Designing Materials with modeFRONTIER

An application of modeFRONTIER to the optimization of physical and chemical properties of polymers

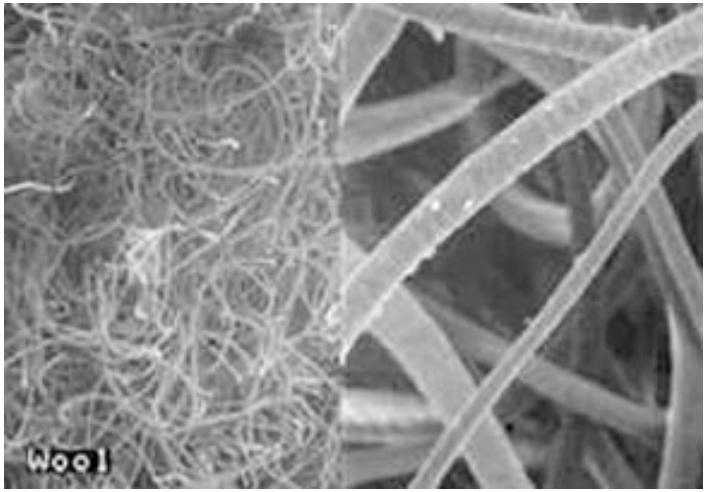
Danilo Di Stefano
danilo.distefano@esteco.com

What Polymers are

- Polymers are macro-molecules composed by hundreds or possibly thousands subunits called monomers. The polymer presents a regular repetition of its monomer in such a way to build regular structures, especially long chains organized in sheets, elices,…
- There are two very general and broad classes of polymers: biopolymers (e.g. proteins) and synthetic industrial polymers (e.g. plastics, resins,…)
- They have very different chemical composition and physical-chemical properties

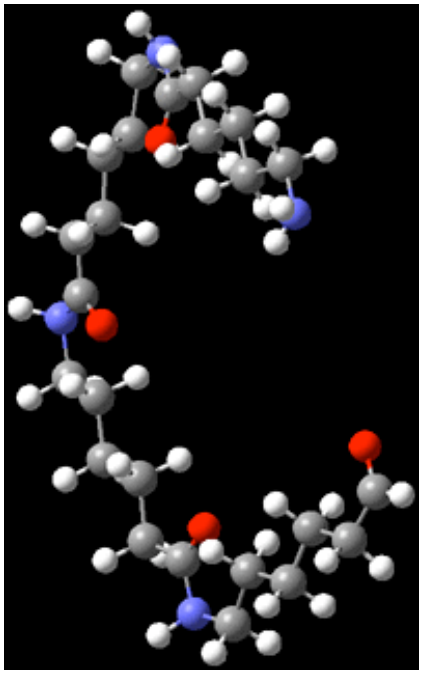
How Polymers look

Polyethylene fibers by Optical Microscopy

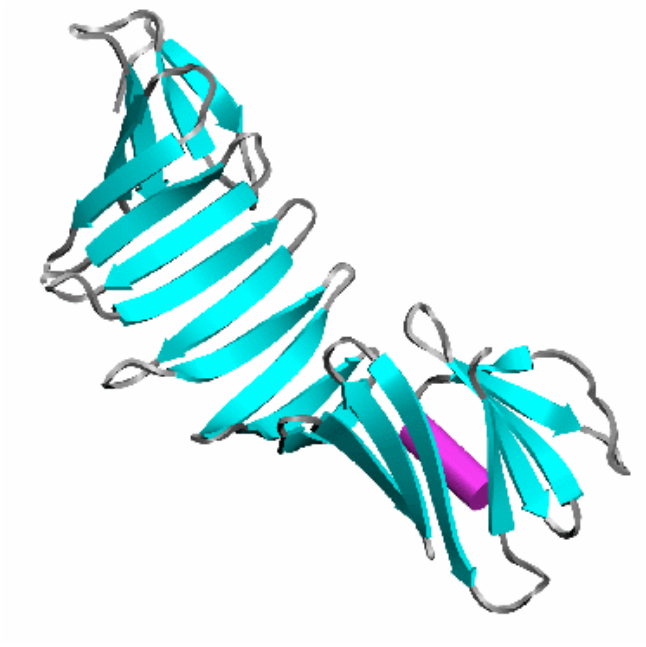


Wool fibers by Scanning Electron Microscopy

Structural Models for Polymers



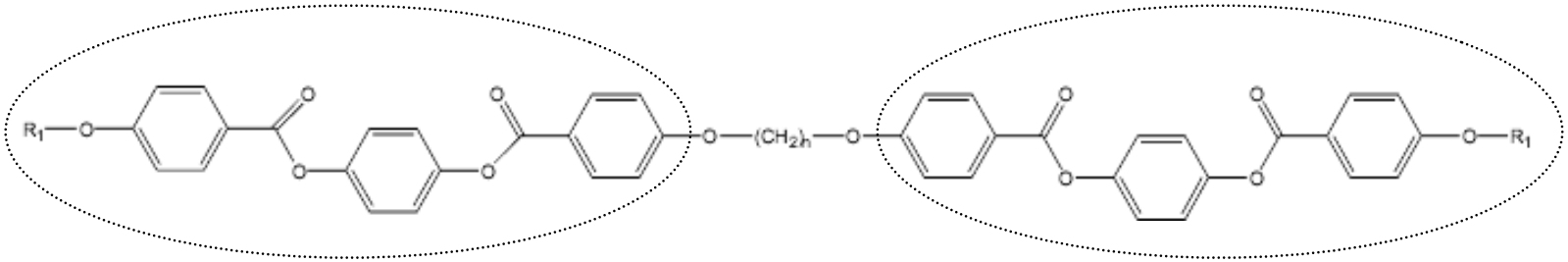
Ball and Stick Model



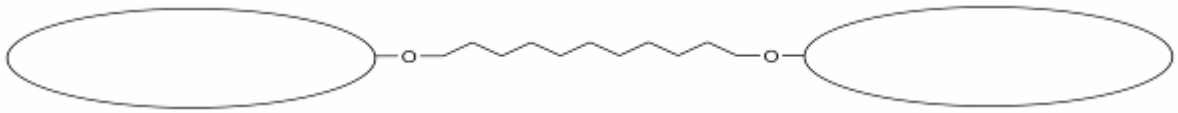
Ribbons Model

Models can be built at different resolutions so capturing several aspects of structural properties

An example: a Liquid Crystal



Rotations around C-C bonds are the main kind of internal motion for this molecule



Terminal groups are conformationally rigid: an ellipsoidal rigid rotor can model it

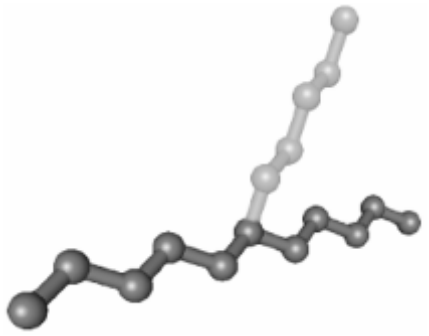
The Dynamic Picture

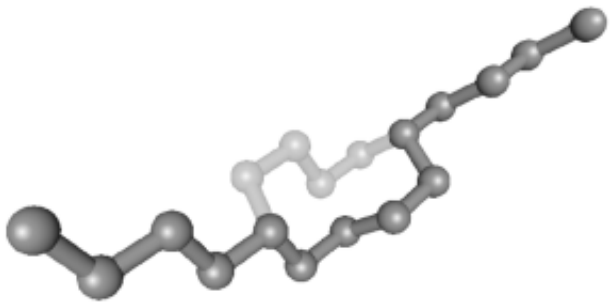
A stochastic model based on Langevin equation permits the calculation of kinetic constants for conformational transitions and the relative displacement of single particles

Cranklike conformational transitions in polyethylene, G.J Moro, B. Nigro, D. Di Stefano, A. Rassu
Journal of Chemical Physics, 2004 Sep 1;121(9):4364-76

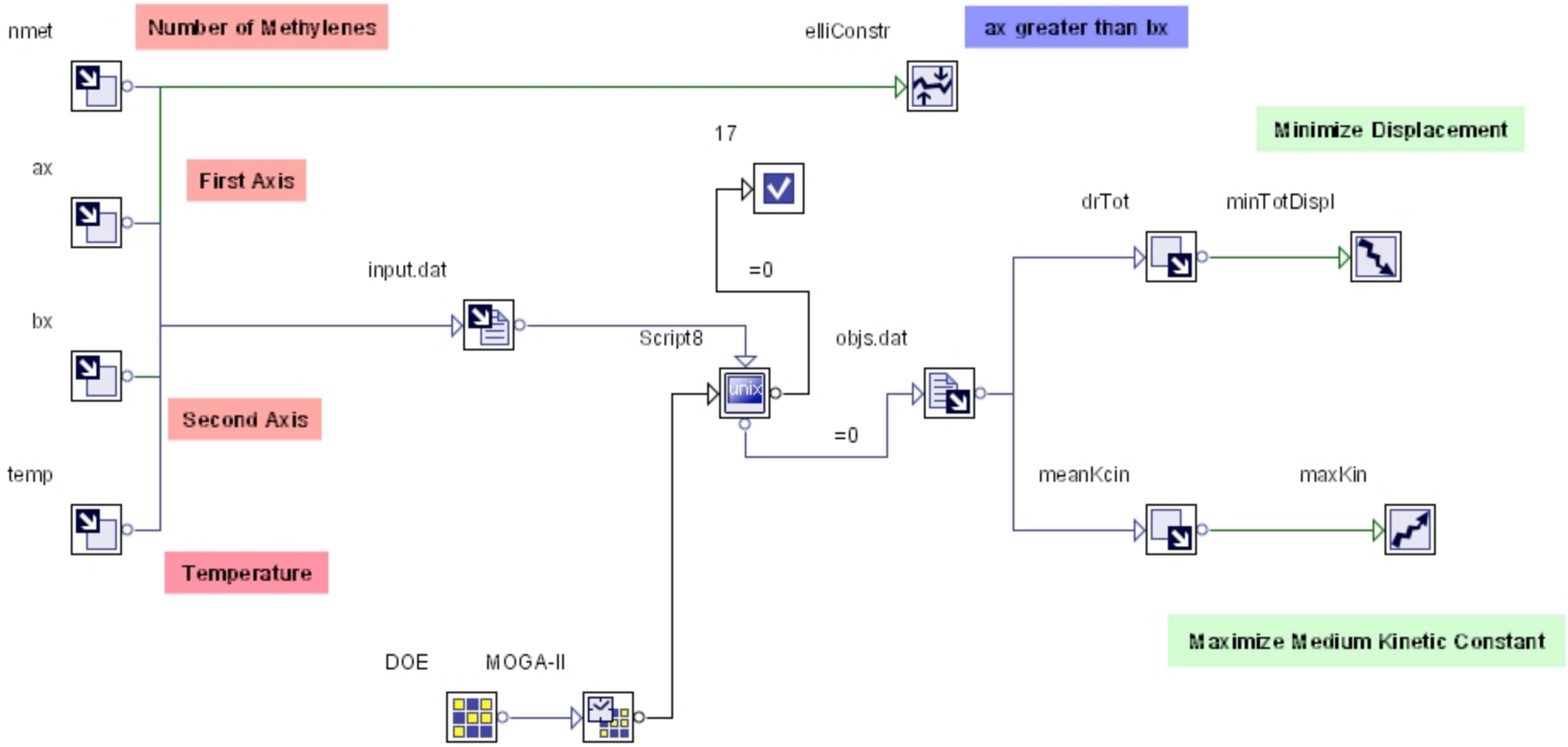
Optimization of Dynamic Properties

- An interesting property of this kind of molecules is their ability to regularly orient themselves with respect to an electrical field and to preserve this orientation into a somewhat large temperature interval
- Optimizing such a property, from a point of view of the stochastic model, implies to minimize the total displacement of the molecule and to maximize the mean value of the kinetic constants, so preserving the possibility to equilibrate with the environment



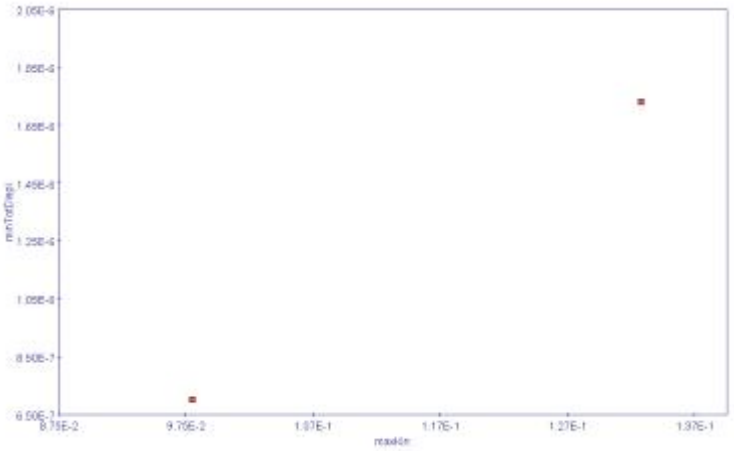


modeFRONTIER WorkFlow



Sobol DOE with 10 designs. MOGA-II with 150 generations.

Best Solutions

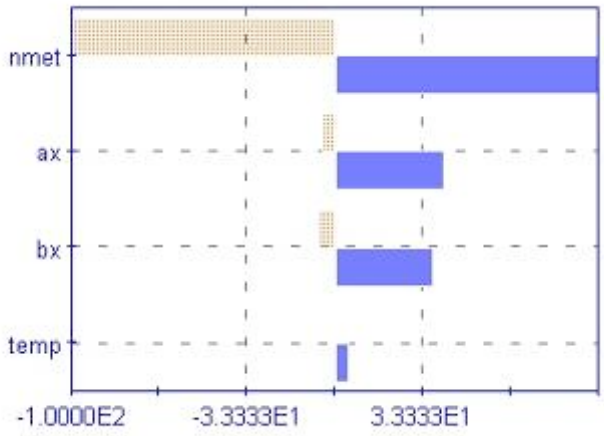


The best solutions tend to push the temperature on its upper limit and the ellissoid on its minimum dimensions. The length of the spacer can be 14 or 22 methylene groups.

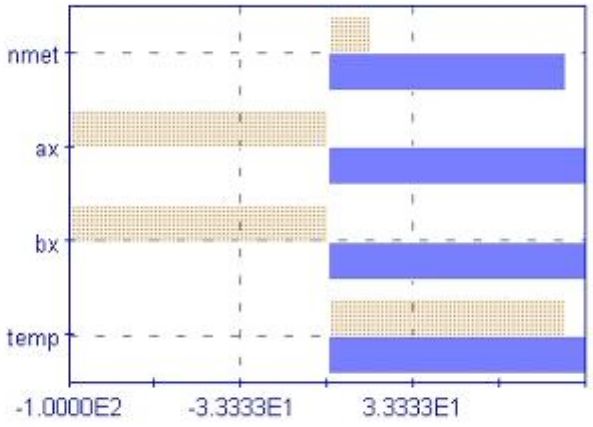
Best Designs

ID	M	C	nmet	ax	bx	temp	drTot	meanKcin	minTotDispl	maxKin	elliConstr
161	☐		14	1.0000E1	1.5290E0	3.1000E2	1.7310E-6	1.3318E-1	1.7310E-6	1.3318E-1	8.4710E0
382	☐		22	1.0000E1	1.5290E0	3.1000E2	7.0464E-7	9.7920E-2	7.0464E-7	9.7920E-2	8.4710E0

Considerations on the Results



t-student on mean displacement



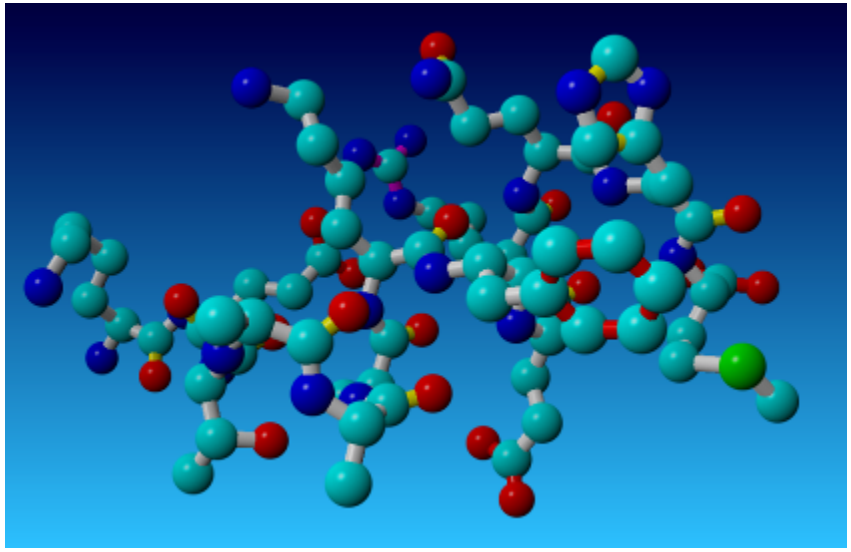
t-student on mean kinetic constant

The number of methylene groups has an inverse strong correlation with the mean displacement. Temperature is strongly correlated with the mean kinetic constant, while ellissoid dimensions have an inverse strong correlation with it.

Conclusions and Future Developments

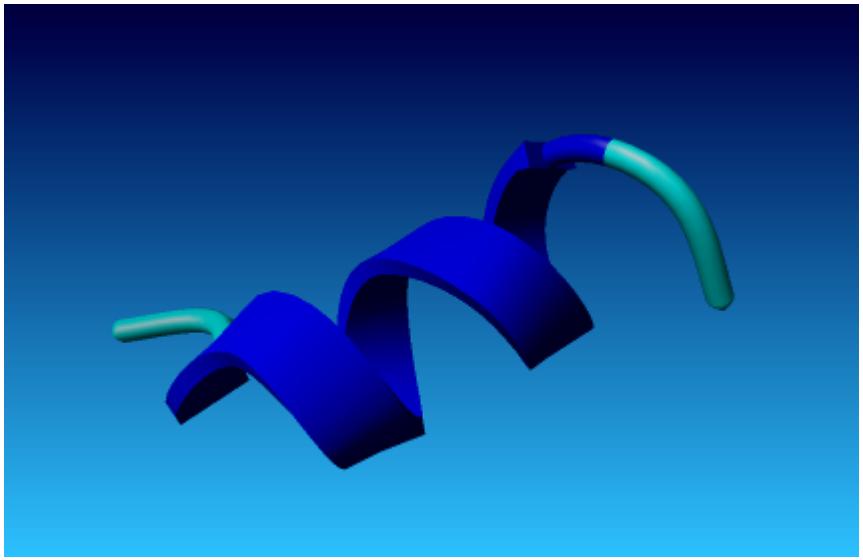
- If the results for the influence of temperature and ellisoid dimensions on design objectives could be expected based on Boltzman kinetic theory, a precise indication for the length of the spacer is of great importance
- Future devolpments will involve the application of the model to the problem of protein – ligand docking, where modeFRONTIER performs a search for the favourable conformations. The so far presented stochastic algorithm will furnish a scoring methodology for the different candidate solutions

Work in Progress…

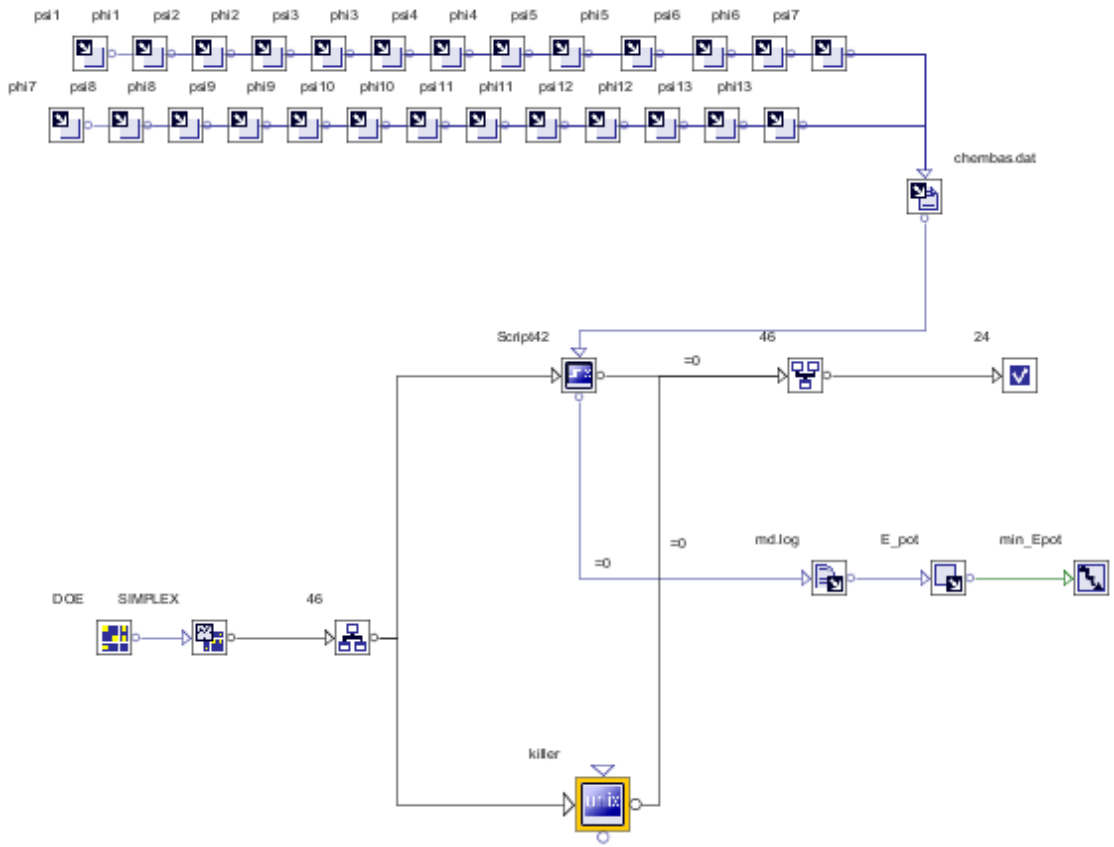


Interfacing **modeFRONTIER** with **Gromacs** molecular dynamics package for the analysis of biological interesting molecules

The aim of the optimization is the minimization of the potential energy of the system formed by a small peptide in water. The design variables are the φ,ψ angles of the peptide.



modeFRONTIER – Gromacs Interface



Treating molecules of biological interest requires a careful choice for the design variables, so avoiding an uncontrolled increase of problem complexity