UNIVERSITY OF TWENTE.

ITC

Department of Applied Earth Sciences

Juan C. Afonso[1,2,3]

[1] Faculty of Geo-Information and Earth Observation (ITC), University of Twente, Enschede, The Netherlands.

[2] Department of Earth and Environmental Sciences, Macquarie University, Sydney, Australia.

[3] Department of Ocean Science and Engineering, Southern University of Science and Technology, Shenzhen 518055, China

Email: j.c.afonso@utwente.nl

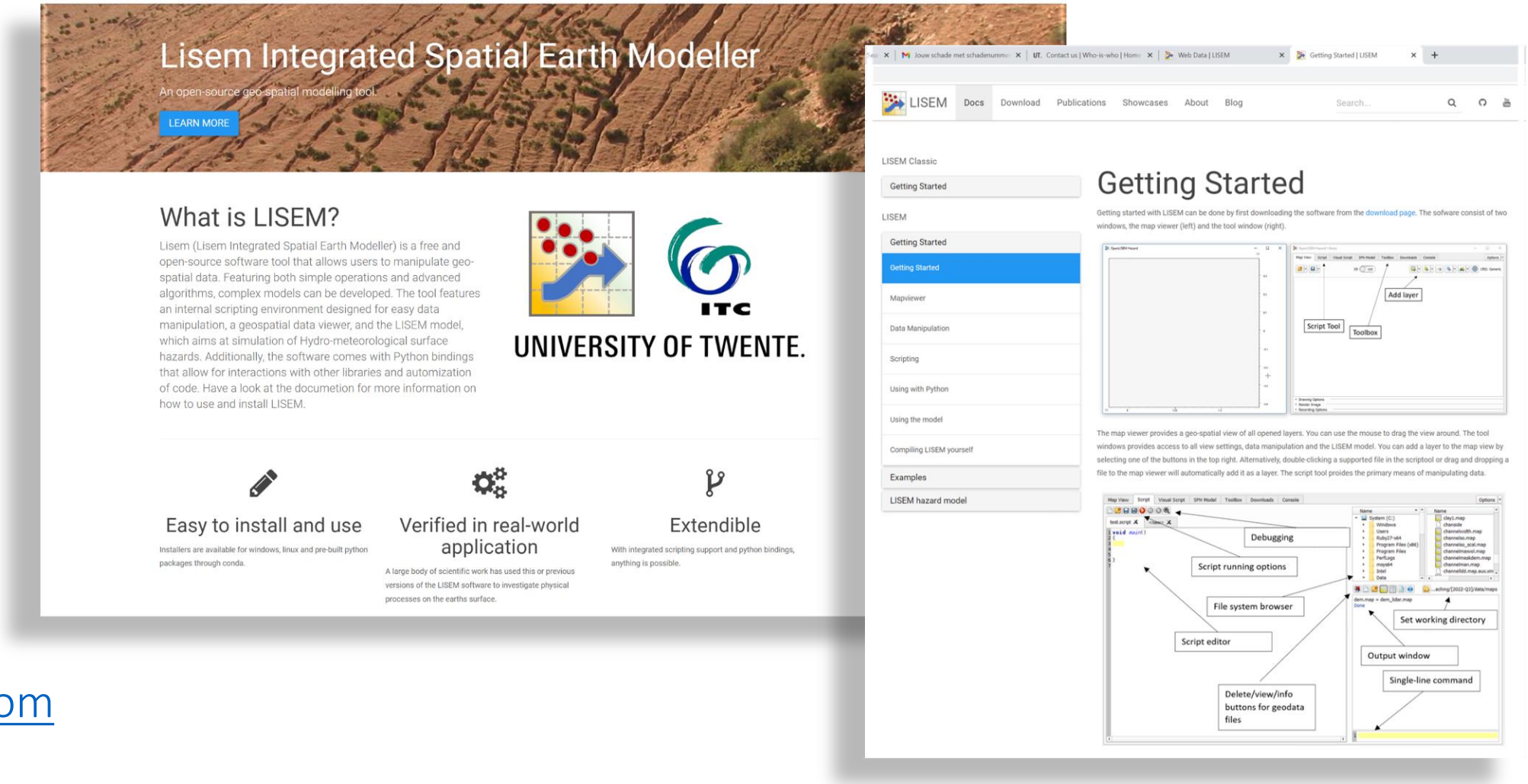
Website: https://www.juanafonso.com

Department of Applied Earth Sciences

- Members of AES have a long tradition in the development of software packages for processing, modelling and manipulating geospatial and hyperspectral datasets for a number of applications (e.g. natural hazards, exploration)

LISEM

Victor Jetten
Bastian van den Bout



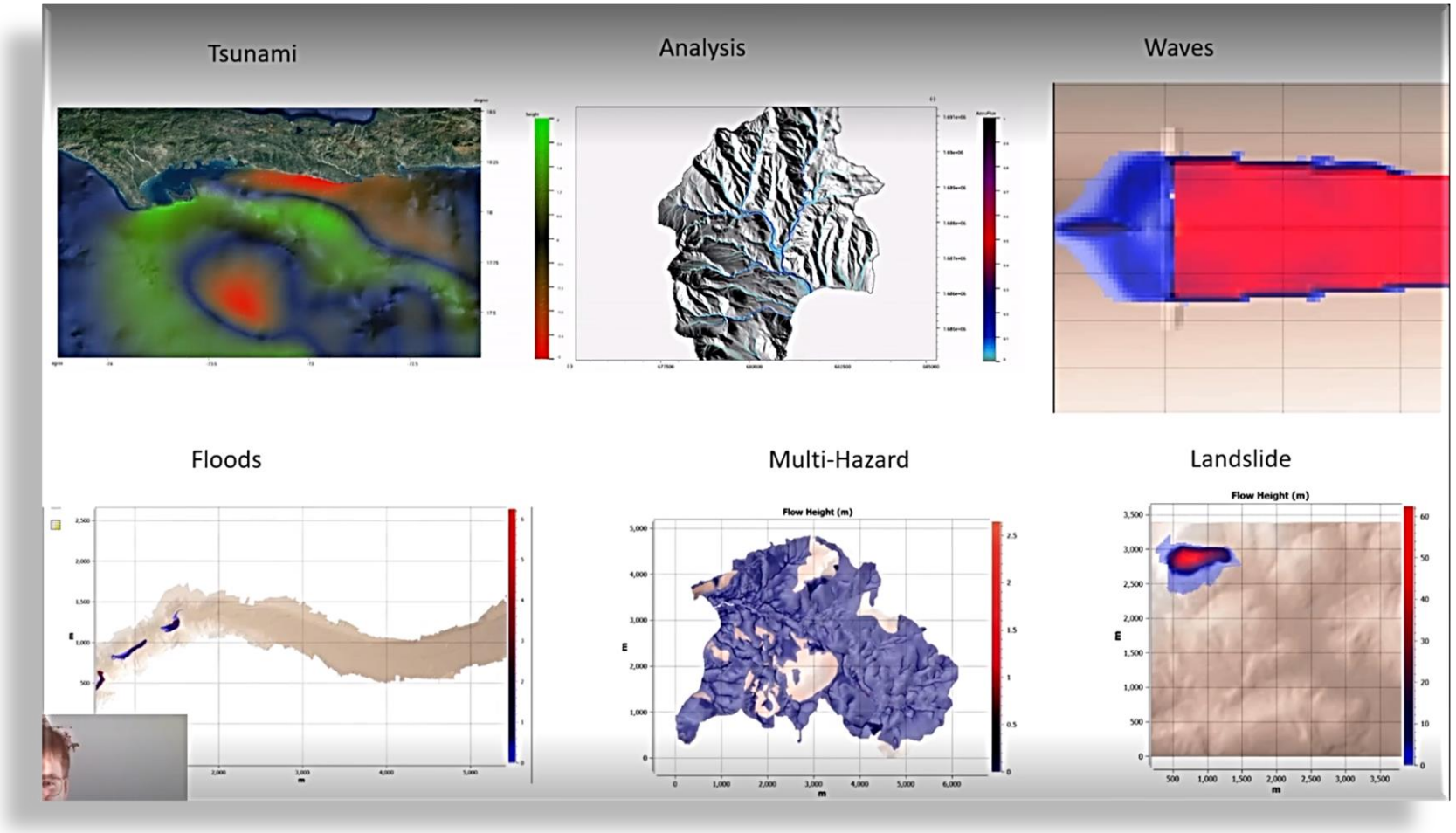
www.lisemmodel.com

Department of Applied Earth Sciences

- Members of AES have a long tradition in the development of software packages for processing, modelling and manipulating geospatial and hyperspectral datasets for a number of applications (e.g. natural hazards, exploration)

LISEM

Victor Jetten
Bastian van den Bout



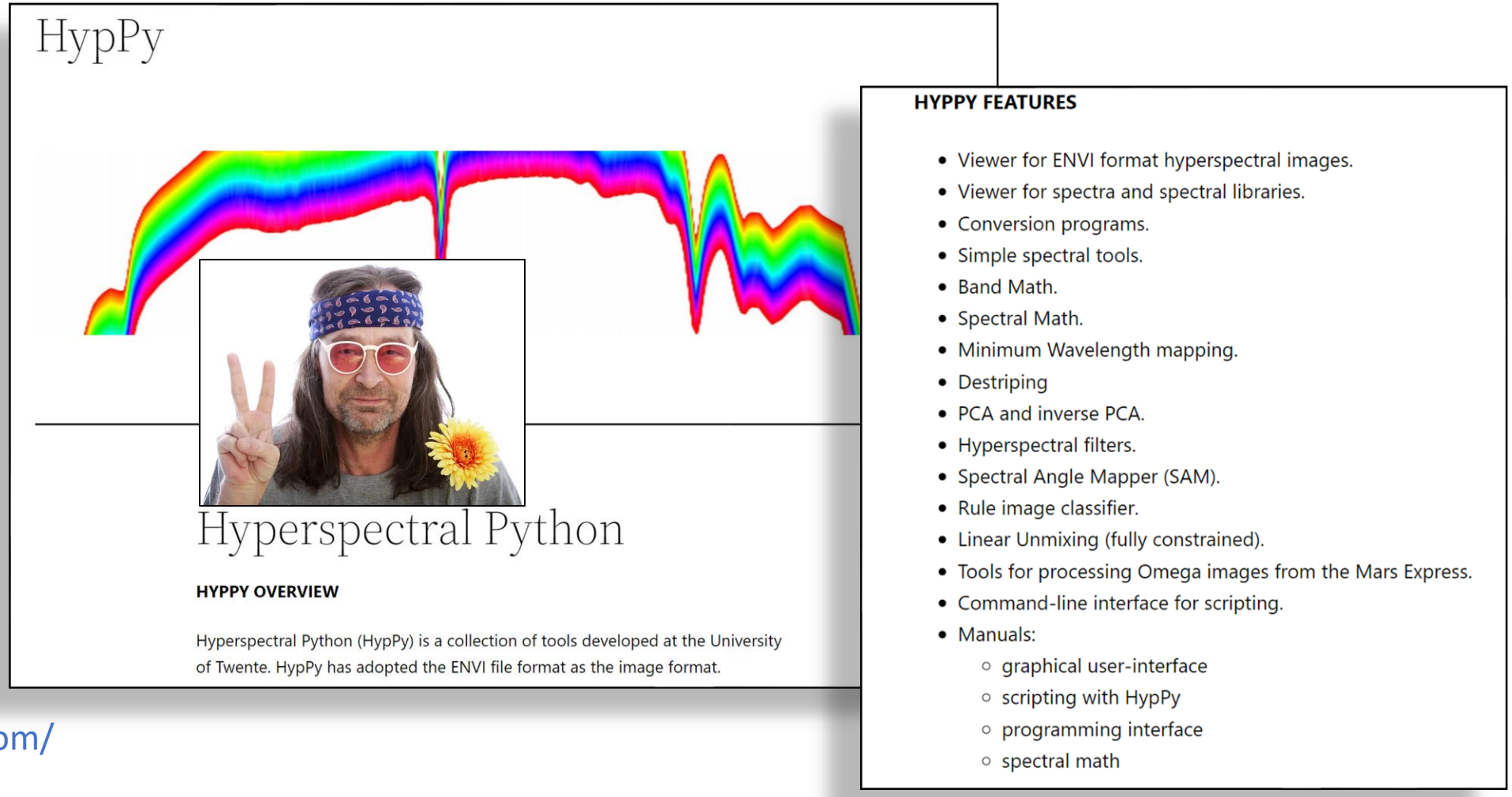
www.lisemmodel.com

Department of Applied Earth Sciences

- Members of AES have a long tradition in the development of software packages for processing, modelling and manipulating geospatial and hyperspectral datasets for a number of applications (e.g. natural hazards, exploration)

HypPy

Wim Bakker
Chris Hecker
Harald van der Werff
Freek van der Meer
Jelmer Oosthoek
Frank van Ruitenbeek



http://hyppy.byethost18.com/

Department of Applied Earth Sciences

- Members of AES have a long tradition in the development of software packages for processing, modelling and manipulating geospatial and hyperspectral datasets for a number of applications (e.g. natural hazards, exploration)

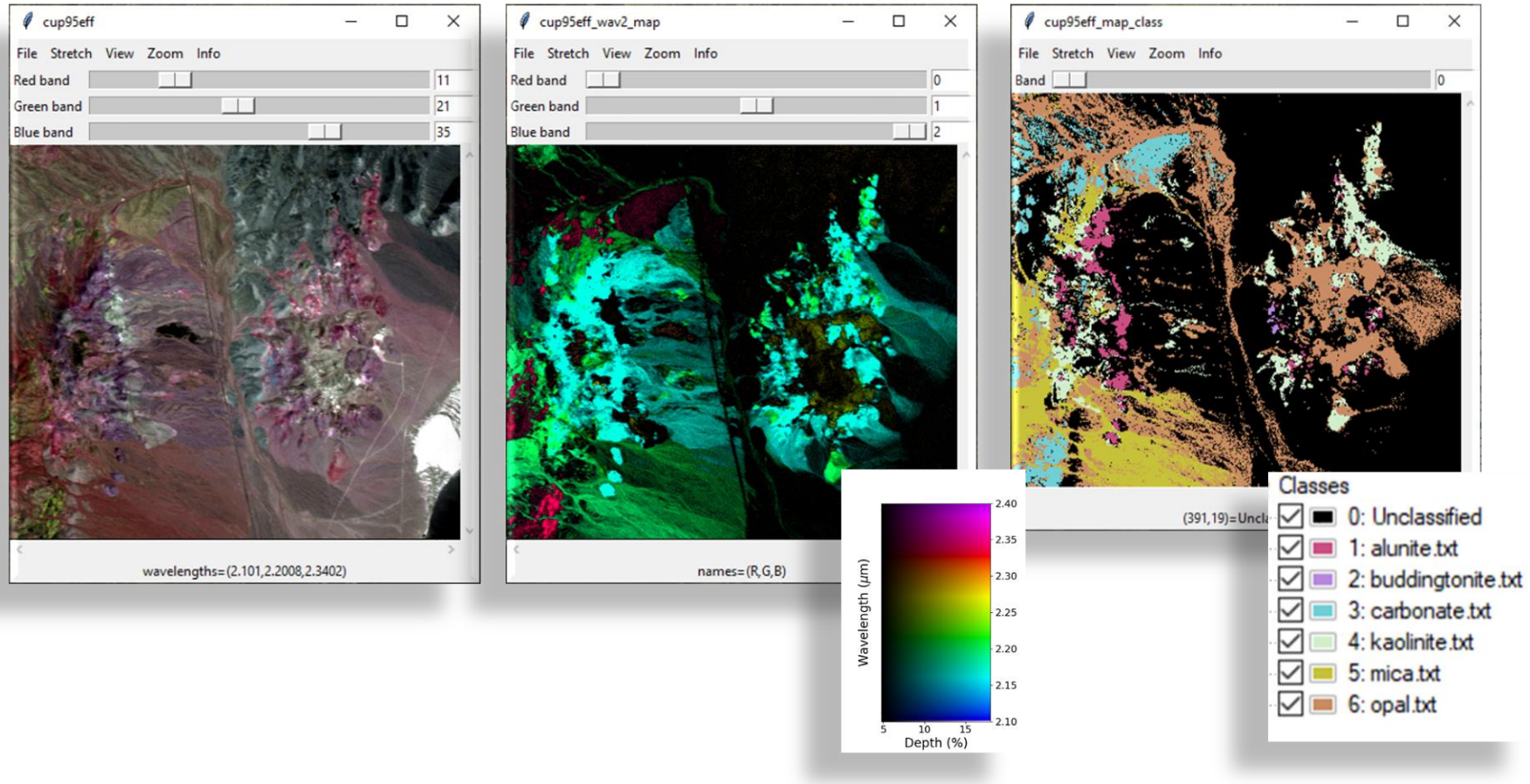
HypPy

Wim Bakker
Chris Hecker
Harald
Freek van der Meer
Jelmer Oosthoek
Frank van Ruitenbeek

Hyperspectral Image

Wavelength Map

Classified Image



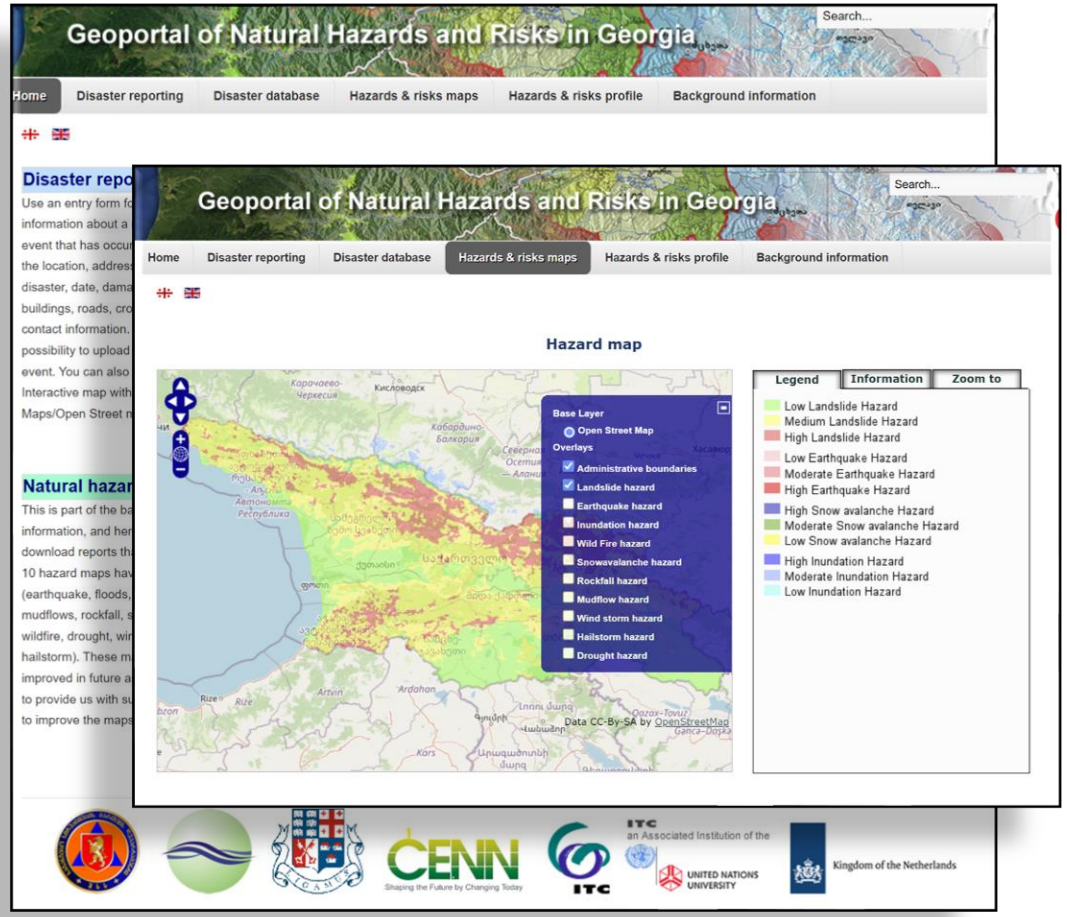
http://hyppy.byethost18.com/

Department of Applied Earth Sciences

- Members of AES have a long tradition in the development of software packages for processing, modelling and manipulating geospatial and hyperspectral datasets for a number of applications (e.g. natural hazards, exploration)

Open Source Portals for Risk Managment

hosts risk management data and information accessible to stakeholders to facilitate analysis, research, greater awareness of risk management and climate change adaptation

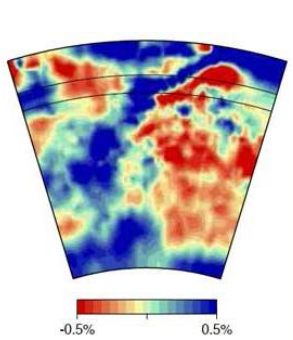


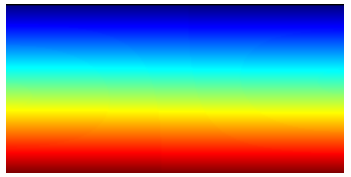
Department of Applied Earth Sciences

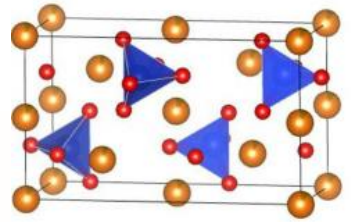
- Members of AES have a long tradition in the development of software packages for processing, modelling and manipulating geospatial and hyperspectral datasets for a number of applications (e.g. natural hazards, exploration)

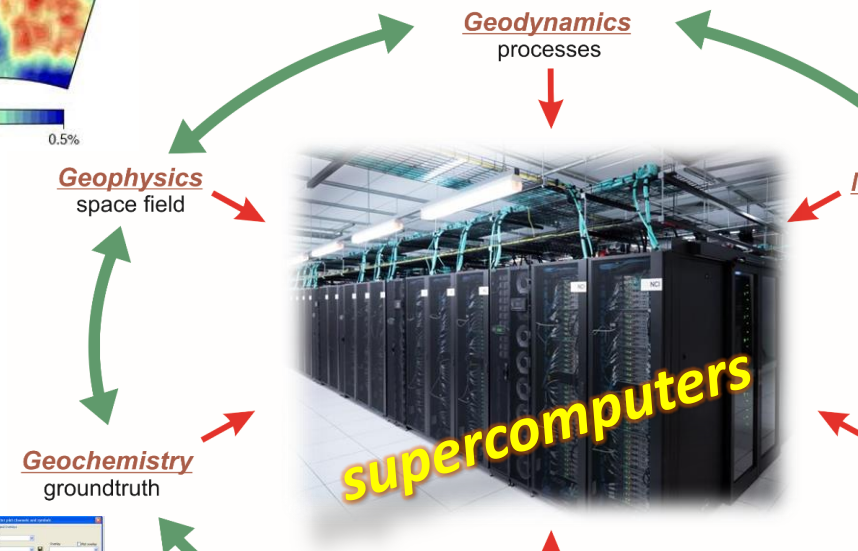
LitMod suite

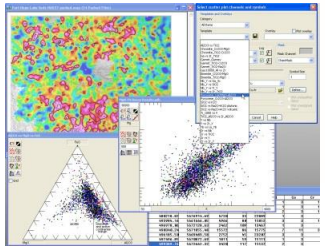
J.C. Afonso
M. Van der Meijde
I. Fadel

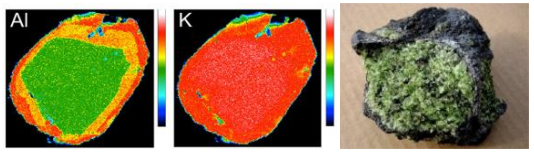


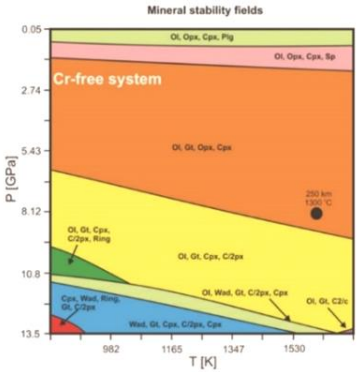






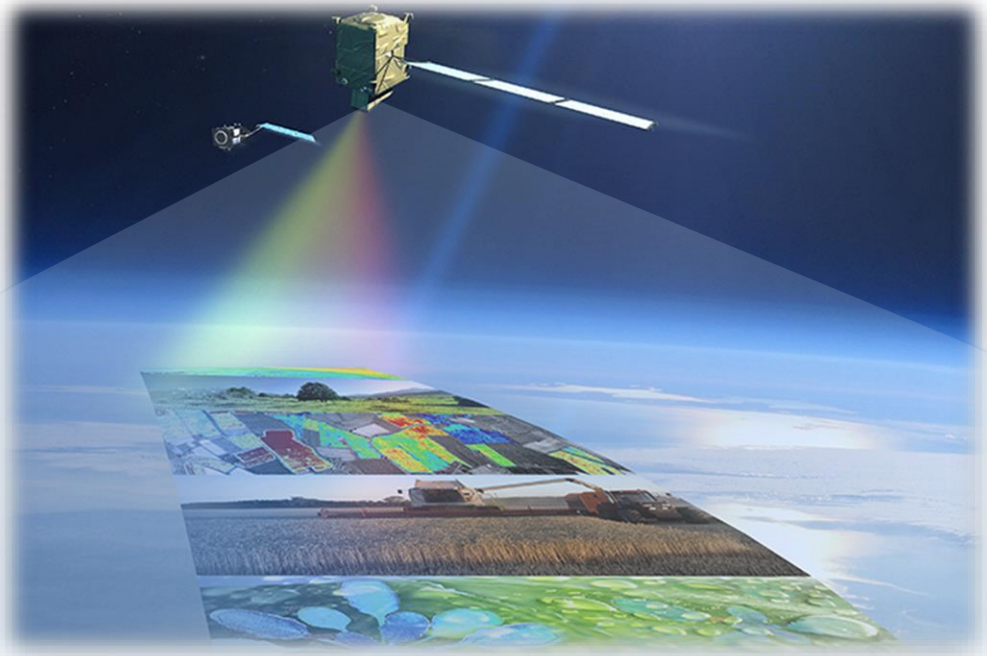




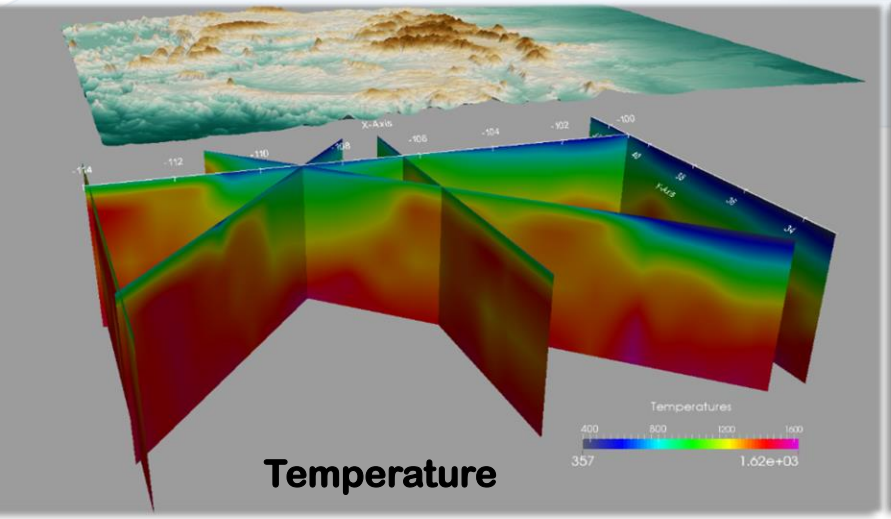


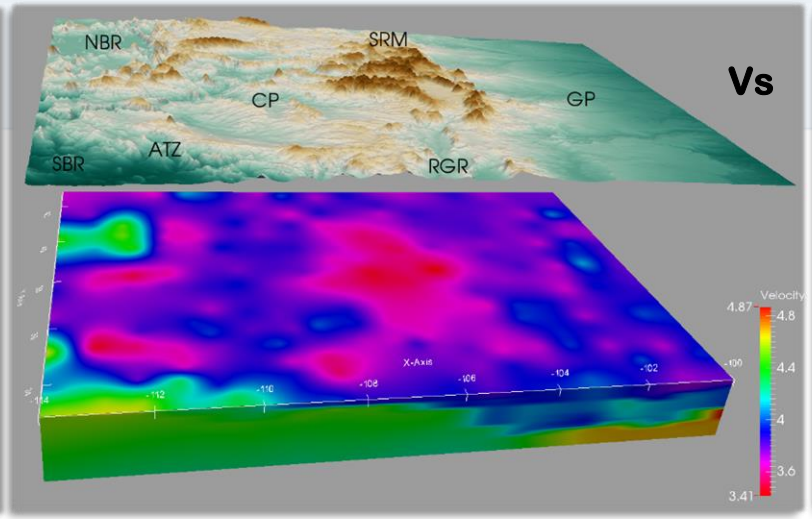
Department of Applied Earth Sciences

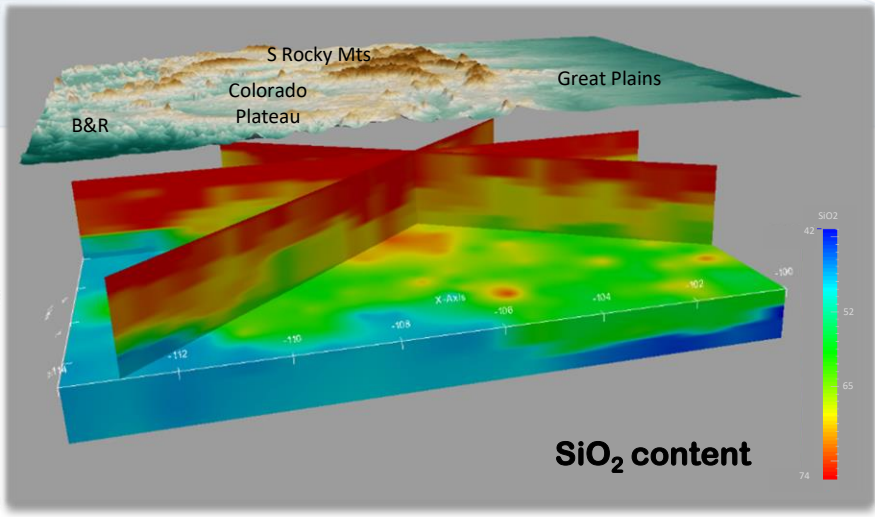
Multi-Observable Thermochemical Tomography (MTT)



State-of-the-art technique to map the entire thermochemical architecture of the crust and lithosphere using *multiple satellite and land-based datasets, probabilistic inverse theory and machine learning*.



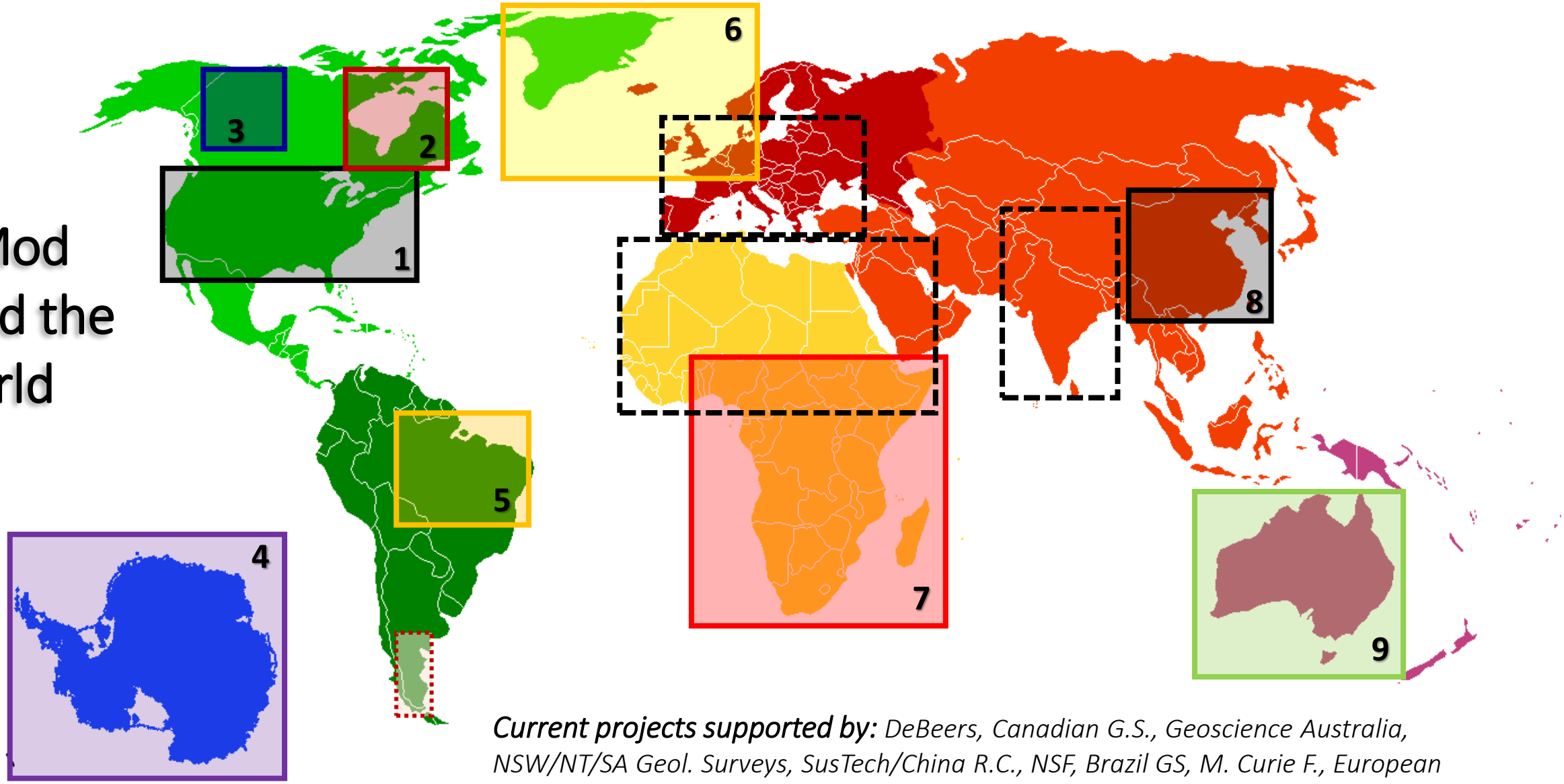




UNIVERSITY OF TWENTE. ITC

Department of Applied Earth Sciences

LitMod around the world

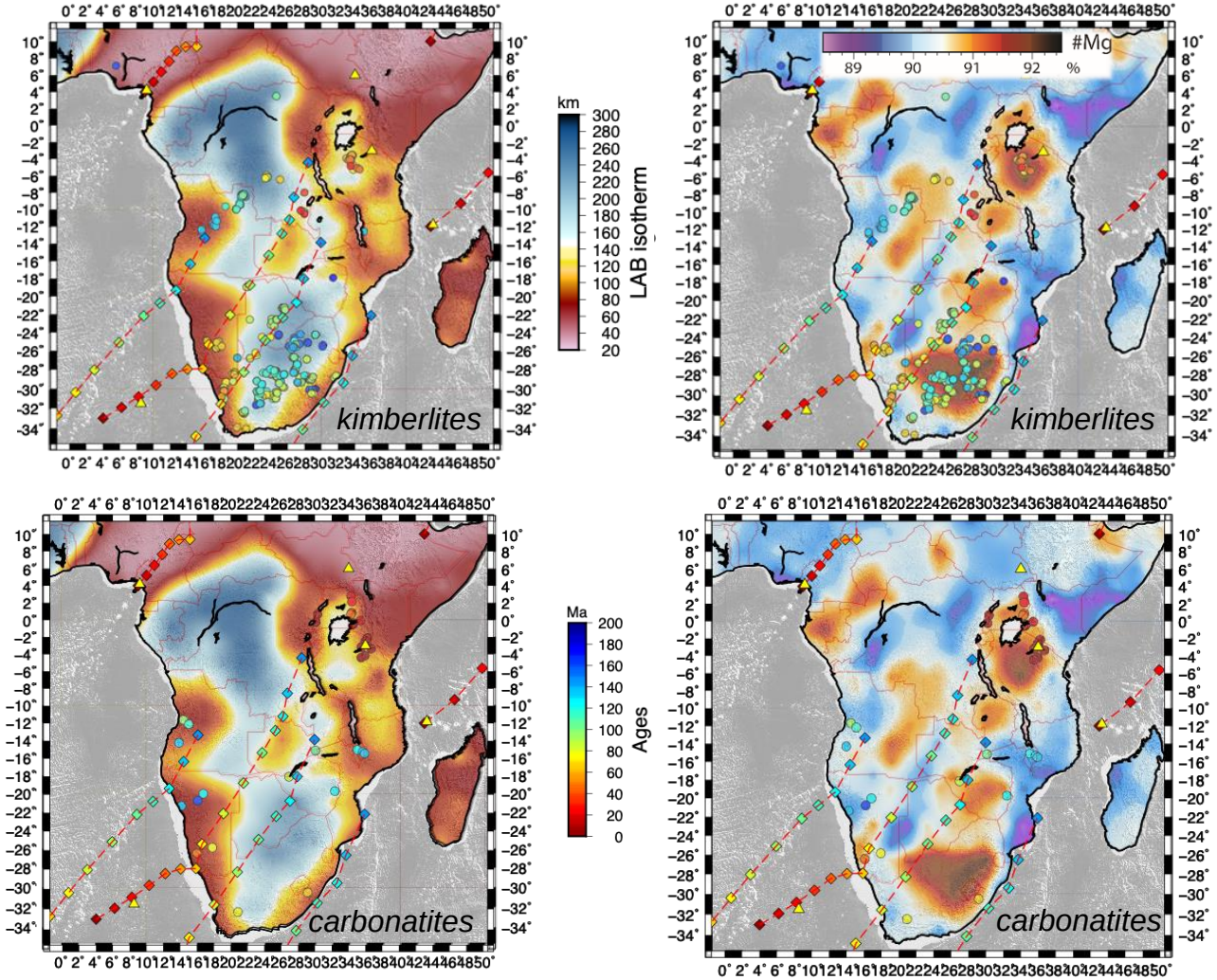


Current projects supported by: *DeBeers, Canadian G.S., Geoscience Australia, NSW/NT/SA Geol. Surveys, SusTech/China R.C., NSF, Brazil GS, M. Curie F., European Space Agency, Clean Air Task Force, ARC, Canadian R.C. and others…*

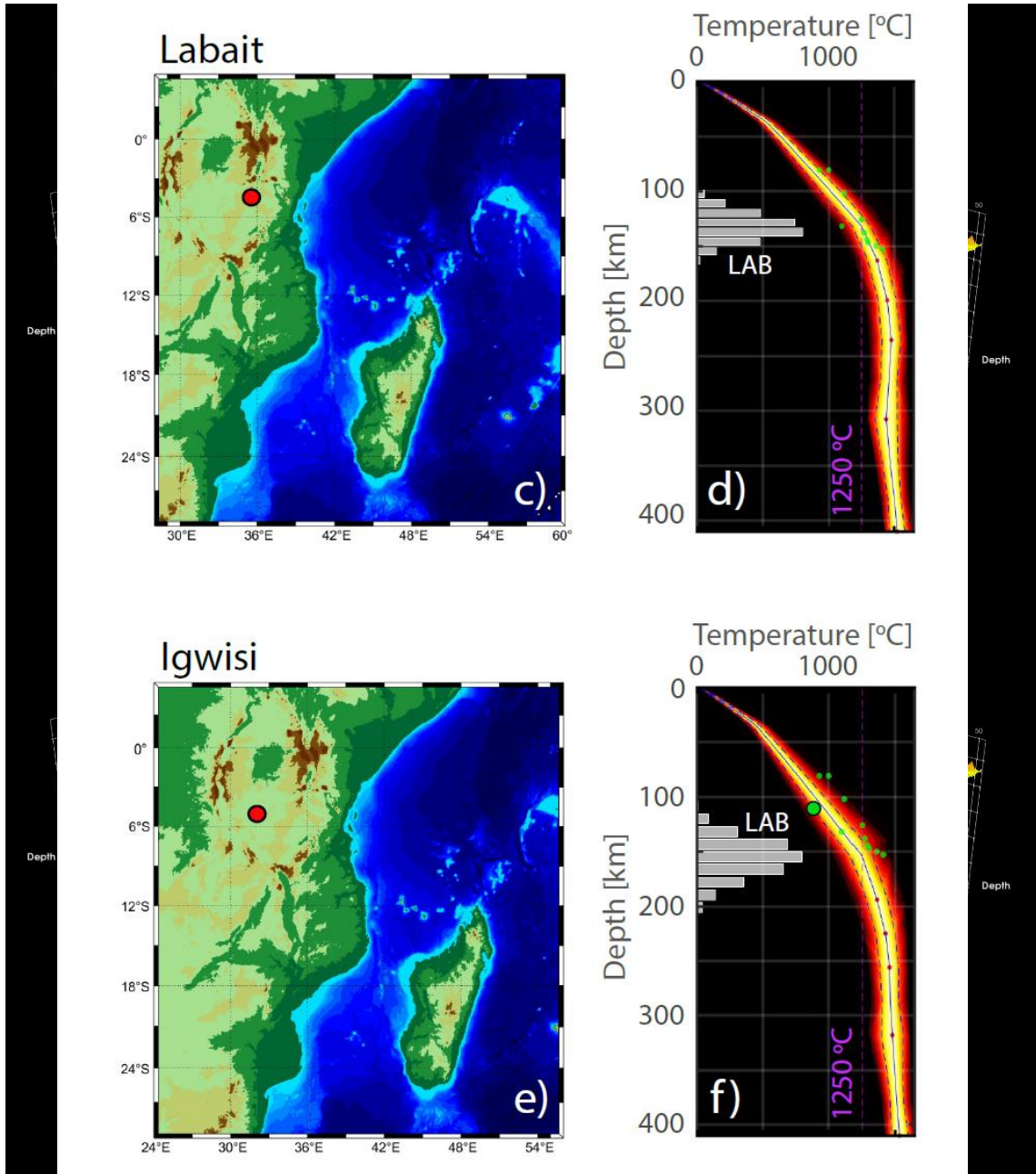
UNIVERSITY OF TWENTE. ITC

Department of Applied Earth Sciences

Central/southern Africa as an example…



Themo-chemical model from surface down to 400 km depth.

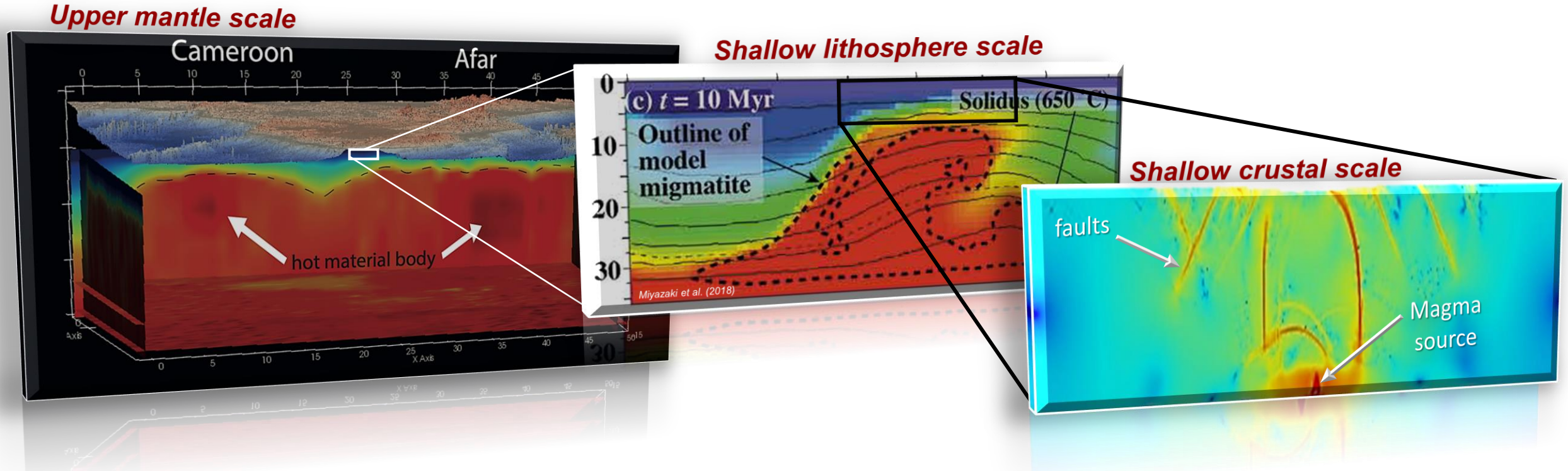


What can we do then for exploration and assessment of geothermal resources at global, regional and local scales?

" Reconstruction of the geologic history of a long-lived magma-hydrothermal system … requires integration of rock-preserved evidence ….with an ensamble of ***increasingly complex computations*** *based on geochemical transport theory…*

…The first step is the construction of a ***reference state*** *model for pure conductive cooling…"*

Denis L. Norton & J. Hulen (2001)



Department of Applied Earth Sciences

- ***Multi-method approach*** *(Multiple-Try-Metropolis, Parallel interacting chains, Tempering, Block Sampling, Adaptation, domain splitting, DE, among others)*

Manual (man pages)

```
      -misfitmod [STRING]
             Procedure to compute misfit computation. Example: -misfitmod xi2
             . Available options:

             L2     - L2 norm with sigmas equal to  data  uncertainty:  (obs-
                    calc)^2/sigma.

             xi2    -  [default]  Chi-squared normalised to the observations:
                    (obs-calc)^2/|obs|.

      -misfitrscl [NUMBER]
             Set number of MCMC steps after which individual weights of  mis-
             fit components will be rescaled. Default is -1 (values <= 0 mean
             never rescale).

OPTIONS: PARALLEL TEMPERING
      -ptadaptive [NUMBER]
             Adjust PT temperatures dynamically using Vousden et  al.  (2002)
             approach. Use -ptadaptive 1 to switch it on and -ptadaptive 0 to
             turn it off [default].

      -ptmixdelay [NUMBER]
             Delay (in MCMC steps)  before  PT  swapping  (mixing  of  states
             between  individual  chains)  begins. Default value is -1 (start
             mixing immediately).

      -pttladder [STRING]
             Initial PT temperature distribution. Example: -pttladder power10
             . Available options:
```

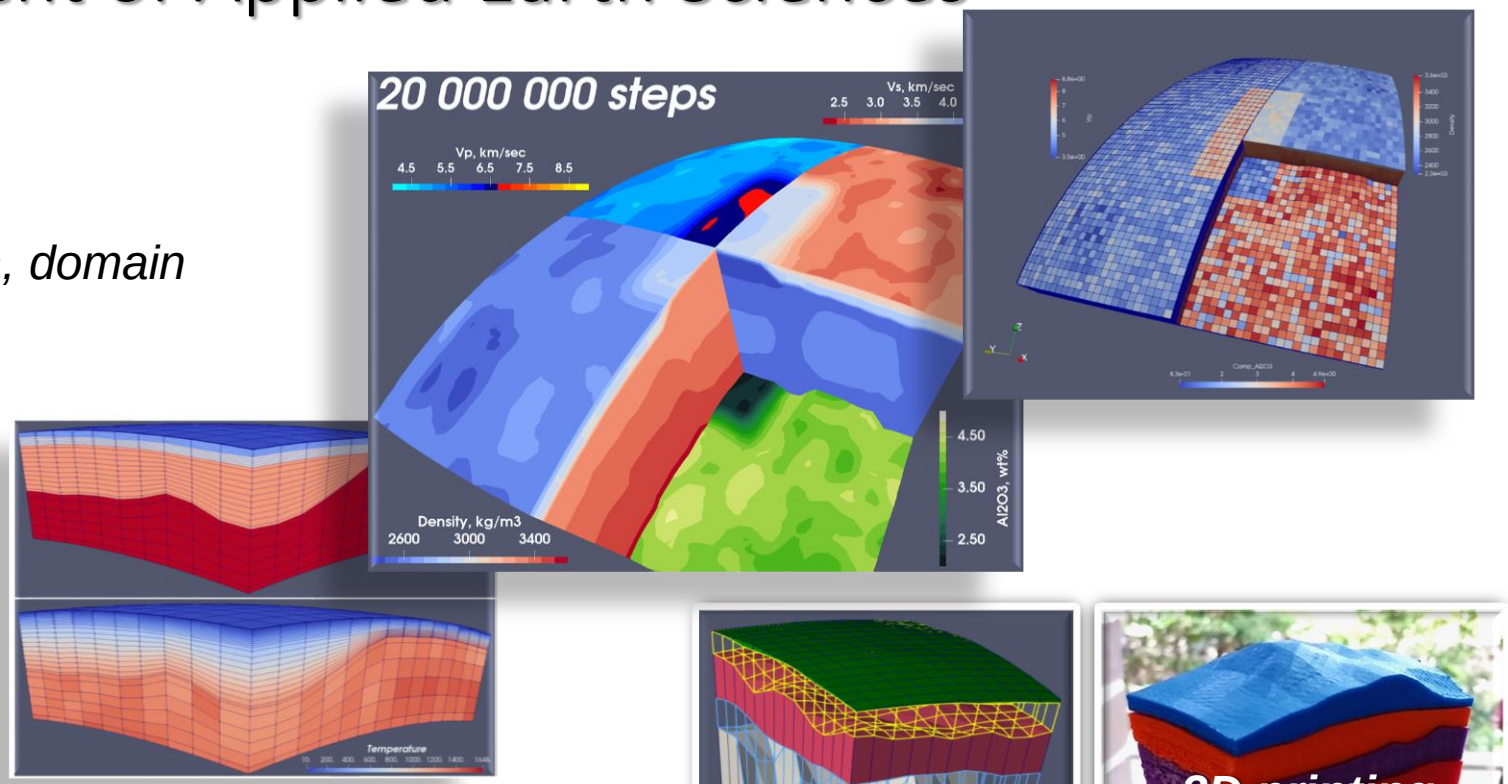
```
          ************************************************
          *                                              *
          *          >>>>  LitMod)4INV v2.0  <<<<        *
          *                                              *
          *                  Written by:                 *
          *                Juan C. Afonso                *
          *                                              *
          *                 Contributors:                *
          *             I. Fomin, F. Salajegheh,         *
          *           N. Rawlinson, J.A.D. Connolly      *
          *                                              *
          * Macquarie University, Australia              *
          * Copyright J.C. Afonso (GNU)                  *
          * Build from Feb 25 2019 14:48:45              *
          *                                              *
          ************************************************


------------------------------------------------------------
LitMod checks the runtime environment before starting...
MPI hydra started without OpenMP directives.
MPI datatypes: real is 64-bit (gravity uses 64-bits) and integer is 32-bit
------------------------------------------------------------
LitMod is parsing command line arguments...
Started with the following command:
./LITMOD.i -i input_inversion -o output -w 2 -misfit 100 -nswap 4 -ptt1chains 4
-nmcmc 6 -mtmis 1 -pttmhmtm 1.5
HDF5 output will be written.
Looking for model input files in folder: input_inversion
Writing outputs in folder: output
------------------------------------------------------------
LitMod started on 8 core(s)
Parallel Tempering environment is setting...
Core #0 (PID3717) with PT-temperature 1.0 (Metropolis-Hastings)
Core #1 (PID3718) with PT-temperature 1.0 (Metropolis-Hastings)
Core #2 (PID3719) with PT-temperature 1.0 (Metropolis-Hastings)
Core #3 (PID3720) with PT-temperature 1.0 (Metropolis-Hastings)
Core #4 (PID3721) with PT-temperature 3.2 (Multiple-Trial Metropolized
Independence Sampler) holds 2 computational samplers
Core #5 (PID3722) with PT-temperature 3.2 is sampler #1 of chain 5
Core #6 (PID3723) with PT-temperature 10.0 (Multiple-Trial Metropolized
Independence Sampler) holds 2 computational samplers
Core #7 (PID3724) with PT-temperature 10.0 is sampler #1 of chain 6
Ordered Tmax value is     10.00 without adaptive tempering
Obtained Tmax value is 10.00 ; Tmin value is 1.00
Geometric sequence used to set PTT
Performing 2 swaps (4 MCMC) per step with probability 100%
Swapping randomly selected chains despite their PT Temperatures
Multiple-Trial Metropolized Independence Sampler tries 10 proposals
OpenMP parallelism for Multiple-Try Metropolis switched OFF
------------------------------------------------------------
```

```
LitMod reads input files...
   reading input_inversion/header.dat ... successfully
   reading input_inversion/structure.dat ... successfully
 ------------------------------------------------------------
 WARNING CRITICAL: Crustal densities are less than 2.16 (halite) or more than
 5.0 g/cm3!
 ------------------------------------------------------------
 ------------------------------------------------------------
 WARNING: LAYER 1 IS THINNER THAN 20 m
 ------------------------------------------------------------
   reading input_inversion/observations.dat ... successfully
   reading TZ and lower mantle data from input_inversion/startmod.dat ...
successfully
 Perple_X reads input files...
   opening ./perplex/inversion.dat
   opening ./perplex/stx08ver.dat
   opening ./perplex/solution_model.dat
   opening ./perplex/perplex_option.dat
 All the model inputs were read!
 ------------------------------------------------------------
 LitMod tries to share domain with size 14 by 10 between 8 CPUs each holding at
least 1 column(s)
 - 4 independent blocks with size 7 by 5 found during Common Divider Grid
Reductions
 - 2 independent blocks in each CDGR subgrid found during Coprime Grid Reduction
 - All the available CPUs will be used to initialize the domain
 ------------------------------------------------------------


 ------------------------------------------------------------
 Simulation mode: solving inversion with MCMC
      Performing 1e6 MCMC steps using uniformly distributed proposals
 ------------------------------------------------------------
 Grid parameters:
   Longitude: 14 nodes from -10.0 to   3.0
   Latitude:  10 nodes from -10.0 to  -1.0
   Grid spacing          dx, dy (degree):  1.000  1.000
         approx    dx1, dx2, dy, dz (km):  110.9 111.3 110.6 2.0
   Thermodynamic nodes:                    16
   Computation nodes:                      194
   Compositional layers:                   6
   Total number of nodes:                  18432
   Total number of property layers:        4
 ------------------------------------------------------------


 ------------------------------------------------------------
                     DOMAIN INITIALIZATION
                       max, min, average

   Crustal properties
       Density, kg/m3:          3125.00  2100.00  2697.64
```

UNIVERSITY OF TWENTE. ITC

Department of Applied Earth Sciences

- ***Multi-method approach*** *(Multiple-Try-Metropolis, Parallel interacting chains, Tempering, Block Sampling, Adaptation, domain splitting, DE, among others)*
- ***Portability, outputs and data mining***
- *Library of benchmarks/examples*



HDF5 *output formats for robust and easy visualization and data mining.Direct output for 3D printing and movies*