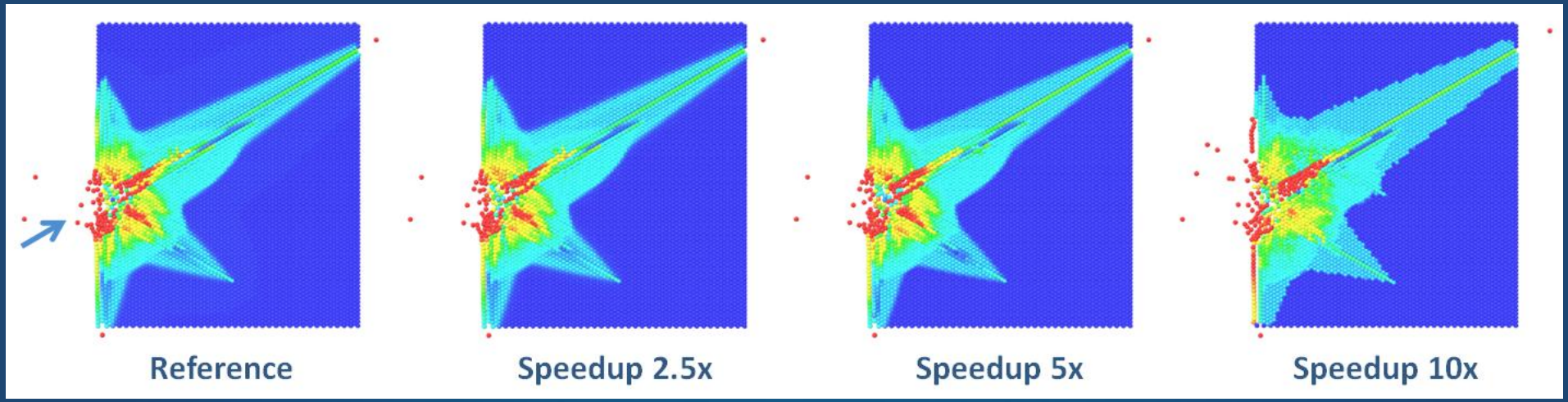
# Theory and Algorithms for Adaptive Particle Simulation


## Stephane Redon

**NANO-D**
**INRIA Grenoble – Rhône-Alpes**

# 1

# Nanoscience is all around

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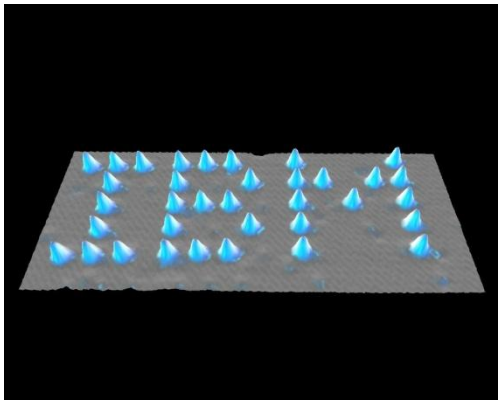
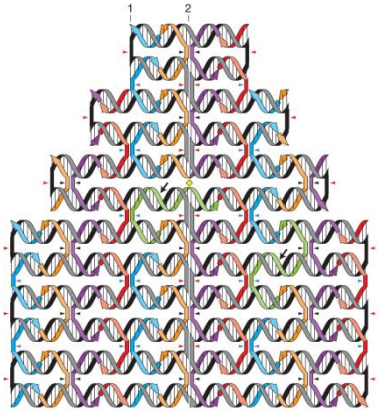
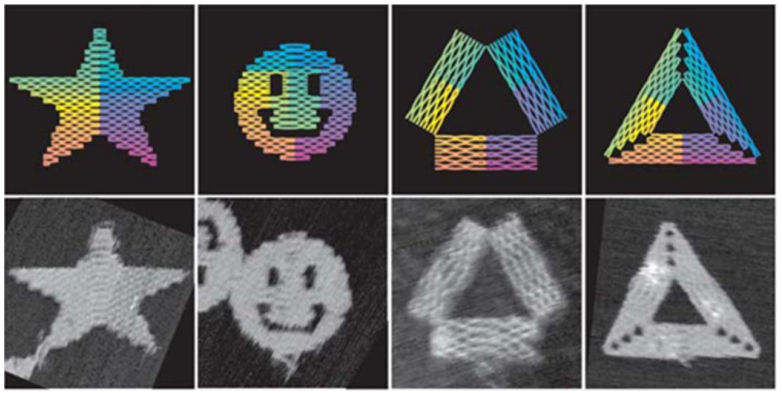
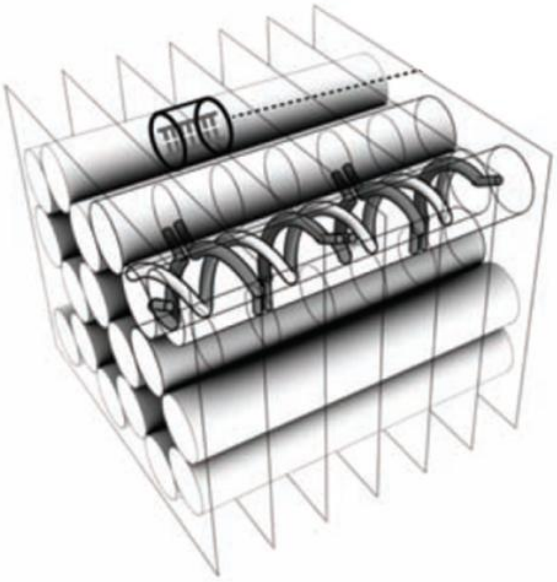


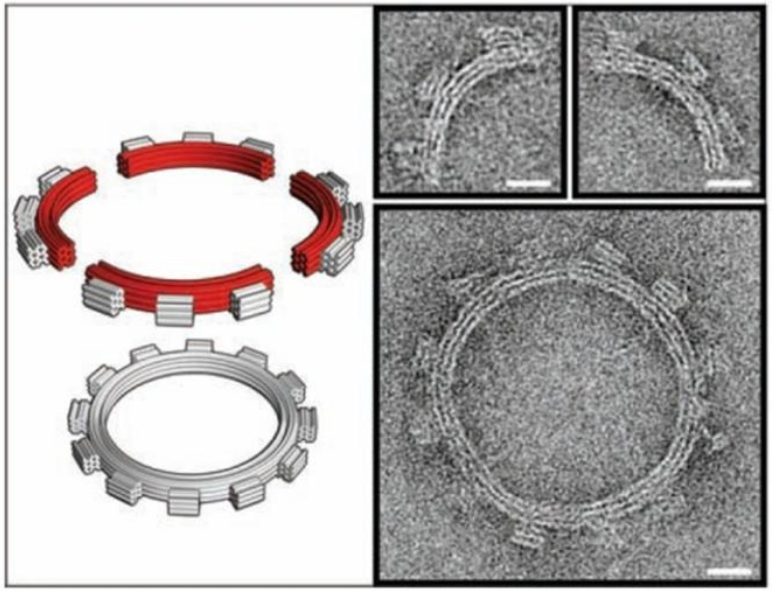
[Eigler and Schweizer, Nature 1990]

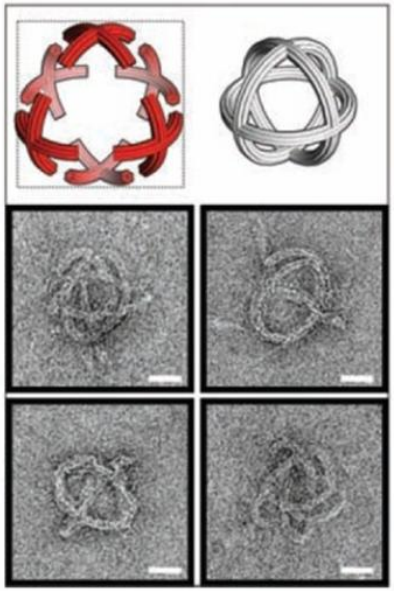




[Rothemund, Nature 2006]

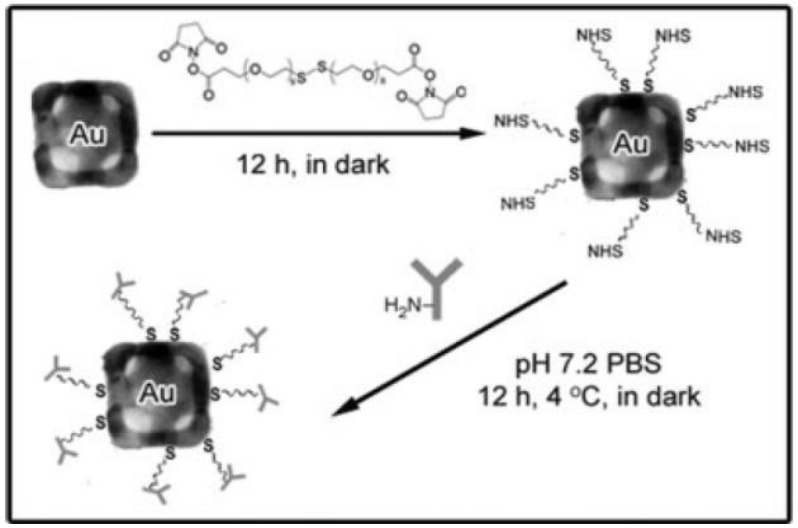




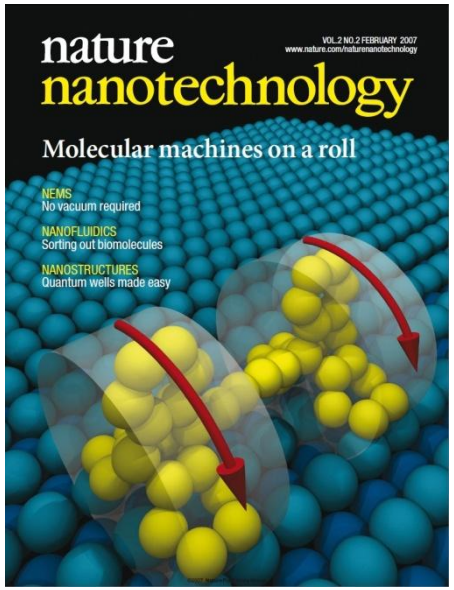


[Dietz et al., Science 2009]

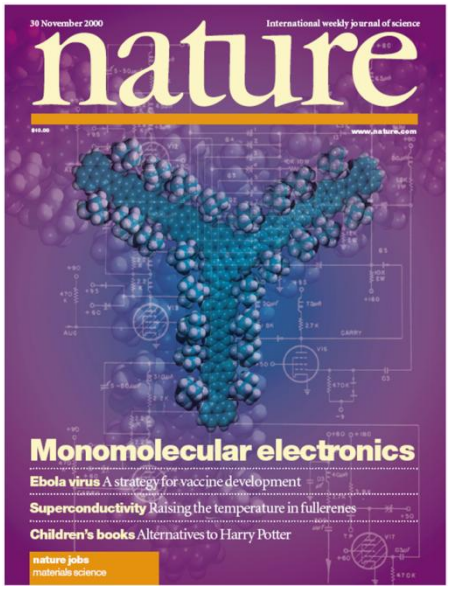
# Nanoscience is all around



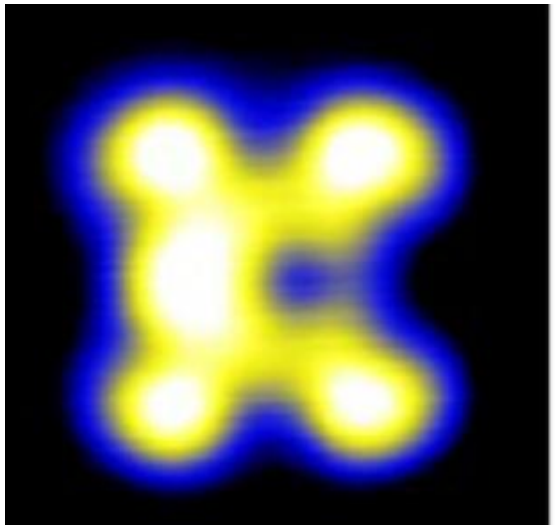

[Chen et al., 2005]

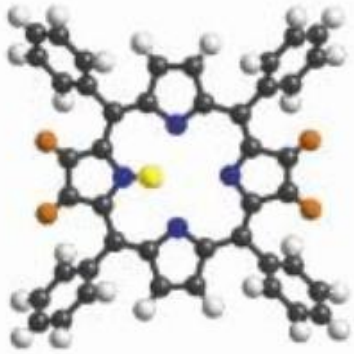



[ Grill et al., 2007]




[Joachim et al., 2000]





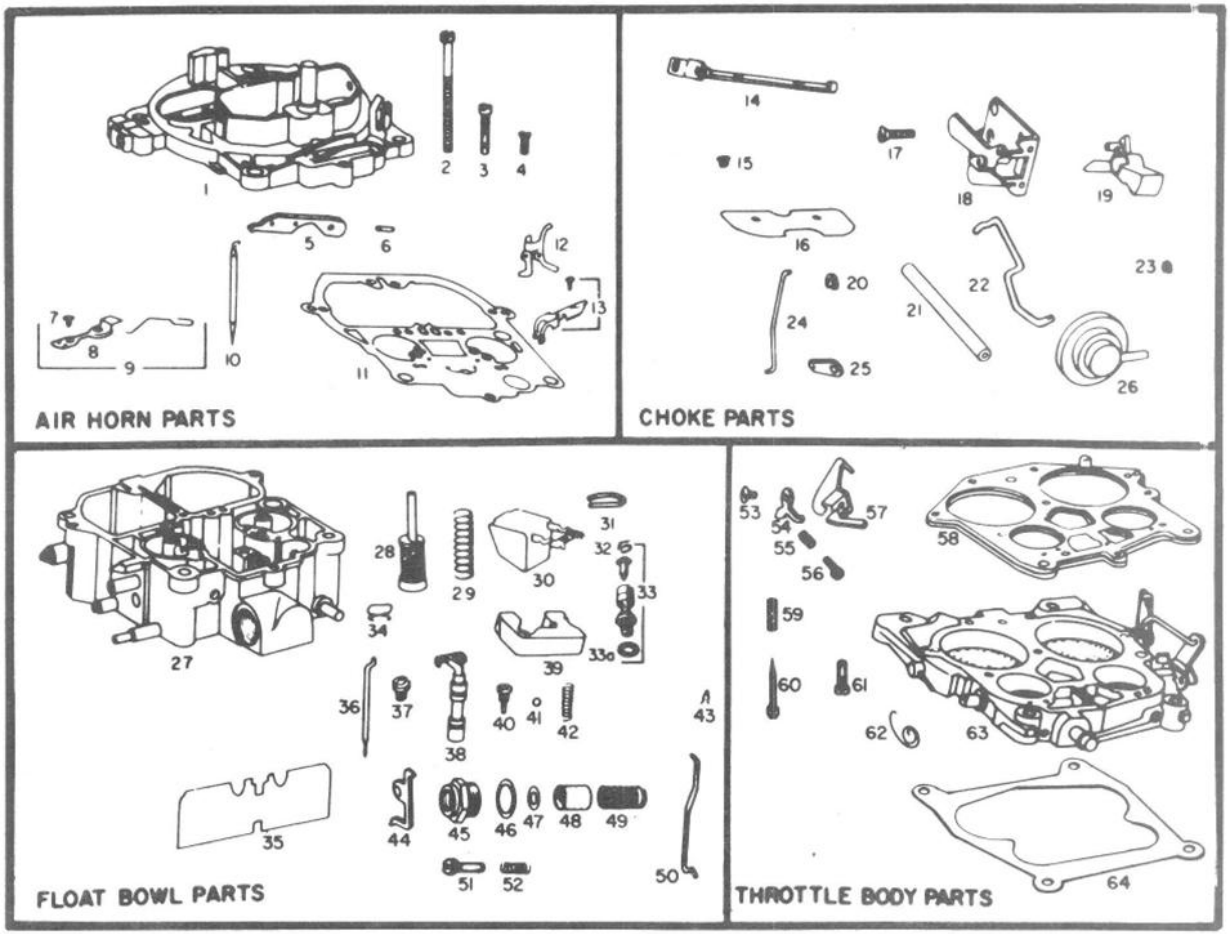
- Drug design
- Materials science
- Chemistry
- Physics
- Electronics
- etc.

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

# 2

## Nanodevices will be designed and prototyped on computers

# MACRO Technology: from schematics…




PARTS SHOWN ARE FOR IDENTIFICATION ONLY. CONSULT PARTS LIST FOR CORRECT PART NAME AND NUMBER

Delco

**Delco Carburetor**

MODEL 4MV QUADRAJET

1971 CHEVROLET, CHEVELLE, NOVA, CAMARO, CORVETTE

350 CUBIC INCH ENGINE

BULLETIN 9C-3058

DATE: NOVEMBER, 1971

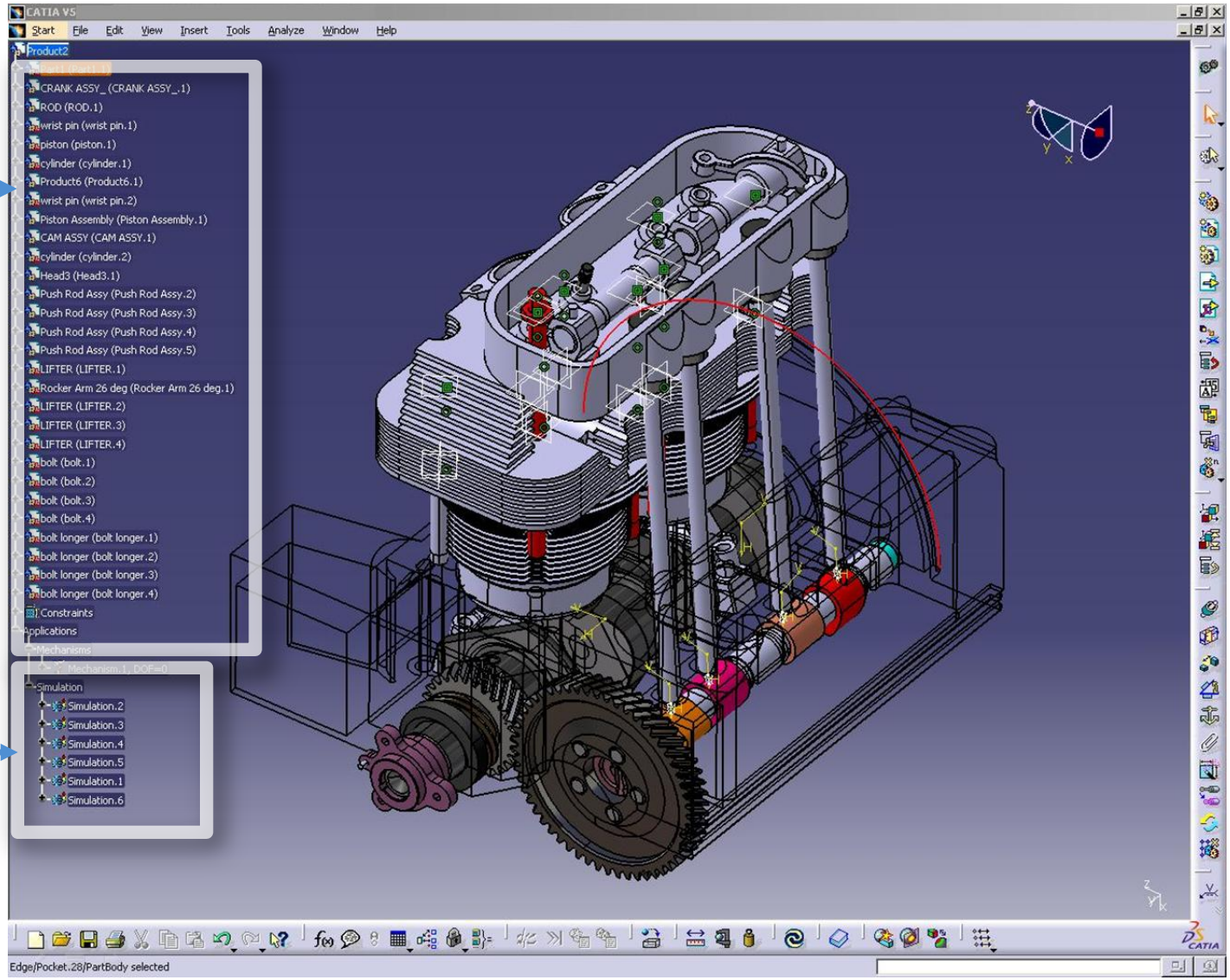
PAGE 1

Inria

# MACRO Technology: …to virtual prototypes

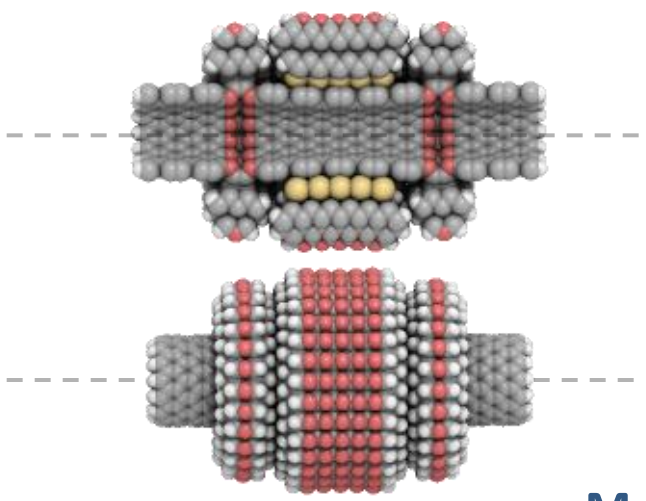
Models

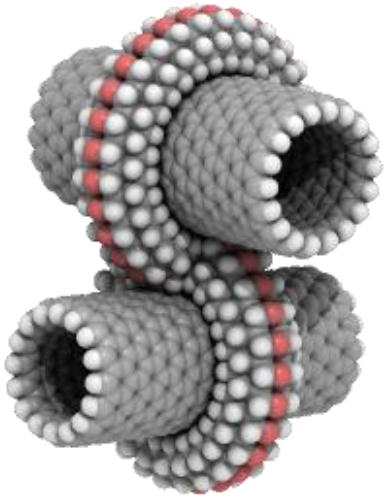
Simulations



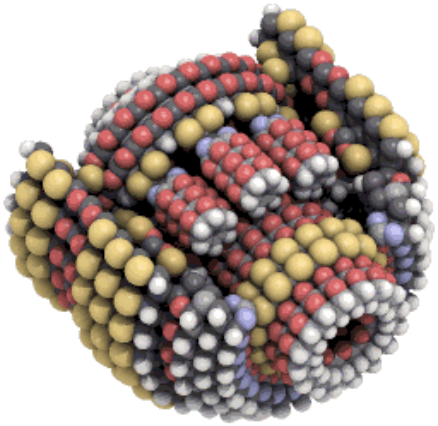

CATIA V5 © Dassault Systèmes

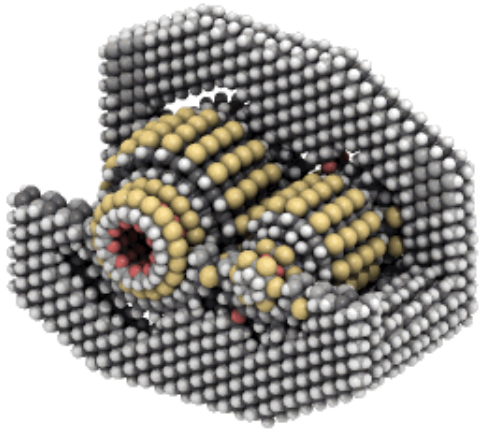
# NANO Science / Technology needs virtual prototyping





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

## Nanosimulation is (very) computationally challenging

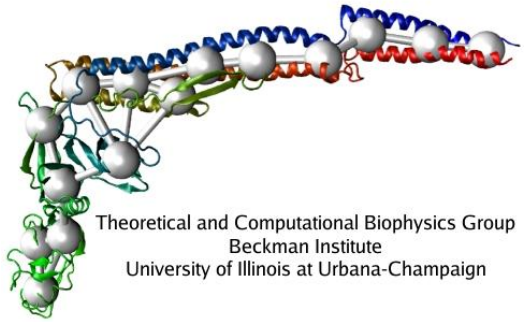
- Complex physics
- Large number of atoms
- Slow physical processes


## 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**

# NANO Science / Technology needs virtual prototyping

## Nanosimulation is (very) computationally challenging

- Complex physics
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## Two standard approaches

- Simulate “everything”
- Simplify

The ADAPT Proposal

## Theory and Algorithms for Adaptive Particle Simulation

- Directly control the cost and precision of a simulation
- Adaptively update classical or quantum interactions
- Integrate into a unified framework for nanosystem design

# 3

# ADAPT

## Theory and Algorithms for Adaptive Particle Simulation

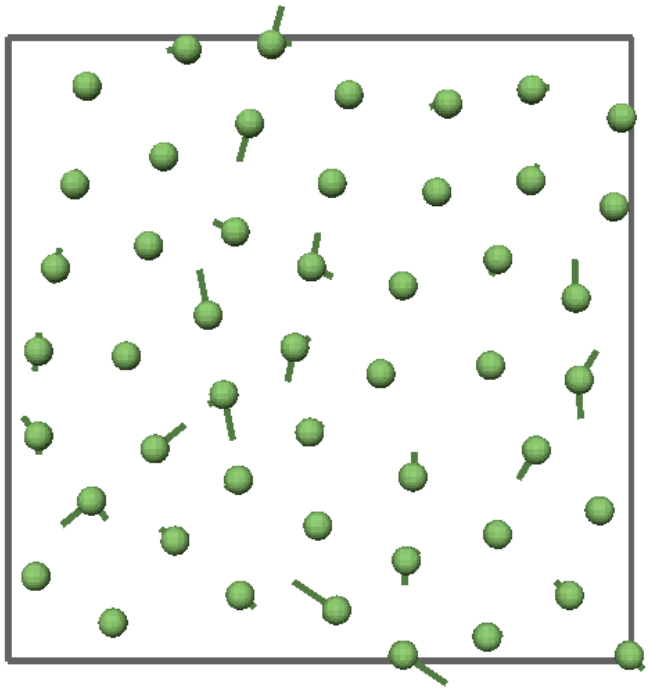
## Overview

# A unified theory for adaptive particle simulation

Positions Momenta Inverse mass matrix

$$H(\mathbf{q},\mathbf{p}) = \frac{1}{2}\mathbf{p}^T\mathbf{M}^{-1}\mathbf{p} + V(\mathbf{q})$$

Hamiltonian Kinetic energy Potential energy



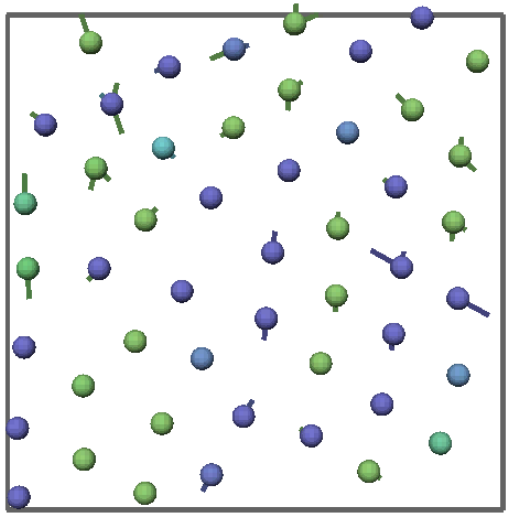
# A unified theory for adaptive particle simulation

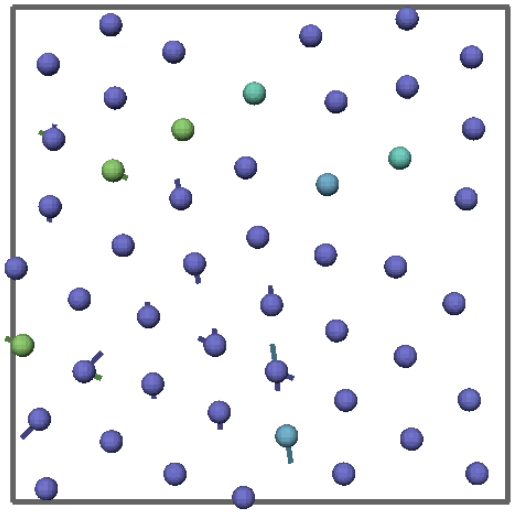
Adaptive inverse mass matrix

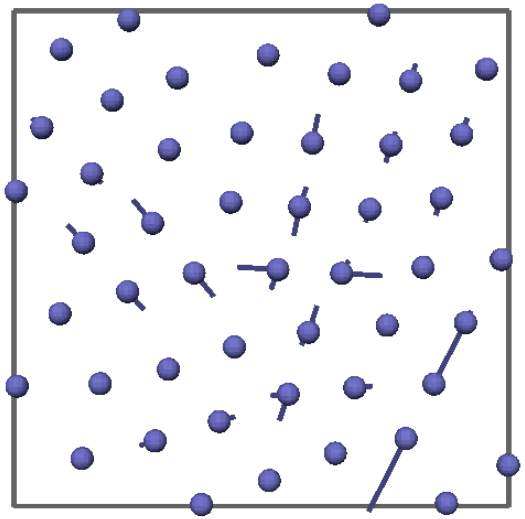
$$H_{AR}(\mathbf{q},\mathbf{p}) = \frac{1}{2}\mathbf{p}^T \Phi(\mathbf{q},\mathbf{p})\,\mathbf{p} + V(\mathbf{q})$$

Adaptively Restrained Hamiltonian

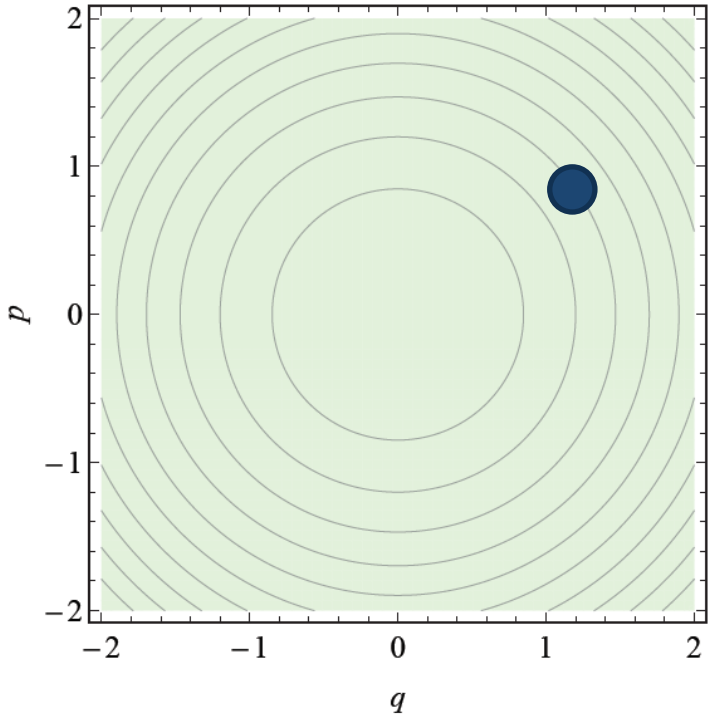
**Depends on momenta**







# A unified theory for adaptive particle simulation




A simple example : the harmonic oscillator

# A unified theory for adaptive particle simulation

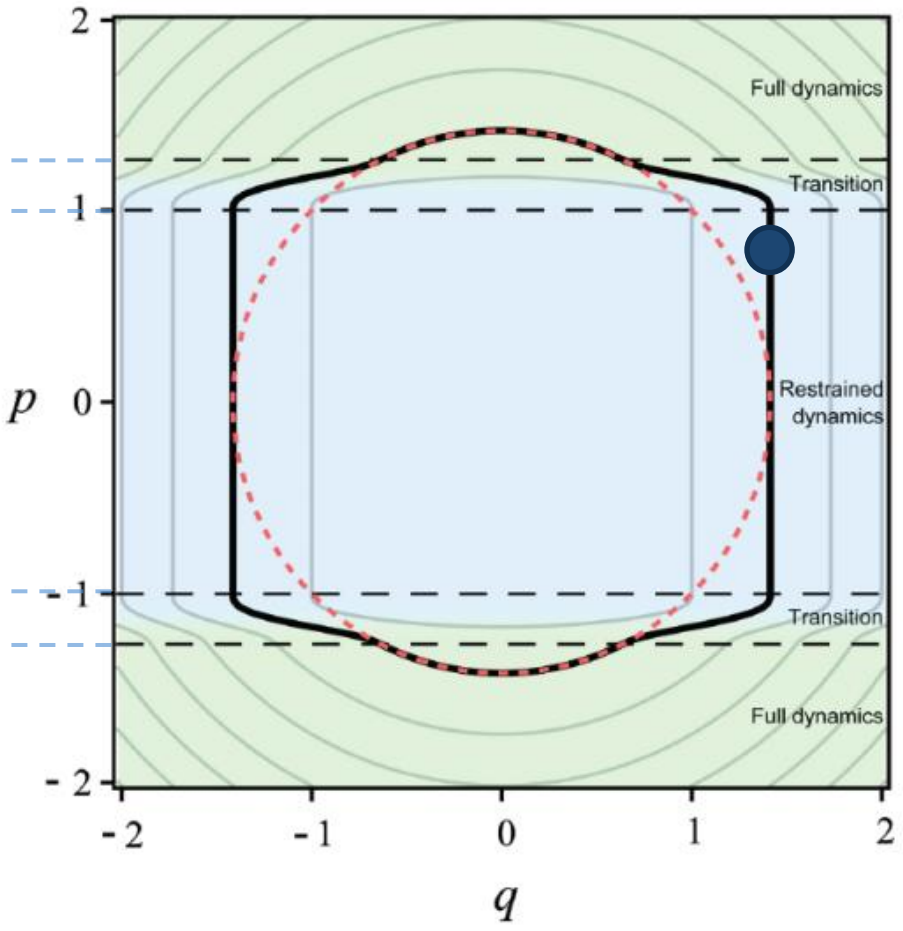
$$\Phi(\mathbf{q},\mathbf{p}) = \mathbf{M}^{-1}$$

Interpolation

$$\Phi(\mathbf{q},\mathbf{p}) = \mathbf{0}$$

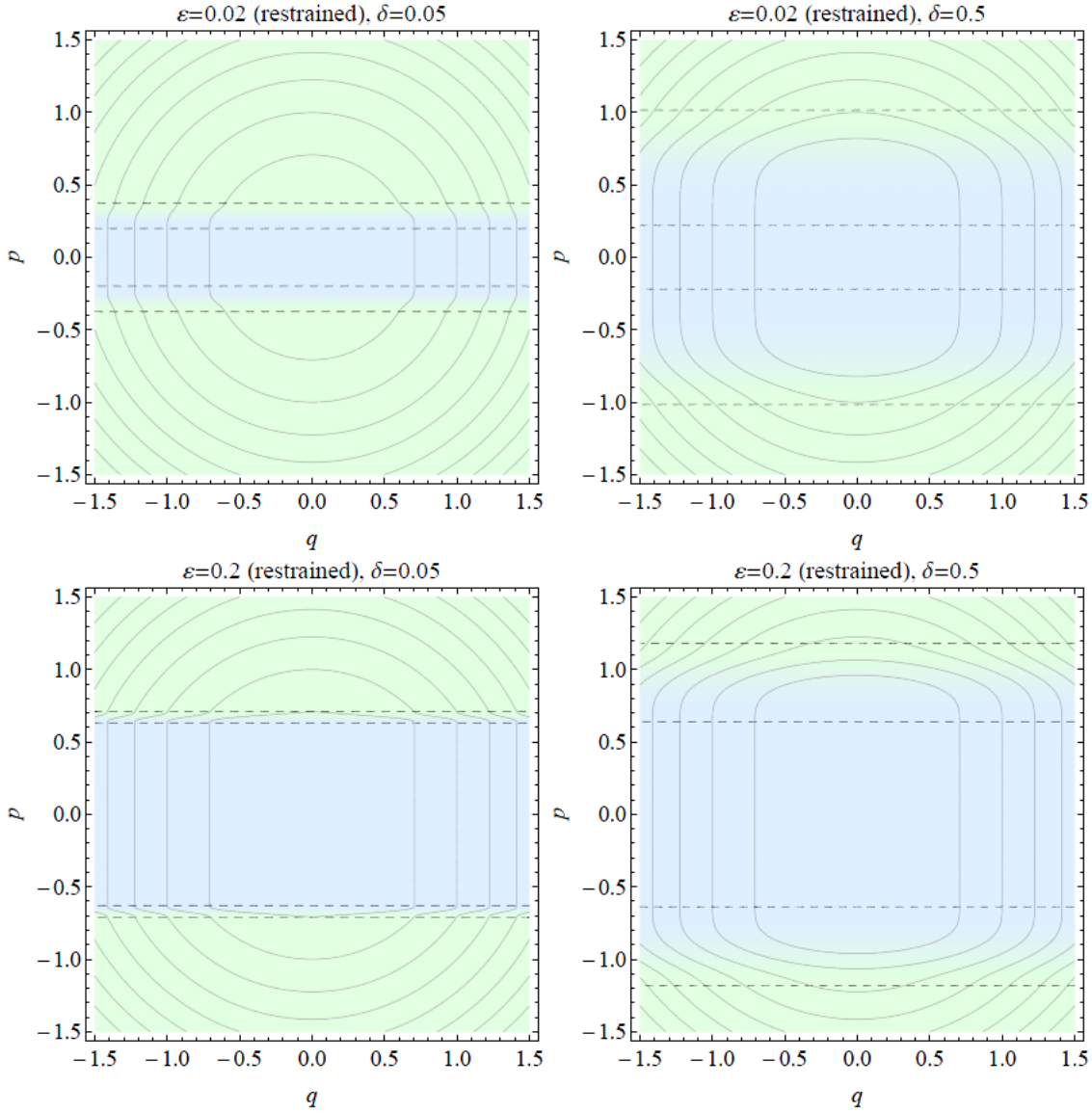
Interpolation

$$\Phi(\mathbf{q},\mathbf{p}) = \mathbf{M}^{-1}$$

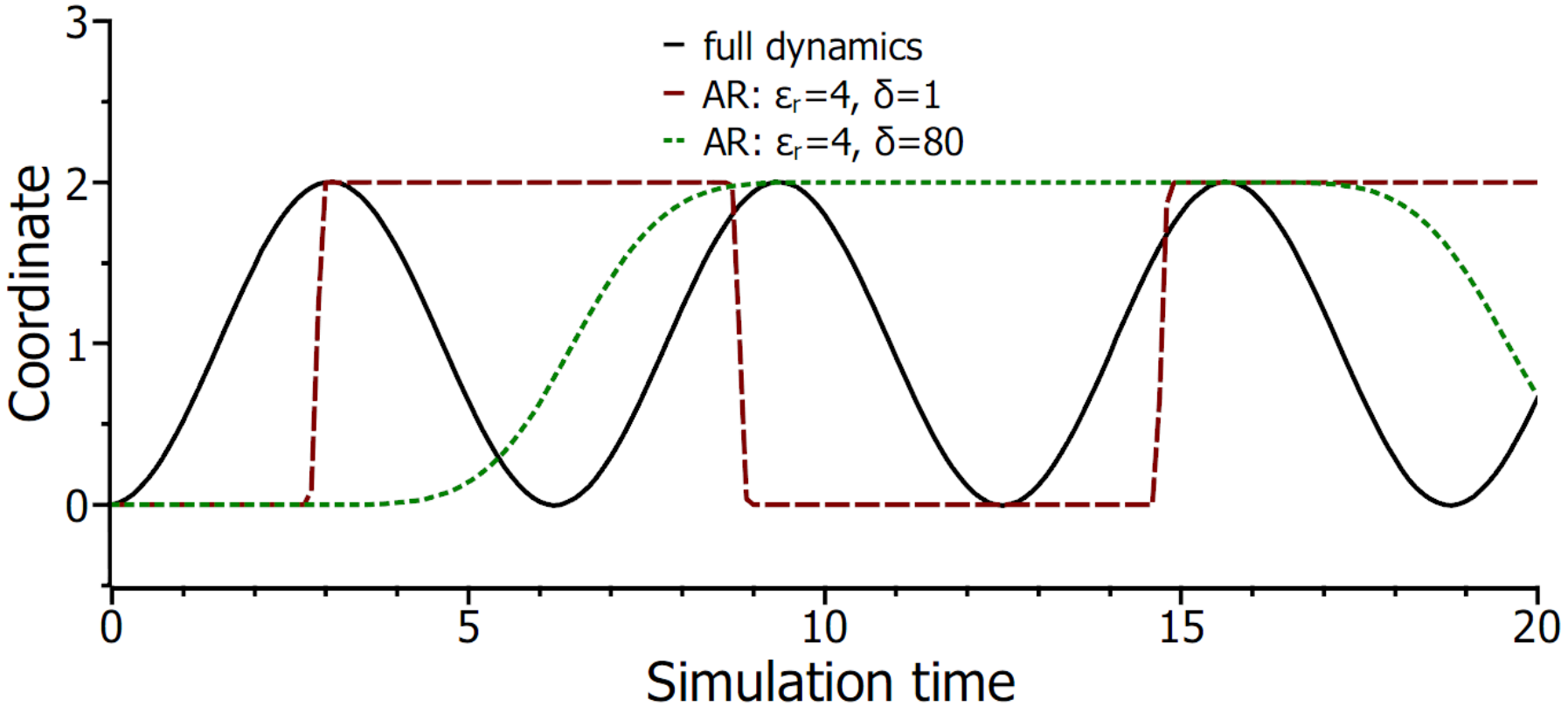



A simple example : adaptively restrained phase portrait of the harmonic oscillator

# A unified theory for adaptive particle simulation



# A unified theory for adaptive particle simulation

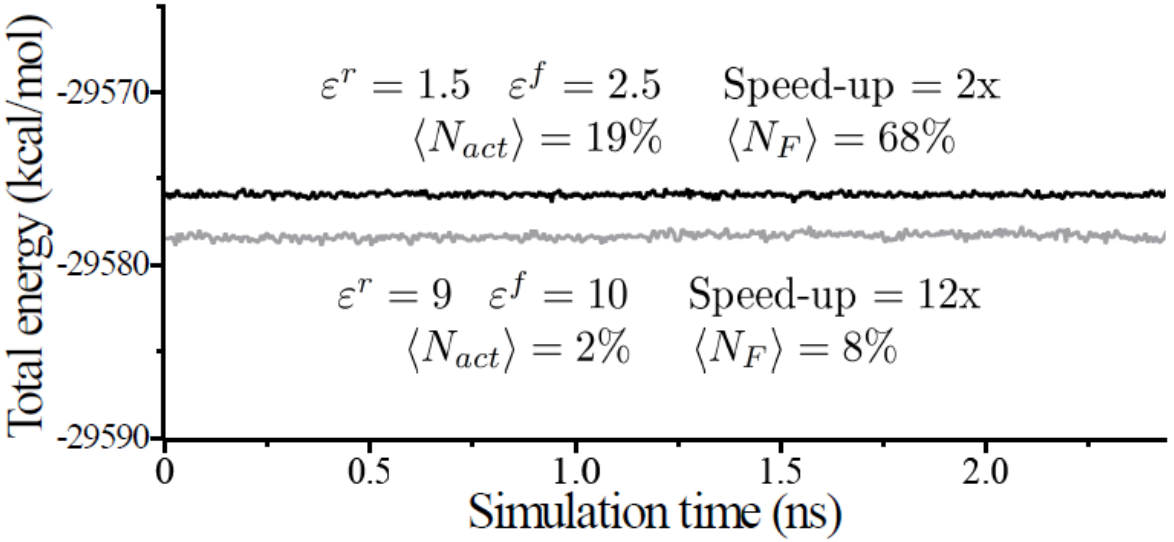



Adaptively restrained trajectories of the harmonic oscillator

# A unified theory for adaptive particle simulation

$$\dot{\mathbf{p}} = -\frac{\partial H_{AR}}{\partial \mathbf{q}} = -\frac{\partial V(\mathbf{q})}{\partial \mathbf{q}} - \frac{1}{2}\mathbf{p}^T \frac{\partial \Phi(\mathbf{q},\mathbf{p})}{\partial \mathbf{q}}\mathbf{p},$$
$$\dot{\mathbf{q}} = \frac{\partial H_{AR}}{\partial \mathbf{p}} = \Phi(\mathbf{q},\mathbf{p})\mathbf{p} + \frac{1}{2}\mathbf{p}^T \frac{\partial \Phi(\mathbf{q},\mathbf{p})}{\partial \mathbf{p}}\mathbf{p}.$$

**Use regular symplectic integrators => stable adaptive simulations**

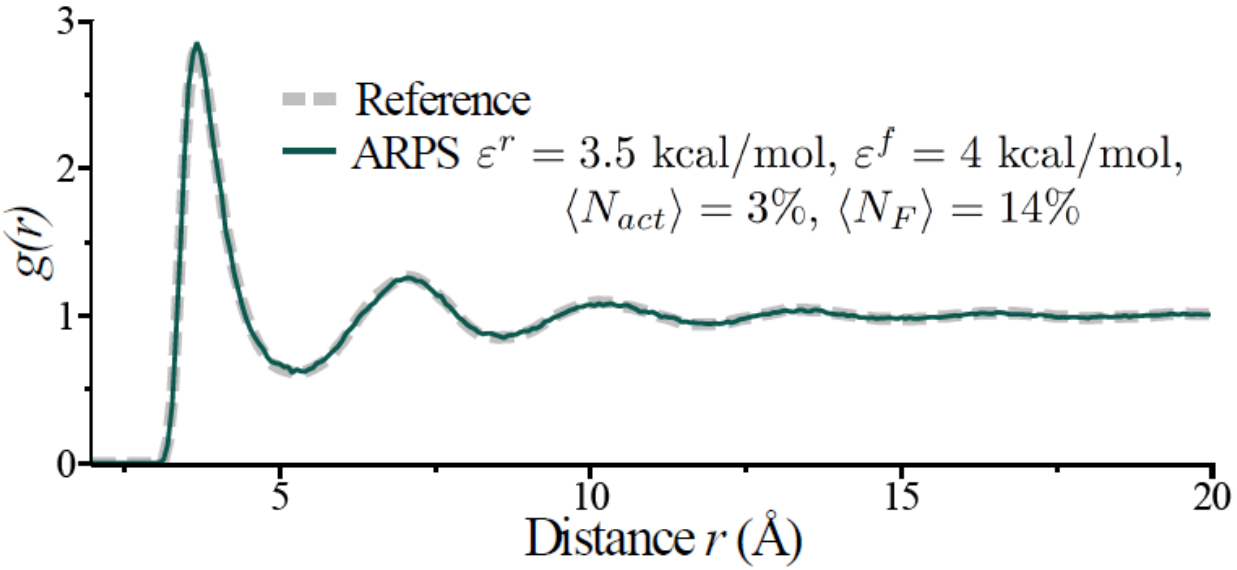



**Conservation of the adaptively restrained Hamiltonian**

# A unified theory for adaptive particle simulation

$$H_{AR} = H + V_{AR}(\mathbf{q},\mathbf{p}) \;\Rightarrow\; \langle \mathbf{A} \rangle_H = \frac{\left\langle \mathbf{A} e^{\frac{V_{AR}(\mathbf{q},\mathbf{p})}{k_B T}} \right\rangle_{H_{AR}}}{\left\langle e^{\frac{V_{AR}(\mathbf{q},\mathbf{p})}{k_B T}} \right\rangle_{H_{AR}}}$$

**Statistics can be recovered !**




**Adaptively restrained simulations may be used to compute statistics**

# 4

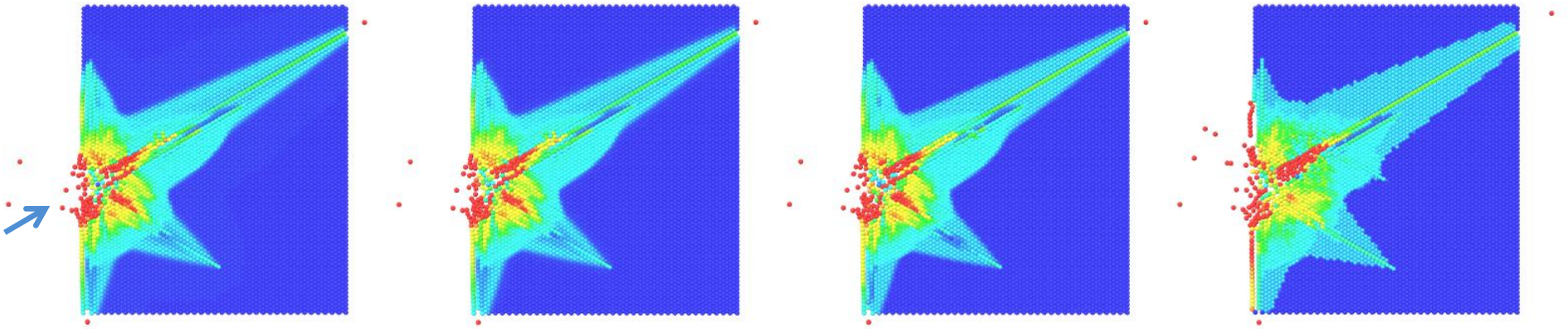
# ADAPT

## Theory and Algorithms for Adaptive Particle Simulation

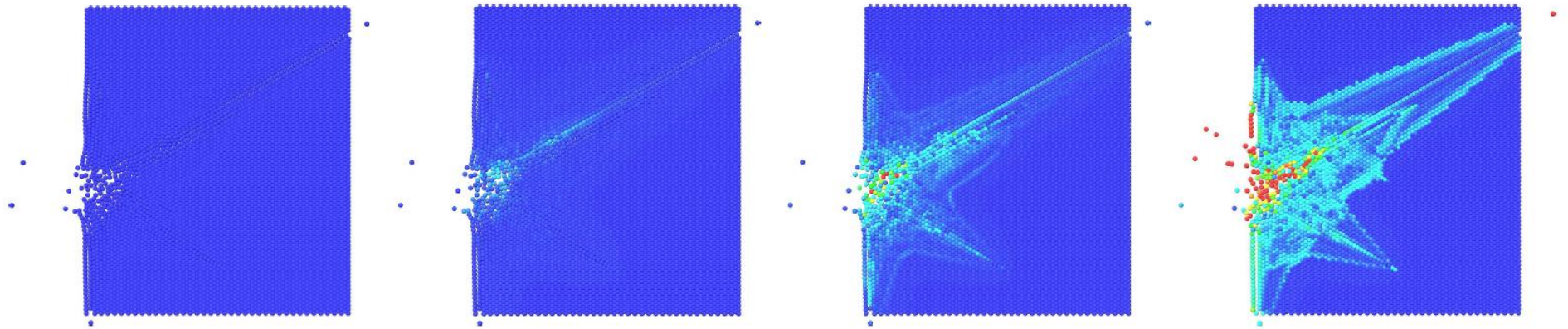
## Preliminary results

# 2D shock propagation with controlled precision

## Particle displacements after the collision cascade



Reference | Speedup 2.5x | Speedup 5x | Speedup 10x



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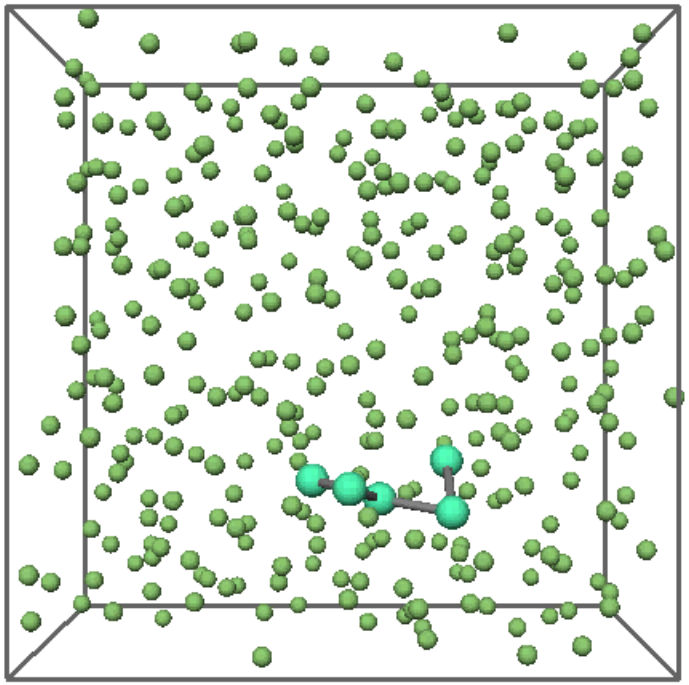
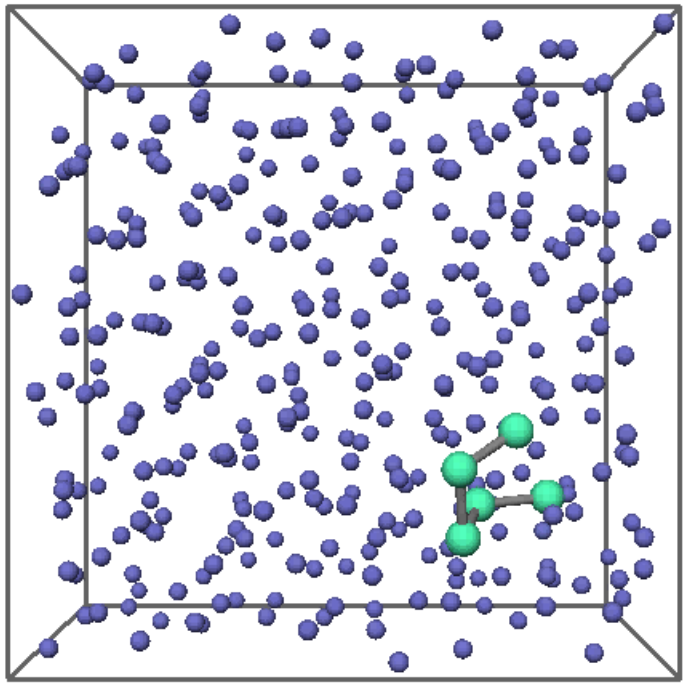
S. Artemova and S. Redon. Physical Review Letters.

# Polymer in solvent – Fast statistics collection





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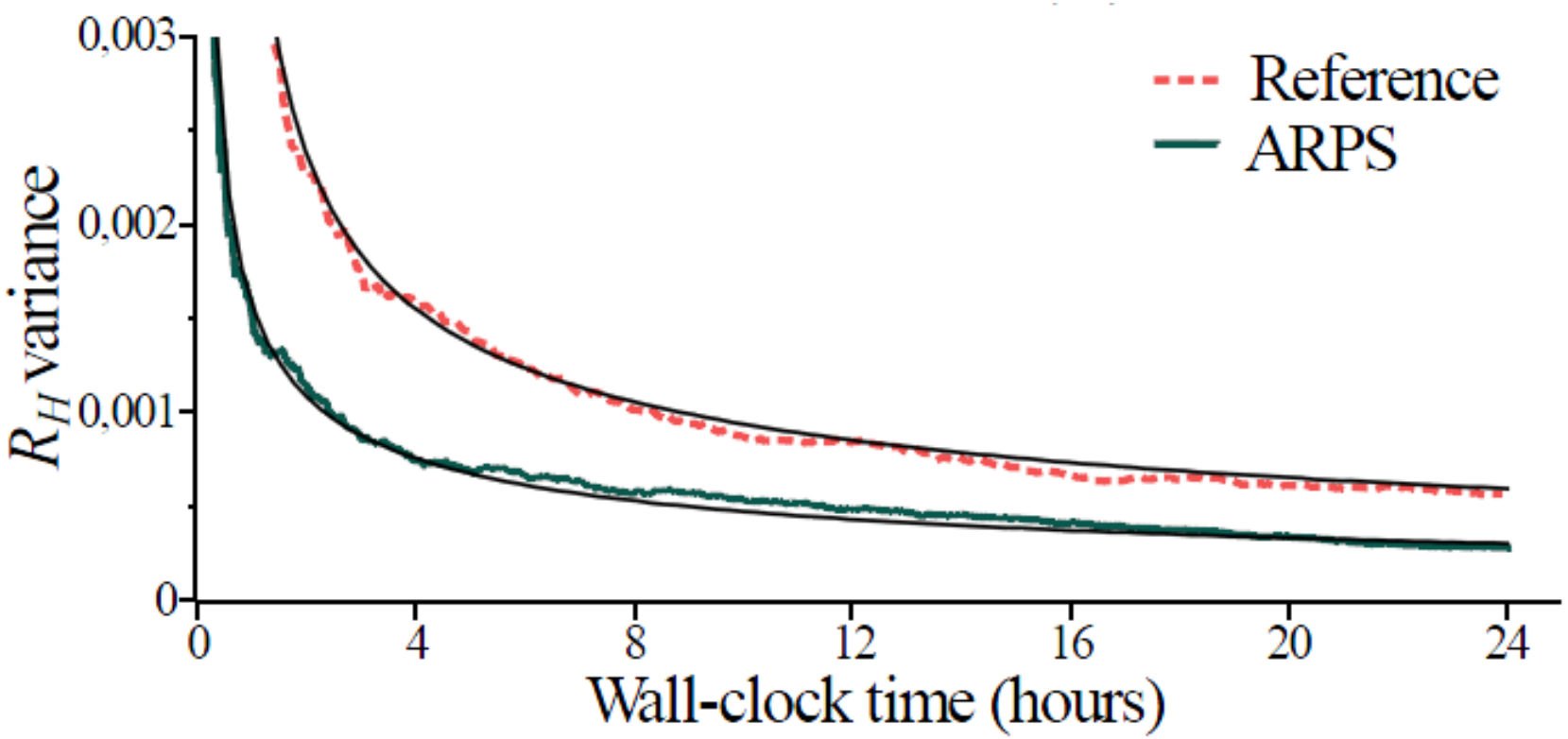
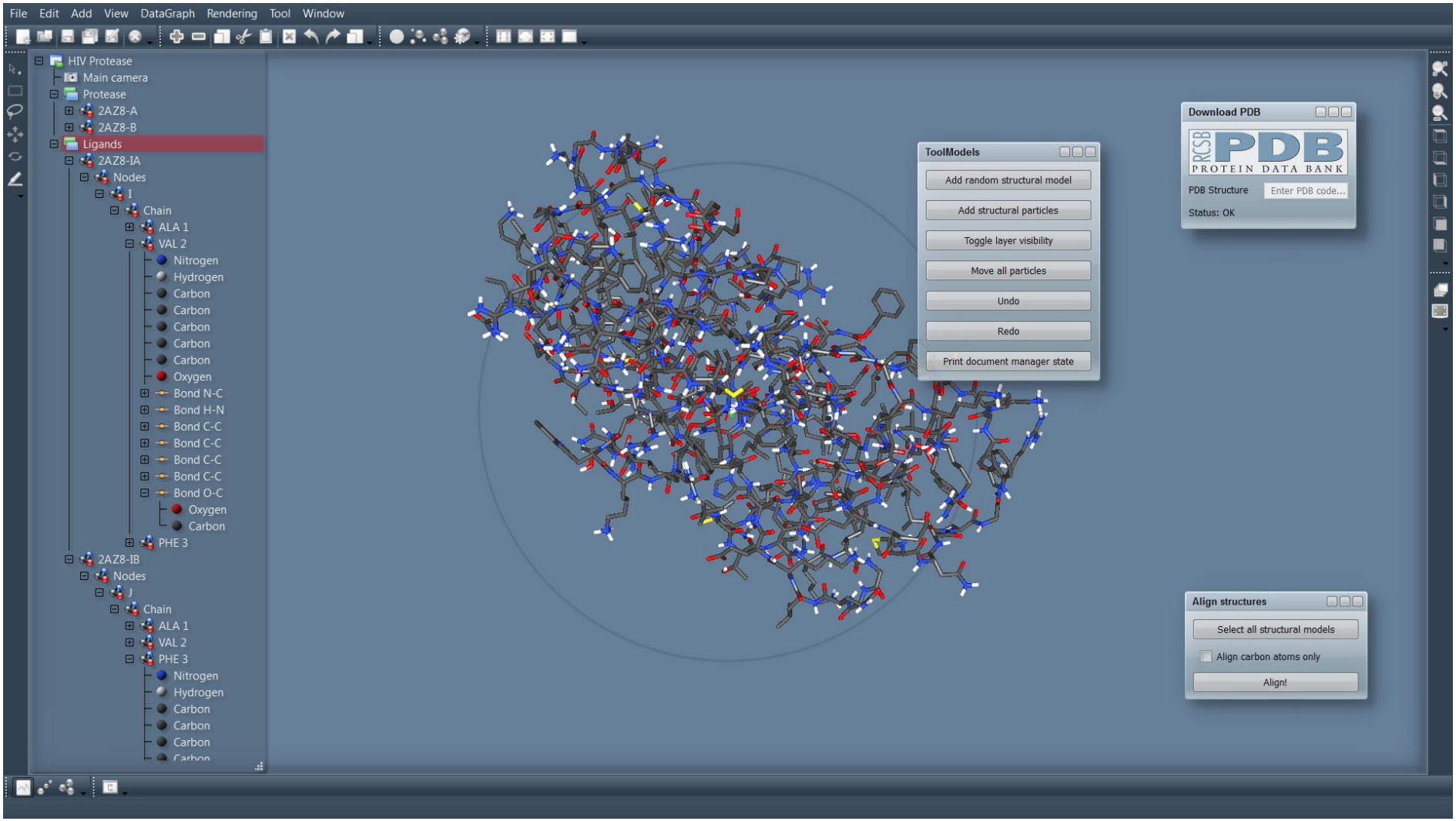



**Polymer statistics are obtained four times faster**

S. Artemova and S. Redon. Physical Review Letters.

# SAMSON: Software for Adaptive Modeling and Simulation Of Nanosystems




Current state of SAMSON

# Thanks for your attention!

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http://nano-d.inrialpes.fr

S. Artemova and S. Redon. “Adaptively Restrained Particle Simulations”. Physical Review Letters.