

NANO-D

Algorithmes adaptatifs pour la modélisation et la simulation de nanosystèmes

Stephane Redon

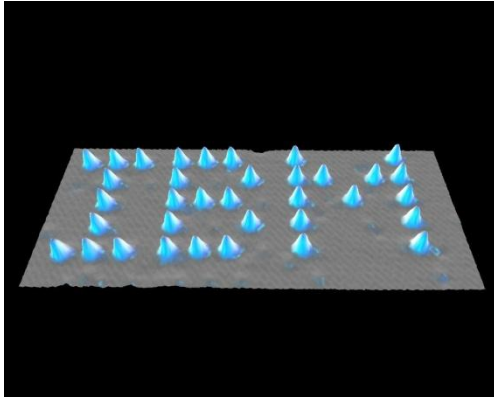
NANO-D

INRIA Grenoble – Rhône-Alpes

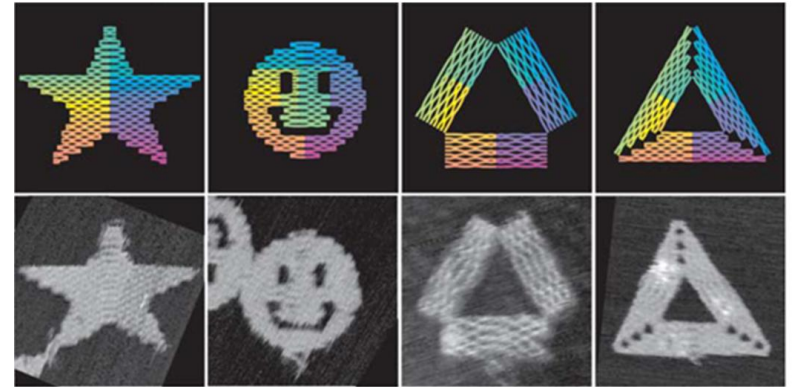
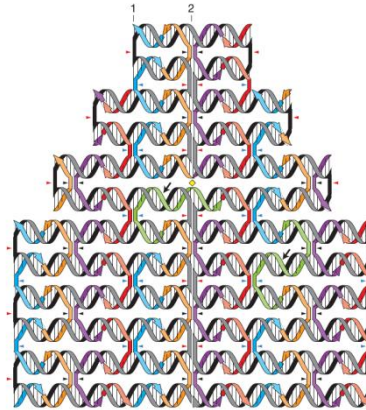
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Nanoscience is all around

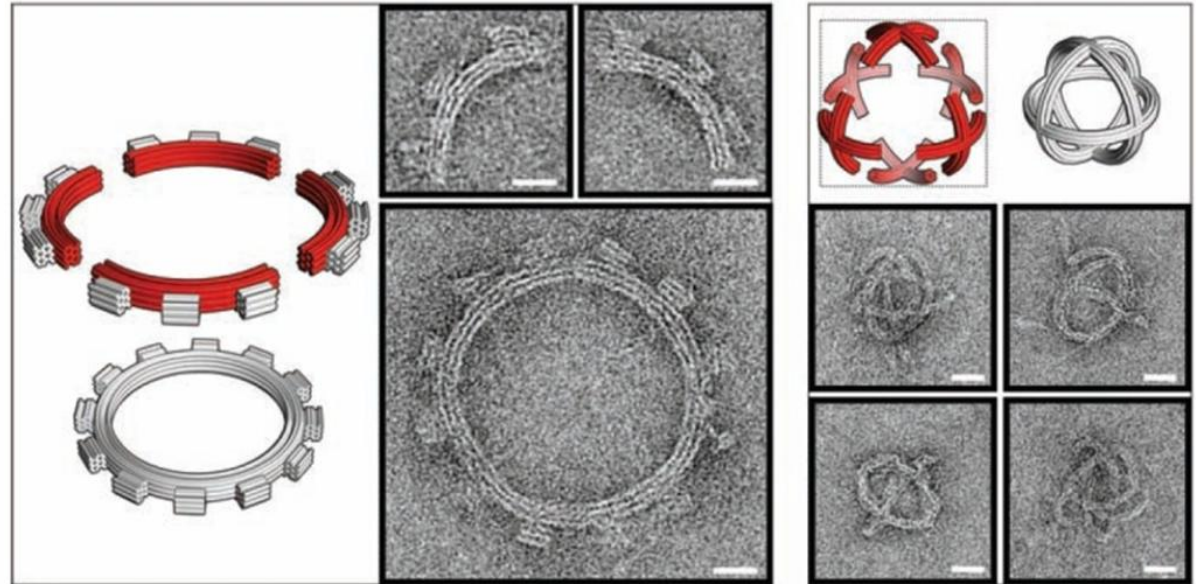
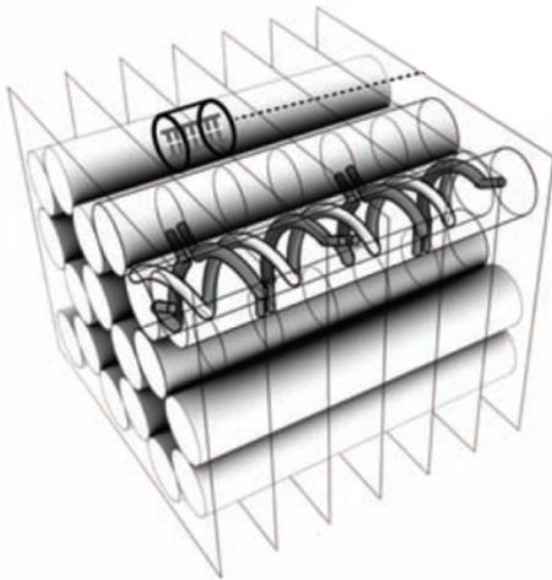
Nanoscience is all around



[Eigler and Schweizer, Nature 1990]

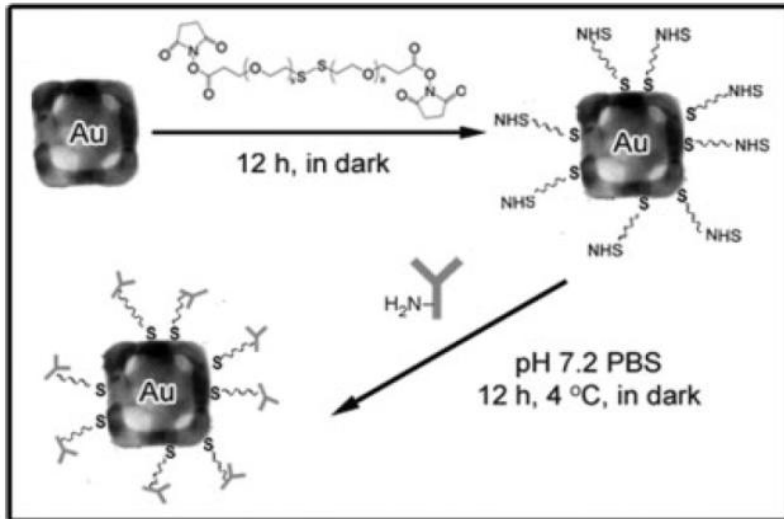


[Rothemund, Nature 2006]

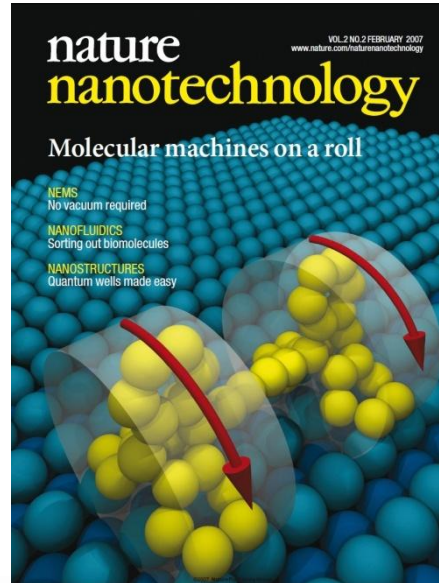


[Dietz et al., Science 2009]

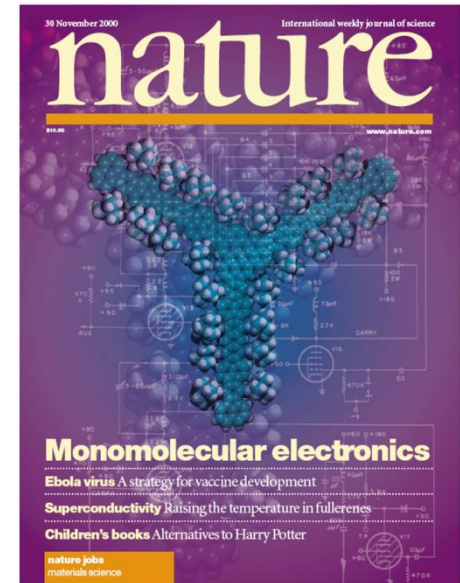
Nanoscience is all around



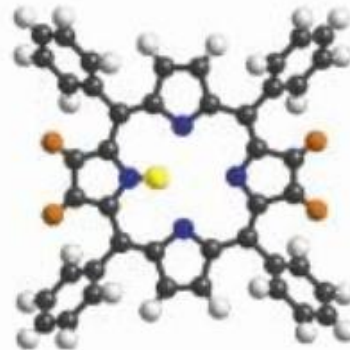
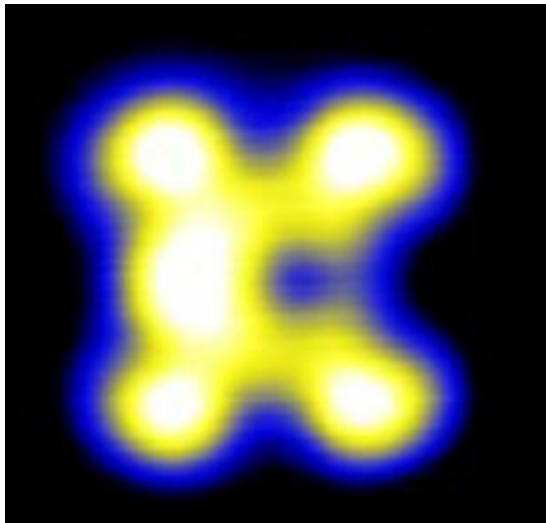
[Chen et al., 2005]



[Grill et al., 2007]



[Joachim et al., 2000]



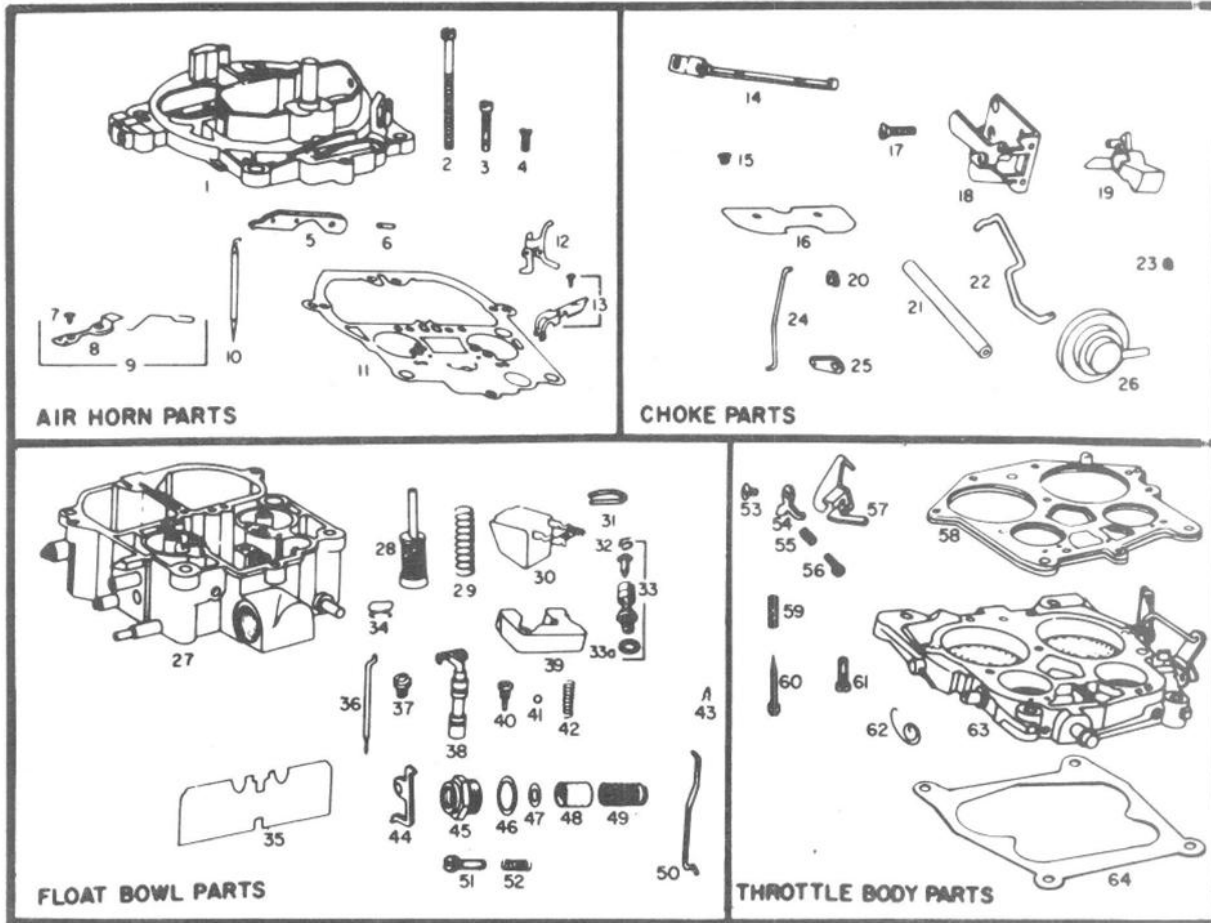
- Drug design
- Materials science
- Chemistry
- Physics
- Electronics
- etc.

[Auwärter et al., Nature Nanotechnology, 2011] (ERC Advanced Grant MolART)

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**Nanodevices will be designed
and prototyped on computers**

MACRO Technology: from schematics...



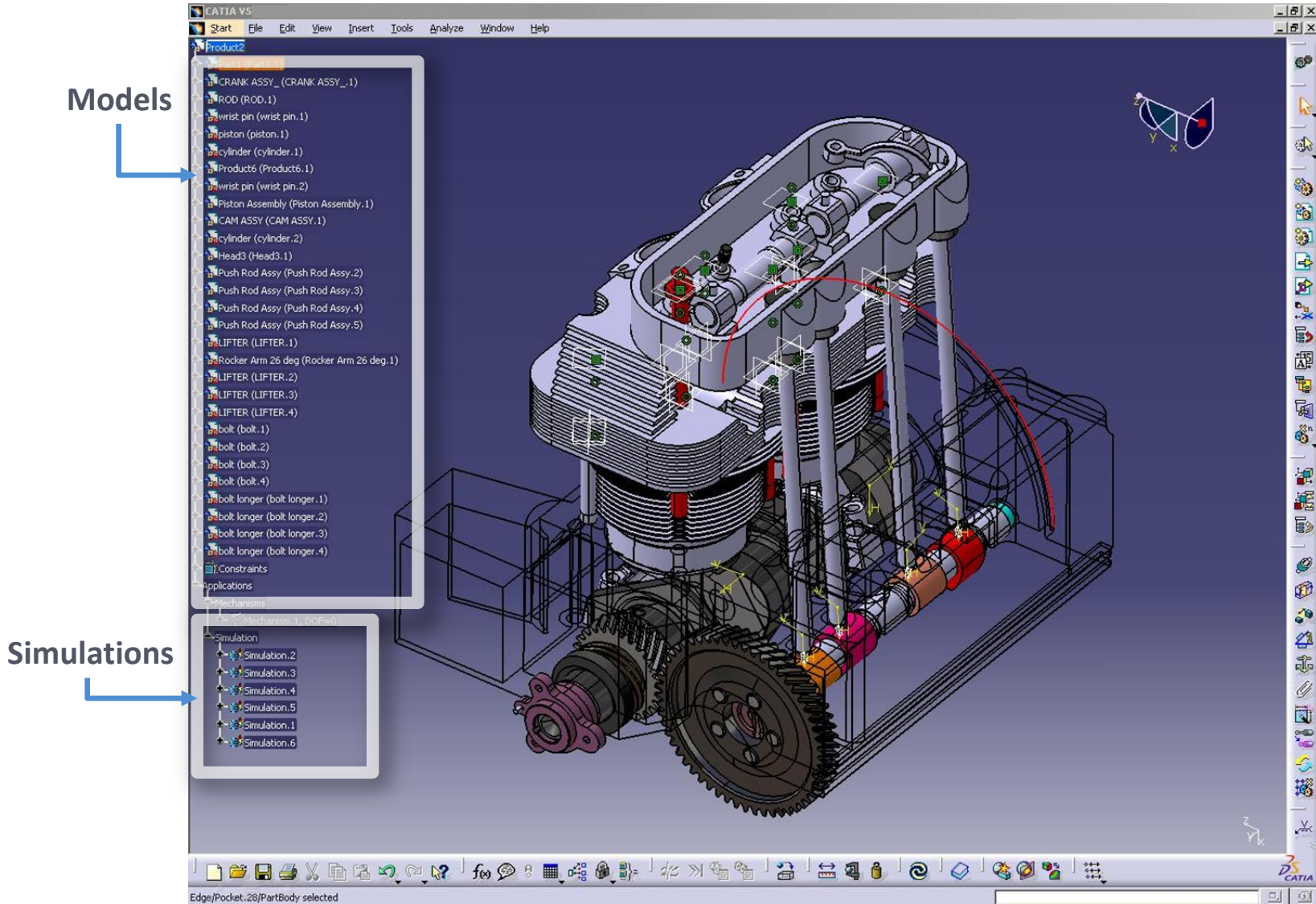
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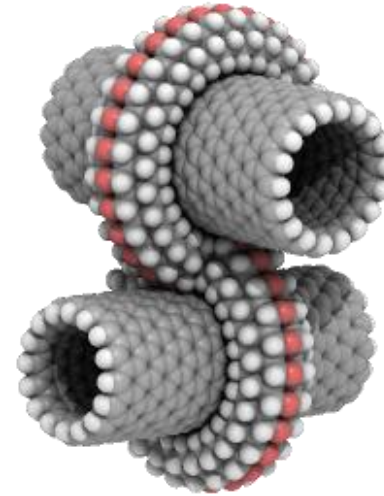
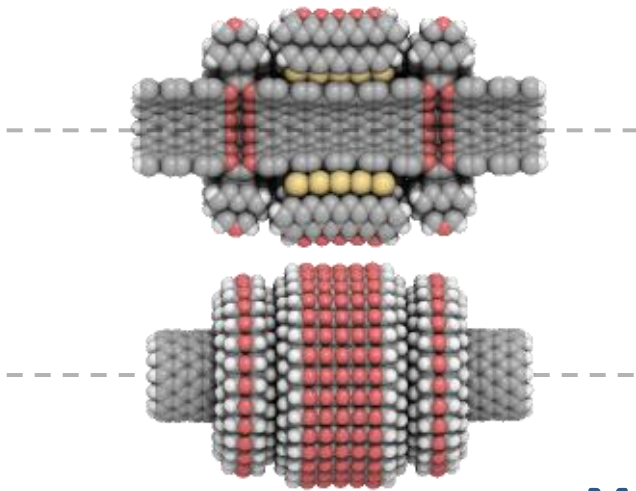
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 MODEL 4MV QUADRAJET
 1971 CHEVROLET, CHEVELLE,
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 350 CUBIC INCH ENGINE

BULLETIN 9C-3058
 DATE: NOVEMBER, 1971
 PAGE 1

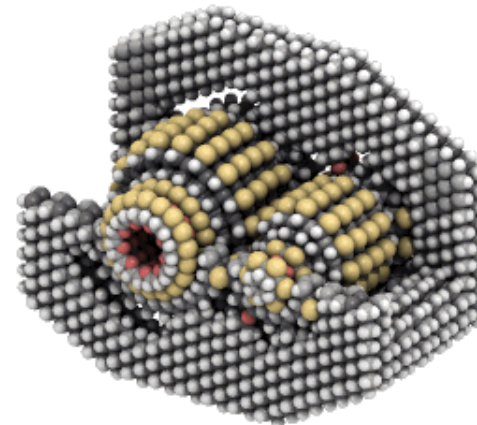
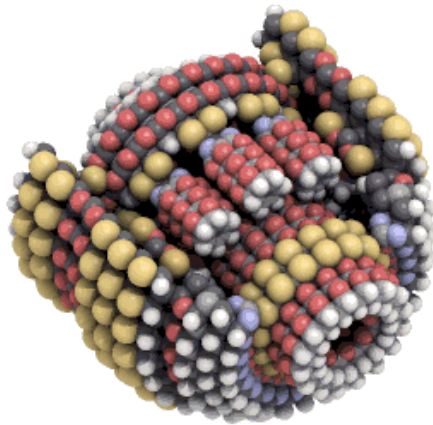
MACRO Technology: ...to virtual prototypes



NANO Science / Technology needs virtual prototyping



Modeling



Simulation

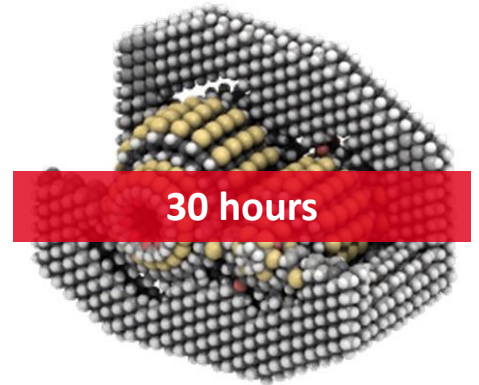
NANO Science / Technology needs virtual prototyping

Nanosimulation is (very) computationally challenging

- Complex physics
- Large number of atoms
- Slow physical processes

Two standard approaches

- Simulate “everything”



IBM BlueGene

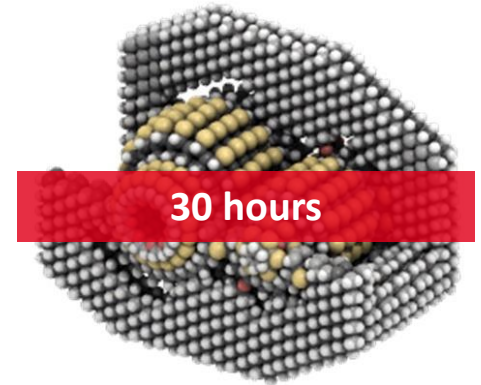
NANO Science / Technology needs virtual prototyping

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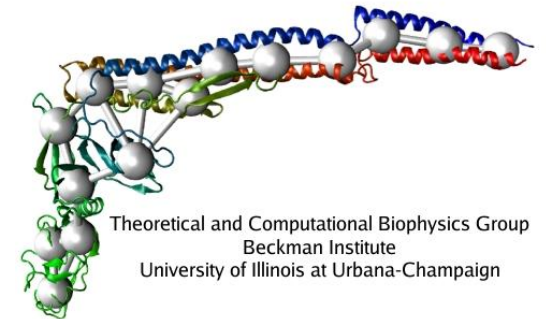
Two standard approaches

- Simulate “everything”
- Simplify



$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right) \psi(\mathbf{r}, t) = i\hbar \frac{\partial \psi}{\partial t}(\mathbf{r}, t) \Rightarrow \mathbf{F} = m\mathbf{a}$$

Simplify the physics



Simplify the structures

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SAMSON

Software for Adaptive Modeling and Simulation Of Nanosystems

Live demos

Thanks for your attention!

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