



**Integrated simulation system
for soft materials**

J-OCTA

August 15, 2019

JSOL Corporation

Engineering Technology Division

<http://www.j-octa.com>

JSOL



- Tokyo, Osaka, Nagoya office in Japan
- System Integration and CAE, Simulation
- 1,300 employees (150 for Simulation field)
- More than 20 CAE, Simulation Software packages

NTT DATA Global IT Innovator
NTT DATA Group

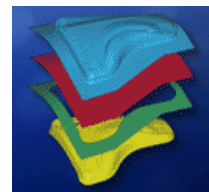


Structure, Production

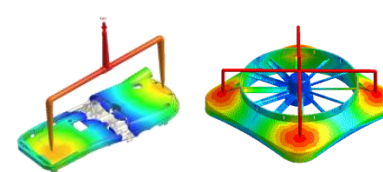
LS-DYNA



JSTAMP

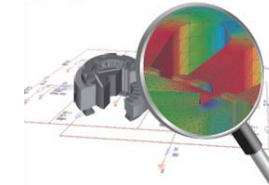


Moldex3D



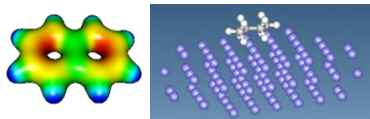
Electro Magnetic

JMAG

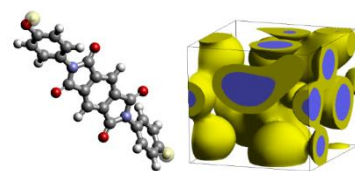


Material Simulation

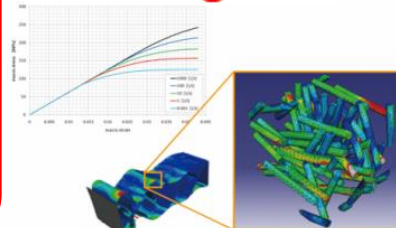
siestaTM



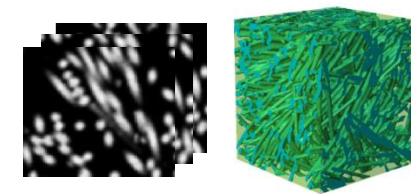
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digimat



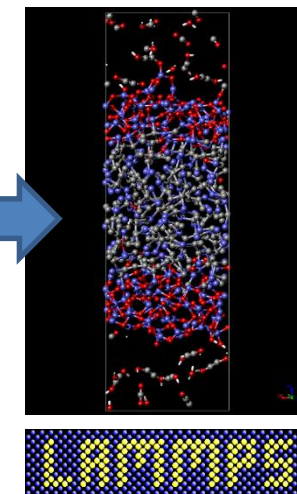
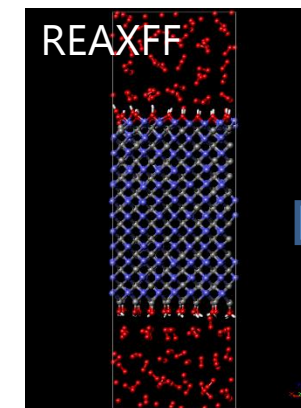
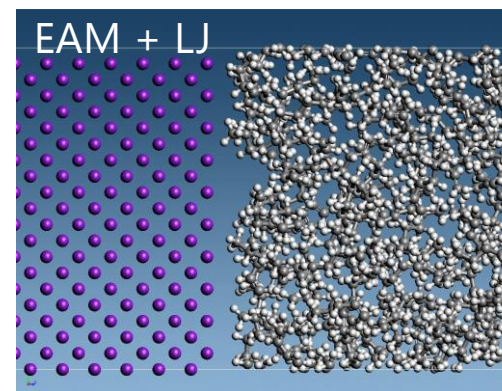
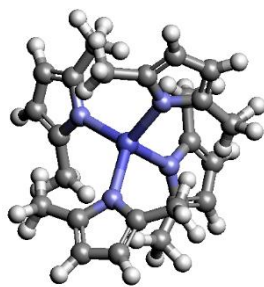
SimplewareTM Software





Force Field DB

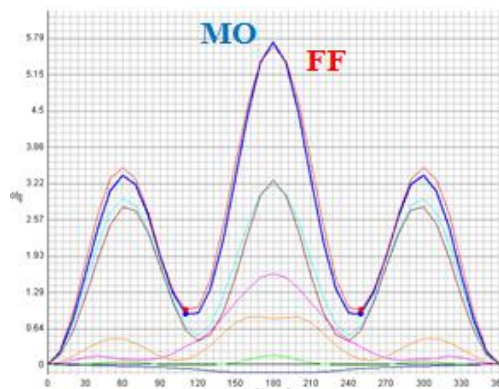
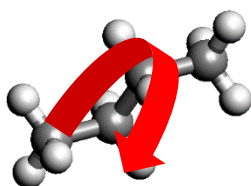
- OPLS (AA,UA), LOPLS
- DREIDING (AA, UA)
- UFF
- AMBER
- GAFF
- CLAYFF
- I/F with Direct Force Field (TEAM-LS&MS)



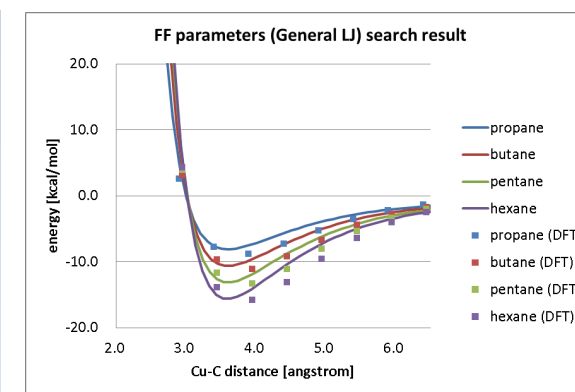
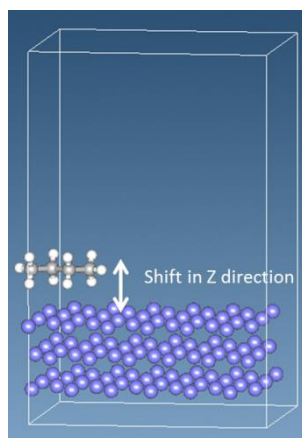
Point charge can be calculated by direct running of ABINIT-MP, Firefly, Gaussian, and MOPAC

Force Field Estimation and Optimization

Optimization of Bond/Angle/Torsion potential
Comparison with QM calculation



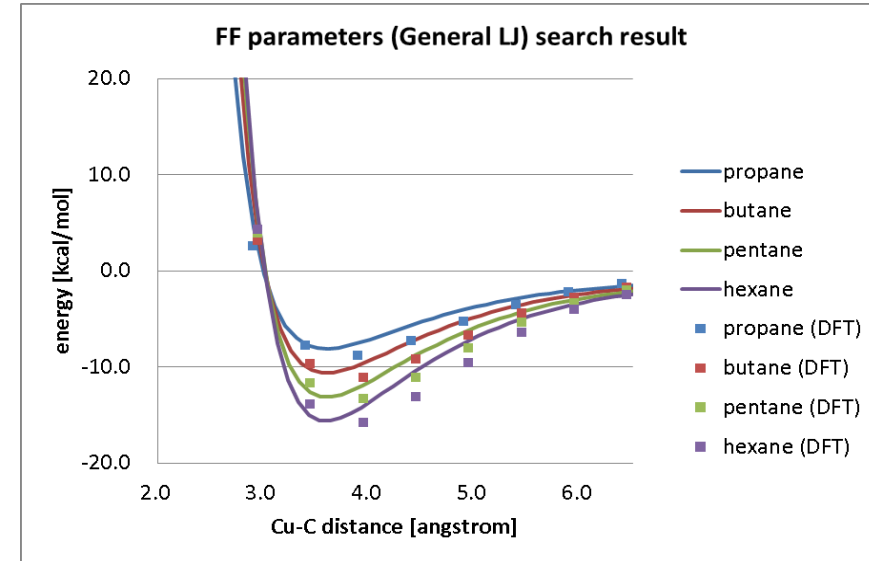
SIESTA Interfacial Energy Tool
LJ Potential for Inorganic/Organic interface



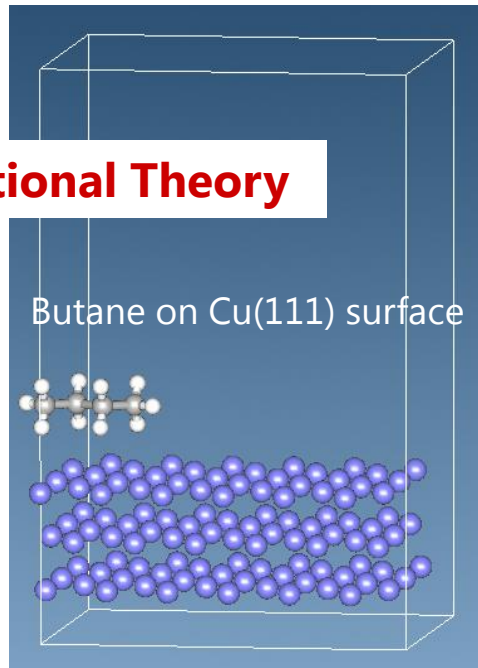
Multi-scale simulation : DFT to Molecular dynamics



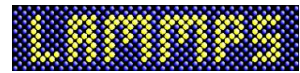
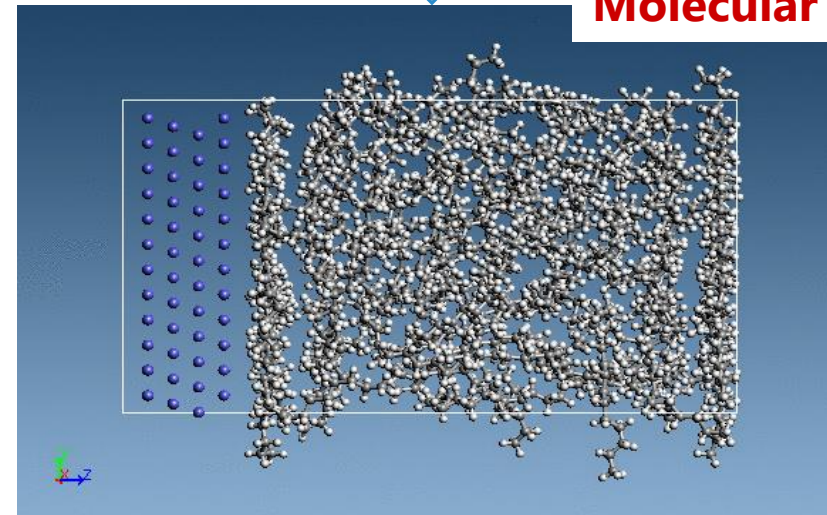
- SIESTA Interfacial Energy Tool
- Adsorption of Butane molecules onto Cu surface
- Results of DFT was fitted with Generalized Lennard Jones inter-atomic potentials
- The obtained LJ potentials were used in the classical MD calculation
- Composite materials, Adhesive, Electrode, etc.



Density Functional Theory



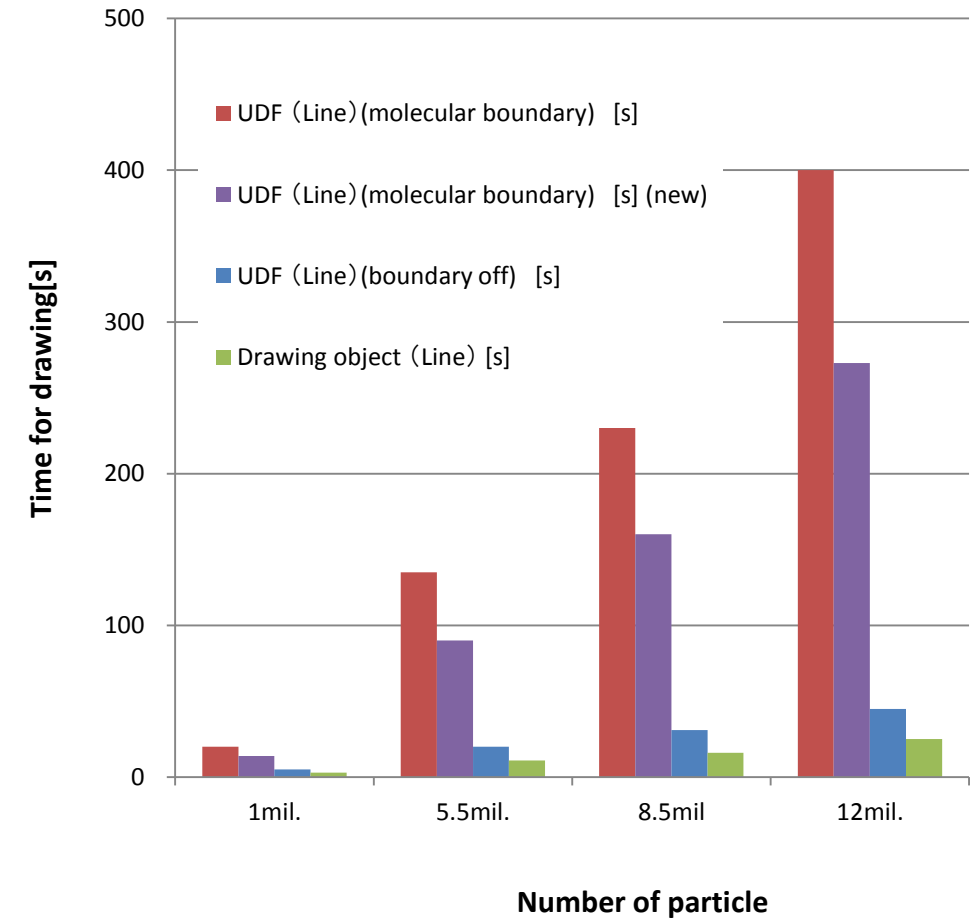
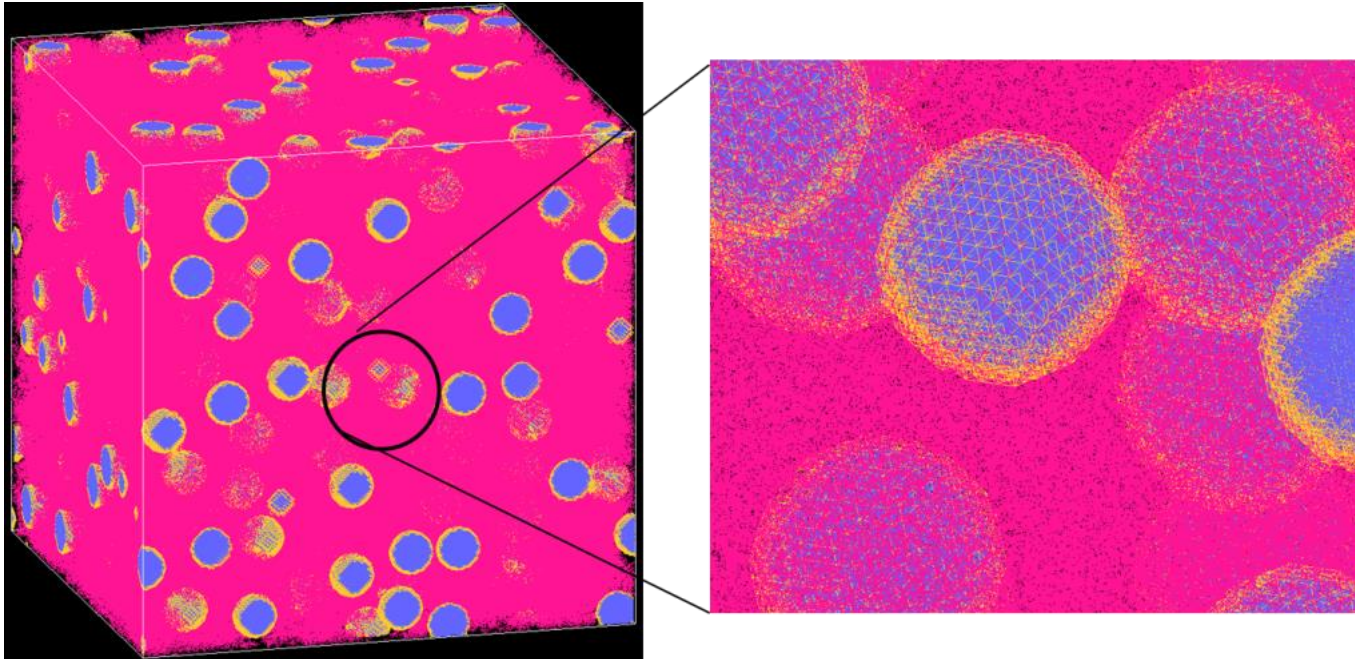
Molecular Dynamics



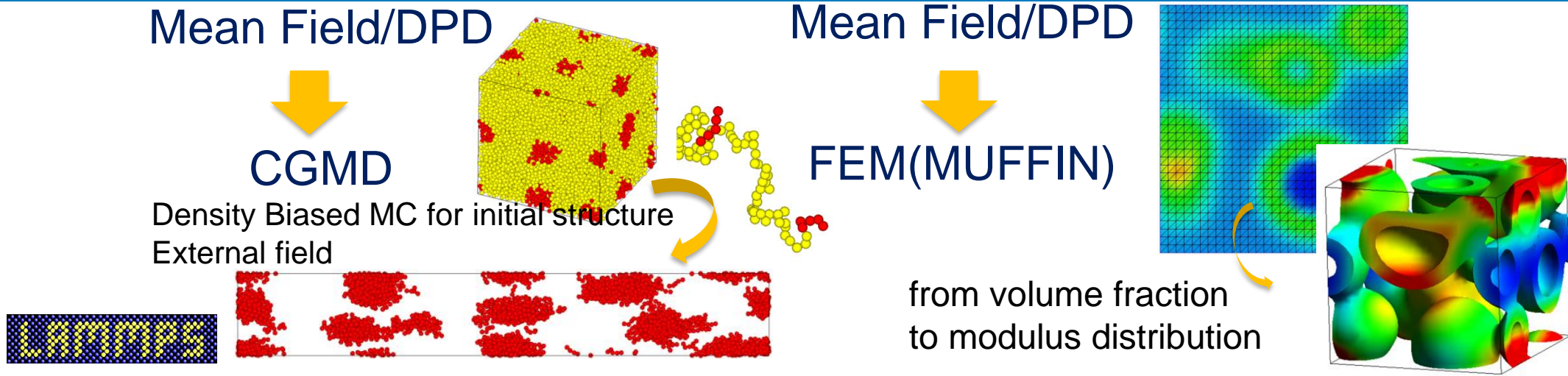
Create large systems and draw those systems



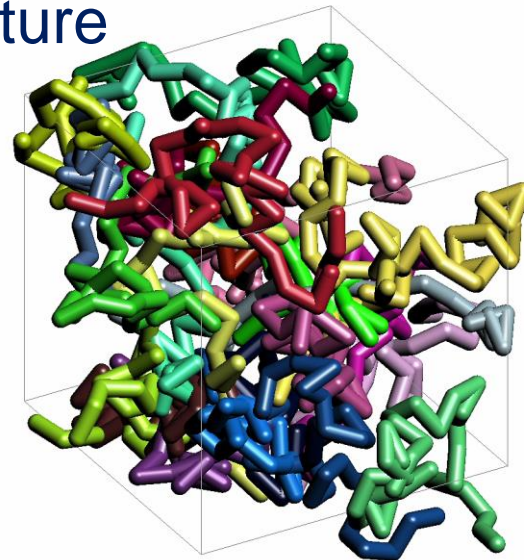
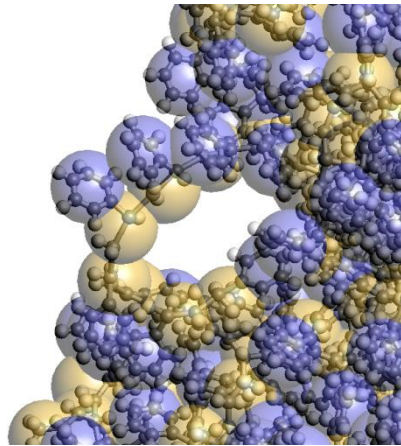
- Create large models
- High-speed drawing



Multi-scale modeling: Zooming



Reverse mapping from Kremer-Grest model and CGMD to FAMD for the relaxed amorphous structure



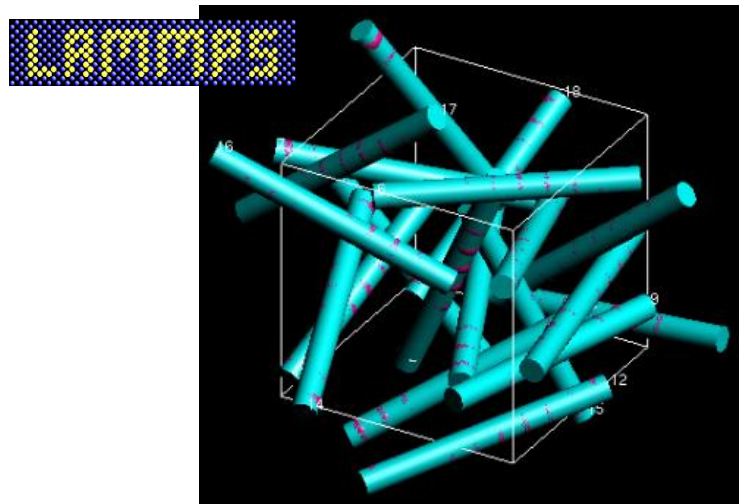
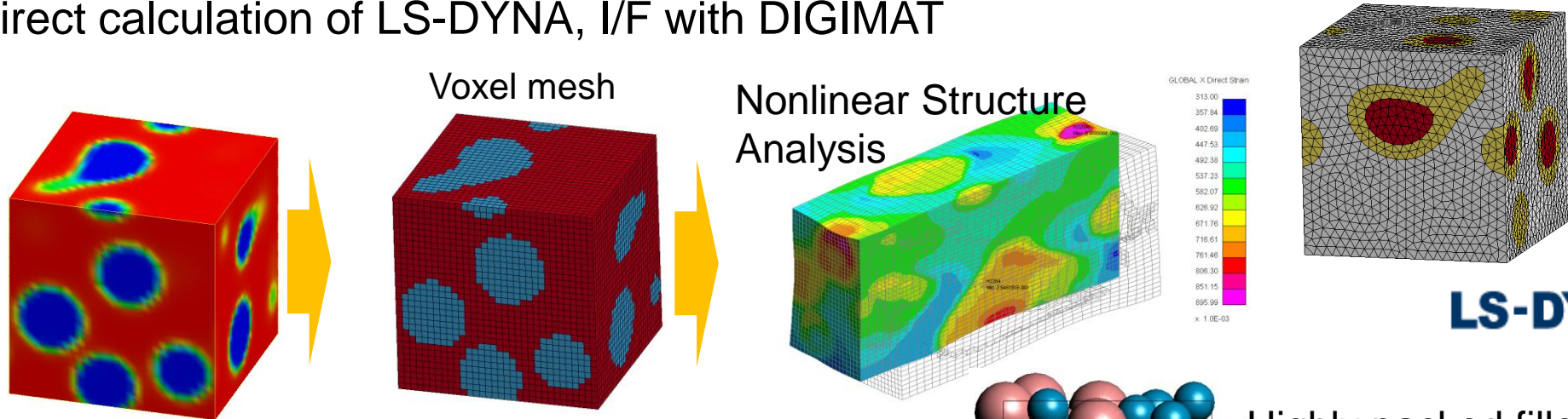
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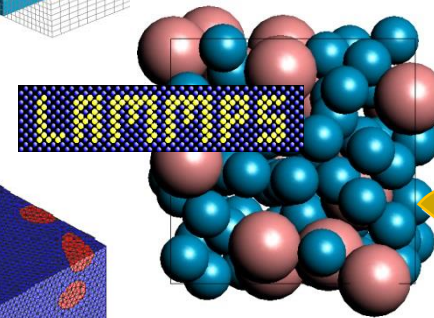
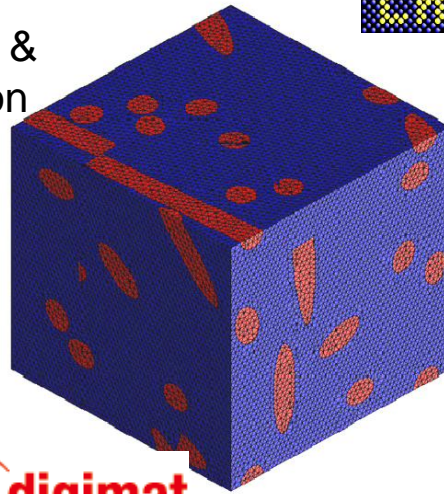
Finite Element Modeling: RVE



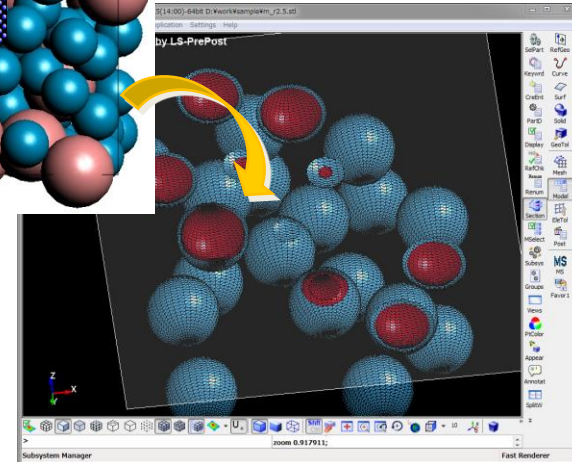
- From phase separation to STL of interface or Voxel mesh.
- Creating filler dispersion (MD or RMC) to STL or position information.
- Direct calculation of LS-DYNA, I/F with DIGIMAT



shape & position



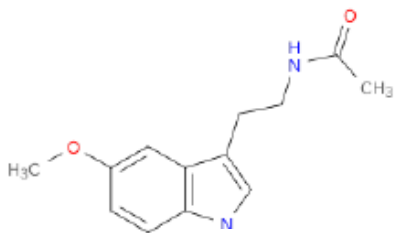
Highly packed fillers





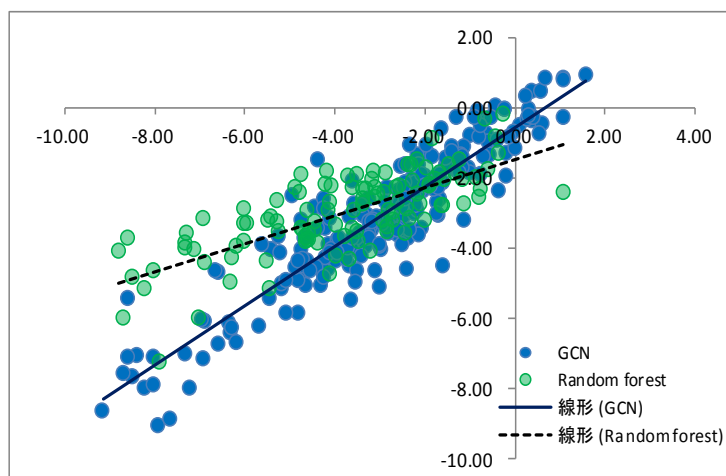
SMILES

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CC(=O)NCCC1=CNc2c1cc(OC)cc2
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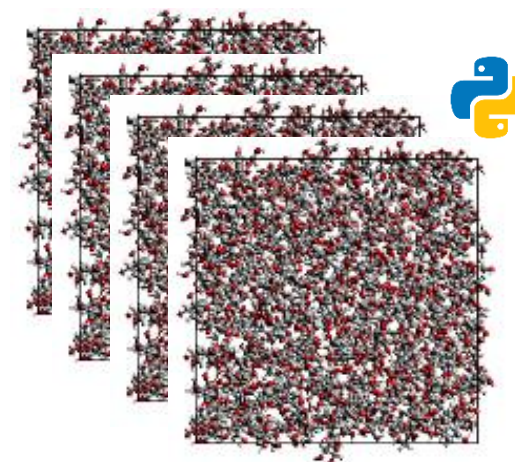
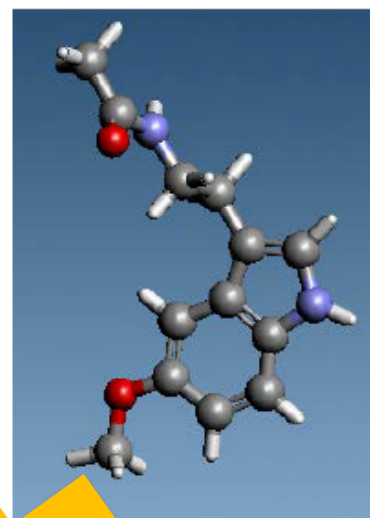


Convert to
3D model

From SMILES to 3D structure
on J-OCTA, automatically



Many MD systems are prepared and
properties (density, modulus, Tg) are
calculated.



High-throughput MD simulation
using python and J-OCTA API

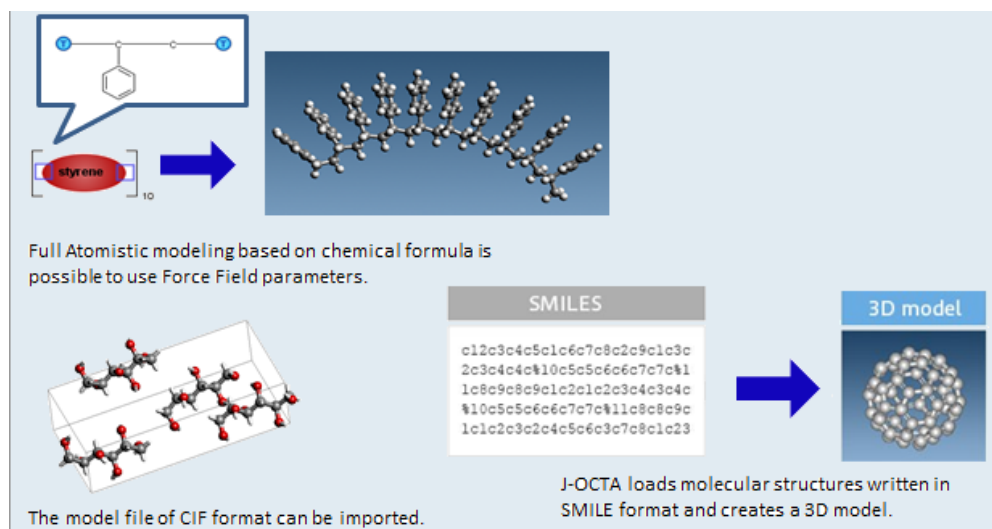
Results are stored in DB.

QSPR (Quantitative Structure Property Relationship)
With Deep Learning (Tensorflow/DeepChem by Google)



- Multi-scale simulations from microscopic to mesoscopic.
- Large systems for modeling and drawing.
- Academic price & student edition

<http://49.212.191.63/phpBB/> (<http://octa.jp/>)





Thank you for your attention.

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