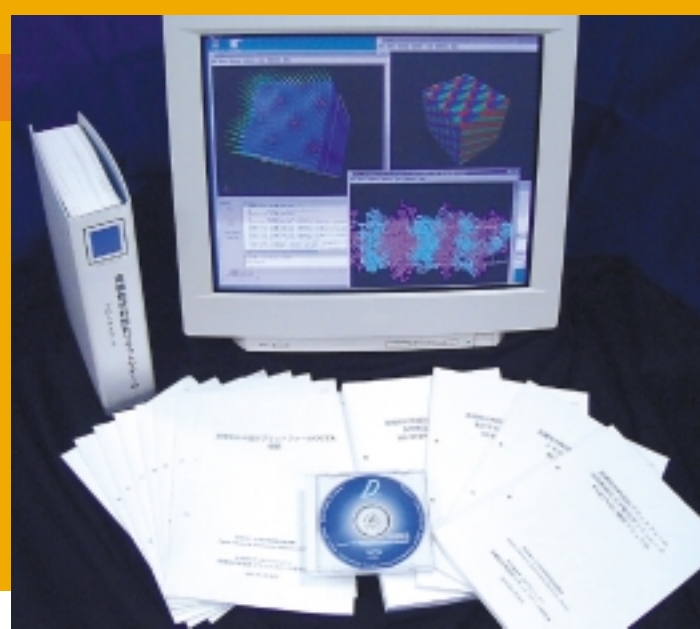


# APPLICATIONS

- Stiffness of polymeric materials
- Spin coating
- Soft actuators
- Micro-reactor chips
- Morphology of tapered polymers
- Morphology of 3-component systems
- Reaction-induced phase separation
- Deformation of crystalline lamellae
- Morphology near a surface
- Morphology of tri-block copolymers
- Rheology of linear and star polymers
- Cross linked polymers
- Confined systems
- Topological gels
- Clay-polymer composites
- Liquid crystals
- .... etc.



# What is OCTA?

OCTA is an integrated simulation system for soft materials developed by the joint project of industry and academia funded by Ministry of Economy, Trade and Industry (METI), Japan. The objective of the project is to bridge microstructural (or molecular) characteristics of soft materials with their material characteristics by simulation and modeling. This objective was quite challenging.

Soft materials are made of complex molecules consisting of millions of atoms, having internal structures at many levels, and exhibiting complex responses over time scales ranging from nano-seconds to years. Theoretical models for soft materials are quite diverse: atomistic models, coarse-grained models, continuum models, and other hybrid models have been proposed to deal with mesoscopic phenomena of soft materials. They are based on different physical concepts and have disparate data structures. Our task was to construct a simulation system by integrating such diverse models. This is the so called multi-scale, multi-physics problem in computational science and engineering.

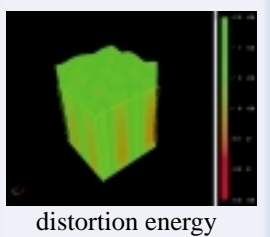
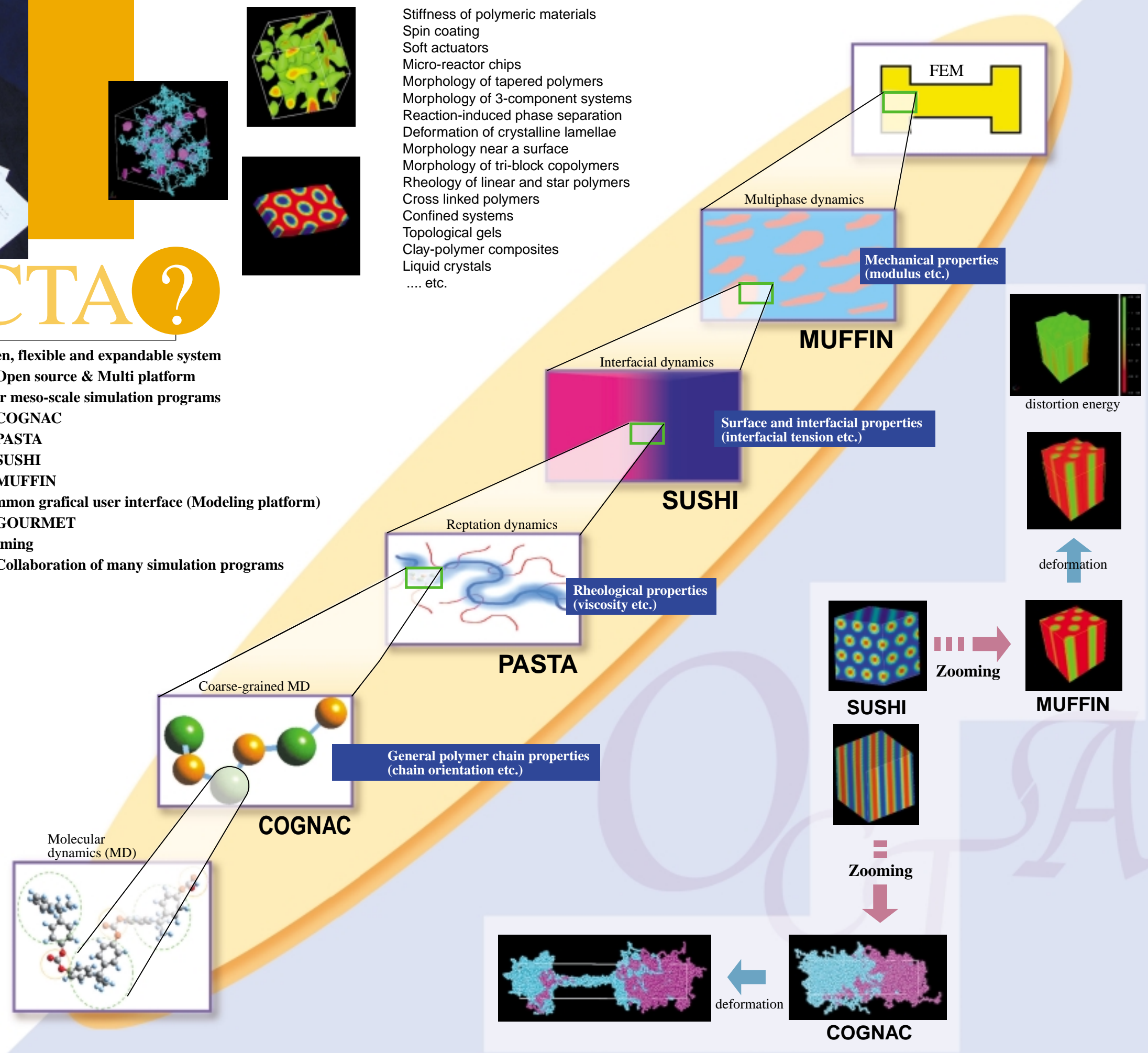
In this project, we tried to solve this problem by relying on the power brought by the collaboration of human beings. Rather than producing a software package dedicated to do a limited number of physical problems, we focused our attention on constructing a system which can grow in the future.

OCTA consists of four simulation engines (COGNAC, PASTA, SUSHI, MUFFIN) and a simulation platform (GOURMET). The simulation engines can carry out the simulations of molecular dynamics, reptation dynamics, interfacial dynamics, gel dynamics, two-fluid dynamics etc, and the simulation platform gives a common graphical user interface to all engines, providing an environment for various engines to work together.

In Japanese, the word "OCTA" means growth for future. OCTA is by no means complete: to cover the whole area in soft materials, engines need to be enhanced and the platform needs to be brushed up. We paid special attention to make the system customizable and expandable, so that the system can grow on its own. We very much hope that the system is useful for your research, and welcome any comments you have regarding the system.

**Masao Doi**  
Project Leader, Nagoya University

- Open, flexible and expandable system**
- Open source & Multi platform
- Four meso-scale simulation programs**
- COGNAC
- PASTA
- SUSHI
- MUFFIN
- Common graphical user interface (Modeling platform)**
- GOURMET
- Zooming**
- Collaboration of many simulation programs



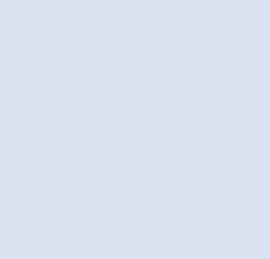
↑ deformation



Zooming



Zooming



← deformation