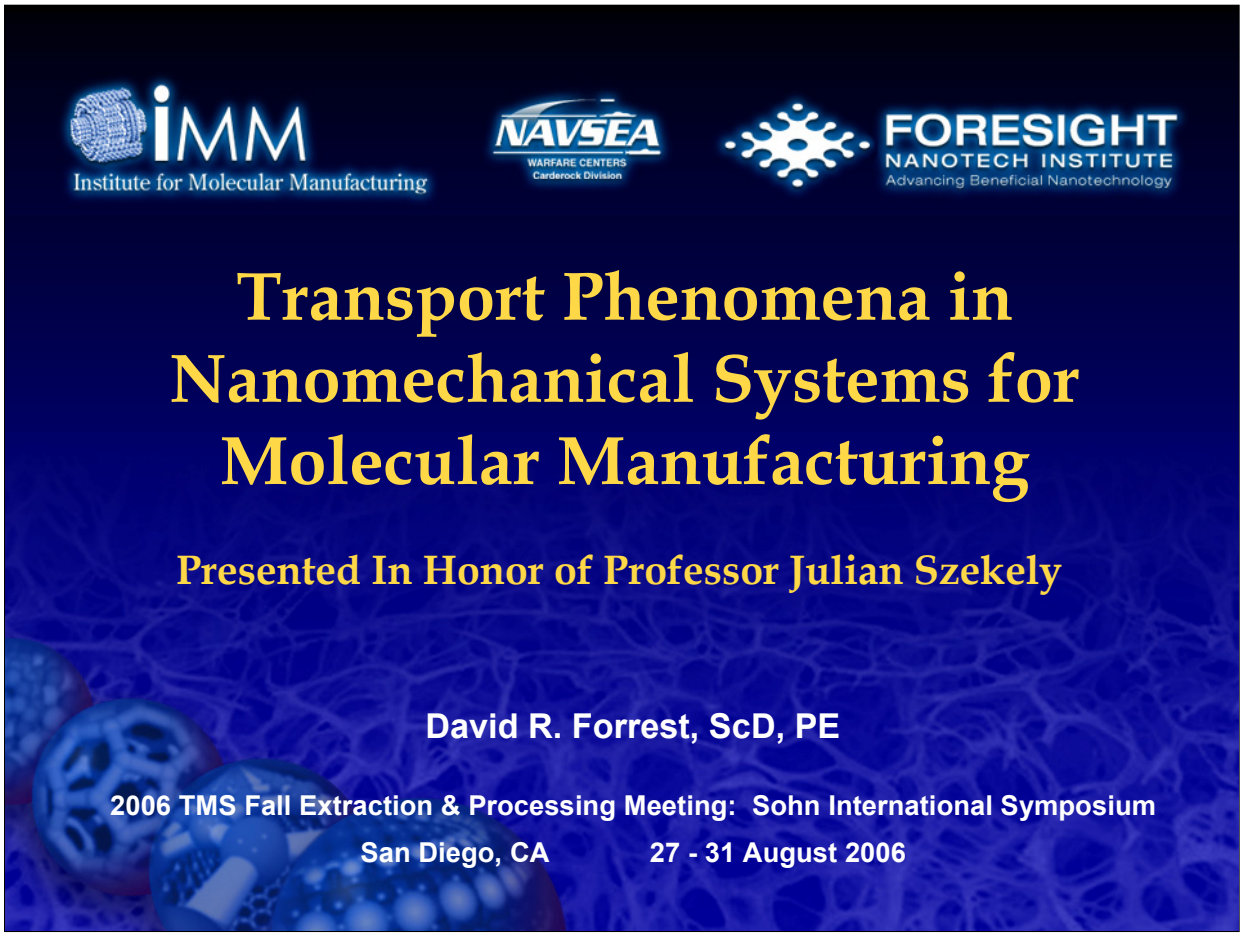
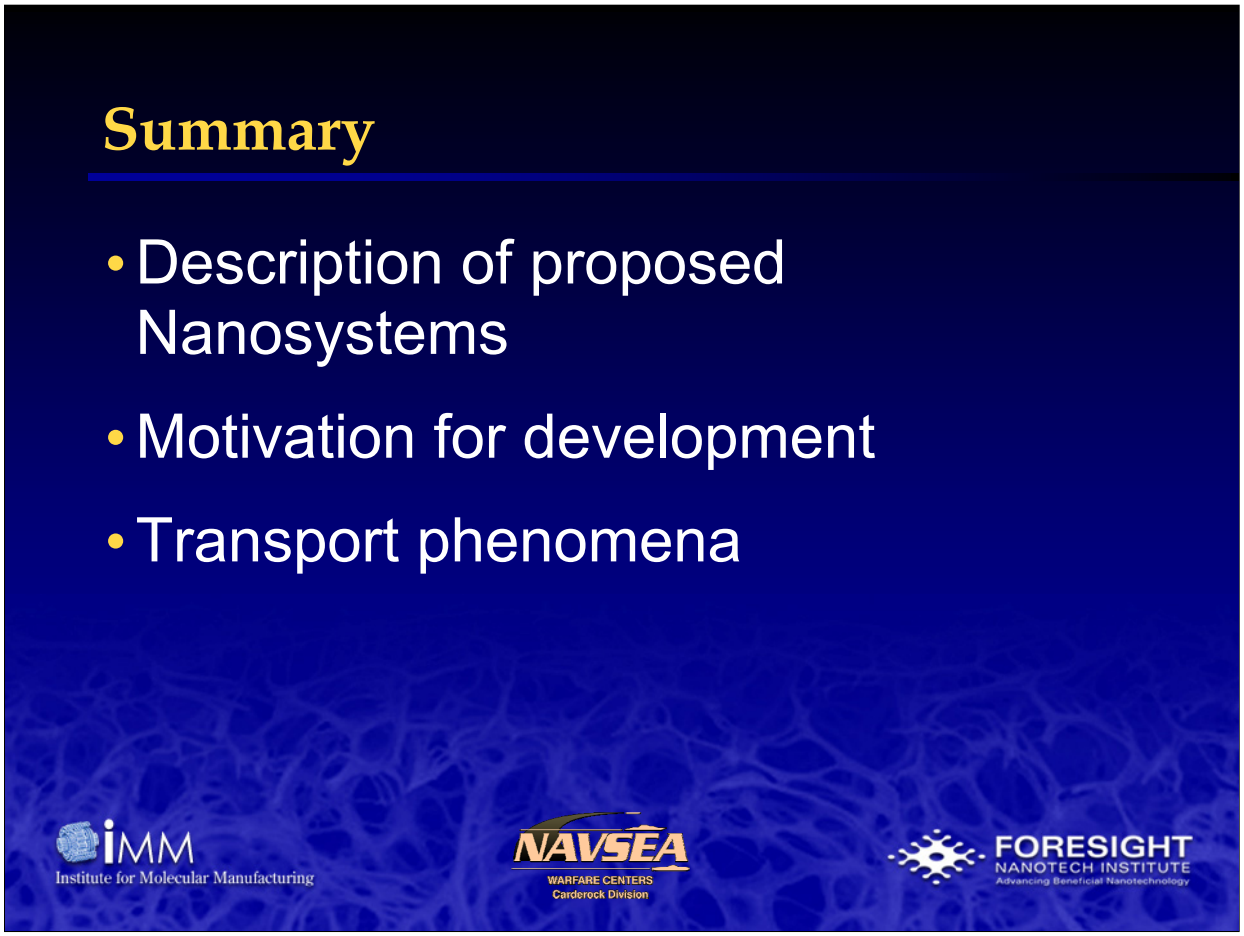



I'd like to acknowledge the three organizations that sponsor and support me: the Naval Surface Warfare Center in Bethesda, Maryland, where I work, the Institute for Molecular Manufacturing (a non-profit in California, of which I'm President), and the Foresight Nanotech Institute, where I'm a Senior Fellow.


Before I dig into the technical content, I'd like to say a few words about the motivation for the topic that I chose to speak about this afternoon. Julian Szekely's legendary work--applying the mathematical analysis of continuum transport phenomena to materials processing systems--has certainly been an inspiration to me in my career, and I'm proud to have played a small part in that effort while I was in his lab at MIT from 1985 to 1991. I know that he was frustrated with me from time to time because I would lose focus on my research to organize talks and seminars on molecular nanotechnology, but he never discouraged me from that pursuit. And now, 20 years later, groups are building molecular machines, ushering us into a new age of manufacturing technology. When I heard that there would be a Szekely reunion session at this conference, I couldn't resist the chance to honor Julian Szekely's legacy with a talk on transport phenomena in nanosystems.


I'll be flipping quickly through these slides, but don't worry if you miss something. This presentation is available online at my website.




Molecular mechanical devices

There are compelling reasons to develop Nanosystems

Can't apply continuum assumptions when analyzing transport phenomena

# Overview

## Vision for Molecular Manufacturing

- Molecular robotic systems
- Large products built to atomic precision
- High performance
- Low cost

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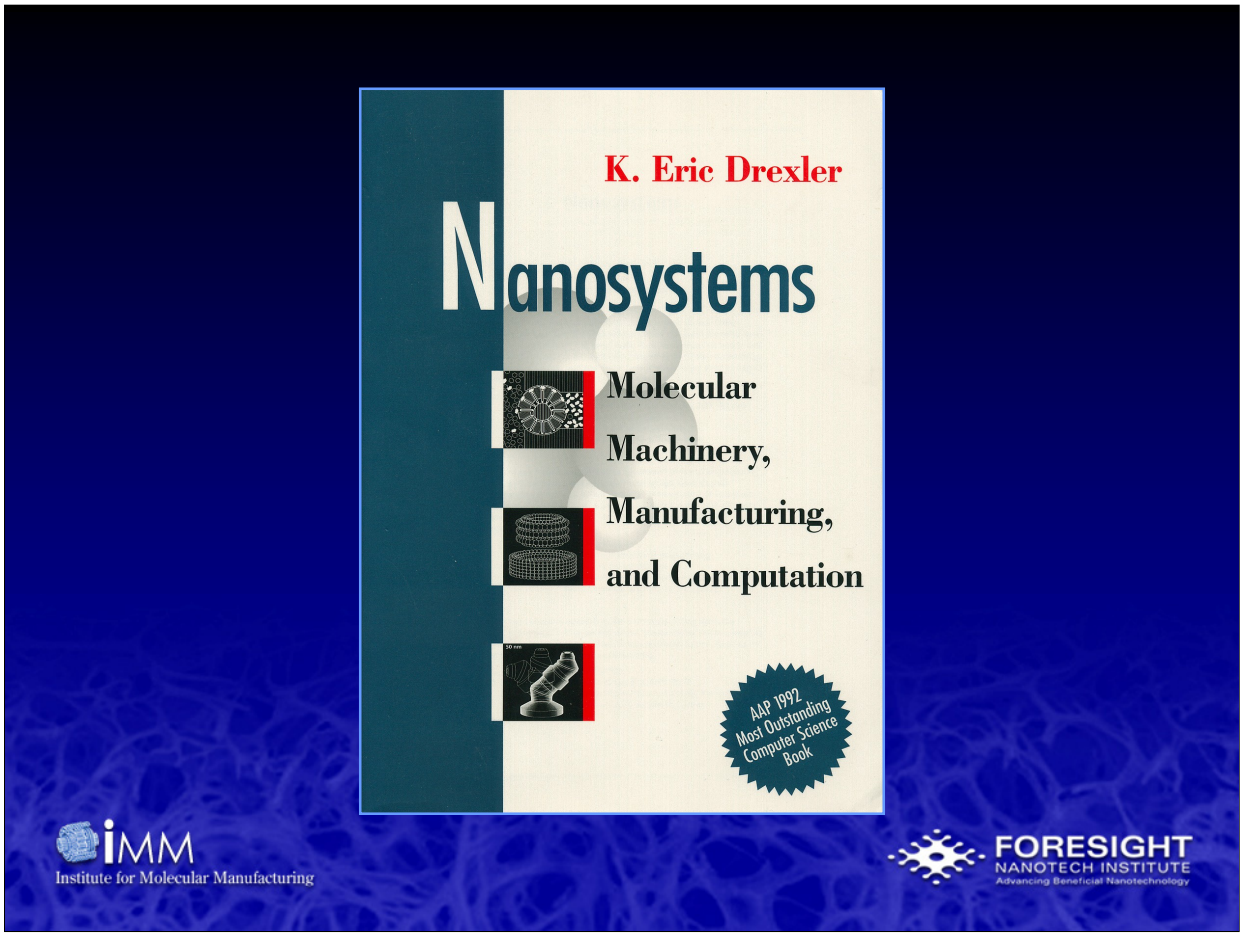
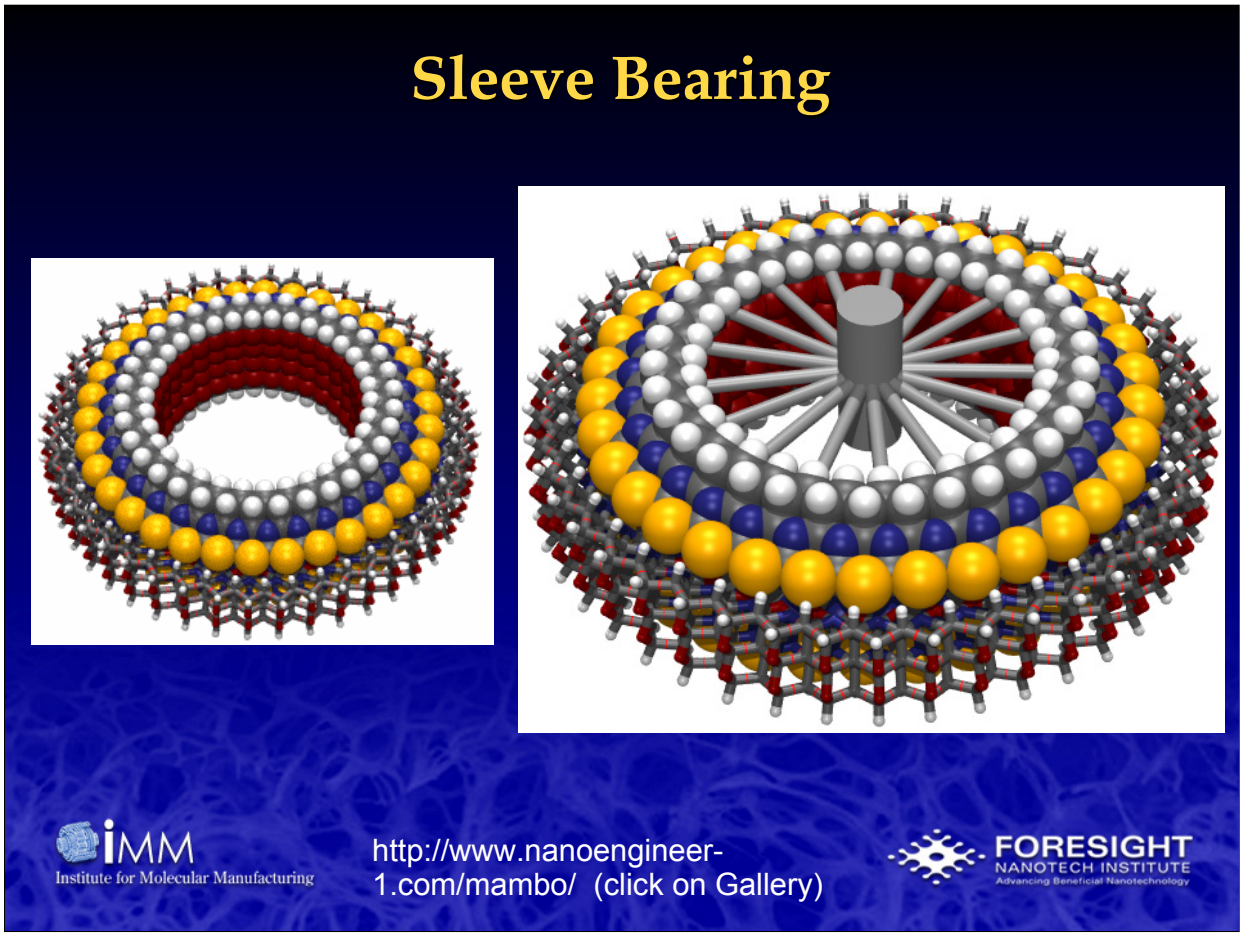
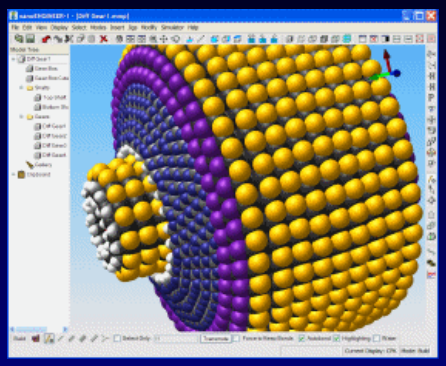

K. Eric Drexler
Nanosystems
Molecular Machinery, Manufacturing, and Computation
AAP 1992 Most Outstanding Computer Science Book
iMM
Institute for Molecular Manufacturing
FORESIGHT
NANOTECH INSTITUTE
Advancing Beneficial Nanotechnology

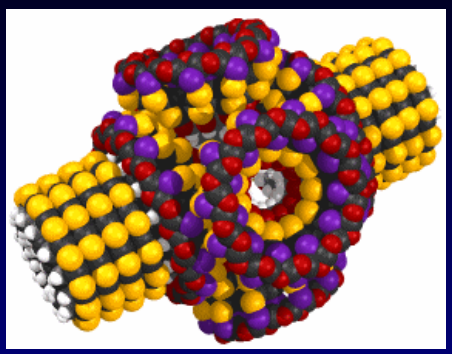



This is the ***strained-shell sleeve bearing*** from Nanosystems (page 296) designed by K. Eric Drexler and Ralph Merkle while they were working together at Xerox PARC The model comprises two molecular components; the *inner shaft* and the *outer sleeve* and contains a total of 2,808 atoms.

With practice, an experienced user can create this bearing in 10-15 minutes. NanoEngineer-1 includes an extrusion tool for creating rods and rings from a molecular fragment (called a *chunk* in NanoEngineer-1). The contraption with spokes connected to the inner shaft is called a ***rotary motor***. This is a type of jig in NanoEngineer-1 that applies torque to the atoms to which it is attached during a molecular dynamics simulation, driving the inner shaft. The rotary motor here had a torque setting of 100 nN-nm and a speed of 500 GHz. These values are extreme and were used to produce an interesting simulation as quickly as possible. A serious engineer assessing the operating conditions of this bearing would have used more reasonable numbers.

# Differential Gear





Name: Differential Gear
Designers: K. Eric Drexler and Ralph Merkle
Date: 1995
Number of components: 7

Number of atoms: 8,292
Width: 5.8 nm
Height: 5.8 nm
Depth: 5.8 nm

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http://www.nanoengineer-1.com/mambo/ (click on Gallery)

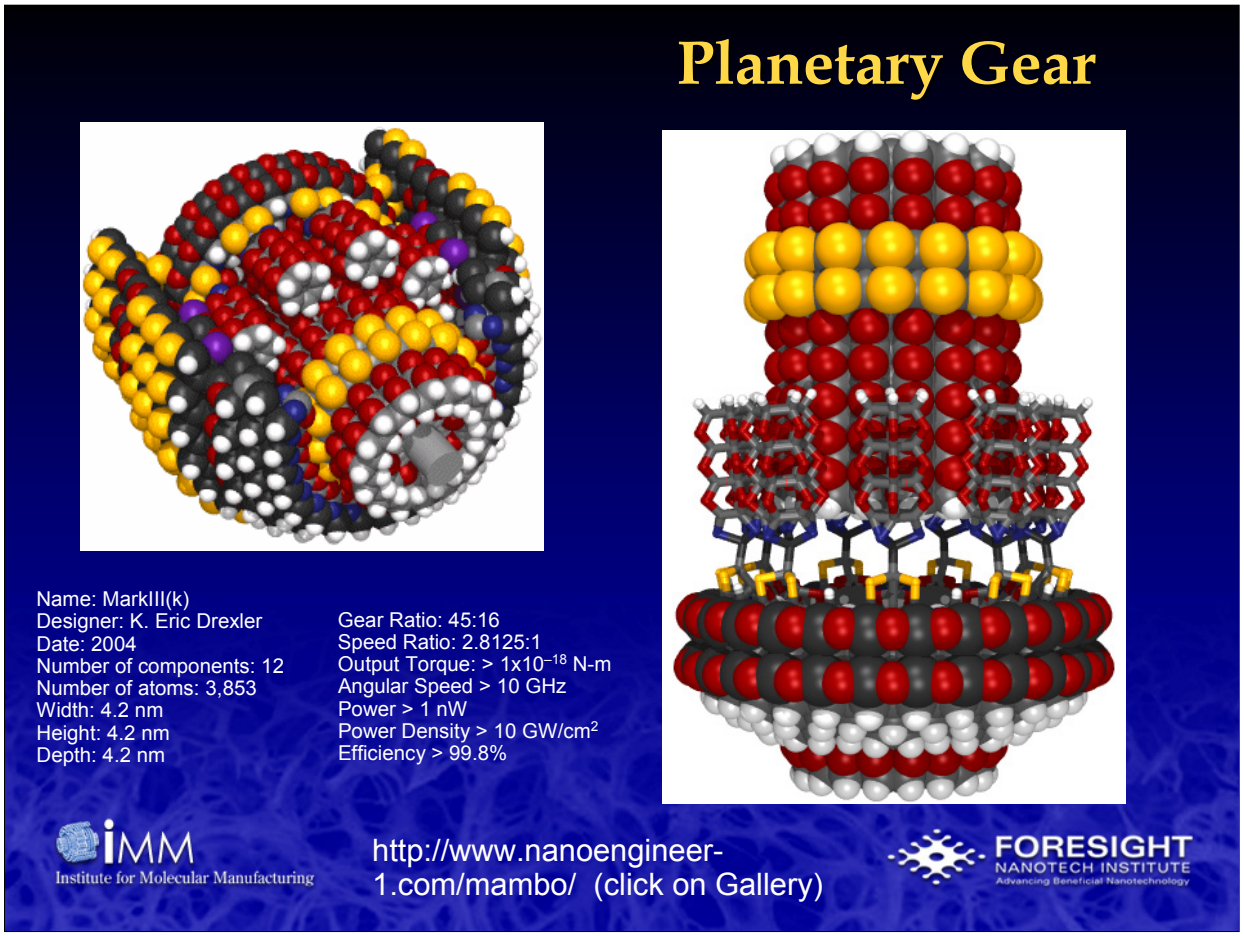
FORESIGHT NANOTECH INSTITUTE Advancing Beneficial Nanotechnology

This animation loop shows the results of a molecular dynamics simulation done with NanoEngineer-1. It is the first time the Drexler-Merkle differential gear has ever been simulated. While the individual frames of the animation loop were rendered using POV-Ray, NanoEngineer-1 generated the POV-Ray files automatically. The gearbox casing was hidden to expose the internal gearing mechanism. Notice that the front and back shafts rotate in opposite directions. If you'd like to see how this was done, click "How I Simulated the Drexler-Merkle Differential Gear".

Dr. Drexler provides the following brief description of the differential gear:
In this view the two cylindrical shafts and their facing bevel (conical) gears are shown, along with two of the four casing-mounted pinion gears that mesh with both shaft-gears. Acceptably smooth motion (despite the atomic granularity of the building blocks) is made possible by geometry and symmetries. For example, the shaft-gears have 14-fold symmetry, while the casing has 4-fold symmetry; if one pinion gear is exactly opposite a shaft-gear tooth, its 90-degree partners will be opposite shaft-gear *grooves.* Thus, energy fluctuations at the tooth-meshing frequency will cancel, leaving only higher-frequency, lower-amplitude fluctuations as barriers to rotation. The shafts rotate in the casing on standard sliding-interface bearings, using the same principle to achieve smooth motion. The lowest quality bearings are those between the pinion gears and the casing, which lack the regularity required for high smoothness.

The structure is designed to be built chiefly of hydrogen (white), carbon (gray), silicon (black), nitrogen (blue), phosphorus (purple), oxygen (red), and sulphur (yellow). The larger size of second-row atoms helps in constructing tapered gears and reduces the number of atoms needed to construct the outer cylinder of the casing. Such structures are far beyond the state of the art of chemical synthesis today, but their design and modeling is becoming straightforward.

*- K. Eric Drexler*



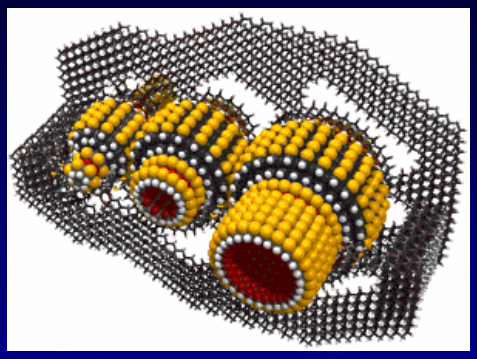

This is the MarkIII(k), a planetary gear created by K. Eric Drexler. A planetary gear couples an input shaft via a sun gear to an output shaft through a set of planet gears (attached to the output shaft by a planet carrier). The planet gears roll between the sun gear and a ring gear on the inner surface of a casing. The animation below was produced from a NanoEngineer-1 molecular dynamics simulation. A section of the casing atoms have been hidden to expose the internal gearing assembly.

Planetary gears are attractive targets for molecular modeling because (with careful choice of planet numbers and sun- and ring-gear symmetries) the overall symmetry of the system virtually guarantees low energy barriers along the desired motion coordinate. They also pack considerable complexity into a small structure.

Planetary gears are common mechanical systems used for speed reduction (= torque multiplication). Macroscale versions are found in automobile transmissions, electric screwdrivers, and Mars landers.
The MarkIII(k) gear updates an early 1990s design by Drexler and Merkle, modified to reduce interactions between the sun gear and the bases of the planet gears. The original version was designed with very small moving parts in order to fit the computational constraints of the time. The planet gears are near the lower limits of diameter for functional gear components, and because of this, the "gear teeth" in this system are better thought of as smooth, low-amplitude corrugations in the gear surfaces.

# Speed Reducer Gears

Designer: Mark Sims
Date: August 31, 2005
Number of components: 4
Number of atoms: 15,342
Width: 11.3 nm
Height: 7.5 nm
Depth: 5.6 nm
Gear Ratio: 13:6
Speed Ratio: 2.167:1
Torque (large gear): 10 nN-nm



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http://www.nanoengineer-1.com/mambo/ (click on Gallery)

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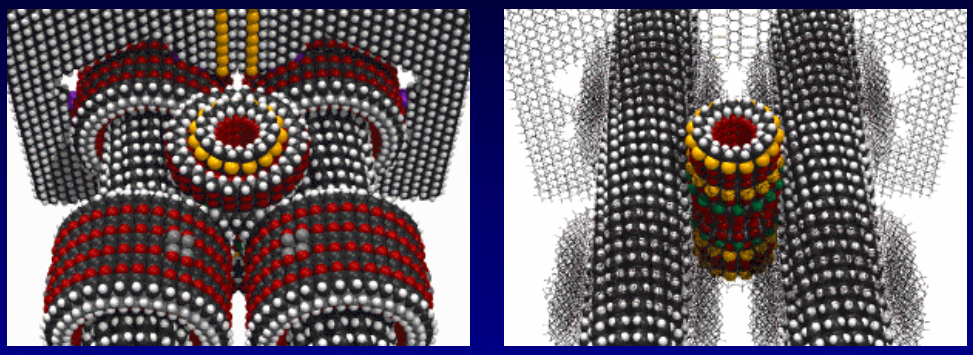
The SRG-III is the third parallel-shaft speed reducer gear created by Mark Sims. A hybrid of the SRG-I and SRG-II, it is the first molecular gear train ever designed. With 15,342 atoms, the SRG-III is the second largest nanomechanical device ever modeled in atomic detail.

# Worm Drive Assembly



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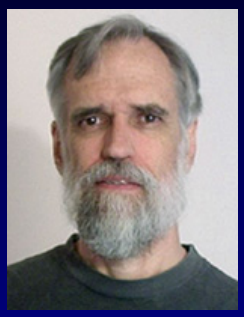
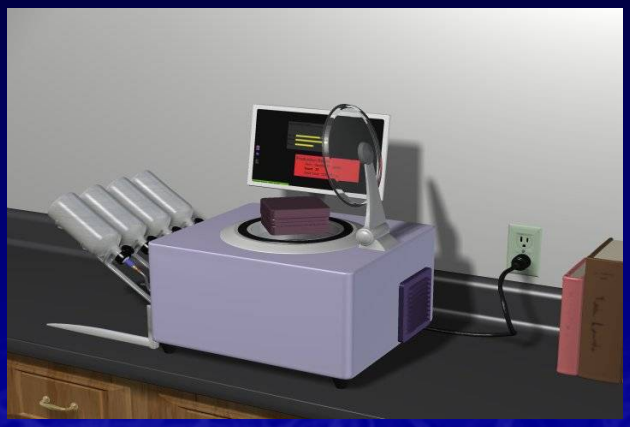
This worm drive assembly designed by K. Eric Drexler, Josh Hall, Ninad Sathaye and Mark Sims includes 11 components totalling 25,374 atoms. The animations below have been created from simulation results using NanoEngineer-1 Alpha 7, taking just over 370 hours to complete on a Dell laptop running WindowsXP. It is the largest model ever simulated with NanoEngineer-1.

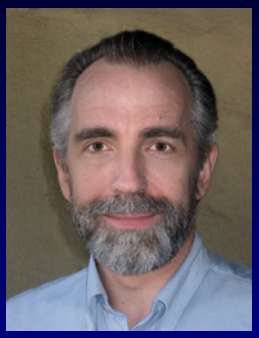
http://www.nanoengineer-1.com/mambo/index.php?option=com_content&task=view&id=60&Itemid=57

# Desktop Assembler Animation



John Burch





Eric Drexler

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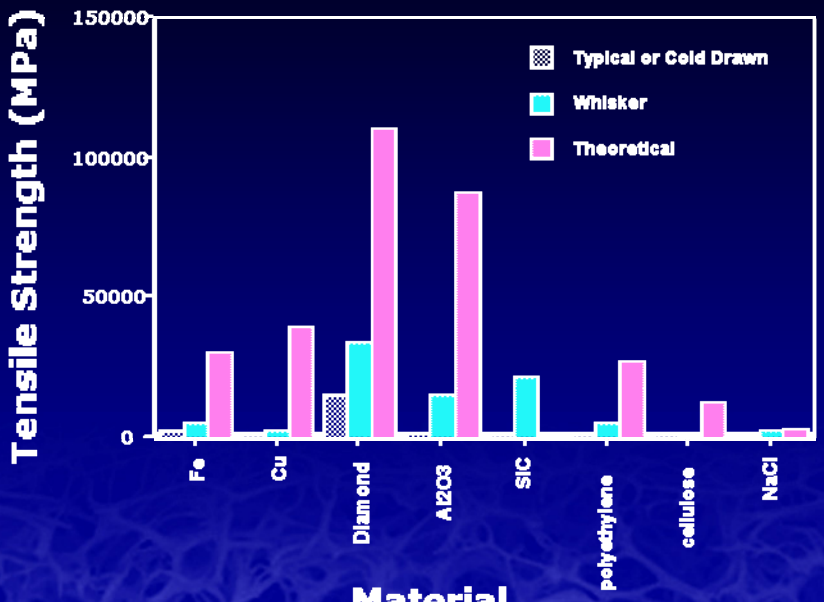
Switch to Animation

http://www.foresight.org/nanofactory.mov

# Stronger Materials

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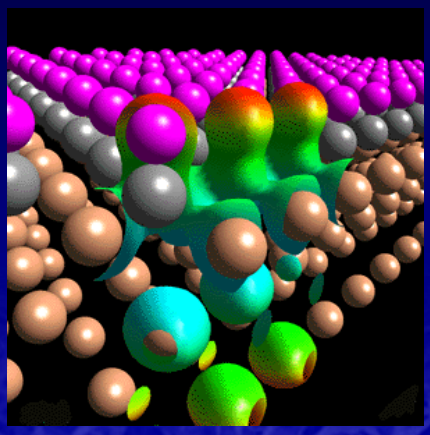
# Property Improvements

- Near-Perfect Structures
  - Excellent toughness (initiators gone)
  - Low friction, low wear (atomically smooth surfaces, contaminants sealed)
  - Good corrosion resistance (initiators gone; coherent, inert terminating surfaces)
  - Good fatigue strength (initiators gone)
  - Reduced creep (no initial dislocations, hard to form)
  - Good oxidation resistance (intermetallics, practical oxides)



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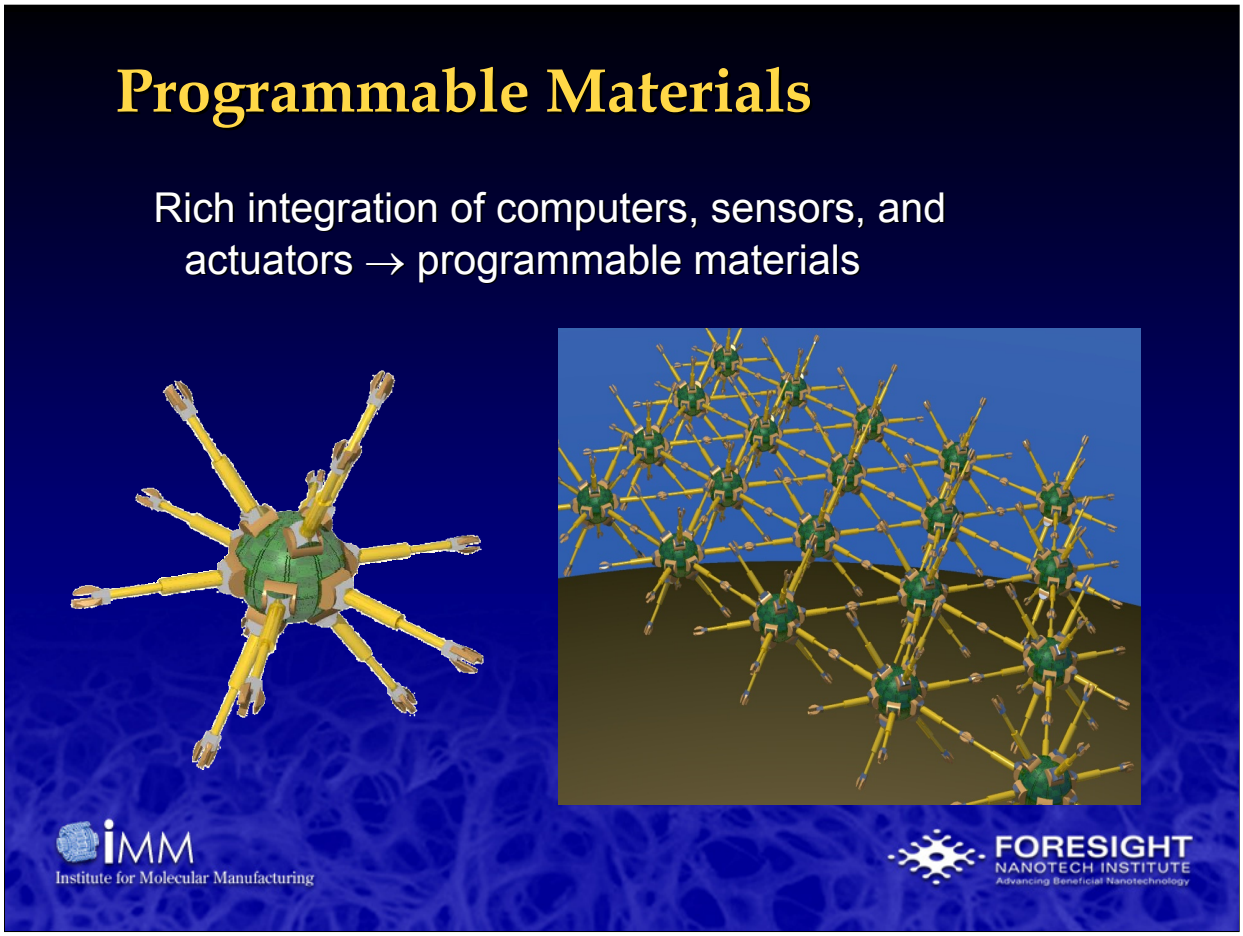
http://www.accelrys.com/gallery/sstate.html




http://www.foresight.org/Nanomedicine/Gallery/Artist/Hall.html

# Envisioned Products

- Powerful desktop computers ~ billion processors
- Abundant energy (solar)
- Cures for serious diseases using medical nanorobots
- New materials 100 times stronger than steel
- A clean environment
- More molecular manufacturing systems

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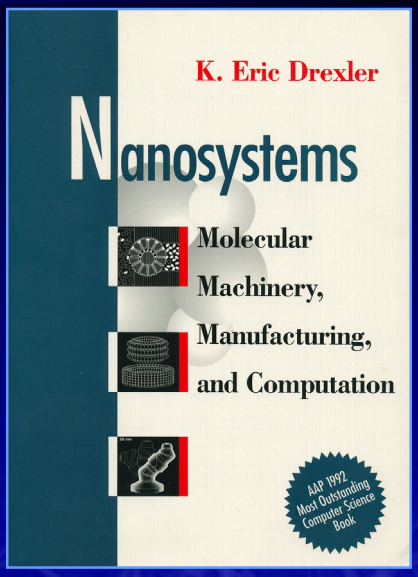
# Friction Between Sliding Surfaces

- Drexler,
  Molecular Gears and Bearings

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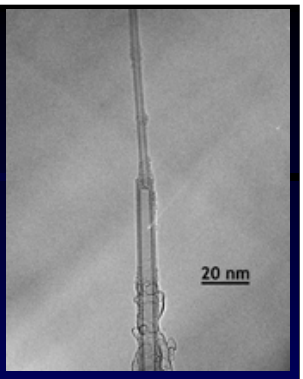
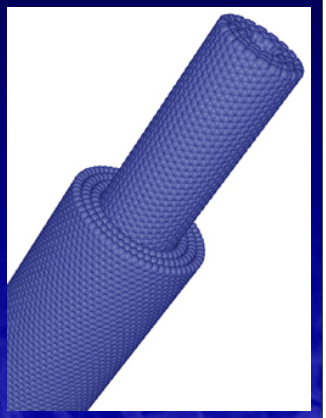
# Friction Between Sliding Surfaces

- Cumings and Zettl, Nested Carbon Nanotubes
- Static friction force < $2.3 \times 10^{-14}$ N/atom
- Dynamic friction force < $1.5 \times 10^{-14}$ N/atom
- About 1000 times less than atomic-scale measurements for conventional materials



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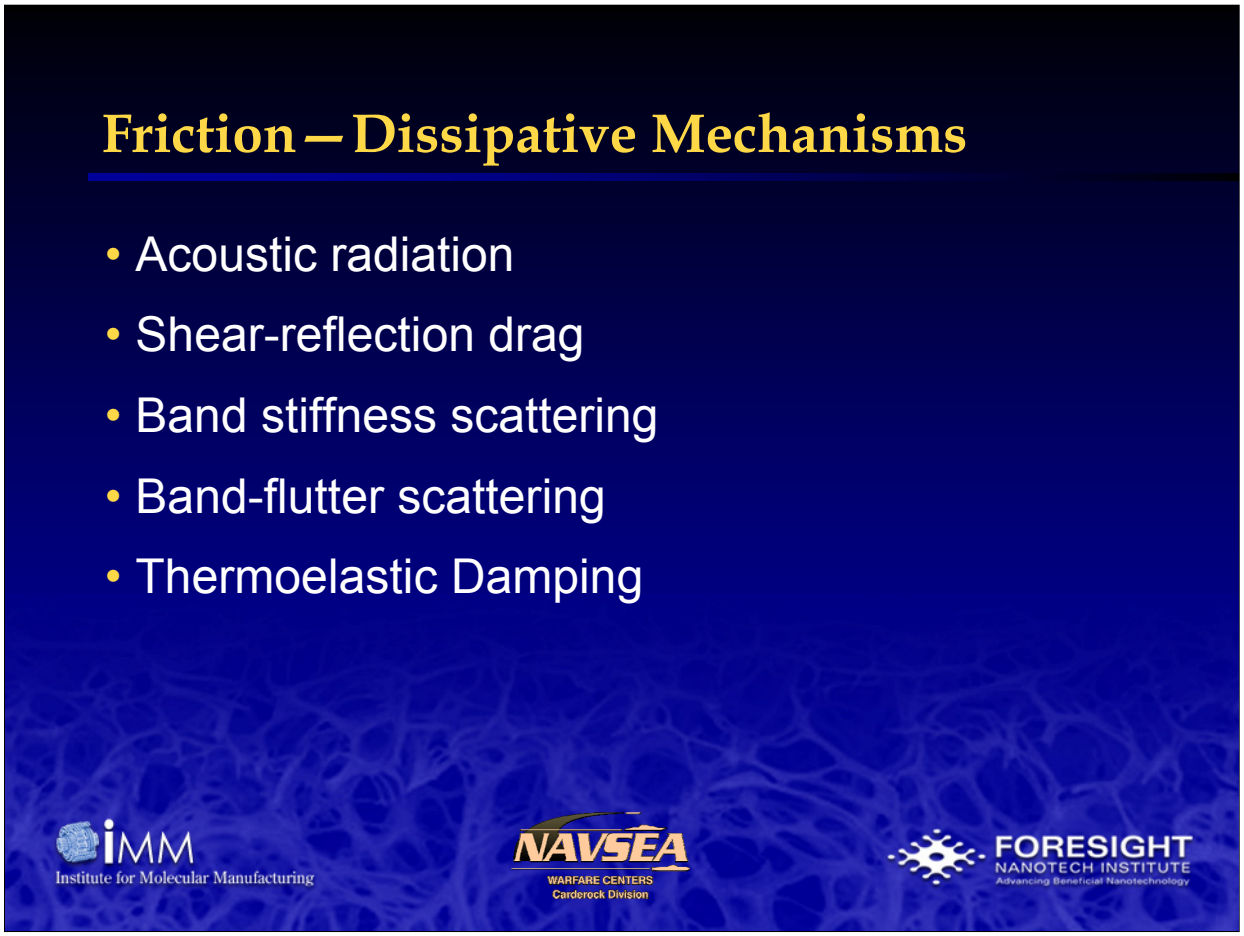


***Nanosystems: Molecular Machinery, Manufacturing, and Computation***
http://e-drexler.com/p/idx04/00/0411nanosystems.html
http://www.foresight.org/Nanosystems/toc.html

# Fluid Flow — Molecular Dynamics

- Newtonian mechanics applied to particles, conservation of potential and kinetic energy

$$F = ma = -\frac{dU}{dr}$$

- Interactions via Lennard-Jones, REBO

$$U_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right],\ \sigma_{C-He} = 3.191\text{Å},\ \varepsilon_{C-He} = 0.26646\,zJ$$

$$U(r) = \frac{1}{2}\sum_{\alpha,\beta}\left[V_R(r_{\alpha\beta}) - B_{\alpha\beta}V_A(r_{\alpha\beta})\right],\ B = f(\text{bond angles, torsional angles, bond lengths, atomic coordination})$$

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**Dynamics of fluid flow inside carbon nanotubes,** Robert E Tuzun *et al* 1996 *Nanotechnology* **7** 241-246

www.physics.unc.edu/~zhou/muri/pubfiles/Brenner_JPCM.second.generation.pdf

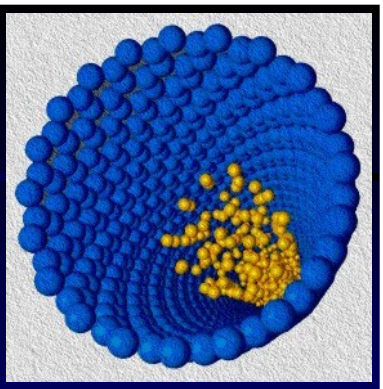
http://phelafel.technion.ac.il/~syanivg/nanotubes/molecular_dynamics.html

http://sinnott.mse.ufl.edu/sub05_nano-fluid-mech.html

http://sinnott.mse.ufl.edu/sub05b_nanomechanics.html

http://phjoan5.technion.ac.il/~talimu/rebo1.html

# Fluid Flow



Molecular Dynamics Studies of Tuzon, *et al.* (1996)

- Helium and Argon in carbon nanotubes
  - Flow rate reduced with higher fluid density
  - Helium flowed faster than Argon
  - Flexing of tubes (resonant modes) impeded the flow

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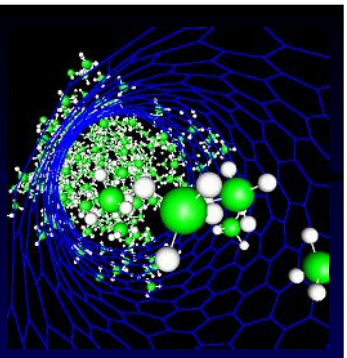
**Dynamics of fluid flow inside carbon nanotubes,** Robert E Tuzun *et al* 1996 *Nanotechnology* **7** 241-246

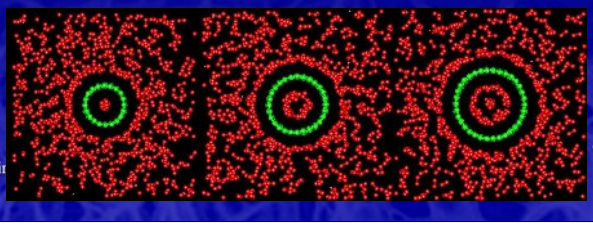
# Fluid Flow
# Sinnott (U. Florida)



Molecular Dynamics Studies

- Methane in carbon nanotubes
  - Single file when diameter too small
  - Implications for gas separation
- Oxygen in nanotubes
- Open source code (REBO)

QuickTime™ and a YUV420 codec decompressor are needed to see this picture.



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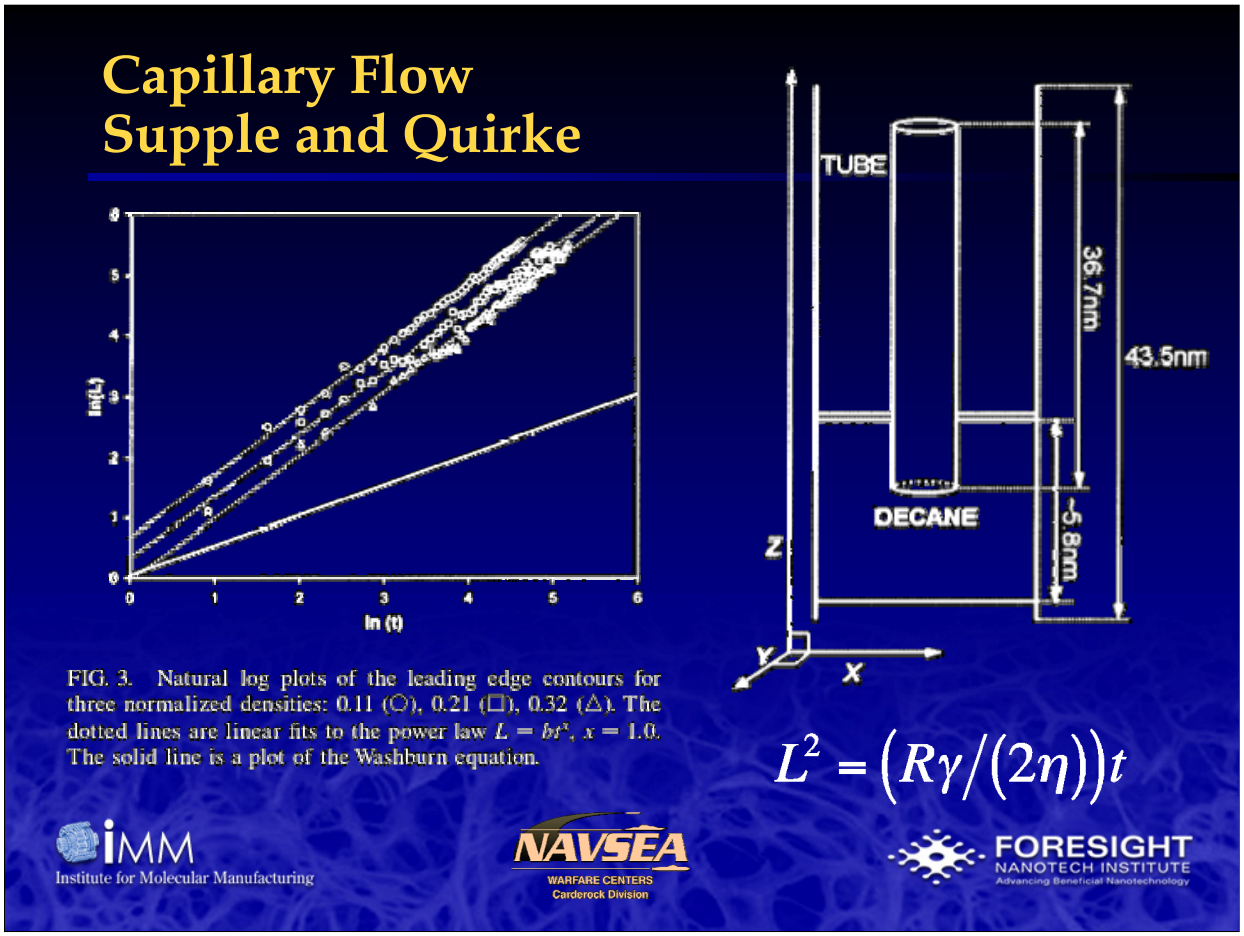
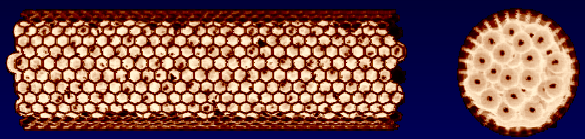
http://sinnott.mse.ufl.edu/sub05a_nanofluidics.html
http://sinnott.mse.ufl.edu/sub05_nano-fluid-mech.html
http://www.caer.uky.edu/energeia/PDF/vol14_2.pdf




S. Supple and N. Quirke, " Rapid Imbition of Fluids in Carbon Nanotubes," Physical Review Letters, v. 90, no. 21, 30 May 2003 , 214501 (4).

# Continuum Approximations
# Sokhan, Nicholson, Quirke



$g_z \longrightarrow$

$$F_y = -\tau_o^{-1} m \frac{2\alpha}{2-\alpha} u_w$$

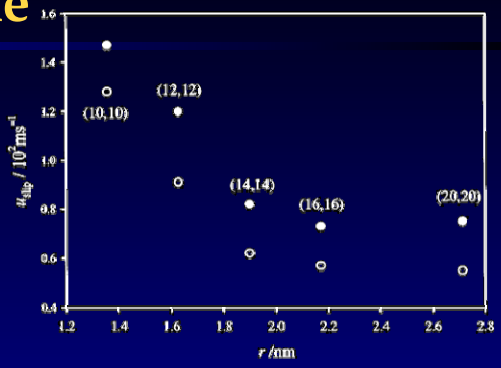



FIG. 7. Slip velocity for rigid and thermal nanotubes as a function of the nanotube diameter.

- Methane in nanotubes
- Compared approach using Maxwell coefficient $\alpha$ to MD-derived friction
- Maxwell slip velocities about 40% higher than MD-derived
- Using MD-derived friction field, can apply continuum approximations

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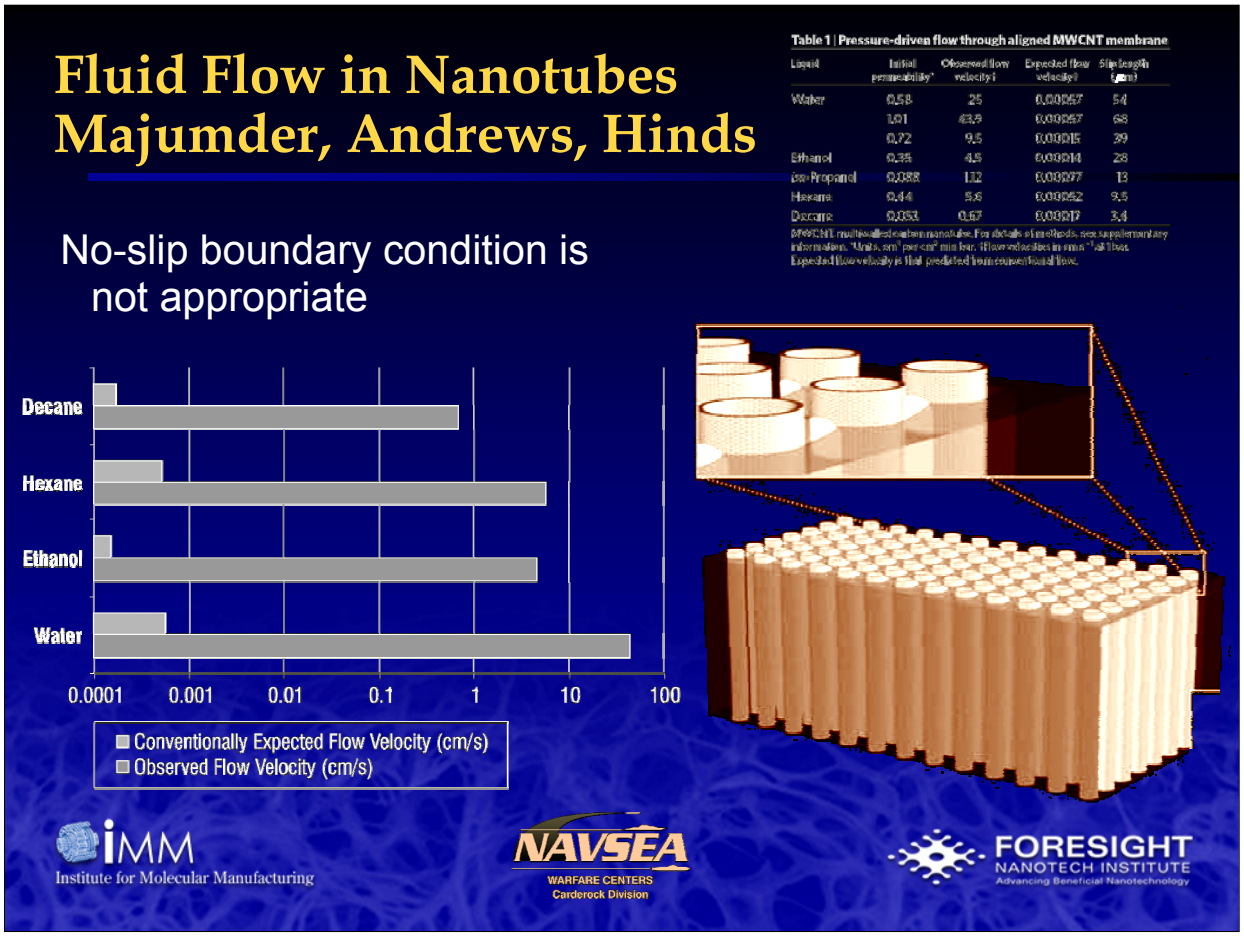
Sokhan, et al., "Fluid flow in nanopores: Accurate boundary conditions for carbon nanotubes," J. Chemical Physics, v. 117, no. 18, 8 November 2002, p. 8531-8539.



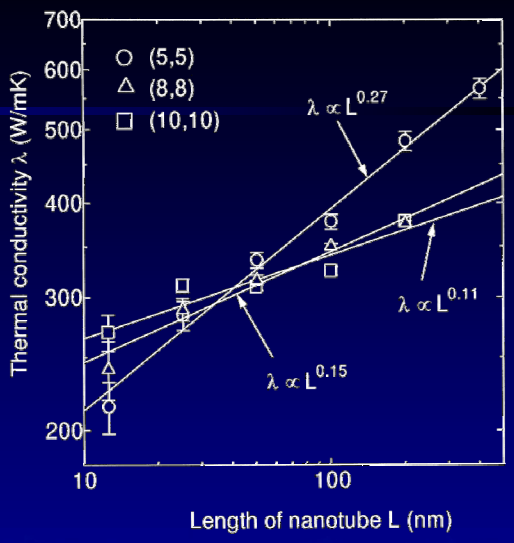

http://www.caer.uky.edu/**energeia**/PDF/vol17_2.pdf

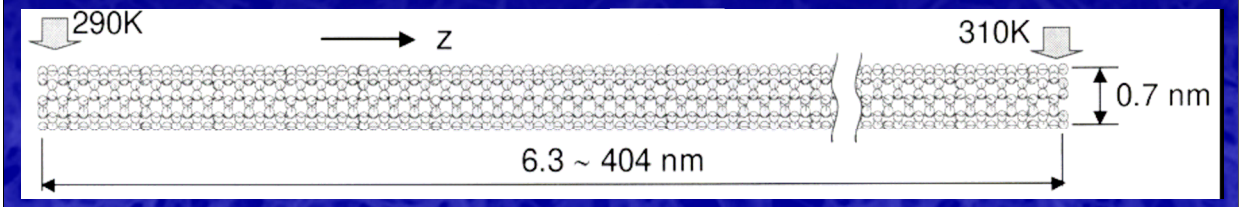
Majumder, et al., "Enhanced Flow in Carbon Nanotubes," Nature, v. 438, 3 Nov. 2005, p. 44.

# Heat Transfer in Carbon Nanotubes

Maruyama (2003)

- Lattice vibration transport dominant
- Increases with length
- Mean free path of energy-carrying phonon




**A MOLECULAR DYNAMICS SIMULATION OF HEAT CONDUCTION OF A FINITE LENGTH SINGLE-WALLED CARBON NANOTUBE, *Shigeo Maruyama,* Microscale Thermophysical Engineering, 7:41–50, 2003**

**This has implications for all nanomachine components.**

# Computational Tools — DFT

- Abinit
- ADF
- AIMPRO
- Atomistix Toolkit
- CADPAC
- CASTEP
- CPMD
- DACAPO
- DALTON
- deMon2K
- DFT++
- DMol3
- EXCITING
- Fireball
- GAMESS (UK)
- GAMESS (US)
- GAUSSIAN
- JAGUAR
- MOLCAS
- MPQC
- NWChem
- OCTOPUS
- ORCA
- OpenMX
- ParaGAUSS[1]
- Q-Chem
- Quantum-ESPRESSO
- SIESTA
- TURBOMOLE
- VASP
- PWscf
- WIEN2k
- Spartan
- FSatom, dozens of free and proprietary DFT programs

http://www.wikipedia.org/wiki/Density-functional_theory

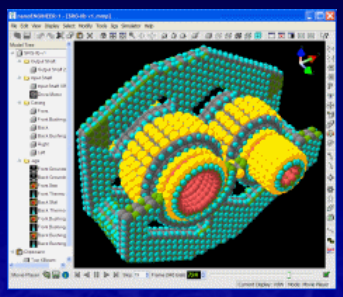
# Computational Tools—Molecular Dynamics

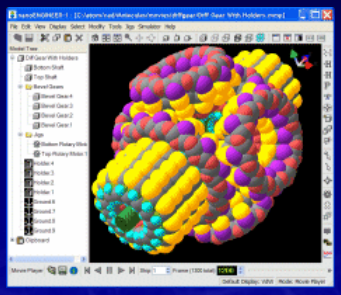
- ABINIT (DFT)
- AMBER (classical)
- CPMD (DFT)
- CHARMM (classical)
- DL_POLY (classical)
- ESPResSo (classical coarse-grain MD, specialized for polymer dynamics)
- GROMACS (classical)
- GROMOS
- LAMMPS [1]
- MOE
- NAMD
- PWscf
- QUANTUM 3.1
- SIESTA (DFT)
- VASP (Ab-initio)
- TINKER (classical) http://dasher.wustl.edu/tinker/

http://en.wikipedia.org/wiki/Molecular_dynamics

# Computational Tools—NanoRex

http://www.nanoengineer-1.com/mambo/





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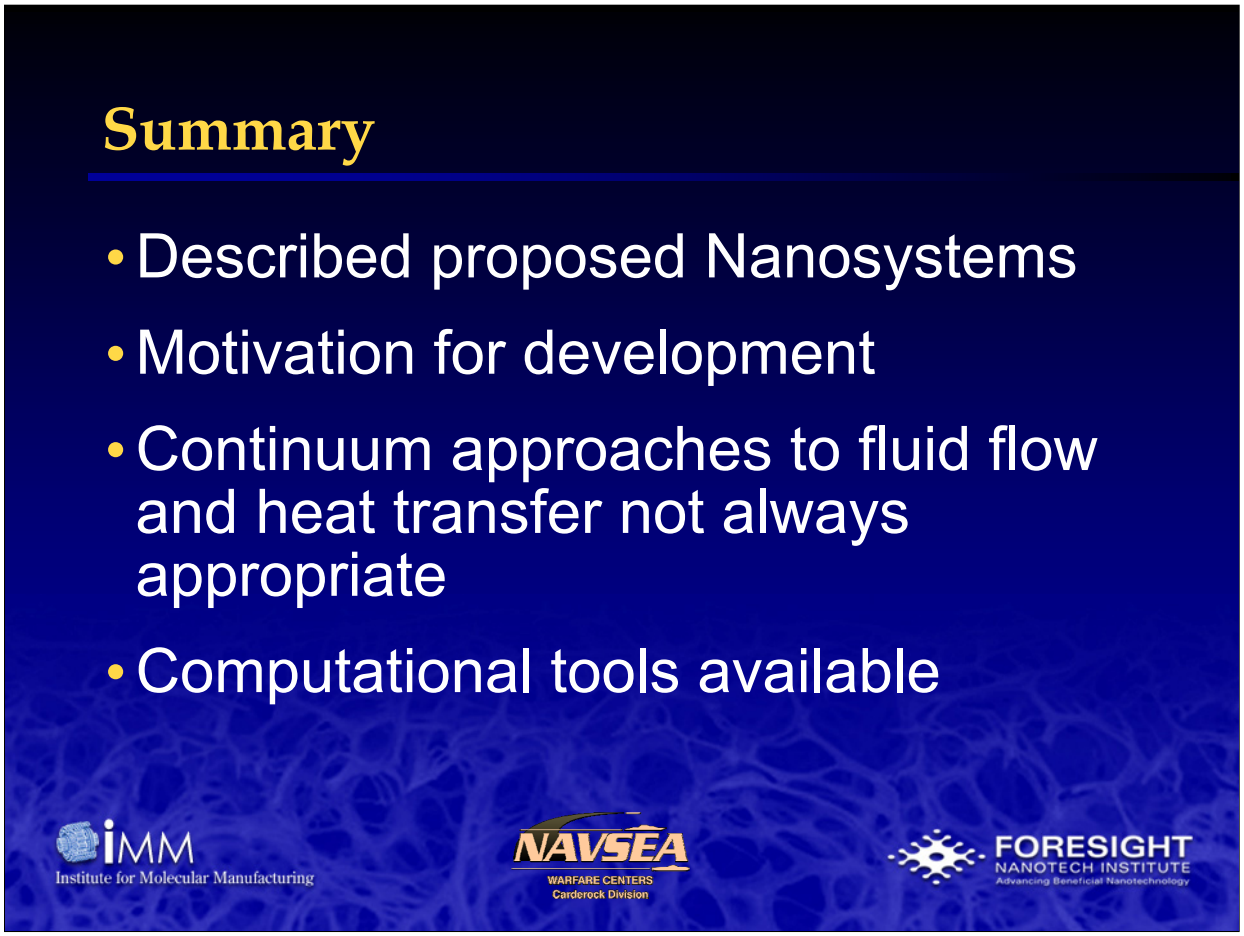


Molecular mechanical devices

There are compelling reasons to develop Nanosystems

Can't apply continuum assumptions when analyzing transport phenomena

http://davidrforrest.com/szekely

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NEMS: http://nano.caltech.edu/papers/Ekinci-RSI2005.pdf

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