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Title:	Scripting ToolKit (STK) 2.0 for Granta Database. Model Calibration Examples
Author(s):	Benedikt, Bartlomiej Jozef
Intended for:	Share it with Granta MI (company that provides Granta database to LANL)
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Scripting ToolKit (STK) 2.0 for Granta Database
Model Calibration Examples

2-12-2020

Motivation

Multiple stress cushion (SX-358) uniaxial compression tests are performed.

There are 640 (= *4 cycles x 160 tests*) compression test curves coming to Granta.

Find CHIP-Foam material model parameters.

Efficient method is needed to process test data to calibrate custom material models.

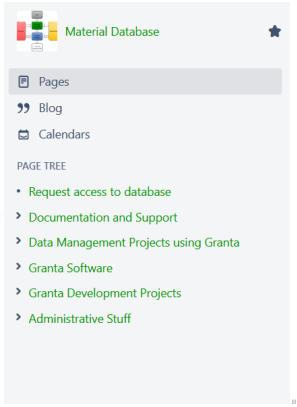
Agenda

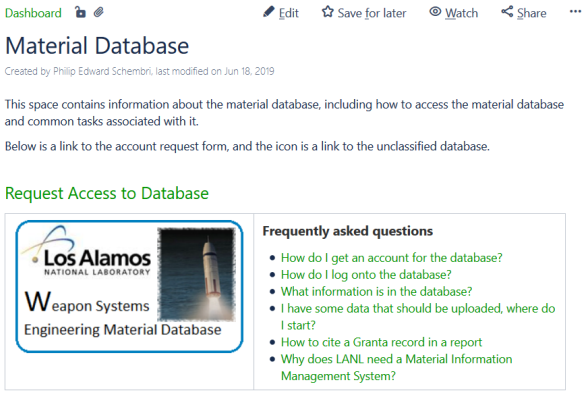
1. What is Python STK 2.0?
2. How can to access and use it?
3. Example 1: How to export data from Granta?
4. Example2: Model Calibration
   - CHIP-Foam Model
   - Updates to Driver
   - Calibration Example
5. Conclusions and Current Projects that Use STK 2.0

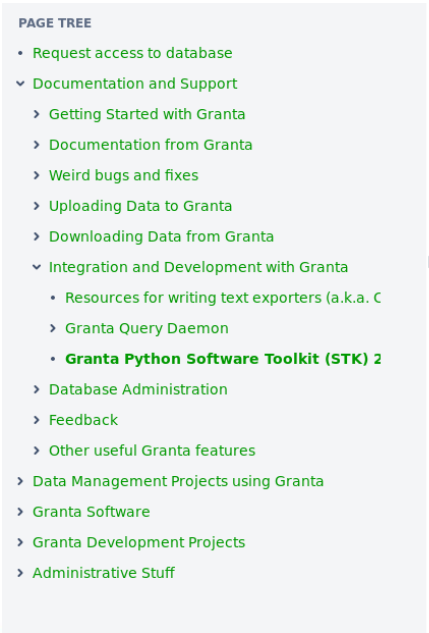
What Is Python STK 2.0?

Python STK 2.0 is an interface for accessing Granta records from Python script.
It is similar to what Prabhu did a few years ago (Granta Query Daemon, GQD), however it has more features and it is supported by Granta MI.

What Is Python STK 2.0?







Granta Python STK 2.0 Example Scripts

File	Description	Author
STKv2_Test_WildcardAttrib.py (Windows/Euphrates-vm) STKlnx_Test_WildAttrib.py (Linux)	Return all records in database that match a wildcard in any attribute. The initial script search criterion uses the attribute "Material Name" to search for records.	Clay
STKv2_Test_SpecificHeat.py (Windows/Euphrates-vm) STKlnx_Test_Cv.py (Linux)	Get specific heat from a record in Material Universe	Clay
STKv2_Test_YoungsModulus.py (Windows/Euphrates-vm) STKlnx_Test_Modulus.py (Linux)	Get Young's Modulus from a Common Material Property record in the LANL database	Clay
STKv2_pbx9502_EngSE_plot.py (Windows/Euphrates-vm) STKlnx_Test_EngSEplt.py (Linux)	Get stress-strain curve from a PBX 9502 uniaxial test record in the LANL database	Clay
STKv2_Test_FileDownload.py (Windows/Euphrates-vm) STKlnx_Test_FileDownload.py (Linux)	Download a file that is part of a record in granta	Clay
STKv2_Test_Images.py (Windows/Euphrates-vm) STKlnx_Test_Images.py (Linux)	Download a picture that is part of a record in granta	Clay

Several examples of how to perform basic tasks with STK 2.0 can be found on the Granta Confluence page.

Where STK 2.0 Is Used:

- CHIP-Foam project (calibration of material model)
- TIMS: provides interface between TIMS database and Abaqus models
- DC-745: used to calibrate hyperelastic models (e.g. polynomial models)

How Can I Access/Use STK 2.0?

```
# Import STK 2.0 module:
import GRANTA_MIScriptingToolkit as GrantaToolkit
from GRANTA_MIScriptingToolkit import granta as mpy
```

Import STK 2.0

```
#### Imput your username ( z# + "@lanl.gov")
user_name = "193644@lanl.gov"
#### Input your password (crypto-card)
cred = getpass.getpass("Password: ")
#
#
# Define INPUT for connecting to Granta, setting the units, etc:
# ----------------------------------------------------------
#
#### Connect to Granta MI:
mi = mpy.mi.Session("http://grantami/mi_servicelayer", user_name, cred)
#### Connect to Database:
my_db = mi.get_db("LANL Weapon Systems Engineering Materials Database")
###### Set Unit System for Database:
my_db.set_unit_system('MPa-mm-s-K', absolute_temperatures=True)
#### Find Table in Database:
my_tbl = my_db.get_table("Testing - Uniaxial")
```

Open database and open the Table you want to access

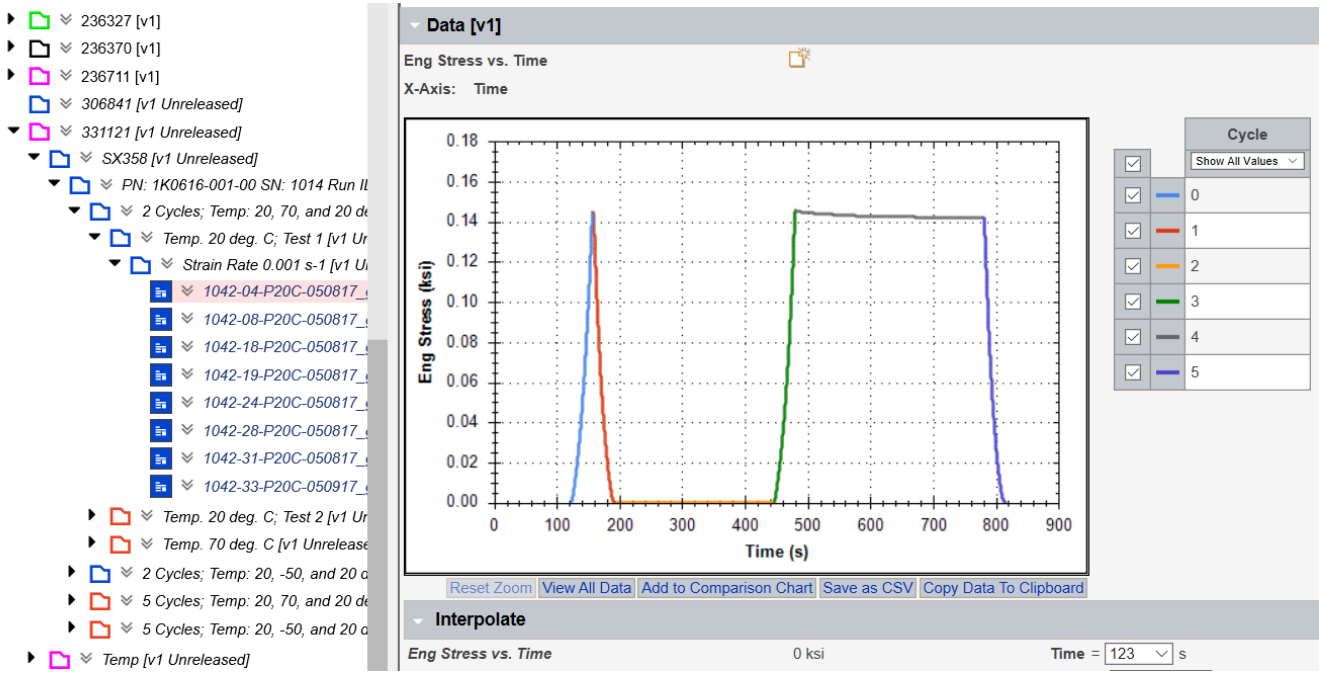
STK 2.0 module is saved in beta version of Toolbox.
Beta toolbox can be accessed by *sv3b*.

STK 2.0 has also been installed on Windows *vm-euthrates*

Example 1: How to Export Data from Granta?

Goal:

Need to export to Python stress vs. strain data from selected records.



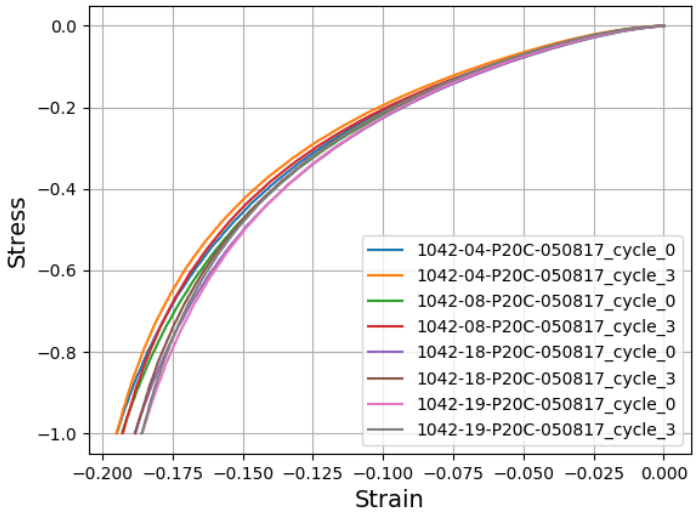
Example 1: How to Export Data from Granta?

Specify what records to search, what functional data to export, units, etc.

```
# Define search criteria:
list_of_IDs = [ '1042-04-P20C-050817_granta_cycles', '1042-08-P20C-050817_granta_cycles', \
                '1042-18-P20C-050817_granta_cycles', '1042-19-P20C-050817_granta_cycles']
#
# Cycles definition:
# ------------------
cycles_to_use = [0, 3]
#
# Functional Data:
# ----------------
attributes_list = [ 'Eng Stress vs. Eng Strain', \
                    'Strain []', \
                    'Y min (Eng Stress vs. Eng Strain [MPa])', \
                    'Density']
```

Import data to Python, arrange the data

```
# Find records that meet search criteria and save them in list:
# -------------------------------------------------------------
records_found = []
for _ in list_of_IDs:
    records_aux = my_tbl.search_for_records_by_text(_)[0]
    records_found.append(records_aux)
#
# Define dictionary with strain and stress data for each record:
# --------------------------------------------------------------
#
data_dict = create_dictionary_from_records(records_found, attributes_list, cycles_to_use)
#
attrib = 'strain'
strain_test_Dict = create_flat_dictionary_from_nested_dict(attrib, data_dict)
#
attrib = 'stress'
stress_test_Dict = create_flat_dictionary_from_nested_dict(attrib, data_dict)
#
```



Example 2: Model Calibration

CHIP-Foam

Constitutive equation ⇒ $\sigma = \frac{1}{J}\frac{\partial W_{foam}}{\partial F} \cdot F^T$

σ – Cauchy stress
J – Jacobian
F – deformation gradient
W_{foam} – strain energy density

Strain energy density function for CHIP-Foam formulation is given by the following formula:

$$W_{foam} = \underbrace{\frac{\hat{G}}{2}(\bar{I}_1 - 3) + \hat{K} f_1(J, J_b)}_{\text{Small deformation response}} + \underbrace{C_{10} f_D(\varphi_0, \bar{I}_1, J_m)}_{\text{Pore deformation (Danielsson)}} + \underbrace{(1-\varphi_0)K(J_m ln J_m - J_m + 1)}_{\text{Compressibility of parent material}}$$

Material parameters such as ρ_s, *K*, C_{10}, *G_hat*, and *K_hat* are determined for a foam material by fitting the model to the experimental data

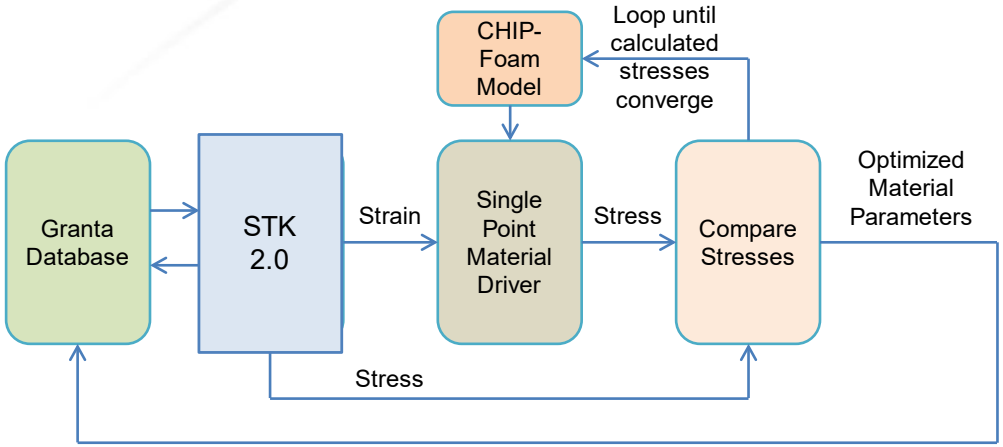
Example 2: Model Calibration

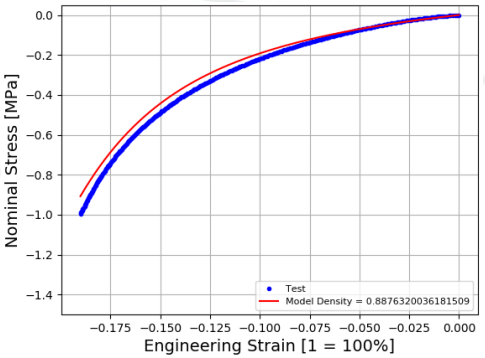
Updates to Driver

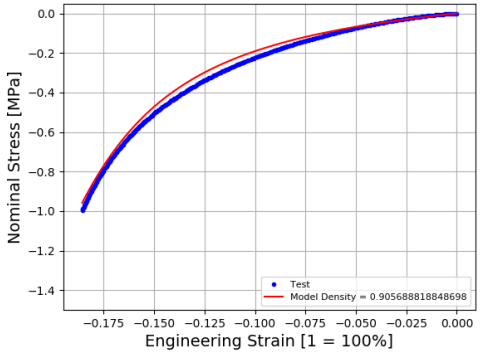
- STK 2.0 interface added to export data from Granta and use it with the material driver
- Driver can use deformation gradient as well as strain as input
- Most commonly used deformation gradient generators implemented:
  - ✓ uniaxial strain
  - ✓ pure shear
  - ✓ simple shear
  - ✓ volumetric
- Uniaxial stress loading case added

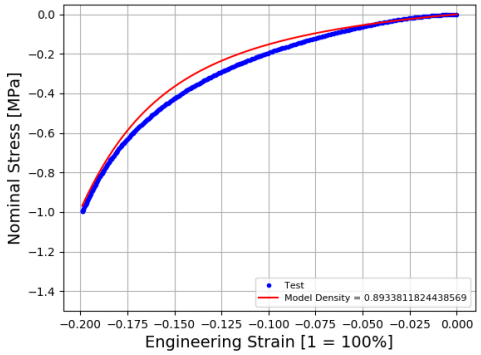
Example 2: Model Calibration

Numerical Example









Material model calibration process is automated

Conclusions and Current Projects that Use STK 2.0

Conclusions:

- STK 2.0 is user friendly and it is faster than GQD
- STK 2.0 is supported by Granta MI
- STK 2.0 has many additional features: plotting, changing units of individual attributes, several database searching options, and more
- Documentation of STK 2.0 exists and it is helpful
- If there is need to convert the exported data into another data structures (e.g. datanode), this can be accomplished relatively easily
- STK 2.0 can also be used to import data to database (not yet tested)