

From Molecules to Computers

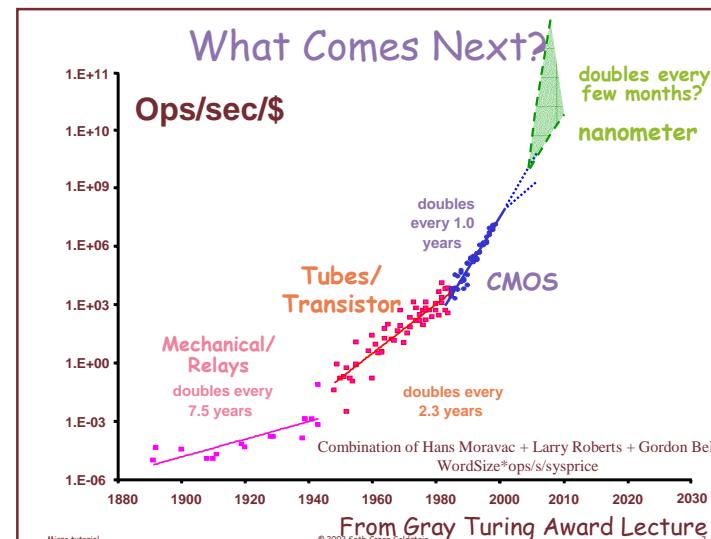
Seth Copen Goldstein
Carnegie Mellon University

Istanbul, Turkey
November 19, 2002

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Technology Shifts

- Size of Devices
⇒ Inches to Microns to **Nanometers**
- Type of Interconnect
⇒ Rods to Lithowires to **Nanowires**
- Method of Fabrication
⇒ Hammers to Light to **Self-Assembly**
- Largest Sustainable System
⇒ 10^1 to 10^8 to 10^{12}
- Reliability
⇒ Bad to Excellent to **Unknown**

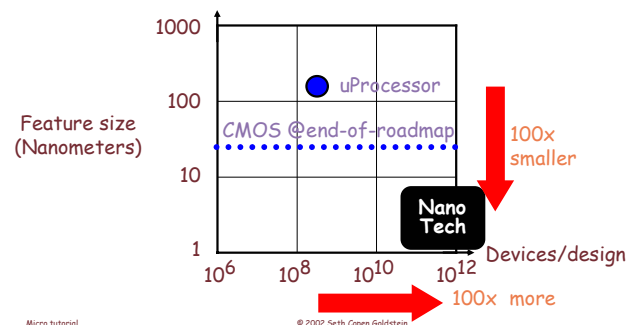
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On the cusp of Major Technology Change

- Devices will be *very* small & numerous
- Scale is new: **100x smaller**, **100x more**



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Outline

- The current path
- Molecular Electronic Devices
- Fabrication
- Implications
- Circuits
- Architectures
- Compilation
- Defect Tolerance

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Current Approach

- Today's Approach
 - CMOS
 - Photolithography (Top-down manufacturing)
 - ITRS "roadmap"
- Requires every increasing investment of
 - Time
 - Power
 - Money

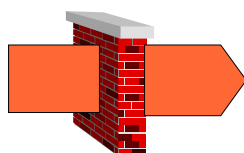
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Customer Relationship Management	57	58	59	58	59	60	61	62	63
Netzeitung/Onlinezeitung	0	0	2	2	2	2	2	2	2
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Online-Advertising (Pop-ups)	56	57	58	57	58	59	60	61	62
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Online-Advertising (Native Advertising)	56	57	58	57	58	59	60	61	62
Online-Advertising (Sponsored Content)	56	5							

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From ITRS Roadmap

Scaling Is Getting Harder

- For the first time, scaling appears to have reached fundamental limits in several areas.
- Current ITRS contains major barriers with no known solutions.
- Red Brick Wall is getting closer!
- Overcoming these barriers requires:



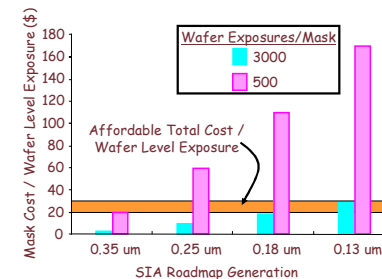
- **New** materials
- **New** types of devices
- **New** physical models
- **New** types of processing
- **New** design tools & methodology

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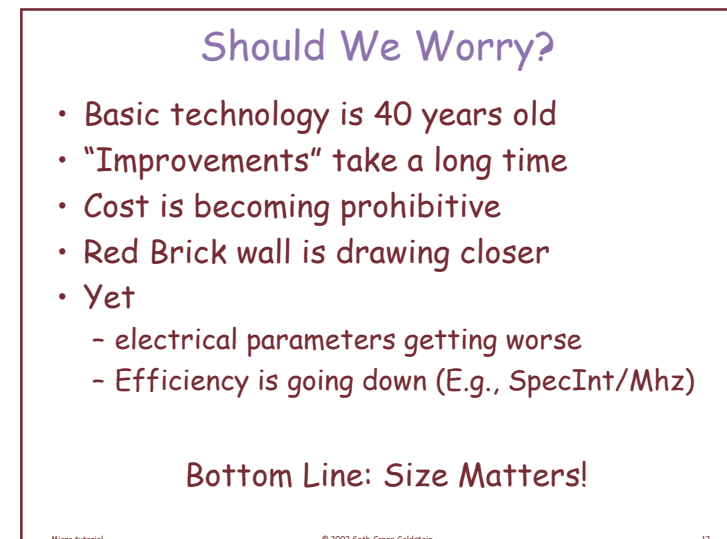
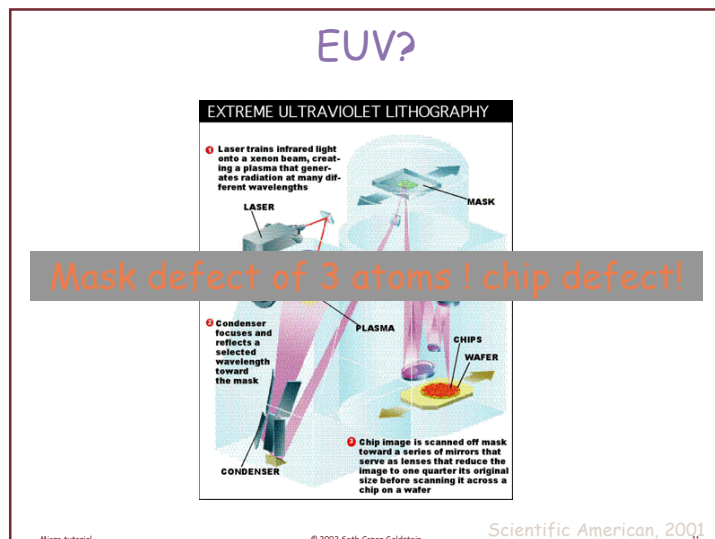
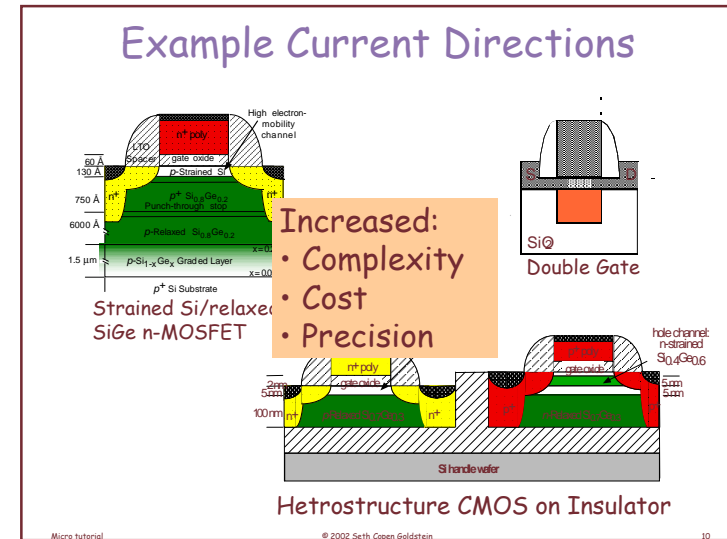
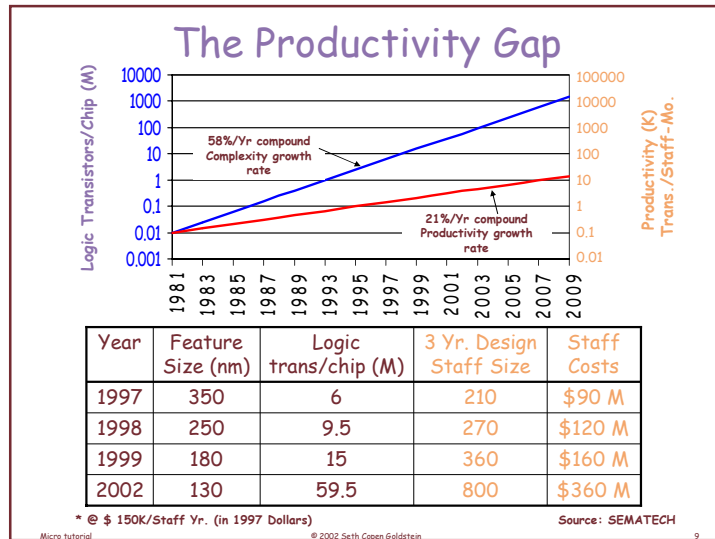
Cost Is a Driving Force

- Costs are increasing
 - Development
 - Fabrication plants
 - Wafers
 - Tools
 - Masks
 - Design



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Karen Brown, NIST



CMOS Too ...

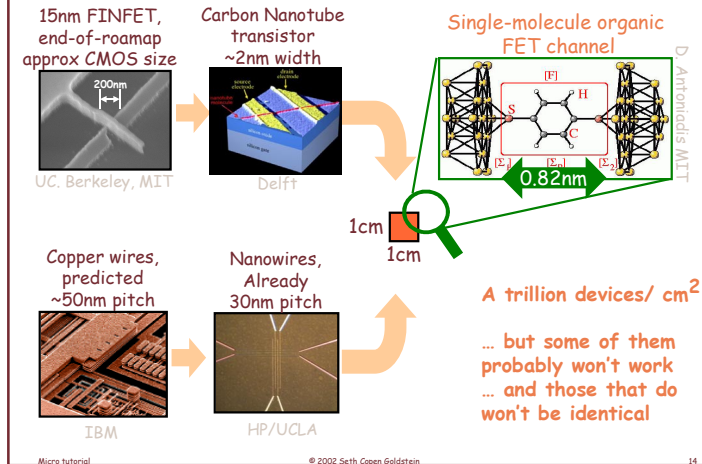
- Precision is expensive
- Current Abstractions have a major impact on cost
 - Requires process engineers to deliver robust devices
 - Requires perfect devices
- CMOS is becoming just another nanoscale component
- Process rules and mask costs are already eliminating arbitrary patterns

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Size Matters



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Consequences of Smallness

- Variability
 - 25 nm
 - 50 nm
 - IBM 1 dopant atom
- Single-event upsets
 - 0 0 1 1
- No Arbitrary Connections
 - CMOS MIT
 - Nano HP
- Solutions:
 - post-fabrication reconfiguration
 - Computation
 - redundancy

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Independent of Technology

- As we scale down
 - Devices become
 - more variable
 - more faulty (defects & faults)
 - numerous
 - Fabrication becomes
 - More expensive
 - More constrained
 - Design becomes
 - More complicated
 - More expensive
- Requires:
- Defect tolerant architectures
 - Higher level specification
 - Universal substrate

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Defect Tolerant Architectures

- Features:
 - Regular topology
 - Homogenous resources
 - Fine-grained?
 - Post-fabrication modification
- Example from today: DRAM
 - Requires external device for testing
 - Requires external device for repair
- Logic? **FPGA**

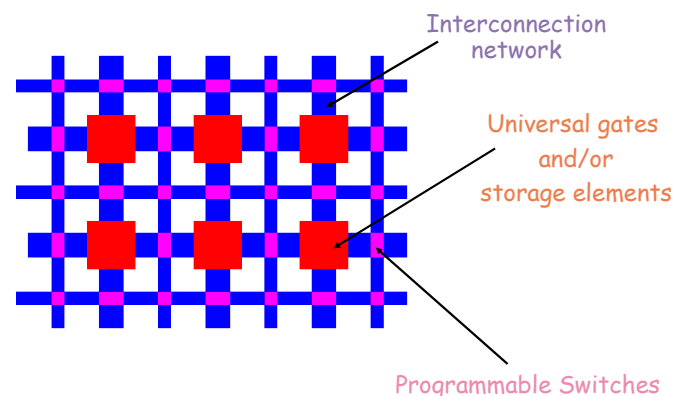
Key is redundancy

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Island-Style FPGA



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Dealing With Defects

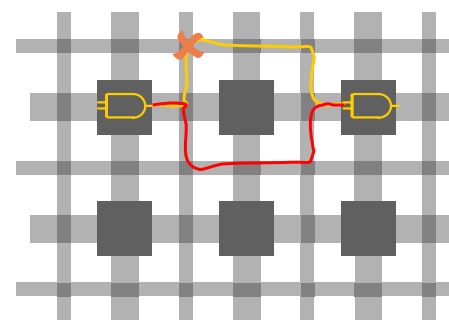
- Assume there exists a map of the defects.
 - Broken connections (stuck-open)
 - Shorted wires (stuck-closed)
 - Bad devices
- Only use the good devices
 - Route around defects
 - Use good devices
- Sometime, no loss in logic density

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Routing Around Defects



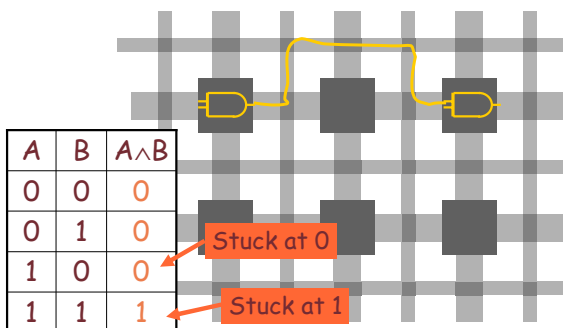
- Choose new channels
- Choose new wires in the same channels
- Re-place destination or source

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Configure Around Defects



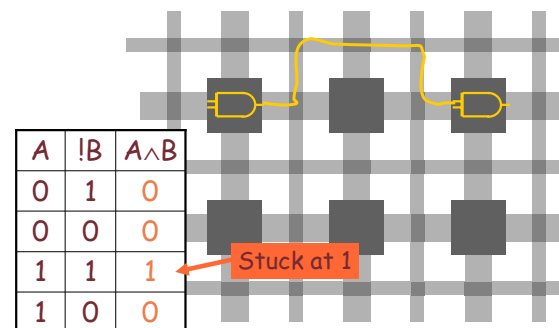
- See if stuck-open or closed fits function

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Configure Around Defects



- See if stuck-open or closed fits function
- See if complement is available

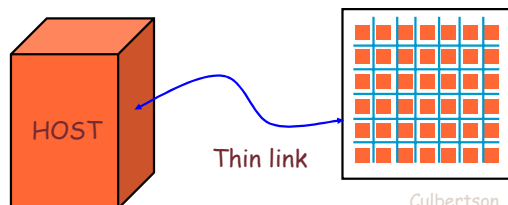
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Finding Defects

- Need to discover the characteristics of the individual components, but
- Can't selectively stimulate or probe the components
- Download test machines



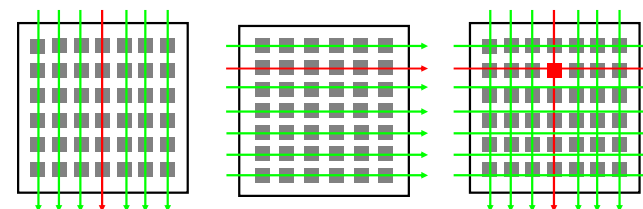
Culbertson, et al, FCCM'97

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Built-In Self-Test



Configure the device to test itself!

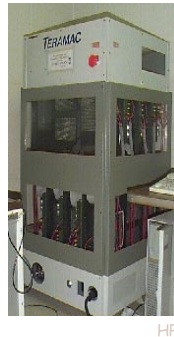
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Defect Tolerance Realized: Teramac

- Largest defect-tolerant system ever built
 - 8 PCBs, 4 MCMs each, 27 FPGAs each
 - 8 million total resources, 3% defective
- Compile around the defects
 - 10% of all logic cells
 - 10% all interchip wires
- Demonstrated years of reliable operation of large-scale defect-tolerant programmable hardware



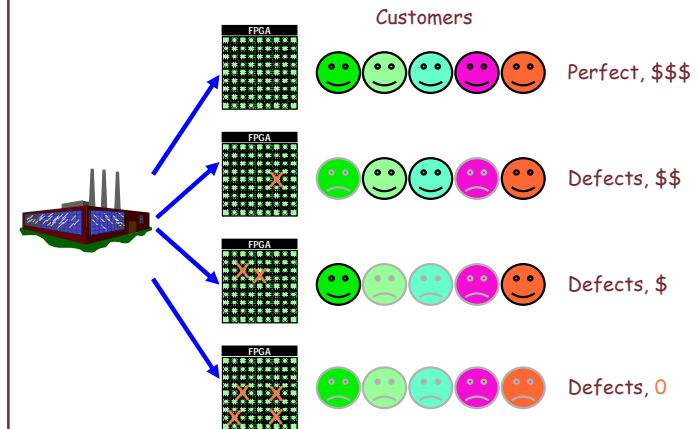
HP

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Coping With Defects

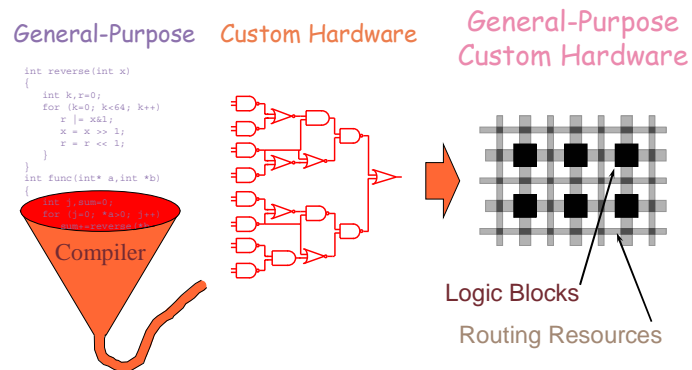


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Reconfigurable Computing



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Advantages of Reconfigurable

- Flexibility of a processor
- Performance of custom hardware
 - Reduce time to market
 - Reduce design cost
 - Built-in
 - Dynamic fault tolerance
 - Self-test
 - Defect tolerance
 - Low power

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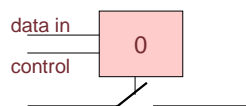
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Heart of an FPGA

The cost of the FPGA:
Increased Area-Delay Product

Universal gate = RAM



Switch controlled by a 1-bit RAM cell

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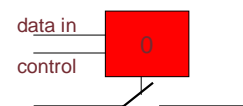
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Heart of an FPGA

The cost of the FPGA:
Increased Area-Delay Product

• RAM cell



Switch controlled by a 1-bit RAM cell

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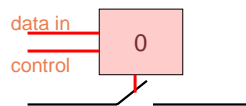
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Heart of an FPGA

The cost of the FPGA:
Increased Area-Delay Product

- RAM cell
- Wires to program RAM cell



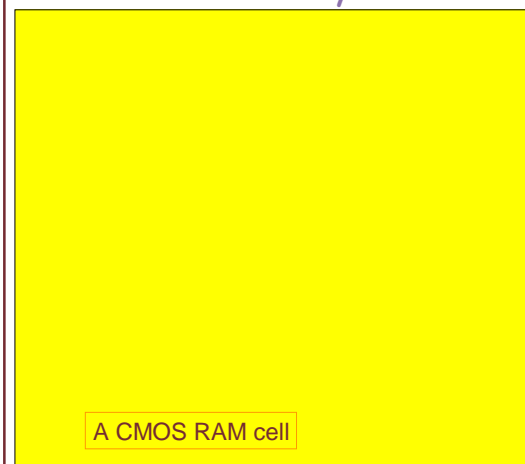
Switch controlled by a 1-bit RAM cell

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Another Way to scale down



A CMOS RAM cell

Technology
Molecules
Self-assembly

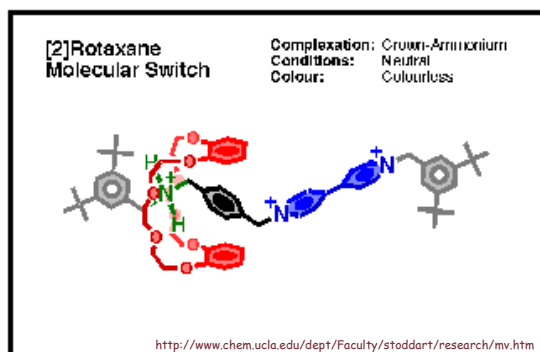
NanoRAM cell
↓

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Key Component: Reconfigurable Switch

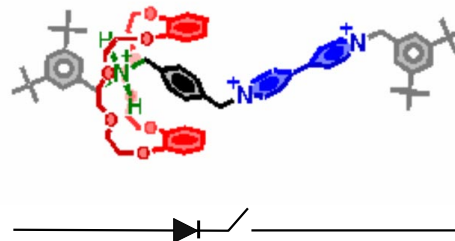


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Key Component: Reconfigurable Switch

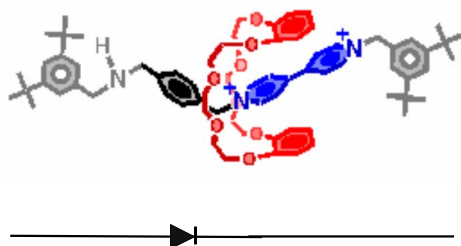


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Key Component: Reconfigurable Switch

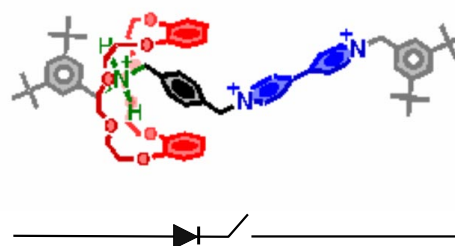


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Key Component: Reconfigurable Switch



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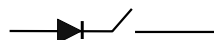
Key Component: Reconfigurable Switch

[2]Rotaxane
Molecular Switch

Complexation: Crown-Ammonium
Conditions: Neutral
Colour: Colourless

Reconfigurable Molecular Switch

- Holds its own configuration state
- Can be programmed with the signal wires



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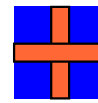
37

Using The Reconfigurable Switch

- Create a crossbar (perfect for FPGA)
- Programmable crosspoint fits in wire crossing!
- Compare to CMOS crosspoint (even with same dimension devices)

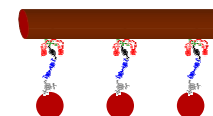
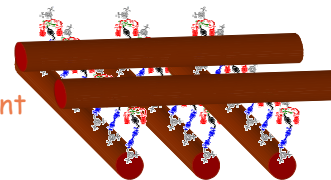


nano



CMOS

(to scale)



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Molecular Device Characteristics

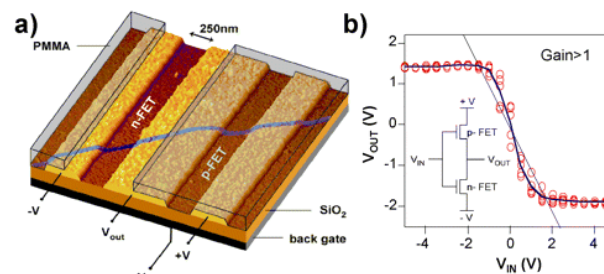
- Have useful and novel features
 - I-V curves
 - Devices with integrated state
 - Huge variety possible
 - Amenable to thermodynamic-assembly
- State of the art is changing rapidly!
- Requires new circuit methodologies

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Carbon Nanotube Inverter



Nano Letters 1, 453 (2001)

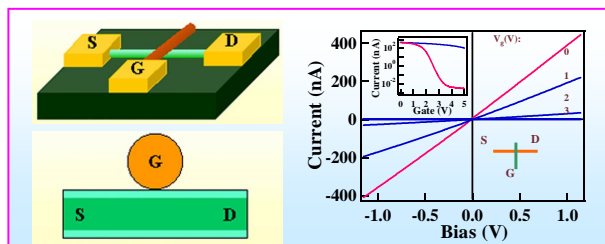
- Two Carbon nanotube FETs
- Doped on substrate
- Not all dimensions are nanoscale

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Crossed Nanowire FETs



Science 294, 1313 (2001)

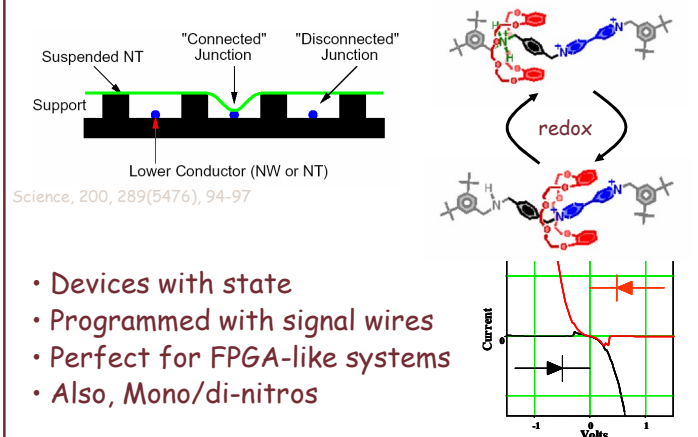
- A crossed nanowire FET
 - channel width by the active nanowire diameter (to 2 nm)
 - channel length by the gate nanowire diameter (to 1-2 nm)
 - gate dielectric oxide coating on the nanowires (to 1 atomic layer)
- The conductance of cNW-FETs can be changed by more than 10^5 -times with less than 0.1 V variation in the nano-gate.

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Molecular Switches



Science, 200, 289(5476), 94-97

- Devices with state
- Programmed with signal wires
- Perfect for FPGA-like systems
- Also, Mono/di-nitros

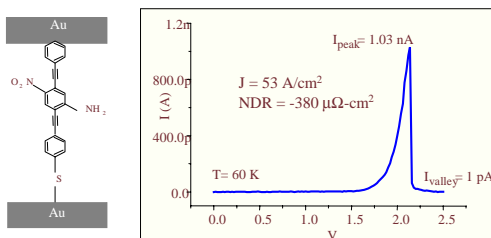
Angew. Chem. Int. Ed. Engl., 1997, 36, 1904-1907

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Negative Differential Resistor (NDR)



Mark Reed

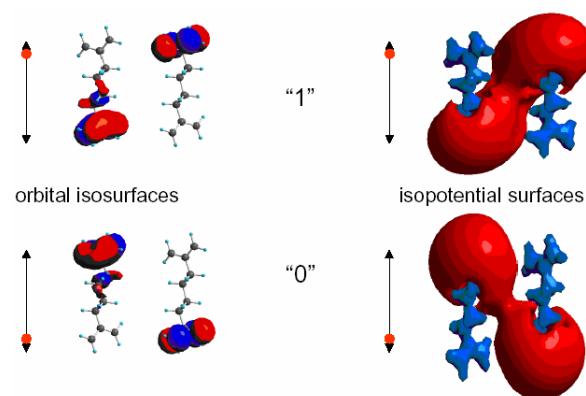
- NDR with 1000:1 Peak-to-valley ratio
- Similar to RTDs
- Heavily explored in the 70s!

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QCA Cell



Information carrier is NOT current or voltage

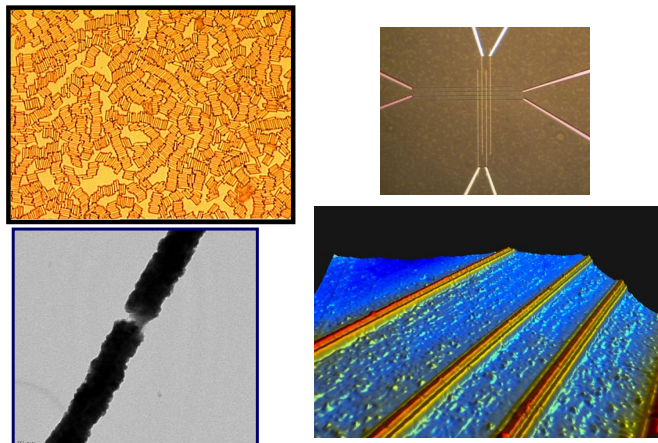
Notre Dame, Lieberman

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Some Nanoscale Wires



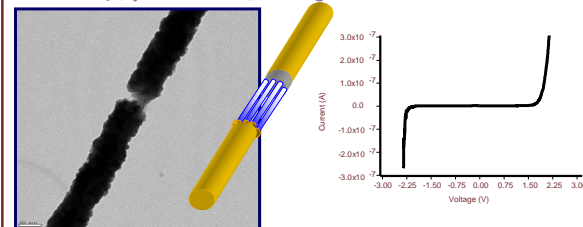
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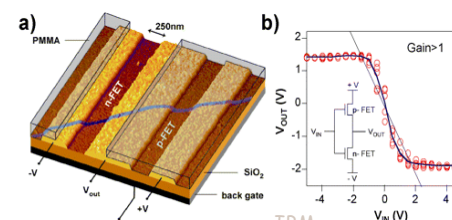
Penn State, HP, UCLA

45

More than Just Conductors



PSU

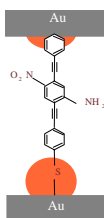


IBM

46

Contacts

- Contacts are still a problem
- Ohmic contacts are just part of the solution.
- Molecular devices and contacts cannot be analyzed in isolation
- E.g. DNA measured as
 - Conductor
 - Insulator
 - Semi-conductor
 - Proximity-induced superconductor

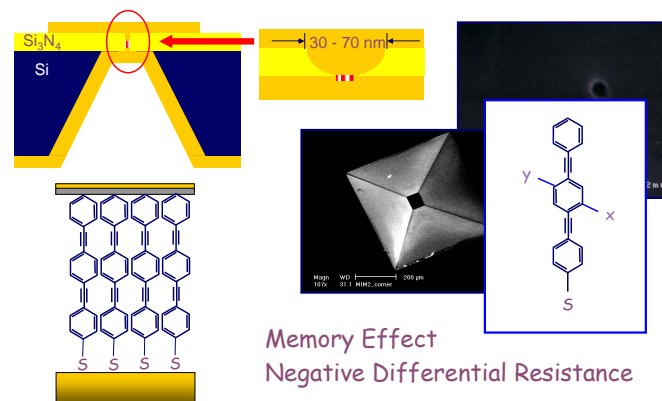


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NanoPore



Memory Effect
Negative Differential Resistance

♦ Zhou, C., M. R. Deshpande, M. A. Reed, L. Jones, and J. M. Tour, *Appl. Phys. Lett.*, 71 (5) 1997

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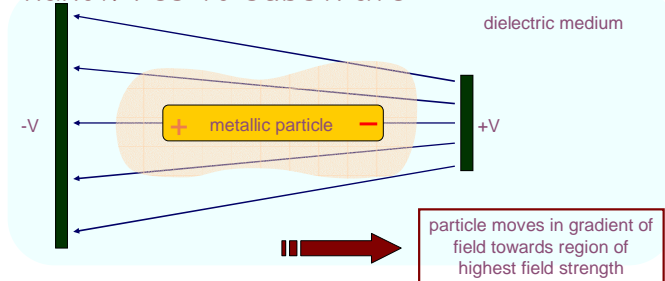
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Theresa Mayer, PSU

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Electrofluidic Assembly of Nanowires

- Long-range forces used to attract nanowires to substrate



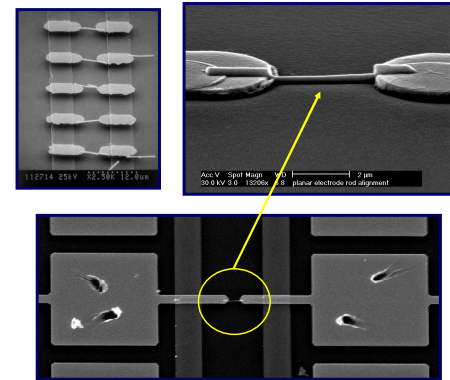
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Theresa Mayer, PSU

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Characterizing Nanowires



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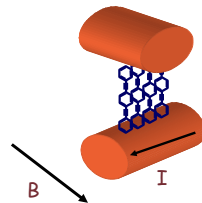
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Theresa Mayer, PSU

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Measuring Devices

- Break Junction (Reed, Yale)
- Individual Molecules with STM (Weiss, PSU)
- Crossed-Wire Tunnel Junction (Kushmerick, NRL)



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Fabrication Is Different!

- Electronic nanotechnology separates:
 - Manufacturing of devices
 - Fabrication of the circuit
- Manufacture wires and devices
- Somehow glue them together

Assembly, Assembly, Assembly

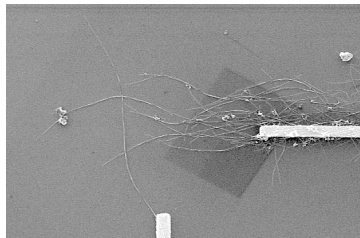
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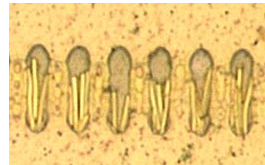
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Parallel Wires

- Can align wires
- Can mix types of wires
- Not precise



UCLA (2000); PSU(2000)



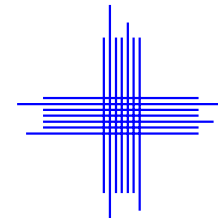
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Fabrication Primitives

- Parallel wires
- 2-D grids

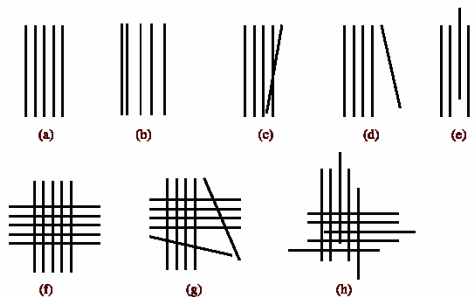


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Some Possible Outcomes



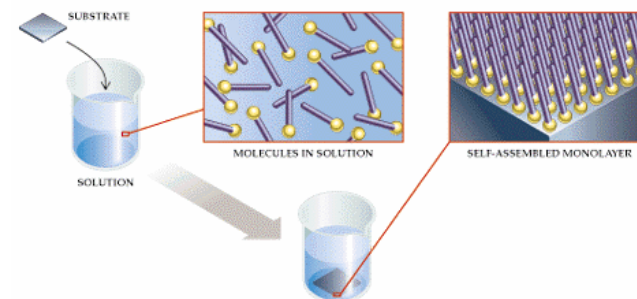
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Fabrication Primitives

- Parallel wires
- 2-D grids
- Self-assembled monolayers



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Fabrication Primitives

- Parallel wires
- 2-D grids
- Self-assembled monolayers
- Connections between orthogonal wires



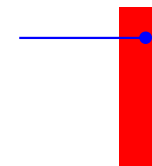
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Fabrication Primitives

- Parallel wires
- 2-D grids
- Self-assembled monolayers
- Connections between orthogonal wires
- Connections to CMOS



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Fabrication Primitives

- Parallel wires
- 2-D grids
- Self-assembled monolayers
- Connections between orthogonal wires
- Connections to CMOS
- Non-deterministic placement



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Fabrication Primitives

- Parallel wires
- 2-D grids
- Self-assembled monolayers
- Connections between orthogonal wires
- Connections to CMOS
- Non-deterministic placement
- Selective variability on a lithographic scale



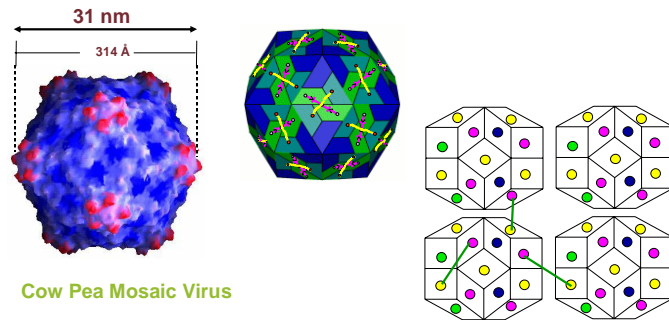
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Viral Crystals

Directed self-assembly in 3-D



- Scaffolding for 3-D assembly

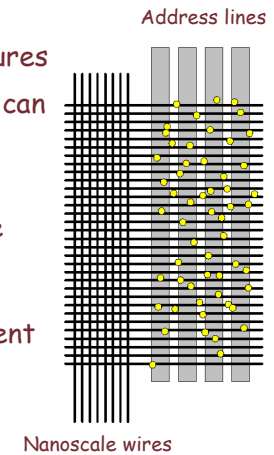
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Paul Franzen

Harnessing Randomness

- Fab primitives prefer low information content structures
- Can we design circuits that can exploit this?
- Example: Scale Matching
 - Address 1 nanoscale wire with $5\log(N)$ micronscale wires
 - Based on random placement of molecules

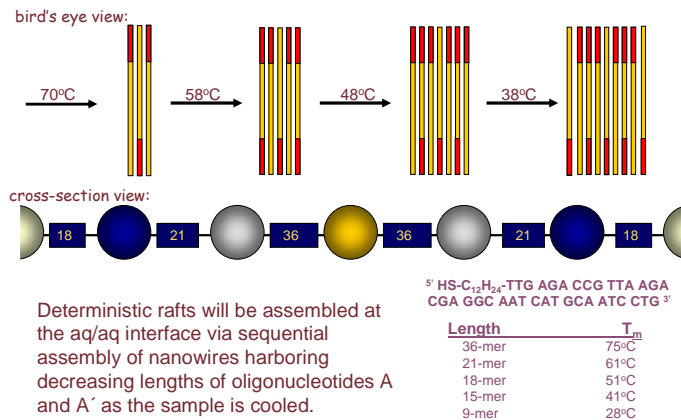


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Temp-programmed Raft Assembly



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Keating, PSU

Nanoimprinting

- Create master
 - Ebeam
 - CVD & then break
- Stamp into "soft" material
- Stamp and leave behind molecules

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Assembly, Assembly, Assembly

Wires alone are not useful
scale computing is **bottom-**

FLUIDIC SELF ASSEMBLY

Alien Technology

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Computing Crystals

- A reasonable medium-term position
 - No end-to-end connections
 - Maybe multi-terminal devices
 - No complex predetermined patterns
 - Quasi-regular & non-deterministic
 - Hierarchical assembly

Assembly \Rightarrow Computing Crystals

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Computing Crystals

- A reasonable medium-term position
 - No end-to-end connections
 - Maybe multi-terminal devices
 - **No complex predetermined patterns**
 - Quasi-regular & non-deterministic
 - Hierarchical assembly

With defects

Assembly \Rightarrow Computing Crystals

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Building a Computing Crystal

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Some Implications

- Restricted set of manufacturable patterns
 - Current uncompressed single layer mask data is 70GB, (90nm → 220GB)
 - Can we even do 3-terminal devices?
- Increased defect densities
- Increased fault rates
- Efficient Programmable crosspoints



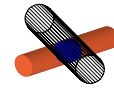
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Some Implications

- Restricted set of manufacturable patterns
 - Current uncompressed single layer mask data is 70GB, (90nm → 220GB)
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- Increased fault rates
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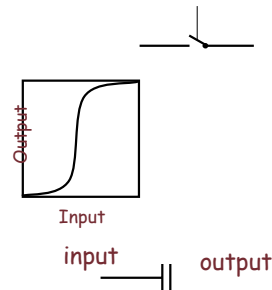
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Good Computing Devices

- Requirements:
 - Complete Logic Family
 - Restoring Logic
 - Fan-out
 - I/O-isolation
 - Gain
 - Inexpensive
 - Expend power only when computing
- Lithographically created CMOS MOSFET practically perfect



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Requirements: Nano-Circuits

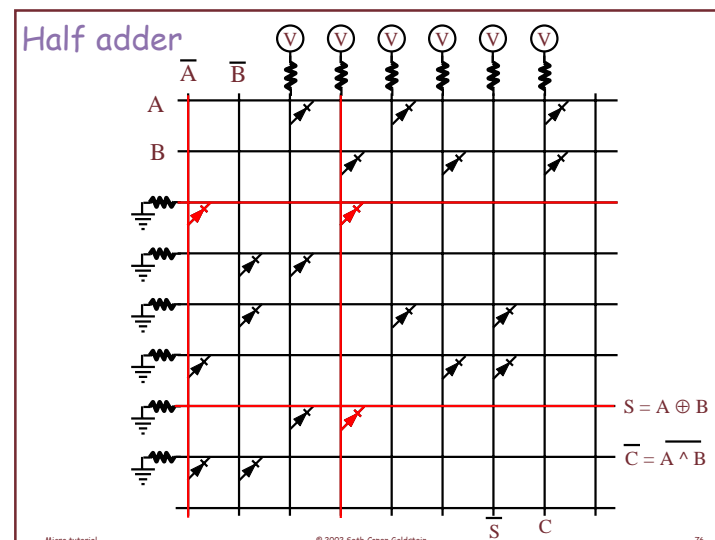
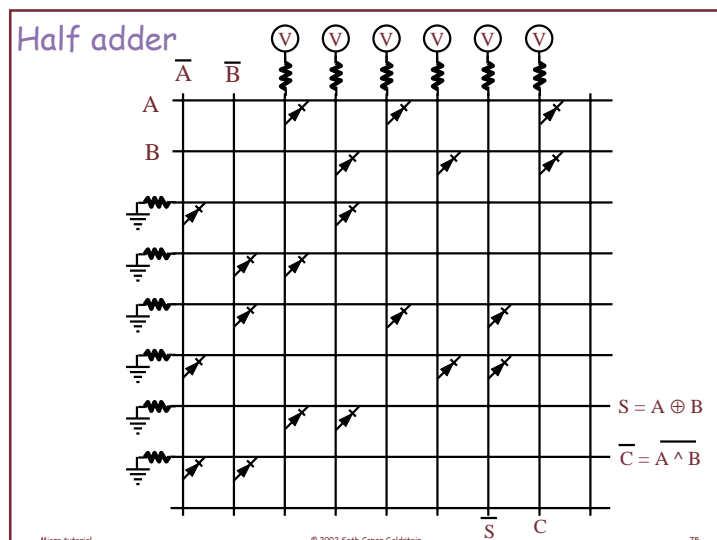
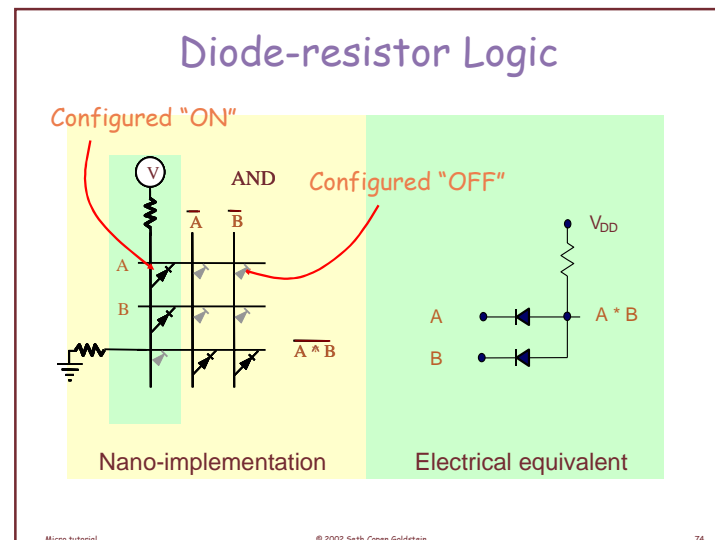
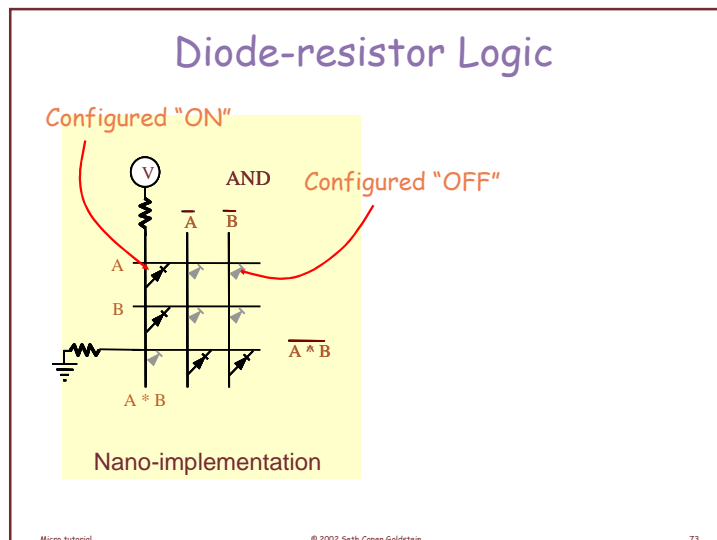
- Complete logic family
- Composable Circuits
 - Gain
 - Input/Output isolation
 - Fan-out
- Fabrication friendly
- Low variability
- Device/Wire ratio
- Energy-Delay product
- Harness Novel IV curves

CMOS	Nano
😊	😞
😊	😞
	😞
😞	😞
😞	😞
😊	😞
😞	😞
😊	😞
😞	😊

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But, Wait

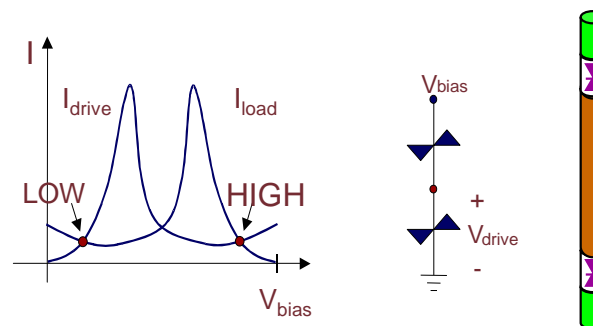
- Noise immunity?
- Signal restoration?
- Restoring logic?
- I/O isolation?
- Gain?
- Latches?

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Molecular Latch Using NDRs



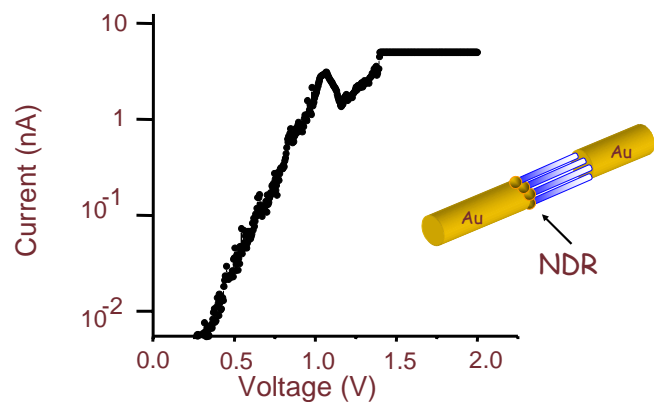
High and Low States of Bistable Latch

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Recent in-wire measurements



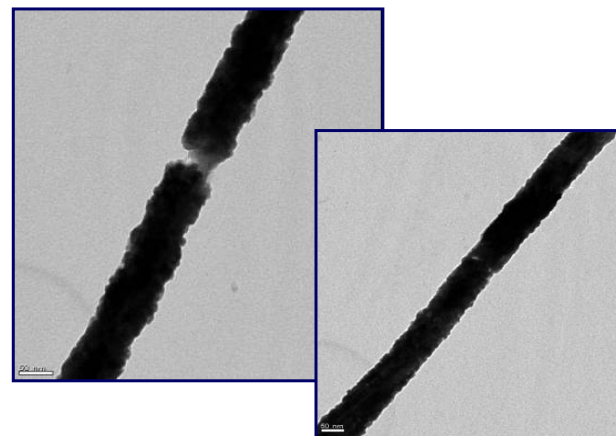
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Mallouk, Mayer, Mattzela, Kratochvilova, Mbindyo, Zambaya

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Inwire devices

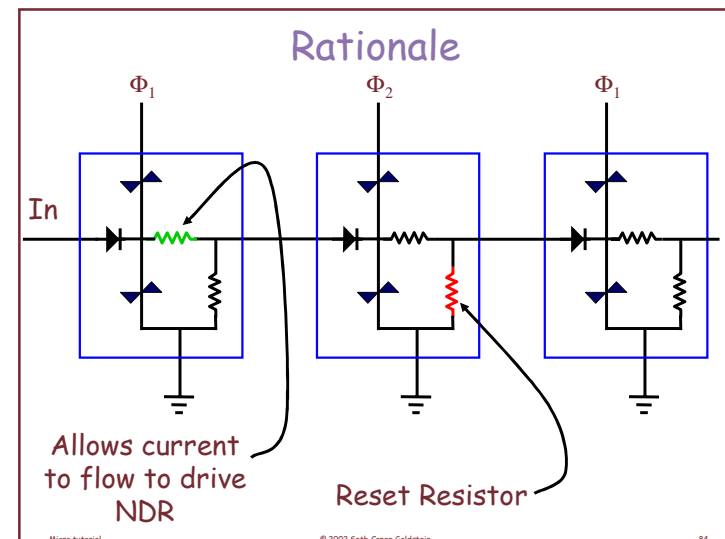
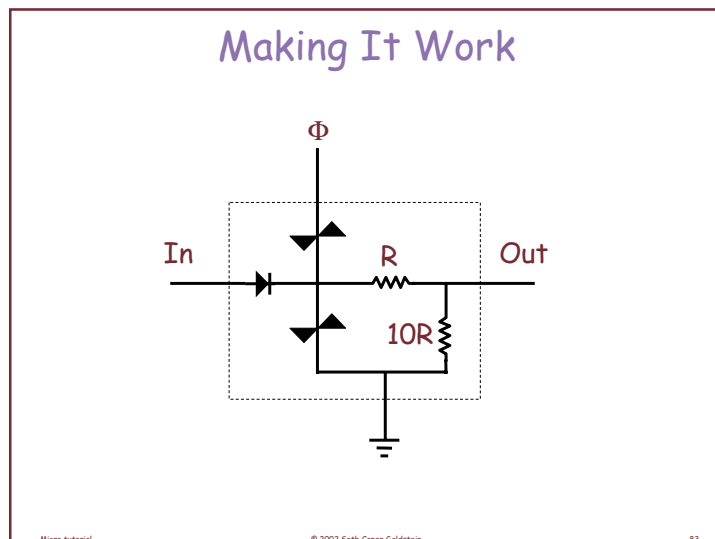
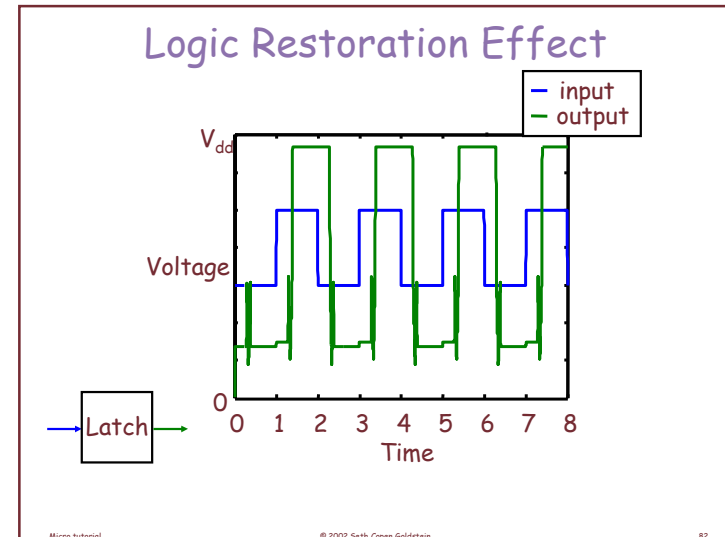
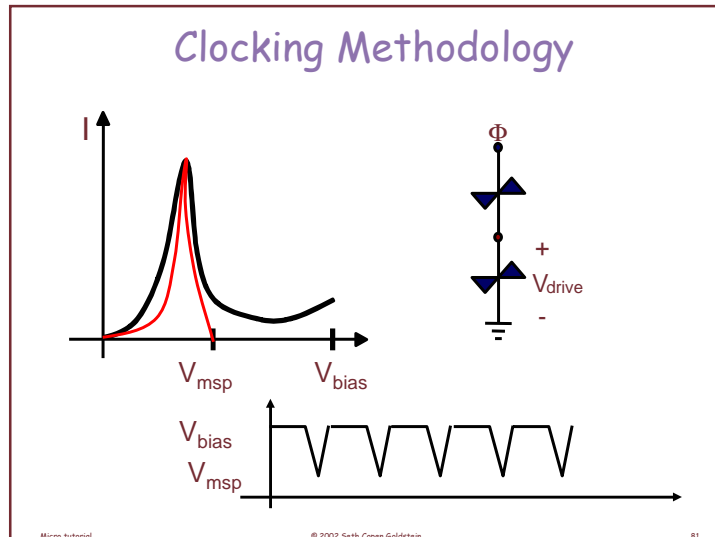


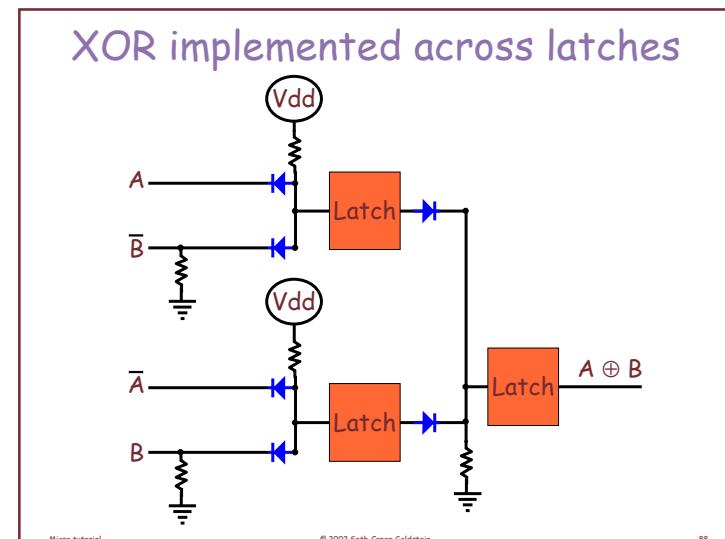
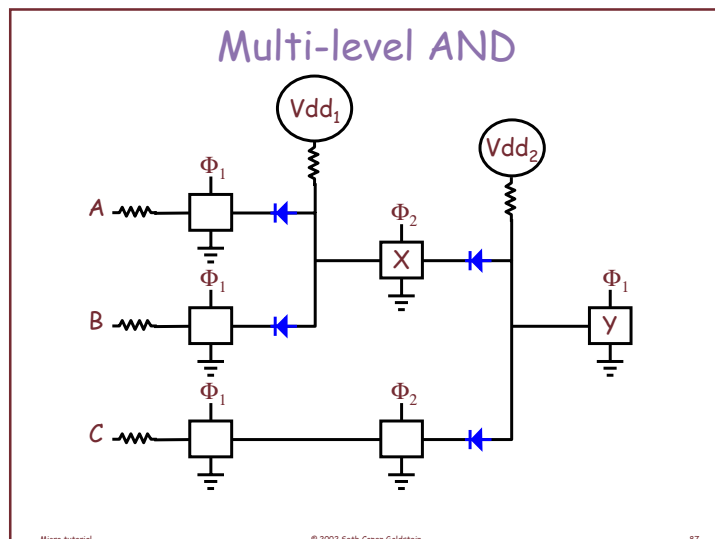
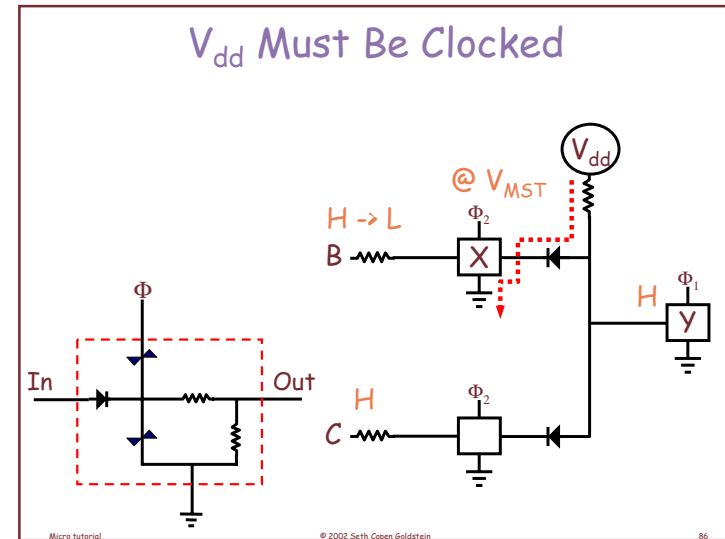
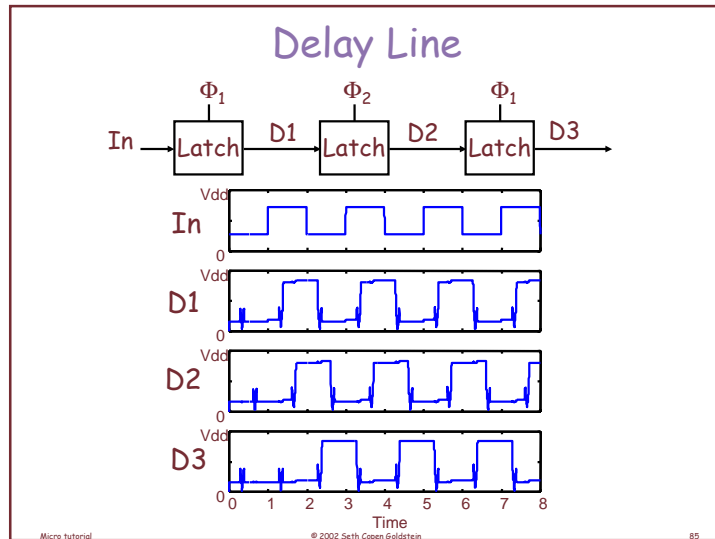
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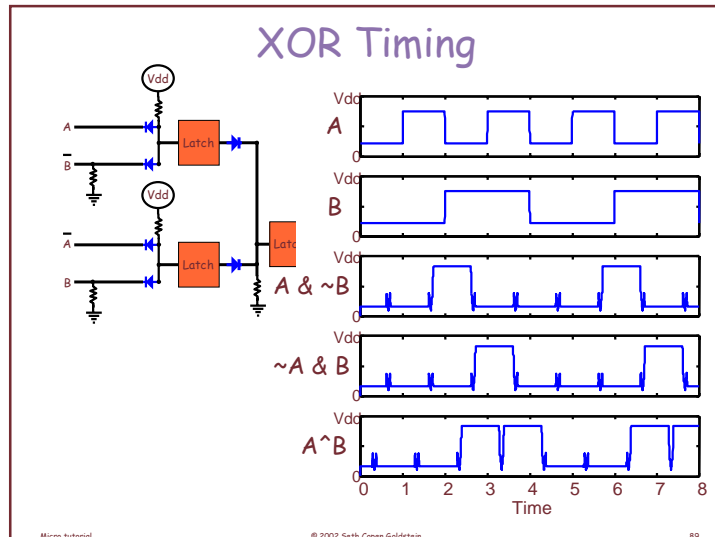
Mallouk, Mayer, Mattzela, Kratochvilova, Mbindyo, Zambaya

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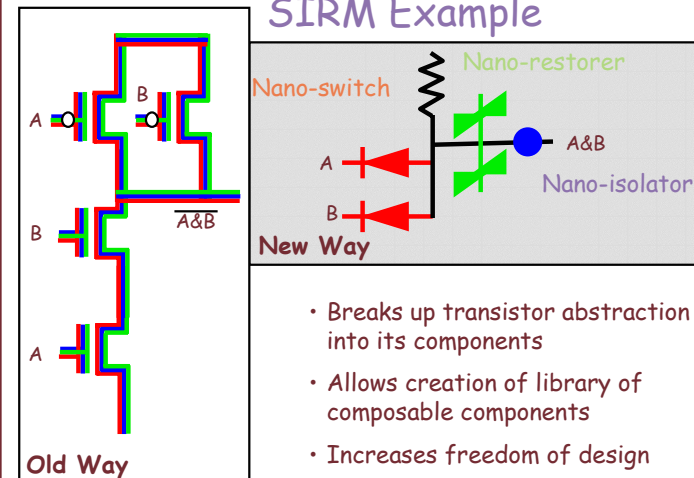
Necessary Device Abstraction

- Transistor provides it all
 - Switch
 - Fan-out
 - I/O isolation
 - Signal restoration
- Replace single abstraction with multiple abstractions: SIRM
- Enables an incremental path to direct nano-circuits

SIRM

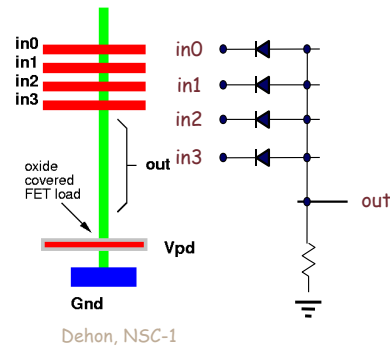
- SIRM allows multiple devices to replace a single transistor
 - Switch
 - Isolator
 - Restorer
 - Memory
- SIRM already in use
- Allows circuit designers to explicitly manage the different components of a scalable circuit technology

SIRM Example



Diode Logic From Crossing NWs

- Another example of DR-logic
- Or gate shown
- The S from SirM



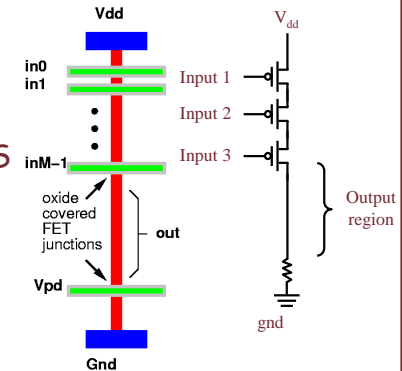
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PMOS-like Restoring FET Logic

- Crossing Doped NWs to build NOR
- Similar to N-MOS logic of old. (Static load)
- Sir of SirM



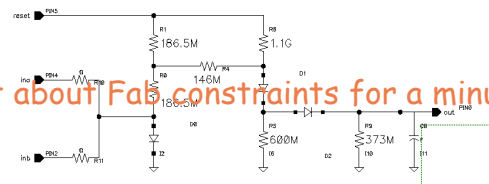
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NDR-based Circuits - 1

Forget about Fab constraints for a minute.



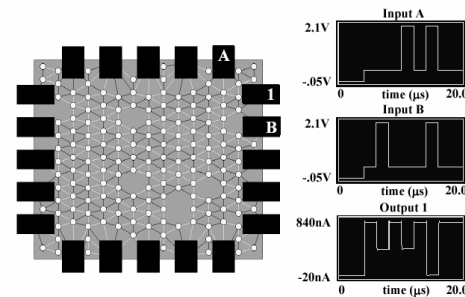
- 2-Input Current-mode NAND gate
- Gate is first reset to place the NDR diodes in the low impedance state
- If both input currents reach threshold, the output transitions from a low impedance state to a high impedance state
- Complex, low noise immunity, poor power-delay product, little manufacturing tolerance, poor isolation

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NDR-based Circuits - 2



- Nanocell (Husband, Tour, Reed, et. Al.) Husband, 2002
- Easy to fabricate
- S of SirM
- Will come back to this

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Review

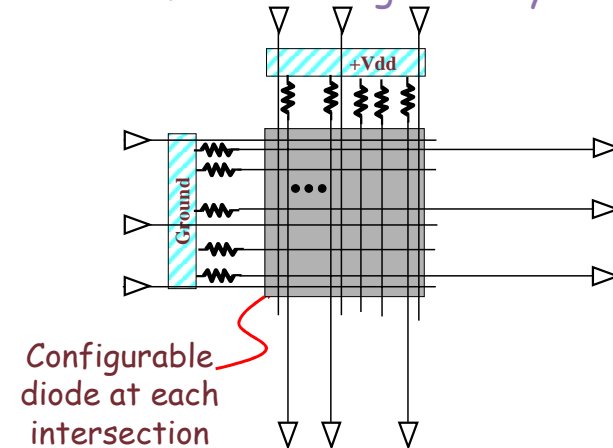
- Devices
 - Diodes, resistors, programmable switches, memory devices, wires, NDRs, latches
- Fabrication Constraints
 - Regular
 - Low-information content structures
 - Defects
- Need post-manufacturing modification
- Crosspoints are cheap.

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Molecular Logic Array

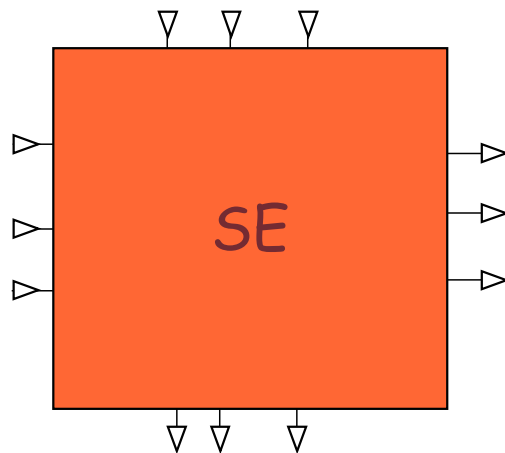


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Abstract

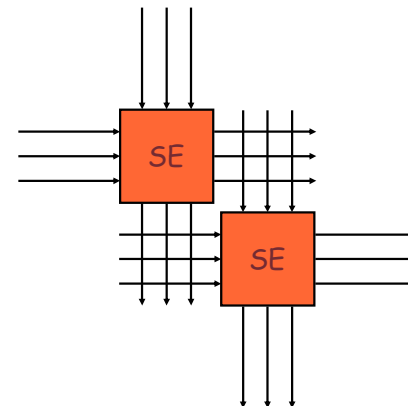


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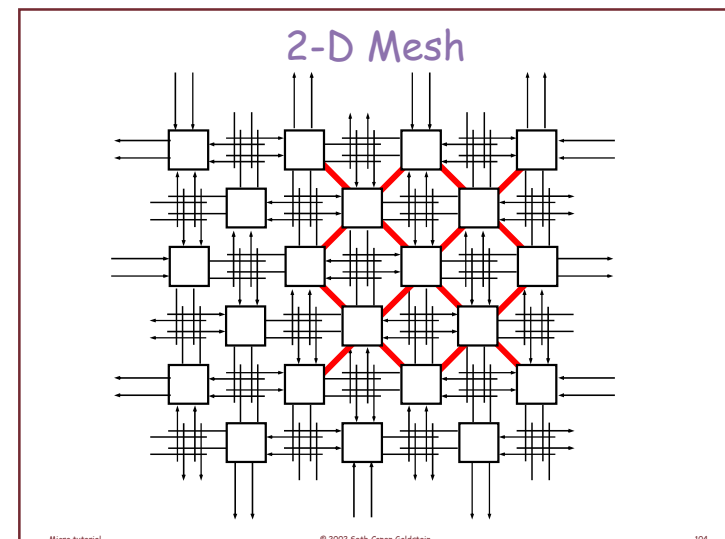
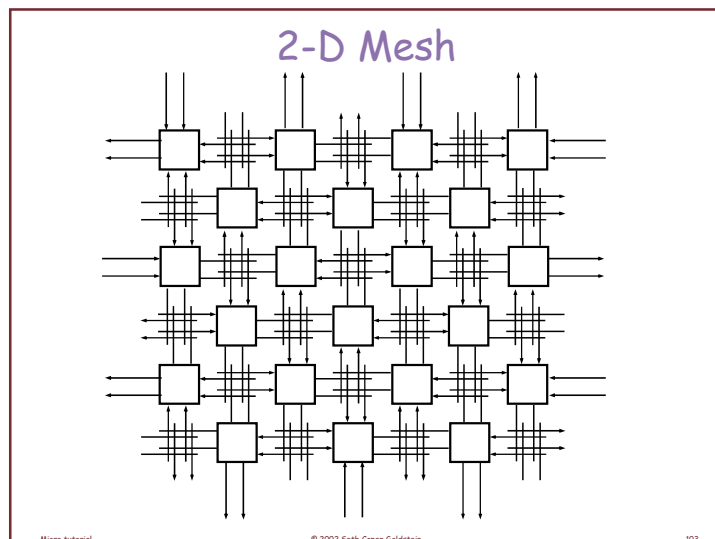
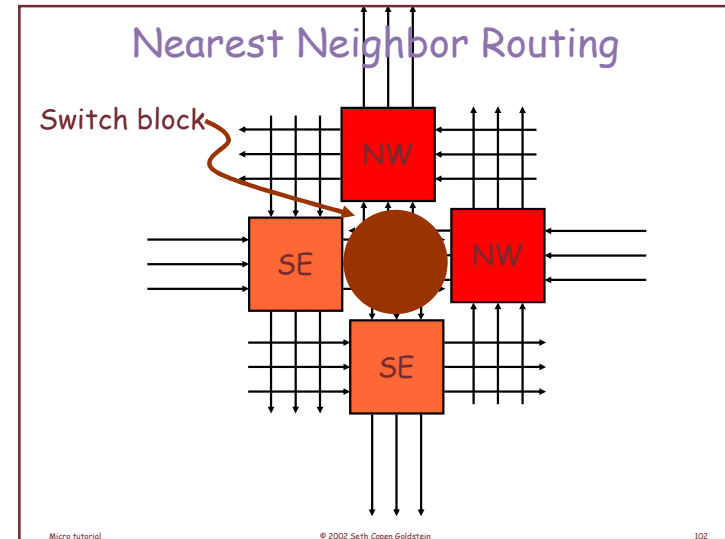
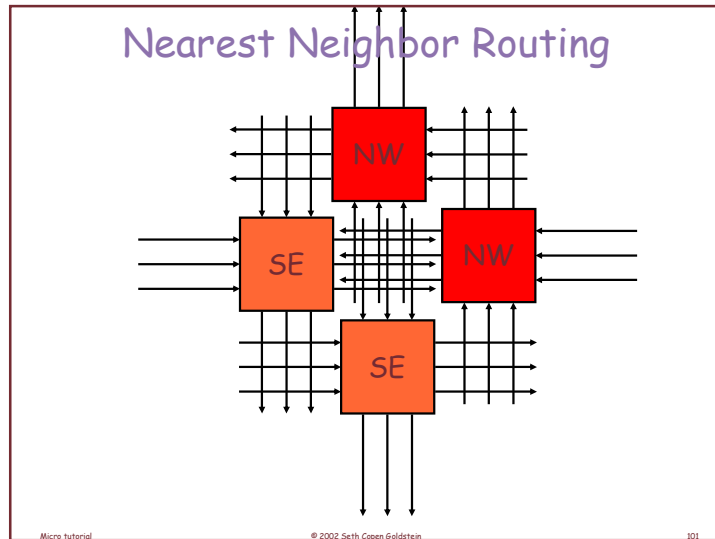
Nearest Neighbor Routing



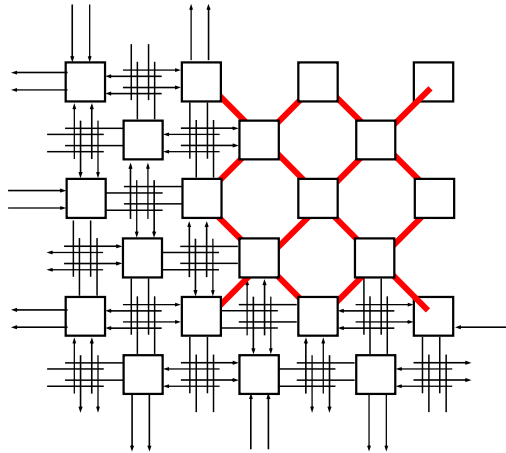
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2-D Mesh



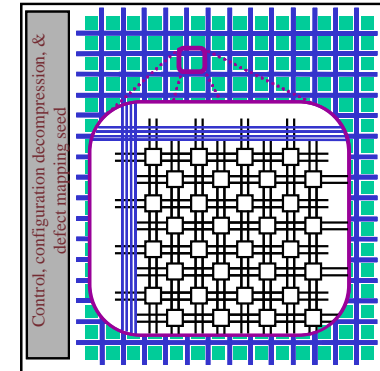
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The NanoFabric

- Nanoscale layer put **deterministically** on top of CMOS
- Highly regular
- $\sim 10^8$ long lines
- $\sim 10^6$ clusters
 - Cluster has 128 blocks



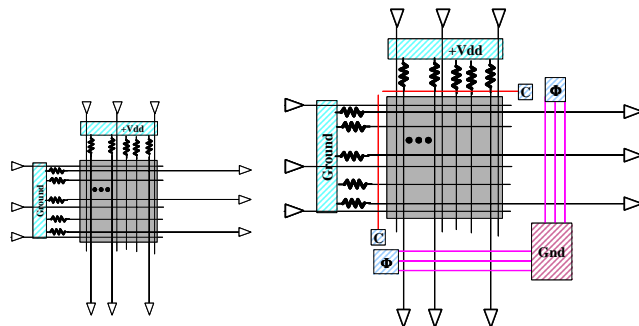
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Lets Fill in some details

- Need to be able to configure crosspoints
- Need to restore logic signals



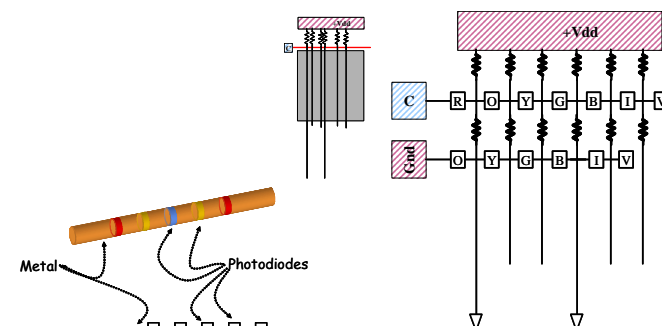
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Interfacing Micro & Nano

- Nanoblock strategy uses single-wire demux
- Enables small nanoscale array



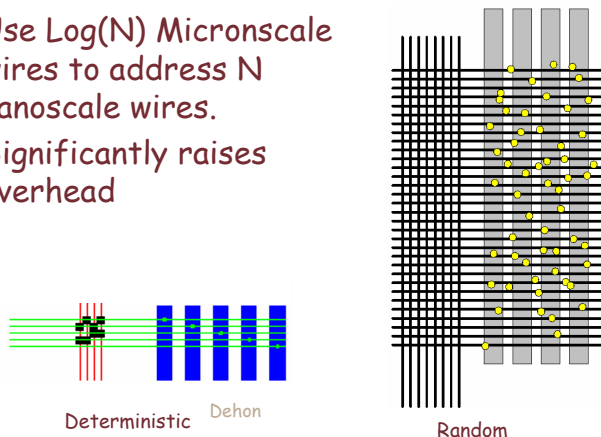
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Log(N) Demuxes

- Use $\text{Log}(N)$ Micronscale wires to address N nanoscale wires.
- Significantly raises overhead



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Choosing an array size

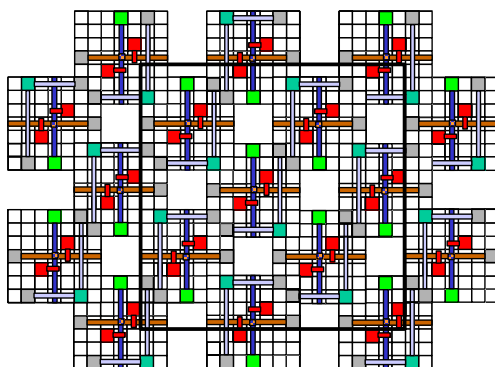
- Prefer large array
 - To amortize overhead
- Prefer small array
 - To reduce hit from defects
 - To isolate defects
 - To increase speed
 - To increase utilization

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Putting Nanoblocks on CMOS

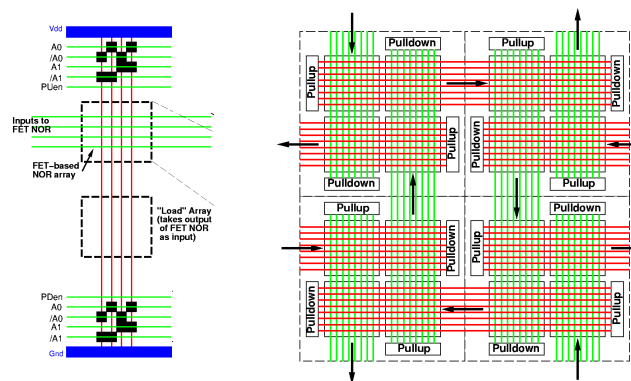


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Another Array-based Architecture



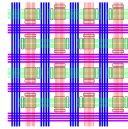
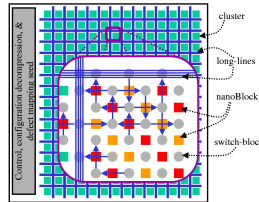
Dehon, NSC-1

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Array-based Architectures

- Both
 - Regular
 - Built on CMOS
 - Based on reconfigurable non-volatile switch
- Nanofabric
 - Does not require precise nanoscale placement
 - Uses light for programming
- ABAME
 - Requires precise placement for decoders
 - Can program electrically

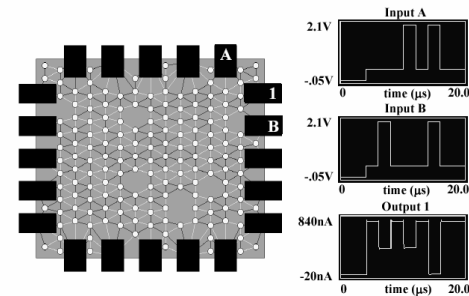


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Nanocell architecture



Husband, 2002

- Random deposition of particles
- Determine functionality after manufacture
- Requires significant CMOS

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NanoFabric Attributes

- Hierarchical fabrication
 1. Manufacture devices
 2. Non-deterministically align wires
 3. Self-assemble monolayers onto wires
 4. Create meshes
 5. Deterministically align w/CMOS
- Reconfigurable
- Defect tolerant

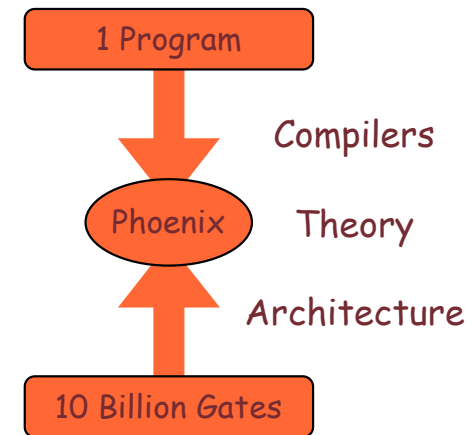
How do we use it?

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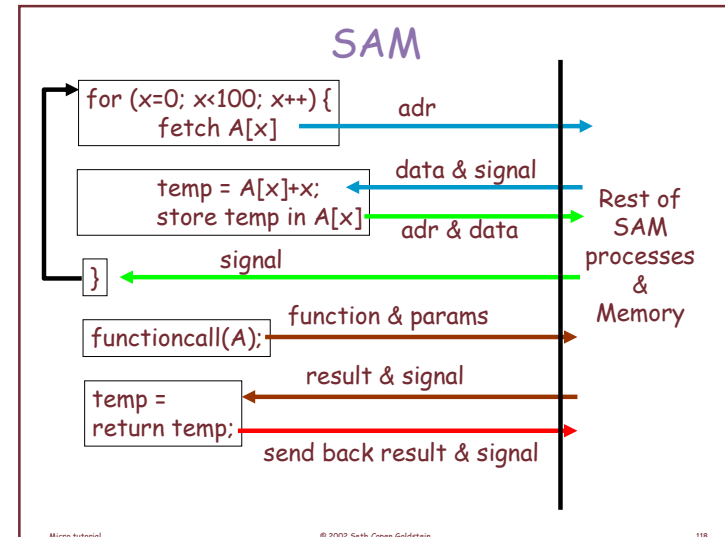
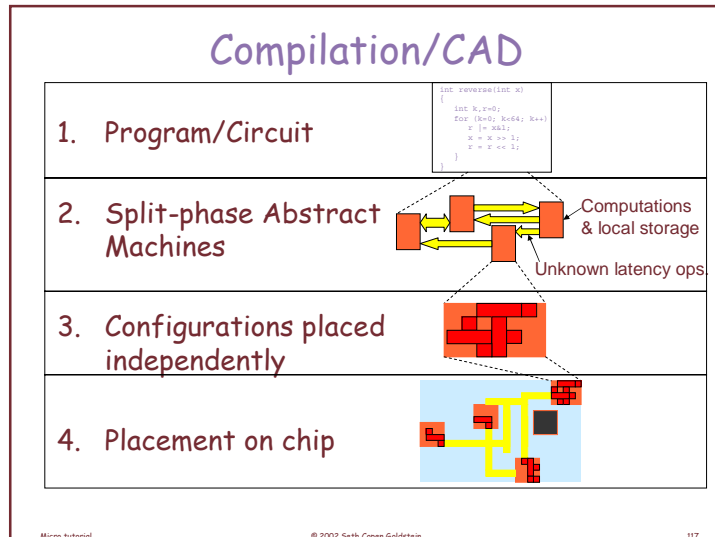
Spanning 10-orders of Magnitude



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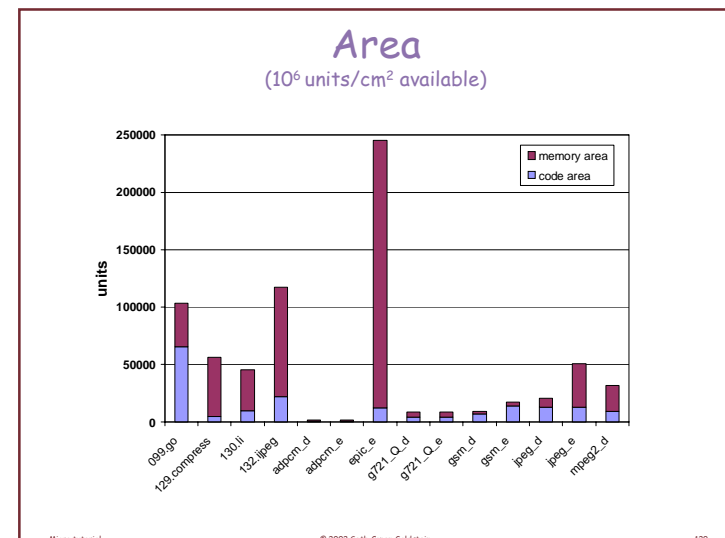
116



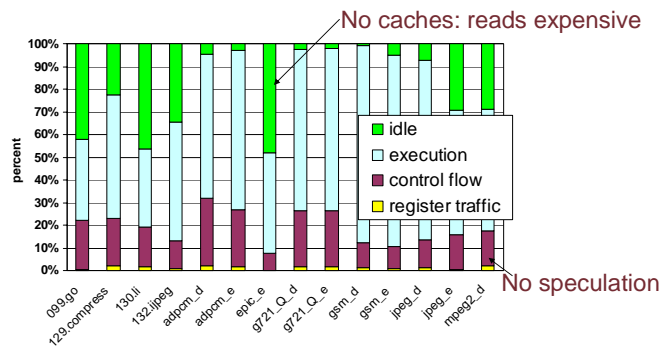
Limit Study

- We investigate using the nanoFabric as a computing substrate
- Mapping
Programs \Rightarrow SAM \Rightarrow nanoFabric
- We discover:
 - Programs and data fit on 1 cm² (From SpecInt95 & MediaBench)
 - Single-threaded performance is fair
 - Spatial computing requires different tradeoffs and compilation techniques

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How Time Is Spent

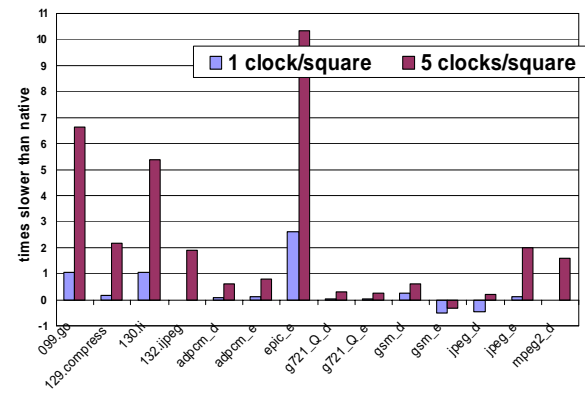


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Application Slowdown

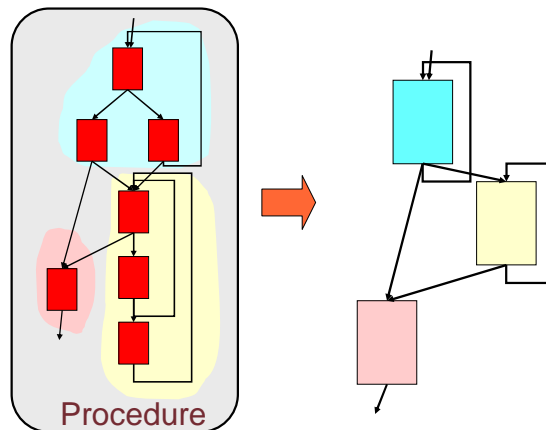


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Hyperblocks

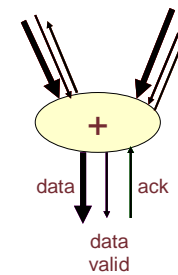


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Asynchronous Computation



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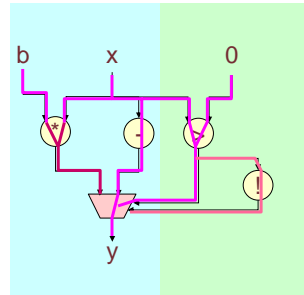
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Lenient Operations

```

if (x > 0)
    y = -x;
else
    y = b*x;

```



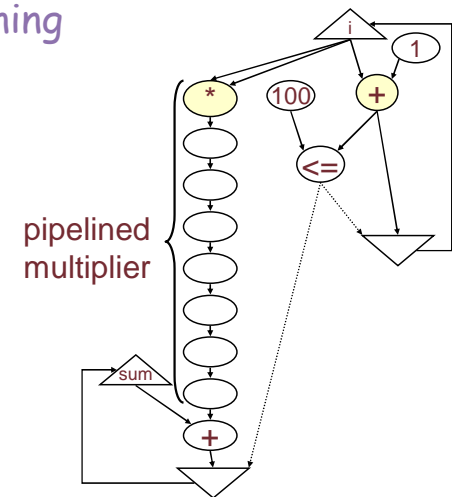
Solve the problem of unbalanced paths

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Pipelining

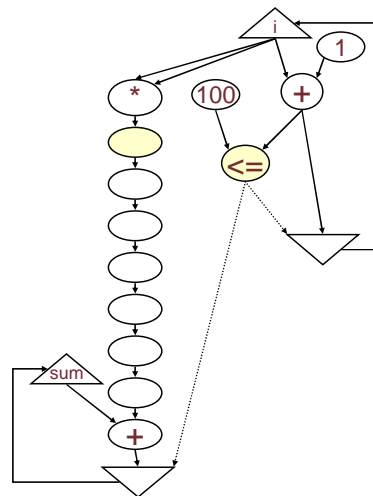
pipelined
multiplier

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Pipelining

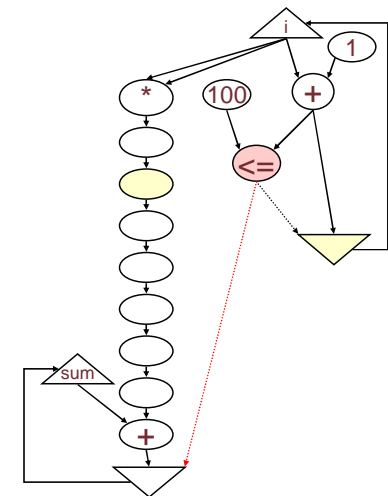


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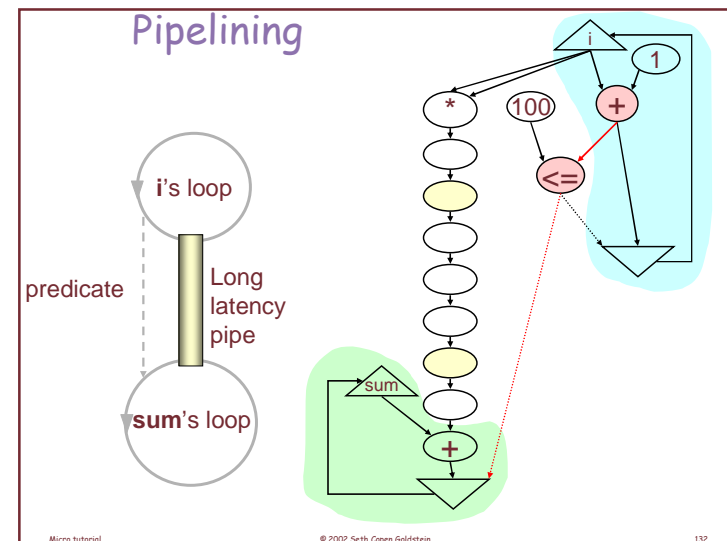
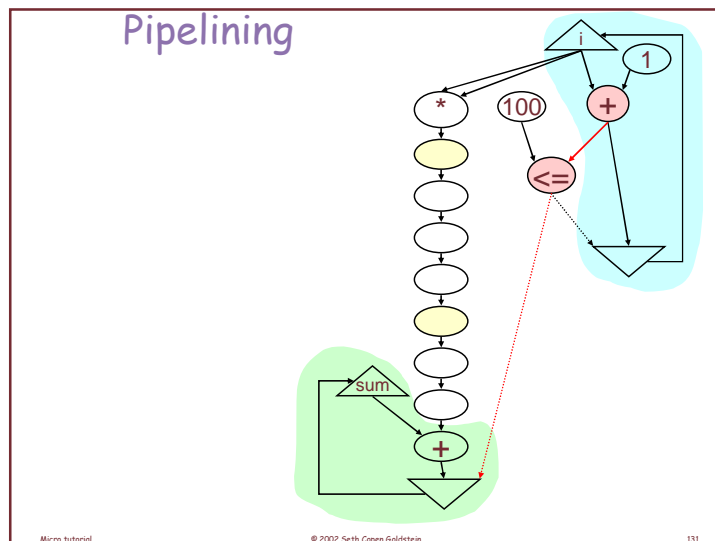
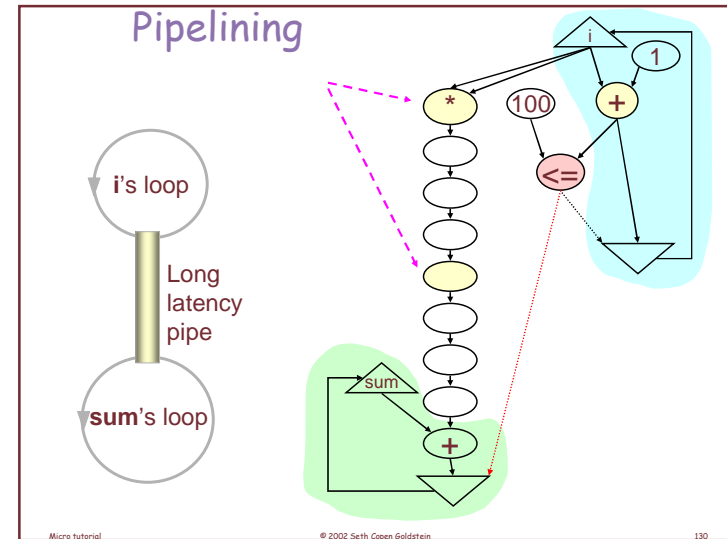
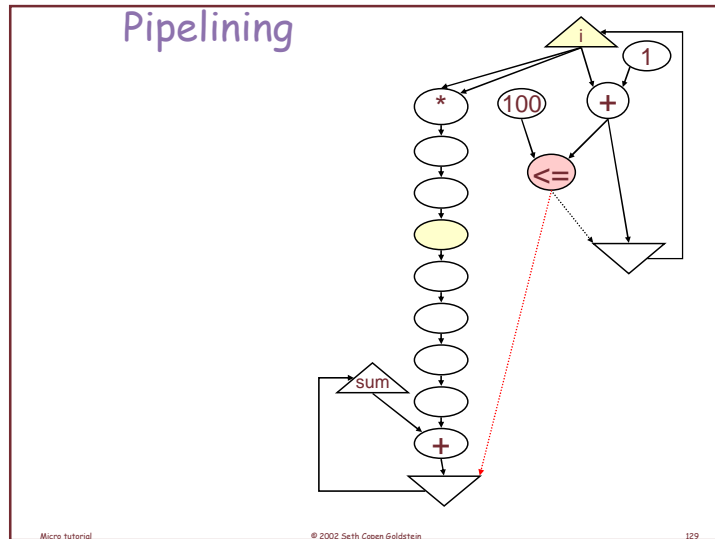
Pipelining

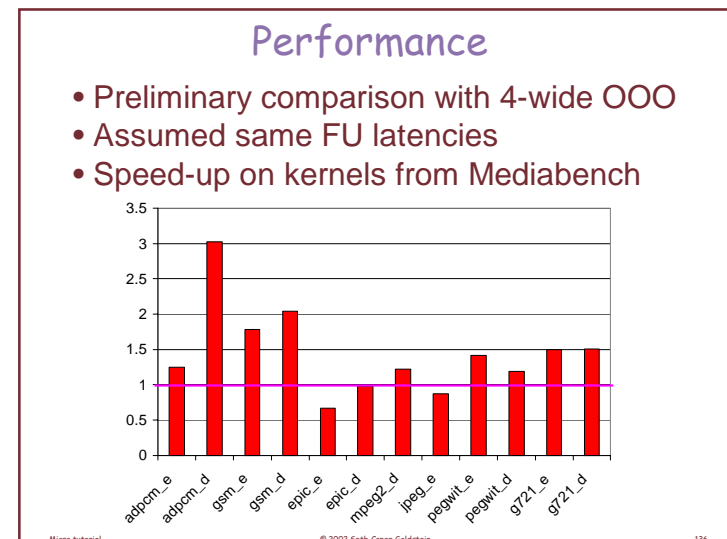
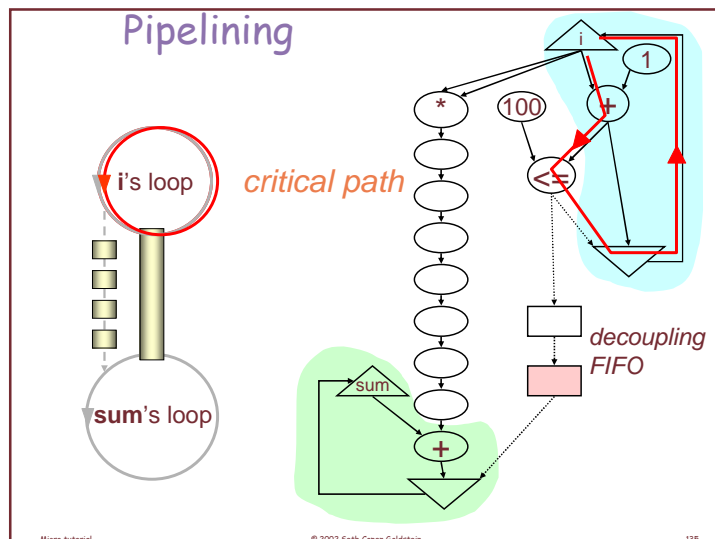
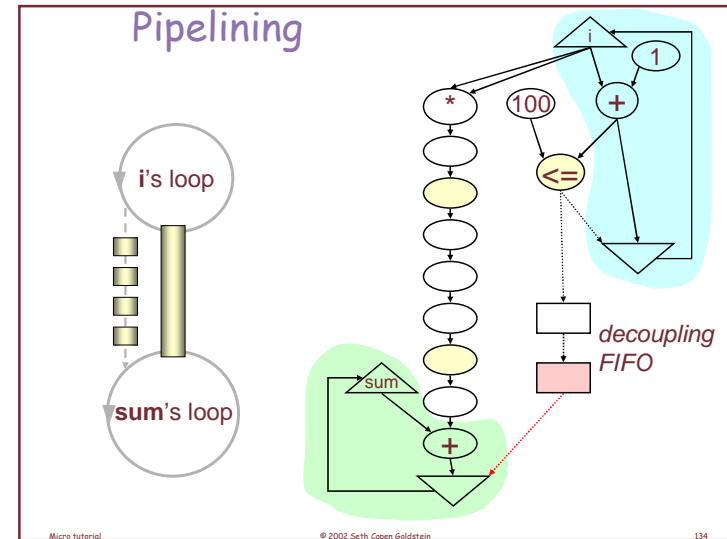
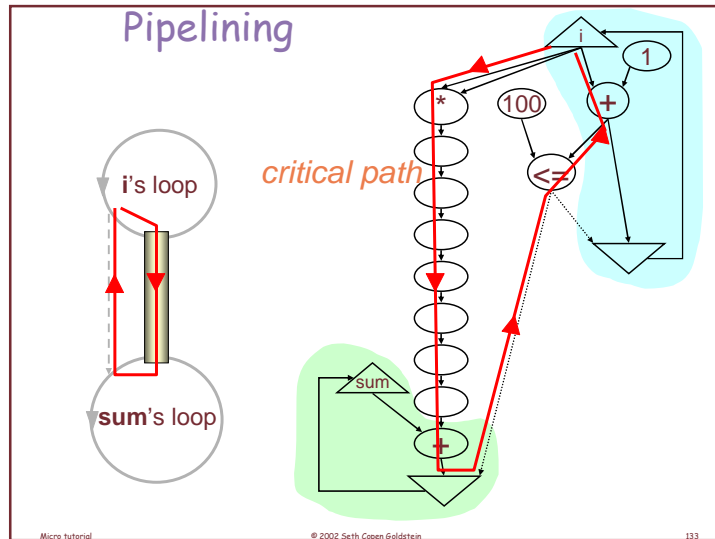


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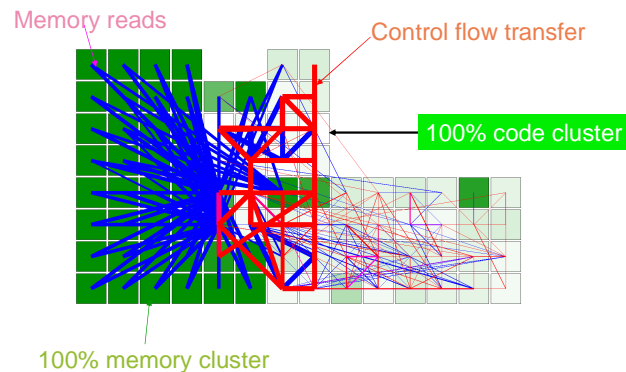
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Typical Program Graph (g721_e)

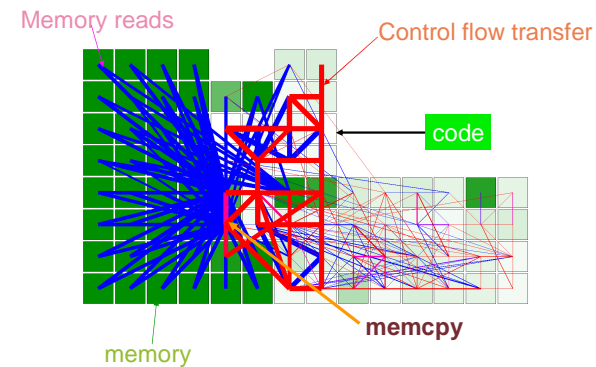


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Typical Program Graph (g721_e)

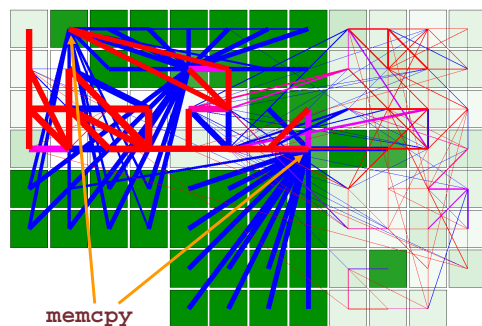


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Program Graph After Inlining memcpy



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Return to Defect Tolerance

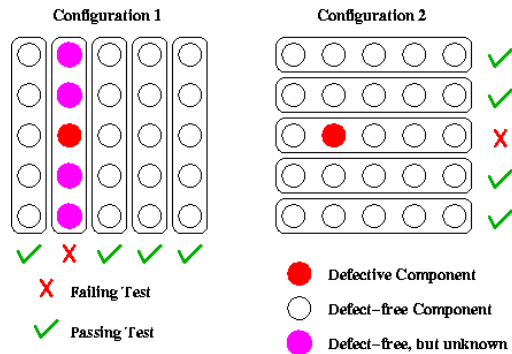
- Expect faulty components
 - Broken wires
 - Shorted wires
 - Bad contacts
 - unprogrammable configuration bits
- Strategy
 - Locate defects
 - Must scale with defect densities
 - Must scale with number of devices
 - Cannot probe individual components
 - Place&route around them

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Test-circuits in action



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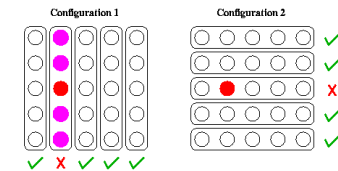
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Some terminology

- n components being tested
- Probability of defect p
- Each test circuit has k components
- Circuits arranged in various orientations, or *tilings*
- % of good components recovered: *yield*

In the example,

- $n=25$
- $k=5$
- 2 tilings
- yield is 100%.



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Assumptions

- Permanent defects
 - defective component always displays faulty behavior
 - defect in one component does not affect others
 - i.e., no short-circuits between wires
 - manufacturing process biased to ensure this
 - no Byzantine failures

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Assumptions (cont.)

- Arbitrary, unlimited connectivity
 - any component can be connected to any other, including non-adjacent ones
 - makes large number of tilings possible
- Above assumption: to simplify analysis

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Scaling with defect density

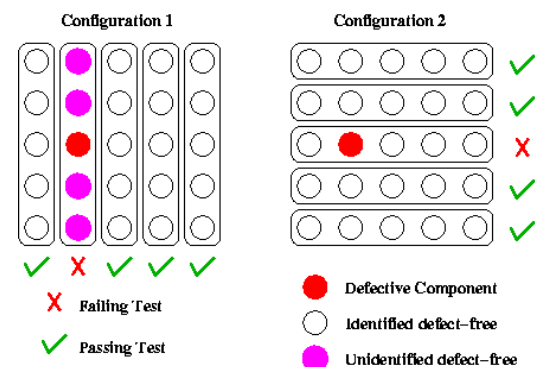
- Expected $k \cdot p$ defects/test-circuit
- Fewer defects/circuit:
easier to locate
- We examine the following 3 cases:
 - $k \cdot p \ll 1$
 - $k \cdot p \approx 1$
 - $k \cdot p \gg 1$
- Remember, k cannot be too small

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Example with very low defect rate

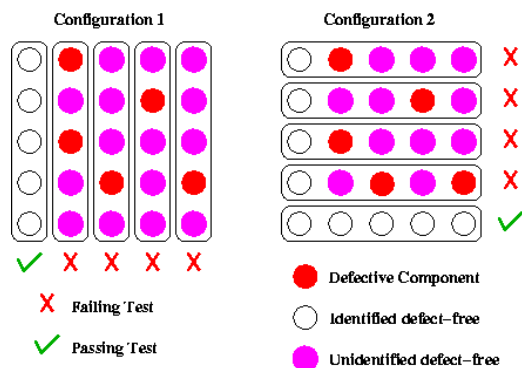


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Example with higher defect rate

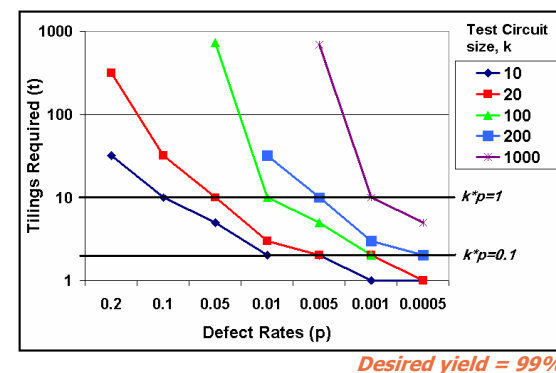


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Tilings required for low defect rates



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High defect rates: $k \cdot p \gg 1$

- Many defects/test-circuit
- Finding a defect free circuit is extremely unlikely
 - e.g., for $k=100$, $p=0.1$, probability of finding a defect-free circuit = $1.76 \cdot 10^{-5}$
- The previous approach does not work: something new is needed

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Making test circuits more powerful

- Use test-circuits which *count* defects
 - error in output depends directly on number of defects
 - e.g., use error-correcting, fault-tolerant circuit designs
- These can return correct counts only upto a certain threshold
 - must indicate when threshold is crossed
 - use *two* different test circuits simultaneously!

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New testing methodology

- Split into two phases:
 - *probability-assignment* phase
 - *defect-location* phase
- First phase: identifies components with high probability of being defect-free
- Second phase: tests these components further to pin-point defects
 - each phase: uses many different tilings

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Probability-assignment phase

- Each component made a part of many different test circuits and defect counts are obtained
- Find probability of each component being good using Bayesian probabilistic analysis
- Discard components with low probability of being good

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This works, but why?

- Intuitively, a defective component increases defect counts of all circuits it is a part of
- If a component is part of many circuits with a high defect count, our analysis assigns it a low probability of being good

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Defect location phase

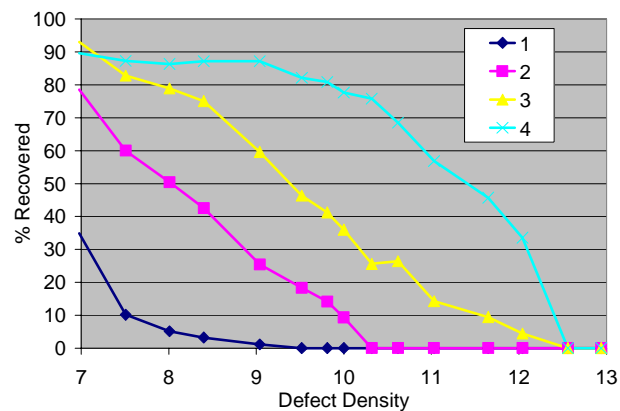
- Remaining components have low defect rate
- Configure into test circuits, mark all the components good if circuit has no defects
- Repeat for many different tilings
- Everything left is marked bad

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Perfect Counting Circuits



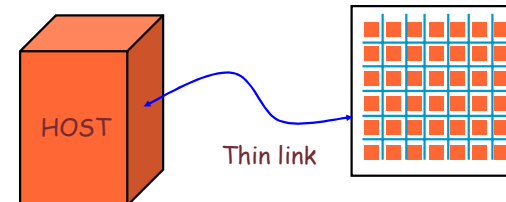
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Scaling to 10^{11}

- Eliminate Host
- After initial area is found, configure chip to act as host
- At end of complete test, upload entire defect map.
- For proposed device <1 day to map



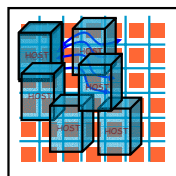
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Scaling to 10^{11}

- Eliminate Host
- After initial area is found, configure chip to act as host
- At end of complete test, upload entire defect map.
- Goal: <1 day to map



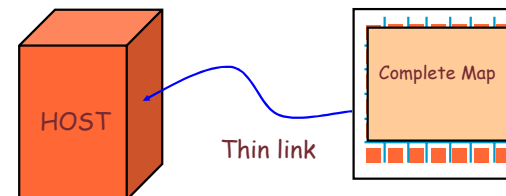
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Scaling to 10^{11}

- Eliminate Host
- After initial area is found, configure chip to act as host
- At end of complete test, upload entire defect map.
- Goal: <1 day to map



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Predicting the Future

Imagine Computers:

- *Small* enough to fit inside cells
- *Cheap* enough to be disposable
- *Dense* enough to embed a supercomputer
- *Smart* enough to assemble themselves

Computers from atomic scale components



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Summary

- Significant progress in nanoscale
 - Devices
 - Wires
 - Fabrication
- Independent of Technology
 - Loss of arbitrary patterns at fab time
 - Increase in defects and faults
 - Reconfigurable fabrics look good
- Molecular electronics is reconfigurable friendly

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Plenty of Interesting Research

- Devices Abstractions
- Circuits
- Architectures
- Cad Tools
- Compilers
- Defect Tolerance
- Fault Tolerance

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