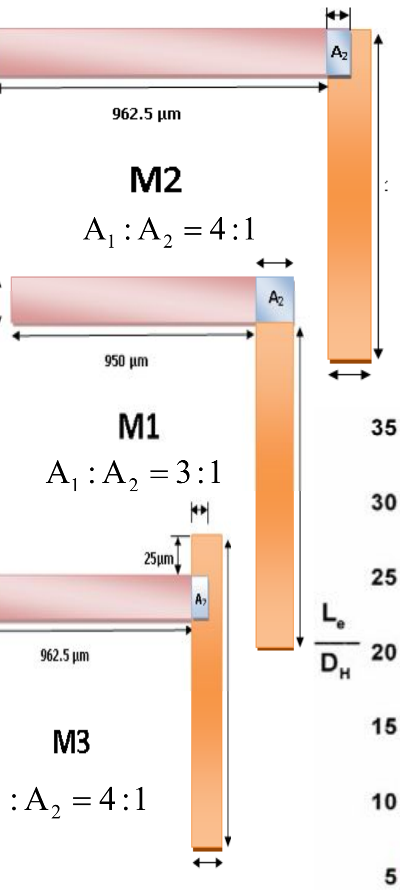
effect for
s
metrical
match



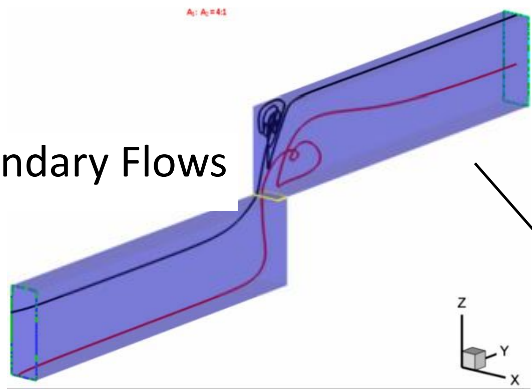


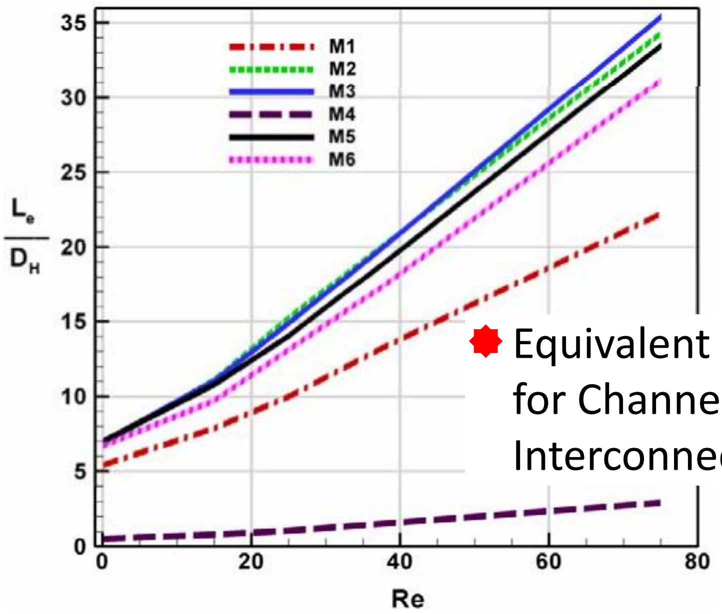
Plug re-concentration after PMMA-PC material mismatch

Interconnects: Channel Overlap Configuration (Jason Emory, LSU)

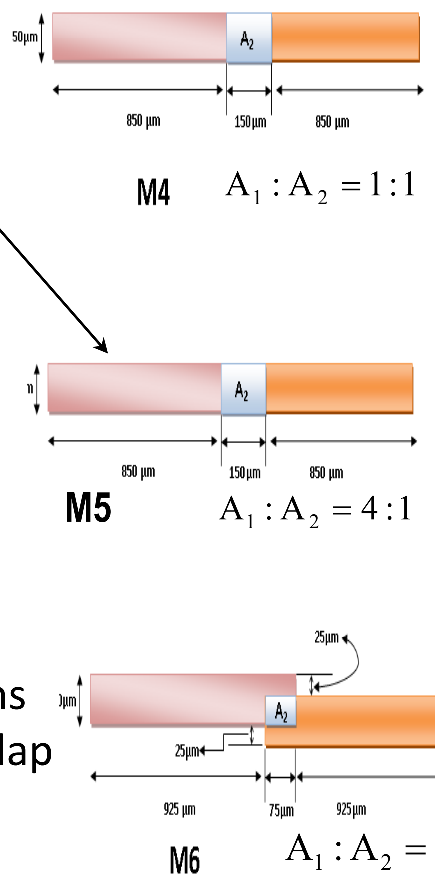


- Secondary Flows



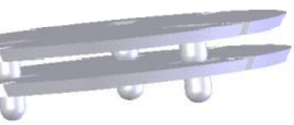


- Equivalent Lengths for Channel-Overlap Interconnects

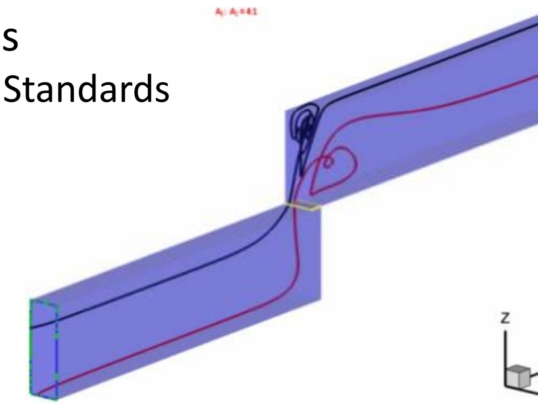


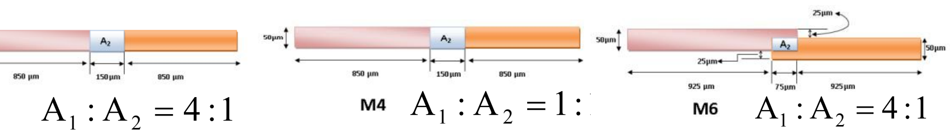
Poster
S. Rani

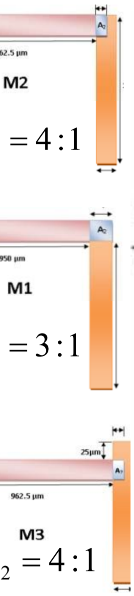
Design Knowledge Base & Rules Through Simulation (Dimitris Nikitopoulos, LSU)

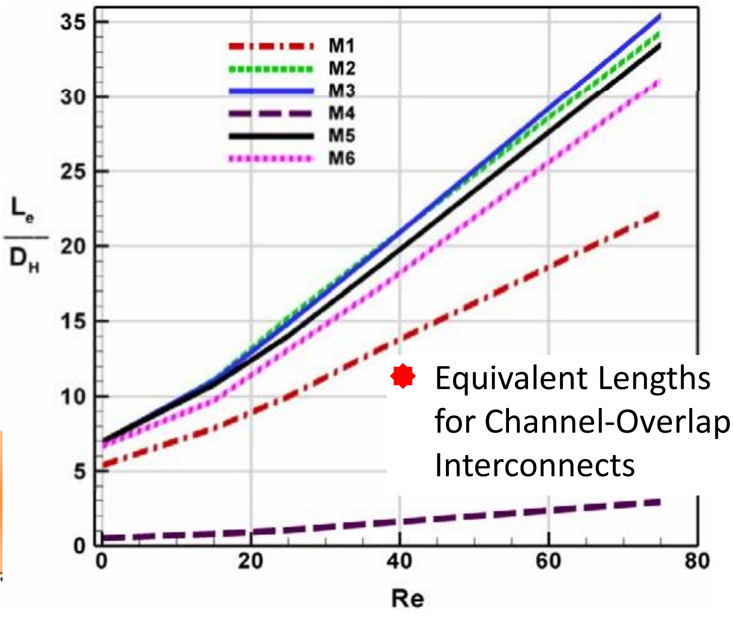


- Pressure Loss Through Interconnects
  - Determined according to ANSI/ASME Standards
  - Equivalent length dependence on
    - Reynolds number
    - Interconnect Configuration









- Equivalent Lengths for Channel-Overlap Interconnects

- HPC Utilization and Benefit
  - Migrate commercial codes on Queenbee (WP4)
  - Parametric study parallelization (W
  - Interactive Post-processing and Dat Management
  - *Full-system simulation* when component-by-component approac fails (e.g. processes involving heat a mass transfer)

Posters
. Kim (Exp.)
. D. Walker (Sim.)

Understanding Multi-phase Micro-Fluidics (Dimitris Nikitopoulos)

de adapted to handle wall-interface interaction and break-
/coalescence

rallelization – Code (Walker; WP4 - Tyagi) – Run (WP1)

vanced interactive visualization tools (WP3 - Ullmer)

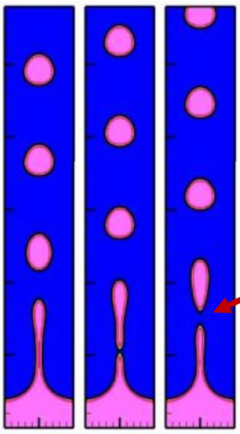
provement of Accuracy/Performance

Multi-Grid algorithm for elliptic eqns. with discontinuous coefficients (Walker; WP4 – Aksyolu, Tyagi)

ndle complex Cartesian geometries (Walker; WP4 - Tyagi)

mputational Steering (WP1, WP3, WP4)

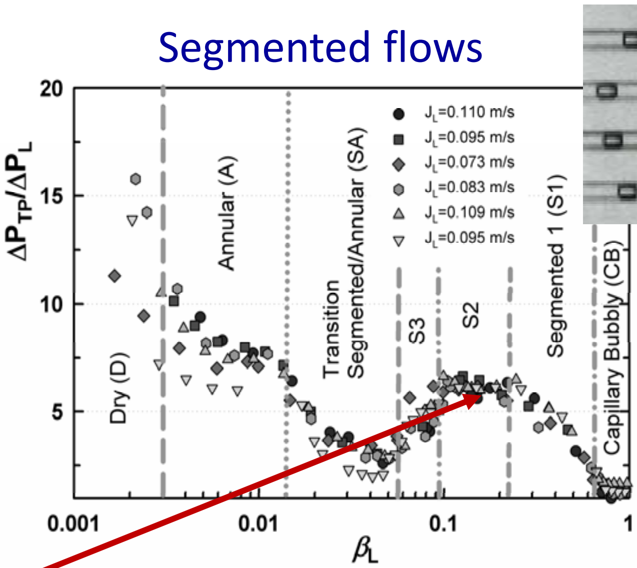
njection

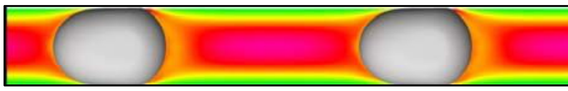


Scientific Challenges

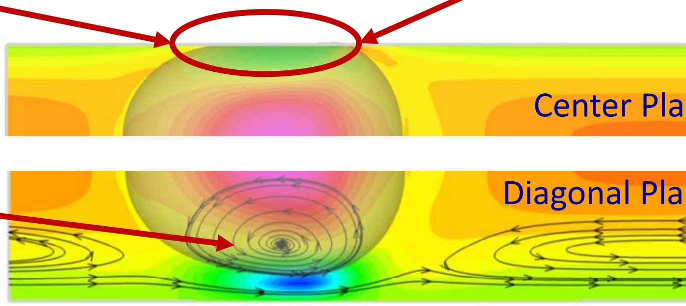
- Pressure drop prediction
- Understand and model the physics
  - Interface/wall interaction
    thin films - wettability
  - Break-up (injection)
  - Coalescence

Segmented flows





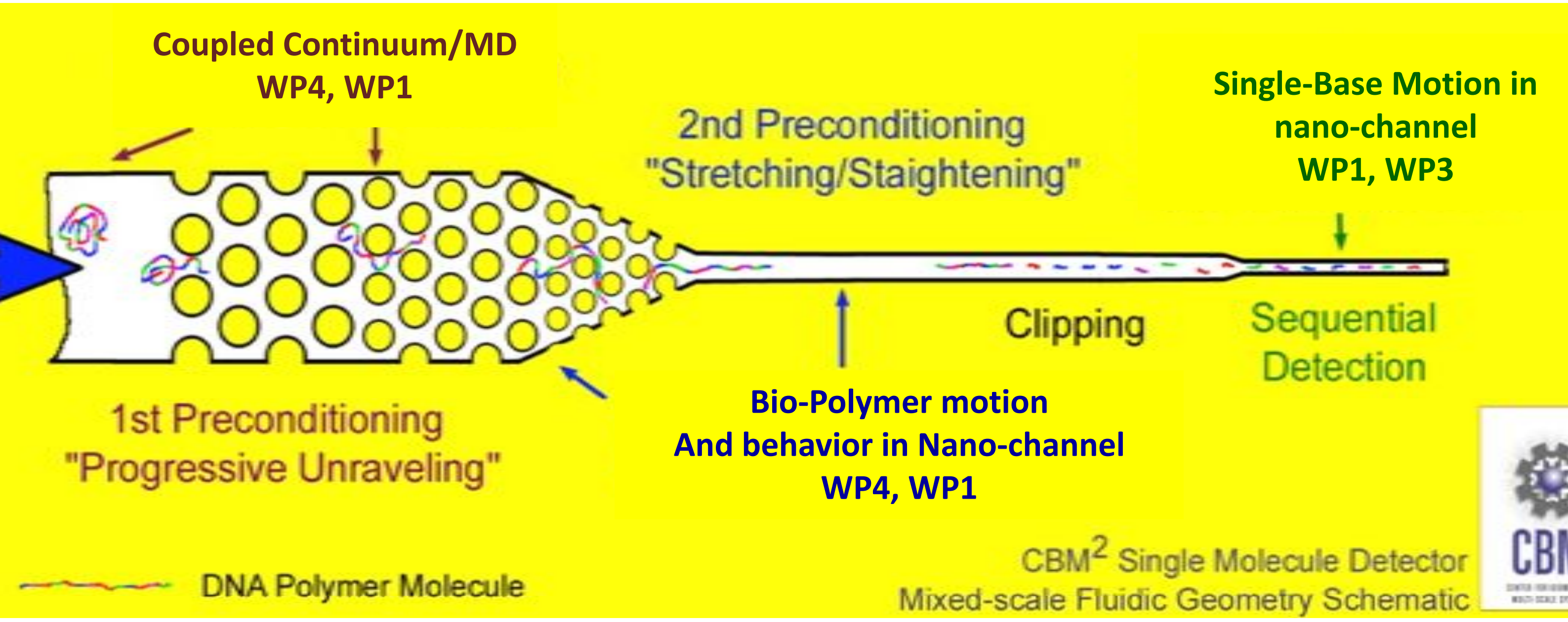
film break-down = contaminatior



secondary flows
aid mixing

Multi-scale Application Test-Bed Example (Dimitris Nikitopoulos)

- Single-Molecule Multi-Scale Sensor
  - 1st Preconditioning: Milli- micro- to nano-scales
  - 2nd Preconditioning & Bio-polymer length meas.: micro- to nano-scale
  - Nano-channel Small Molecule Sensor: nano-/molecular scales



Poster
. Dufaud

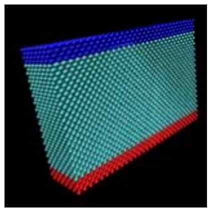
Multi-scale Coupled MD-Continuum Simulation Tool (Dimitris Nikitopoulos)

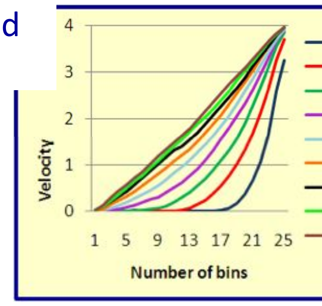
sic in-house MD code
- Developed, parallelized, Tested (Couette, Poiseuille)
- Documentation of the code for delivery to WP4
- Migration to CACTUS (New Student, WP4-Tyagi, Schnetter, Kim)

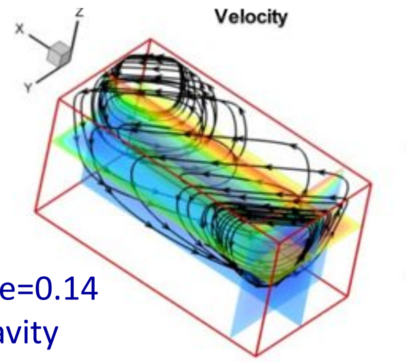
ntinuum 3D N-S Parallel Code (Velocity/Vorticity)
- Developed, parallelized (T.-Dervout*, Dufaud)
- Tested on 3D driven cavity test problems (Dufaud)
- Documentation of the code for delivery to WP4 (Dufaud)
- Migration to CACTUS (New Student, WP4-Tyagi, Schnetter)

ntinuum-MD Coupling
- Parallelization issues (Dufaud, New Student; WP4-Tyagi)
- MD-Continuum code coupling using constrained dynamics under CACTUS (New Student; WP4-Tyagi, Schnetter, Kim; WP1)

Test Results: Impulsively Started Couette Flow

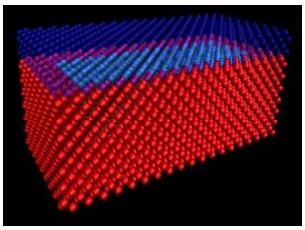




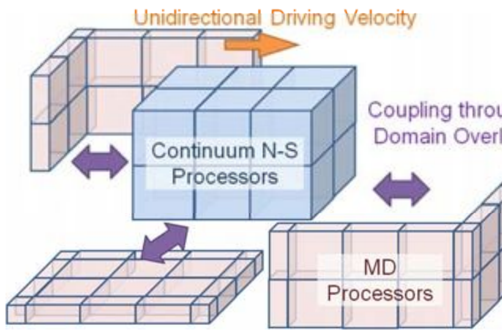


Test Results: Re=0.14 xy-driven cavity

MD Domain Layout for Driven- Cavity Test Problem

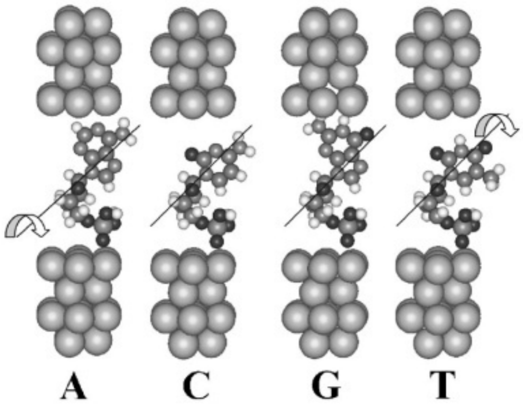


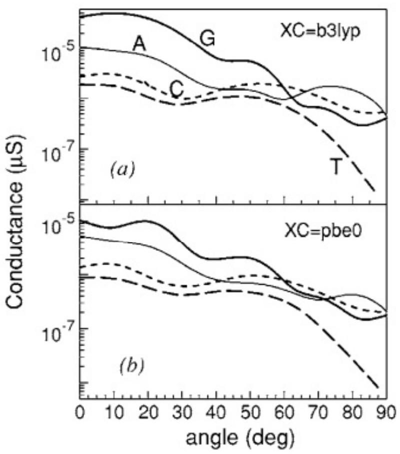
Problem Distribution Schematic for Coupled MD-Continuum Driven-Cavity Test Problem



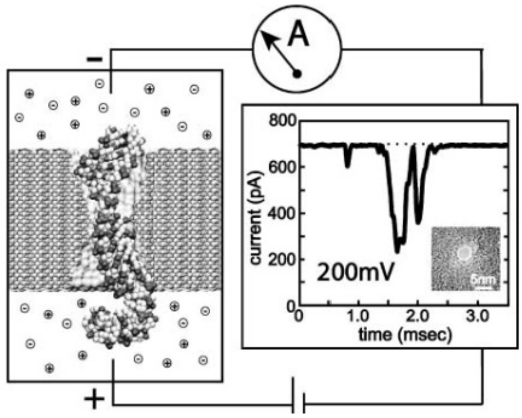
omistic Simulation of Biopolymer Transport
rough Nano-Domains (Dorel Moldovan, LSU)

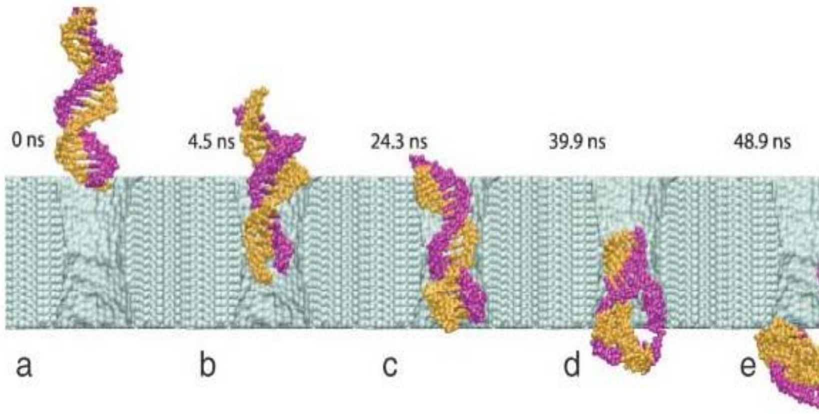
Motivation





R. Zikic et al. , Characterization of the tunneling conductance across DNA bases, Phys. Rev E 74, 011919 (2006)





A. Aksimentiev et al., et al. , Microscopic kinetics of DNA translocation through synthetic nanopores, Biophys. J. 87 (200 2086

tomistic Study of Biopolymer Transport ough Nano-channels (Dorel Moldovan, LSU)

Methodology and Simulation System

- MD simulations were performed with the software package LAMMPS

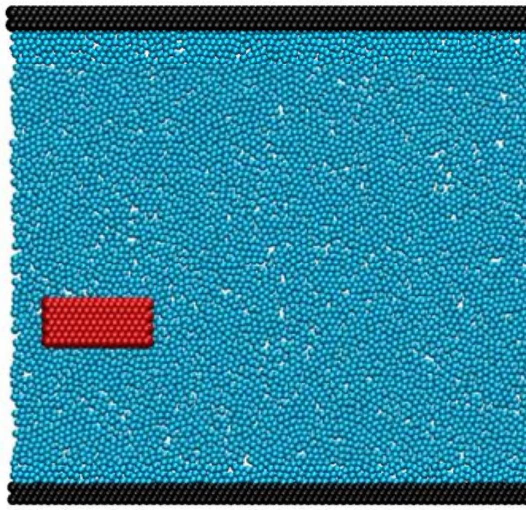
- The interactions between any pair of atoms are described by the Lennar-Jones potential.

- The two-dimensional system consists of ~6000 atoms and the nolecule has an elongated shape of aspect ratio 2.6

- The simulations were conducted and analyzed in reduced units. The distances are expressed in units of σ, the energy in ε, the emperature in ε/k_B, the time in, $1/\sqrt{\varepsilon/m\sigma^2}$ the force in ε/σ, the lensity $1/\sigma^2$, etc.

- The simulations were carried out at temperature $k_B T/\varepsilon = 1.2$ nd density $\rho/\sigma^2 = 0.81$.

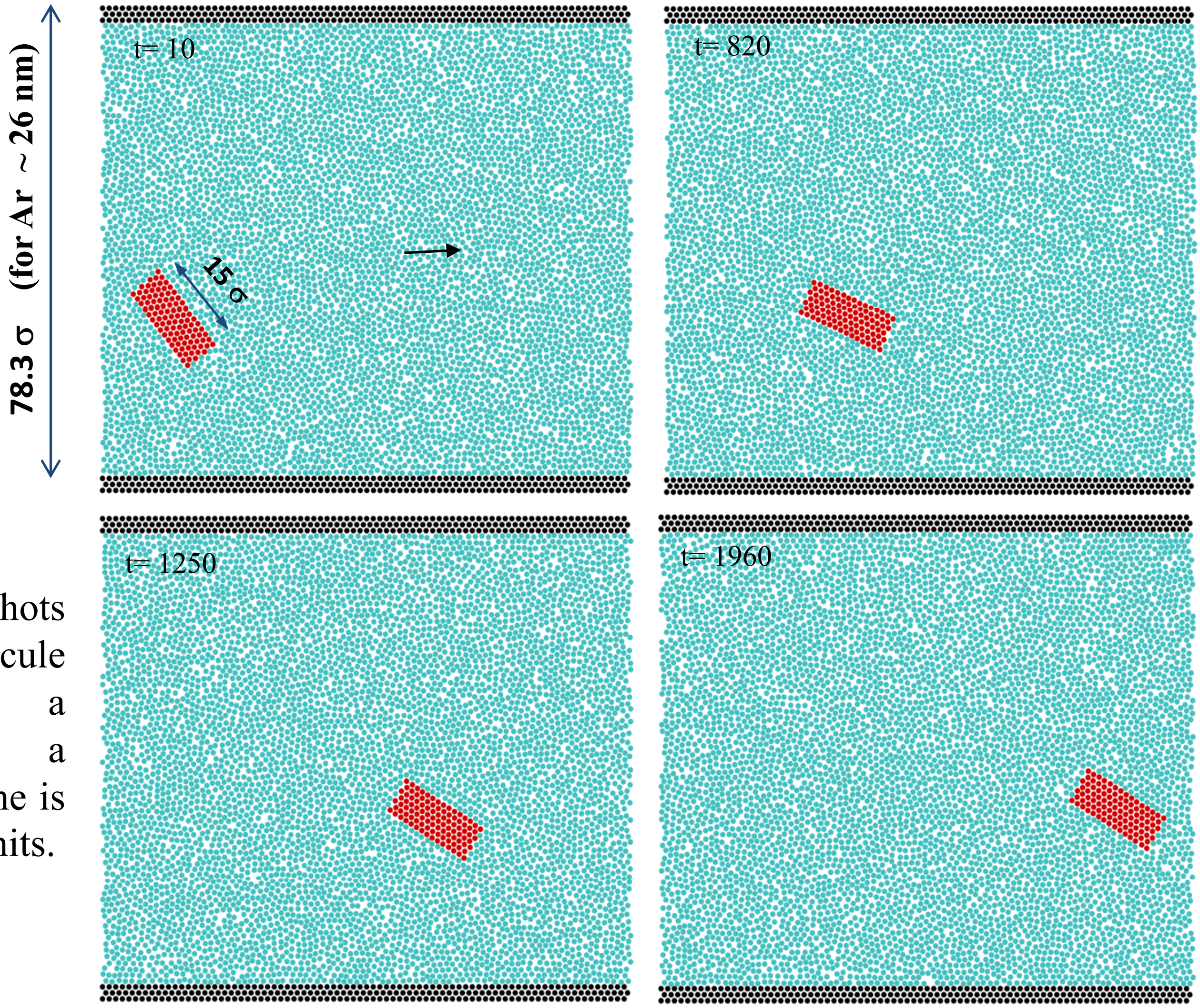
- The Poiseuille flow was induced by introducing a "gravity" orce that is applied parallel to the channel axis to each atom of he liquid and molecule.



$$V_{LJ}(r_{ij}) = 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]$$

For Ar: σ = 3.4 Å, ε/k_B = 120K, m=40 a.u.
accordingly the natural time unit is = 2.16 p

MD Simulation Results

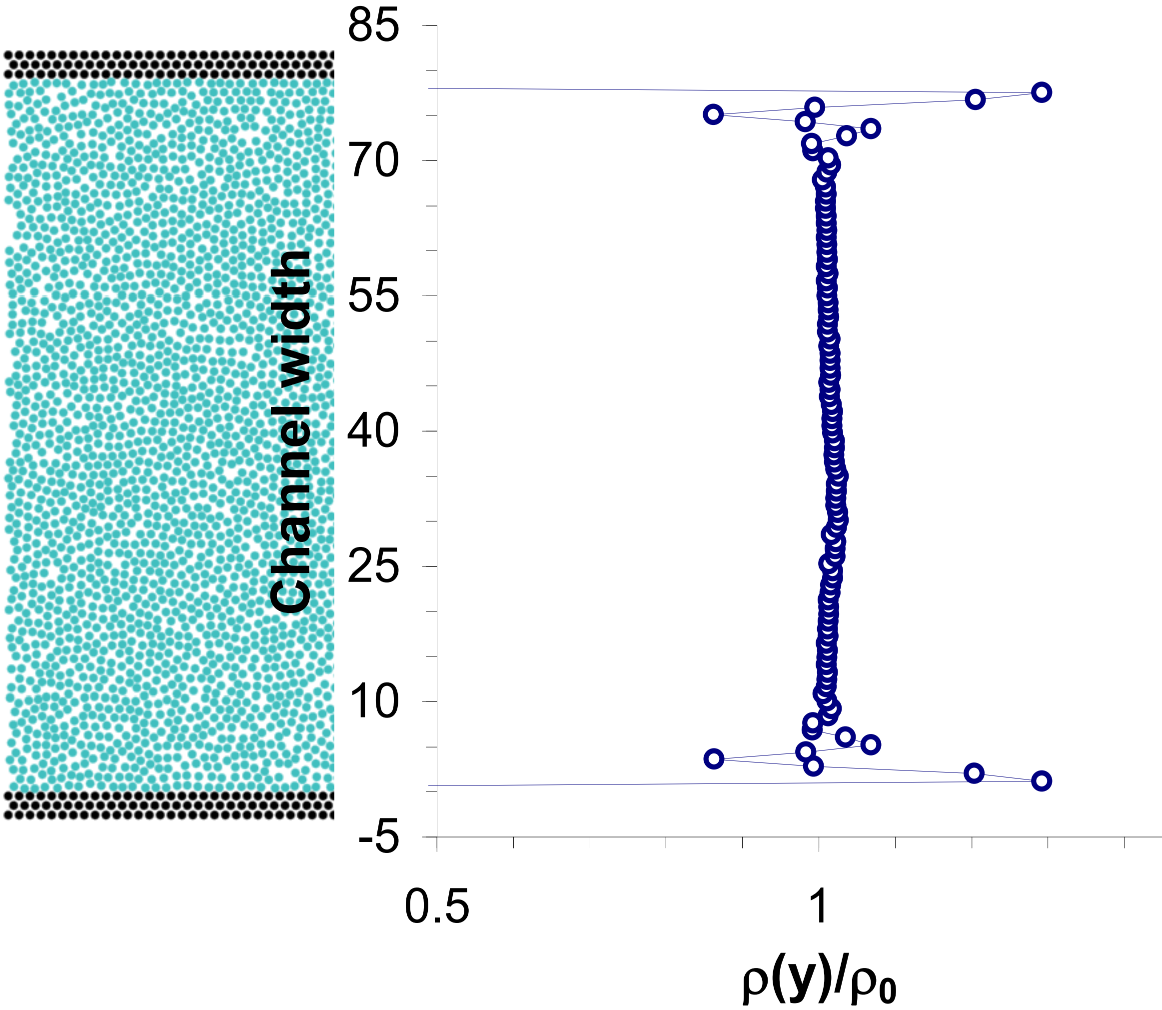


ulation snapshots the molecule ving in a ochannel in a seulle flow. Time is en in reduced units.

Atomic Layering Close to Walls (Dorel Moldovan, LSU)

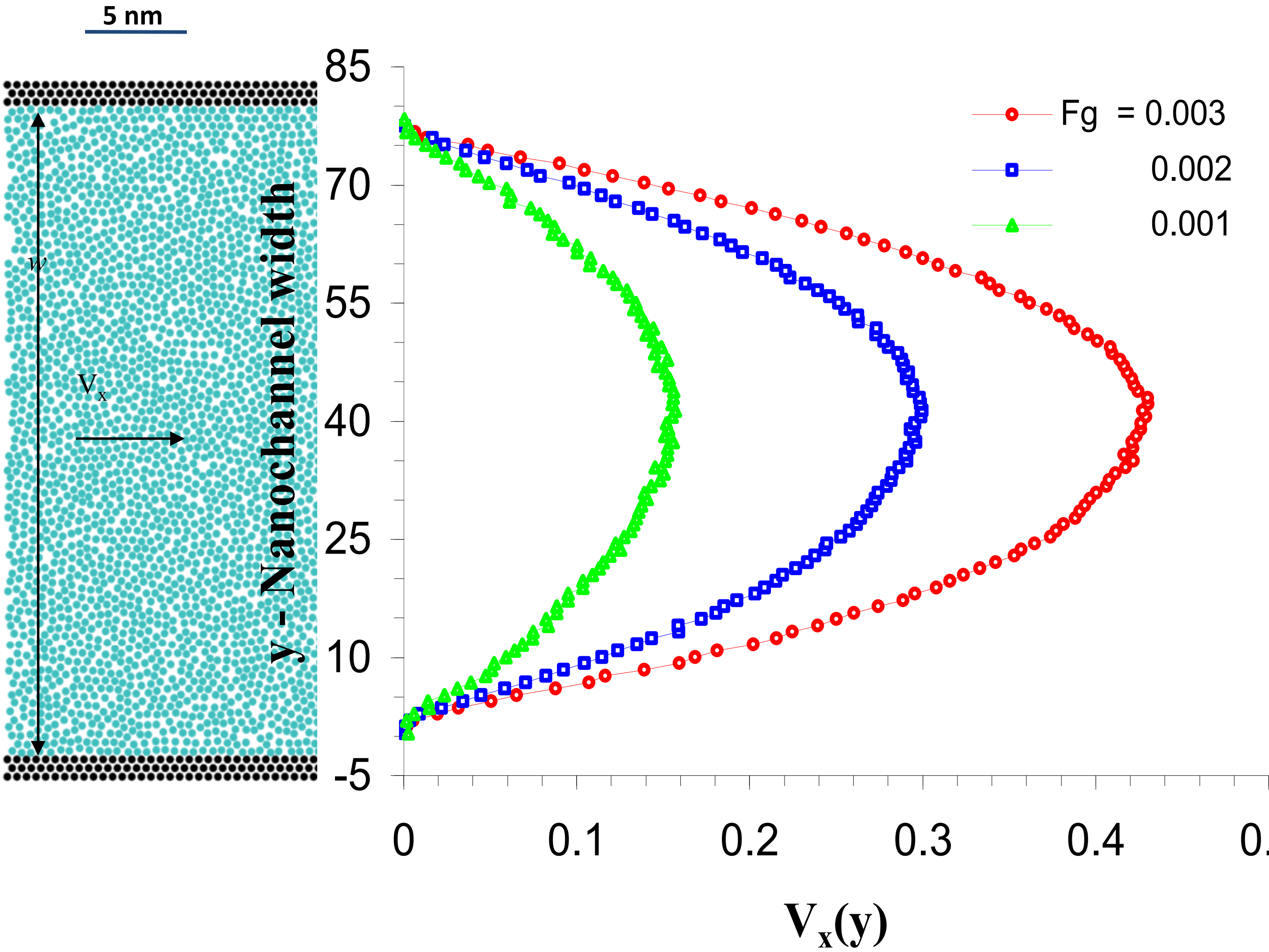
5 nm

ormalized atomic ensity in the liquid hase across the width f the nanochannel. The quid bulk atomic ensity is $\rho_0 = 0.81$.

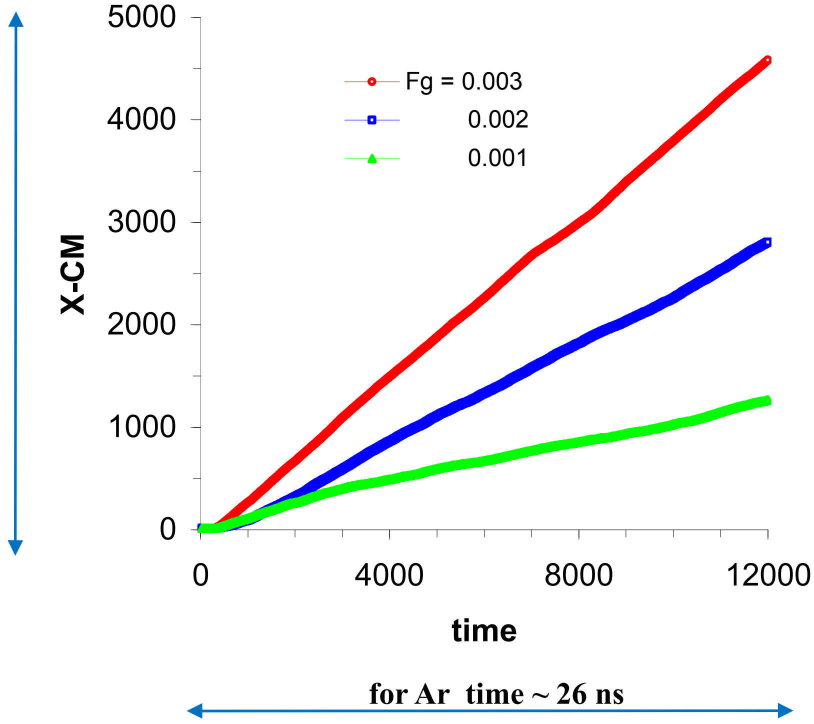


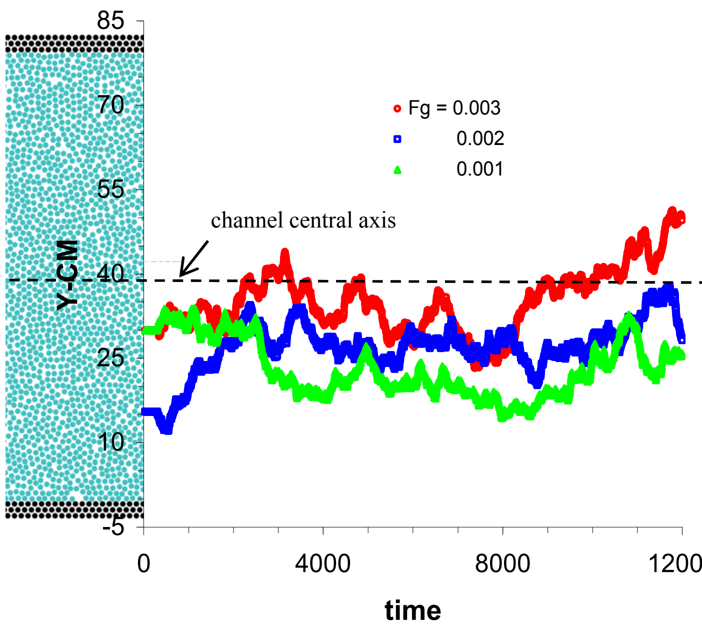
Transverse Velocity Profile (Dorel Moldovan, LSU)

…ty profiles …ed from MD …ations of …uille flow. … result are … for three … of the …onal constant F_g=0.003, …002, and …001, applied …ach "liquid" … to generate …ow.



Time Evolution of Molecular CM during Translocation (Dorel Moldovan, LSU)





Variation of the x-component of the position of the molecule center of mass vs time for three flow regimes controlled by gravity forces: F_g=0.003, F_g=0.002 and F_g=0.001

Variation of the y-component of the position of the molecule center of mass vs time for three flow regimes controlled by gravity forces: F_g=0.003, F_g=0.002 and F_g=0.001

Education and Outreach: Professional Development Seminars for GS, PDF

CBM² Seminar Series

"Using LSU's High-Performance-Computers to Simulate Merging Stars"

by **Prof. Joel E. Tohline**

Department of Physics and Astronomy and Coast to Cosmos (C2C) Focus Area Lead
at Center for Computation and Technology (CCT)
Louisiana State University

Astronomers understand that the internal structure of individual stars, like our Sun, as well as the interactions between pairs of stars that orbit one another in so-called "binary star systems" is governed by essentially the same set of mathematical equations that govern fluid flows here on Earth. However, generally speaking, very large and very fast computers are required to solve this complex set of equations, especially in the case of strongly interacting binary systems. We are using high-performance-computers (HPCs) at LSU and across LONI (Louisiana Optical Network Initiative) to study the evolution of binary stars whose interactions are so strong that they eventually collide and merge. Such violent events in nature are thought to give rise to certain types of supernovae or even more energetic phenomena referred to as gamma-ray bursts (GRBs). Research by various groups within LSU's Center for Computation and Technology (CCT) has aided us in our pursuit of this challenging astrophysics goal, and is guiding our plans to effectively use future generations of HPC hardware.

Wednesday, June 25, 2008
Presentation at 4:00 pm
Life Sciences Annex A101
followed by refreshments at 5 pm

For more info contact: Dr. Maggie A. Witek mwitek@lsu.edu

CBM² Seminar Series

Scientific and Professional Writing

by **prof. Malcolm Richardson**

Dr. J.F. Taylor Professor of English
Department of English
Louisiana State University

Methods to create good scientific writing are not complex or mysterious but require certain kinds of preparation which are typically not taught during English writing courses either in the U.S. or abroad. These methods, which should be fully understood before the first word is written, include first an understanding of basic rhetorical principles of audience analysis and second an understanding of both the purpose of the entire scientific document and of its different parts (introductions, results, discussion, etc.). This presentation will focus on writing theses, dissertations, and academic articles, and will suggest practical ways to be a more efficient writer by planning ahead.

Monday, October 16 th 2006
Refreshments at 4:30 pm
Presentation at 5:00 pm
Life Sciences Annex A101

Contact: Dr. Maggie Witek mwitek@lsu.edu

Other E&O Activities

Science Adventure Camps (Audubon Girl Scouts) –

Goal: increase interest in science/engineering in females; one-week summer camps with experiments in chemistry, biology, environmental engineering, mechanical engineering, biological engineering.

Project Science (Cain Center, LA Dept. Education) –

Goal: provide linkages to university and community resources to build synergistic relationships among scientists and educators.

You Be the Chemist Challenge (Exxon)

Goal: Provide middle school students the opportunity to be exposed to rigorous chemistry concepts and gain experience in participating in academic exercises.

Other E&O Activities

Science and Engineering Day @ LSU (08/01/08)

- Formal presentations and panel discussions on biological/medical technology needs; computational capabilities in microfluidics design; poster session

High School/Undergraduate Research Experiences

- *Ginger Granville* – Louisiana Arts and Science Academy High School, Microchip separation of *Alu* elements
- *Jenny Hsu* – Princeton University, Novel Near-IR Fluorescent Dyes for Drug Discovery

Numerous Graduate Student Presentations at National/International Meetings

2007

2008

- Pin-Chuan Chen; Paul Okagbare; Jason Emory; Samuel Njorge; Matt Hupert (µTAS)

Publications (10 faculty - 4 CHEM; 3 BS; 3 ME)

- Team faculty members and their students published 68 papers in 07/08

Other Activities (Patents and Entrepreneurship, Center Grants)

- **Statistics for Technology Transfer** – 10 disclosures and 4 Provisional Patents were filed in 2007/2008
- BioFluidica Microtechnologies, LLC – Commercial venue for new technologies emanating from CBM^2 (won two business plan competitions; CEO – Yohannes Desta, Ph.D. with Prof. Michael Murphy) – Development of point-of-use systems for human identification
- **CBM^2 submitted an ERC application in 2007** – of ~155 pre-proposals submitted, CBM^2 was selected at one of 34 for full proposal submission; was not selected for site-visit
- **CBM^2 submitting STC in 2008**