Parameter Studies and High Performance Computing with GeoDict

Jürgen Becker

GeoDict User Meeting 2012

MATH 2 MARKET

Motivation

Graphical user interface requires interaction:

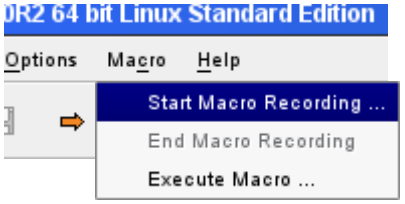
- Set parameters in dialogs
- Click 'run'
- Do the same thing again and again (with one different parameter)
- Computer can work 24/7

Don't spent your time watching progress bars!

History I

2007:

- Macros (*.gmc) introduced
- Command line introduced: geodict *.gmc
  - Cluster batch queue



2008:

- VaryMacro command introduced
  - Replaces %1, %2 placeholders in another .gmc file
  - Allows parameter studies from command line

2010

- GeoDict Vary Macro (*.gvm) format introduced (in SinterGeo)
  - Add, Subtract, etc possible in *.gvm
  - Define variables in *.gvm (enhancement of placeholders)

History II

2012R1

- Merged .gmc and .gvm format (*.gmc now has the enhanced syntax)
- Merged VaryMacro and VaryGvm command
- 'Save Image' works in macros (when executed from GUI)
- Record movies uses macro syntax (no *.anim files anymore)
- UserModule added
  - Parameter studies from GUI
- Execute Macro allows to Step, Skip, Extract

2012R2:

- Compatibility: can execute *.gmc recorded with 2012R1

The Basic Idea: Record & Play

Idea:

I. Record all actions ("Commands") done by the user in a text file ("Macro").

II. GeoDict can execute macro files:

- exactly the same actions happen again
- exactly the same results are produced

Sound boring at first, but

- useful to log your project work

  (Which part of the tomography did I crop?)
  (Maybe I forgot to set the correct viscosity?)

- with Skip & Extract you can get parameters from the macro into the dialogs

But there is more...

- Edit macro files
- Define variables
- Call shell scripts

Example

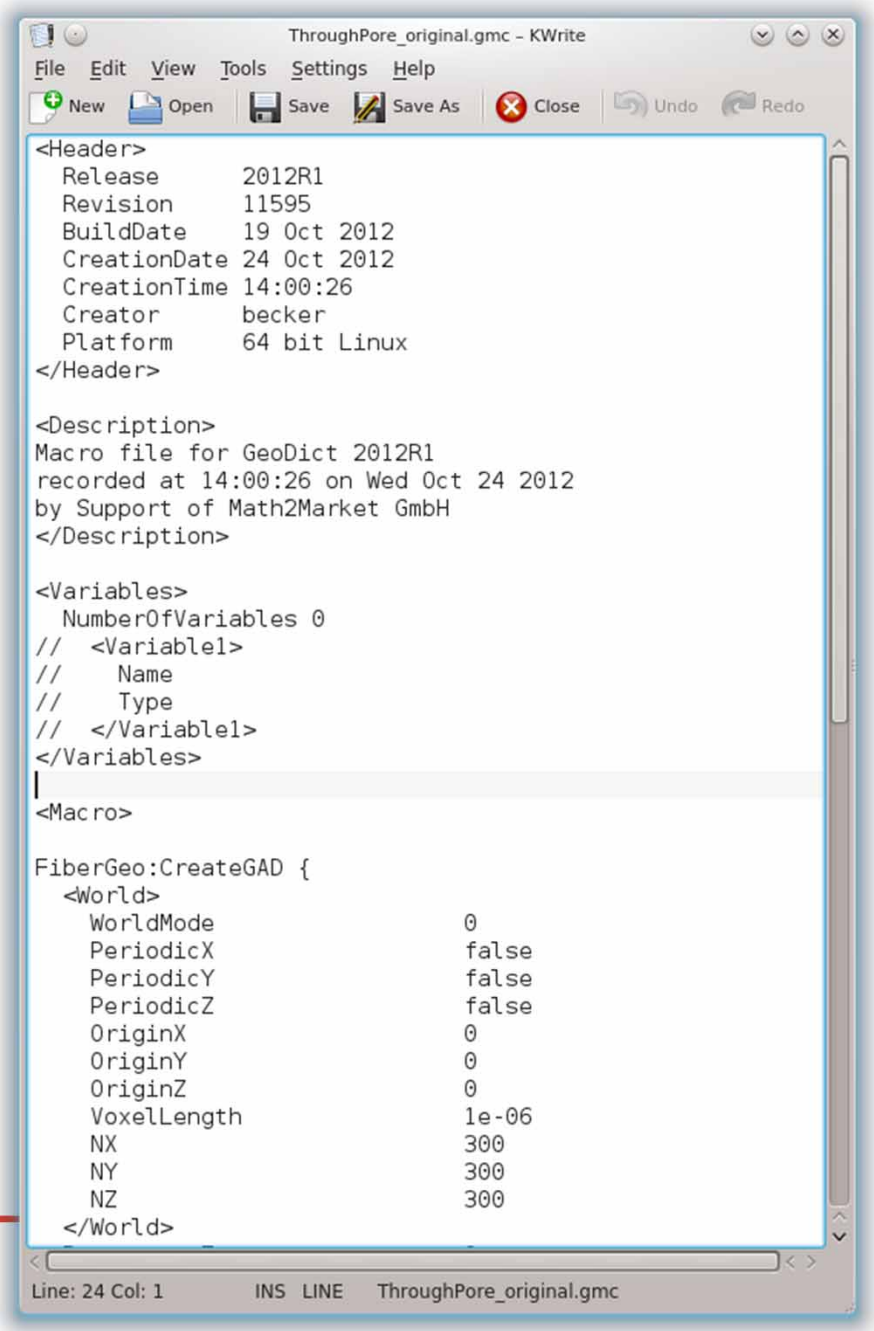
Task:

- Create a structure with FiberGeo
- Determine percolation path with PoroDict

Vary:

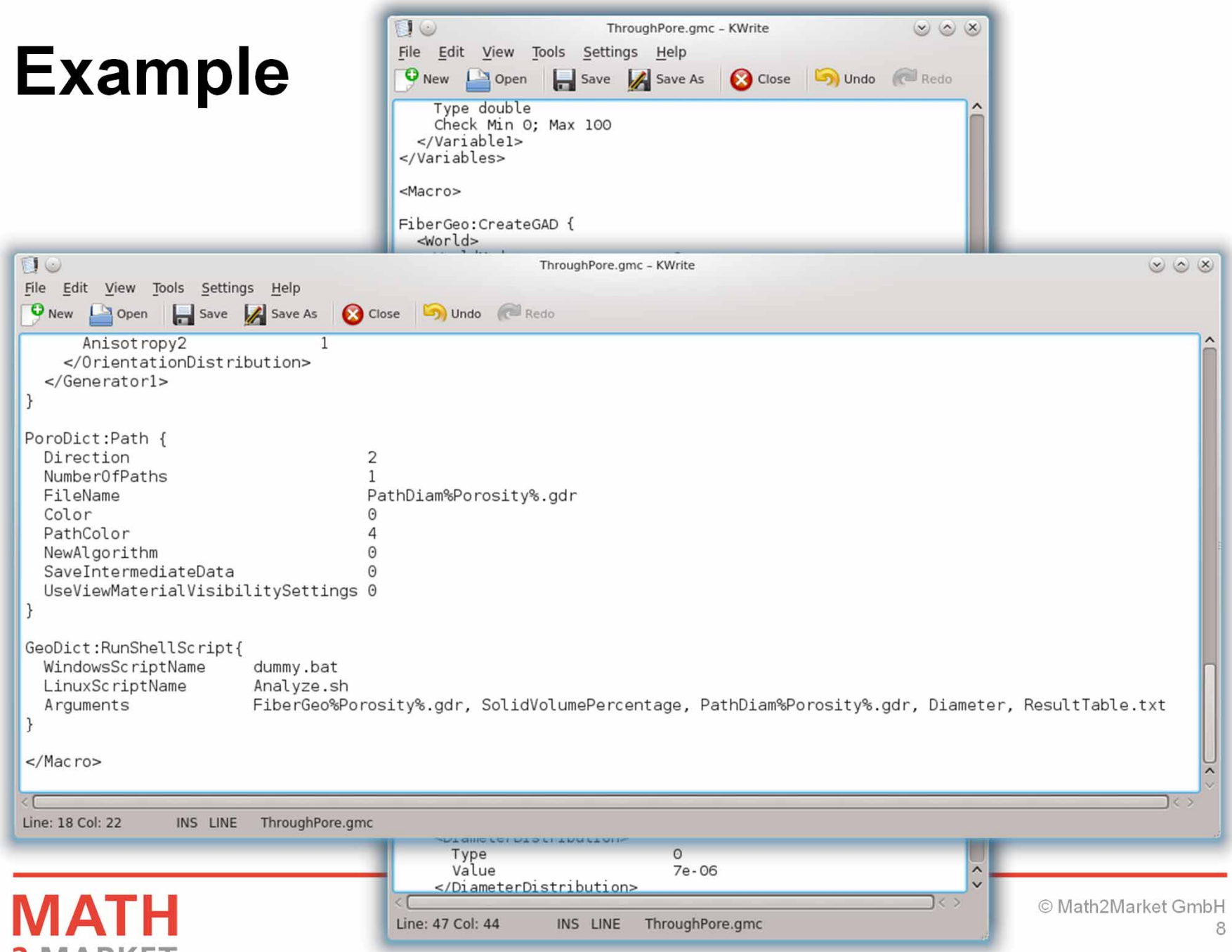
- Porosity (or solid volume fraction)

First step: record macro with FiberGeo:Create and PoroDict:PercolationPath



MATH 2 MARKET

Example



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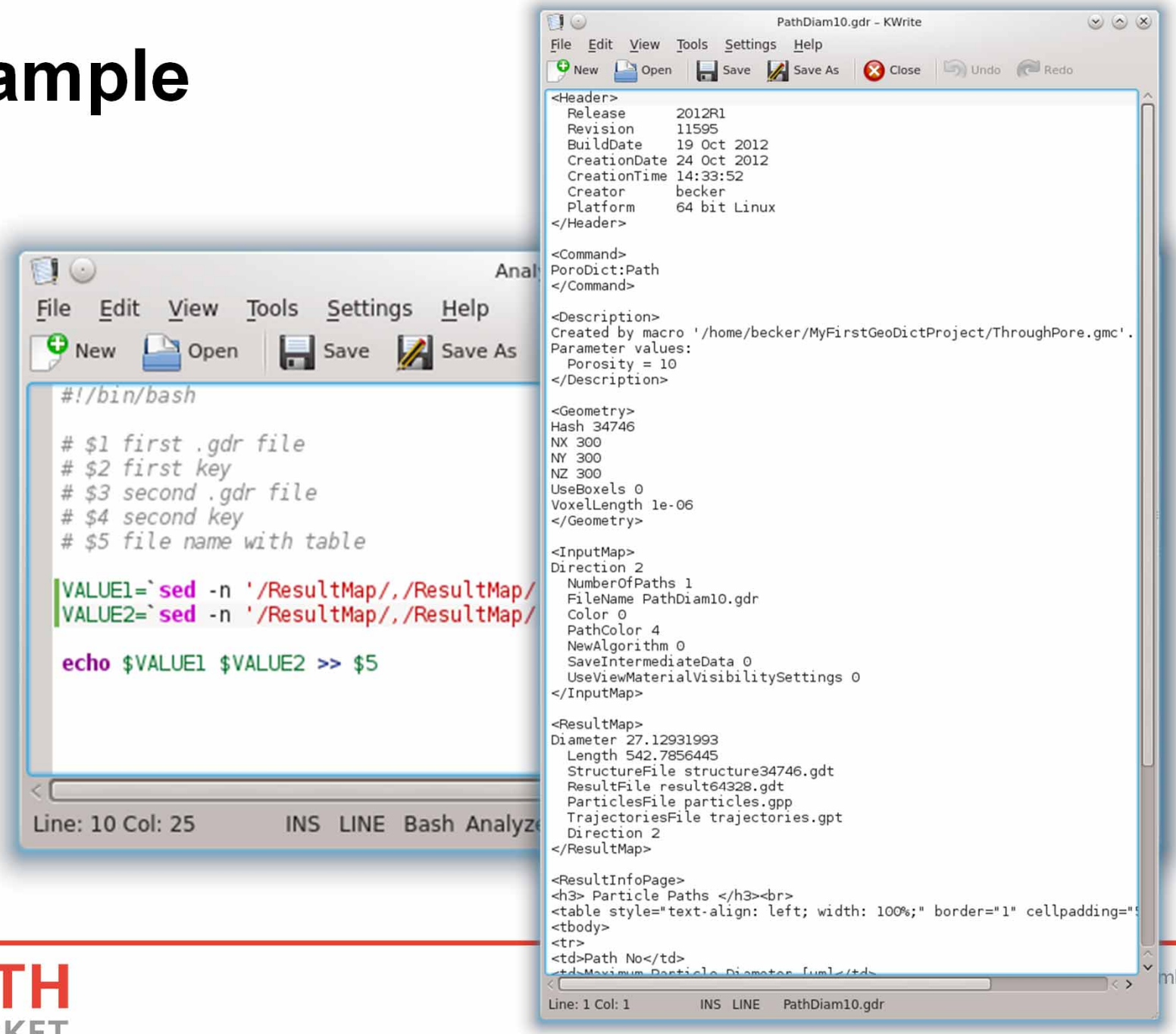
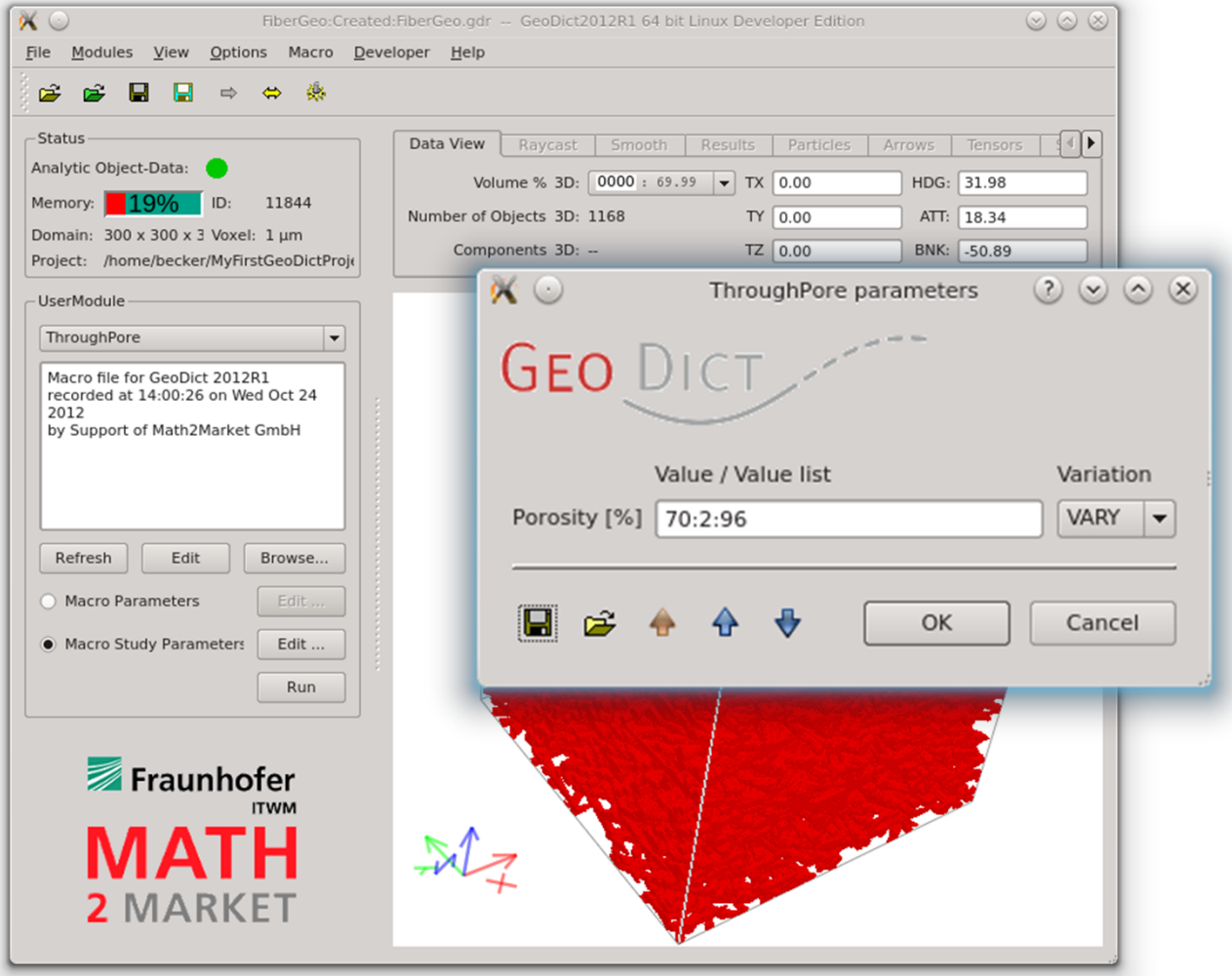
Example

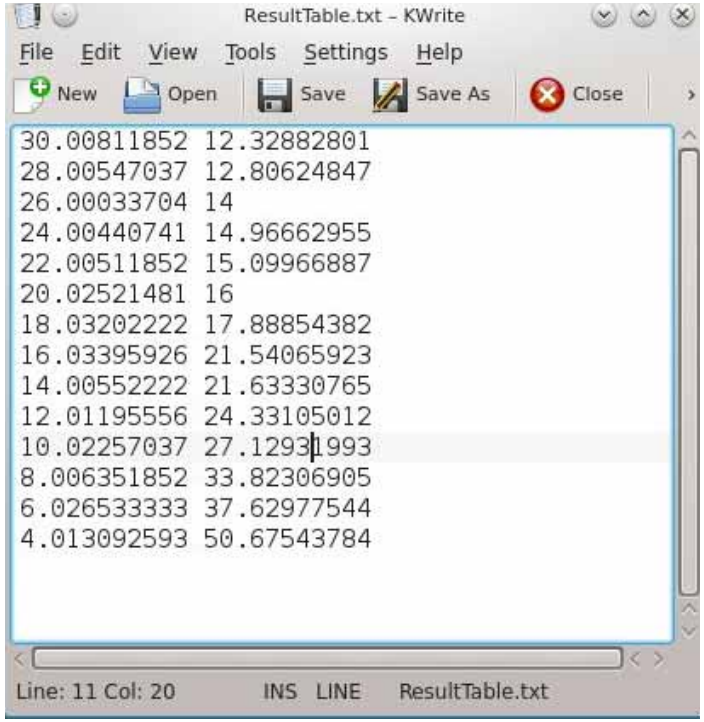

PathDiam10.gdr – KWrite
File Edit View Tools Settings Help
New Open Save Save As Close Undo Redo
<Header>
Release 2012R1
Revision 11595
BuildDate 19 Oct 2012
CreationDate 24 Oct 2012
CreationTime 14:33:52
Creator becker
Platform 64 bit Linux
</Header>
<Command>
PoroDict:Path
</Command>
<Description>
Created by macro '/home/becker/MyFirstGeoDictProject/ThroughPore.gmc'.
Parameter values:
Porosity = 10
</Description>
<Geometry>
Hash 34746
NX 300
NY 300
NZ 300
UseBoxels 0
VoxelLength 1e-06
</Geometry>
<InputMap>
Direction 2
NumberOfPaths 1
FileName PathDiam10.gdr
Color 0
PathColor 4
NewAlgorithm 0
SaveIntermediateData 0
UseViewMaterialVisibilitySettings 0
</InputMap>
<ResultMap>
Diameter 27.12931993
Length 542.7856445
StructureFile structure34746.gdt
ResultFile result64328.gdt
ParticlesFile particles.gpp
TrajectoriesFile trajectories.gpt
Direction 2
</ResultMap>
<ResultInfoPage>
<h3> Particle Paths </h3>
<table style="text-align: left; width: 100%;" border="1" cellpadding="
<tbody>
<tr>
<td>Path No</td>
Line: 1 Col: 1 INS LINE PathDiam10.gdr
File Edit View Tools Settings Help
New Open Save Save As
#!/bin/bash
# $1 first .gdr file
# $2 first key
# $3 second .gdr file
# $4 second key
# $5 file name with table
VALUE1=`sed -n '/ResultMap/,/ResultMap/
VALUE2=`sed -n '/ResultMap/,/ResultMap/
echo $VALUE1 $VALUE2 >> $5
Line: 10 Col: 25 INS LINE Bash

Example



Example

- Creates FiberGeo70.gdr ... FiberGeo96.gdr
- Creates PathDiam70.gdr ... PathDiam96.gdr
- ResultTable.txt



Cluster Usage

Record the macro on your desktop (with GUI):

1. Start macro recording
2. Choose project folder
3. Load or generate the structure model
4. Record only: FlowDict/FilterDict etc

Edit the macro:

- Check file path in ChangeProjectFolder (should be absolute)
- Check that file paths in other commands are ok (should be relative)
- Check that NumberOfProcesses are ok in ****Dict commands

Run the macro on the cluster (without GUI).

Example: *hercules* Cluster at ITWM

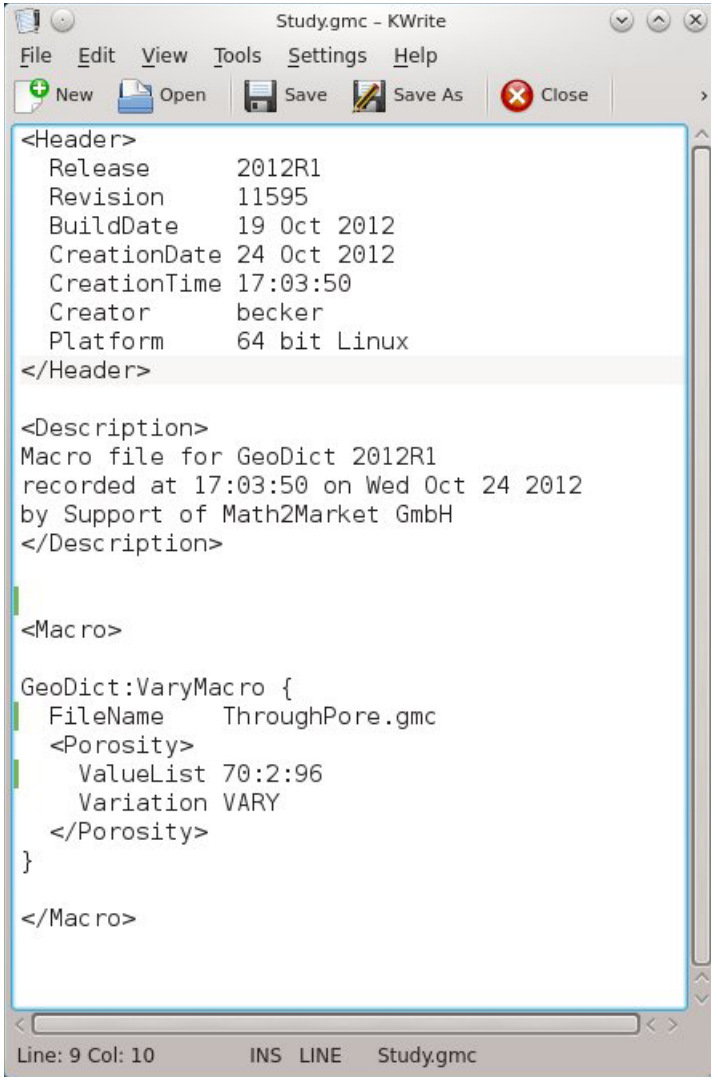
1. Have GeoDict and MPI installed on Cluster,
   adjust path to mpiexec in GD2012_externals.sh file

2. Create a file geodict.sh in ~/bin/ (directory should be in $PATH):
   /u/herc/becker/GeoDict2012R1Linux64/geodict2012 -s $MACRO

3. Submit jobs to batch queue, e.g.:
   qsub -l nodes=8:ppn=4,walltime=24:00:00
    -v MACRO=/u/herc/becker/test/testmacro.gmc geodict.sh

Tips and Tricks

- Running a parameter study is a command (this is recursive!)
- If you do not know the syntax: record it!
- Have a look at the example *.gmc files provided with the UserModule



Future Developments

1. Master *.gdr file
   (Running a parameter study is a command and could produce a *.gdr file)
   - knows variables used in study
   - knows all *.gdr files produced in study (and can relate them to variables)

2. Analyzing this *.gdr with GeoDexcel
   - Aim: create charts like
     Fiber diameter - filter efficiency
     Porosity - permeability

Thank You!