Using TEMPER's Genetic Algorithm and MSIAC Databases to fit SDT Model Parameters

Emmanuel LAPÉBIE, Heloise VIGIÉ (trainee), CEA/DAM/Gramat

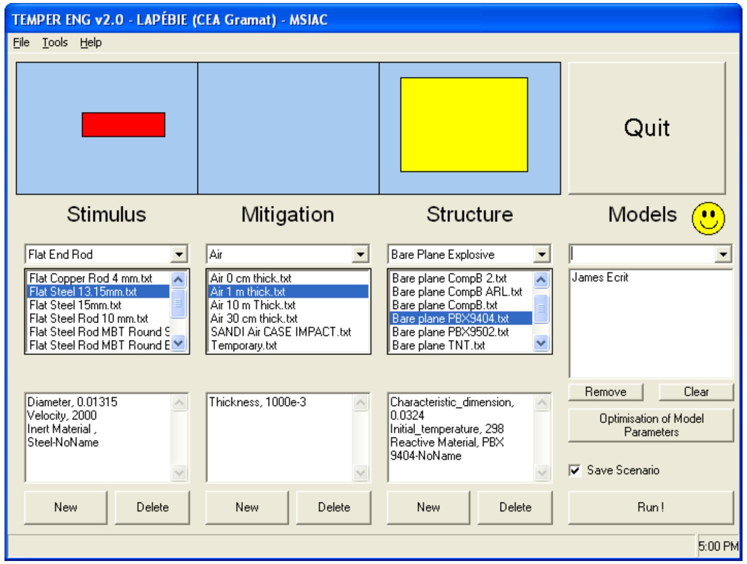
Pierre-François PÉRON, NATO/MSIAC

Outline of presentation

- TEMPER and FraID
- Genetic Algorithms
- How to ?
- Conclusions

TEMPER (1/2)

- TEMPER (Toolbox for Engineering Models to Predict Explosive Reactions)
  - Is a “Library” of analytical / empirical / 1D models dedicated to ammunition safety
  - Has been originally developed by CEA/Gramat (formerly DGA/CEG)
  - Is now available through NATO/MSIAC (Munition Safety Information and Analysis Centre)
    - Version 2.0 has been released in October 2007, Version 2.2 is currently under test at MSIAC
- A TEMPER “Scenario” consists in:
  - A “Stimulus” / A “Mitigation” / A “Structure” / At least one “Model”
  - Single / Multiple / Statistical runs
- Output is an embedded Excel™ workbook
  - One or more charts
    - Threshold curves
    - Initial / Residual stimulus data points
  - A summary worksheet
- Other features
  - Models comparison
  - Material Editor
  - Help
  - **Model-fitting tool**

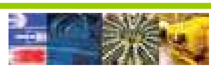


TEMPER GUI

energie atomique • energies alternatives

TEMPER (2/2)

- TEMPER's models are mainly SDT (Shock-to-Detonation Transition) ones:
  - Held's criterion expressed either as v^2d or u^2d,
  - Jacobs-Roslund original and MSIAC-modified threshold velocity models,
  - several approaches based on the "critical energy" concept
    - Walker-Wasley, James, Peugeot,
  - Yactor's model, based on pop-plot results,
  - generic $P^n.\tau$ criterion.
- SDT models may be used for a quick assessment of ammunition safety …
  - Fragment impacts (NATO fragment, Spherical fragment …)
  - Shaped Charge Jet Impacts
  - Sympathetic Detonation
- … provided that model parameters are available somewhere!
  - Scarce literature data, and only for a few compositions
  - We should take benefit of the large amount of experimental results …
    - MSIAC databases



energie atomique • energies alternatives

FraID

- FraiD (Fragment Impact Database)
  - Is one of the NATO/MSIAC results databases
  - Contains more than 1700 impact results (1.8 version)
    - On bare or covered HE, and also on systems,
    - For different fragment shapes
  - For 89 HE compositions
- How to use these data?
  - If sufficient data is available for a given HE, we can draw an experimental "threshold curve".
  - This experimental curve should be compared to a TEMPER's threshold curve from one SDT model.
  - The discrepancies between these two curves is a measure on how well the model performs with its current set of parameters.
  - If we could find a way to reduce the discrepancies to a minimum, then the model parameters will be fitted.
- We need an optimization procedure!

FraID's interface

Optimization techniques

- First we need to define a « fitness function » with values in [0,1]
  - It measures the difference between experimental and computed threshold curves
  - The fitness function tends to 0 if both curves are far apart from each other
  - It tends to 1 when both curves match perfectly
- Then we need an optimization technique
  - It is a mathematical way to let the fitness function tends to 1 (perfect fit)
  - It modifies model parameters to do so…

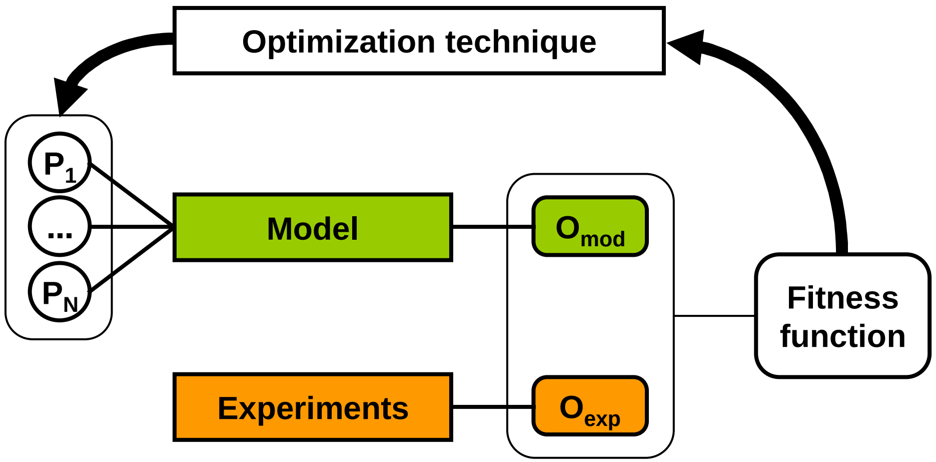
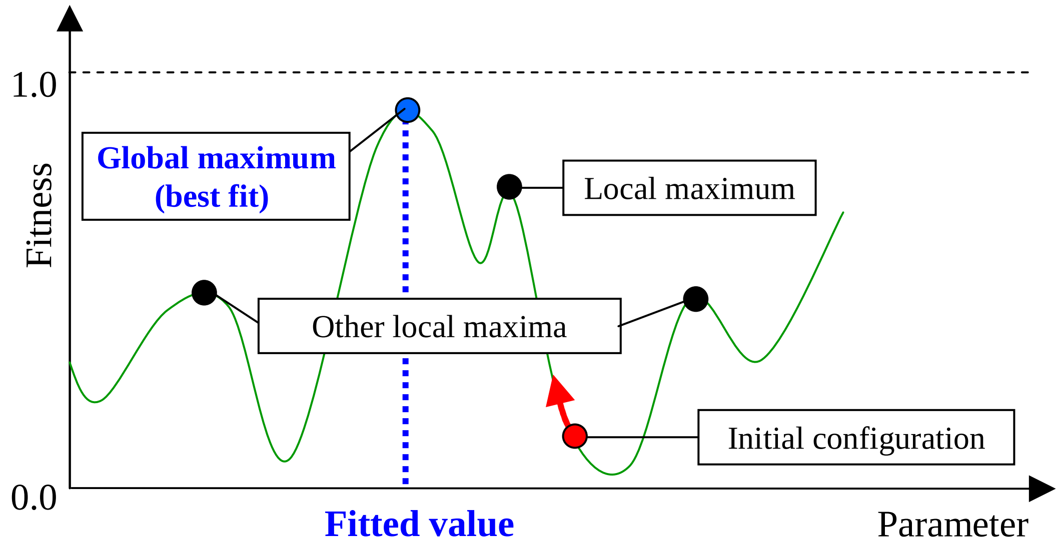


Illustration of the optimization procedure



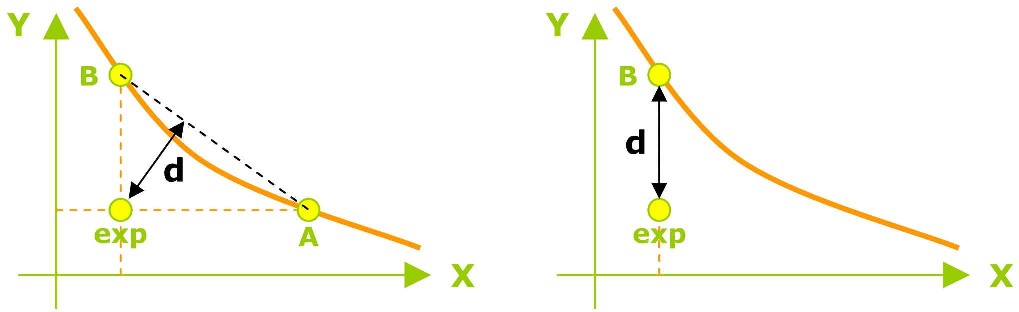
From an initial parameter value to a fitted one …

Fitness function

- The fitness value in TEMPER is the total scaled distance between experimental points and the computed threshold curve
  - A SDT model threshold curve is expressed as Y=f(X), usually:
    - Threshold velocity as a function of projectile diameter in the **[Ø,V]** plane,
    - Threshold pressure as a function of shock duration in the **[τ,P]** plane.
  - Case 1: the reverse function $X=f^{-1}(Y)$ has been coded in TEMPER
    - The distance of each point to the threshold curve may be computed
  - Case 2: the reverse function has not been coded
    - Only the Y-distance is computed
- The X (resp. Y) distances are scaled by DeltaX (resp. DeltaY), the range of experimental results in X (resp. Y) to avoid unit problems.

$$\text{Fitness} = \frac{1}{1+\frac{\sum_{i=1}^{N} d_i}{N}}$$

N = Number of experimental points



Computing the distance : Case 1 (Left) and Case 2 (Right)

energie atomique • energies alternatives

Optimization technique

- Many optimization techniques have been described in the literature
  - Gradient search algorithms,
  - Simplex method,
  - Simulated annealing,
  - Neural networks,
  - Genetic algorithms, …
- A Genetic algorithm (GA) technique has been chosen for TEMPER
  - GA have a small number of parameters,
  - GA are robust, all-purpose methods,
  - GA are straightforward to code,
  - Despite a limited theoretical background, GA usually perform very well!

energie atomique • energies alternatives

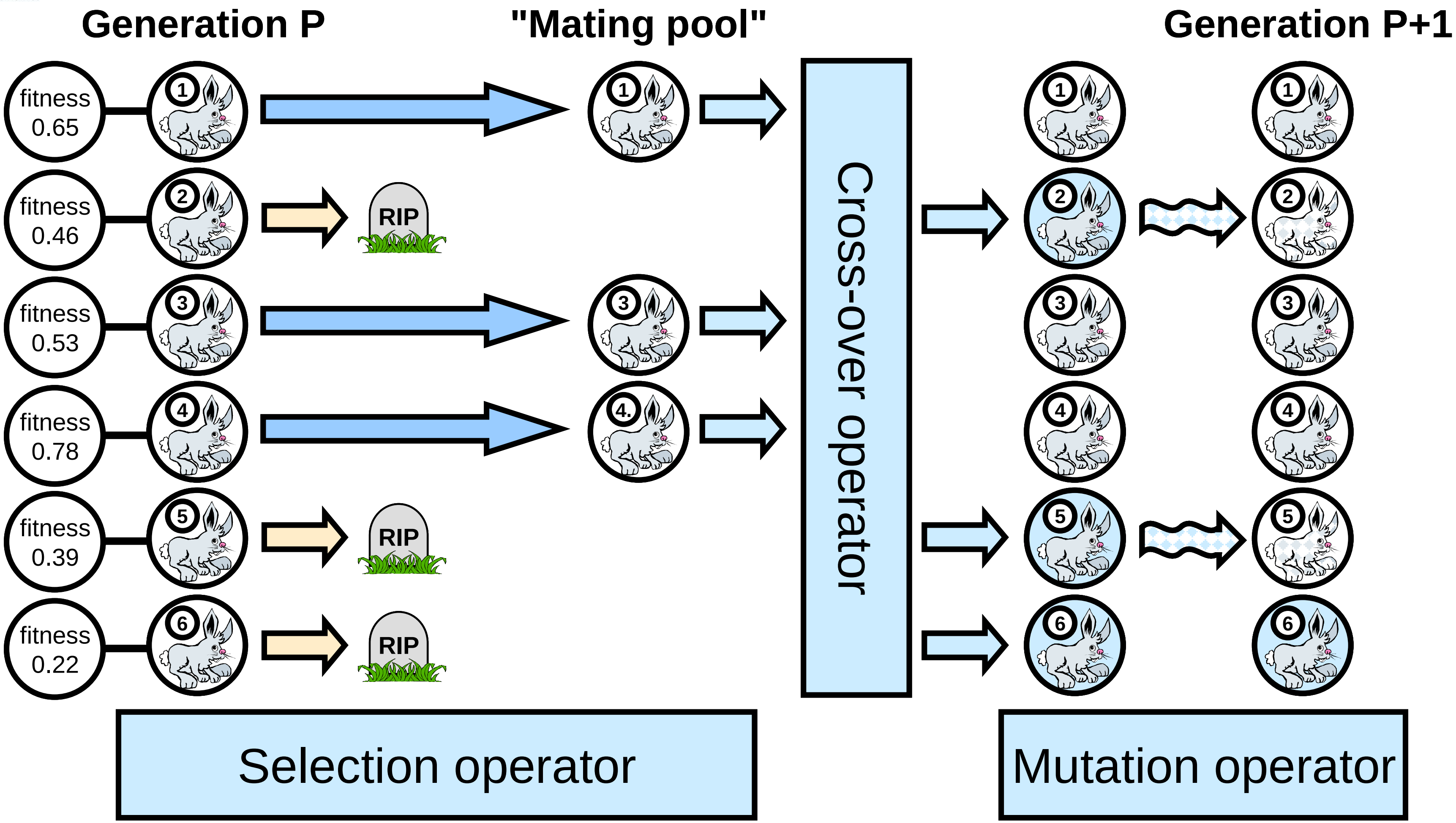
Genetic algorithms in words

- Non-sequential paradigm (evolution of a population)
- The model parameters (P_1, …, P_N) are linked to the "genes" of "individuals"
  - In TEMPER, each parameters is coded on two "half-genes"

$G_{2i-1} \in [0,1]$ $G_{2i} \in [0,1]$ $P_i = P_{i,min} + (G_{2i-1} \times G_{2i})^{1/2} \times (P_{i,max} - P_{i,min})$

- A "population" of individuals evolves through "generations" :
  - Selection (the most viable are allowed to mate) and Crossover
  - Mutation (to avoid a quick "freeze" of genes in local minima)
  - Stops when population is uniform, or when $F > 1-\varepsilon$, or when generation > G_{max}
- Few parameters :
  - Population size and maximum number of generations
  - Selected fraction (fraction of the current generation allowed to survive)
  - Mutation rate (sometimes it decreases through generations)
  - Selection and Cross-over strategies
- Mathematical background : Schemes theory
  - Only for binary coding [Holland, 1975; Goldberg, 1989 & 1990]
- Extension to real numbers [Christine Lapébie, 1995]

Genetic algorithms in pictures



Genetic Algorithms : Selection, Crossover and Mutation operations

energie atomique • energies alternatives

Step 1 : Reformatting FraID results

Microsoft Excel - PBX9404.xls

PBX-9404 (92% HMX, 3% Nitrocellulose and 3% CEF)

Bare

EXPLOSIVE			COVERING/CASING				PROJECTILE					RESULTS	REMARKS	REFERENCE
density (g/cm³)	process	state	thickness (mm)	diameter (mm)	length (mm)	nature	shape	nature	incidence (°)	velocity (m/s)	diameter or side (mm)	(detonation no detonation type III, IV, V, XDT,		
1.84	-	solid	0	-	-	-	sphere	steel	0	1140	13	detonation threshold	Data from reference 107 See Chart - Bare	3 107
-	-	solid	0	100	25	-	sphere	aluminium	0	1250	18	detonation threshold	See Chart - Bare	10
1.84	-	solid	0	25.4	25.4	-	flat	steel	0	2200	1.27	detonation	Special set-up to perform three or seven experiments with each gun shot; 0.94 L/D flat projectiles; Acrylic target holder to isolate the high explosive targets from each other; See Chart - Bare	38 4
										1940	1.016	no detonation		
										1620	1.27	no detonation		
										1620	1.778	detonation		
										1130	2.794	no detonation		
										1130	3.556	detonation		
										1040	3.81	no detonation		
										750	7.62	detonation		
										740	7.62	no detonation		
										650	10.16	detonation		
										500	16.51	no detonation		
										500	19.05	detonation		
1.84	-	solid	0	25.4	25.4	-	round	steel	0	1950	4.445	detonation	Special set-up to perform three or seven experiments with each gun shot; 0.62 L/D round projectiles; Acrylic target holder to isolate the high explosive targets from each other; See Chart - Bare	38 3
										1870	3.556	no detonation		
										1740	4.445	no detonation		
										1700	5.08	detonation		
										1530	5.715	no detonation		
										1530	7.62	detonation		
										1210	10.16	no detonation		
										1210	11.43	detonation		
										1160	11.43	no detonation		
										1160	12.7	detonation		
										1040	15.24	no detonation		
										1040	17.78	detonation		
										880	20.32	no detonation		
1.83	-	solid	0	76	76	-	flat	steel	0	2070	1.14	detonation threshold	6.4 mm thick brass casing Data used for the determination of Jacob-Roslund model parameters	23
										589	12.7	detonation threshold		
										500	19.05	detonation threshold		
1.83	-	solid	0	76	76	-	round	steel	0	1910	4	detonation threshold	6.4 mm thick brass casing Data used for the determination of Jacob-Roslund model parameters	23
										1615	5.4			
1.844	-	solid	0	-	-	-	shaped charge jet	copper	0	2870	2.04	detonation	$V^2D = 16 \pm 2\ mm^3/\mu s^2$	125
										2510	2.25	no detonation		
										2760	2.11	no detonation		
										3070	1.95	detonation		
										3070	1.95	detonation		

Al | Bare | Steel | Tantalum | Composite | Chart - Bare | Chart- Tantalum | Chart - Composite

FraID PBX-9404 Workbook

Flat steel projectile / Bare PBX-9404 values

PBX-9404 (92% HMX, 3% Nitrocellulose and 3%

Bare

PROJECTILE					RESULTS
shape	nature	incidence (°)	velocity (m/s)	diameter or side (mm)	(detonation no detonation type III, IV, V, XDT, ...)
flat	steel	0	2200	1,27	detonation
			1940	1,016	no detonation
			1620	1,27	no detonation
			1620	1,778	detonation
			1130	2,794	no detonation
			1130	3,556	detonation
			1040	3,81	no detonation
			750	7,62	detonation
			740	7,62	no detonation
			650	10,16	detonation
			500	16,51	no detonation
			500	19,05	detonation
flat	steel	0	2070	1,14	detonation threshold
			589	12,7	detonation threshold
			500	19,05	detonation threshold

Flat Steel Projectile - Bare PBX9404 for GA.tx...

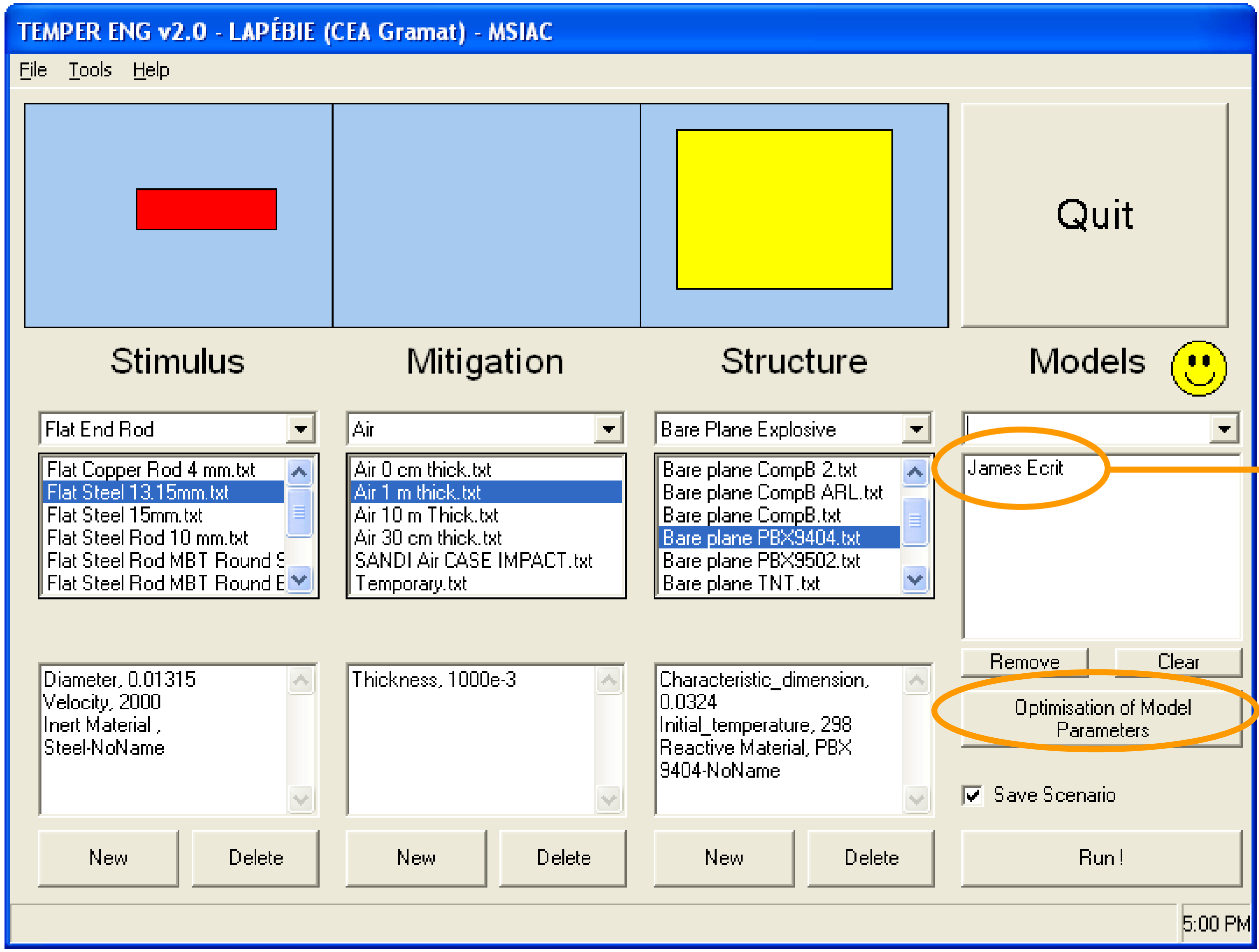
Fichier Edition Format Affichage ?

```
0.00127;2200;go
0.001778;1620;go
0.003556;1130;go
0.00762;750;go
0.01016;650;go
0.01905;500;go
0.001016;1940;nogo
0.00127;1620;nogo
0.002794;1130;nogo
0.00381;1040;nogo
0.00762;740;nogo
0.01651;500;nogo
```

TEMPER file (in international units)

energie atomique • energies alternatives

Step 2 : Preparing the scenario in TEMPER



We want to fit parameters for this model.

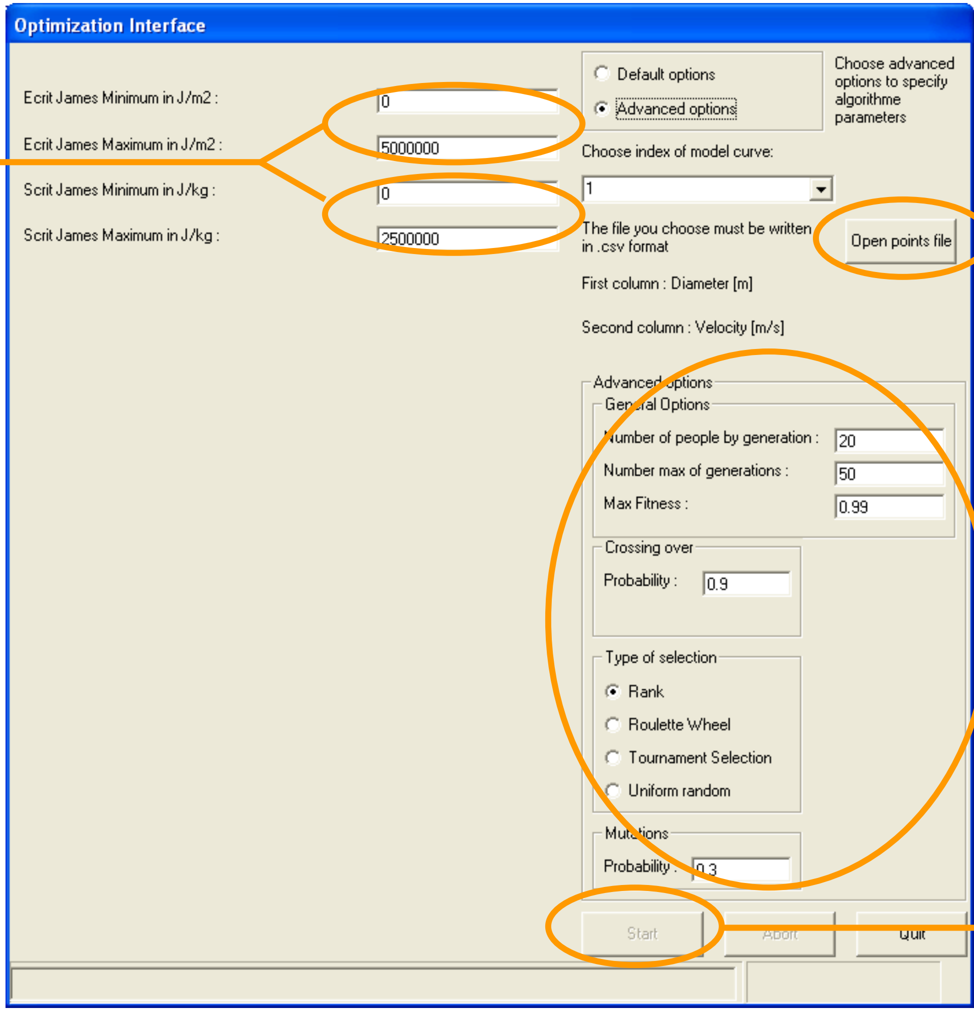
Clicking on this button opens the optimization interface

Preparing the scenario: Flat steel rod / Bare PBX9404

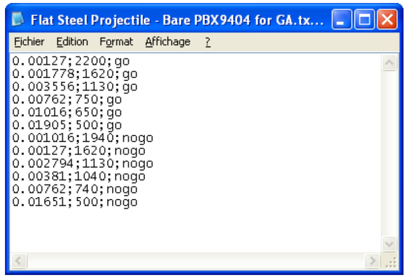
energie atomique • energies alternatives

Step 3 : Launching the optimization …

Min and max values for each parameters are required



Selection of the file with "experimental points"



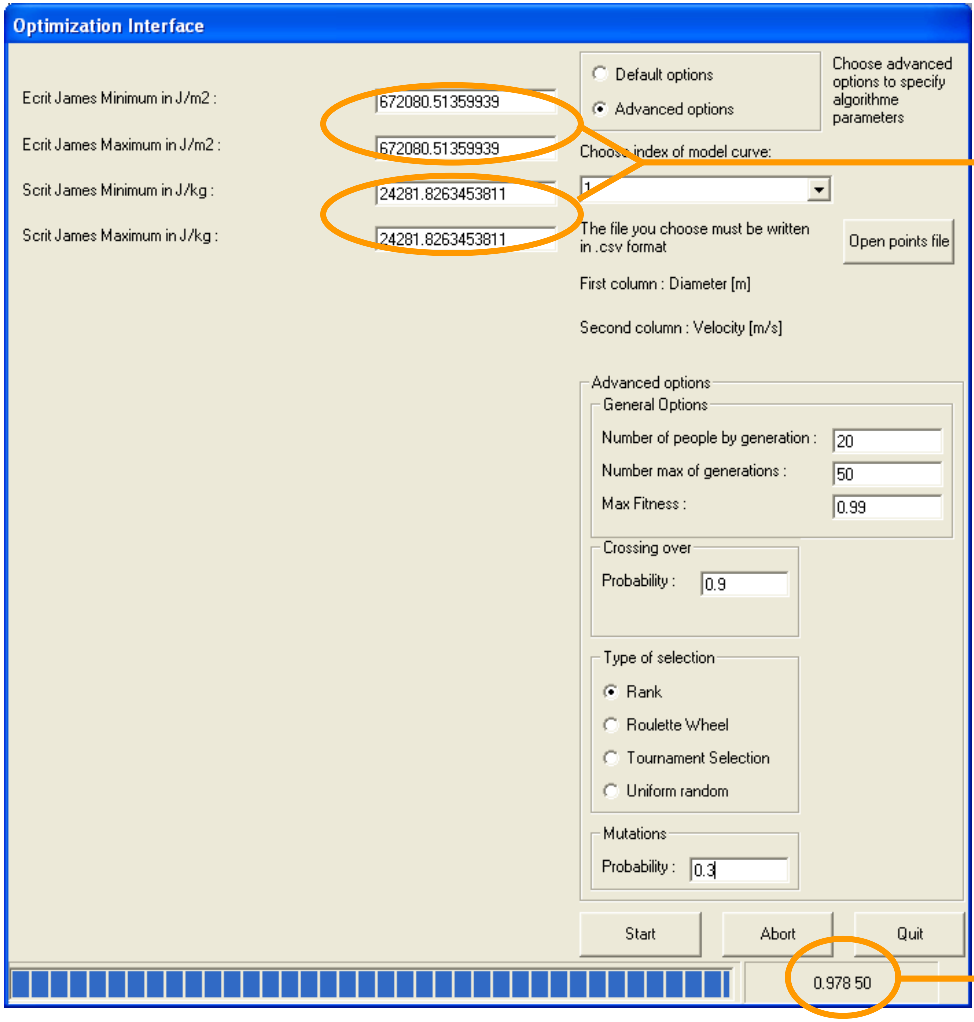
"Advanced" options

If everything is fine, the "Start" button is enabled

Preparing for the optimization

energie atomique • energies alternatives

Step 4 : Processing the results (1/2)



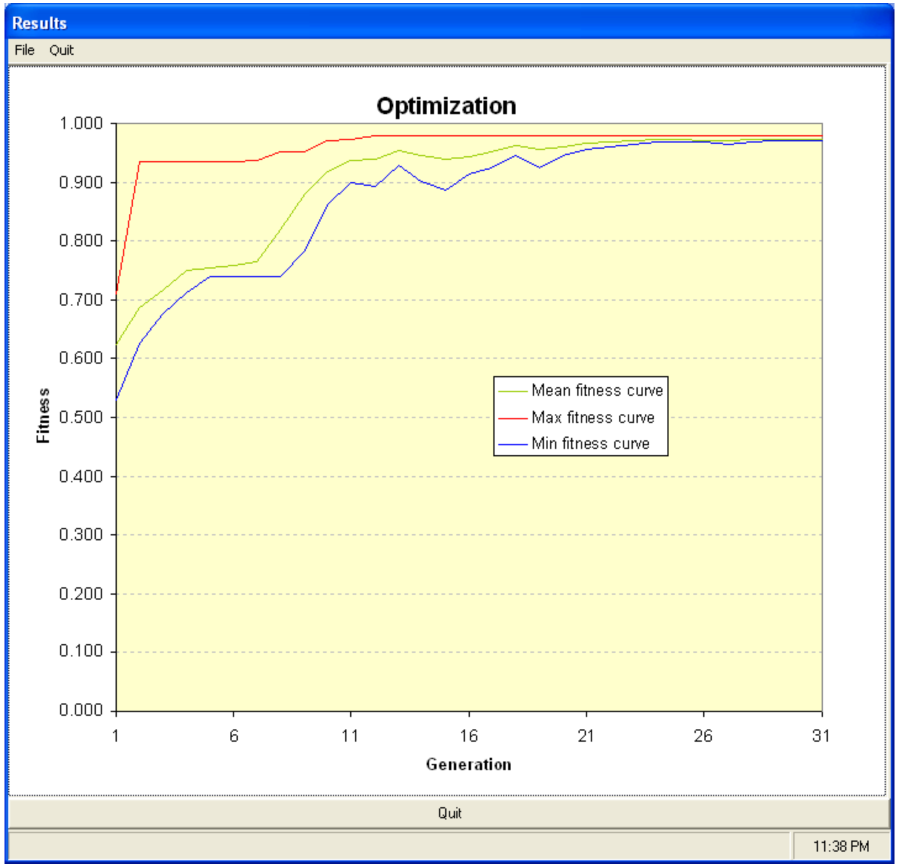
The optimization interface once the optimization is over

The fitted parameter values are indicated

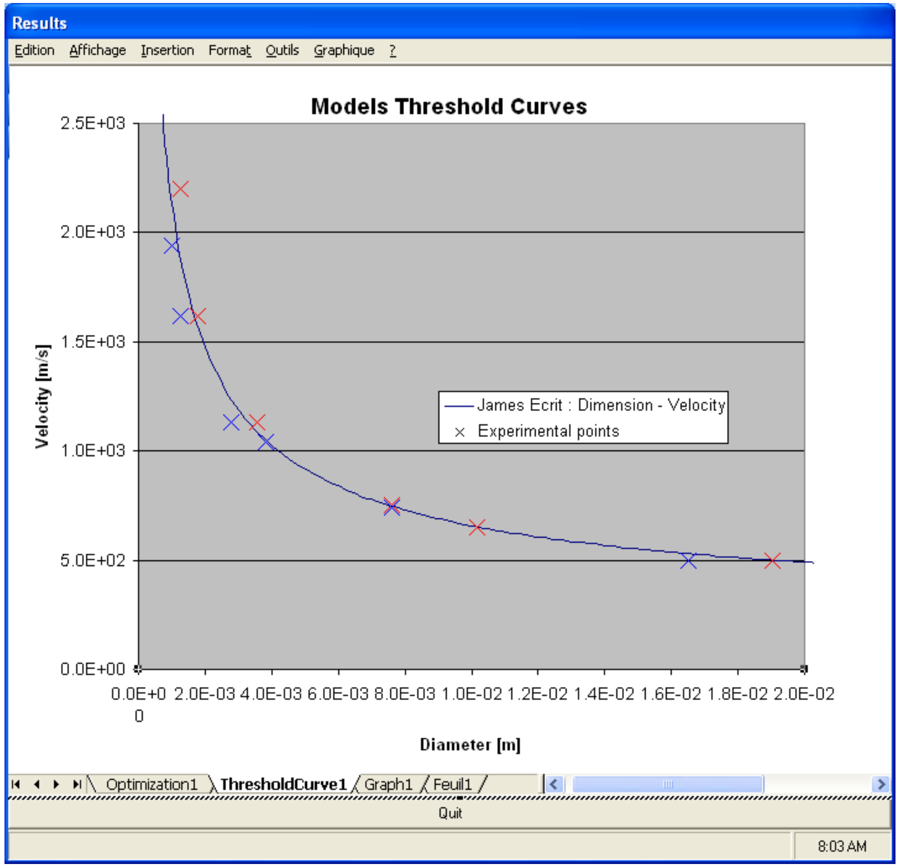
Current best fitness and generation number

Step 4 : Processing the results (2/2)

The Excel™ optimization workbook



Evolution of Max, Average and Min fitness through the generations

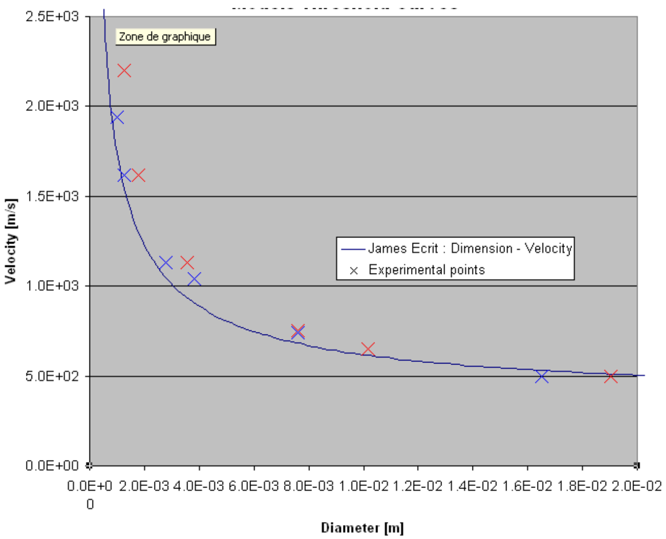


Comparison of experimental points (markers) with the computed threshold curve (best fit)

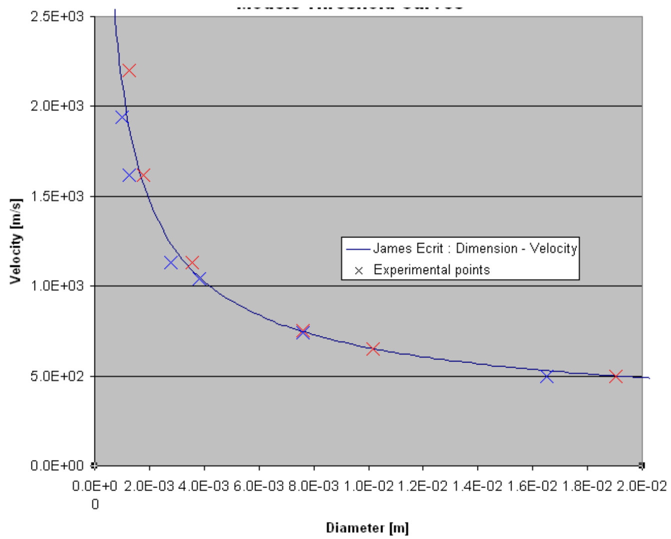
energie atomique • energies alternatives

Work done so far …

- First set of tests on 10 HE compositions and 6 SDT models (H. Vigié)
  - Advantages:
    - The technique is easy to use and converges quickly to an optimum.
    - If it freezes in a local minimum, changing GA parameters usually solves the problem



Flat steel projectile impact on bare PBX9404 James original parameters (Left) TEMPER's GA fit (Right)



  - Limits :
    - A small set of experimental results hinders the optimization from finding a good fit
    - There is no way to perform a global optimization on different scenarios at the same time (for instance round and flat projectile, bare and covered HE, …).
- Extension to 30 HE formulations under completion at CEA/Gramat
  - The results will be published in 2011 (MSIAC report)

energie atomique • energies alternatives

… and work still to be done

- Linking the optimization to the material editor
  - Direct cut & paste of fitted parameters into the reactive material file.
- Adding another optimization technique to TEMPER
  - The Genetic Algorithm works even for 1-parameter models, but simpler methods (gradient search) would do it as well, and much more quickly.
  - As everything in TEMPER, the optimization techniques are “Objects”, so the addition of a new technique should not be a problem.
- Extending the optimization to multiple scenarios
  - The main limitation of the optimization procedure is its inability to handle more than a single scenario.
  - For HE formulation with few experimental results, it could be interesting to fit at the same time “flat end rod” and “round end rod” scenarios …
  - For covered explosive, results with different cover thicknesses have to be considered as different scenarios, which for instance makes impossible the direct fit of Jacobs-Roslund parameters.
  - **This is not as simple as it may seem …**

energie atomique • energies alternatives

Thank you for your attention !