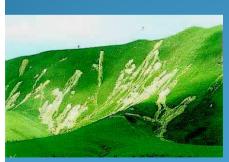
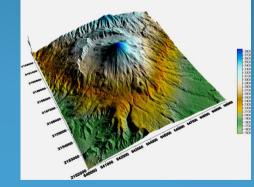
# Differential Evolution (DE) algorithms for optimal solutions search: micromacro scale applications in Earth Sciences

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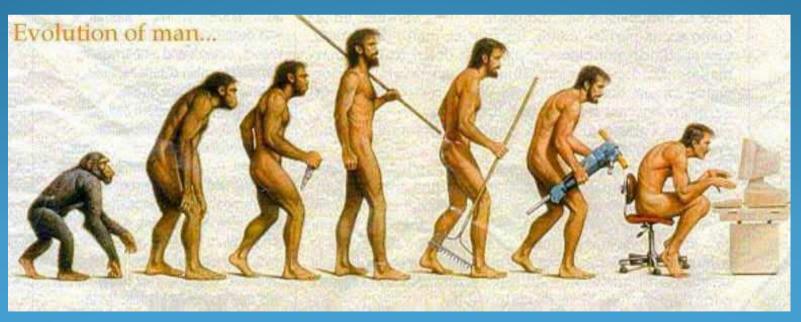
This seminary have as subject the optimization techniques based on a class of genetic algorithm named DIFFERENTIAL EVOLUTION and their application in the context of earth sciences research.

#### synopsis

- 1) Optimization and general concepts in real world and earth sciences.
- 2) Differential Evolution algorithms and for application in earth sciences research fields.
- 3) Presentation of examples of application in various fields (micro and macro scale):
  - •Particle shape analysis.
  - Sedimentology,
  - Hydrology,
  - •Stability of natural slopes,
  - Volcano's DTM analysis

Optimization and evolution ....
...Or how to obtain the BEST RESULT
(e.g. maximum food production) with a MINIMUM
COST in terms of resources, time, energy....etc.

The human being aspires to the best possible performance. Both individuals and enterprises are looking for optimal - in other words, the best possible - solutions for situations or problems they face.



Optimization is fundamental in technological processes and in the progress of science which is the product of a long way of trials and errors in experiments, theories and models.

Typical examples of current optimization algorithms applications in technology include:

- •Protein structure prediction (minimize the energy/free energy function)
- •Traveling salesman problem and optimal circuit design or network (minimize the path length)
- •Chemical engineering (e.g., analyzing the Gibbs free energy)
- •Safety verification, safety engineering (e.g., of mechanical structures, buildings)
- •Model calibration (many engineering fields..)
- •Many .. many others...

Most of these problems can be expressed in mathematical terms, and so the methods of optimization undoubtedly render a significant aid in applications in science (earth science):

- •Fitting of nonlinear models to data
- Data mining
- Data clustering
- •Inversion procedures
- •Numerical Approximation of roots of functions
- New model paradigm validation and testing
- •Image processing ...

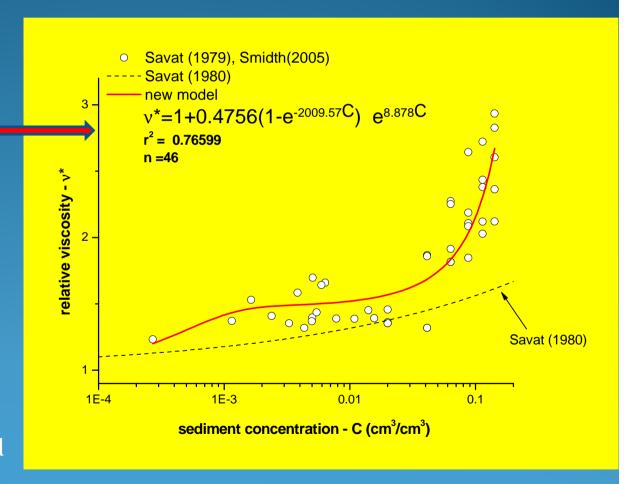
Subject of optimization procedure:

#### **Example non linear fitting**

To fit nonlinear model to data In the example we need to find 3 parameters

When the non linear function is Simple the fitting can be done With common statistical Softwares: Statistica, origin.. Matlab, excel solver .....etc.

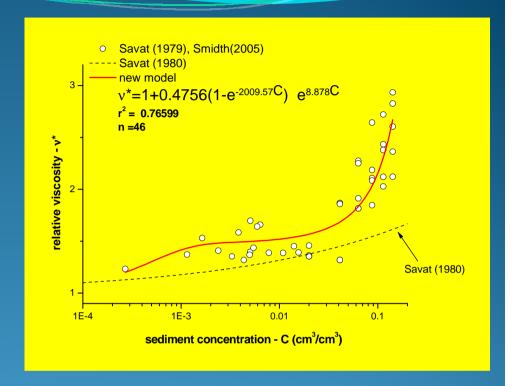
When More complex cases arise we need of special coding ... and Program



#### Goal

Minimize the sum of all the differences between the data and the assumed nonlinear model

The best performance coincide with the minimum possible of this sum of differences.



So our GOAL is to find the optimal 3 parameters in the nonlinear model that ensure the minimum possible difference with respect the data (residuals)

#### Cost or objective functions

$$obj = \sum_{i=1}^{n} (obs_i - pred_i)^2$$

Least squares

$$obj = \sum_{i=1}^{n} |obs_i - pred_i|$$

Sum of absolute deviate

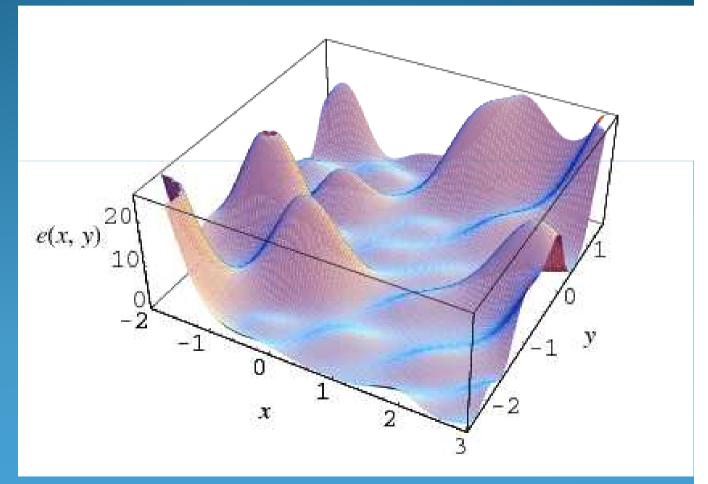
$$obj = \sum_{i=1}^{n} \frac{(obs_i - pred_i)^2}{\sigma^2_{obs}}$$

Reduced Chi square

### Dimension of the problem

In this example the OBJECTIVE function is defined by TWO PARAMETERS

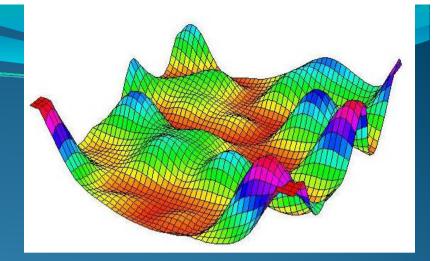
The dimension of the Problems is given by the number of parameters
That in n-dimensional Space define the Objective function



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#### Searching techniques

Algorithms designed to explore the n-dimensional surface of the OBJECTIVE function in order to find the place where the GOAL (minimum, maximum, or close to zero) is satisfied ...



#### Actual methods (best known):

- •Gradient descent aka steepest descent or steepest ascent
- •Nelder-Mead method aka the Amoeba method
- •Simplex method
- •Quasi-Newton methods
- •Interior point methods
- Conjugate gradient method

## Optimization in practice -6 Local optimization versus global optimization Single starting point Vs Multiple starting points (+ interactions between points)

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Others fundamental components in the optimization algorithms are:

**Parameters space** (search space for each parameter ) (e.g.  $[-\infty,+\infty]$ ; [0,100] ...[-20.0,+5.0]).

**Constraints** (e.g.  $A \ge 0$ ; B < 20; C < f(x,y..z)).

**Penalty functions** (to increase the OBJ function of a constant when a constraint is violated). Usually very high or very low constant; E.g. Penalty = 1E+10; ObJ=Penalty if an assigned constraint is violated

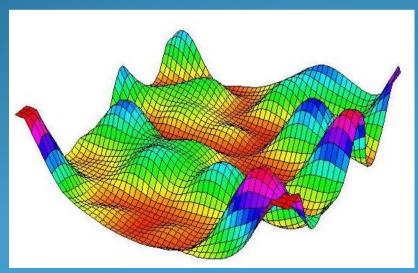
**Termination criteria** e.g. stop the search iteration when the difference in OBJ values between two successive iteration is Lower than a given tolerance value: e.g.  $\varepsilon = 1E-12$ 

Stop if 
$$|OBJ_{n-1} - OBJ_{n}| < \epsilon$$

there are a many other popular methods for mathematical optimization:

- •Simulated annealing
- •Tabu search
- •Genetic algorithms
- •Ant colony optimization
- Evolution strategy
- •DIFFERENTIAL EVOLUTION
- •Particle swarm optimization

•••••



Valid criteria to choose one of them should be based on:

- •Available software (commercial, freeware, open source)
- •Available code for programming in special Complex optimization problems
- •Easy implementation of new problems
- •Good performance (considering comparative benchmarks studies)
- •Global optimization
- Speed of the computation

Differential evolution (DE) is a stochastic parallel direct search evolution strategy optimization method that is fairly fast and reasonably robust. Differential evolution is capable of handling nondifferentiable, nonlinear and multimodal objective functions.

http://mathworld.wolfram.com/DifferentialEvolution.html

DE algorithm Born in the middle of 90's from some Ideas from K.Price and R. Storn. (Storn and Price 1997a,b)

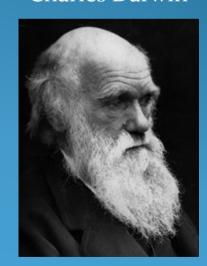
This algorithm uses some paradigms from the theory of evolution but use also use many stochastic components to implement these concepts.

Since 1996-1997 appeared more than 3000 papers and technical Reports with studies and implementation of DE.

Many scientists consider the DE algorithms as one the best Optimization algorithm and useful in many applications



Charles Darwin



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#### General field of application:

In all cases where there are many local optima; intricate constraints; mixedtype variables; or noisy, time-dependent or otherwise ill-defined functions, the usual methods don't give satisfactory results the DE may be a solution

DE implementations exist for well known software and programming languages

Mathematical –numerical analysis software as interpreted scripts or compiled toolboox Mathematica (wolgram resarach) Matlab (mathworks) Scilab R Programming languages
high level (procedural or OOP)
C++
Fortran 90
Java
Pyton
Pascal

Object Pascal (by L.B)

And many compiled or specialized Software..

<u>See :</u>

http://www.icsi.berkeley.edu/~storn/code.html

#### Basic steps in DE algoritms

Preliminary steps

iterative loop Initialization

Evaluation

Repeat

Mutation

Recombination

Evaluation

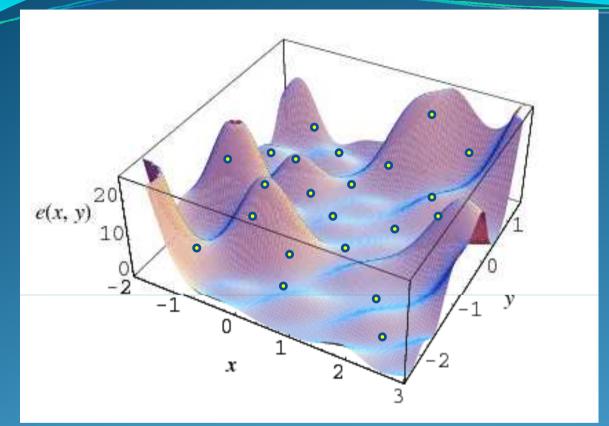
Selection

Until (termination criteria are met)

**Initialization** – random filling the population of vectors that contains The parameters (a,b,c,d,e,f) to calculate the given OBJ function obj = f(a,b,c,d,e,f)... (6 parameters vectors - Population of n vectors )

	V <sub>1</sub>	V <sub>2</sub>	V <sub>3</sub>	V <sub>4</sub>		Vn
a	200	153	99	34		170
b	20.2	32.4	9.5	4.3	•••••	18.2
С	0.01	2.3	4.3	1.3		3.4
d	45.3	32.1	46.3	34.8		39.6
e	435	82	293	91	•••••	103
f	349	294	673	830		327
	obj 1	obj 2	obj 3	obj 4		obj n

Fittness Calculation for each individuals (EVALUATION)



Vector initialization

In a population of potential solutions within an n-dimensional search space, a fixed number of vectors are randomly initialized, then evolved over time to explore the search space and to locate the minima of the objective function.

The Kernel of DE algorithm is a sequence of operations (or use of some operators) at each iteration:

- Mutation (casual mutation of genes)
- Recombination (or Crossover exchange genes)
- Selection (the best survive the worst die)
- •Age evaluation (and individual can't survive more than a given number of generations (age) this is recent addition to solve stagnation problems)

mutation –At each iteration, called a generation, new vectors are generated by the combination of vectors randomly chosen from the current population

	Vr1	Vr2	Vr3		Vi mutar	ıt
a	200	153	99		254	
b	20.2	32.4	9.5		43.1	
c	2.6	2.3	4.3	mutation	0.6	
d	45.3	32.1	46.3	With Assumed F=1.0	31.1	
e	435	82	293		224	
f	399	294	673		20	

For each i in (1, ...n) population of vectors, form a 'mutant vector' using simple Vi(mutant) = Vr1+F(Vr2-Vr3) or Vi(mutant) = Vr1+rand F(Vr2-Vr3) Where r1, r2, and r3 are three mutually distinct randomly drawn indices from (1, ...n), and also distinct from i, and 0.0 < F < = 2.

**Recombination** (or Crossover) -The new generated vectors are then mixed with the parent vector (Vparent) of the old population. This operation is called **recombination** and produces the final **trial vector** 

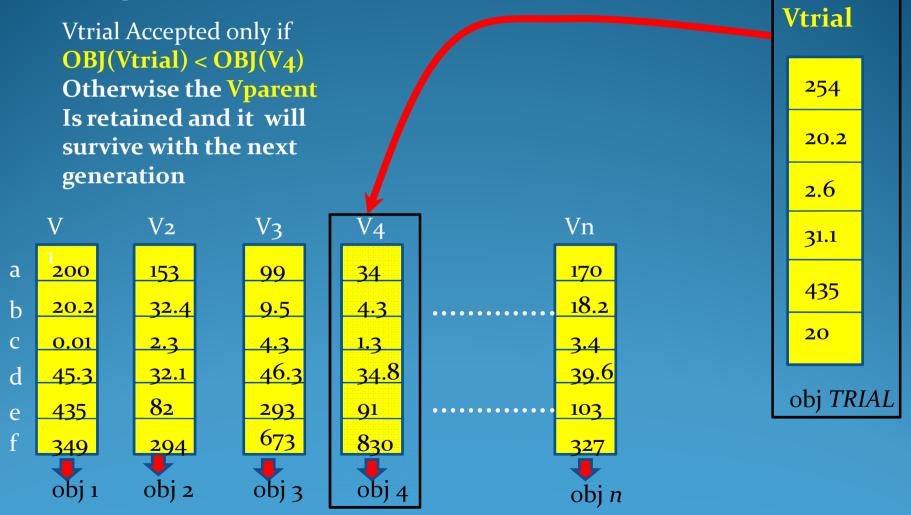
	Vpare	nt CR V	<sup>7</sup> i mutan		Vtrial
a	200	0.34	254	CR=0.5	254
Ь	20.2	0.89	43.1		20.2
С	2.6	0.72	0.6		2.6
d	45.3	0.14	31.1	OK	31.1
e	435	0.53	224		435
f	399	0.23	20	OK	20

For each component of vector, draw a random number in U[0,1]. Call this rand<sub>j</sub>. Let  $0 \le CR \le 1$  be a cutoff.

If rand<sub>i</sub><=CR, then Vtrial<sub>i</sub>=Vmutant<sub>i</sub>, else Vtrial<sub>i</sub>=Vparent<sub>i</sub>...

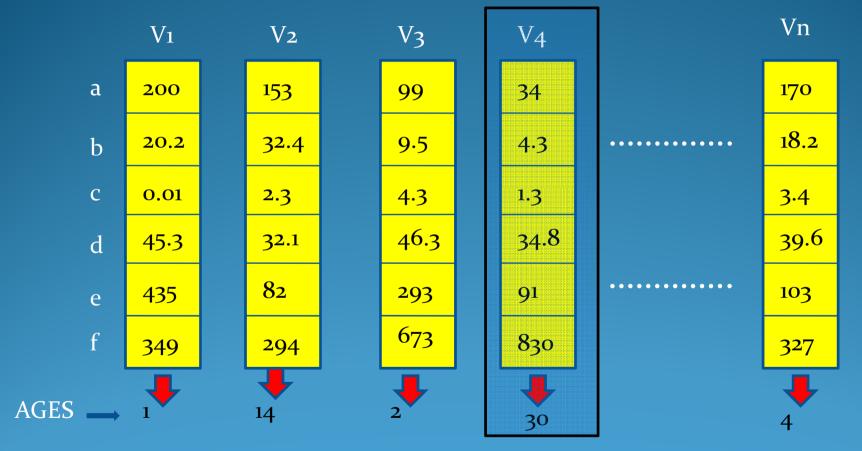
**SELECTION** – Finally, the trial vector is accepted for the next generation if and only if it yields a reduction in the value of the objective function.

This last operator is referred to as a **selection** 



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Ageing – vectors that stay unchanged for a long time after several generations will have a too OLD age (e.g use a Cutoff age AG=30). In this case the vector Is substituted with a new one with a random in initialization



Age counter for each vector increase 1 at each new generation...

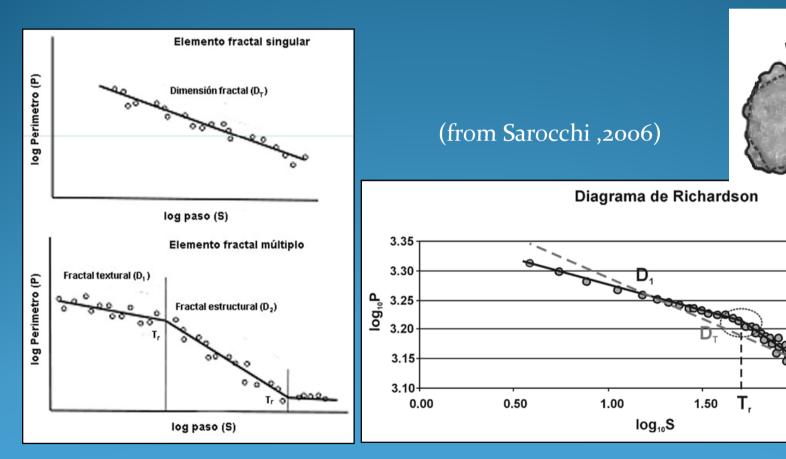
Termination criteria – the iterations Terminate when, for example, the variance of all the OBJ function values is lower than a predefined tolerance (e.g 1E-10). The vector with BEST performance contains the OPTIMUM set of the 6 parameters.



- Exist several variants for DE algorithms, mainly in the MUTATION operator.
- •The F parameter (weight for mutation) usually is assumed in the range F=[0.5, 1.5].
- •The CR cutoff value for CROSSOVER is assumed in the range [0.5,1.0] (usually 0.8-0.9)
- •The number of vectors in a population usually should be at least 10 times the number of parameters to optimize (e.g. a 6-parameters problem should have a population of 60 vectors).. But in some case these value may be higher (200-300) to guarantee GLOBAL OPTIMIZATION.
- •<u>Ageing cutoff value</u> is usually low (AG =20-30) but this should be evaluated for each specific problem

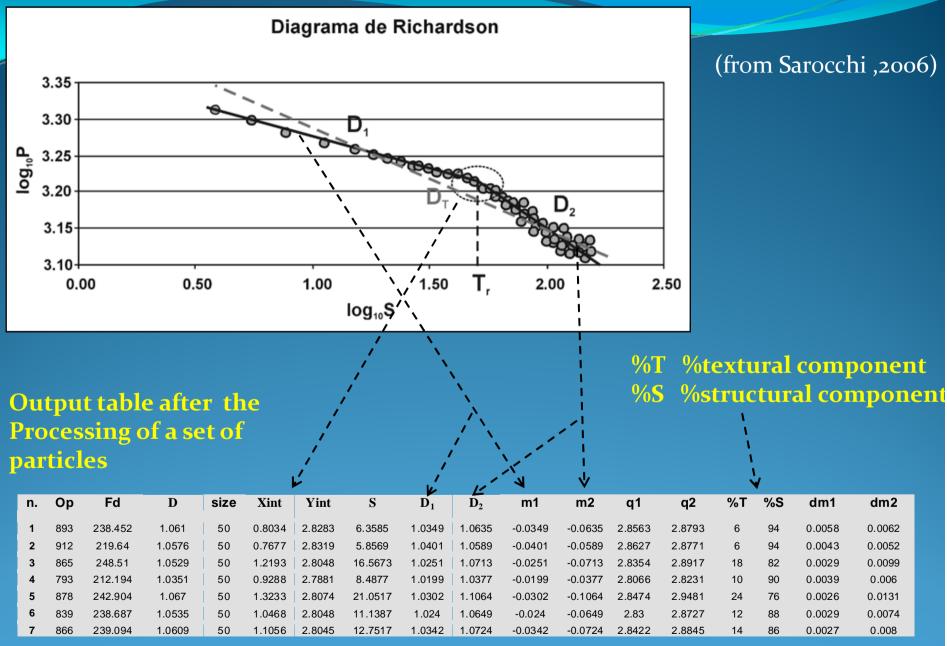
#### DE example of application -1 - PARTFRACT software (Borselli & Sarocchi 2005,2006)

PARTFRACT calculate, after a <u>DE Global optimization of with 5 parameters</u>, The fractal dimension textural (D<sub>1</sub>), structural (D<sub>2</sub>) of particle's perimeter. The perimeter value are obtained with several approximantion using segments of different length S. So that the perimeter is approximated with a irregular poligon . Reducing the length S of the segment we have a longer perimeter P.



2.50

#### DE example of application – 1 - PARTFRACT software (2)



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#### DE example of application – 1 - PARTFRACT software (3)

DE optimization parameters

D=5 (number of parameters)

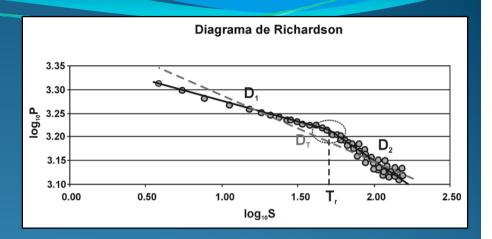
N=150 (No. Of vectors in the population)

F=0.9 (weight factor in the mutation)

**CR=0.9** (crossover probability)

AG=50 (age cutoff)

Tolerance 0.001



#### Constraints:

- •The slopes of the textural and structural components must be included in the range -1E-19 and -1.0
- •The Xm, Ym must be in the range of the observed data

#### **OBJECTIVE FUNCTION**

$$obj = \sum_{i=1}^{tr-1} (obs_i - pred_i)^2_{text} + \sum_{i=tr}^n (obs_i - pred_i)^2_{strut}$$

#### DE example of application - 2 - DECOLOG software (Borselli L., Sarocchi D., 2006)

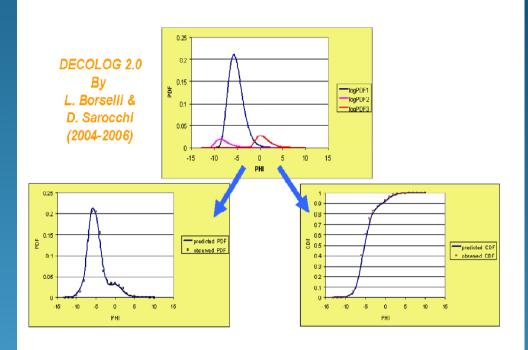
#### WWW.DECOLOG.ORG

Aim of DECOLOG software is develop a solution to decode the information present in the natural mixture of particles/sediments using, as paradigm, the 3-paramters log-normal distribution and particularly a defined mixture of these distributions.

DE algorithm is the Kernel of the Optimization procedure.

The optimization process in this case is MULTI-OBJECTIVE because the optimization proceeds in parallel with the best fitting of PDF(mixture) and CDF(mixture) to Experimental data....

#### DECONVOLUTION OF MIXTURES OF LOGNORMAL COMPONENTS FROM PARTICLE SIZE DISTRIBUTIONS



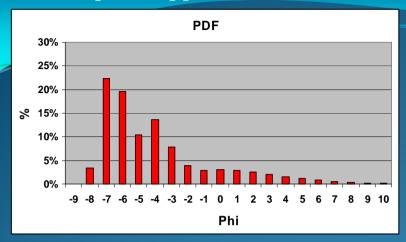
**DECOLOG** (rel 2.0 - 2004-2006):

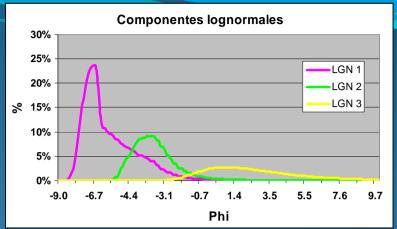
#### LORENZO BORSELLI

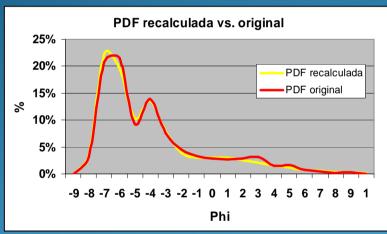
Research Institute for Hydrogeological Protection (CNR-IRPI)
Piazzale delle Cascine 15, 50144 Florence (ITALY), borselli@irpi.cnr.it

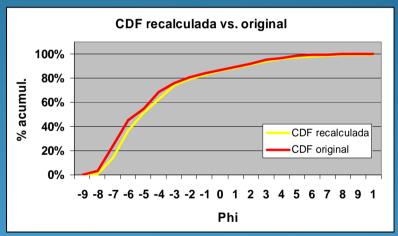
DAMIANO SAROCCHI
Instituto de Geofisica - UNAM (Mexico), d.sarocchi@mclink.it

#### DE example of application – 2 - DECOLOG software (2)









#### Natural MIXTURE of distributions

$$f(x)_{mix} = w_1 f_1(x) + w_2 f_2(x) + \dots + w_n f_n(x)$$

$$F(x)_{mix} = w_1 F_1(x) + w_2 F_2(x) + \dots + w_n F_n(x)$$

PDF

$$\sum_{i=1}^{n} w_i = 1$$

Weights of the mixture (fraction of each component)

#### DE example of application – 2 - DECOLOG software (3)

Global fitting statistics for CDF -----
Model efficiency coefficient EF: 0.9968002

Coefficient of Determination R^2: 0.9987997

Kolmogorov-Smirnoff difference Ks: 0.0684153

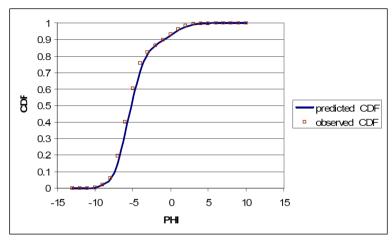


Fig 3.: global fitting performance on the observed CDF

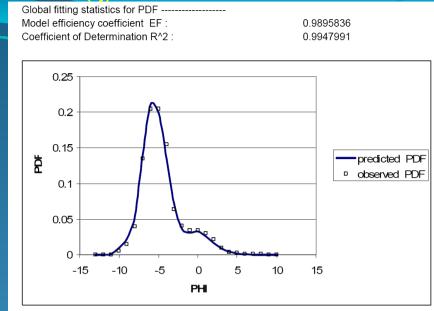
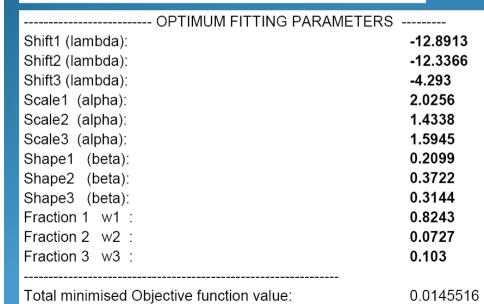


Fig 4.: global fitting performance on the observed PDF



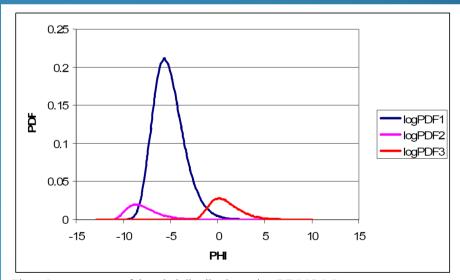


Fig.1: 3 components of decoded distribution using DECOLOG.

#### DE example of application – 2 - DECOLOG software (4)

Decoding with non linear multiobjective global optimization

A non linear multiobjective global optimization procedure has been developed to complete in efficient and robust way the decoding process. The optimization process allow to obtain the parameters  $\alpha_i, \beta_i, \lambda_i, w_i$  for each distribution.

We established a concurrent fitting of the observed PDF and CDF by way of a multiobjective optimization minimizing at the same time the errors in the PDF and CDF. Because the tho objective are concurrent each optimum may be partially in conflict with the other establishing dominance.

So to obtain a result we transform the multiobective process for a computation purpose in a single objective optimization (Andersson, 2000).

$$obj = W_{cdf} K + W_{pdf} E_{ff}$$

Where K is the Kolmogorov-Smirnov maxmum difference between observed and computed CDF;  $E_{ff}$  is the model efficiency parameter developed by Nash and Sutcliffe (1970) that has a well recognized performances for non linear fitting, In this case we apple it to PDF part

$$W_{pdf} = 1 - W_{cdf}$$

$$W_{cdf} = f(E_{ff})$$

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#### DE example of application – 2 - DECOLOG software (5)

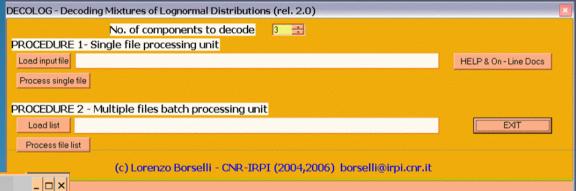
DE optimization parameters

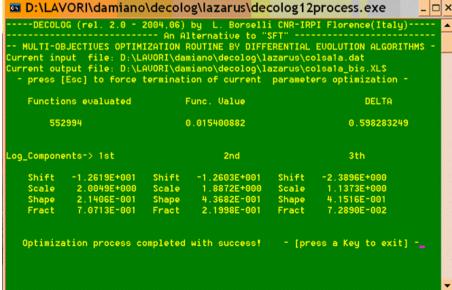
D=11 (number of parameters for 3 component mixture)

N=330 (No. Of vectors in the population)

F=0.9 (weight factor in the mutation)

CR=0.9 (crossover probability) AG=30 (age cutoff) Tolerance 0.0001





The decolog software is a freeware tool It can be downloaded at

www.decolog.org

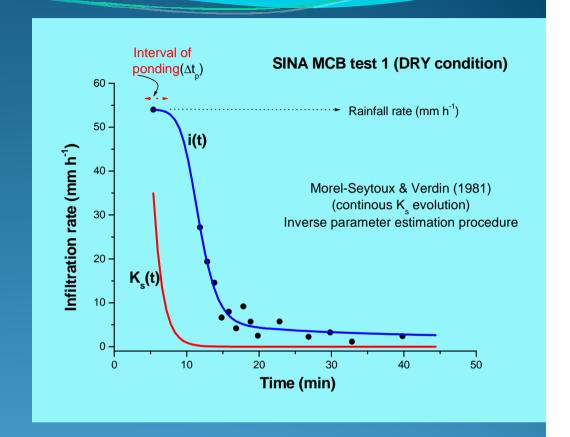
The next update at 3.0 will be in 2009

#### DE example of application – 3 - INFIT software (Borselli 1998,2002)

#### INEIT 1.2

Software for inversion procedures and determination of soil hydraulic parameters in condition of strong dynamic of the surfeces as for high rainfall, runoff intensity, severe soil erosion soil surface degradation due to reduction of porosity, sealing and a consequent reduction of saturated conductivity.

Parameters to estimate  $G, Ks_0, Ks_f, a$ 



Dynamic infiltration model (non linear):

Morel-Seytoux & Verdin (1981) Borselli (1998):

$$i(t) = f(r, t_p, K_s, G, \Delta\theta)$$

If typ 
$$K_s(t-t_p) = (K_{s0} - K_{sf})e^{-a(t-t_p)} + K_{sf}$$

#### DE example of application – 3 - INFIT software (2) Rainfall simulator/infiltrometer •full cone nozzles [int. 25 to 120 mm/h] ∆tp .∧tr..... •height of fall 4.5 m. 70 Effective infiltration rate •plot with buffer areas, Apparent infiltration rate •runoff & subsurface flow collection 60 Infiltration rate - mm/h area o5Xo.8 m •CCD camera I = r•laser microprofilometer i = r - qNozzle **CCD** camera 20 20 25 30 10 35 40 Time (min) INFILTRATION RATE is computed by: Infiltration rate= Rain. Rate - Runoff rate Runoff Subsurface flow

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# DE example of application – 3 - INFIT software (3) Initial surface Dynamic of soil surface subject to intense rainfall and runoff and erosion Decay or roughness Erosion /re-deposition sealing and reduction of water conductivity reduction of porosity Soil (sina mcb)

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#### DE example of application – 3 - INFIT software (4)

DE optimization parameters

D-4 (number of parameters)

N=80 (No. Of vectors in the population)

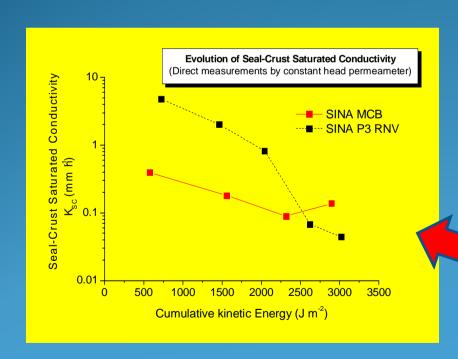
F=0.9 (weight factor in the mutation)

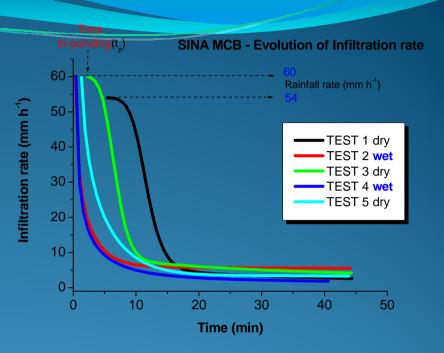
CR=0.7 (crossover probability)

AG=30 (age cutoff)

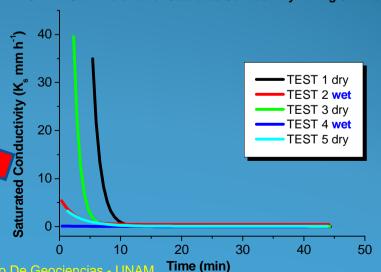
Tolerance o.oooooo1

OBJECTIVE 
$$obj = \sum_{i=1}^{n} (obs_i - pred_i)^2$$









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# DE example of application – 4 - SSAP software (Borselli 1991,2008)

SSAP (SLOPE STABILITY ANALISYS SOFTWARE)

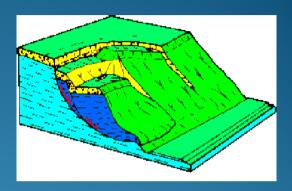
SOFTWARE for stability analysis (by limit equilibrium method) of natural and artificial slopes (soil and rock mass) with many components able to analyze hydraulic conditions and artificial Reinforcement effects, seismic action etc.

Users: geomorphologists,

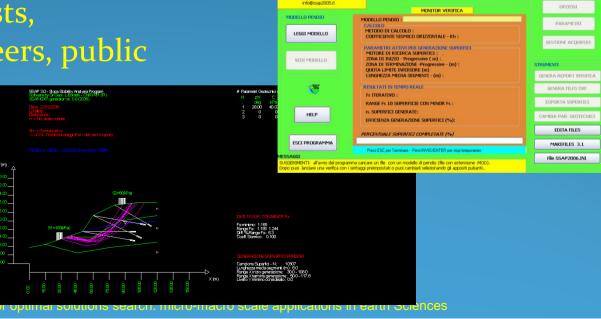
geologists, civil engineers, public

institutions...

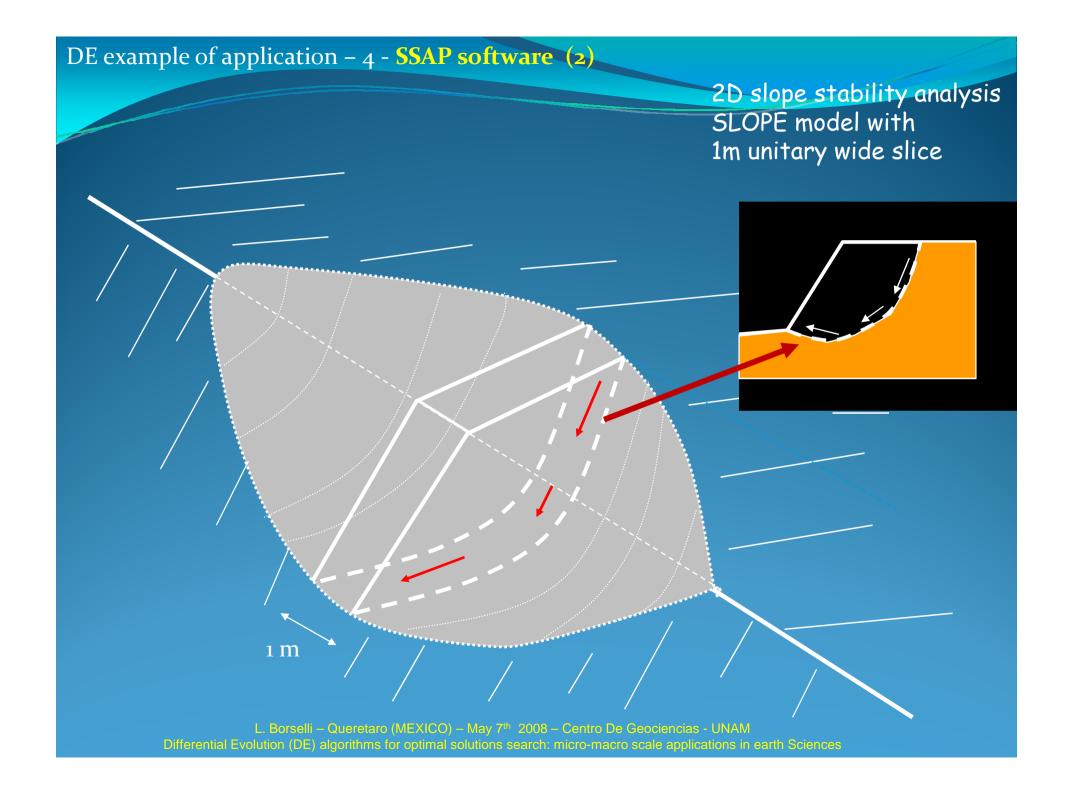
# http://www.ssap2005.it



SSAP version: 3.0.2 2008



SSAP 2006 (rel. 3.01 - 2007)



#### DE example of application – 4 - SSAP software (3)

#### ITERATIVE procedure to FIND Stability factor Fs INSTABLE if Fs < 1.0

$$F_{S} = \frac{\sum_{i} \{ [W_{i} \cos \alpha_{i} - U_{i} l_{i}] \tan \phi'_{i} + c'_{i} l_{i} \} m_{\alpha}}{\sum_{i} W_{i} \sin \alpha_{i} m_{\alpha} + E_{a} - E_{d} + \sum_{i} \Delta Q_{i} + I_{ff}}$$

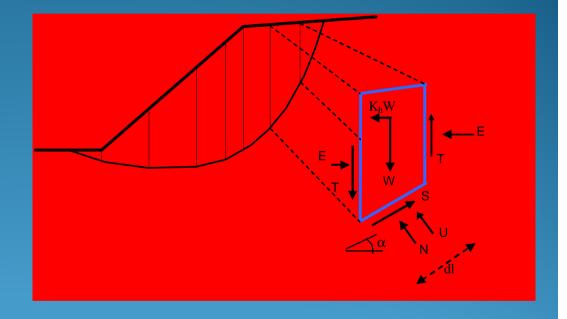
Equilibrium
Horizontal
forces
components

Generalized form Espinoza (1994)

where:

$$m_{\alpha} = \frac{\sec \alpha_i}{1 + \frac{\tan \alpha_i \tan \phi'_i}{Fs}}$$

$$I_{ff} = \sum_{i} \left[ \Delta T_{i} \tan(\phi'_{m} - \alpha_{i}) \right]$$





Seismic coefficient
To account of sesmic effect on stability
Kh,Kv=f(a<sub>g</sub>max)

#### DE example of application – 4 - SSAP software (4)

DE is used in SSAP 3.0.2 only to find The value of Kh (seismic coefficient) that put Stable slopes (FS>1) in critical condition of instability FS=1.0 due to the seismic action.

$$\mathbf{Obj} = |\mathbf{Fs-1.0}| \qquad F_S = \frac{\sum_i \{ [W_i \cos \alpha_i - U_i l_i] \tan \phi'_i + c'_i l_i \} m_{\alpha}}{\sum_i W_i \sin \alpha_i m_{\alpha} + E_a - E_d + \sum_i \Delta Q_i + I_{ff}}$$



We have to find, by numerical method, the root of a equation where one term of it (FS) also must be obtained by a separate iterative numerical method

The DE algorithm applied to minimize the Given OBJ function allows to find the optimal *Kh*. In this case the minimum coincides with e Zero of the OBJ function

Special attention and management for the condition Where the FS computation don't Converge...

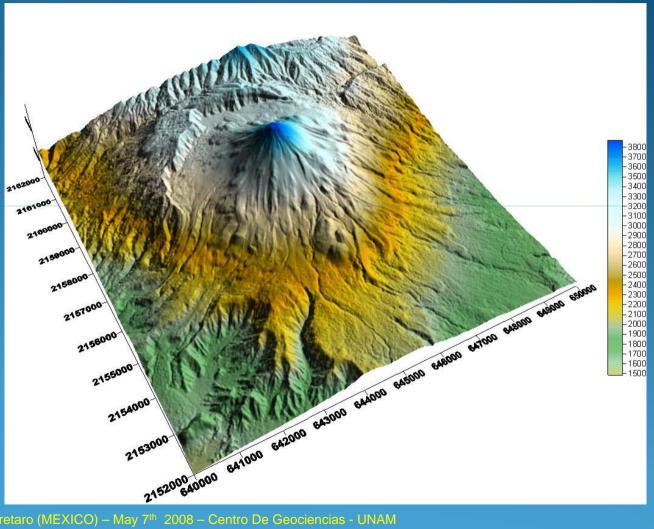
DE optimization parameters
D=1 (number of parameters)
N=50 (No. Of vectors in the population)
F=0.9 (weight factor in the mutation)
CR=0.9 (crossover probability)
AG=80 (age cutoff)
Tolerance 0.0001

#### DE example of application – 5 - VOLCANOFIT software (Borselli; 2005,2006)

VOLCANOFIT - is a special surface fitting software made in occasion of a study, with D. Sarocchi, ans C. De la Crux, on the stability of the volcan de fuego de Colima Using also SSAP...

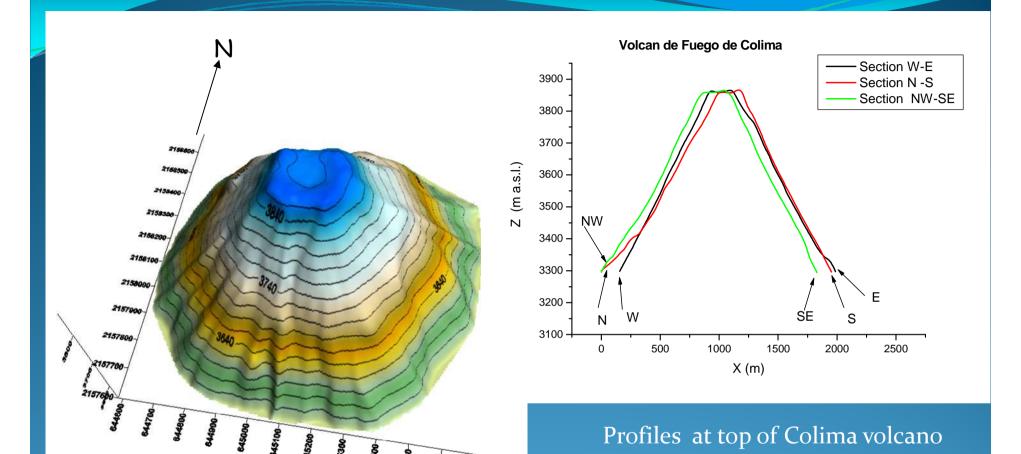
•Fitting of original DEM with a Truncated conical surface

•The analysis of local Mass excess, or deficit, in this portion of volcanic edifice is finally done by the computation of the residual surface after the fitting



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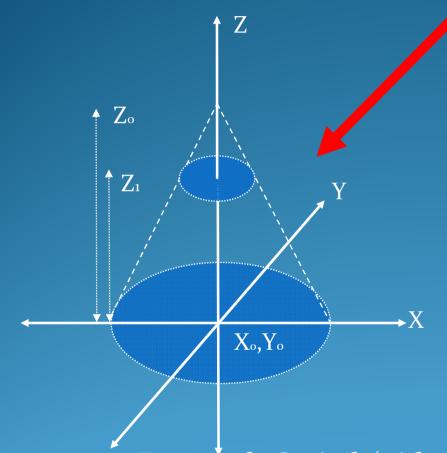
#### DE example of application – 5 - VOLCANOFIT software (2)



Top of Colima volcano Above 3540 m s.l.m.

## DE example of application – 5 - VOLCANOFIT software (3)

VOLCANOFIT fitting function (case of Colima volcan de fuego)

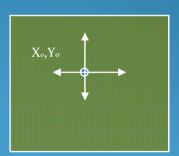


$$Z = z_0 - c\sqrt{\frac{(X - x_0)^2}{a} + \frac{(Y - y_0)^2}{b}}$$
if  $Z > z_1 \to Z = z_1$ 

OBJECTIVE 
$$obj = \sum_{i=1}^{n} |obs_i - pred_i|$$
FUNCTION

Centered on coordinate X<sub>o</sub>, Y<sub>o</sub>

Yutm

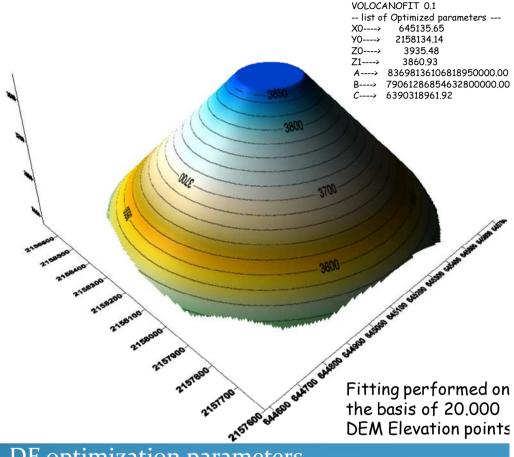


Truncated - Conical (with ellliptic base) fitting surface
Seven parameters:

 $X_0,Y_0,Z_0,a,b,c$  and  $Z_1$ 

Xutm

#### DE example of application – 5 - VOLCANOFIT software (4)



## DE optimization parameters

D=7 (number of parameters)

N=250 (No. Of vectors in the population)

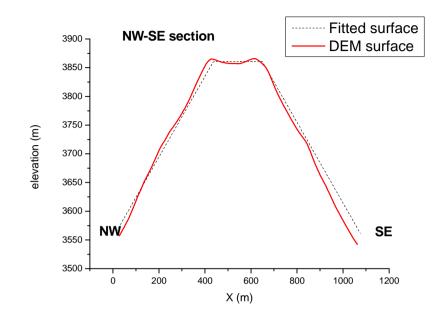
F=0.9 (weight factor in the mutation)

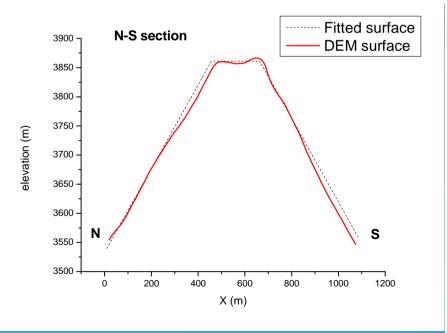
CR=0.9 (crossover probability)

AG=30 (age cutoff)

Tolerance 0.0005

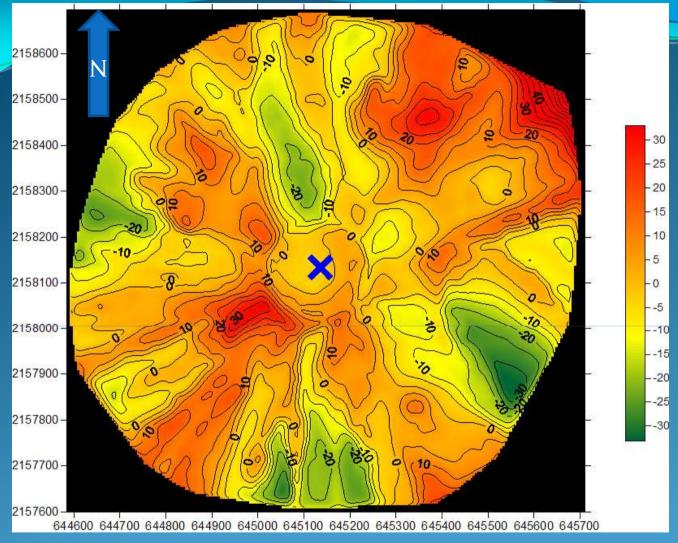
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Differential Evolution (DE) algorithms for optimal solutions search: micro-macro scale applications in earth Sciences

## DE example of application – 5 - **VOLCANOFIT software** (5)



In RED the major local excess of mass.

In GREEN the local deficit of mass

The Blue Cross is the centre of the reference fitted conical surface. It is assumed as the centre of simmetry of the upper part of the volcano

Residual surface = DEM surface NOV. 2004 - Fitted truncated cone surface)

#### Basic REFERENCES for Differential evolution algorithm and global optimization

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