Introduction to

GOURMET

version 3.4.4

Show Window...

Graphical Open User interface_foR
Multi-scale_analysis EnvironmenT

Today's Menu

Appetizer

 ... What is GOURMET?   (powered Pre/Post processor)

Fish

 ... What is your favorite?   desired Pre/Post processor)

Main dish

 ... Recommendation from chef   feature of GOURMET

Dessert

 *... Gourmet Demo with Python & gnuplot flavored*

What is GOURMET?

Pre/Post processor which continues evolving

- *Free to specify the structure of data*
- *Free to change the operation of data*
- *Easy to control the supported engines*
- *Easy editing and drawing of analysis data*
- *Easy to understand other researchers' intention.*
- *The same operations to all engines*

=> *GOURMET*

Graphical Open User Interface foR Multiscale-analysis EnvironmenT
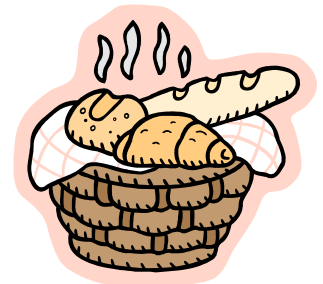
Request from end users

- Existing Pre/Post
  - The interface is made for each engine, and it is difficult(or impossible) to use two or more engines collaboratively.
  - The interface is a fixed program, and it is difficult (or impossible) to customize it.
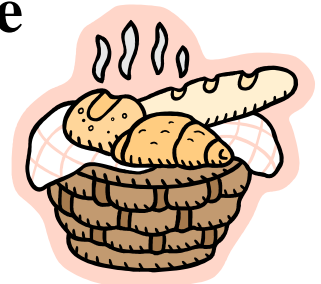
- GOURMET
  - GOURMET is a common interface for all engines, and offers a tool to let two or more engines work together.
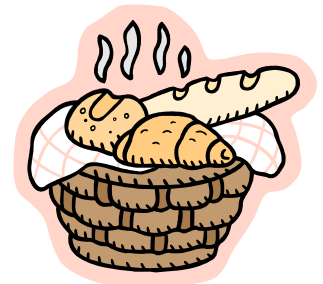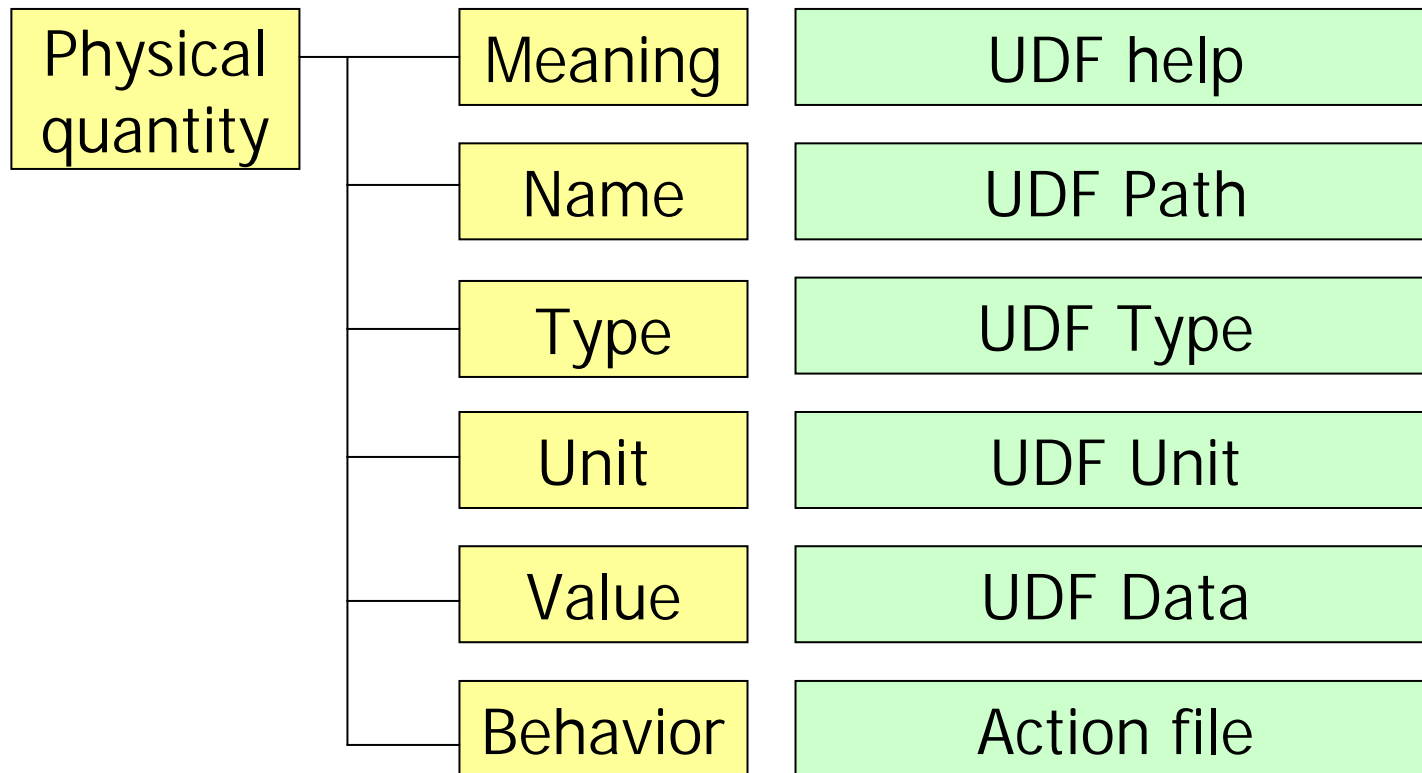 - GOURMET allows users to customize the interface and the analysis tool.
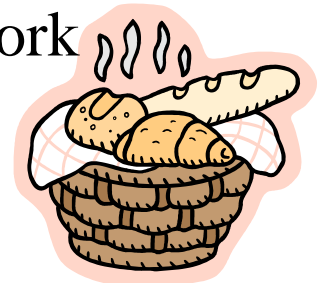
Requests from the engine developers

- **I do not want to spend time to make my engines "user friendly".**
  - GOURMET offers your engine a simple interface instantaneously. You can leave the task of making "user friendly program" to individual users.
- **I do not want to learn things to connect my engines to GOURMET.**
  - The rules to be obeyed to connect to GOURMET is minimal.
- **The data structure of my engine may change as the engine evolves.**
  - GOURMET can adjust the change of the data structure easily.

What is a physical quantity?

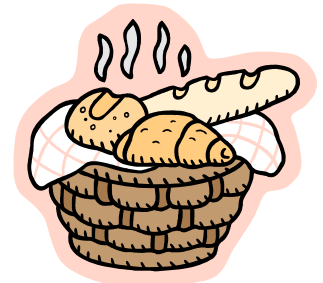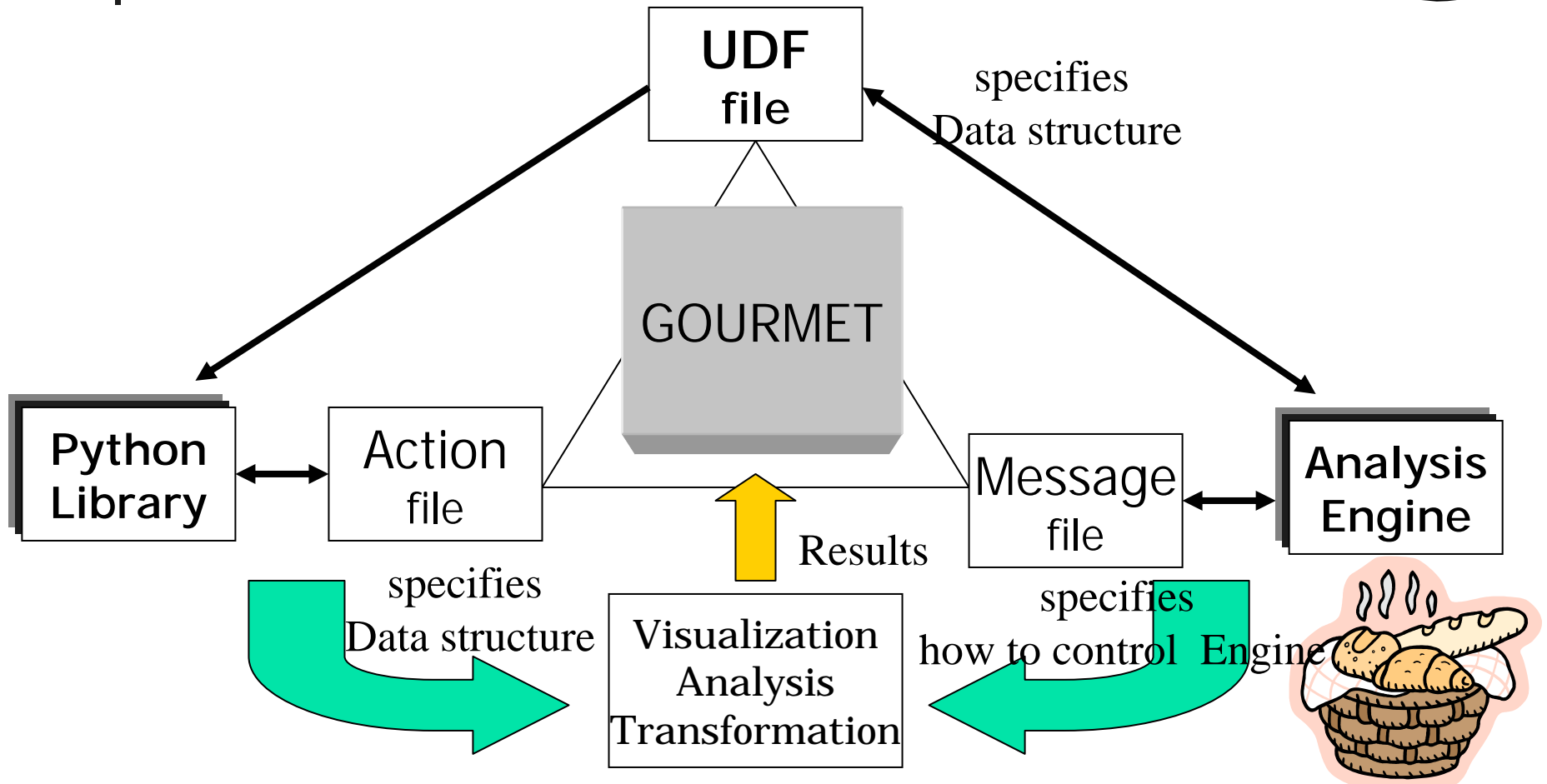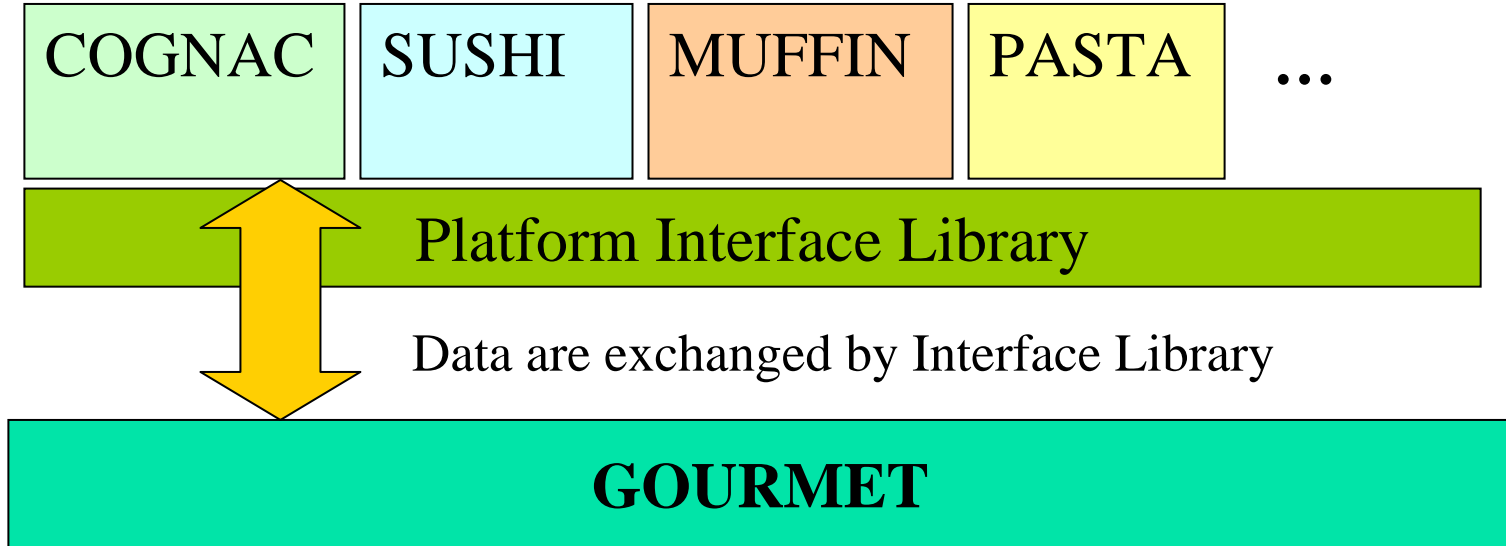| Physical quantity		
	Meaning	UDF help
	Name	UDF Path
	Type	UDF Type
	Unit	UDF Unit
	Value	UDF Data
	Behavior	Action file

Features of GOURMET

- UDF format defines a physical quantity
  - Physical meaning(Help), Name(Path), Type, Unit, Value(Data)
- Action file specifies the behavior of the physical quantity
- Message File controls Analysis engine

How it works

Relationship between GOURMET and Engines

| COGNAC | SUSHI | MUFFIN | PASTA | ... |

Platform Interface Library

Data are exchanged by Interface Library

GOURMET

Coarse grained molecular structure builder

- Specifying rules of the format convention and definition of UDF to be created, the data can be converted to the UDF file.
    - PDB file & mol file are supported.
- Information required by the coarse grained molecular dynamics engine is added automatically.
    - Potential information (Angle, Torsion, etc.)
- Since they are described by python, you can change and advance them easily
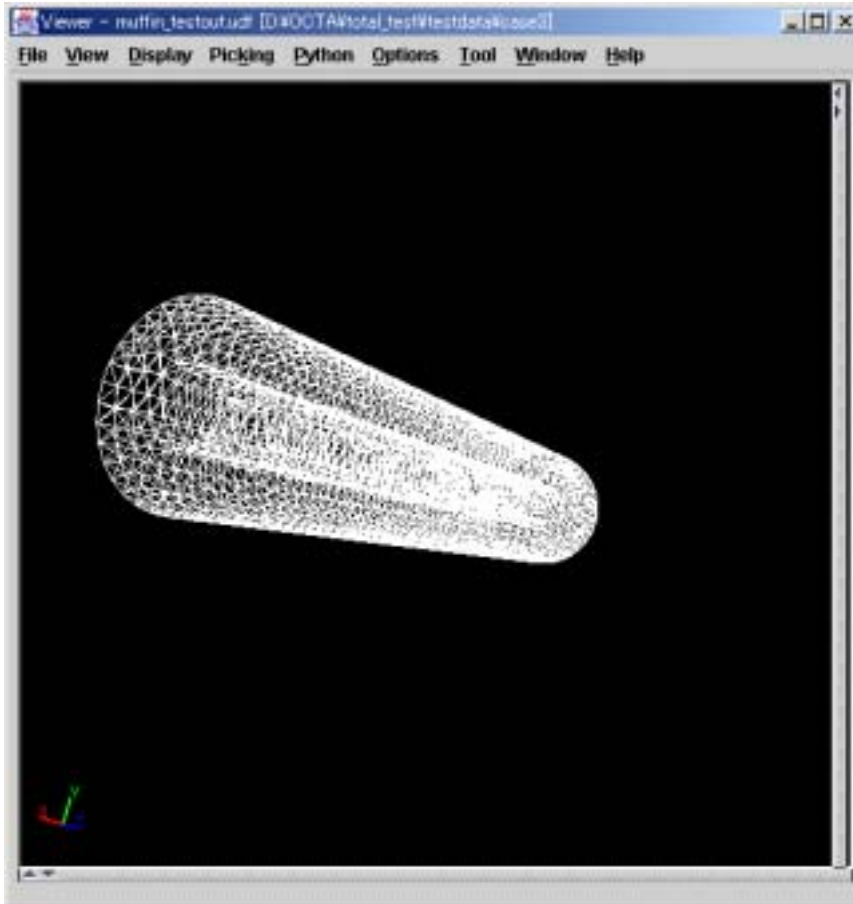   - Support format can be customized freely
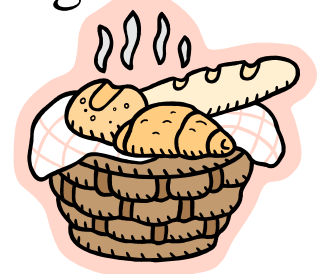
Cooperation with FEM Pre-Processor

- General-purpose data filtering function.
  - The same data-conversion mechanism of the molecular structure builder is used.
  - The complicated mesh data of the bulk data file format of NASTRAN can be read.
  - Extension to a new data structure is also easy.
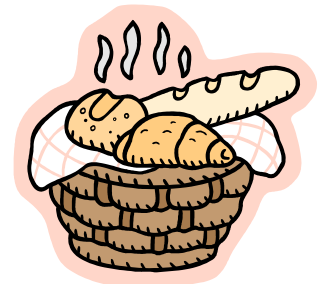
Example of converted mesh data

Transformation was performed to NASTRAN bulk file-MUFFIN3 using the conversion filter which was created as a sample, and it displayed by GOURMET.
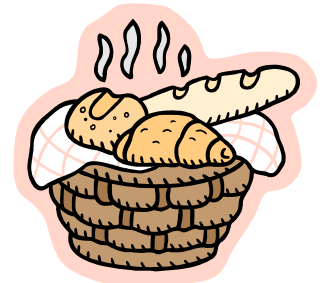
Engine manager

- Starting, pausing, parameter changing, and the situation surveillance of the registered engine on a network are available.

- It works on the server which offers engine execution.

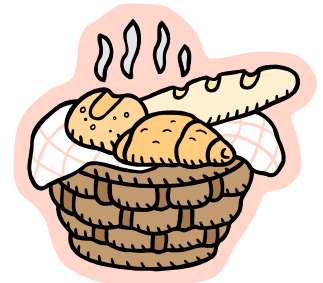- Since the message from/to the engine is UDF, it is easy to extend.

On Client   On Engine Server

GOURMET   ⟷   **Engine Manager**

UDF Files

runs engine

Action

- In GOURMET, programming by python is available.
  - Flexible work can be done at the time of engine development and analysis
- **But …**
  - Many operations are complicated in a completed engine system.
- **Then …**
  - Python script library management has developed.
  - management of the script which is created by the user.
- **From ready-made to easy custom-made!**

Data manager

- Server application.
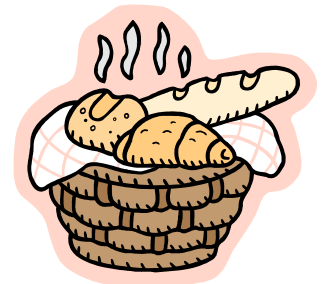- It works on the server which offers a UDF data control function.
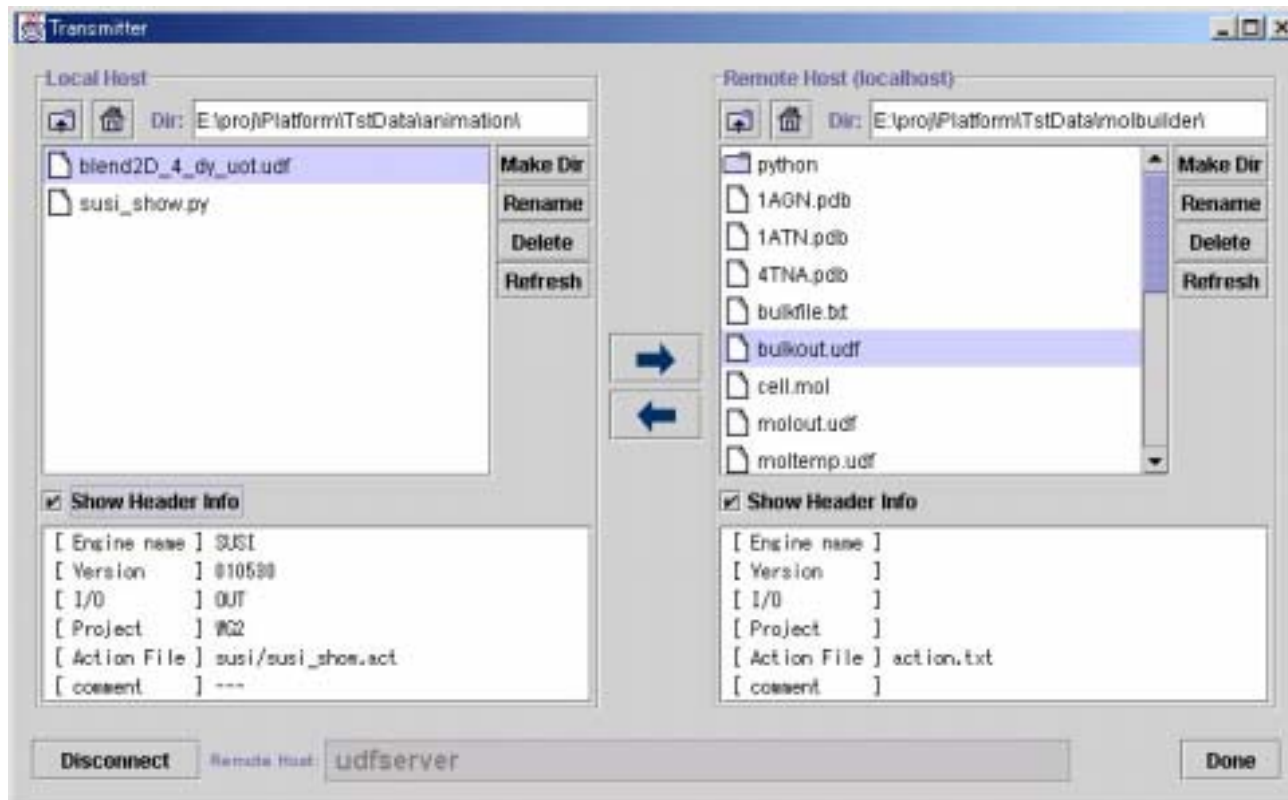
On Client

GOURMET ⟷

UDF Files

UDF Managing Server

Data Manager

Using Data manager

Management, transfer, and information
reference of a UDF file are available.

Improvements on GUI

- **Help**
  - explanations are described in UDF definition, and you can refer it by GUI
- **Select**
  - candidate data are described in UDF definition and you can choose it by GUI.
- **Unit**
  - Unit system conversion function. (It's great!)
- **Picking**
  - Object selecting function.
- **Improvement 2D plot function**
  - data making function for graphs by Built-in GraphSheet
  - Also gnuplot interface library is available
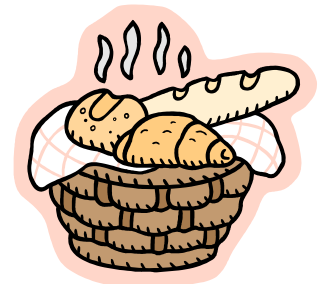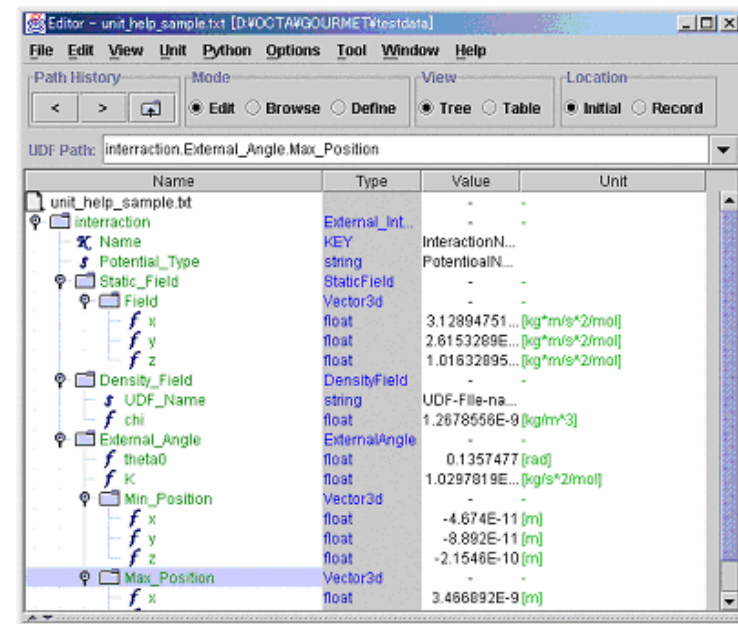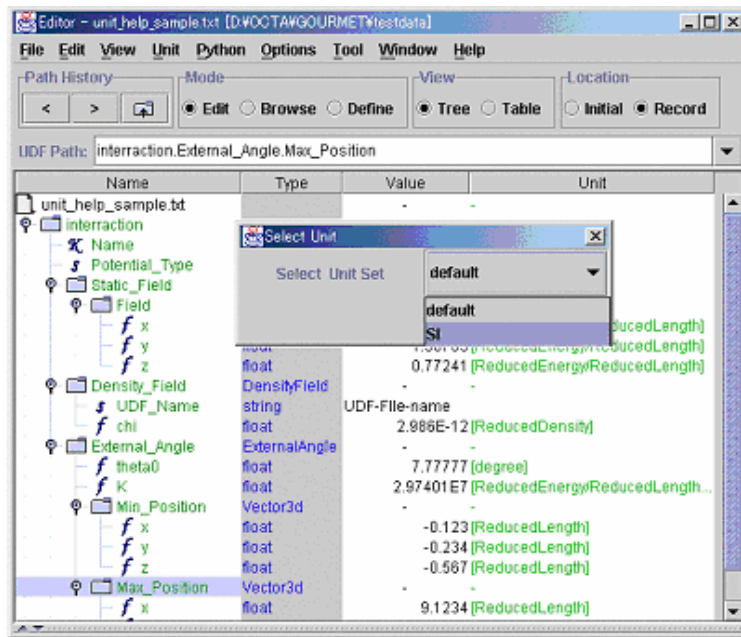
Unit function

- **Many engines use non-dimensional physical-properties value.**

- **But ...**

  - Conventionally, the data conversion to non-dimension unit system are needed.

- **Then ...**

  GOURMET performs the calculation.

  - The conversion method is defined by UDF
  - There is no reason that you learn the conversion process.

Example of unit conversion

Conversion and inverse transformation of unit system is available by GUI.
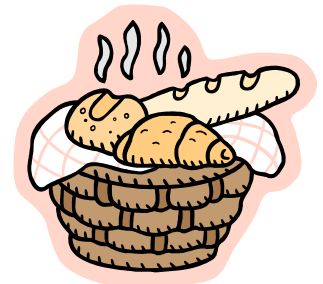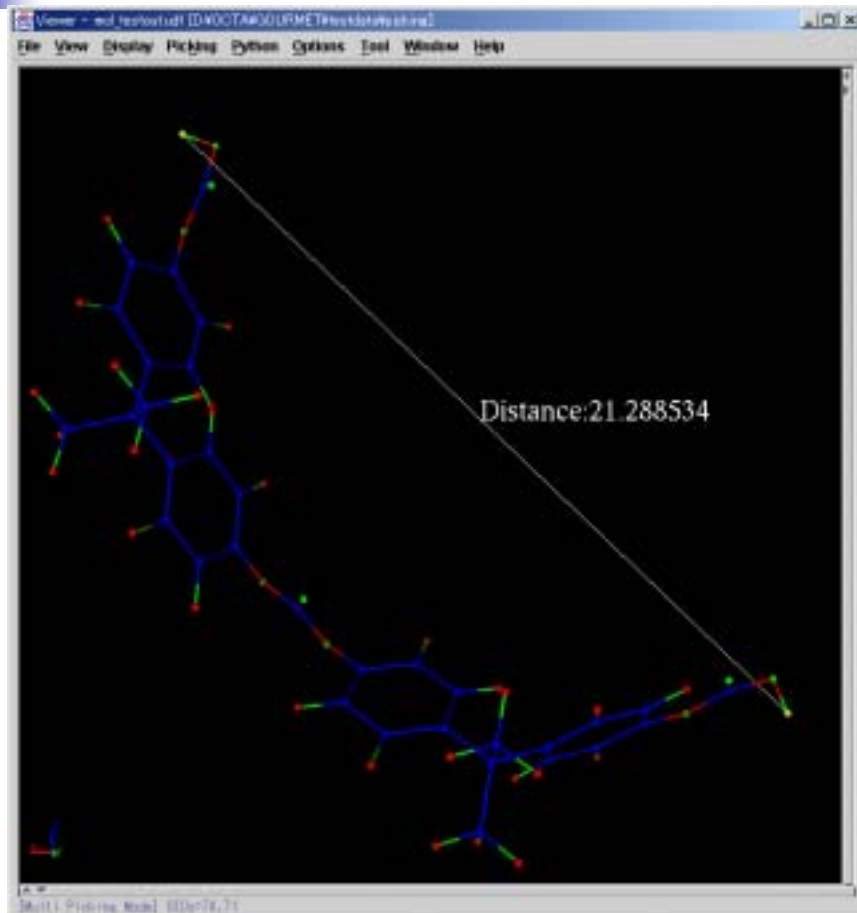(The scale conversion for every data is also available)

Picking function

- By selecting the drawing object displayed in 3D

- Perform the defined action on the object
  - For example, selection, regeneration, etc. of one molecule.

- Supports the work of analysis.
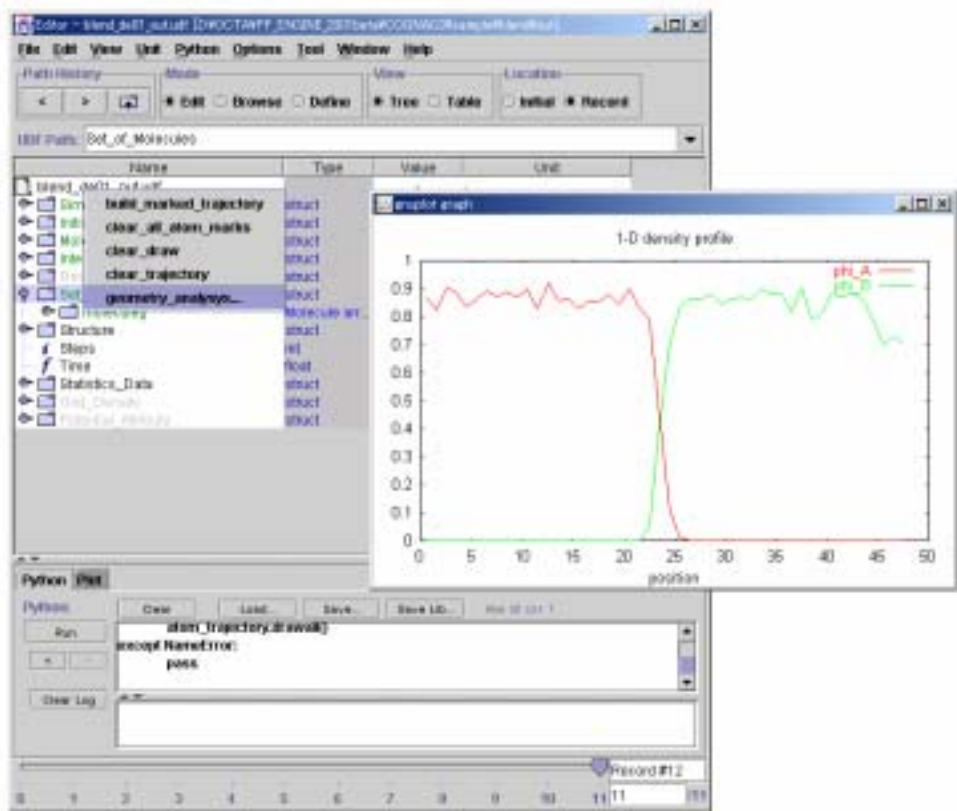
Example of Picking function

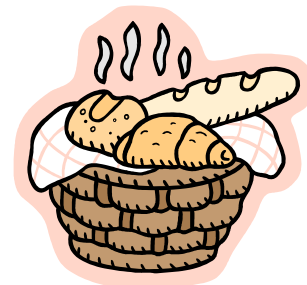display the distance between selected 2 atoms.

(Animation is also possible as it is)
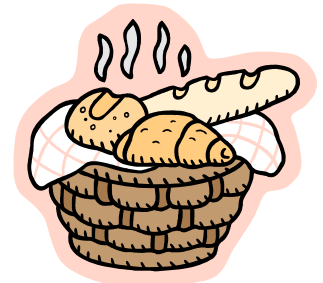
Example of plot action

The example which plots the modulus of a 1-dimensional volume integral from the calculation result by COGNAC.
(Plotting is performed by only three actions)

Released history

- 1999~ start development
- 2000/6 alpha version
  - Many functions with which this platform should be equipped were considered.
- 2001/6 beta version
  - Reconstruction of Architecture for high speed, minimize memory
- 2002/4 Release
  - Improvement for convenience

Improvement
## - To the peoples who used the Alpha / Beta Version -

- ## In speed
  - I/O 20 times faster
  - Drawing:30~500 times faster(when you use memory cache)

- ## In using memory
  - Quarter(architecture has changed from a server-client to local calculation)

- ## Large improvement in operability and convenience

Conclusion

- Cooking materials has been prepared!
  - *COGNAC, SUSHI, PASTA , MUFFIN ...*
- Cooking tool has been prepared!
  - GOURMET with Python & gnuplot
- Have your favorite dish!
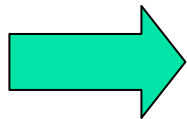
And demonstrations as a dessert