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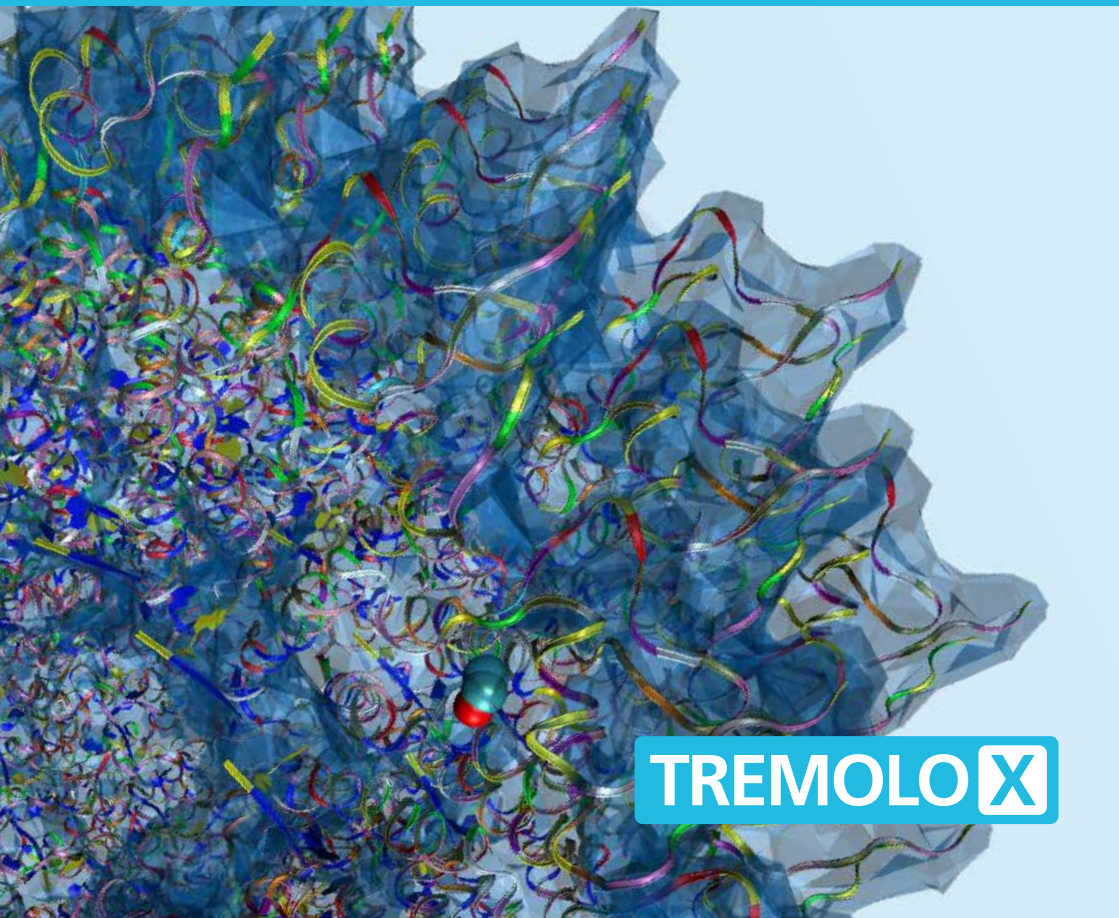
FRAUNHOFER INSTITUTE FOR ALGORITHMS AND
SCIENTIFIC COMPUTING SCAI

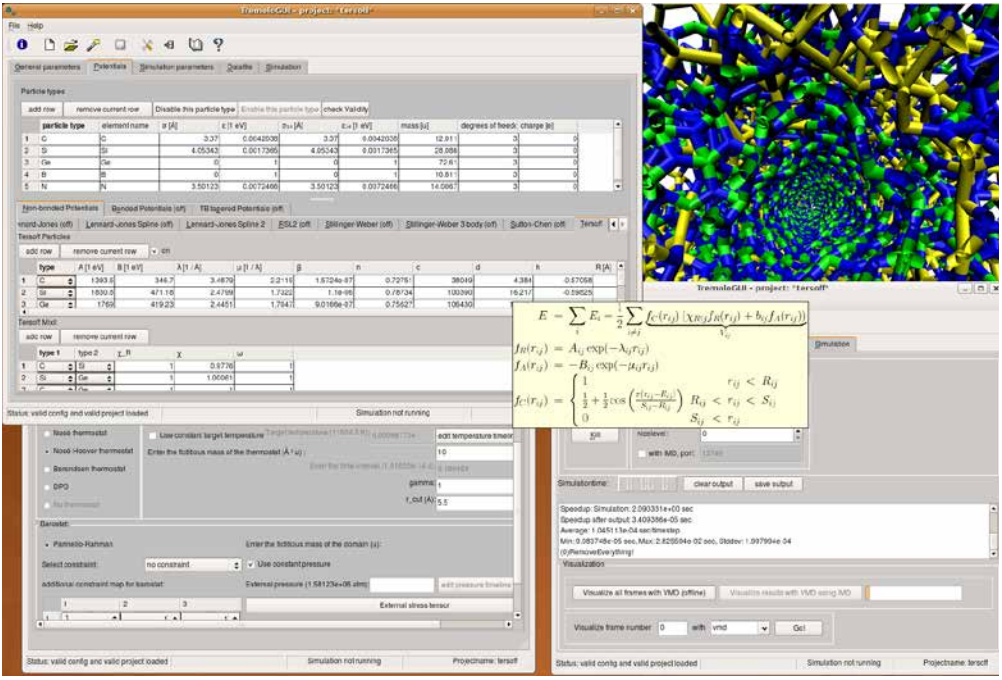
TREMOLO-X:
MOLECULAR DYNAMICS SIMULATION



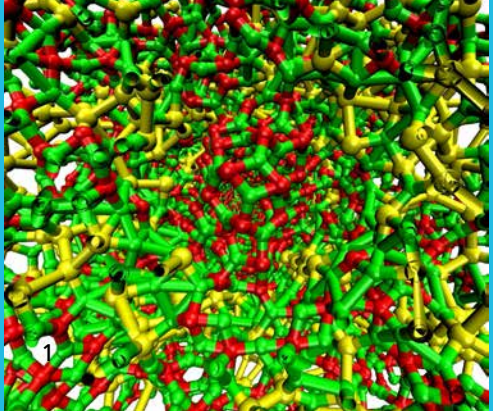
TREMOLO-X
NUMERICAL SIMULATION
OF MOLECULAR DYNAMICS

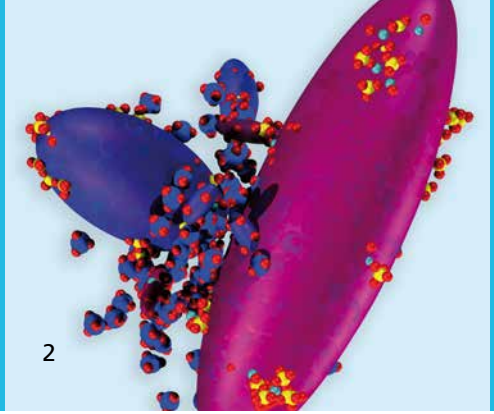
MOLECULAR DYNAMICS SIMULATION

Tremolo-X is a powerful software package used for the numerical simulation of interactions between atoms and molecules, the molecular dynamics. Tremolo-X provides the environment to design new innovative materials.



Screenshot of the Tremolo-X software





1 BN-nanotube reinforced Si-B-N ceramic
2 Building block in cementitious C-S-H-gel

PARALLEL EFFICIENCY

Tremolo-X is particularly optimized for parallel application. It uses tree algorithms for long-range potentials as well as grid algorithms for short- and long-range potentials.

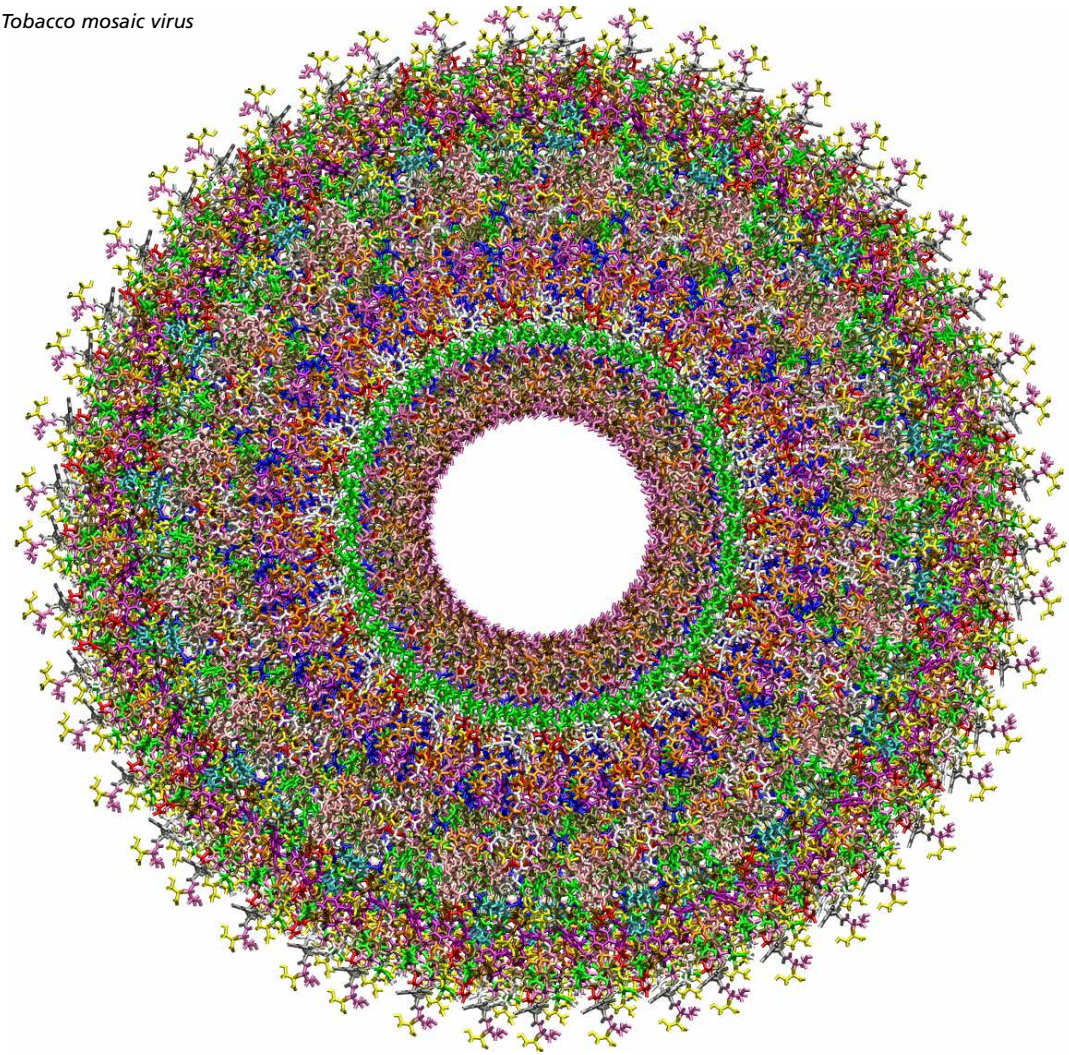
GRAPHICAL USER INTERFACE

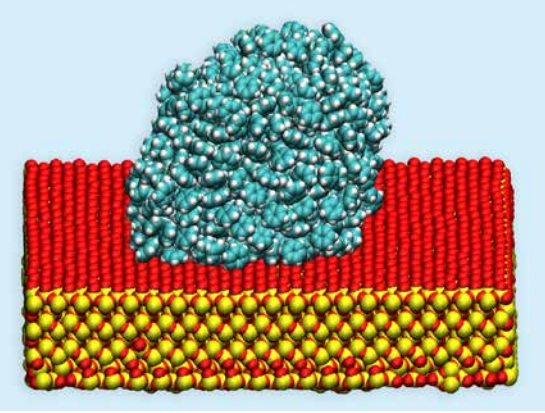
Tremolo-X includes a user-friendly GUI frontend. This provides an easy set-up and analysis of numerical experiments.

MODELING

Tremolo-X includes an efficient implementation of all potential types commonly used for modeling of systems in the areas material science, nanotechnology and biophysics.

Tobacco mosaic virus





Benzene on silica

FEATURES

- User-friendly GUI frontend
- Parallel version for distributed memory computers (MIMD) with the message-passing interface (MPI)
- Parallel implementation of reactive many body potentials of Brenner, Marian, Tersoff, Feuston-Garofalini, Stillinger-Weber and Sutton-Chen
- Parallel implementation of fixed bond, angle, torsion (dihedral) and inversion potentials
- NVE, NVT and NPT ensemble, structural optimization and dissipative particle dynamics (DPD)
- Several time integrators and local optimizers: Verlet, multistep like Beeman-Verlet as well as Fletcher-Reeves and Polak-Ribière
- Computation of many measuring quantities, e.g. diffusion coefficients, stress-strain diagrams, elastic constants, distribution functions, correlation functions and shortest-path-ring statistics
- Fast implementation of short-range potentials via linked-cell method and parallelization by dynamic load-balanced domain decomposition
- Fast algorithms for long-range potentials: Particle-Mesh-Ewald with domain decomposition and parallel 3D-FFT and parallel multigrid. Also Barnes-Hut/fast multiple methods and parallelisation by space-filling curves
- Simply extendible to new potential types by modularity

REFERENCES

PROJECTS AND COLLABORATIONS

Tremolo-X is already successfully applied in many different practical projects in different application areas. Here, the focus is on computations in nanotechnology, material science, biochemistry and biophysics.

A selection of projects and cooperations, which use Tremolo-X for molecular dynamics simulations, is given in the following:

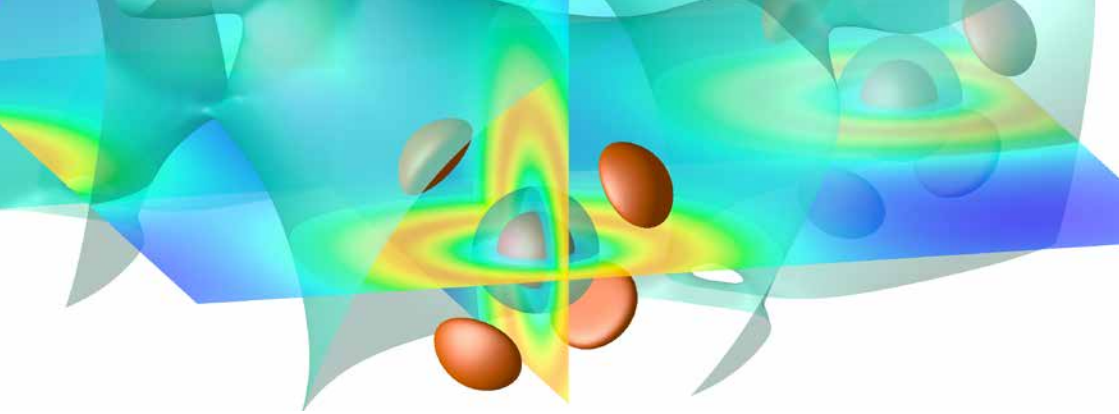
- **ScaFaCoS – Scalable Fast Coulomb Solver**
  This is a network project of German research groups and industrial partners (e.g. IBM and BASF). It is financed by the German Ministery of Education and Science (BMBF).

- **CODICE – Computationally driven design of innovative cement-based materials**
  Research project of international research groups and industrial partners (e.g. BASF and CTG). It is financed by the Seventh Framework Programme (FP7) of the EU.

- **Nanowires and Nanotubes: From Controlled Synthesis to Function**
  Priority Programme 1165 of the German Research Foundation (DFG)

- **Numeric Methods for Multiscale Models and Singular Phenomena**
  Collaborative Research Center 611 of the German Research Foundation (DFG)

- **Inorganic Solids without Translational Symmetry – Synthesis, Structure and Modelling**
  Collaborative Research Center 408 of the German Research Foundation (DFG)



BUSINESS AREA VIRTUAL MATERIAL DESIGN

Applied research and development at the department »Virtual Material Design« is focused on multiscale modelling and numerical simulation in material science and nanotechnology. Massively parallel computers are used to simulate new materials on the nano-, micro- and macroscale by modern multiscale methods in quantum mechanics, molecular dynamics and continuum mechanics. The aim is to create and to study new innovative materials with effective properties in the virtual computer lab in order to propose their structure and design before their synthesis in reality. This approach to material design promises to avoid many expensive prototypes and experiments (in the real lab).

Hence, the costs of development can be substantially reduced with the help of numerical simulation. In addition, completely novel materials can be found.

Offers

Fraunhofer SCAI offers individual solutions to our partners and customers in the following areas:

- Multiscale modeling and numerical simulation for material science and nanotechnology.
- High performance computing in quantum mechanics, molecular dynamics and continuum mechanics.

In particular this includes mathematical modeling and development of algorithms as well as customized software and numerical simulation.

CONTACT

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