Modélisation et simulation de nanosystèmes

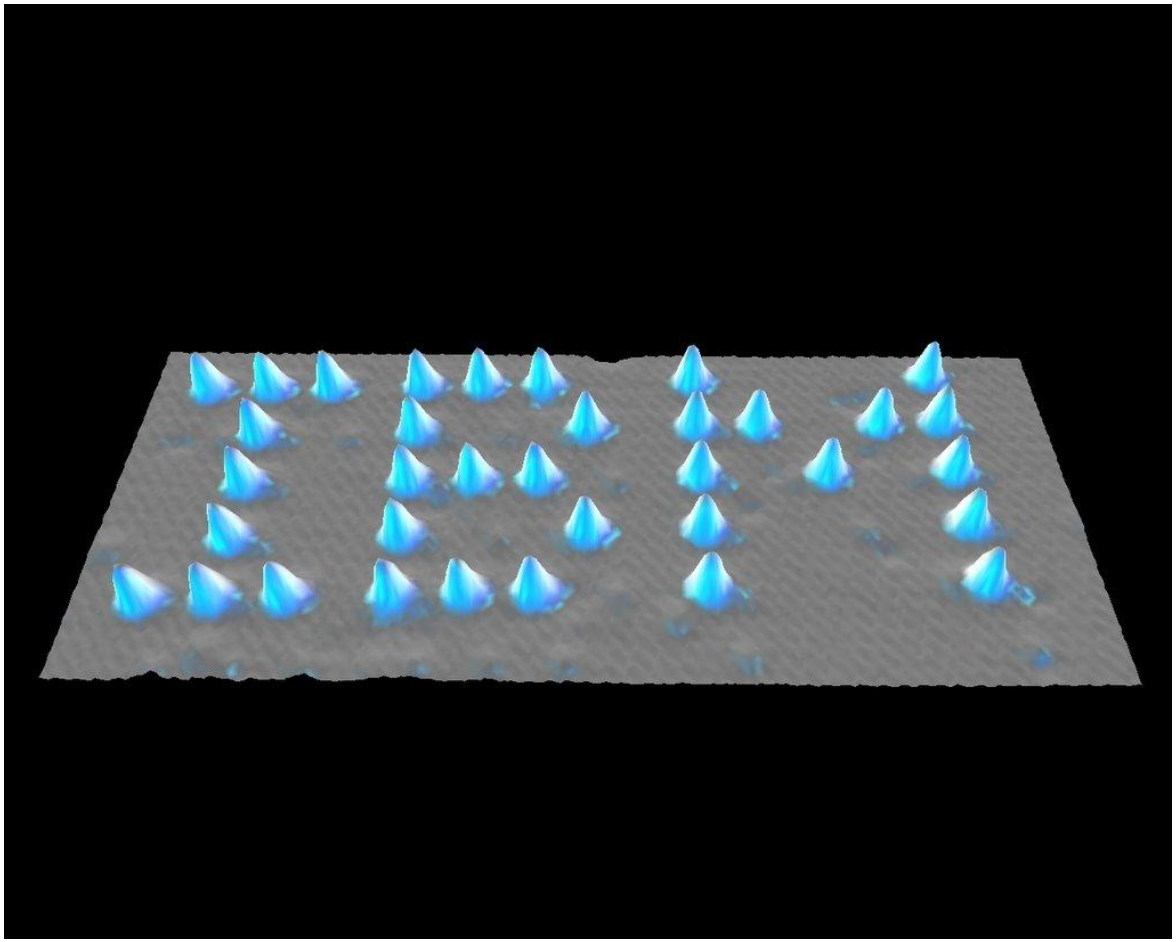
(et de l'utilisation des arbres…)

Stephane Redon
NANO-D – INRIA Grenoble – Rhone-Alpes

Ecole polytechnique – 14 juin 2011

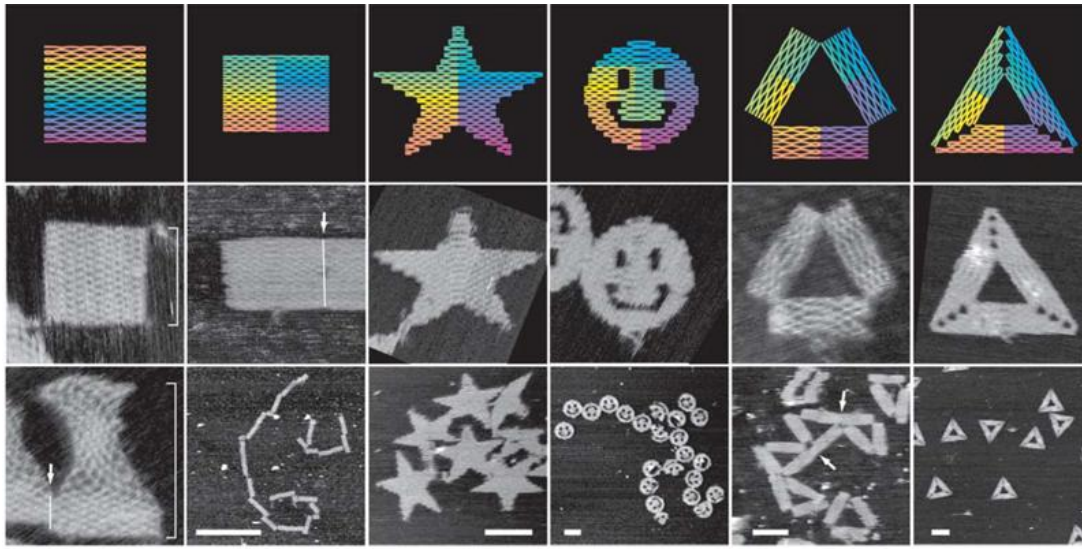
INSTITUT NATIONAL
DE RECHERCHE
EN INFORMATIQUE
ET EN AUTOMATIQUE
INRIA

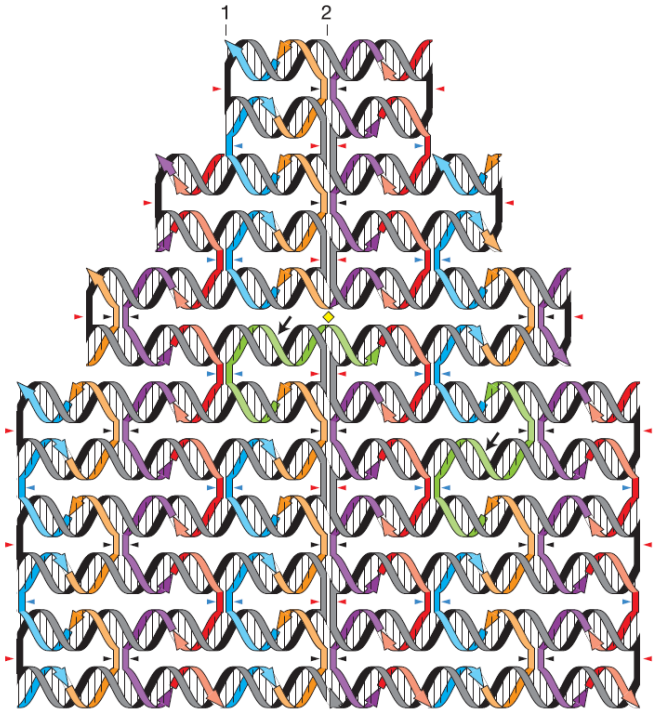
La nanoscience ascendante



Don Eigler – IBM – Fin des années 1980

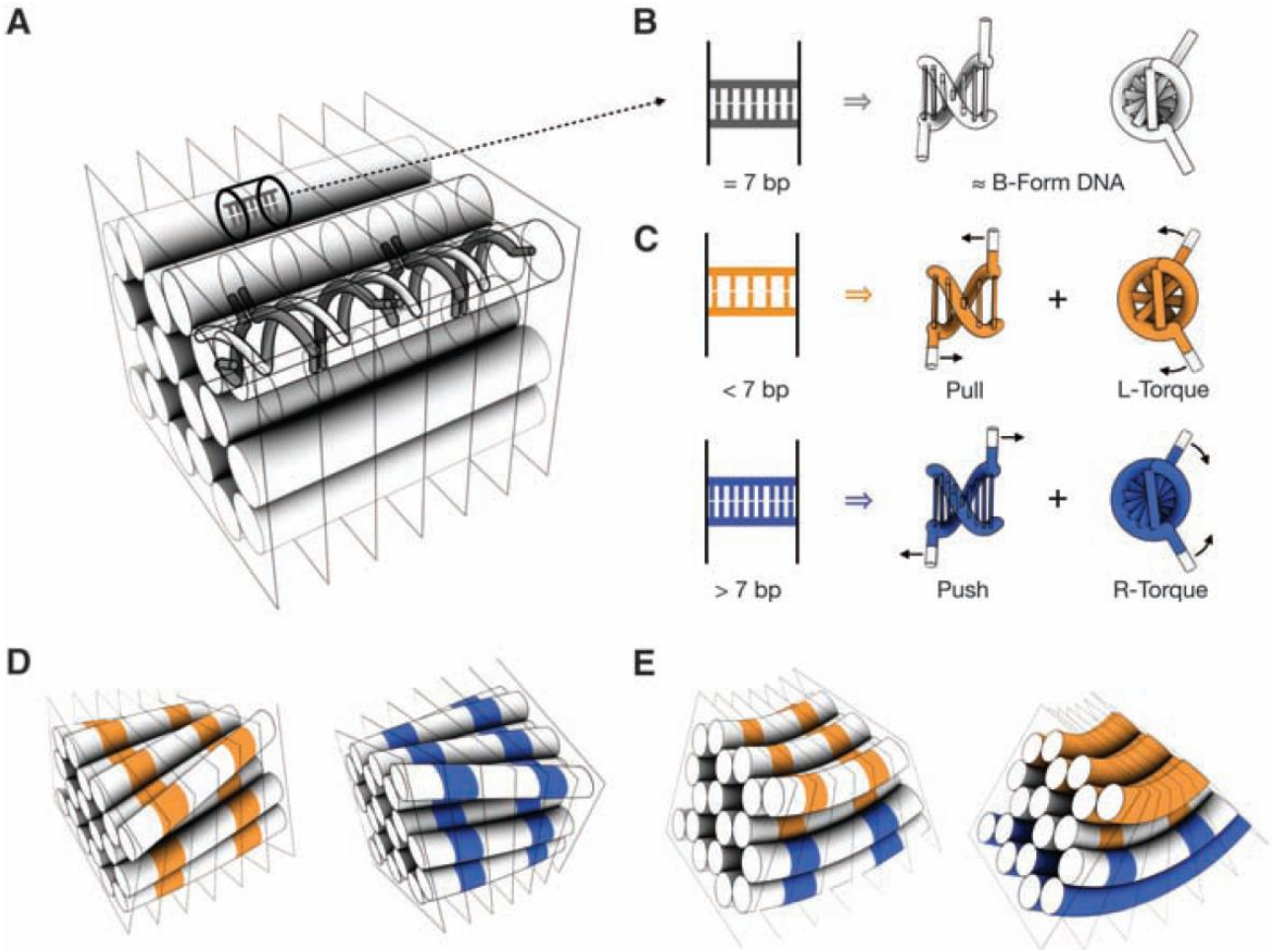
La nanoscience ascendante





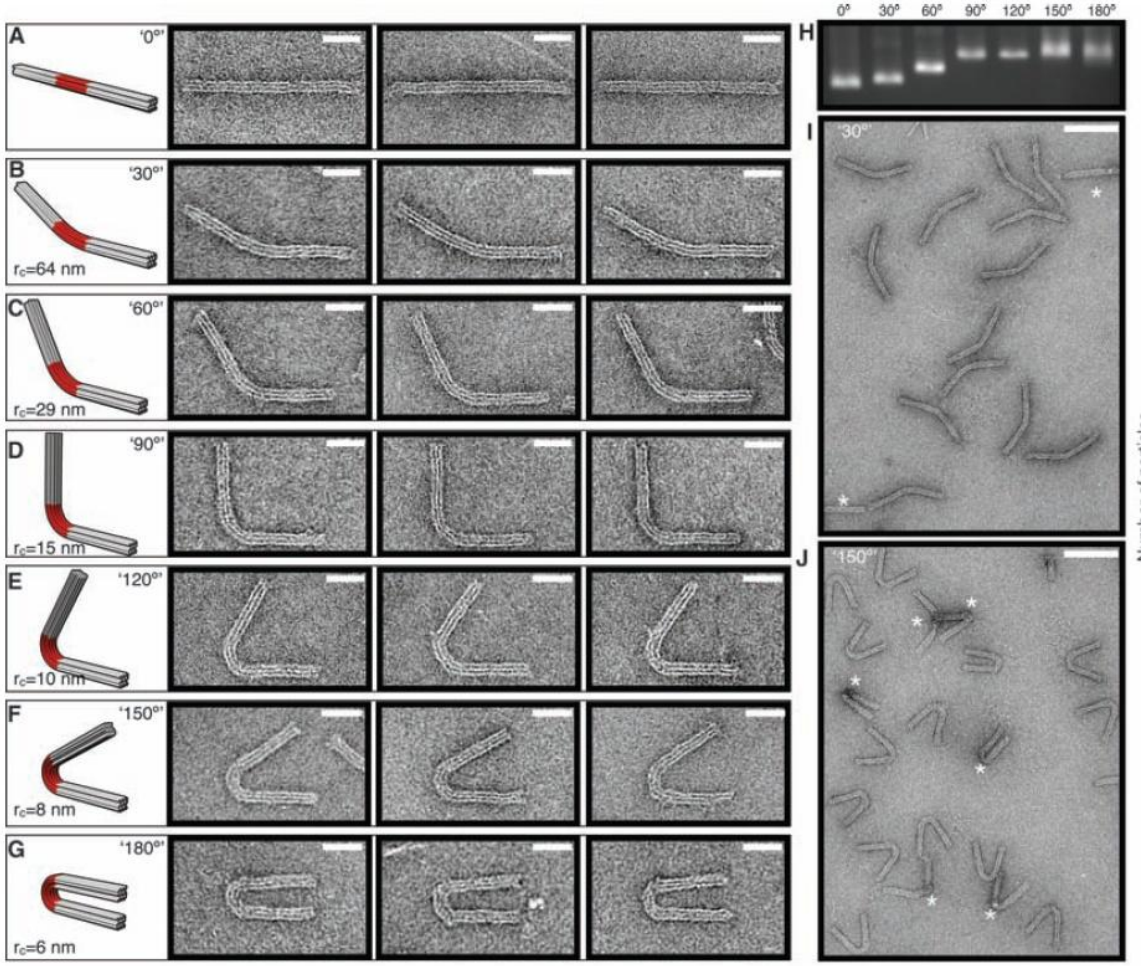
[Rothemund, Nature 2006]

La nanoscience ascendante



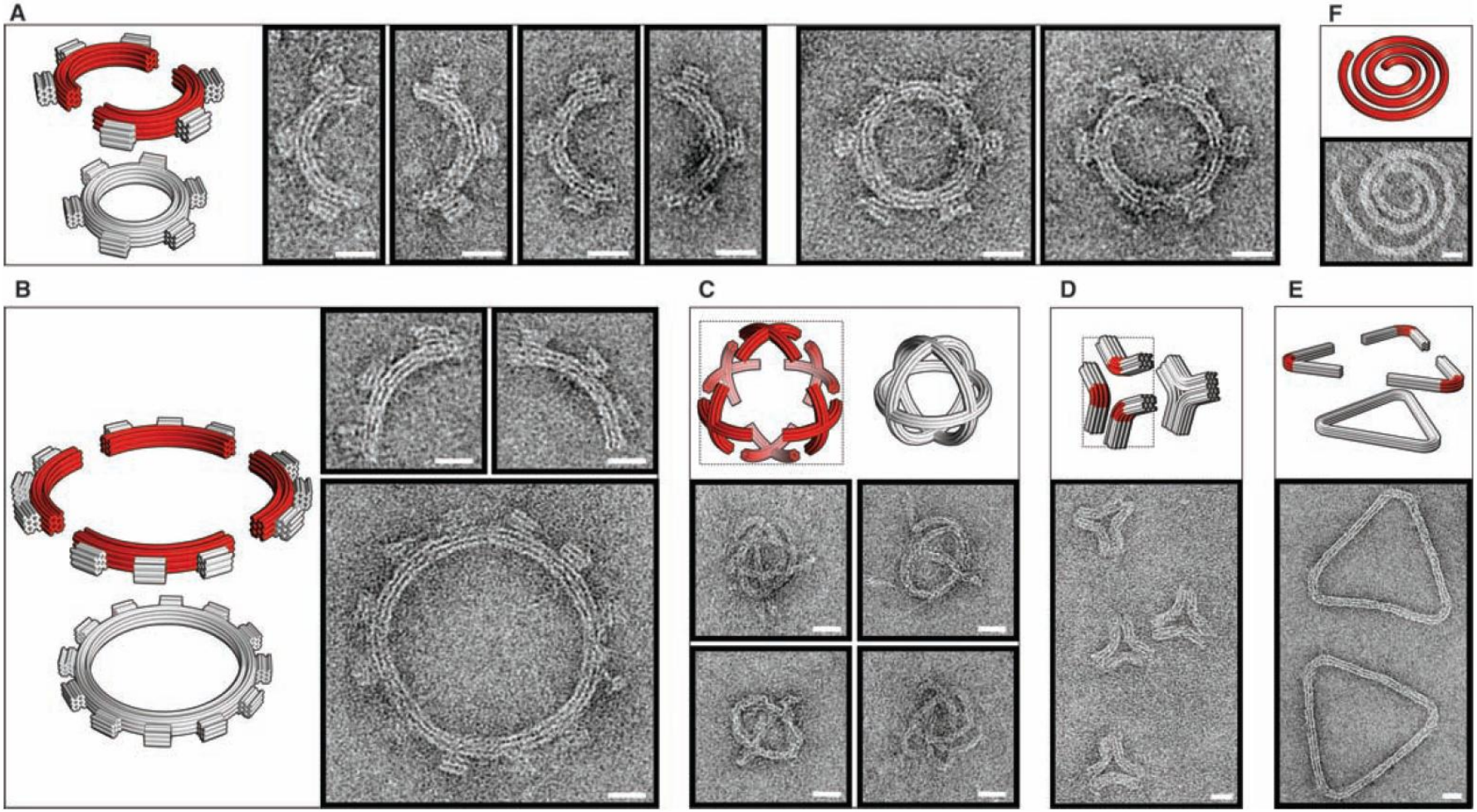
[Dietz et al., Science, August 2009]

La nanoscience ascendante



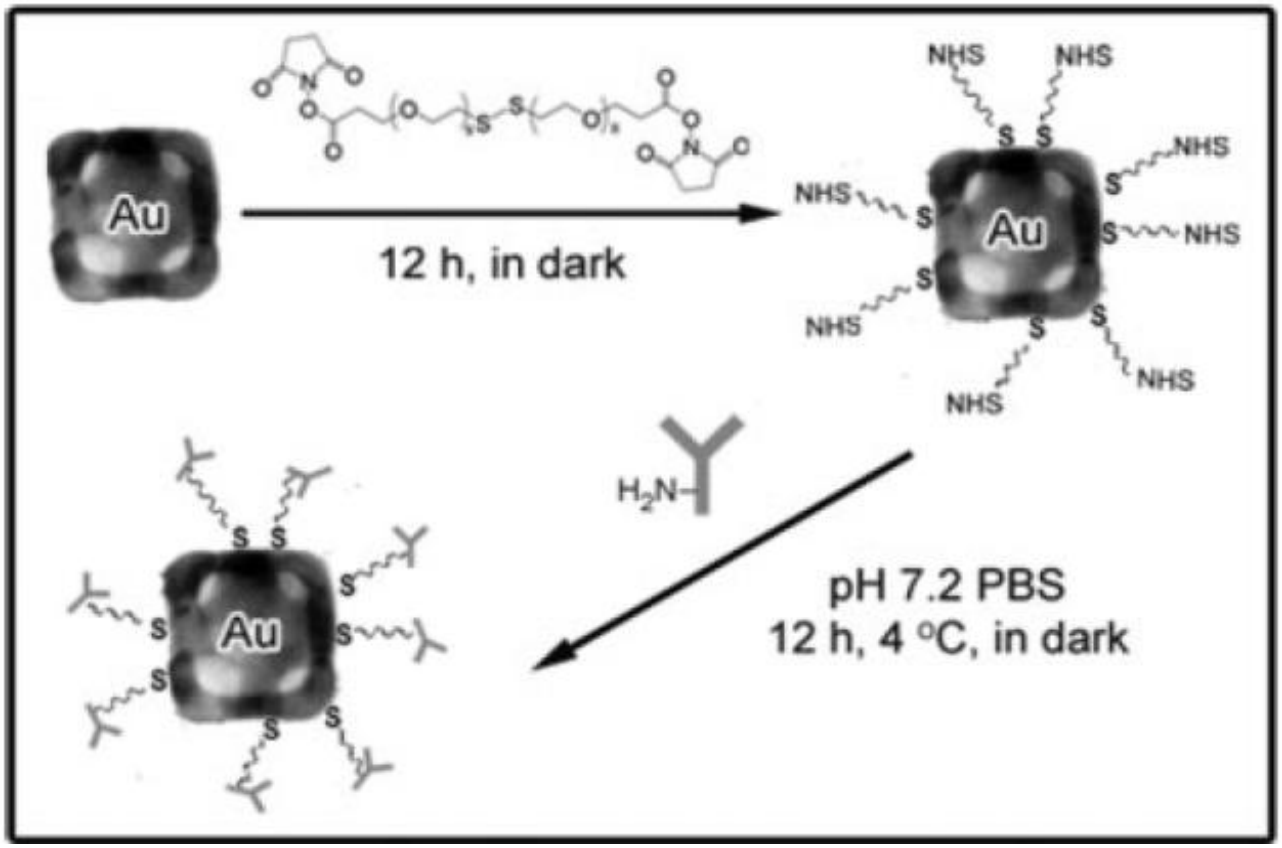
[Dietz et al., Science, August 2009]

La nanoscience ascendante



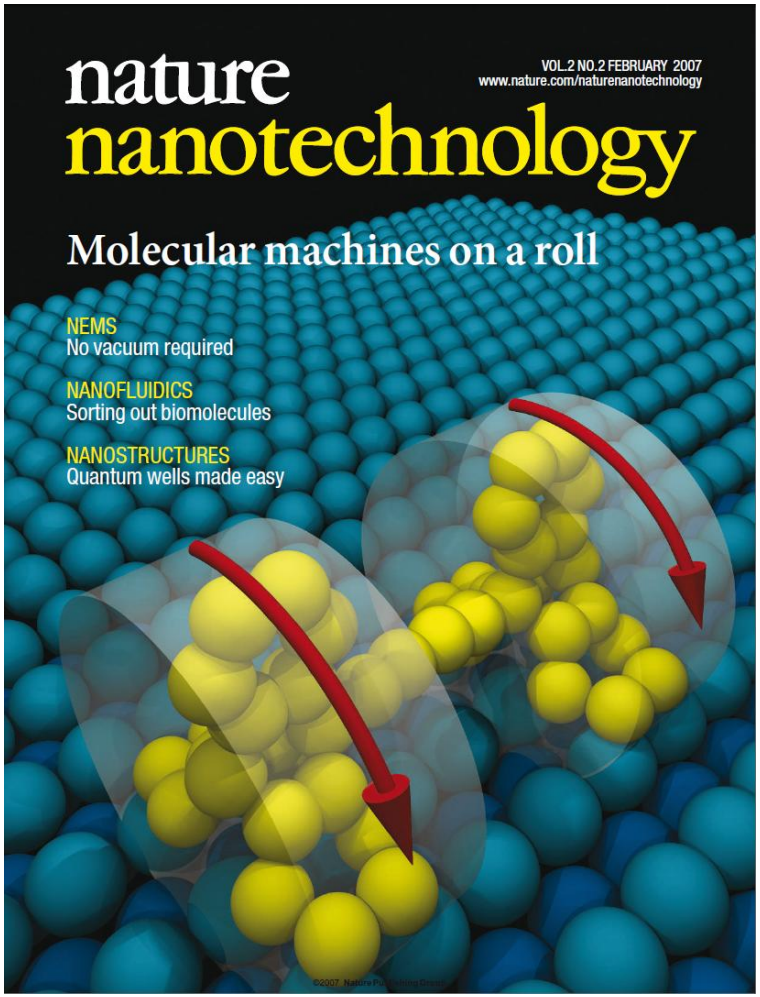
[Dietz et al., Science, August 2009]

La nanoscience ascendante



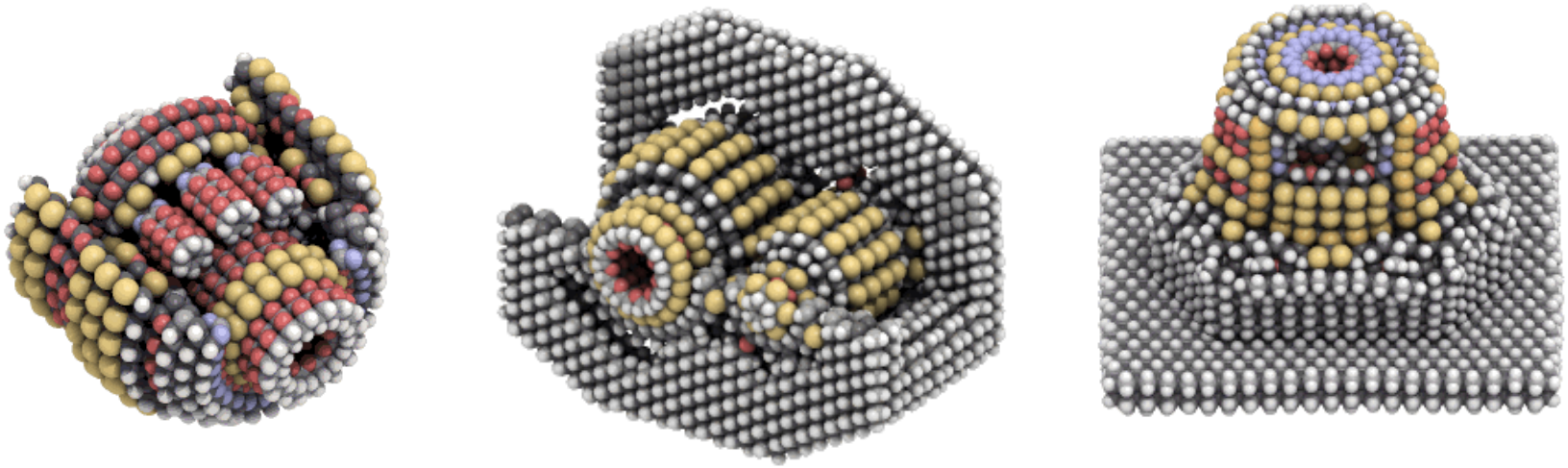
[Chen et al, 2005]

La nanoscience ascendante



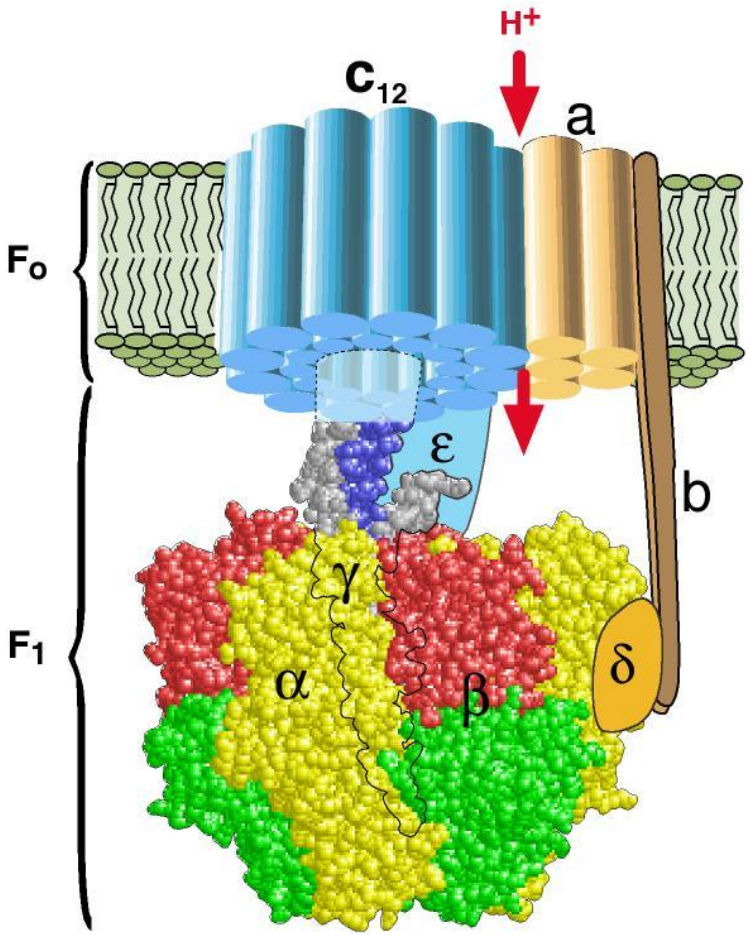
CEMES - CNRS

La nanoscience ascendante



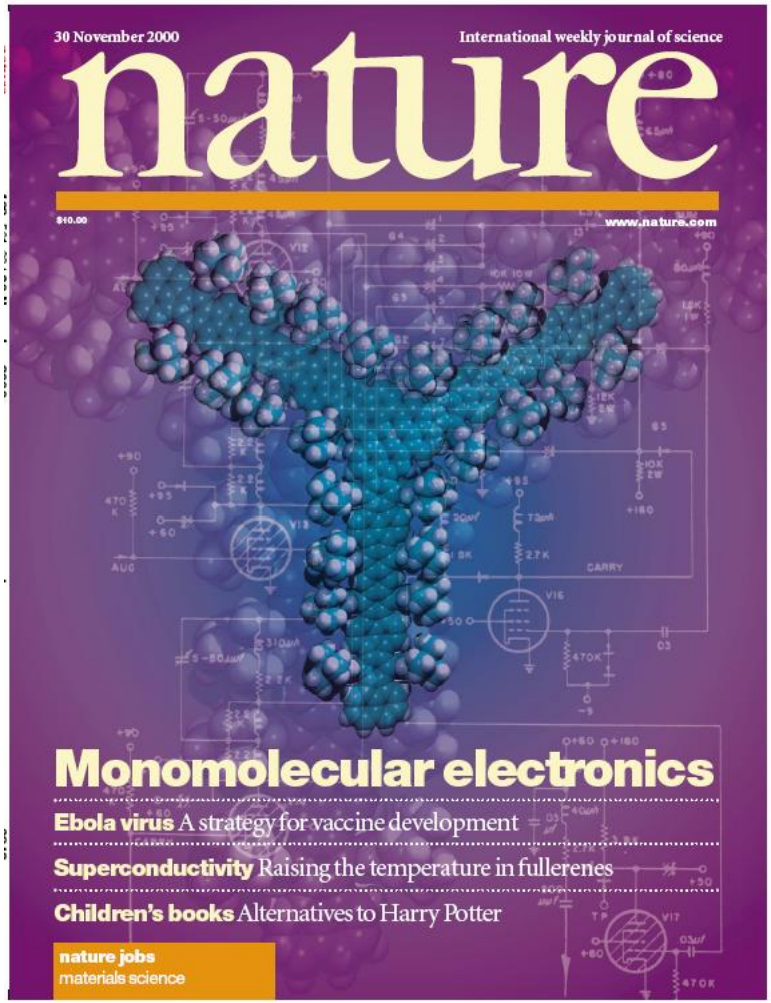
Nanorex

La nanoscience ascendante



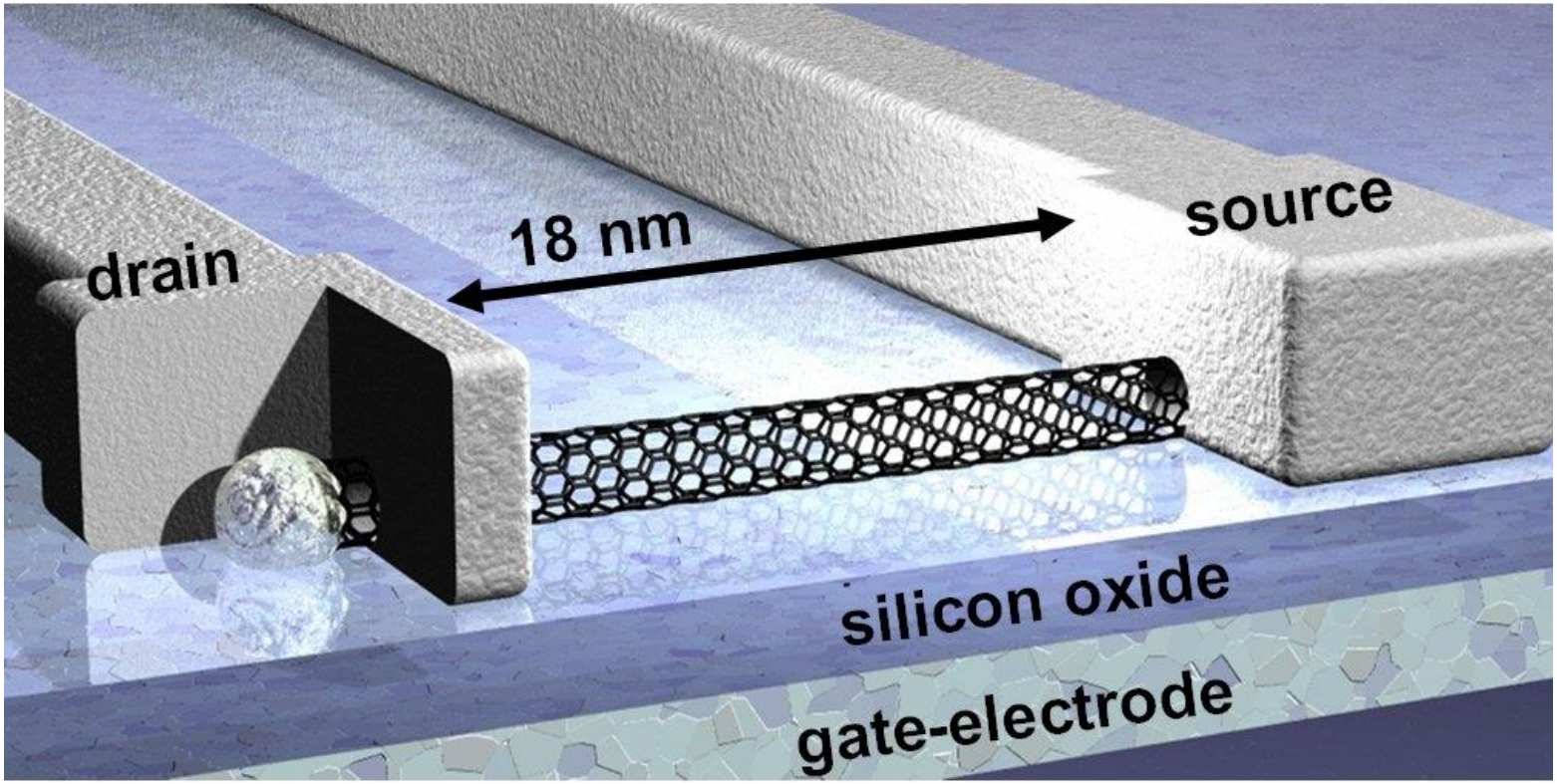
ATP Synthase (transformation de l'ADP en ATP)

La nanoscience ascendante



CEMES - CNRS

La nanoscience ascendante



Nanotube-based transistors – Infineon

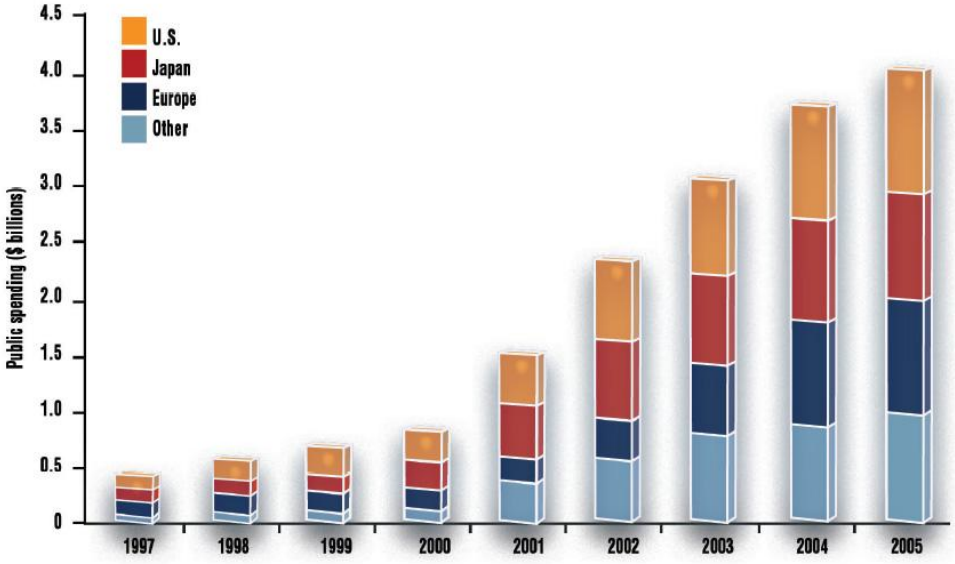
La nanoscience ascendante

- Sur une semaine… (Source: PHYSorg.com)
  - “A step towards better bran implants using conducting polymer nanotubes”
  - “Physicists create first atomic-scale map of quantum dots”
  - “Nanotech researchers develop artificial pore”
  - “Microchip can detect type and severity of cancer”
  - “Twinkling nanostars improve optical imaging of tumors”
  - “Nanodiamonds advance anticancer gene therapy”
  - “Golden nanotubes detect tumor cells, map sentinel lymph nodes”
  - “Engineers produce ‘how-to’ guide to controlling the structure of nanoparticles”
  - …

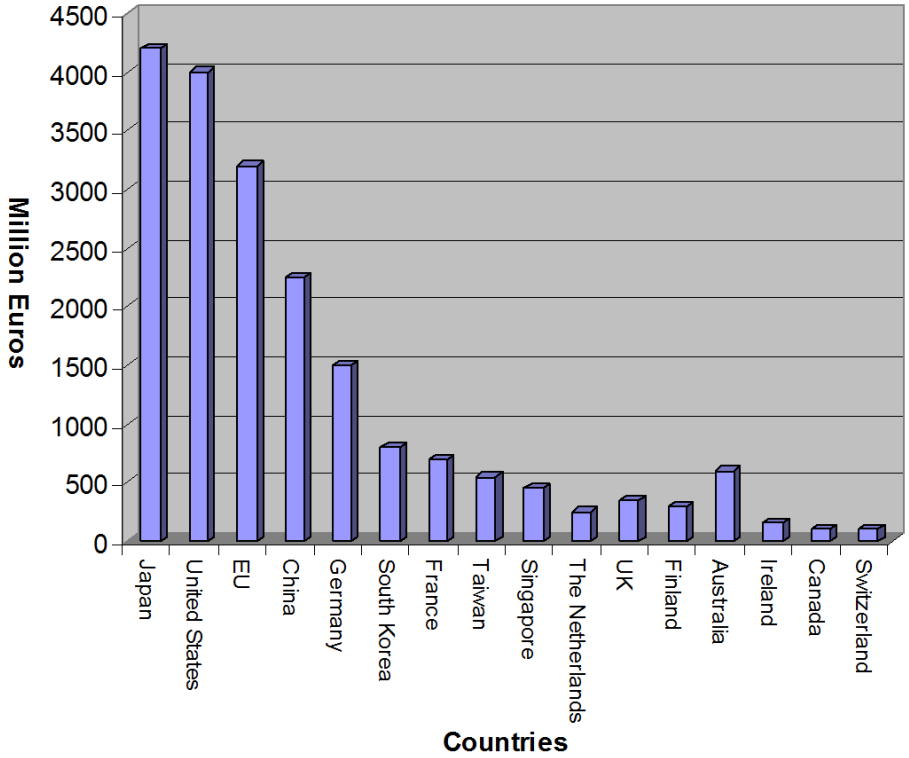
La nanoscience ascendante

- En général
  - Conception de médicaments
  - Science des matériaux
  - Chimie
  - Physique
  - Electronique
  - etc.

Nanosciences



Source: National Science Foundation and Strategies Unlimited

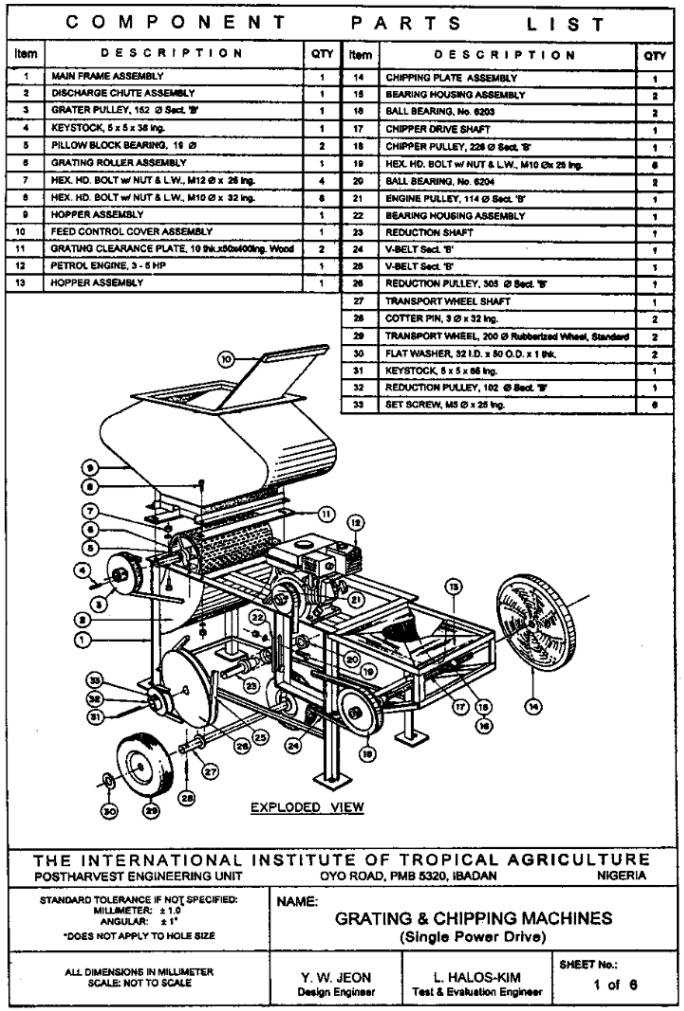


Source: Technology Transfer Centre, 2007

Financement public des nanotechnologies

Left: 1997-2005 – Right: 2006-2010 (projection)

Conception assistée par ordinateur



COMPONENT PARTS LIST

Item	DESCRIPTION	QTY	Item	DESCRIPTION	QTY
1	MAIN FRAME ASSEMBLY	1	14	CHIPPING PLATE ASSEMBLY	1
2	DISCHARGE CHUTE ASSEMBLY	1	15	BEARING HOUSING ASSEMBLY	2
3	GRATER PULLEY, 152 Ø Sect. 'B'	1	16	BALL BEARING, No. 6203	2
4	KEYSTOCK, 5 x 5 x 38 lng.	1	17	CHIPPER DRIVE SHAFT	1
5	PILLOW BLOCK BEARING, 19 Ø	2	18	CHIPPER PULLEY, 228 Ø Sect. 'B'	1
6	GRATING ROLLER ASSEMBLY	1	19	HEX. HD. BOLT w/ NUT & L.W., M10 Ø x 25 lng.	6
7	HEX. HD. BOLT w/ NUT & L.W., M12 Ø x 28 lng.	4	20	BALL BEARING, No. 6204	2
8	HEX. HD. BOLT w/ NUT & L.W., M10 Ø x 32 lng.	8	21	ENGINE PULLEY, 114 Ø Sect. 'B'	1
9	HOPPER ASSEMBLY	1	22	BEARING HOUSING ASSEMBLY	1
10	FEED CONTROL COVER ASSEMBLY	1	23	REDUCTION SHAFT	1
11	GRATING CLEARANCE PLATE, 10 thk.x50x400lng. Wood	2	24	V-BELT Sect. 'B'	1
12	PETROL ENGINE, 3 - 5 HP	1	25	V-BELT Sect. 'B'	1
13	HOPPER ASSEMBLY	1	26	REDUCTION PULLEY, 305 Ø Sect. 'B'	1
			27	TRANSPORT WHEEL SHAFT	1
			28	COTTER PIN, 3 Ø x 32 lng.	2
			29	TRANSPORT WHEEL, 200 Ø Rubberized Wheel, Standard	2
			30	FLAT WASHER, 32 I.D. x 50 O.D. x 1 thk.	2
			31	KEYSTOCK, 5 x 5 x 66 lng.	1
			32	REDUCTION PULLEY, 102 Ø Sect. 'B'	1
			33	SET SCREW, M5 Ø x 25 lng.	6

EXPLODED VIEW

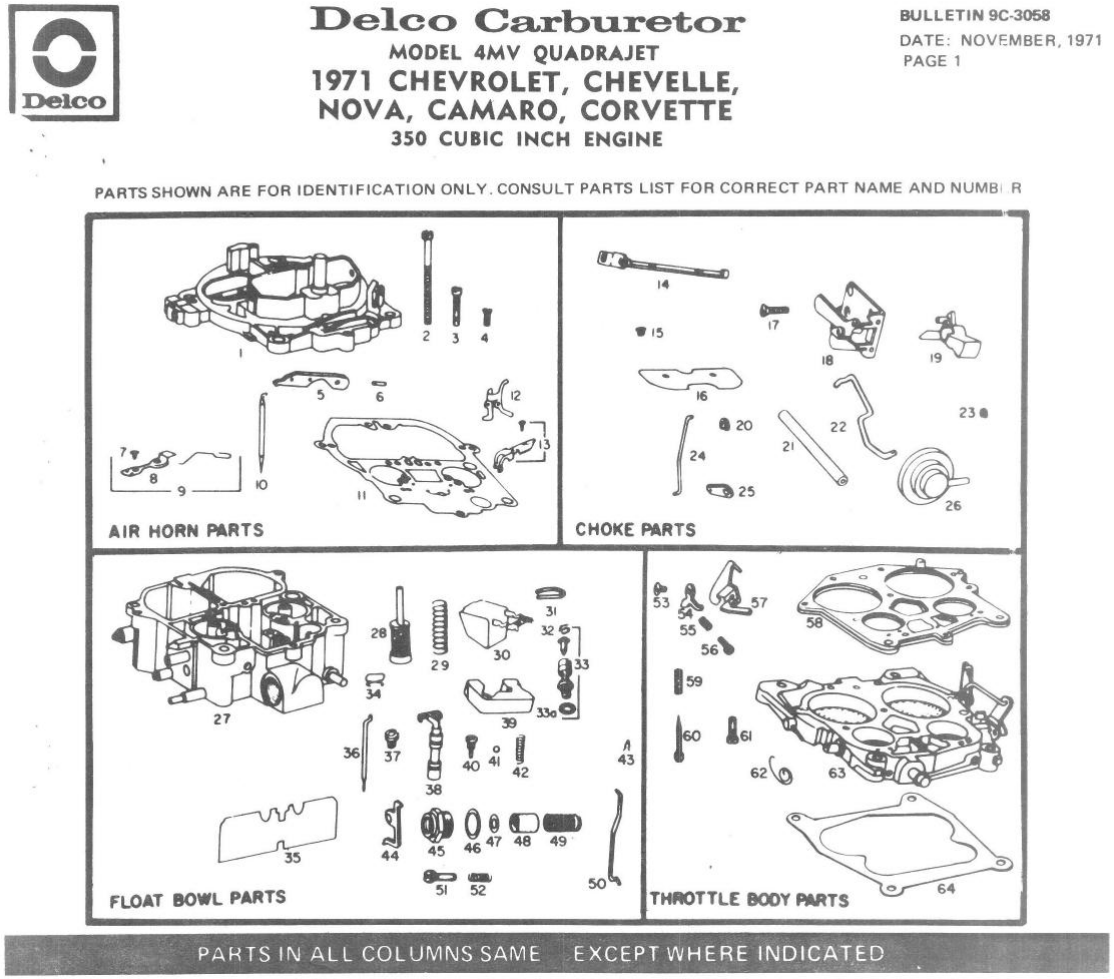
THE INTERNATIONAL INSTITUTE OF TROPICAL AGRICULTURE
POSTHARVEST ENGINEERING UNIT OYO ROAD, PMB 5320, IBADAN NIGERIA

STANDARD TOLERANCE IF NOT SPECIFIED: MILLIMETER: ± 1.0 ANGULAR: ± 1° *DOES NOT APPLY TO HOLE SIZE

NAME: GRATING & CHIPPING MACHINES (Single Power Drive)

ALL DIMENSIONS IN MILLIMETER SCALE: NOT TO SCALE

Y. W. JEON, Design Engineer — L. HALOS-KIM, Test & Evaluation Engineer — SHEET No.: 1 of 6



Delco

Delco Carburetor
MODEL 4MV QUADRAJET
1971 CHEVROLET, CHEVELLE, NOVA, CAMARO, CORVETTE
350 CUBIC INCH ENGINE

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

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

AIR HORN PARTS

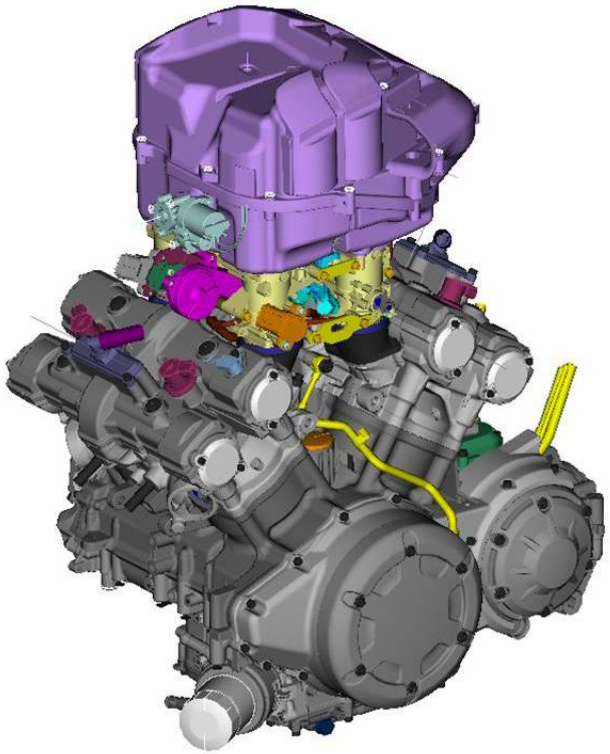
CHOKE PARTS

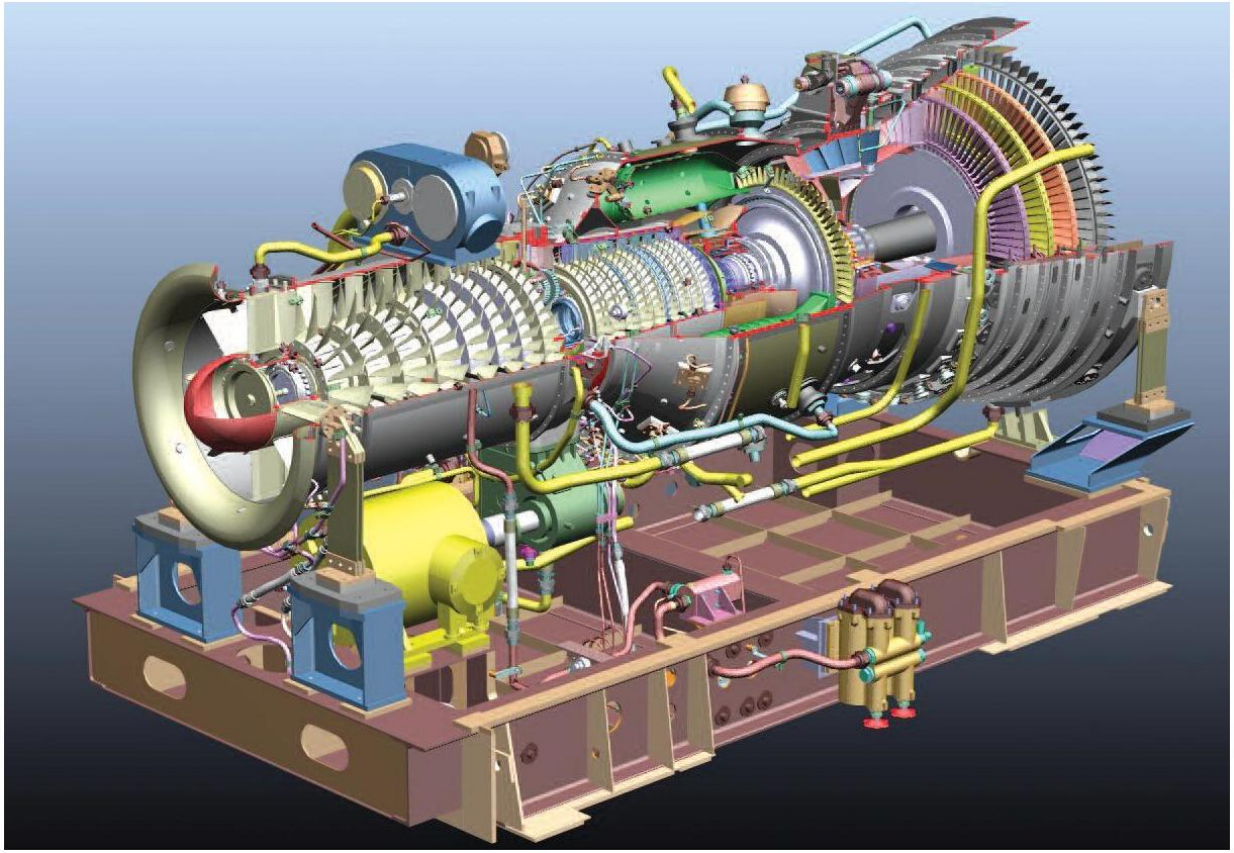
FLOAT BOWL PARTS

THROTTLE BODY PARTS

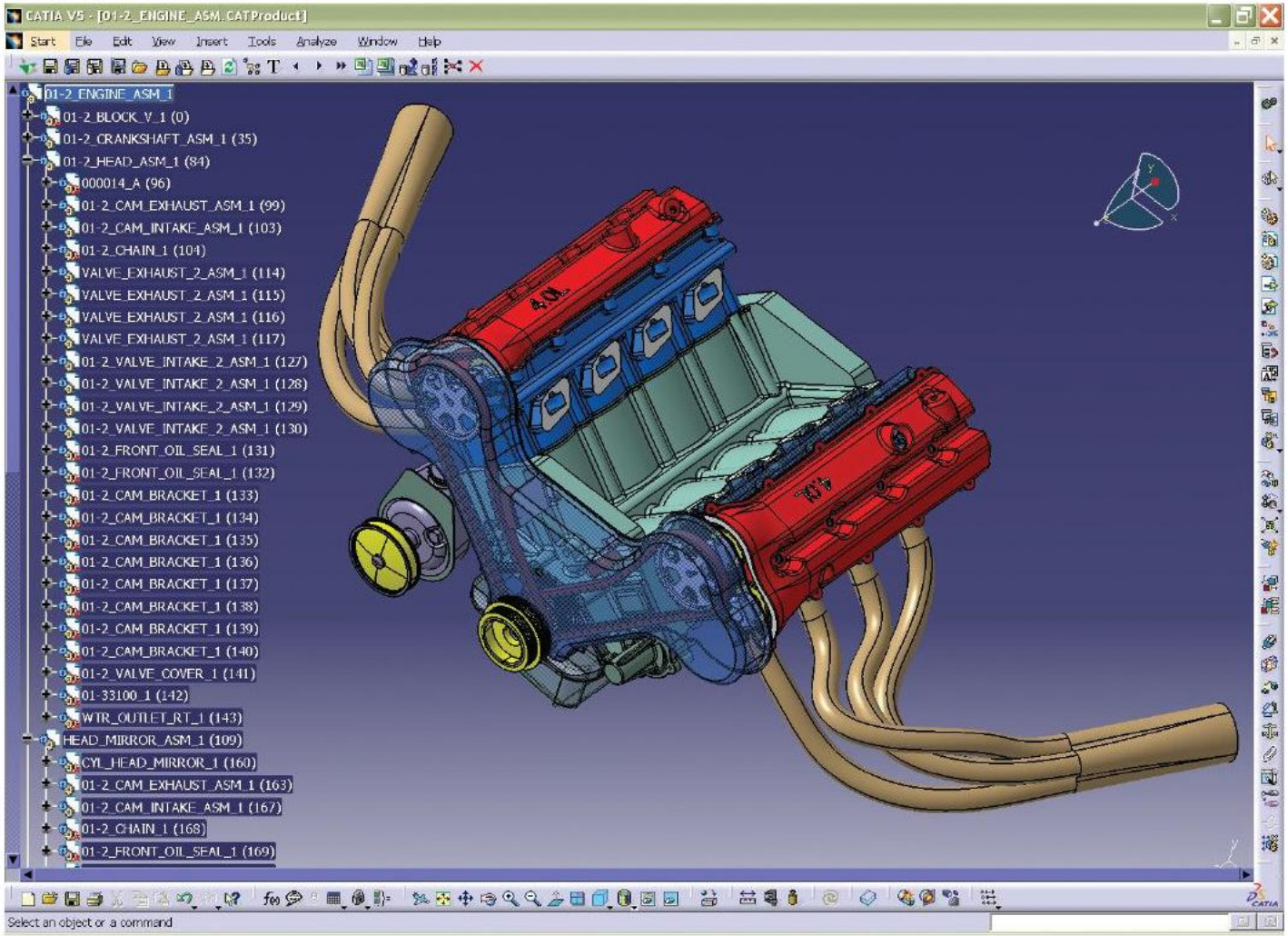
PARTS IN ALL COLUMNS SAME EXCEPT WHERE INDICATED

Conception assistée par ordinateur

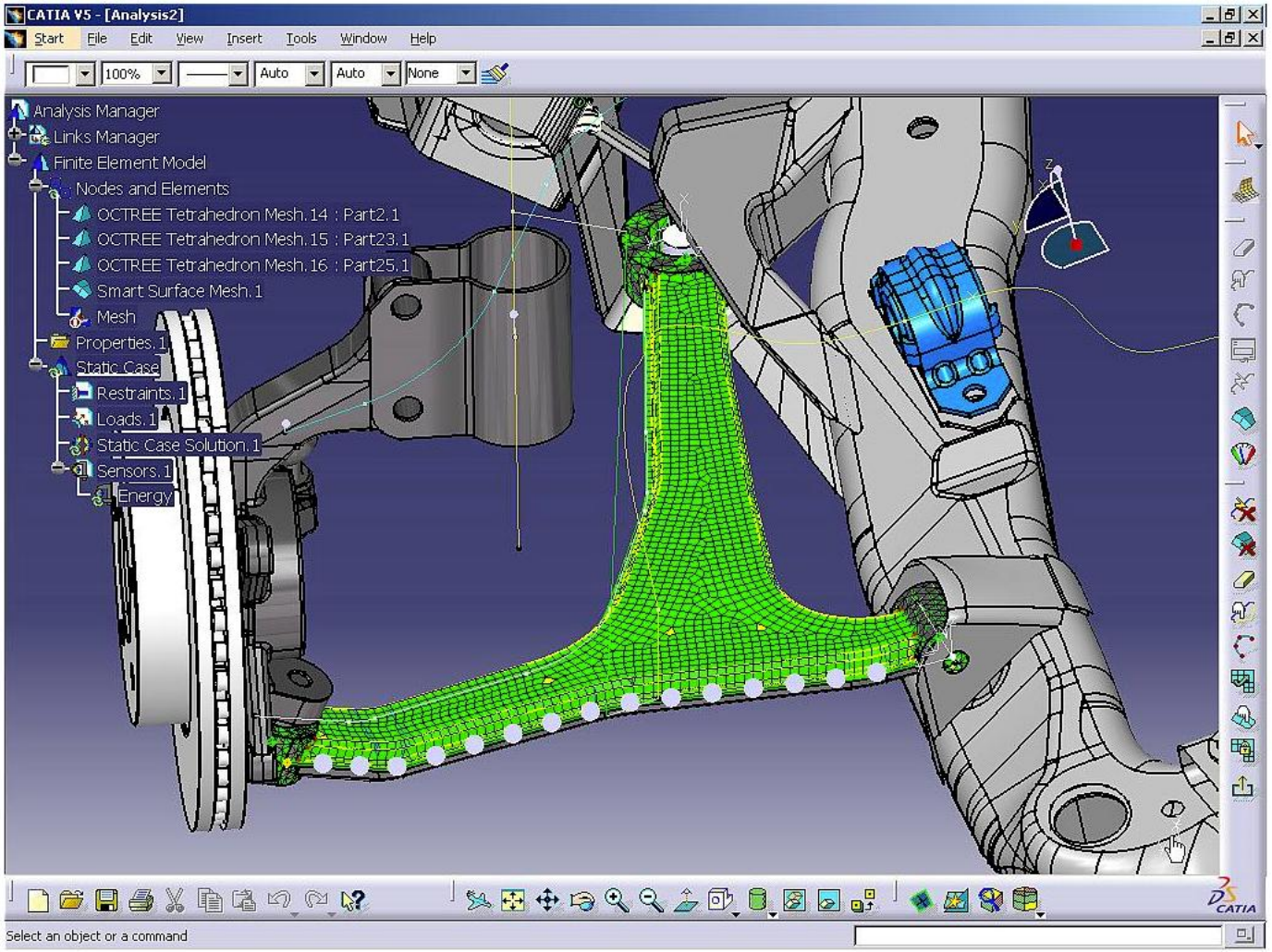




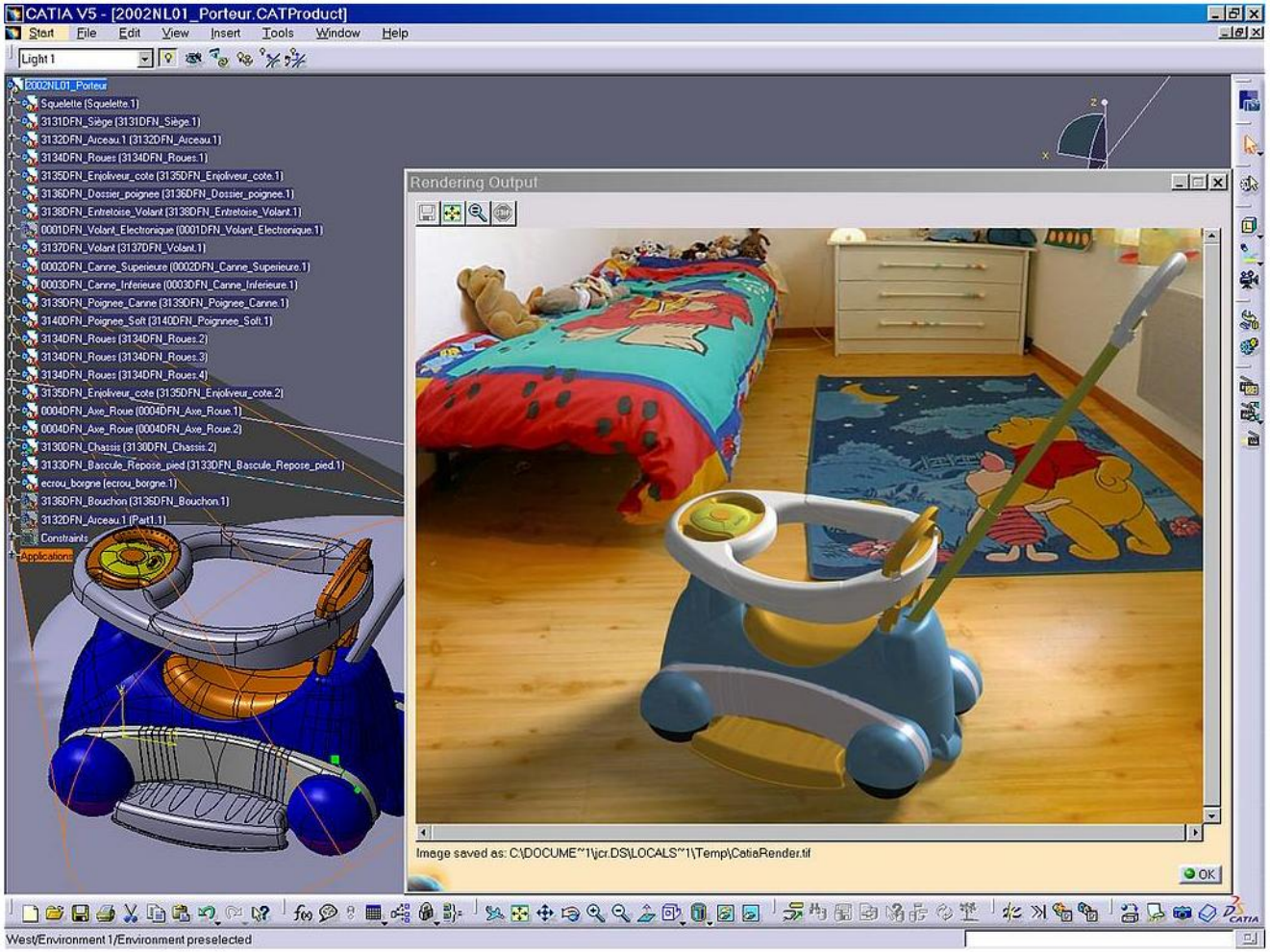
Conception assistée par ordinateur



Conception assistée par ordinateur

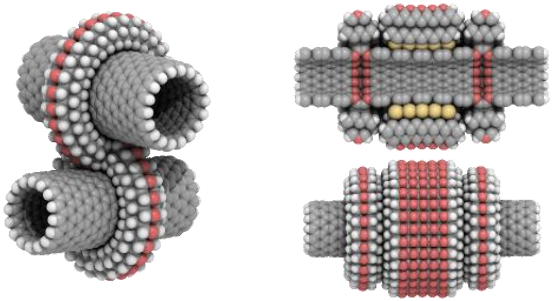


Conception assistée par ordinateur

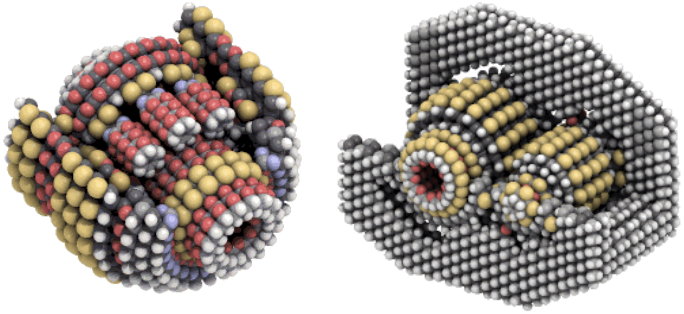


Conception assistée par ordinateur

- Conception assistée par ordinateur
  - Modéliser (dessiner)

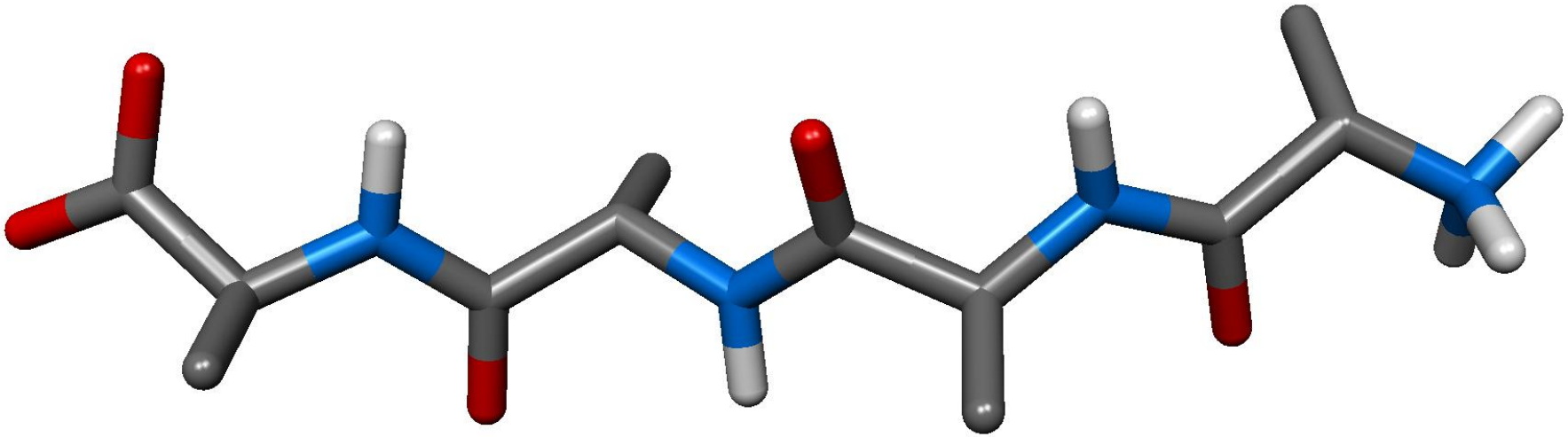


  - …et simuler (calculer le mouvement)



Comment représenter une molécule?

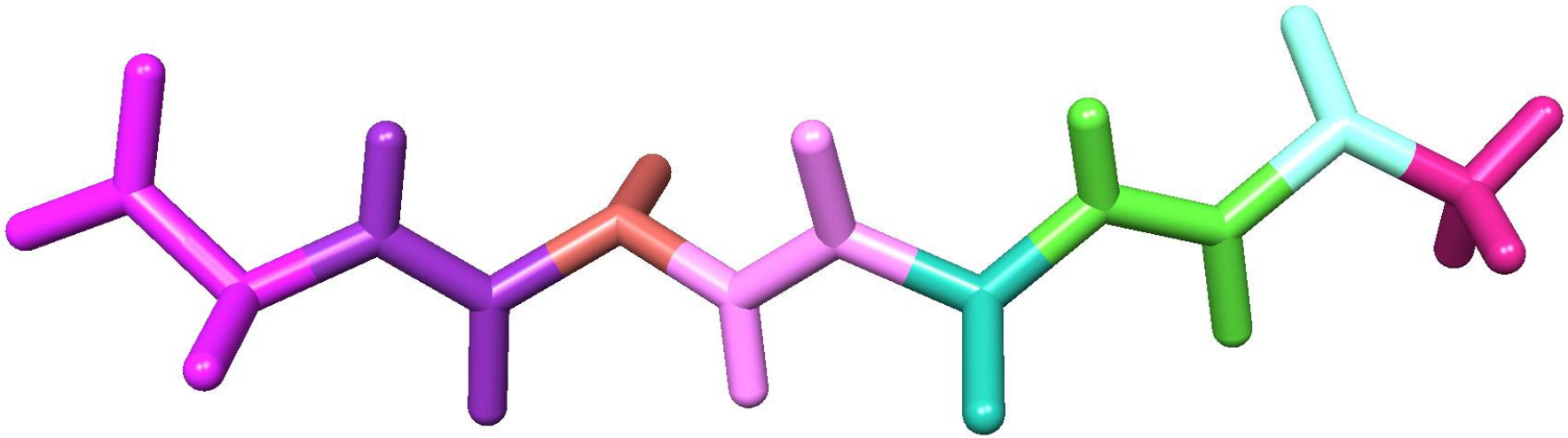
Représenter une molécule



Une petite molécule, la tétra-alanine, est composée de vingt-sept atomes

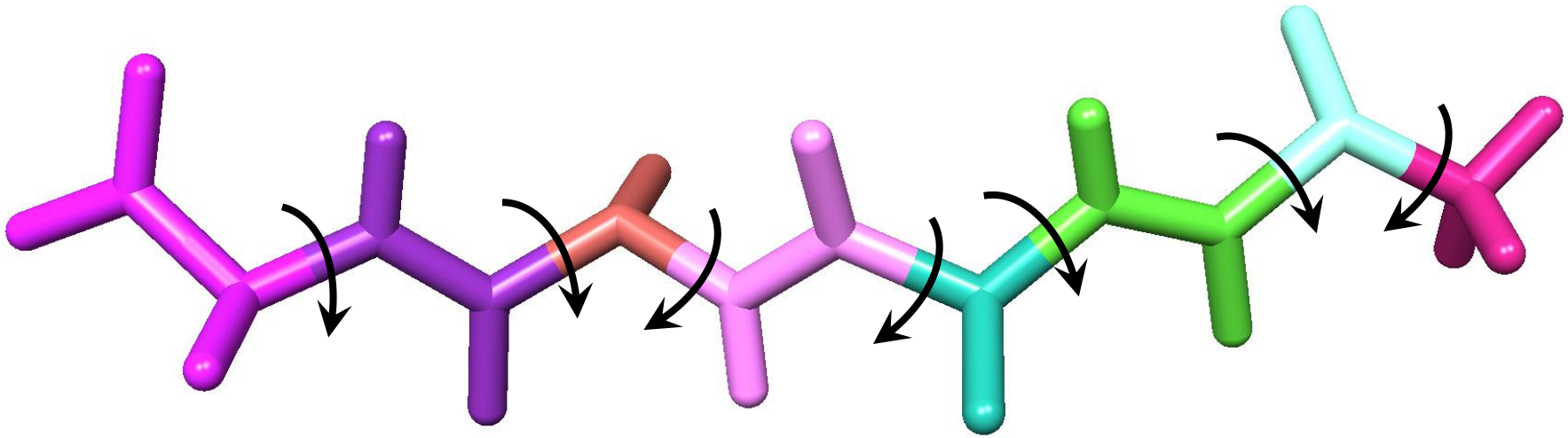
Et le mouvement de la molécule?

Représenter le mouvement d'une molécule



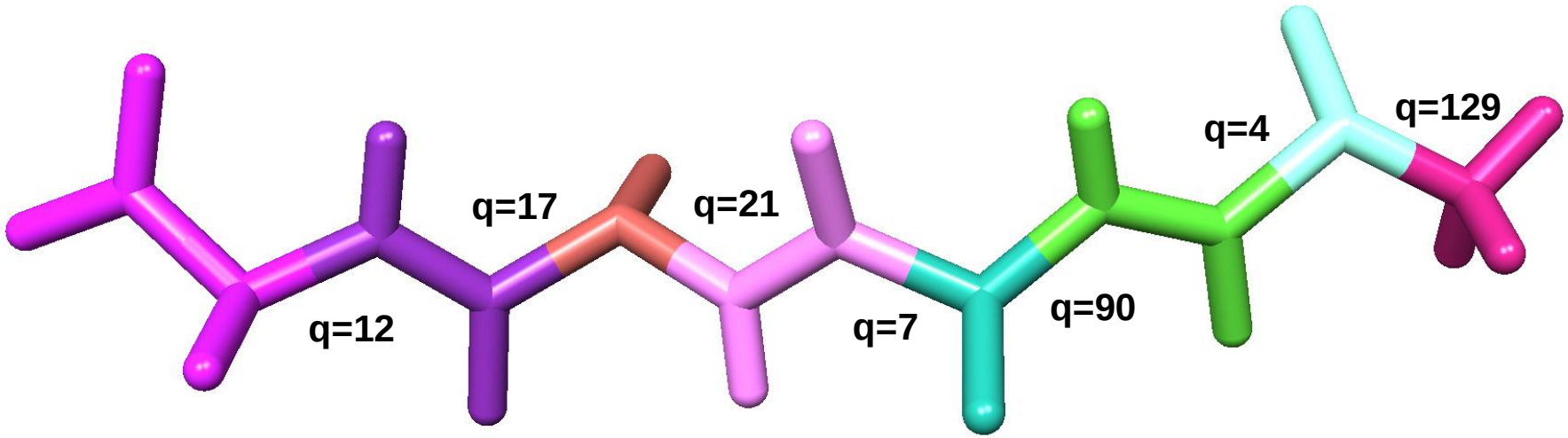
Les atomes sont répartis en huit objets rigides…

Représenter le mouvement d'une molécule



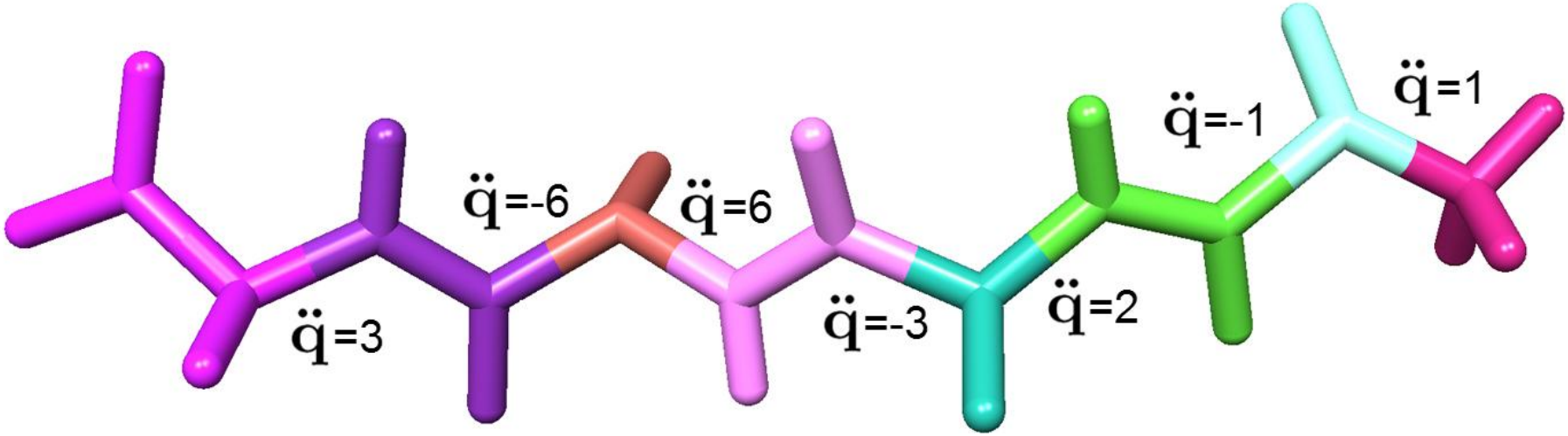
… qui peuvent tourner les uns par rapport aux autres.

Représenter le mouvement d'une molécule



Les angles décrivent la forme de la molécule

Représenter le mouvement d'une molécule



L'inconnue : les accélérations des angles

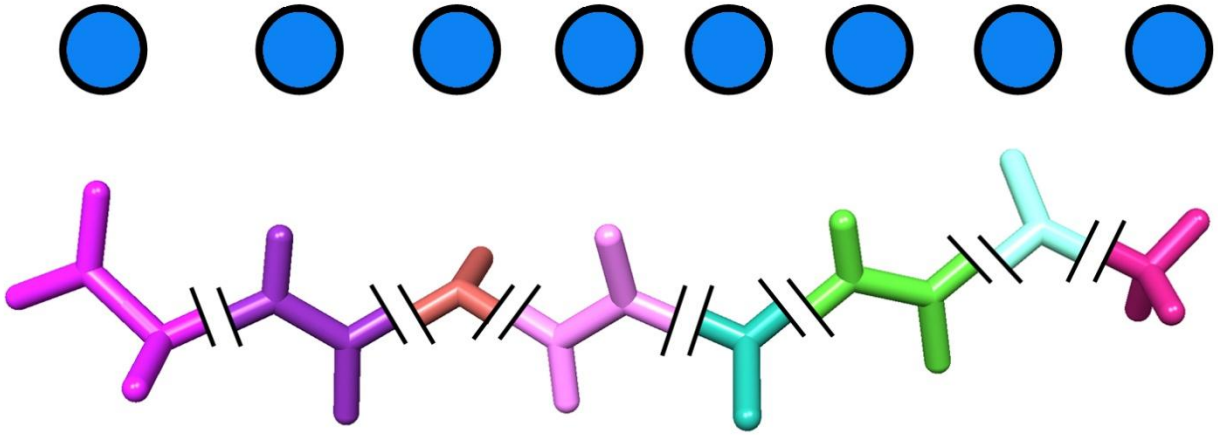
Comment calculer ce mouvement ?

Calculer le mouvement d'une molécule

Idée

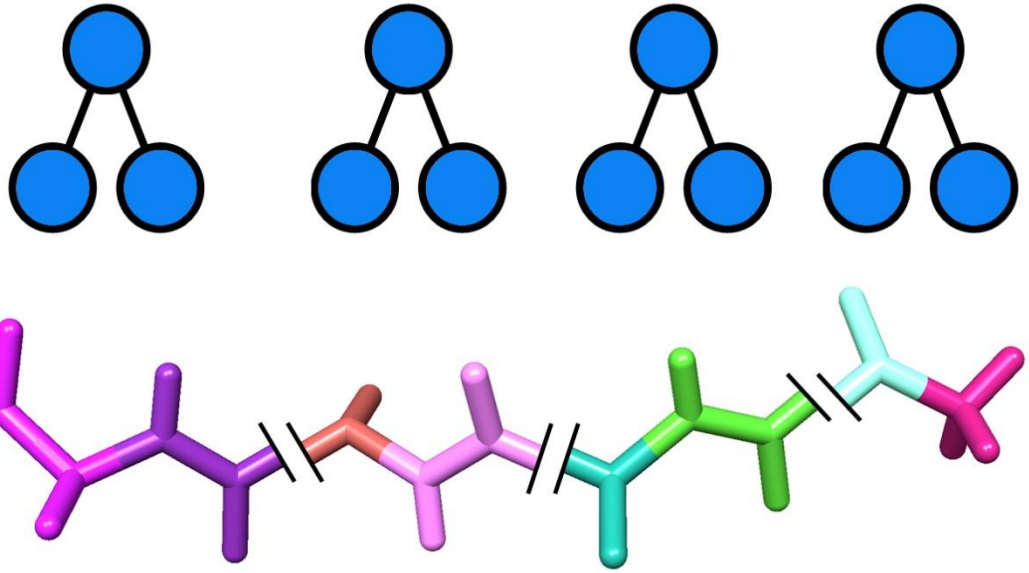
L'approche **diviser-pour-régner** inventée par Roy Featherstone en 1999

Calculer le mouvement d'une molécule



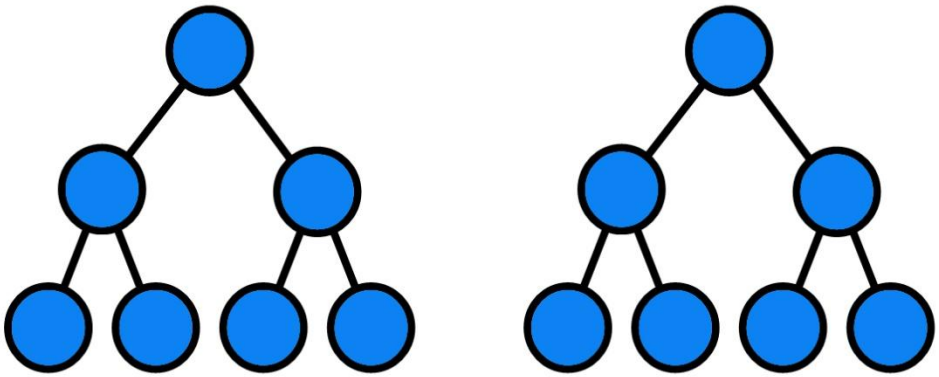
Les objets rigides…

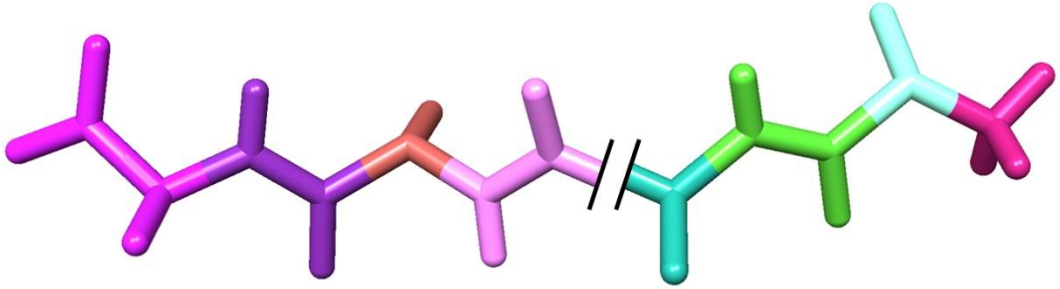
Calculer le mouvement d'une molécule



… sont assemblés deux par deux pour former des paires…

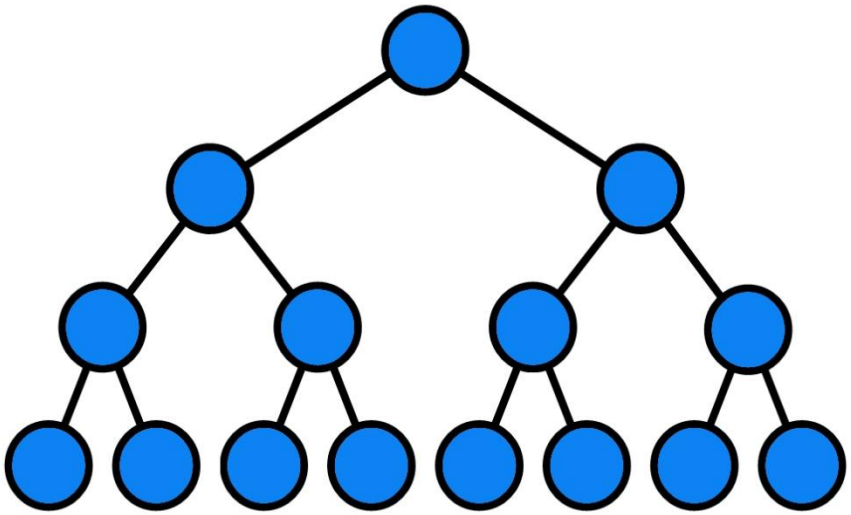
Calculer le mouvement d'une molécule

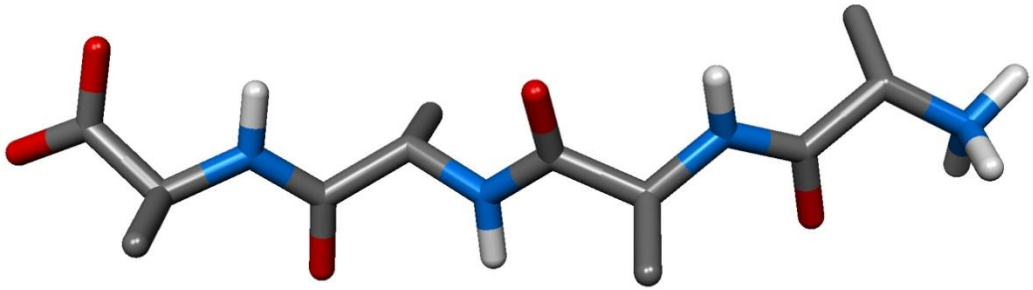




… qui sont assemblées deux à deux…

Calculer le mouvement d'une molécule

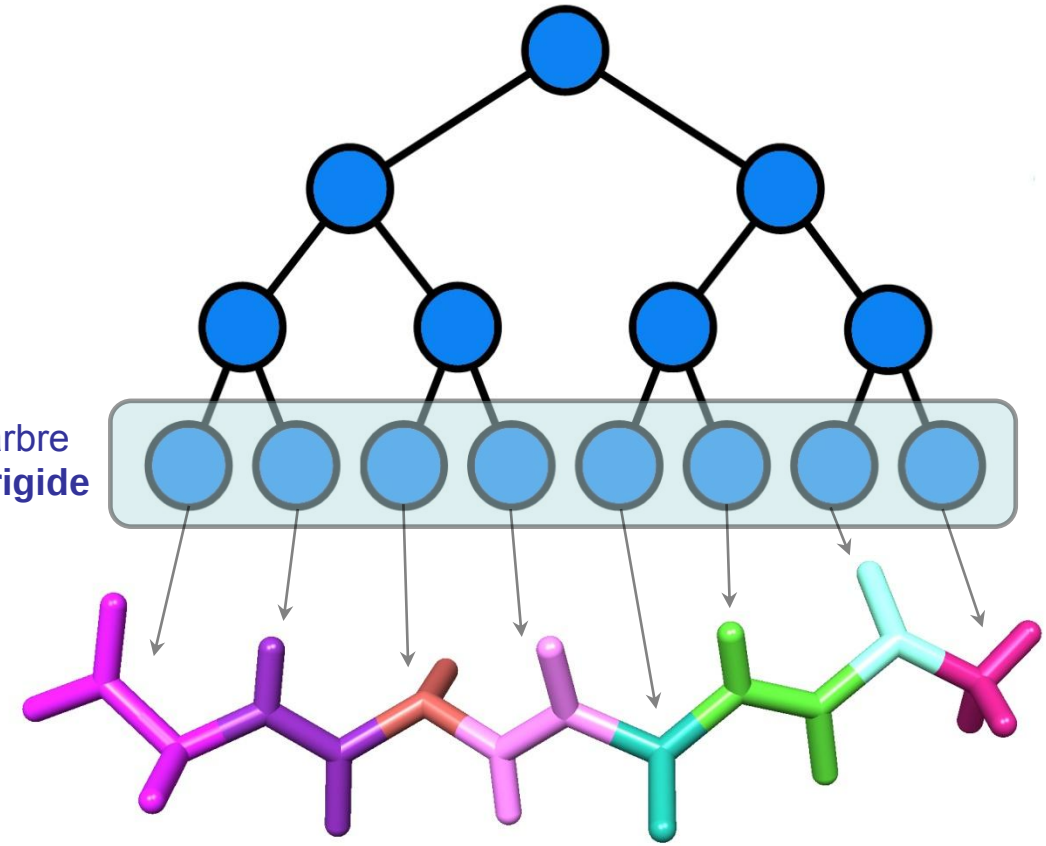




…et ainsi de suite pour former la molécule complète

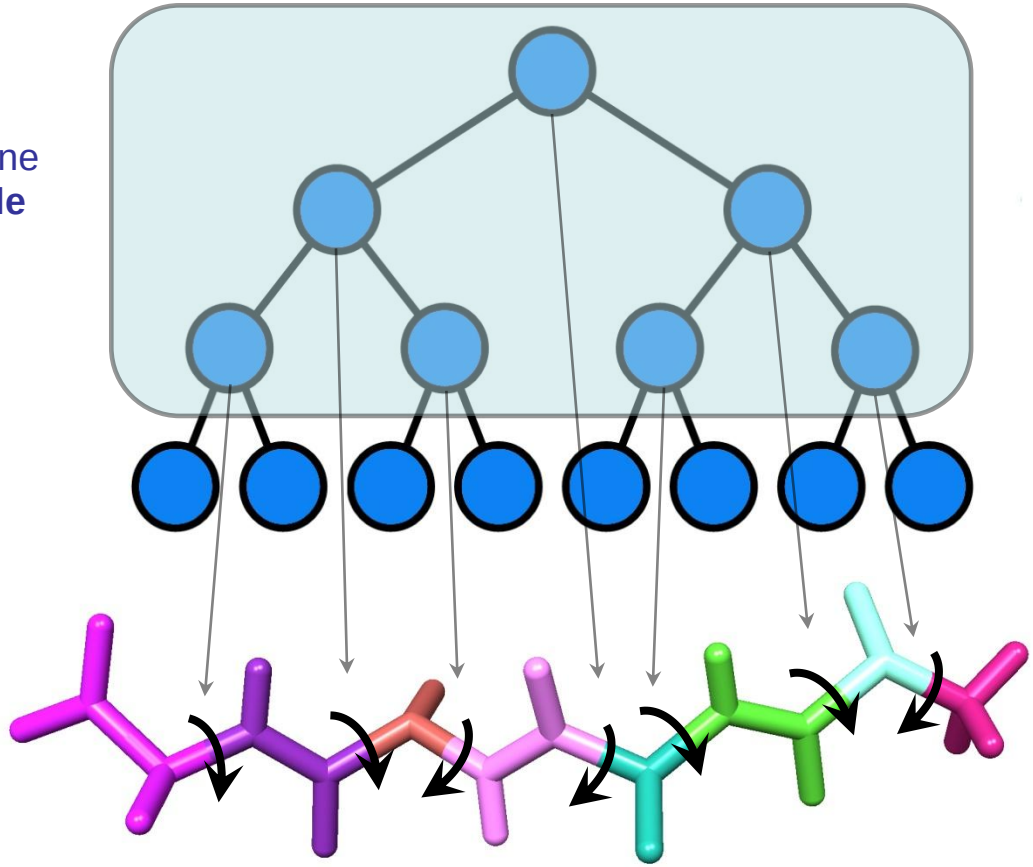
Calculer le mouvement d'une molécule

Chaque feuille de l'arbre représente **un objet rigide**



Calculer le mouvement d'une molécule

Chaque noeud interne représente **un angle**



Calculer le mouvement d'une molécule

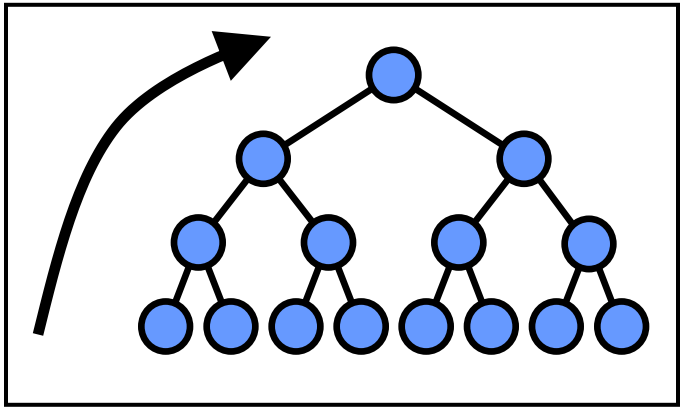
- L'équation des objets articulés (Roy Featherstone, 1999)

$$\begin{bmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \vdots \\ \mathbf{a}_m \end{bmatrix} = \begin{bmatrix} \mathbf{\Phi}_1 & \mathbf{\Phi}_{12} & \cdots & \mathbf{\Phi}_{1m} \\ \mathbf{\Phi}_{21} & \mathbf{\Phi}_2 & \cdots & \mathbf{\Phi}_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{\Phi}_{m1} & \mathbf{\Phi}_{m2} & \cdots & \mathbf{\Phi}_m \end{bmatrix} \begin{bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_m \end{bmatrix} + \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \vdots \\ \mathbf{b}_m \end{bmatrix}$$

Accélérations **Inverse de la masse** **Forces** **Biais**

Calculer le mouvement d'une molécule

- L'équation des objets articulés (Roy Featherstone, 1999)
- L'algorithme de Roy Featherstone
  - On calcule les coefficients des équations (de bas en haut)



Inverse de la masse

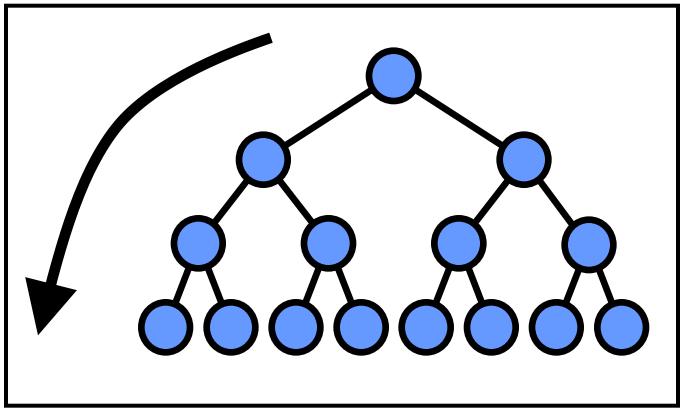
$$\mathbf{\Phi}_1^C = \mathbf{\Phi}_1^A - \mathbf{\Phi}_{12}^A \mathbf{W} \mathbf{\Phi}_{21}^A$$
$$\mathbf{\Phi}_2^C = \mathbf{\Phi}_2^B - \mathbf{\Phi}_{21}^B \mathbf{W} \mathbf{\Phi}_{12}^B$$
$$\mathbf{\Phi}_{21}^C = \mathbf{\Phi}_{21}^B \mathbf{W} \mathbf{\Phi}_{21}^A = (\mathbf{\Phi}_{12}^C)^T$$

Accélérations de biais

$$\mathbf{b}_1^C = \mathbf{b}_1^A - \mathbf{\Phi}_{12}^A \boldsymbol{\gamma}$$
$$\mathbf{b}_2^C = \mathbf{b}_2^B + \mathbf{\Phi}_{21}^B \boldsymbol{\gamma}$$

Calculer le mouvement d'une molécule

- L'équation des objets articulés (Roy Featherstone, 1999)
- L'algorithme de Roy Featherstone
  - On calcule les accélérations et les forces (de haut en bas)



Accélérations

$$\ddot{\mathbf{q}} = (\mathbf{S}^T\mathbf{V}\mathbf{S})^{-1}(\mathbf{Q} - \mathbf{S}^T\mathbf{V}(\mathbf{\Phi}_{21}^A\mathbf{f}_1^A - \mathbf{\Phi}_{12}^B\mathbf{f}_2^B + \boldsymbol{\beta}))$$

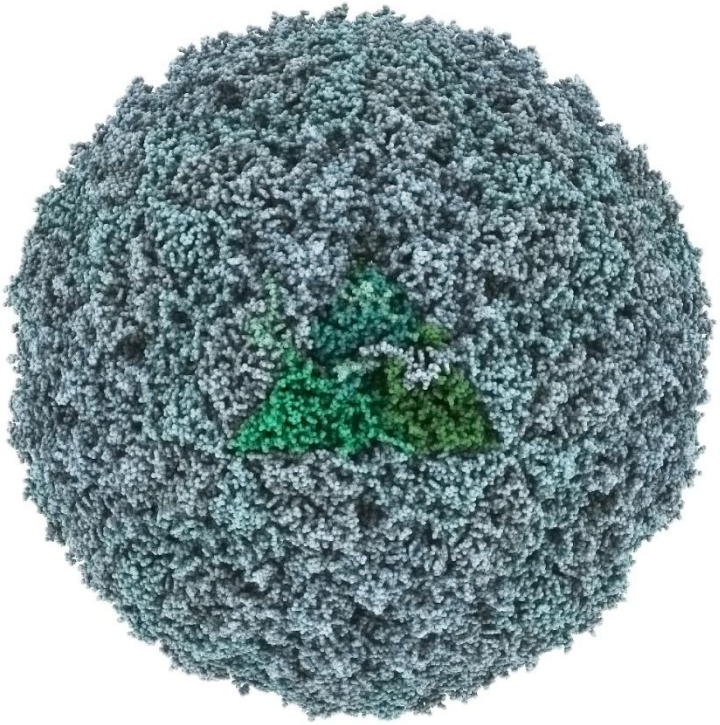
Forces

$$\mathbf{f}_1^B = \mathbf{W}\mathbf{\Phi}_{21}^A\mathbf{f}_1^A - \mathbf{W}\mathbf{\Phi}_{12}^B\mathbf{f}_2^B + \boldsymbol{\gamma}$$
$$\mathbf{f}_2^A = -\mathbf{f}_1^B$$

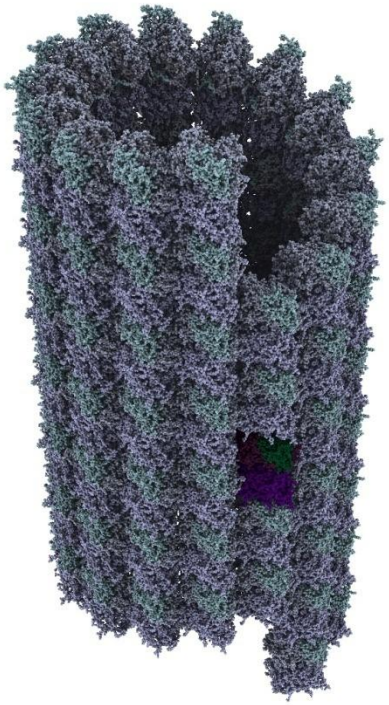
Et ça marche ?

Le problème

Cette méthode est trop lente quand il y a beaucoup d'atomes!



Enveloppe du virus de la fievre aphteuse



Microtubule

Comment faire ?

La simulation moléculaire adaptative

Idée

Seule **une partie** des angles peut changer à chaque instant

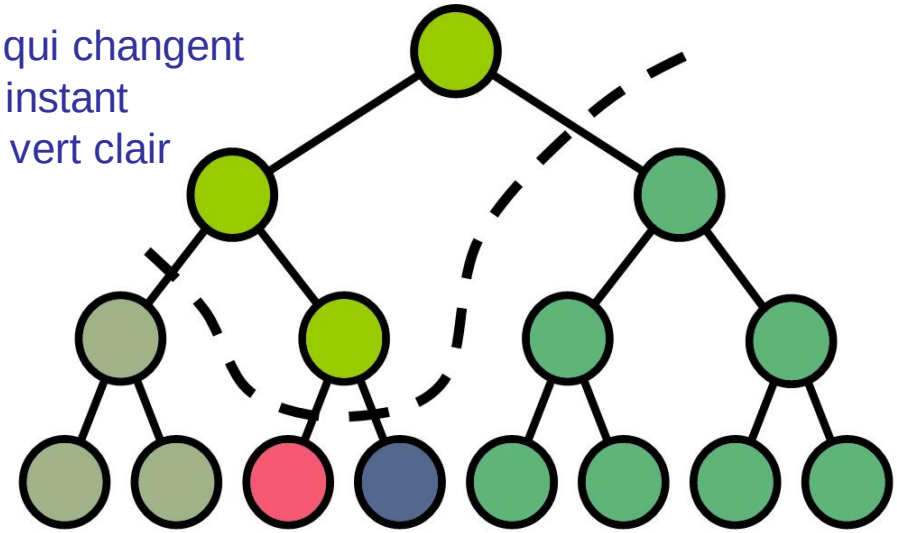
1) L'utilisateur choisit **le nombre** d'angles

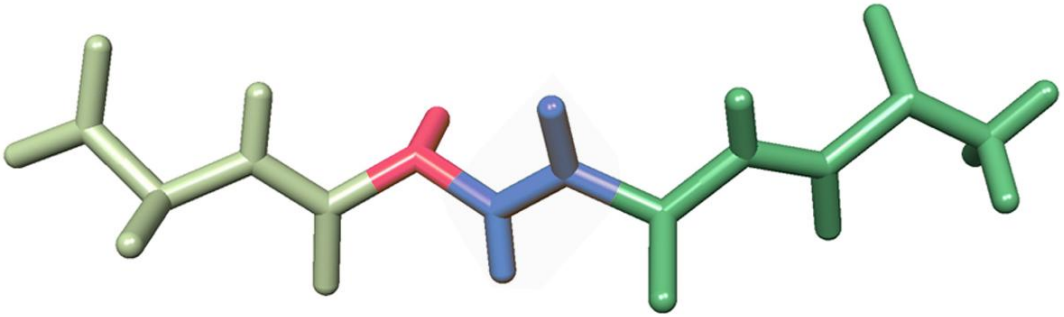
2) L'algorithme choisit **les bons angles**

On obtient un mouvement **approché**, mais **plus rapidement**

La simulation moléculaire adaptative

Les angles qui changent
à cet instant
sont en vert clair





Seule une partie des angles change à chaque instant

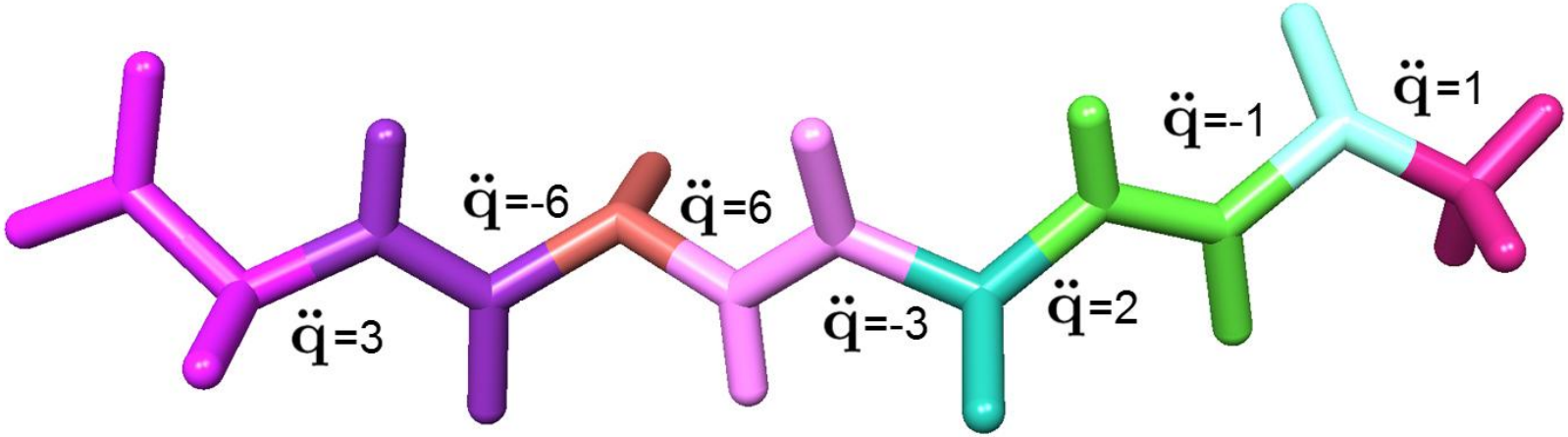
Comment choisir les bons angles?

Choisir les bons angles

$$\mathscr{A}(C) = \sum_{i \in C} \ddot{\mathbf{q}}_i^T \mathbf{A}_i \ddot{\mathbf{q}}_i$$

$\mathscr{A}(C)$ est appelée “accélération de groupe”

Choisir les bons angles



Choisir les bons angles

Théorème

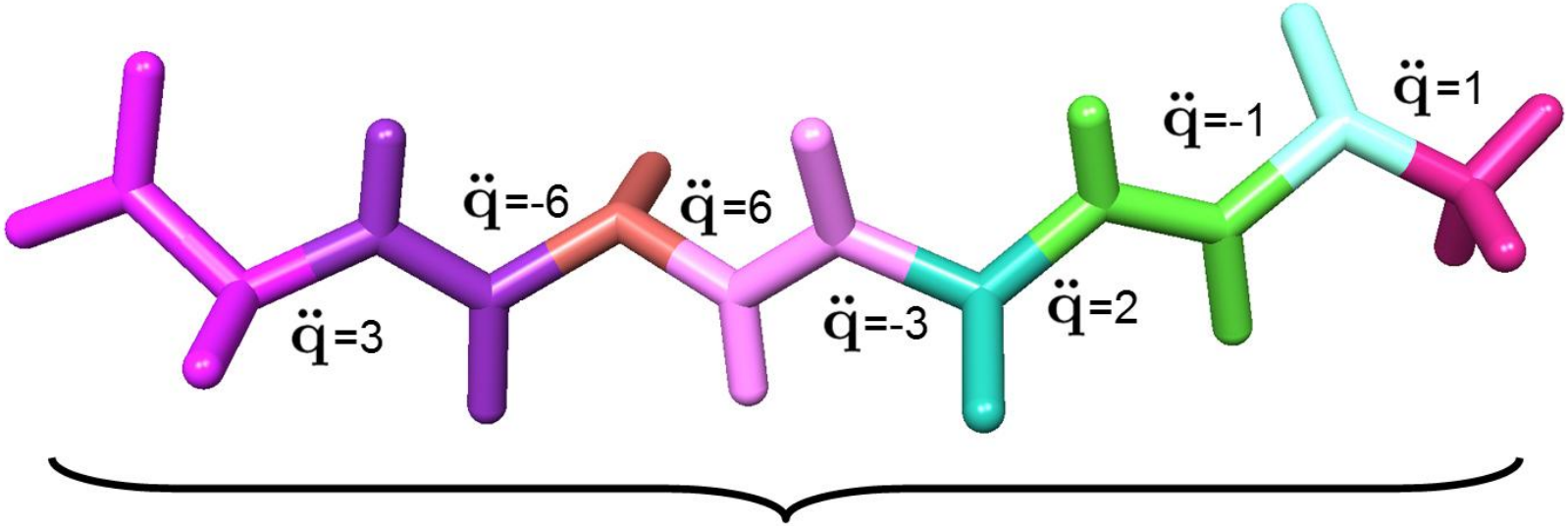
L'accélération de groupe peut être calculée **avant** de calculer chacune des accélérations séparément

$$\mathscr{A}(C) = \begin{bmatrix} \mathbf{f}_1^A \\ \mathbf{f}_2^B \end{bmatrix}^T \begin{bmatrix} \mathbf{\Psi}_1^C & \mathbf{\Psi}_{12}^C \\ \mathbf{\Psi}_{21}^C & \mathbf{\Psi}_2^C \end{bmatrix} \begin{bmatrix} \mathbf{f}_1^A \\ \mathbf{f}_2^B \end{bmatrix} + \begin{bmatrix} \mathbf{f}_1^A \\ \mathbf{f}_2^B \end{bmatrix}^T \begin{bmatrix} \mathbf{p}_1^C \\ \mathbf{p}_2^C \end{bmatrix} + \eta^C$$

(au lieu de $\mathscr{A}(C) = \sum_{i \in C} \ddot{\mathbf{q}}_i^T \mathbf{A}_i \ddot{\mathbf{q}}_i$)

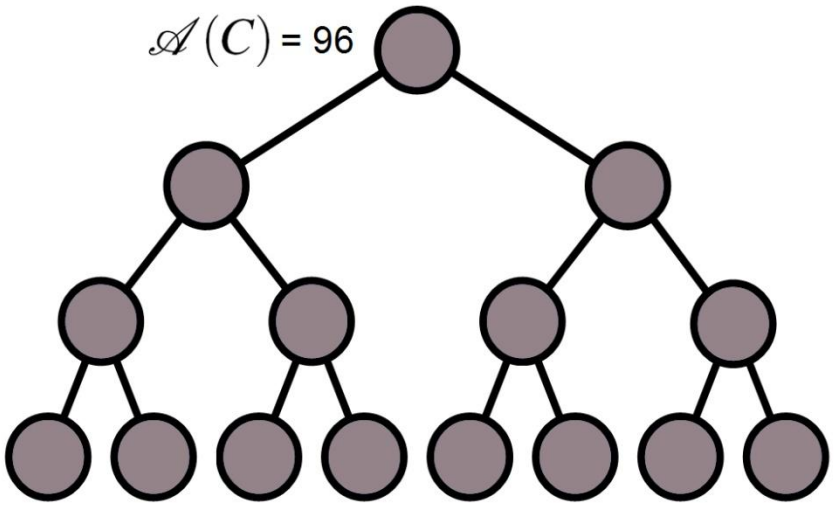
- *S. Redon and Ming C. Lin. "An Efficient, Error-Bounded Approximation Algorithm for Simulating Quasi-Statics of Complex Linkages". In Computer-Aided Design, 38 (2006) 300-314, Elsevier.*
- *S. Redon, N. Galoppo and M. C. Lin. "Adaptive Dynamics of Articulated Bodies". In ACM Transactions on Graphics (SIGGRAPH 2005), 24(3).*
- *R. Rossi, M. Isorce, S. Morin, J. Flocard, K. Arumugam, S. Crouzy, M. Vivaudou and S. Redon. "Adaptive Torsion-Angle Quasi-Statics: a General Simulation Method with Applications to Protein Structure Analysis and Design". Bioinformatics, 2007.*

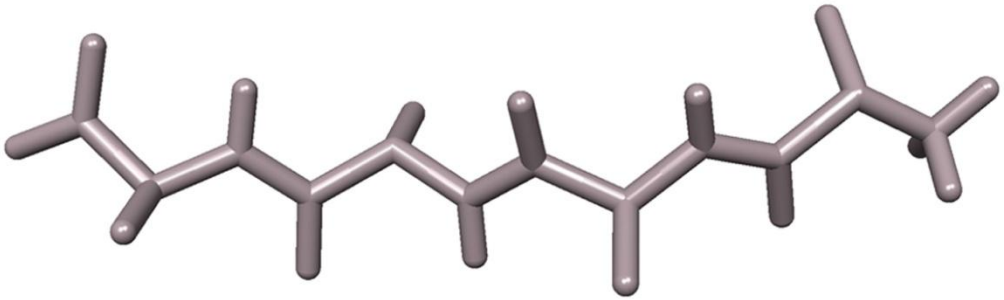
Choisir les bons angles



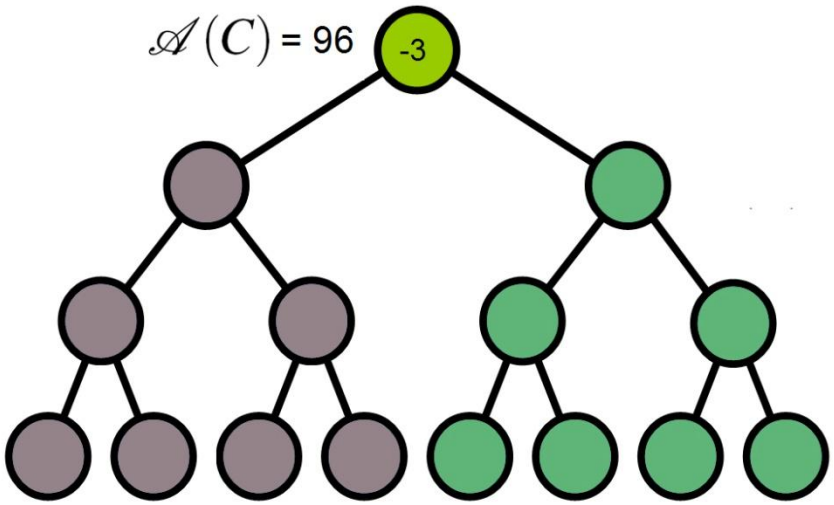
$$\mathscr{A}(C) = 96$$

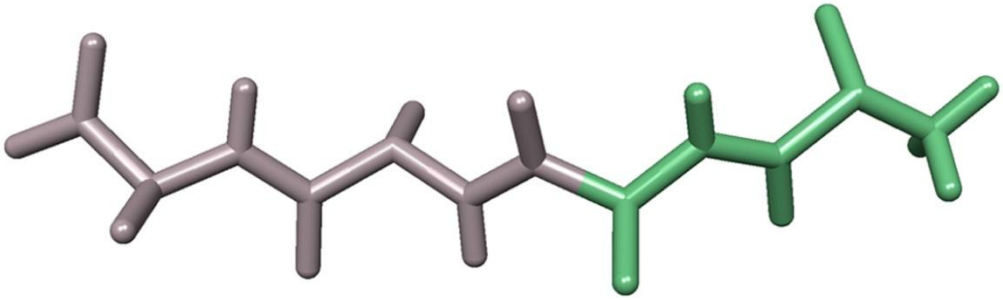
Choisir les bons angles



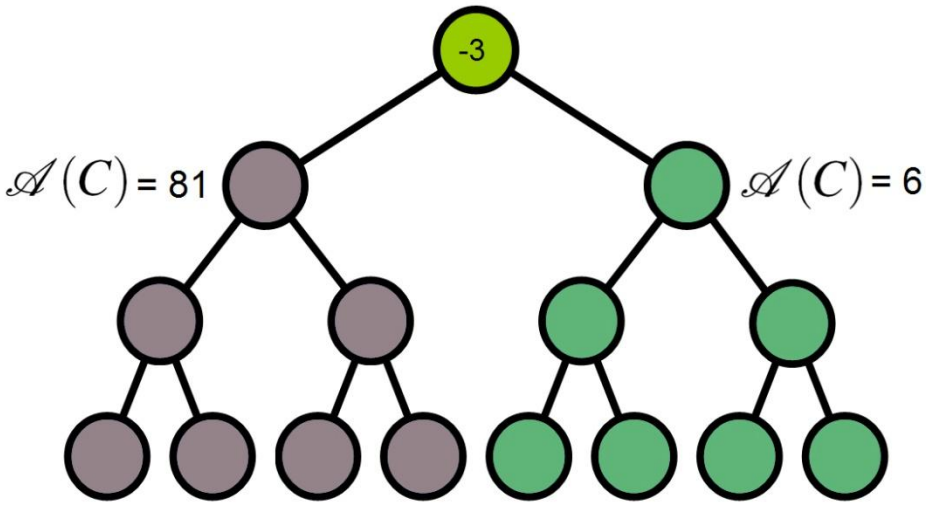


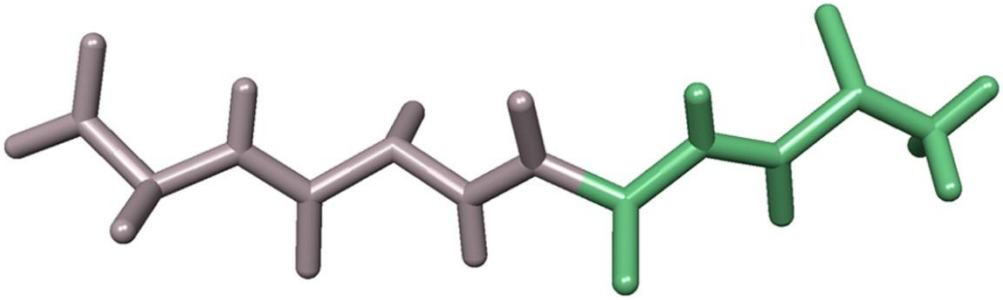
Choisir les bons angles



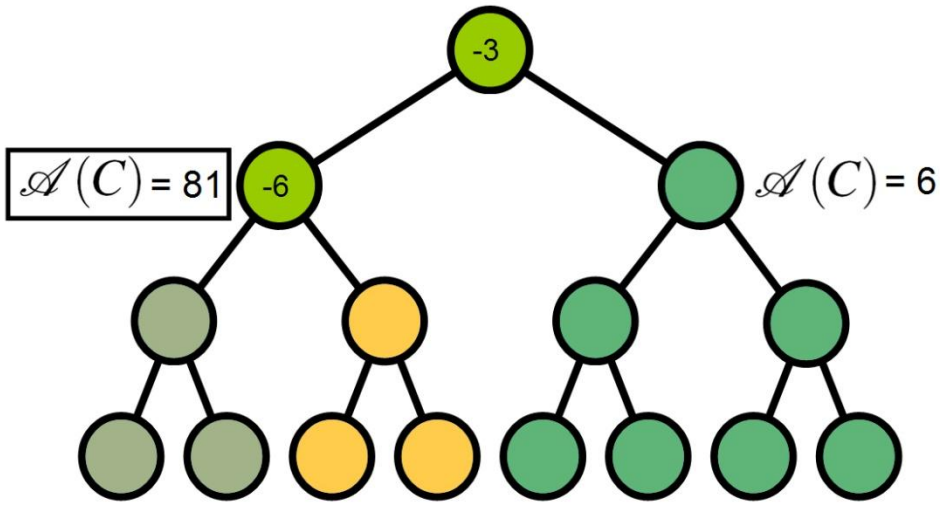


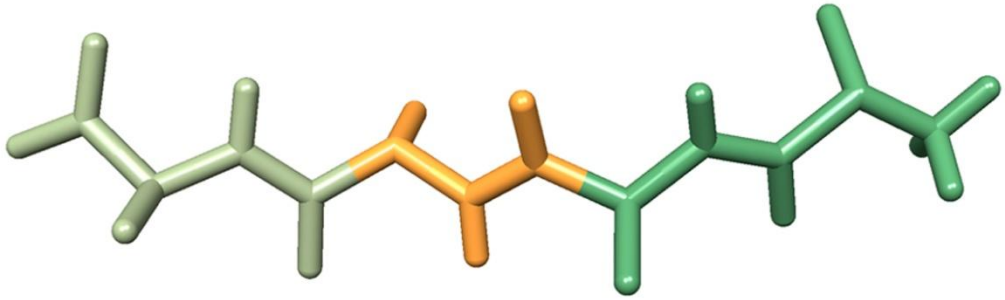
Choisir les bons angles



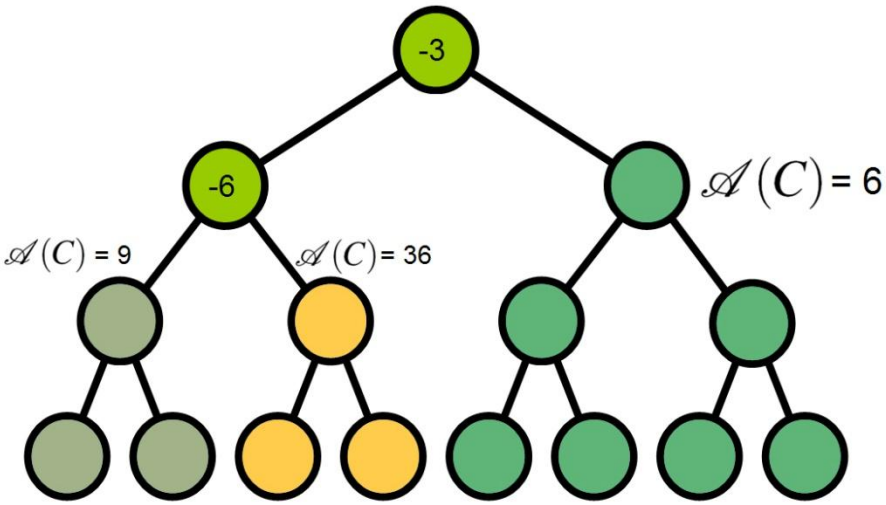


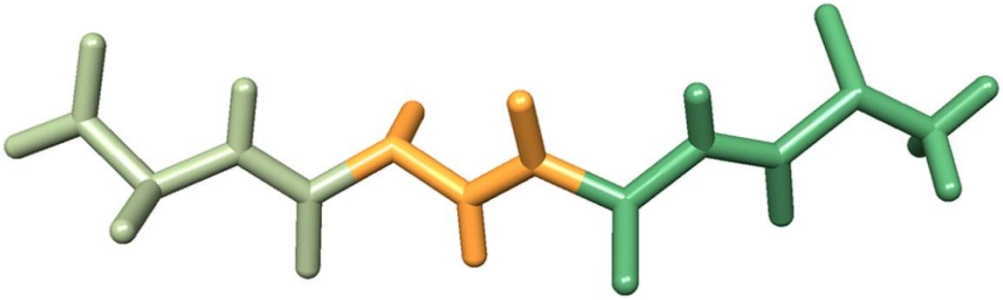
Choisir les bons angles



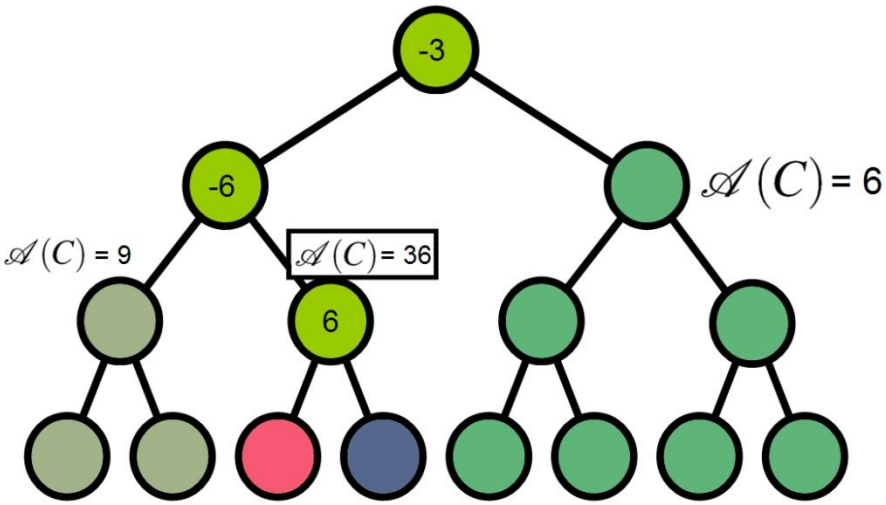


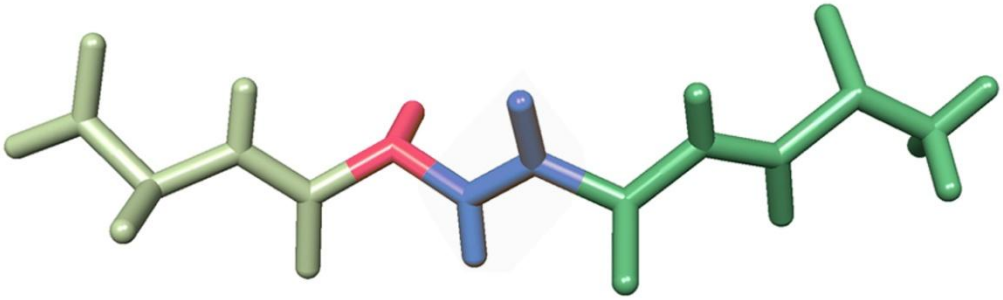
Choisir les bons angles



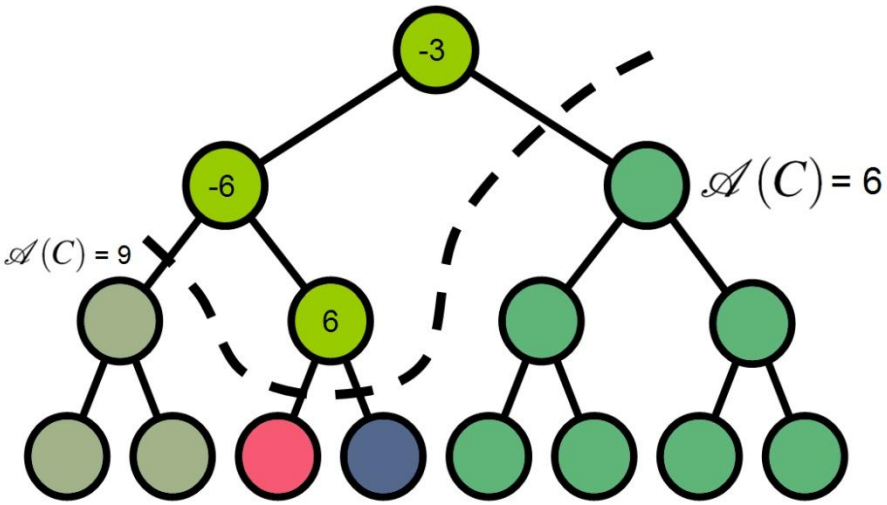


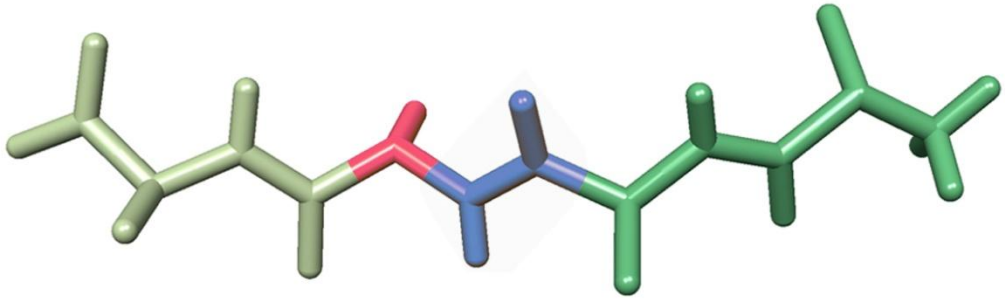
Choisir les bons angles





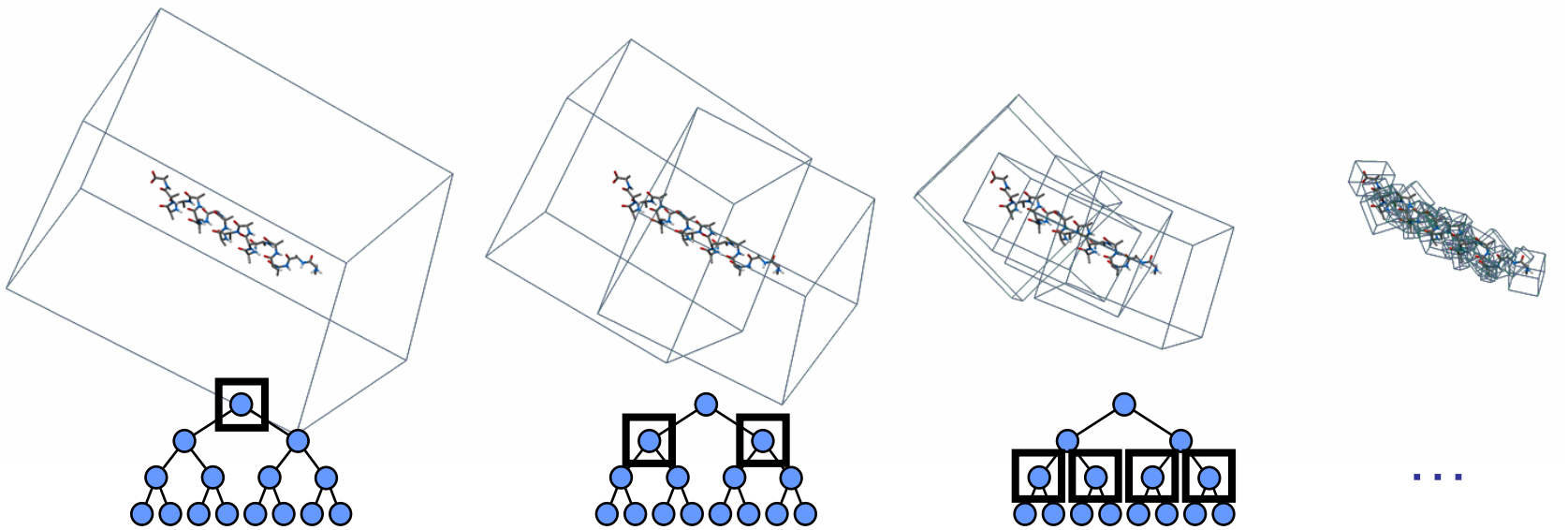
Choisir les bons angles





Et le calcul des forces inter-atomiques?

Détection des paires d'atomes voisins



Démonstration

Démonstration

SAMSON (Collaboration INRIA – CEA)

Système
Adaptatif pour la
Modélisation et la
Simulation d'
Objets
Nanoscopiques

```
    // accessors

    std::string&                    getName() { return name; }
    void                            setName(std::string &n) { name=n; }

    cCHARMMAtomModel*               getModel() { return model; }
    void                            setModel(cCHARMMAtomModel *a) { model=a; }

    double                          getCharge() { return charge; }
    void                            setCharge(double c) { charge=c; }

    unsigned int                    getRigidGroup() { return rigidGroup; }
    void                            setRigidGroup(unsigned int r) { rigidGroup=r; }

private:

    std::string                     name;           // name of the atom
    cCHARMMAtomModel*               model;          // model of the atom
    double                          charge;         // charge of the atom
    unsigned int                    rigidGroup;     // rigid group to which the atom belongs (0 means the atc

};
```

Démonstration

SAMSON (Collaboration INRIA – CEA)

Software for
Adaptive
Modeling and
Simulation
Of
Nanosystems

```
    // accessors

    std::string&                    getName() { return name; }
    void                            setName(std::string &n) { name=n; }

    cCHARMMAtomModel*               getModel() { return model; }
    void                            setModel(cCHARMMAtomModel *a) { model=a; }

    double                          getCharge() { return charge; }
    void                            setCharge(double c) { charge=c; }

    unsigned int                    getRigidGroup() { return rigidGroup; }
    void                            setRigidGroup(unsigned int r) { rigidGroup=r; }

private:

    std::string                     name;           // name of the atom
    cCHARMMAtomModel*               model;          // model of the atom
    double                          charge;         // charge of the atom
    unsigned int                    rigidGroup;     // rigid group to which the atom belongs (0 means the atc

};
```

Démonstration

SAMSON (Collaboration INRIA – CEA)

Videos disponibles **ici**

(http://nano-d.inrialpes.fr/?page_id=59)

Et maintenant?

Le prototypage virtuel de nanosystèmes

Le prototypage virtuel de nanosystèmes

Modélisation physique
(Mise en équations, simplification des équations fondamentales…)

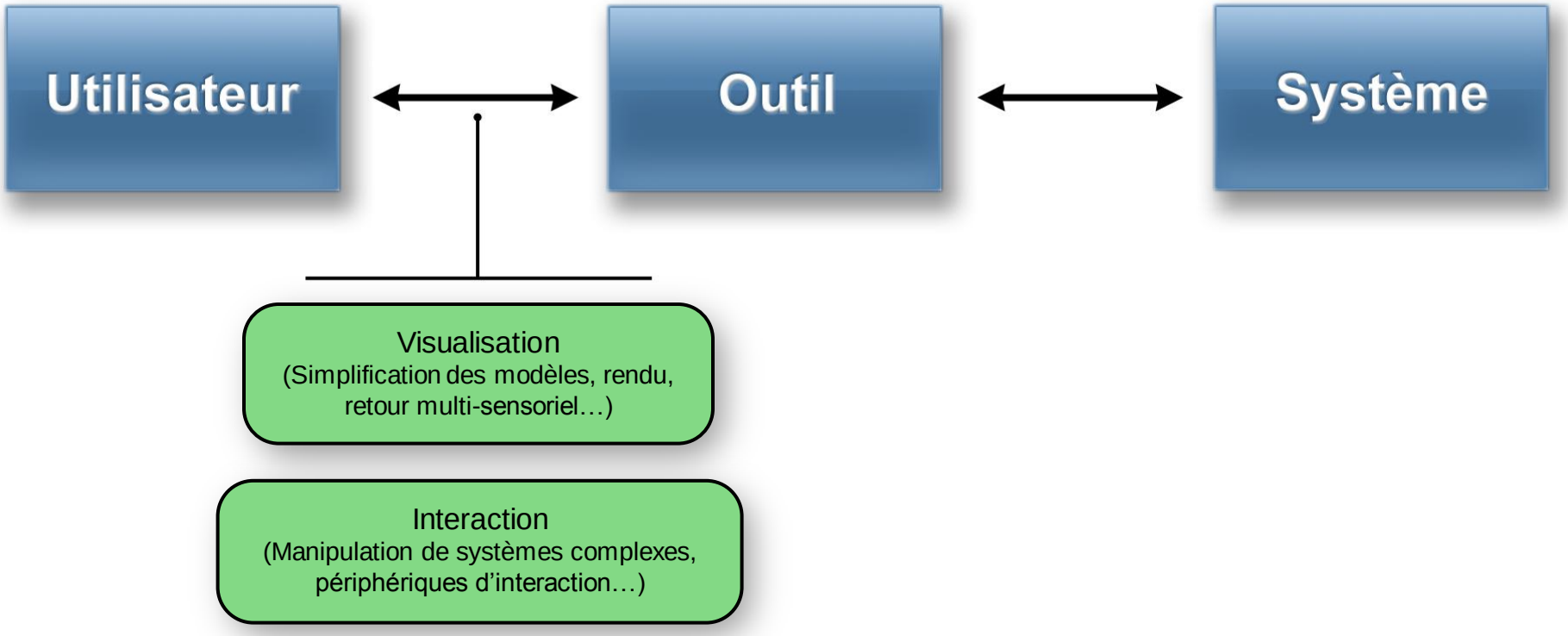
Modélisation mathématique
(Conditions d'existence et d'unicité, analyse des systèmes dynamiques, symplecticité…)

Statistique
(Thermodynamique, minimisation d'énergie, calcul d'énergie libre, Monte-Carlo…)

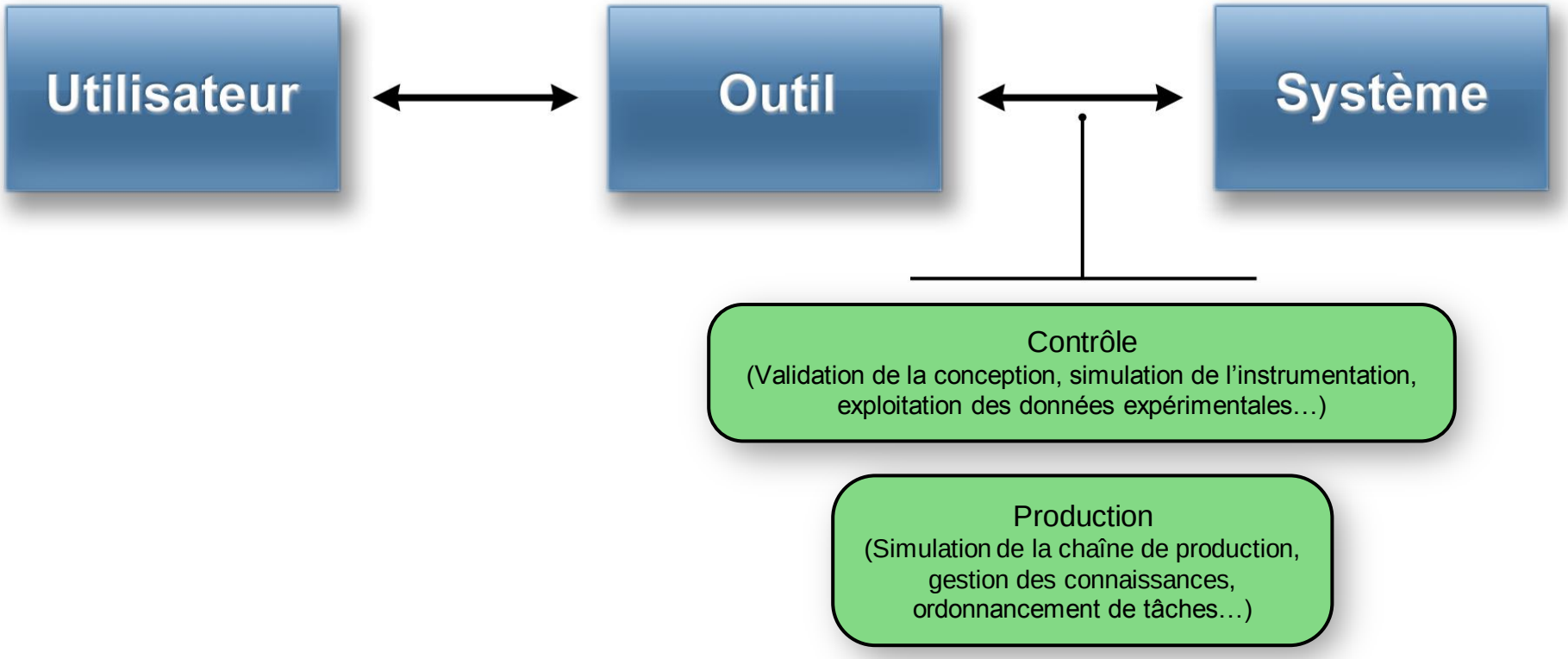
Algorithmique
(Schémas d'intégration, dynamique adaptative Newtonienne et quantique, calcul multi-cœurs, calcul sur cartes graphiques…)

Utilisateur ⟷ **Outil** ⟷ **Système**

Le prototypage virtuel de nanosystèmes



Le prototypage virtuel de nanosystèmes



Merci pour votre attention !

Pour plus de renseignements

Mon adresse : stephane.redon@inria.fr

L'équipe NANO-D : http://nano-d.inrialpes.fr