COBIK
Centre of Excellence for Biosensors,
Instrumentation and Process Control

Investing in your future
OPERATION PART FINANCED BY THE EUROPEAN UNION
European Regional Development Fund

Input - Output Interface Utilities for Batch Calculation of Material Properties with JMatPro

Revision 3, August 2012
(revision 0: November 2011)

Igor Grešovnik

COBIK

Contents:

1   DESCRIPTION OF THE JMATPRO INTERFACE

1.1 Introduction

This technical report contains basic data for using the JMatPro interface for automatic running of material properties calculations for steel and eventually other materials.

1.2 Directory Structure

All JMatPro data is in the JMatPro installation directory; we will usually install the software in the directory
    c:\JMatPro-4.0\
(for version 4.0, which is the last one without the hardware key and is available for use by us).
    Executable is
    c:\JMatPro-4.0\JMatPro-4.0.exe

Other data is contained in the following locations within JMatPro-4.0:
* inits/compos.ini – material compositions

1.2.1 Important files

1.2.1.1   Material composition:

File inits/compos.ini contains all compositons. We will replace the file each time before running JMatPro in such a way that only one composition is contained. We will name the only contained material "0000".

1.2.1.2   Indication for end of calculation:

temp\coldfire.out

1.2.1.3   Calculated material properties

Calculated material properties will be saved to this file:
export/data/0000.dat

- This file can be directly read by Robert Vertnik's simulator (store the file to ss_0000_.dat and state file name in the Sim_main\IN_PUT\SS\dummy___.sim file under MATERIAL PROPERTIES BLOCK (i.e., the text there is "SS_1201_")).

1.3 Running procedures:

Some steps in calculation of material properties include playback of recorded mouse and keyboard events to simulate user interaction. For some of these scripts to work properly, the JMatPro window must always be located at the same position. Normally, JMatPro will on launch open its window at the position where you have last closed it, therefore you can influence the position. The window should be places at the top left corner of the screen and must be precisely aligned with the screen visible area.

Calculation will be performed by play back of recorded keyboard and mouse events, in order to run the program noninteractively. This will be done in three steps described below:
- Starting the JmatPro program
- Running calculation
- Waiting until calculation finishes
- Saving results
- Closing JMatPro

Starting JMatPro and waiting for calculation to finish is done purely programatically while the other tasks are performed by simulated user interaction through playbacks of recorded keyboard and mouse events.

Beside these tasks, there are some sefeguarding and problem resolving tasks:
- Ckecking whether JMAtPro is running
- Killing the JMarPro
- Repairing JmatPro after crash or unintended run

Repairing JMatPro is performed by simulated user interaction while the other two tasks are performed purely programatically.

1.3.1 Launching JMatPro software

Recorded script: **jmatstart.pam** .

1.3.2 Running calculation

Recorded script: **jmatrun.pam** .

To run calculation of material properties:
- Prepare material composition file (*inits/compos.ini*).
- Delete the *temp\coldfire.out* file (used for detection of the end of calculation).
- Launch JMatPro. Its window always opens on the same position that is remembered.
- Chose in the menu Material Types / General Steel, then click the "Extended General" button, set Step to 1.
- Load material data: In the menu, choose File / Load composition (Ctrl-C). Choose "General Steel", then "0000", click the "Choose" button (or tab and then Ctrl-space). When recording mouse & keyboard events, this selection should be performed by keyboard since window positioning may depend on screen resolution.
- Click the »Start calculation« button – the calculation begins.

1.3.3 Waiting for results

End of calculation can be detected by changes in the temp\coldfire.out file. This file is changed several times during calculation, therefore you should check changes in size.

The file is created in the middle of calculation, but keeps its size 0 bytes. When calculation is finished, the data is written to the file and its size increases to a bit over 1 MB. Therefore, the criteria for detection of the end of calculation may be e.g. that the file is <u>more than 5.000 bytes long</u>. It should always be longe;r than this after calculation, and it should not be longer before calculation finished.

Before calculation begins, the file must be deleted in order to enable reliable detection.

Problematic issue and solution:
The coldfire.out file is created a bit before calculation ends, and then increases in size for some time. Criterion for detecting completion of calculations is therefore a bit more complicated. We first delete the file, then wait until it is created and it exceeds the specific size, and then wait until the size does not change any more for some time.

1.3.4 Saving results

User interface script: **jmatsave.pam** .

When calculation finishes, a window opens with title "Extended physical properties". Click on the "Export data" button in the bottom area of this window (icon - press tabulator 12 times, or press Shift-Tab 4 times), choose "More data to worksheet format" (tab and space), choose Save (2x Shift-Tab, then space), under File Name (Alt-N, Ctrl-A) insert "0000.dat", then click on Save (twice tab, space), and click the Yes button (space). That-s all, when done, you can kill JMatPro.

Results are saved to the file **export/data/0000.dat**.

1.3.5 Closing JMatPro

User interface script: **jmatclose.pam** .

This closes JMatPro in an ordinary way by simulating user interaction.

1.3.6 Repairing JMatPro

User interface script: **jmatrepair.pam** .

This repairs JMatPro if something went wrong.
Reparation procedure is necessary after JMatPro has closed abruptly (e.g. by killing the process in a Task Manager) or when somebody else has run the program. In this case, JMatPro must be started, and the "Repair" button must be pressed in the message box that is shown.

There are two important issues related to this. First, interface must detect if such a situation occurs. This is done by executing recorded user interaction for closing of JMatPro software first, then killing the software (which should not run now if everything is normal) and then launching the software. If after this procedure the software is not running, then we know that something is wrong and we need to run reparation procedure. The detection procedure is run as part of launching the JMatPro (launching procedure first tries to close JMatPro, then it kills it just for any case, then it runs it, and finally checks whether the process is running – if this is not the case then the reparation procedure is run).

The next issue is that reparation procedure must work in all possible cases: when JMatPro is already running properly, when it is not running but can not be launched, e.g. because it had been

stopped abruptly, and when it does not run but can be launched normally. The recorded events script will usually try to start JMatPro two times, therefore provoking abnormal situation (and consequently launch of message box with repair option) and pressing the repair button. Where the script is used in a program, the procedure might try to start JMatPro twice in a row and then kill it in order to ensure that the reparation message box is launched.

2 USING THE INTERFACE

2.1 Running Material Calculations

Warning: when running material calculations, do not run java updater or installer on another account on the same computer because JMatPro will hang!

Running is performed in the project directory
```
... \workspaceprojects\12_09_jmatpro
```

Recorded mouse and keyboard events are stored in the directory
```
...\workspaceprojects\12_09_jmatpro\records\
```

Scripts are contained in
```
...\workspaceprojects\12_09_jmatpro\train\jmat\
```

Calculatef material properties are initially contained in the following directory:
```
...\workspaceprojects\12_09_jmatpro\train\jmat\materialdata\
```

The interface is used and manipulated by the internal script class named *IG.Script.S_12_09_jmatpro*.

Scripts are prepared for running material calculations. There are some batch scripts (.bat), but these were used mainly for initial testing. Running is performed by running command-line interpreter's scripts (extension .cmd). The usual procedure is such that one first runs the ANN application with the interpreter in the interactive mode, i.e. by executing the shell by typing the following command in command prompt:

```
Shellext Interactive
```

Then a script containing definitions of variables for specific computer is run in the interactive mode, e.g.

```
Run setvar34.cmd
```

These scripts handle all computer dependent settings, e.g. by defining which setting file is used for reading the settings for the interface. There are several settings files, e.g. `settingsjmat34.json`, and the example command above will cause that precisely this setting file is used.

When computer specific definitions are handled, you can run the script that performs specific calculation, and there is one such script for a given task for all computers (since computer-dependent things were handled by the script containing definitions). For example, calculations of material properties at a number of random compositions (concentrations varying within the appropriate ranges) are run by the following command:

```
Run runjmat.cmd
```

The script `jmat.cmd`, contains some commands for test runs (which can be commented) and the command for running calculations at randomly chosen compositions.

There is another important script, `jmatall.cmd`. This script contains examples of all available internal script commands (accessible through command-line interpreter) so that they can be copy-pasted to the shell's command prompt and executed at will. In this way, different auxiliary tasks are performed, such as printing statistics about calculations performed up to now (for which data as not been moved yet from the original location in the material data directory), or for moving calculation data according to the calculation state (e.g. successfully calculated, unsuccessful, data corrupted, busy flag still set (either calculation is still going on or it has been interrupted)).

2.2 Failures that can occur

Several failures can occur during calculation of material properties. These are mainly a consequence of JMarPro failures or problems with synchronization. Problems with synchronization can not be completely resolved because the java interface (GUI that is managed by recorded key and mouse events) sometimes become quite irresponsive for no known reason, and one can not know how much time should actually be allocated between successive mouse clicks or key presses in order to give the interface enough time. It was also not possible to build in true synchronization procedures that would properly detect when any given part of the interface is ready for the next user input, and this would also be impractical to implement due to excessive segmentation of control scripts.

It seems that synchronization with the availability of results works well now. It is still a question whether synchronization with saving the results works well enough, i.e. the results might still be incomplete when they are transcribed to the storage directory.

If any synchronization between starting material calculation and saving results does not work or JMatPro is not started properly, this is detected and no results will be available in this case (also the flag for successful calculation will not be set).

Many times <u>keyboard does not function properly</u> (when typing, symbols that appear in a text editor or command prompt do not correspond to keys pressed). This can manifest in different ways and is probably due to errors that remain after use of mouse & keyboard emulation scripts. Solution is sometimes to lock the screen, and if this does not help, to log off the account and log on again.

Sometimes, <u>JMatPro just hangs</u> in the middle of calculation or just before writing and results to a file. In this case, timeout occurs. Often calculations become increasingly slower and finally every successive calculation hangs, leading to timeout (noted by a flag). When this occurs, the user running calculations must <u>stop the calculation, log off the account, log in again, and restart the calculation</u>.

Sometimes, <u>units for element fractions are changed from wt% to at%</u> for no apparent reason, which often happens when material composition is loaded. This is solved in such a way that units are changed when saving results.

Sometimes, <u>lowest temperature in result file is higher than 25 C</u>, although calculation proceeds till the end. Maybe this is due to a bug in the interface (e.g. waiting until result file is completely written does not work properly), this still needs to be investigated.

Sometimes <u>the highest temperature in the result file is different than 1600 C</u> (most often it is higher). It seems that this may be related to improper function of the keyboard, since the problem sometimes appears when function of the keyboard is drastically impaired.

<u>Results</u> of JMatPro calculations (temperature dependencies) are becoming <u>more and more noisy</u>. Solution is that you break the batch material properties calculation that is currently going on, log off (even better – restart the machine if this is possible) and restart the calculation.

2.2.1 Chronological list of solutions

Uniqueness of material parameters to storage directory mapping not ensured – procedural bug, detected on December 7. Dismissed on December 11.

By December 16, safety procedures were built in that ensure that there is no successful calculation flag set if there is an error in running JMatPro, if JMatPro hangs during calculation, or there is an error in synchronization after starting calculation and before saving the results.
There may still be undetected error if calculation was not started in the right way, or if results were copied before saving to a file has completed. A check of the results shouls be perform in order to detect such an error.

By January 10, result files are checked for contents, i.e. units and temperature range are checked, and only in directories where result file contents is correct, the flag for successful calculation is set.

By January 6, it seems clear that user must log off and on from time to time when results are becoming more noisy.

References:

[1]   N. Saunders, U. K. Z. Guo, X. Li, A. P. Miodownik, J. -Ph. Schillé: Using JMatPro to model materials properties and behavior. JOM, December 2003, Volume 55, Issue 12, pp 60-65 (Springer).

[2]   Z. Guo, N. Saunders, A. P. Miodownik and J-Ph. Schillé, Modelling of Materials Properties and Behaviour Critical to Casting Simulation. Materials Science and Engineering A, 413-414 (2005) 465-469.

[3]   Introducing JSON. Electronic document at http://www.json.org/ .

[4]   JSON on Wikipedia, http://en.wikipedia.org/wiki/JSON

[5]   I. Grešovnik. IGLib – Investigative Generic Library, library homepage located at http://www2.arnes.si/~ljc3m2/igor/iglib/ .

[6]   I. Grešovnik. IoptLib – Investigative Optimization Library, library homepage located at http://www2.arnes.si/~ljc3m2/igor/ioptlib/ .

[7]   I. Grešovnik. IoptLib user's manual. Electronic document at http://www2.arnes.si/~ljc3m2/igor/ioptlib/doc/optlib.pdf.