IBER-PEST

El comienzo de una hermosa amistad

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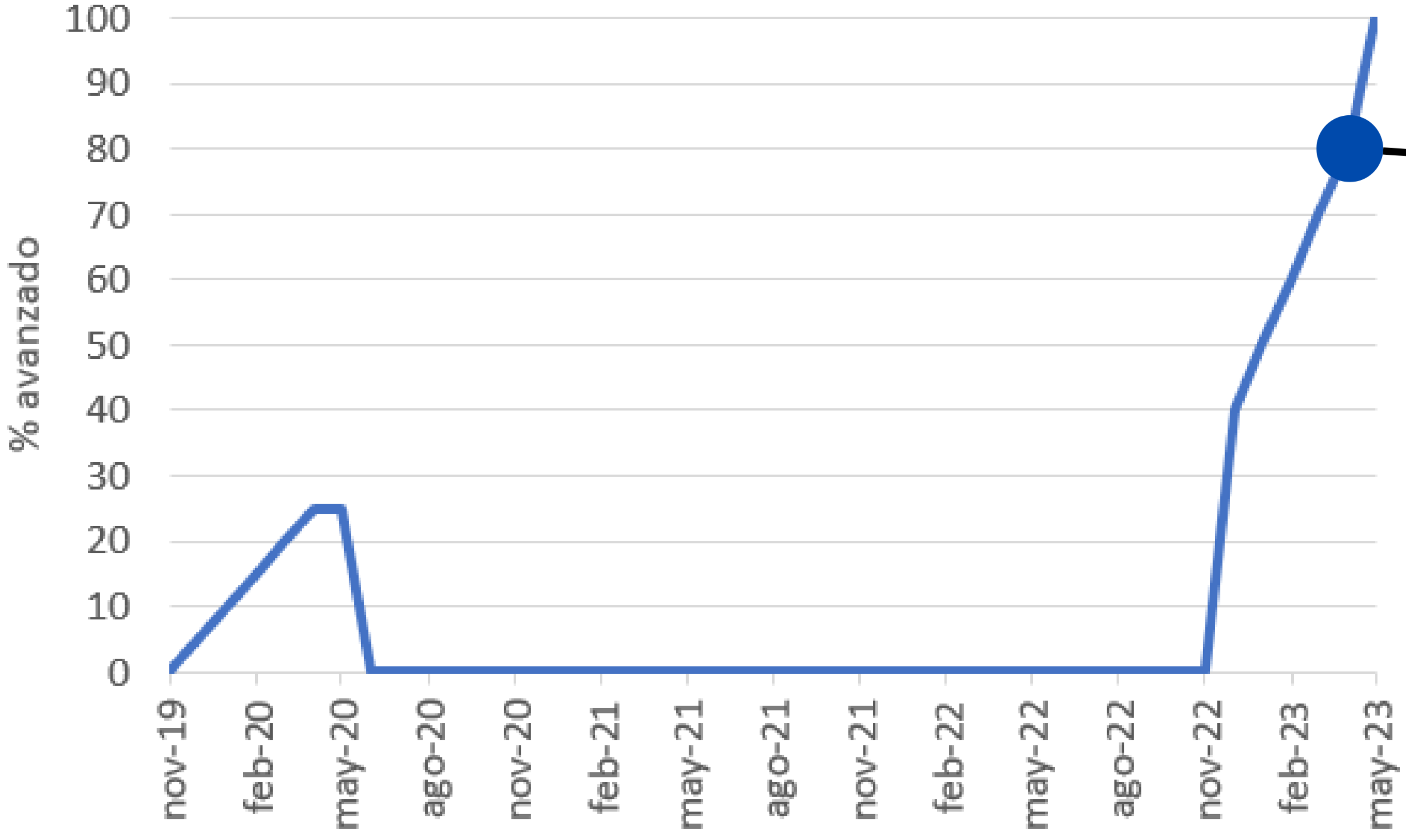
CITEEC
Grupo de Ingeniería del Agua y del Medio Ambiente

Introducción



Curso PEST Burdeos

Dancing with Models

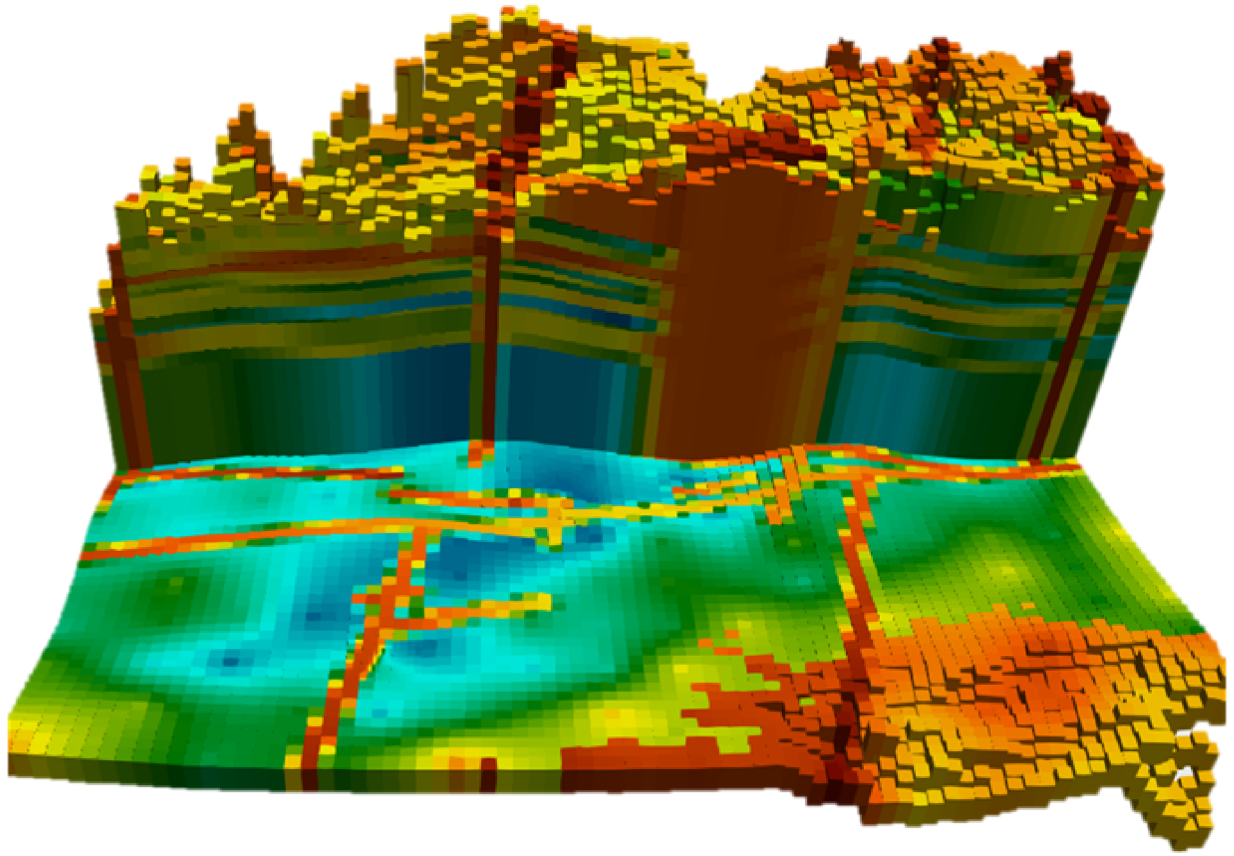
PEST

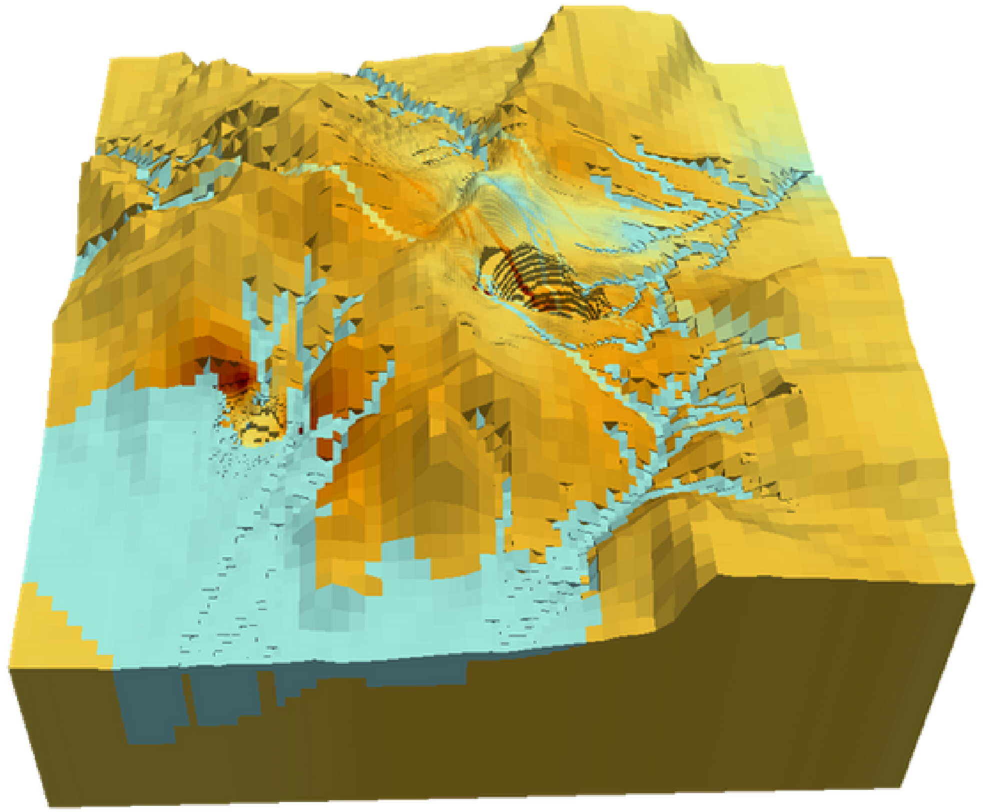
1990 – Universidad de Melbourne, Australia
Watermark Numerical Computing, Australia
Fortran
John Doherty

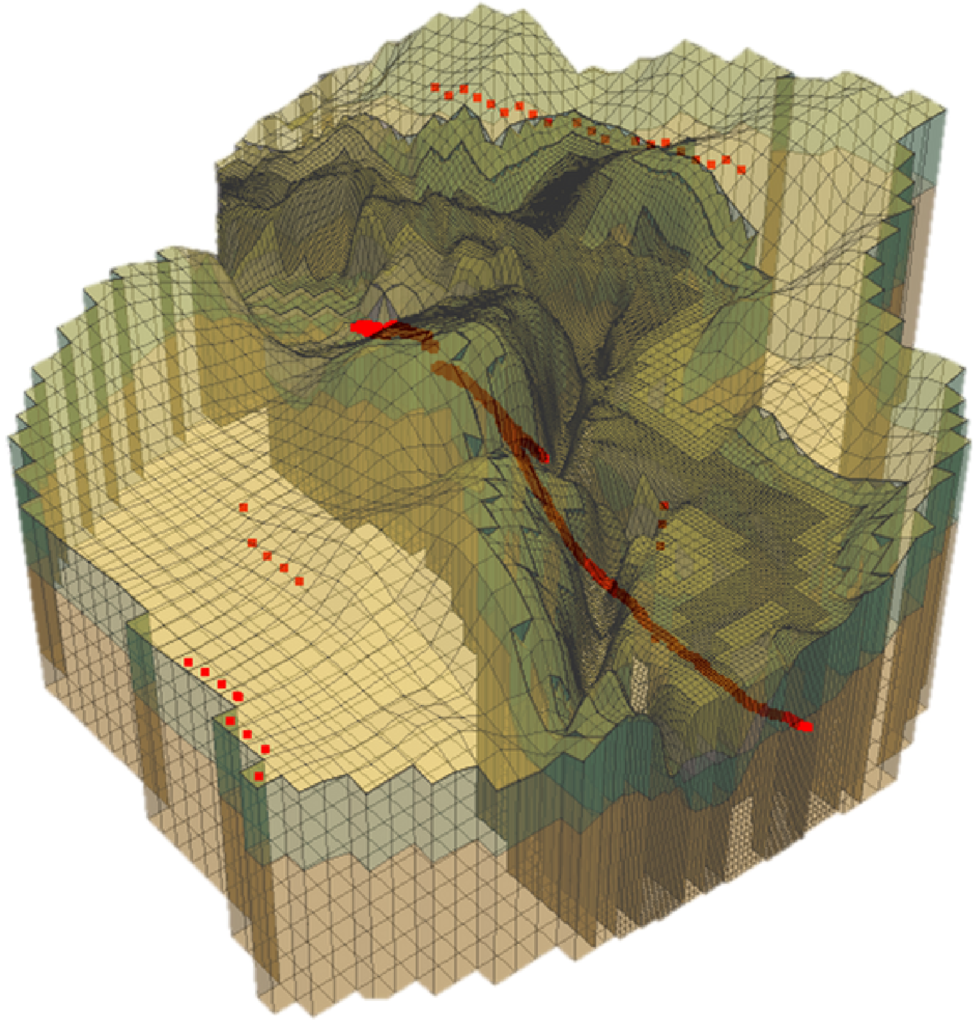
PEST++

2005 – Watermark Numerical Computing, Australia
USGS, USA
C++
Jeremy White, John Doherty, et. al.

Contexto







PEST/PEST++

$$\mathbf{h} = \mathbf{Z}\mathbf{k} + \boldsymbol{\varepsilon}$$

Mediciones de campo

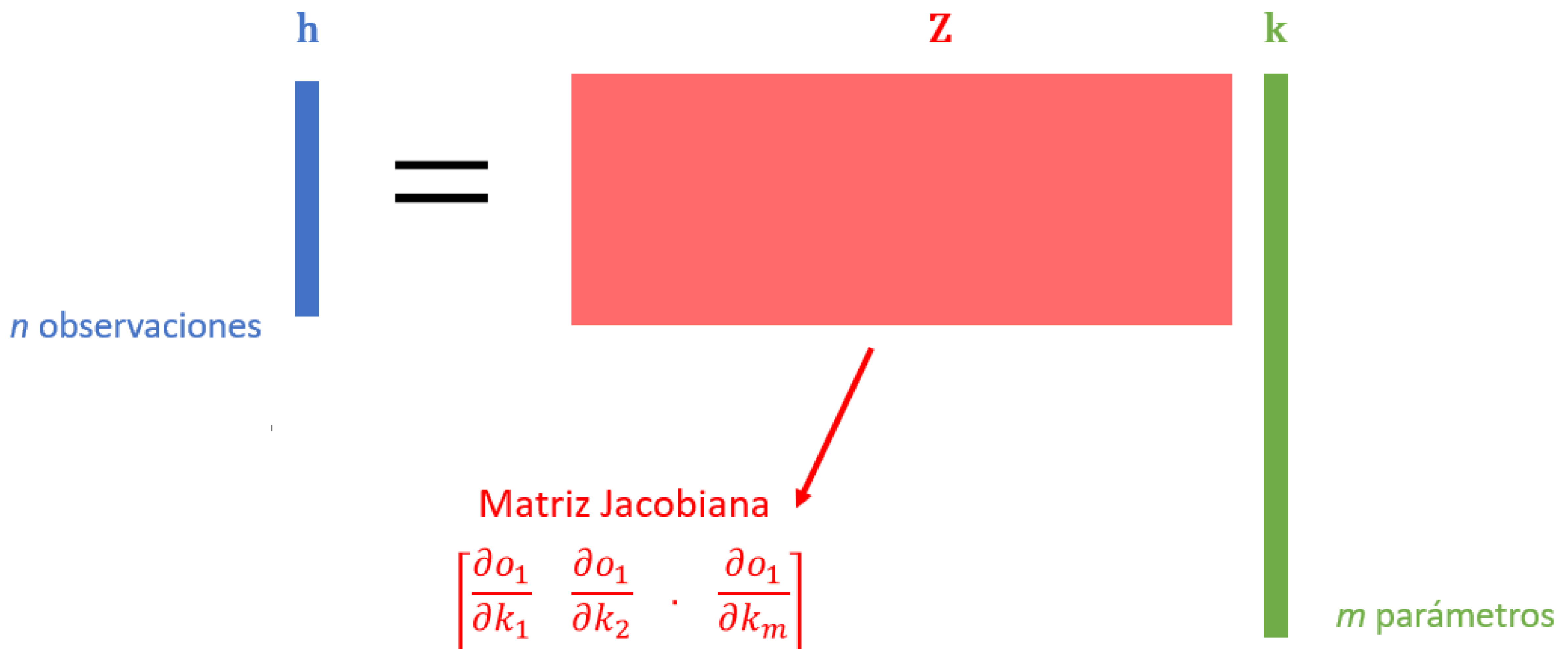
Los procesos hidráulicos y las reglas y condiciones de contorno que los rigen

Propiedades hidráulicas $\bar{\mathbf{k}}$

Asumimos que $\bar{\boldsymbol{\varepsilon}}$ es **0**

PEST/PEST++

$$\mathbf{h} = \mathbf{Z}\mathbf{k}$$

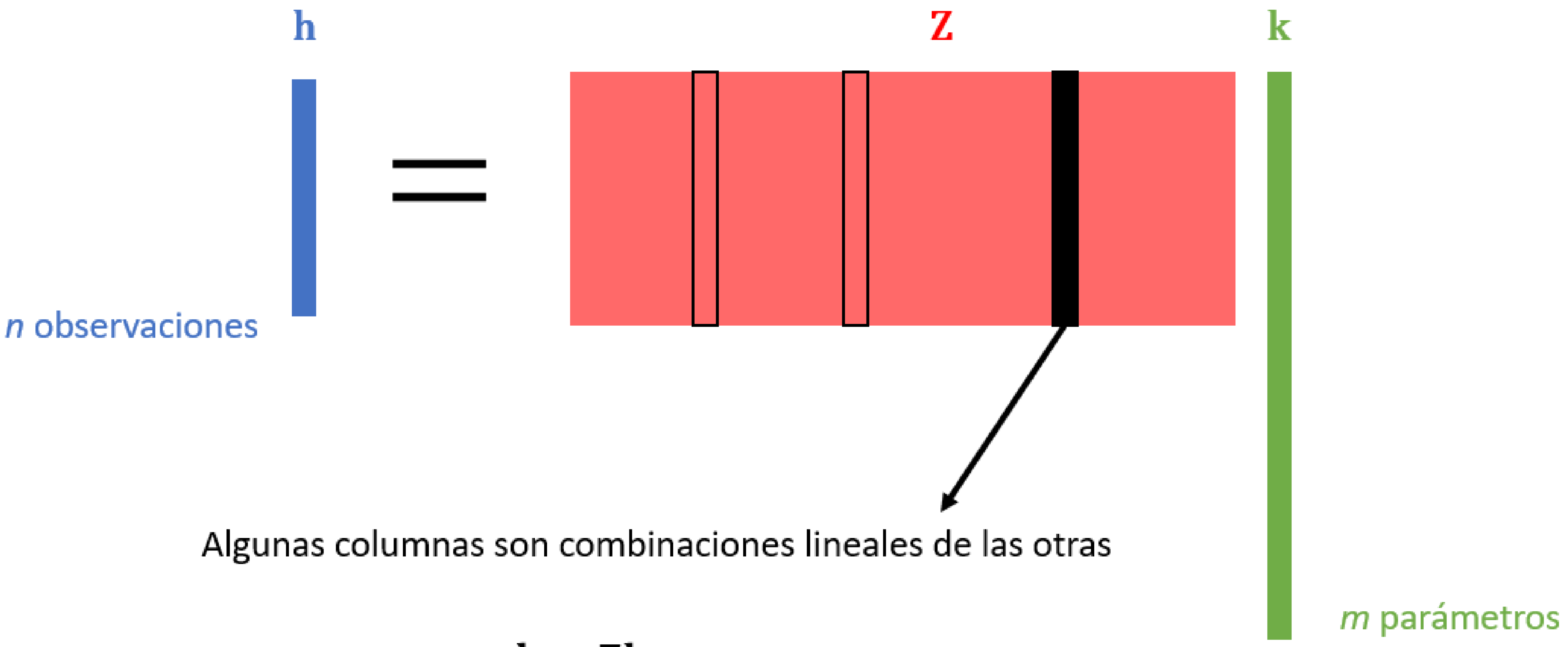


Matriz Jacobiana

$$\begin{bmatrix} \frac{\partial o_1}{\partial k_1} & \frac{\partial o_1}{\partial k_2} & \cdot & \frac{\partial o_1}{\partial k_m} \\ \frac{\partial o_2}{\partial k_1} & \frac{\partial o_2}{\partial k_2} & \cdot & \frac{\partial o_2}{\partial k_m} \\ \frac{\partial o_3}{\partial k_1} & \frac{\partial o_3}{\partial k_2} & \cdot & \frac{\partial o_3}{\partial k_m} \\ \cdot & \cdot & \cdot & \cdot \\ \frac{\partial o_n}{\partial k_1} & \frac{\partial o_n}{\partial k_2} & \cdot & \frac{\partial o_n}{\partial k_m} \end{bmatrix}$$

Espacio nulo

$$\mathbf{h} = \mathbf{Z}\mathbf{k}$$



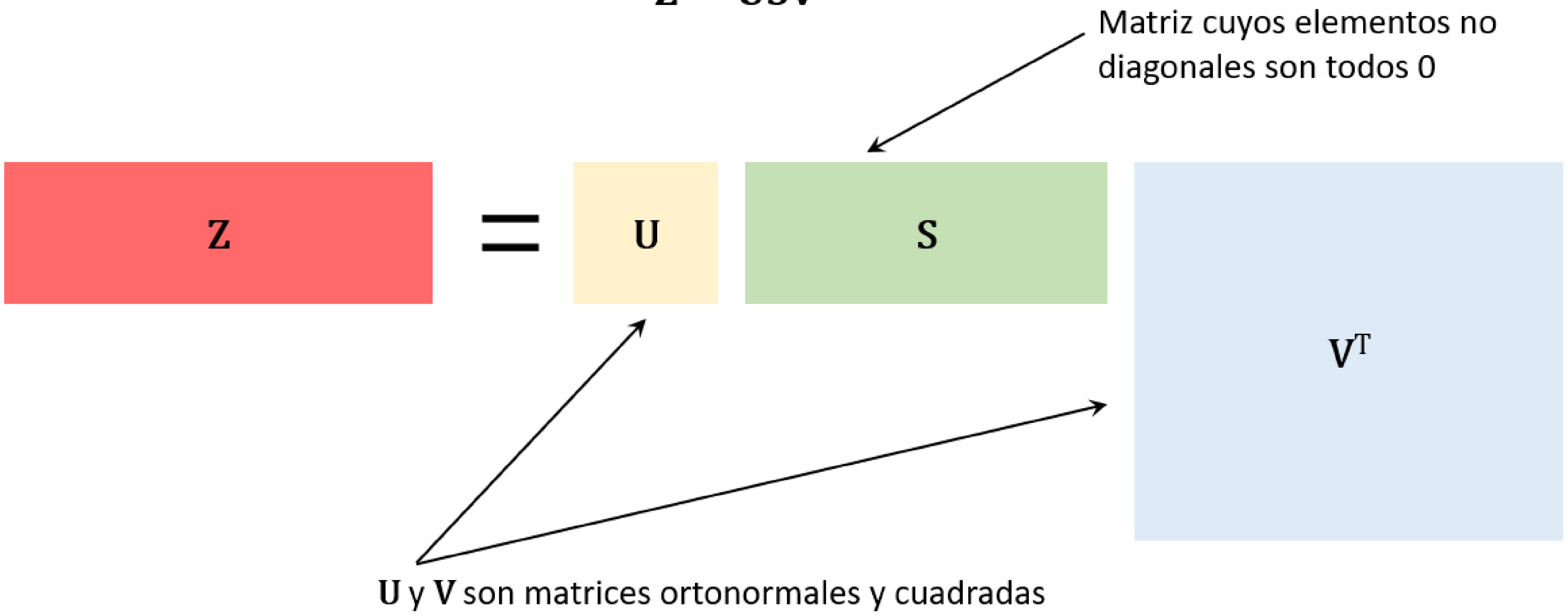
$$\mathbf{h} = \mathbf{Z}\mathbf{k}$$

$$\mathbf{0} = \mathbf{Z}\delta\mathbf{k}$$

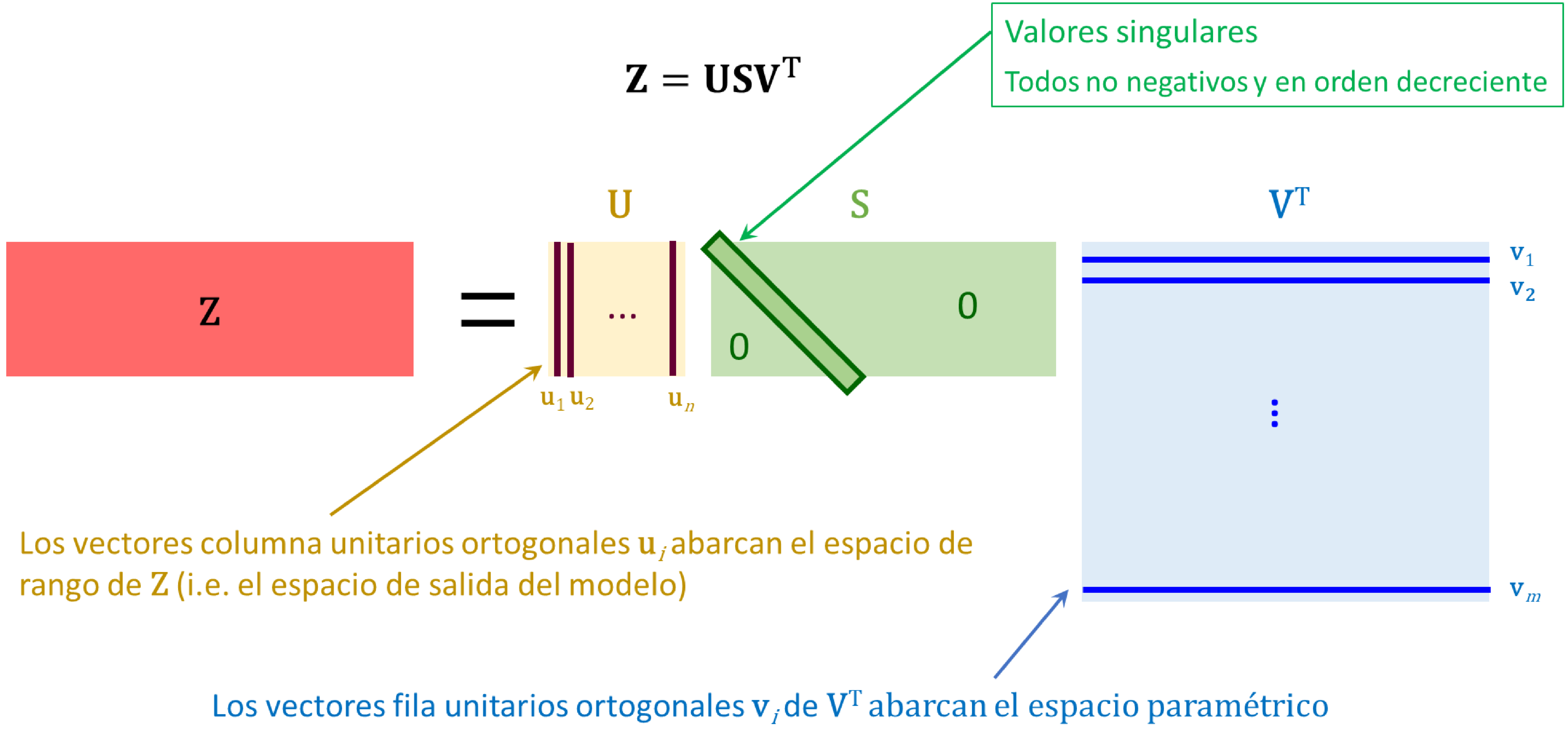
$$\mathbf{h} = \mathbf{Z}(\mathbf{k} + \delta\mathbf{k})$$ → No hay singularidad!
El problema está mal planteado

SVD: Singular Value Decomposition

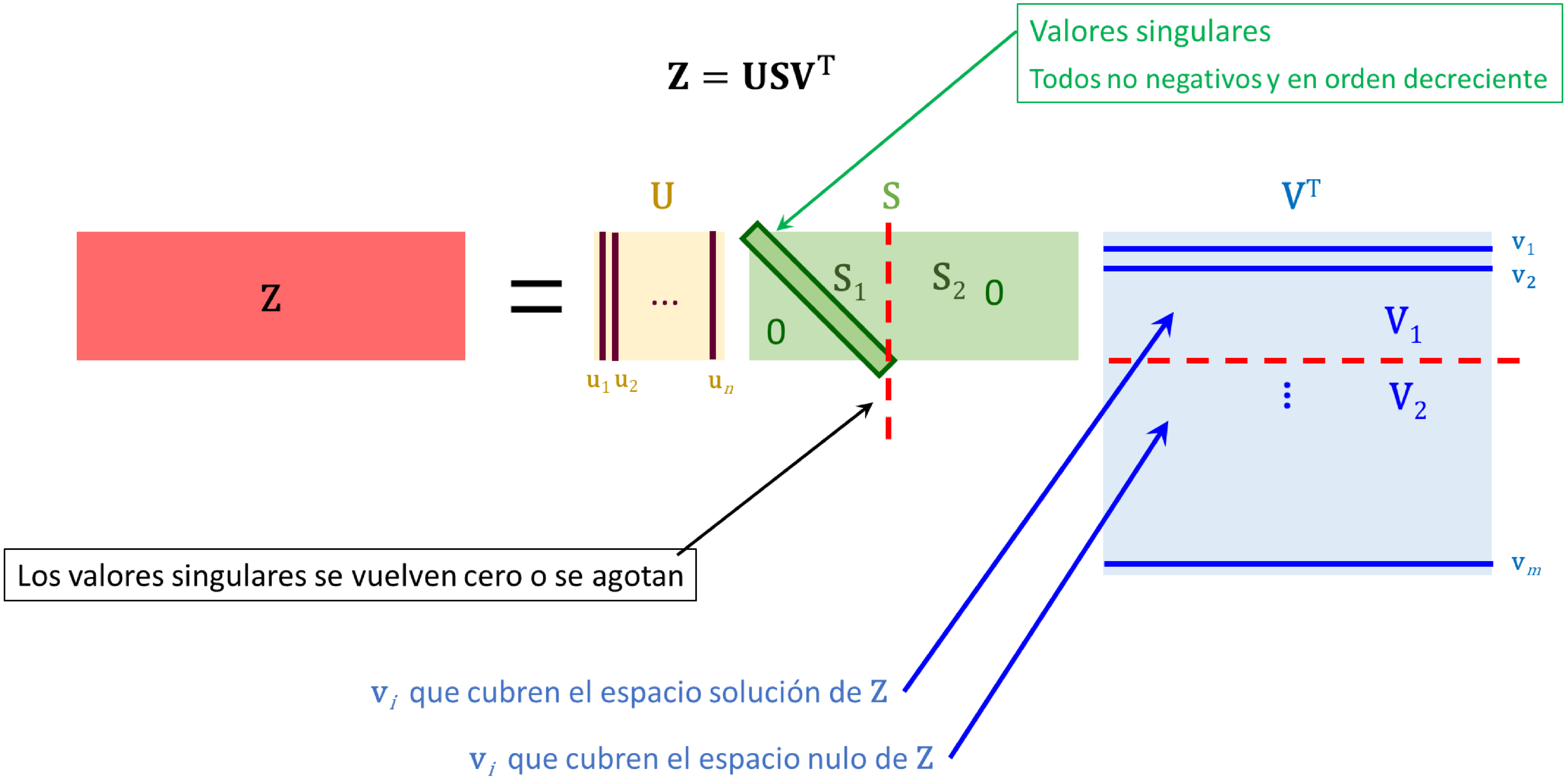
$$\mathbf{Z} = \mathbf{USV}^{\mathrm{T}}$$



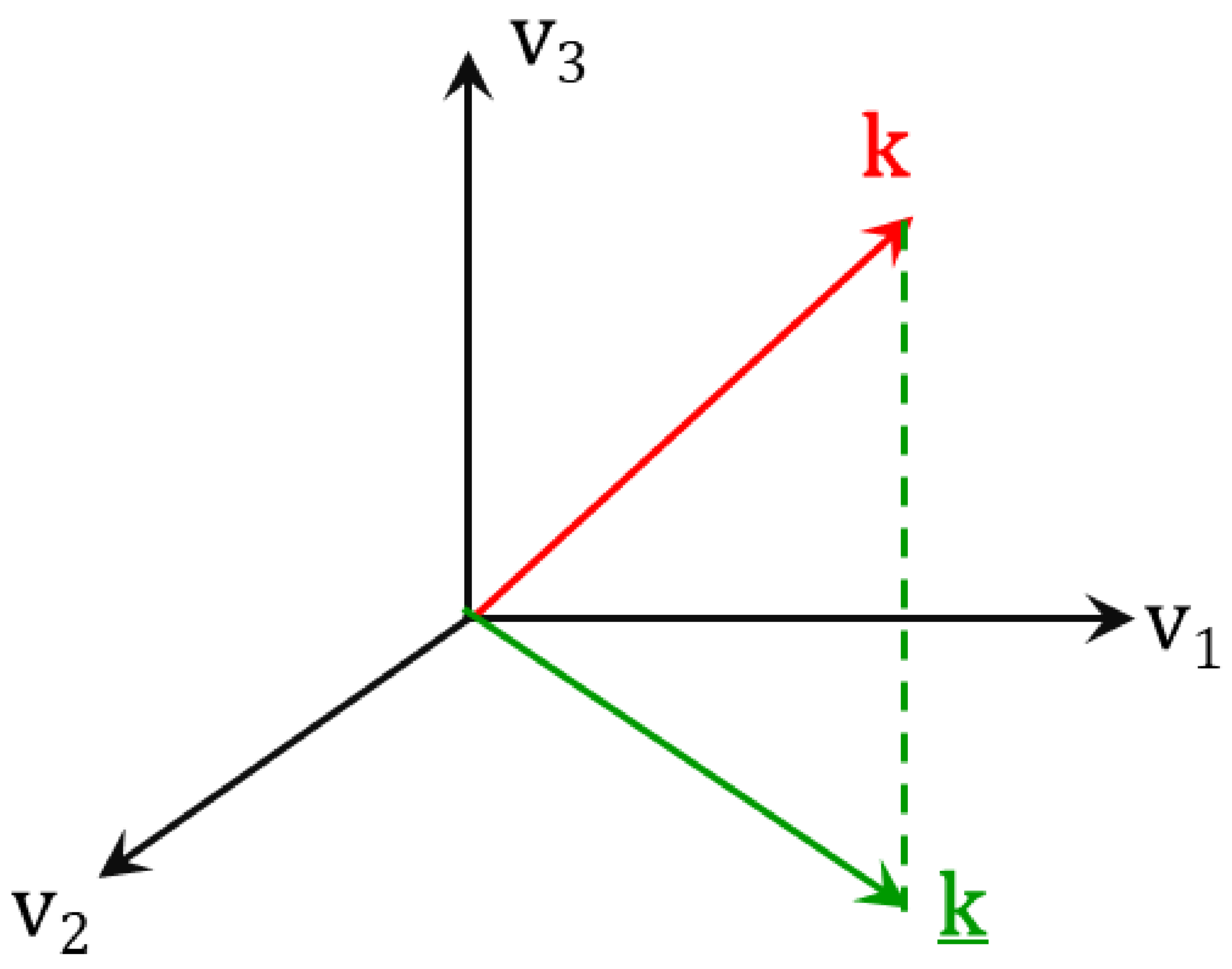
SVD: Singular Value Decomposition



SVD: Singular Value Decomposition

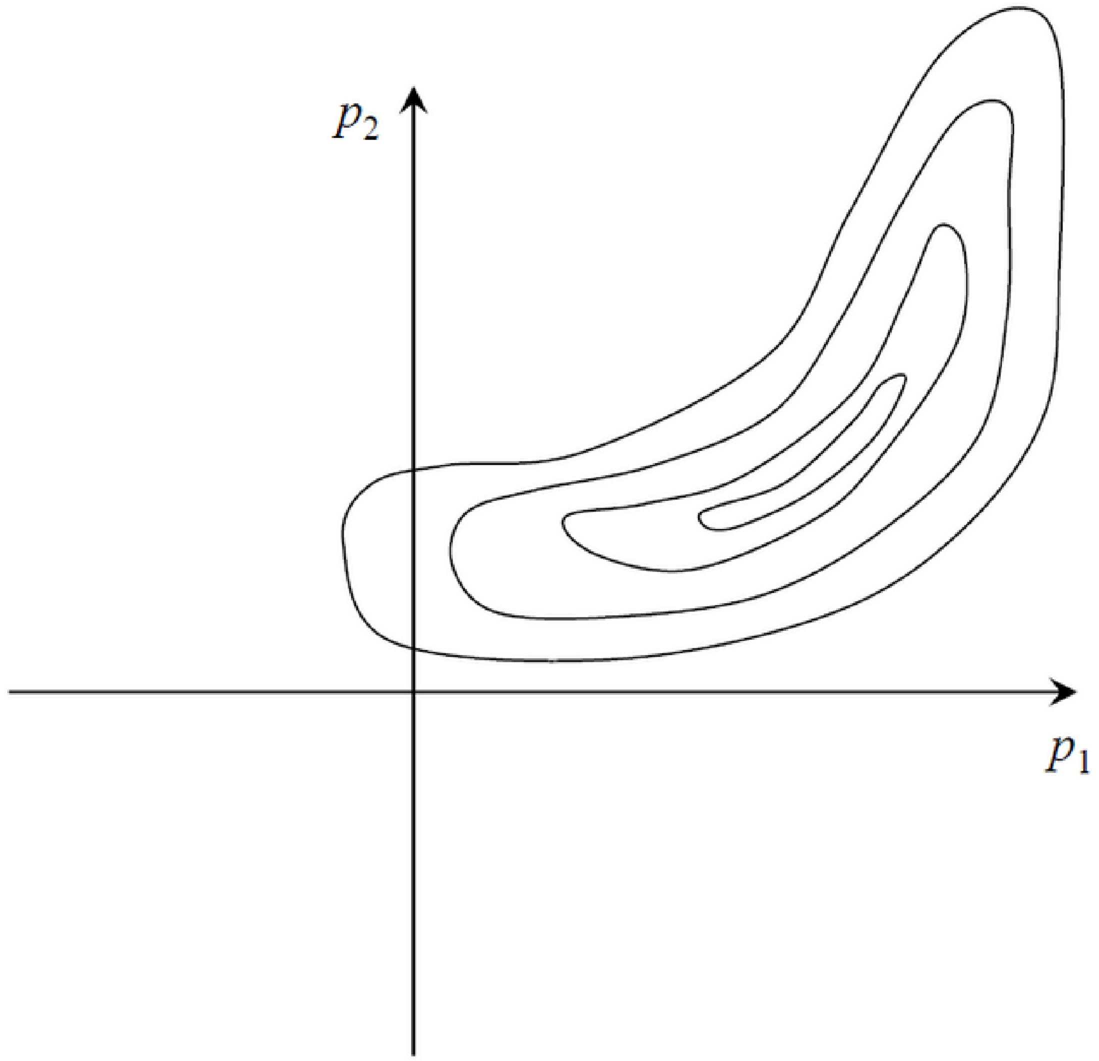


SVD: Singular Value Decomposition



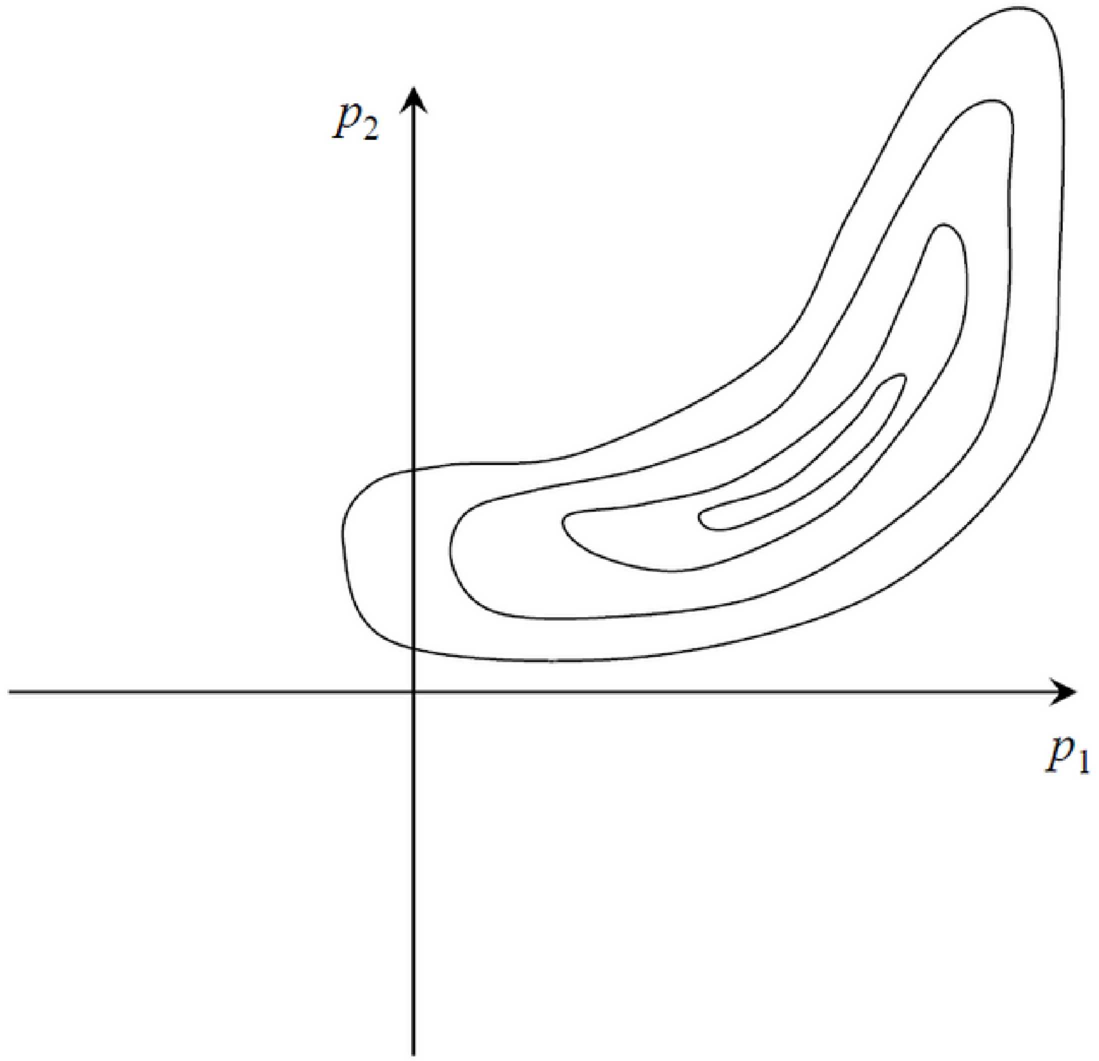
Función objetivo

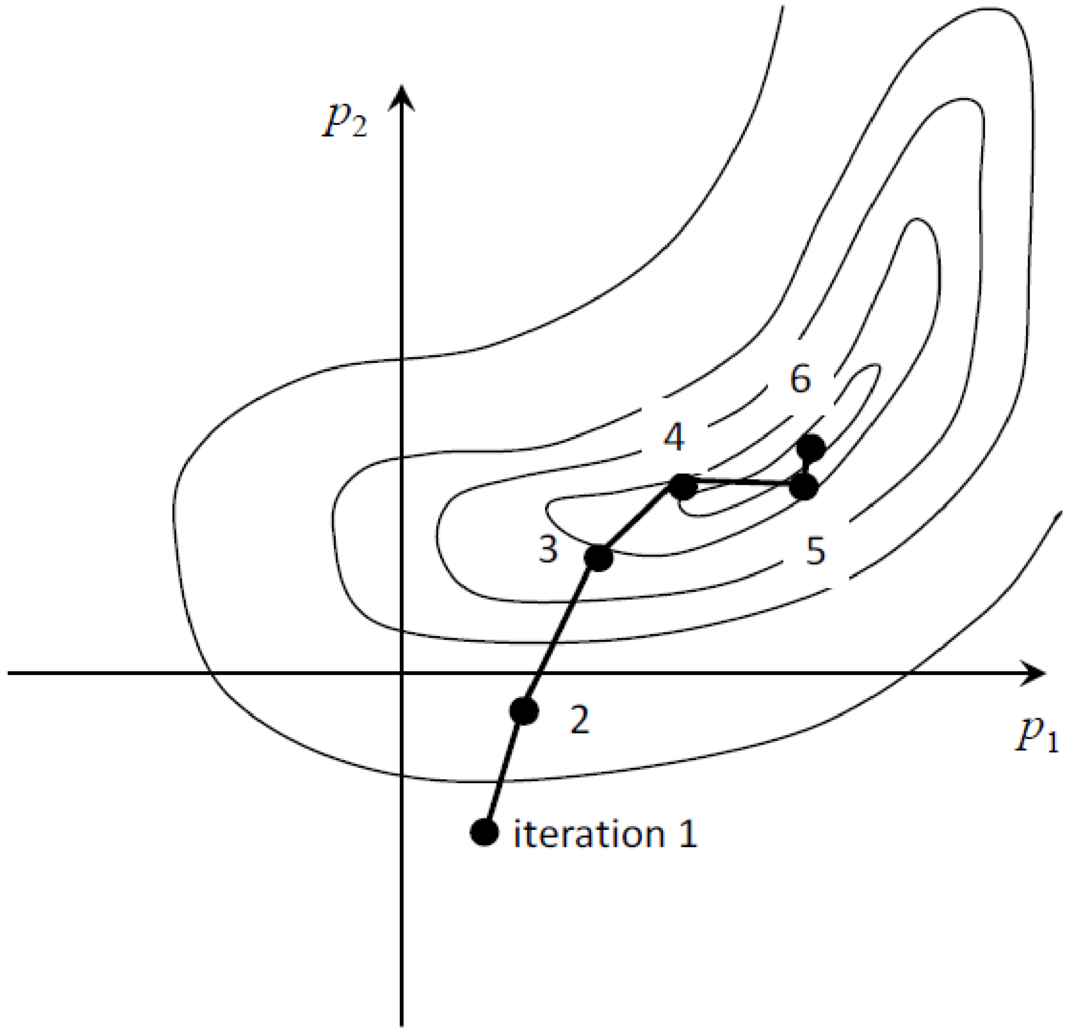
$$\Phi = \sum (w_i r_i)^2$$



Función objetivo

$$\Phi = \sum (w_i r_i)^2$$





$$\Phi = \mathbf{r}^t\mathbf{Q}\mathbf{r} = (\mathbf{h} - \mathbf{X}\mathbf{p})^t\mathbf{Q}(\mathbf{h} - \mathbf{X}\mathbf{p})$$

$$\underline{\mathbf{p}} = (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{h}$$

$$\underline{\mathbf{p}} = (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\mathbf{X}\mathbf{p} + (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\varepsilon$$

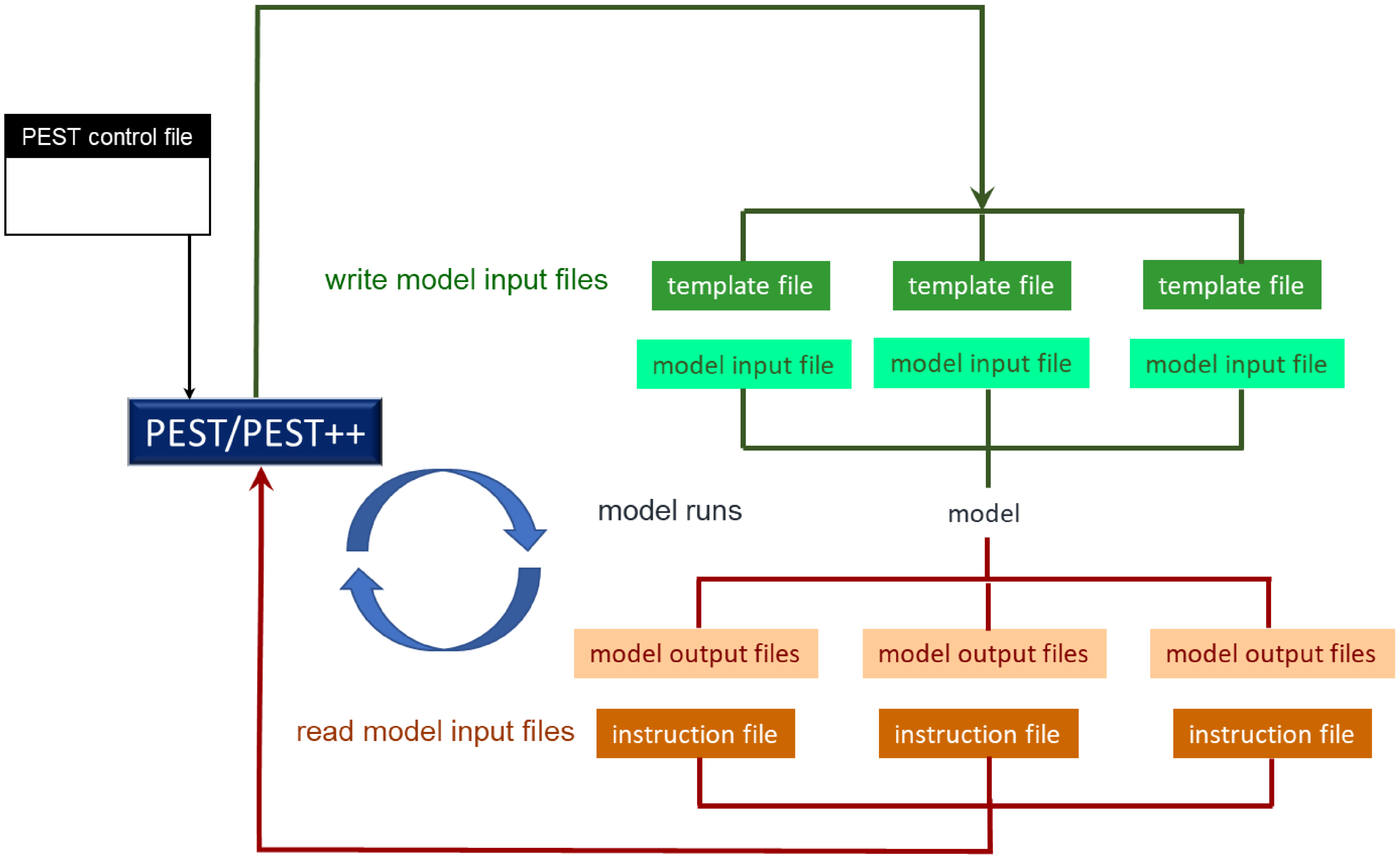
$$\underline{\mathbf{p}} = \mathbf{p} + (\mathbf{X}^t\mathbf{Q}\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Q}\varepsilon$$

$$\mathbf{p} - \mathbf{p}_0 = (\mathbf{J}^t\mathbf{Q}\mathbf{J} + \lambda\mathbf{I})^{-1}\mathbf{J}^t\mathbf{Q}\mathbf{r}$$

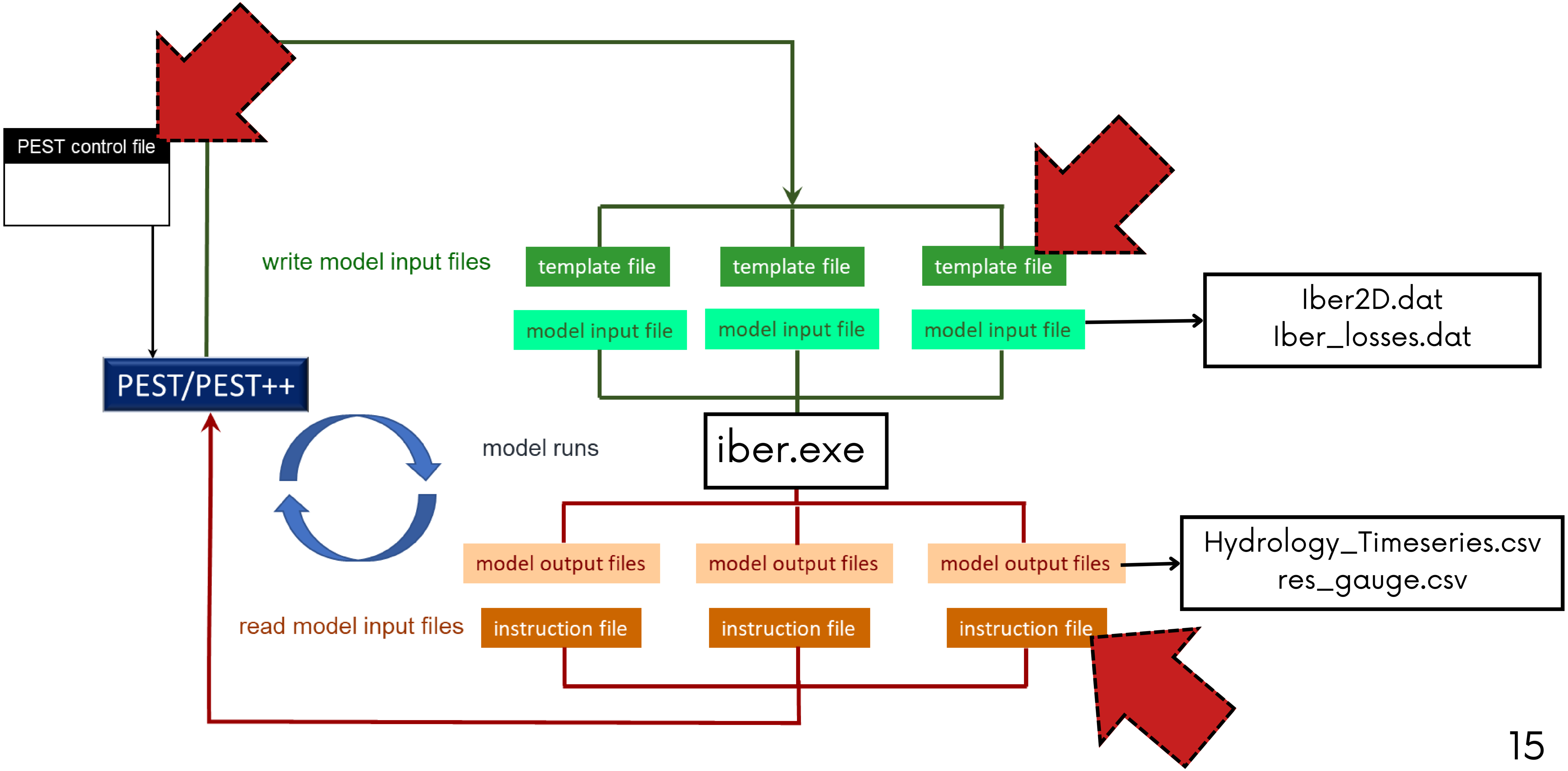
↓

Lambda de Marquardt

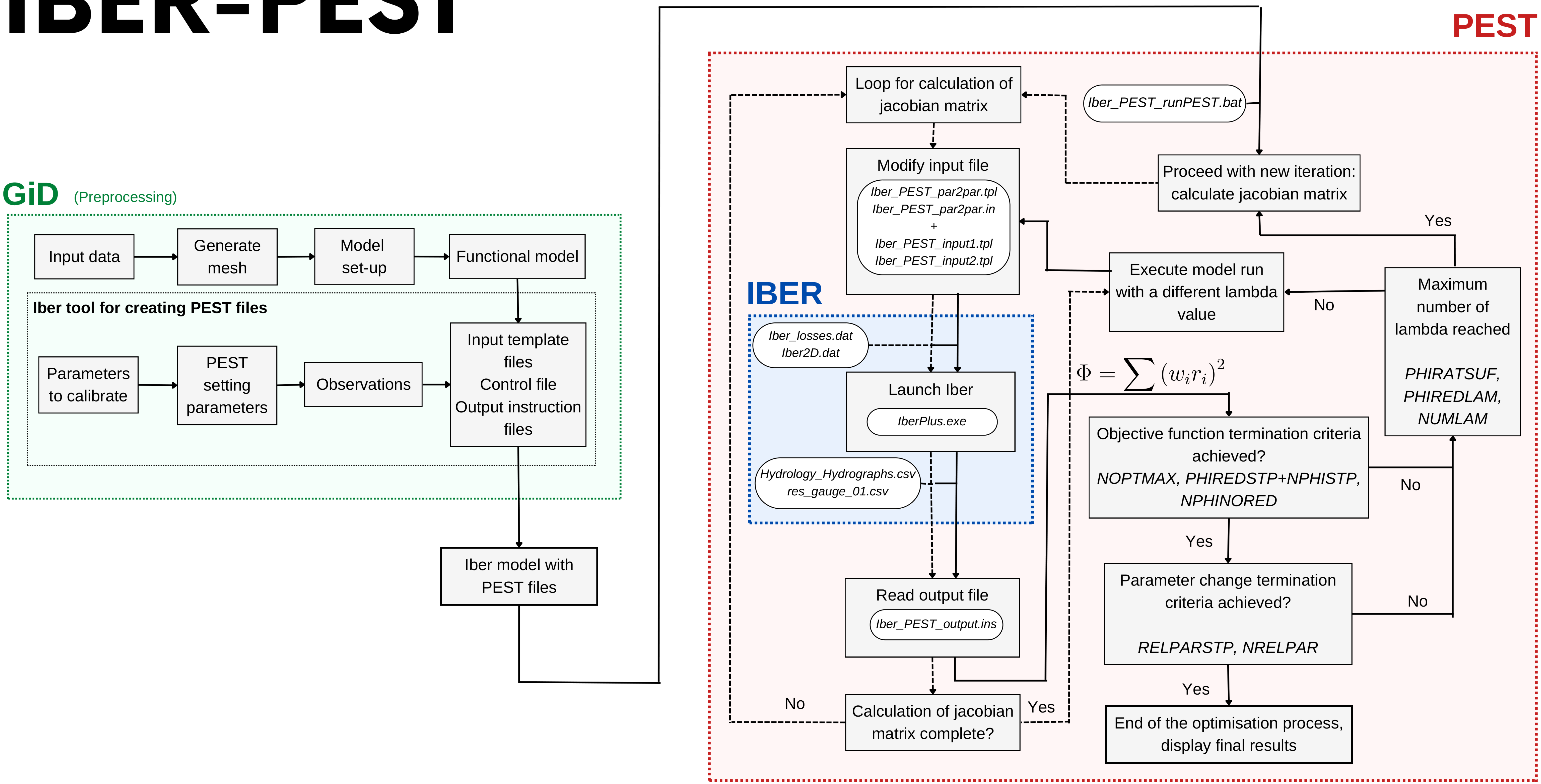
PEST/PEST++


PEST control file
PEST/PEST++
write model input files
template file
template file
template file
model input file
model input file
model input file
model runs
model
model output files
model output files
model output files
read model input files
instruction file
instruction file
instruction file

PEST/PEST++ con Iber

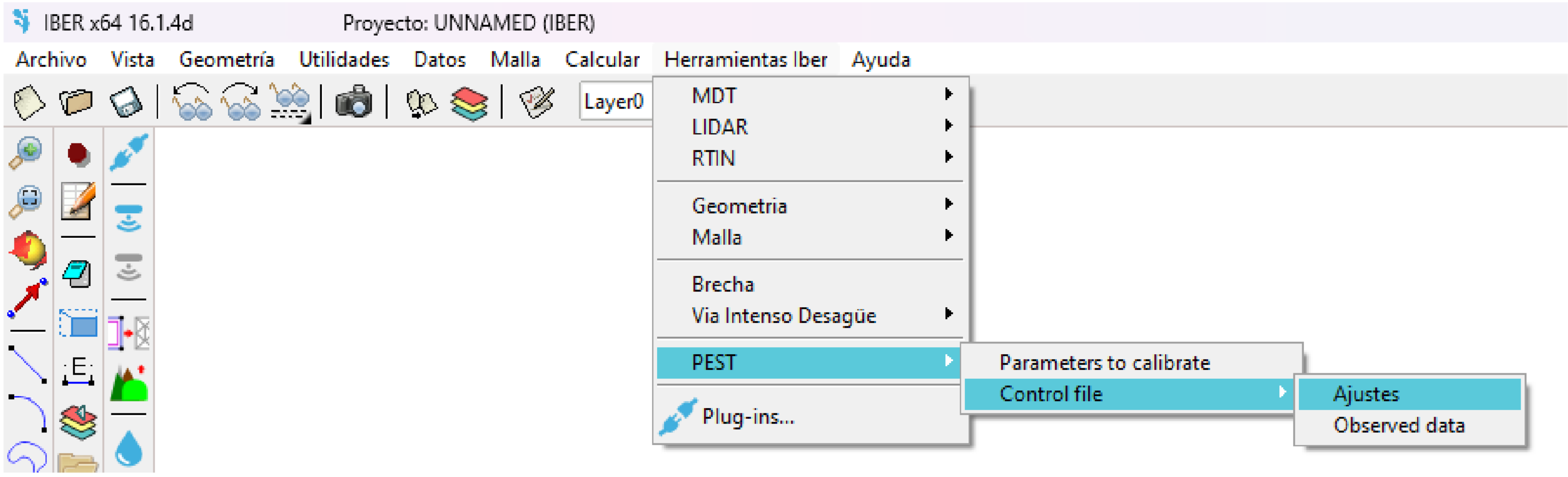


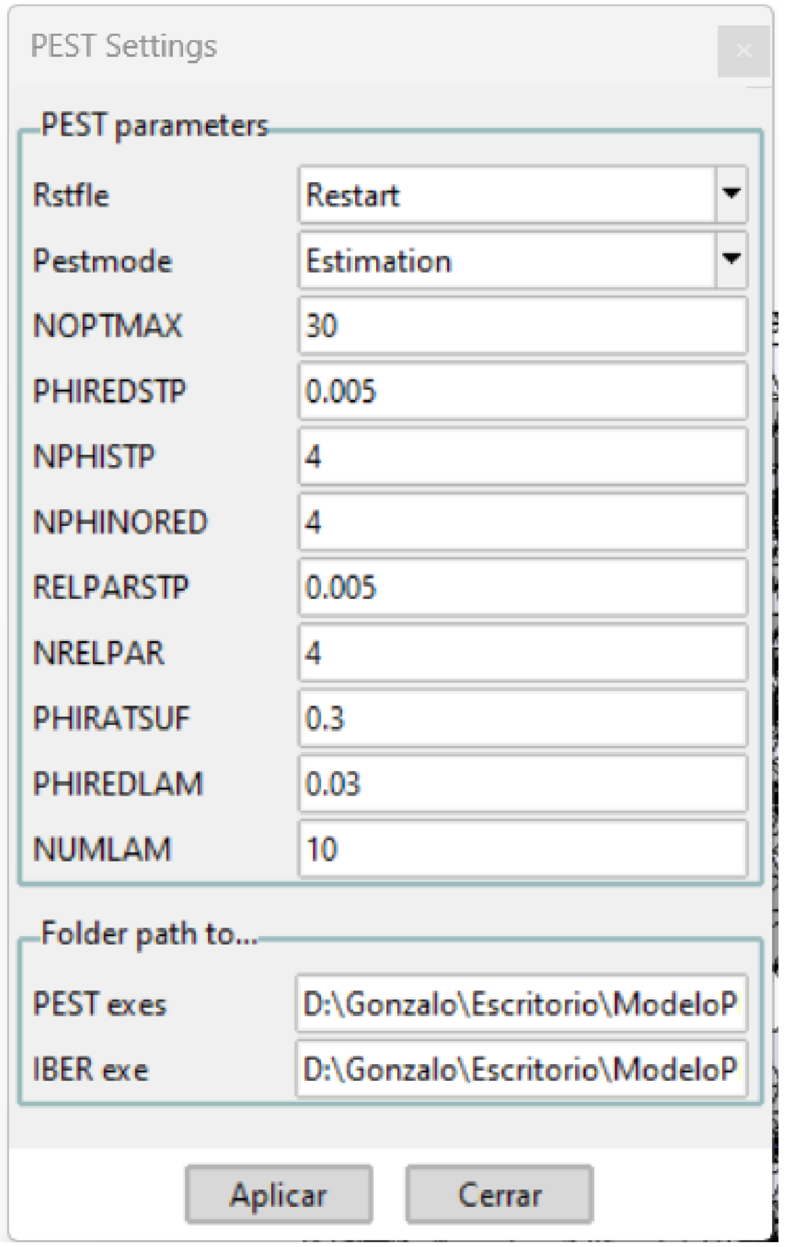
IBER-PEST

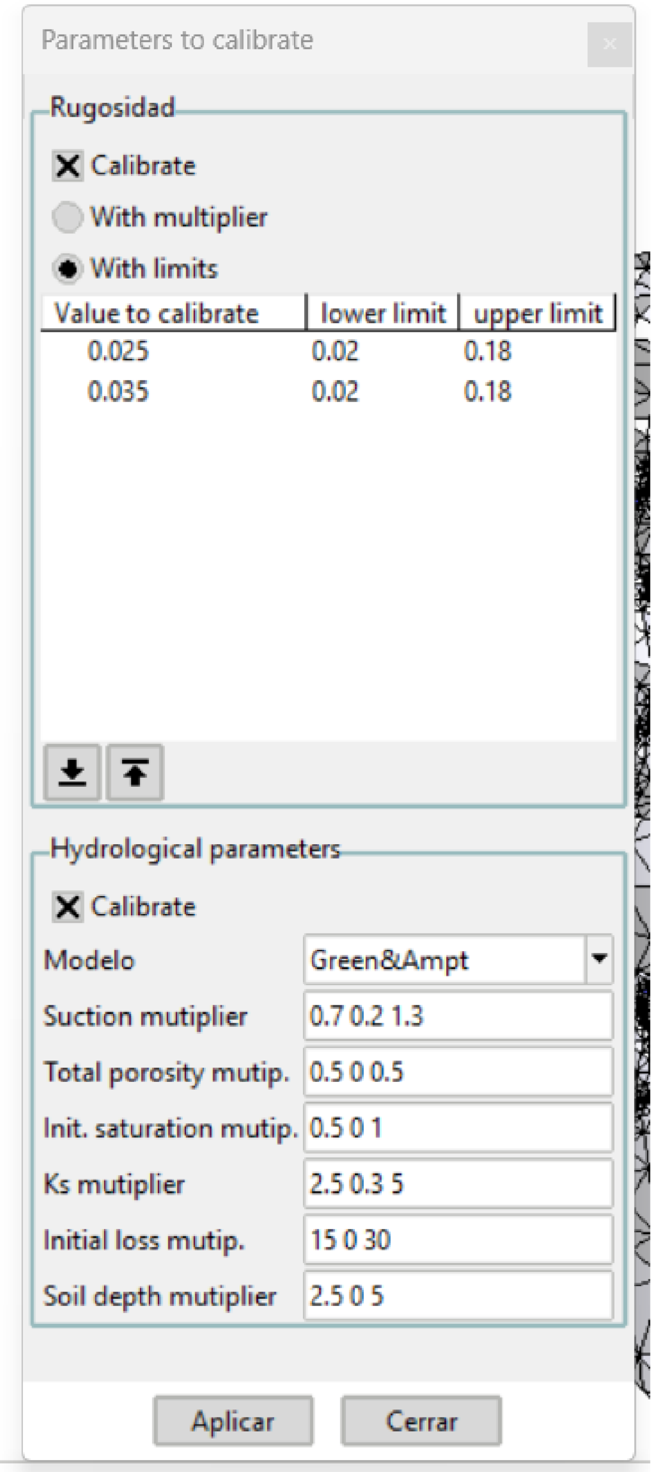


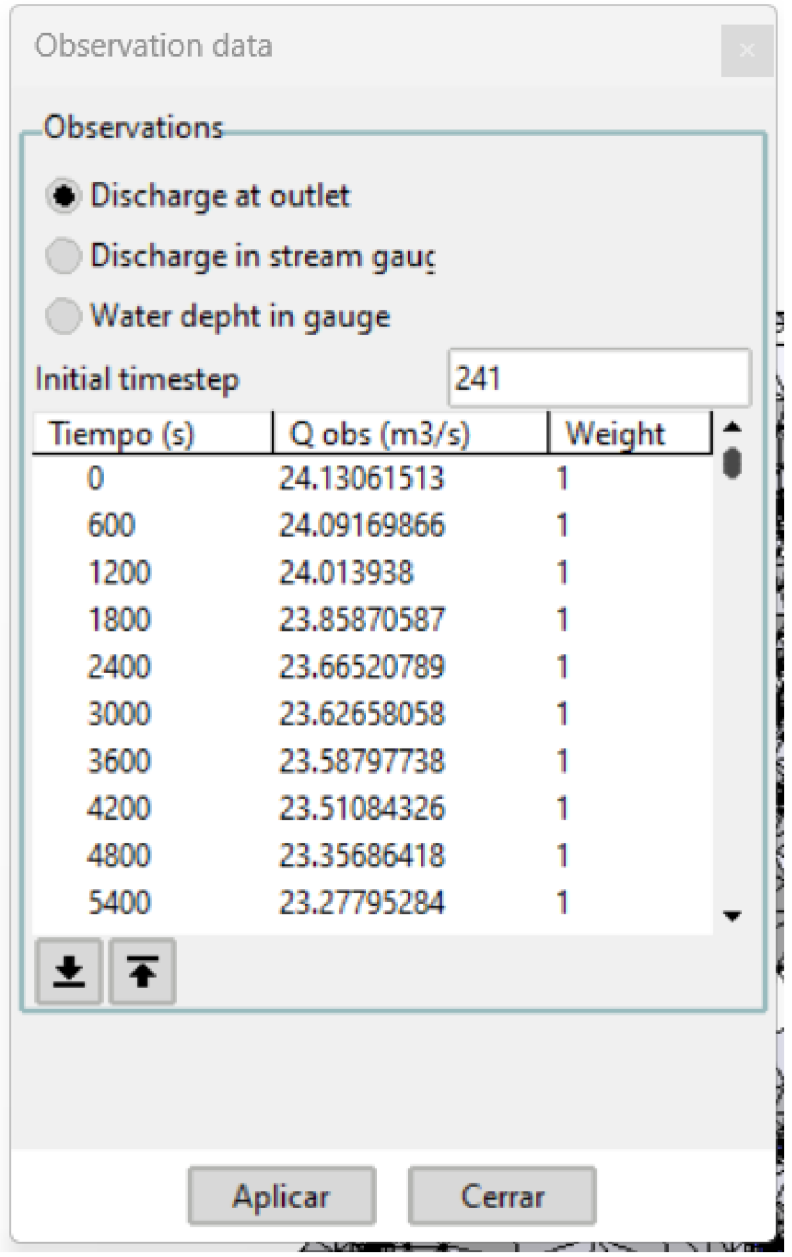
GiD (Preprocessing)
Input data
Generate mesh
Model set-up
Functional model
Iber tool for creating PEST files
Parameters to calibrate
PEST setting parameters
Observations
Input template files
Control file
Output instruction files
Iber model with PEST files
PEST
Loop for calculation of jacobian matrix
Iber_PEST_runPEST.bat
Modify input file
Iber_PEST_par2par.tpl
Iber_PEST_par2par.in
+
Iber_PEST_input1.tpl
Iber_PEST_input2.tpl
Proceed with new iteration: calculate jacobian matrix
Yes
IBER
Execute model run with a different lambda value
No
Maximum number of lambda reached
PHIRATSUF,
PHIREDLAM,
NUMLAM
Iber_losses.dat
Iber2D.dat
Launch Iber
IberPlus.exe
$\Phi = \sum (w_i r_i)^2$
Objective function termination criteria achieved?
NOPTMAX, PHIREDSTP+NPHISTP,
NPHINORED
No
Hydrology_Hydrographs.csv
res_gauge_01.csv
Yes
Read output file
Iber_PEST_output.ins
Parameter change termination criteria achieved?
RELPARSTP, NRELPAR
No
Yes
No
Calculation of jacobian matrix complete?
Yes
End of the optimisation process, display final results

IBER-PEST interfaz

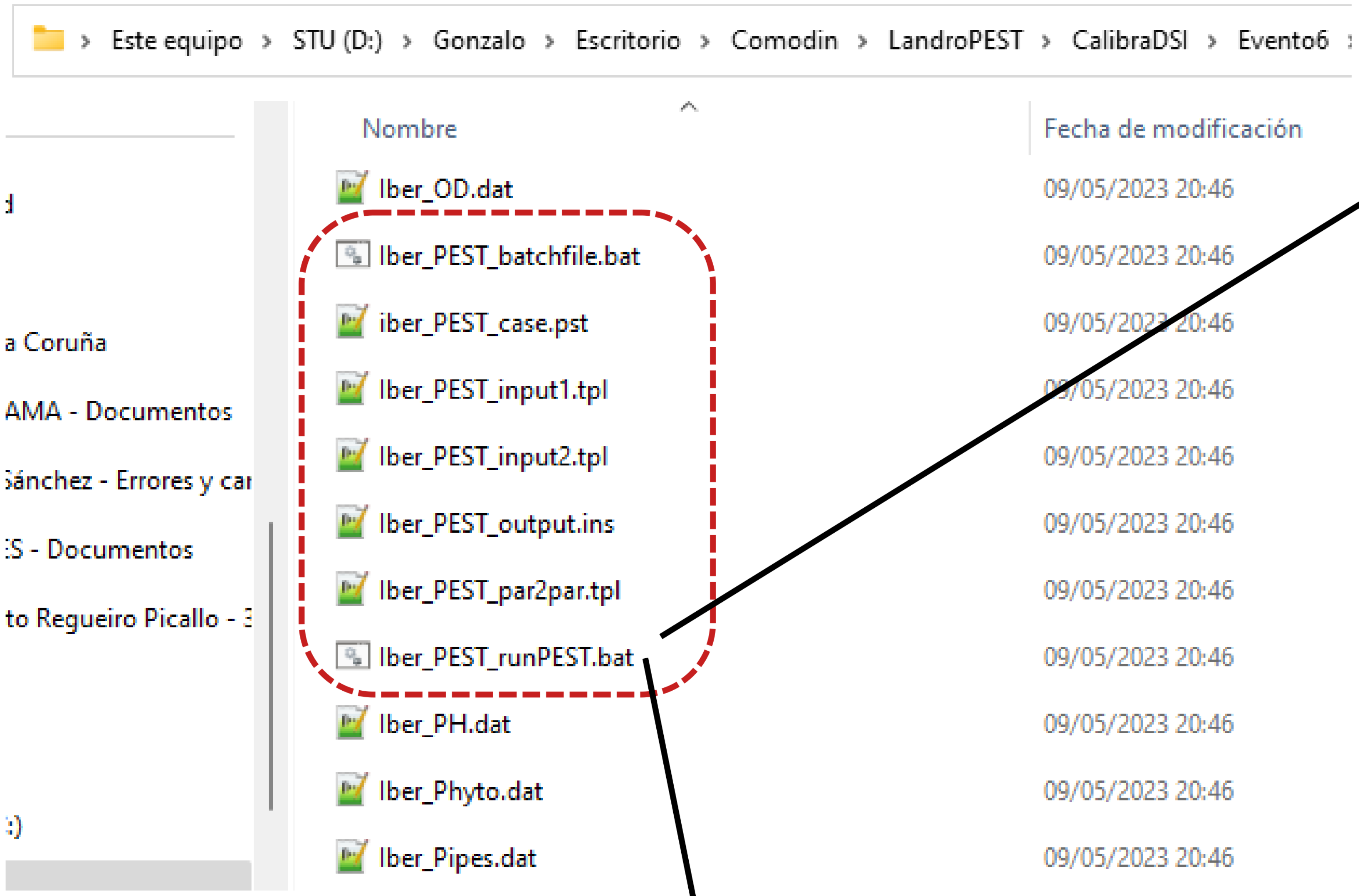








IBER-PEST ejecución

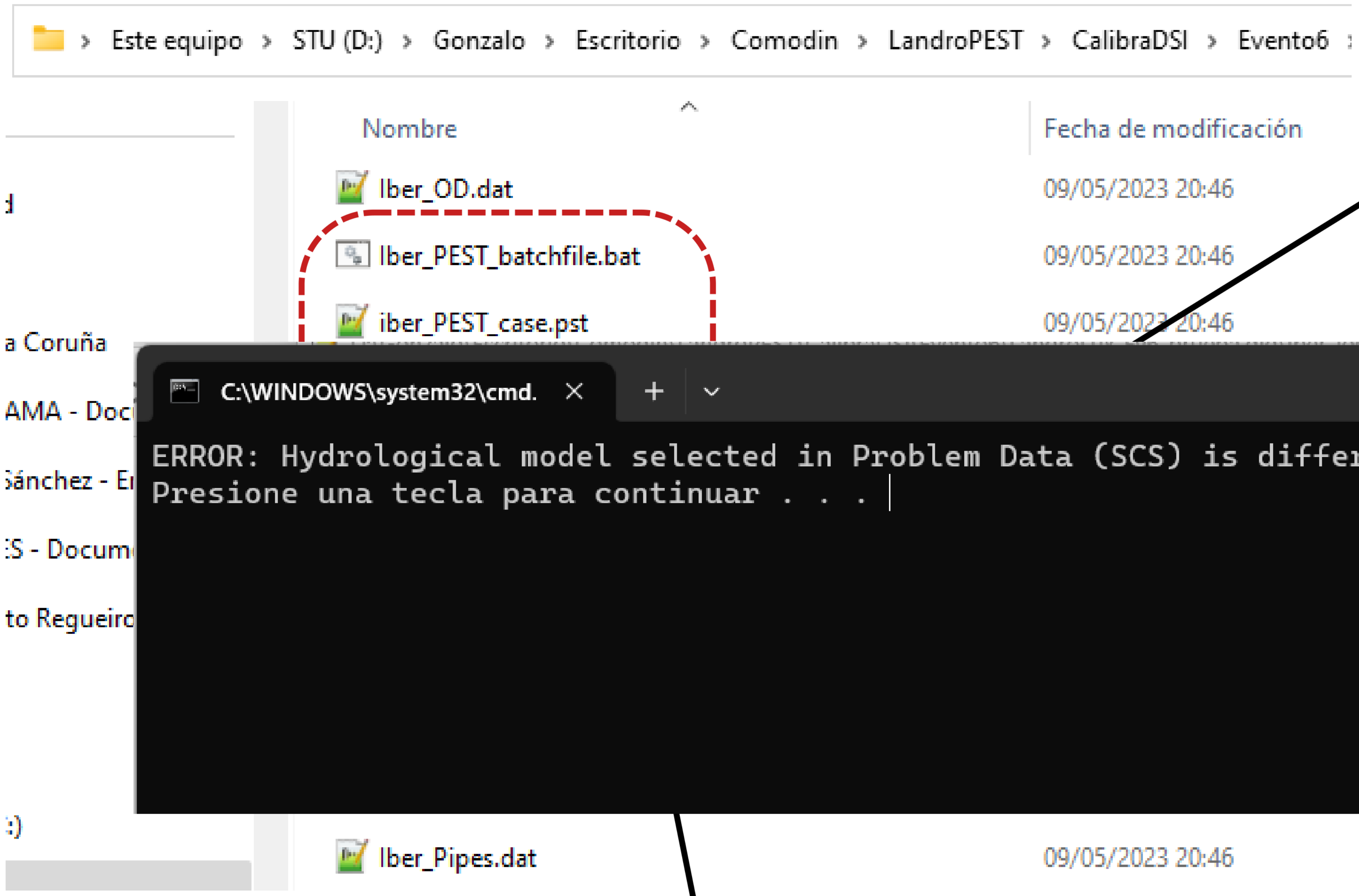


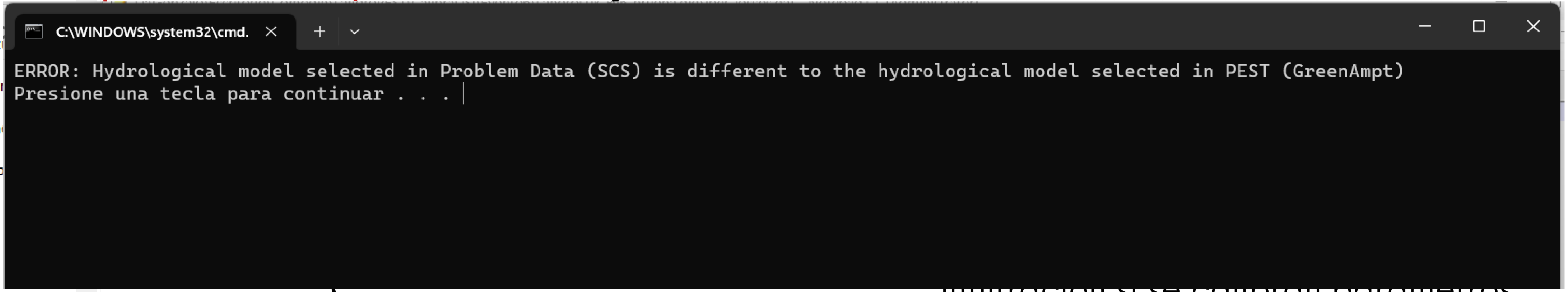
Ejecuto IBER-PEST
haciendo doble click aquí

Comprobaciones:

- Pestchek
- Intervalo de tiempo de observaciones coincide con el intervalo de escritura del modelo
- Número de observaciones coincide con el número de outputs de Iber con los que comparar
- Modelo de infiltración elegido coincide con los parámetros a calibrar
- Activado el cálculo de pérdidas con infiltración si se calibran parámetros hidrológicos

IBER-PEST ejecución





Comprobaciones:

- Pestchek
- Intervalo de tiempo de observaciones coincide con el intervalo de escritura

infiltración si se calibran parámetros hidrológicos

Ejecuto IBER-PEST
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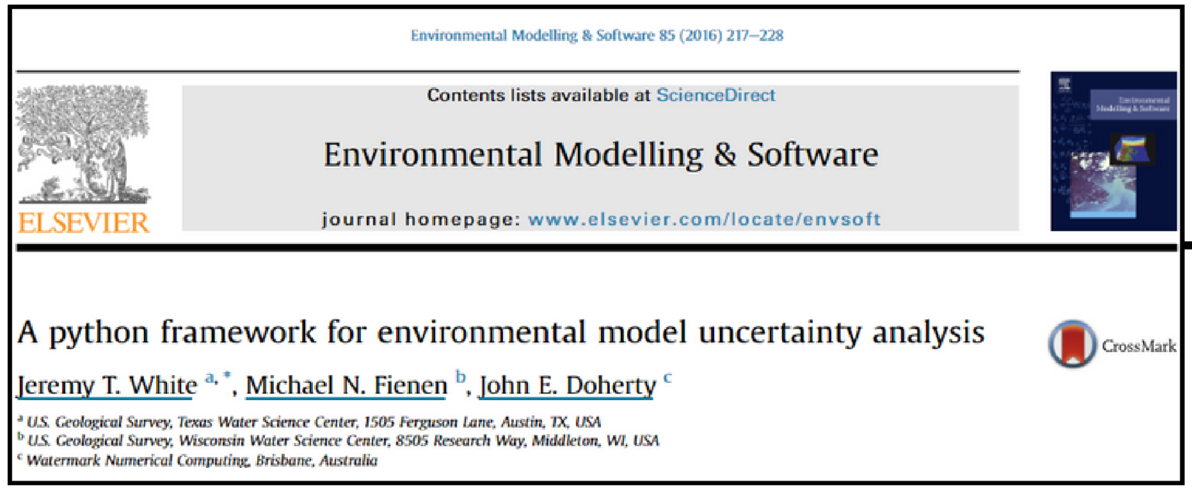
IBER-PEST + PyEMU


Environmental Modelling & Software 85 (2016) 217–228

Contents lists available at ScienceDirect

Environmental Modelling & Software

journal homepage: www.elsevier.com/locate/envsoft

ELSEVIER

A python framework for environmental model uncertainty analysis

Jeremy T. White [a,*], Michael N. Fienen [b], John E. Doherty [c]

[a] U.S. Geological Survey, Texas Water Science Center, 1505 Ferguson Lane, Austin, TX, USA
[b] U.S. Geological Survey, Wisconsin Water Science Center, 8505 Research Way, Middleton, WI, USA
[c] Watermark Numerical Computing, Brisbane, Australia

pyEMU

python modules for model-independent FOSM (first-order, second-moment) (a.k.a linear-based, a.k.a. Bayes linear) uncertainty analyses and data-worth analyses, non-linear uncertainty analyses and interfacing with PEST and PEST++. pyEMU also has a pure python (pandas and numpy) implementation of ordinary kriging for geostatistical interpolation and support for generating high-dimensional PEST(++) model interfaces, including support for (very) high-dimensional ensemble generation and handling

<u>Algunas utilidades para IBER-PEST</u>:

- Representar el resultado de PEST sin tener que bucear entre los txts

```
import matplotlib.pyplot as plt
import pyemu
pst = pyemu.Pst("my.pst")
pyemu.plot_utils.phi_progress(pst)
plt.show()
```

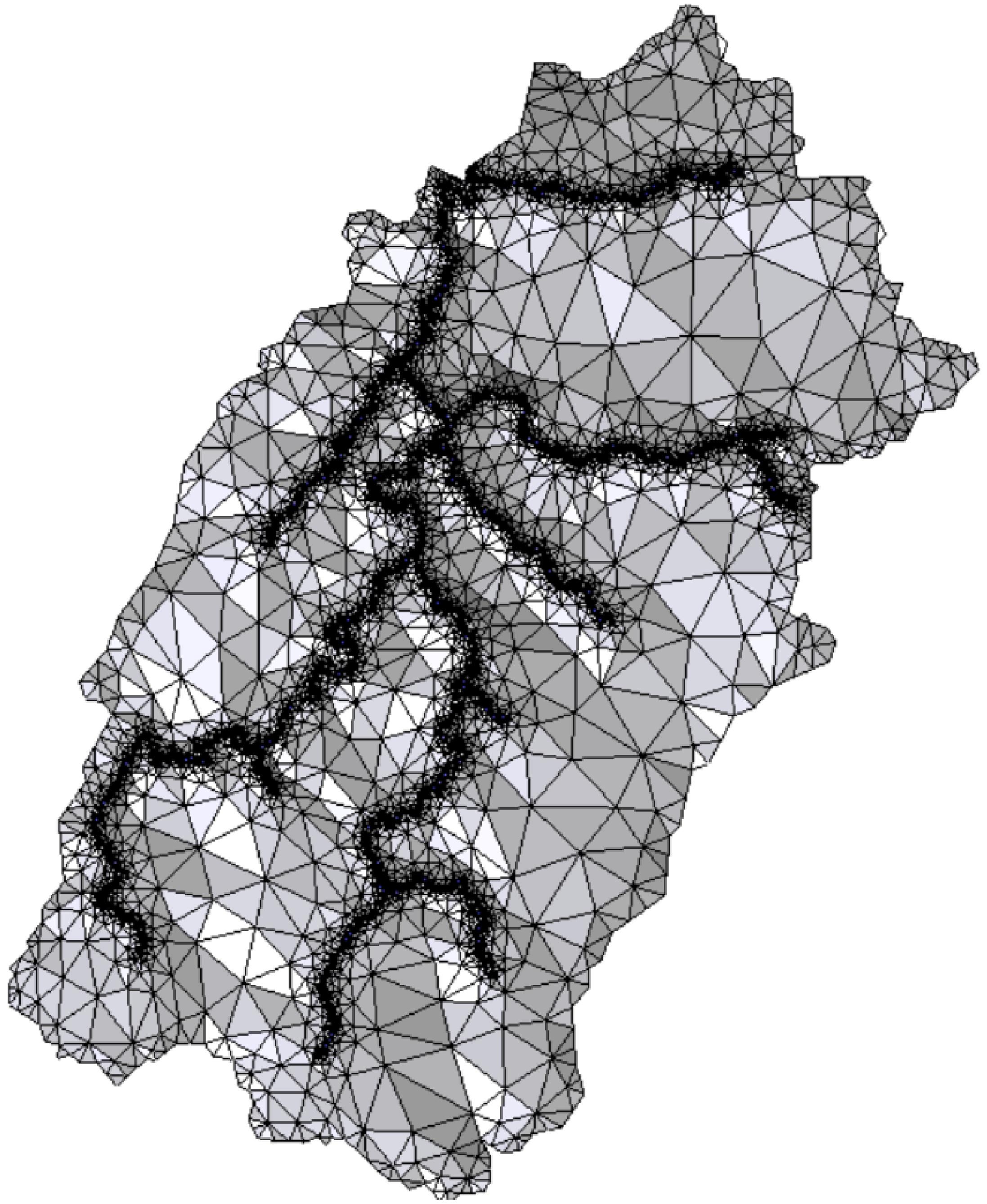
- Editar los txts de PEST sin tener que conocer la posición de cada una de las variables

```
pst = pyemu.Pst("my.pst")
pst.control_data.noptmax = -1
pst.write("my_new.pst")
```

- Crear nuevos txts necesarios para ejecutar otras funciones de PEST

```
cov = pyemu.Cov.from_parameter_data(pst)
cov.to_uncfile("my.unc")
```

Caso de estudio



Río Landro

200 km2
15K elementos
4 parámetros por elemento
1 ejecución = 3-10 min
Observación: caudal a la salida

Parámetro	Rango variación
Ks	[0, 10]
Sro	[0, 1]
Initial losses	[0, 40]
Multiplicador Manning	[0.5, 5]

IBER-PEST: Inputs

iber_PEST_case.pst | iber_pest_case.rec | iber_pest_case.par | iber_pest_case.obs+

```
pcf
* control data
restart estimation
4 289 4 0    1
1    1    single  point    1    0    0
10.0     2.0 0.3 0.03     10
10.0     10.0     0.001
0.1
30   0.005    4    4    0.005    4
1    1    1
* singular value decomposition
1
4 5.0e-7
0
* parameter groups
Satmul  relative    0.01    0.01    switch  2.0 parabolic
Ksmul   relative    0.01    0.01    switch  2.0 parabolic
Losmul  relative    0.01    0.01    switch  2.0 parabolic
Mannin  relative    0.01  0.01  switch  2.0 parabolic
* parameter data
sam log factor  0.5 1e-10 1 Satmul   1.0 0.0 1
ksm log factor  1 1e-10 10  Ksmul    1.0 0.0 1
lom log factor  5 1e-10 40  Losmul   1.0 0.0 1
mam log factor  1 0.5 5 Mannin  1.0 0.0 1
* observation groups
Obs
* observation data
obs1    16.66545708 16.66545708     Obs
obs2    16.56030677 16.56030677     Obs
```

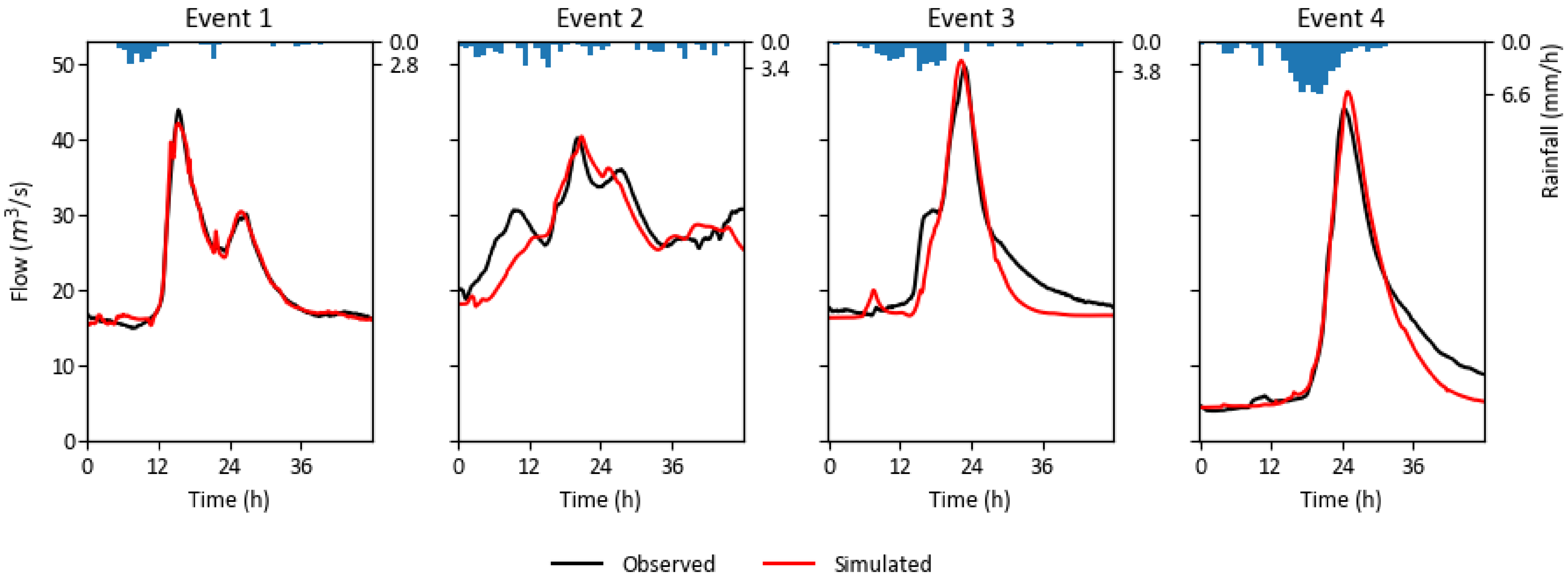
Iber_PEST_par2par.tpl | iber_PEST_case.pst | iber_pest_case

```
ptf $
* parameter data
msa = $    sam  $
mks = $    ksm  $
mlo = $    lom  $
n1 = 0.025 * $   mam  $
n2 = 0.04 * $   mam  $
n3 = 0.035 * $   mam  $
n4 = 0.045 * $   mam  $
n5 = 0.07 * $   mam  $
n6 = 0.065 * $   mam  $
* template and model input files
Iber_PEST_input1.tpl     Iber_losses.dat
Iber_PEST_input2.tpl     Iber2D.dat
* control data
single point
```

Iber_PEST_input2.tpl | iber_pest_control.svd | iber_pest_control.sen | Iber_PEST_output.ins | Hydrol

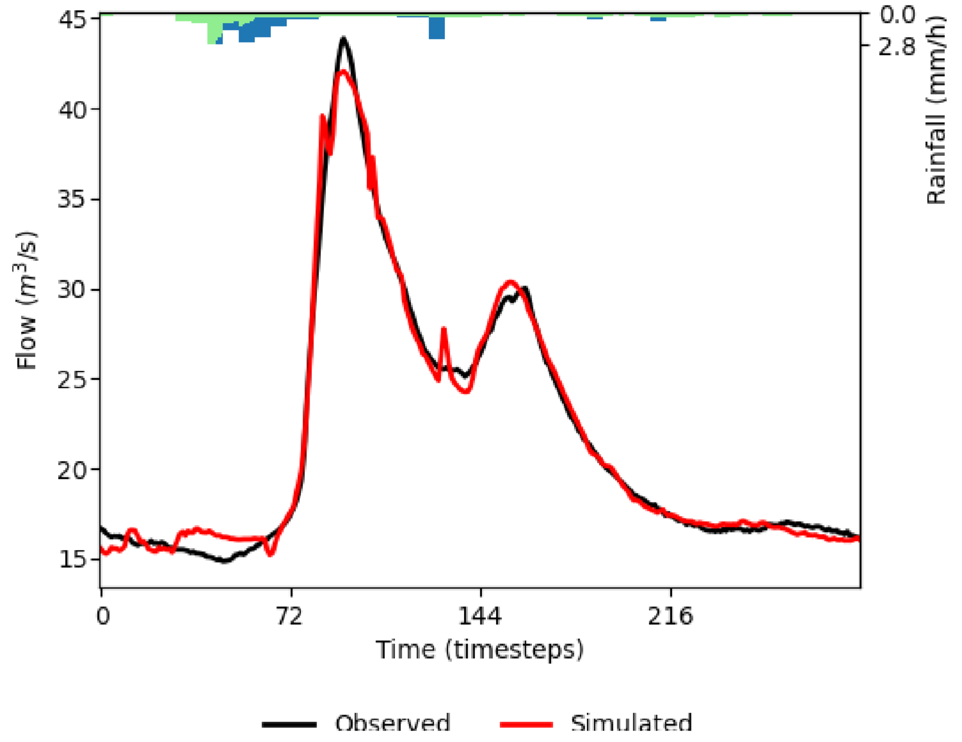
```
ptf #
LandroLux_Ev6
10 388800 600 101 0.7 0.0001 0 0 0 0 0 Disabled 600
MATRIU
     15894
      2851      2858      2860      2851     #n1    #      1
      5472      5475      5474      5472     #n1    #      2
      6011      6022      6027      6011     #n1    #      3
       750       744       754       750     #n1    #      4
      7466      7469      7458      7466     #n1    #      5
      5855      5853      5841      5855     #n1    #      6
      2884      2876      2868      2884     #n1    #      7
      1821      1831      1797      1821     #n1    #      8
      4365      4357      4359      4365     #n1    #      9
      4853      4856      4840      4853     #n1    #     10
       590       591       600       590     #n1    #     11
      5995      6011      6004      5995     #n1    #     12
```

IBER-PEST: Resultados



NSE			
Ev 1	Ev 2	Ev 3	Ev 4
0.989	0.606	0.886	0.950

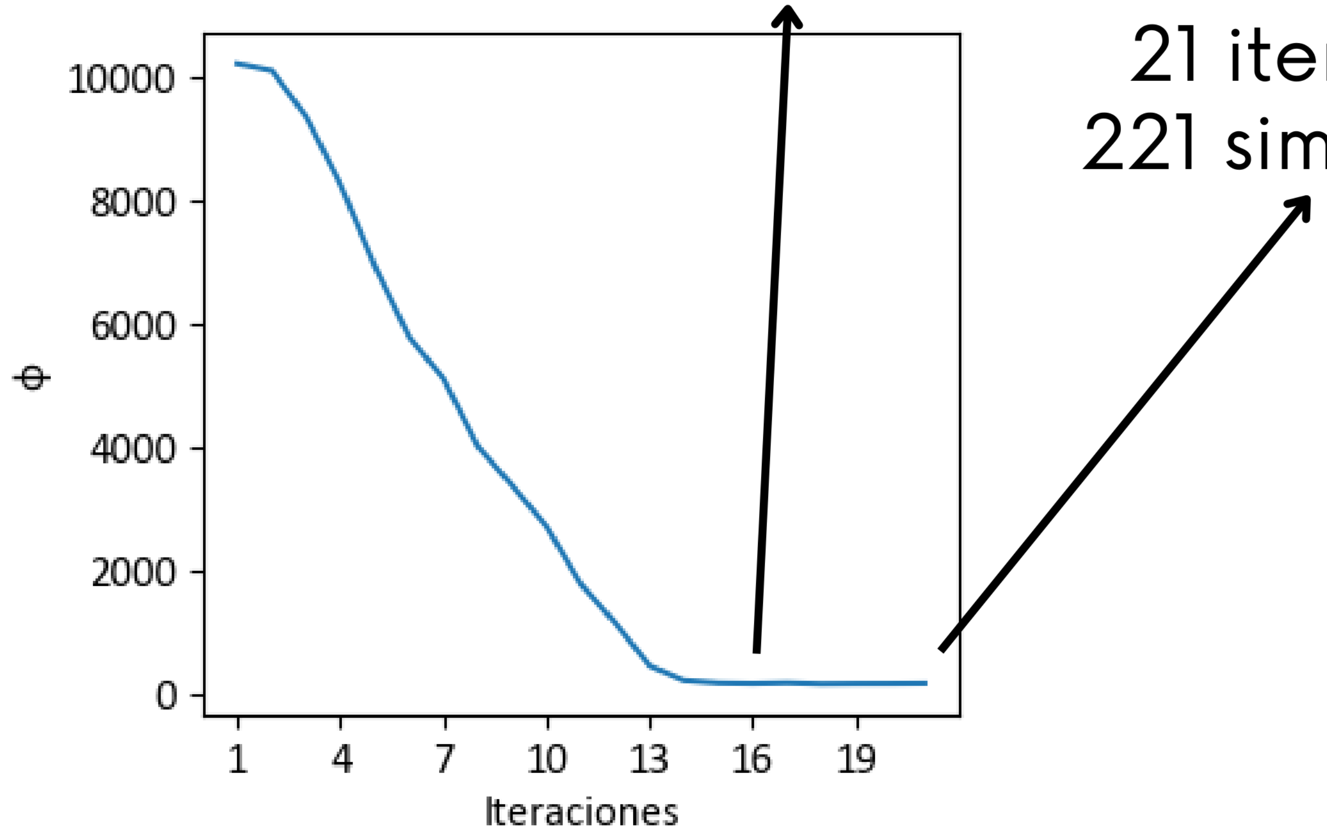
IBER-PEST: Resultados



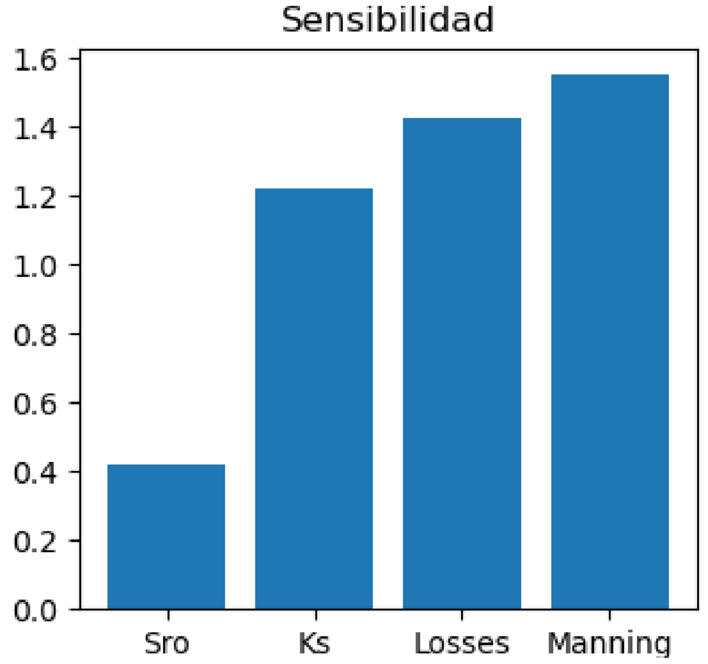
Parámetro	Valor
NSE	0.989
MAE	1.2%
Error rel V	0.5%
KGE	0.990
WNSE	0.993

16iteraciones
157 simulaciones

21 iteraciones
221 simulaciones

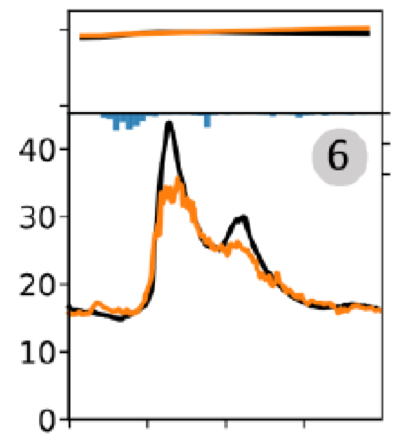


Parámetro	Valor calibrado
Ks	0.383
Sro	0.553
Initial losses	5.996
Multiplicador Manning	1.455




```
---------------------------------------------------------------
OPTIMISATION ITERATION NO.        :   21

CURRENT VALUE OF MARQUARDT LAMBDA =    4.883E-03 ----->

SINGULAR VALUES:-
  373146.9        292994.4        96515.55        15779.27

Number of singular values used in solution = 4


CURRENT VALUE OF MARQUARDT LAMBDA =    2.441E-03 ----->

SINGULAR VALUES:-
  373102.0        292949.4        96470.59        15734.30

Number of singular values used in solution = 4
```

Anteriormente con Renaud...

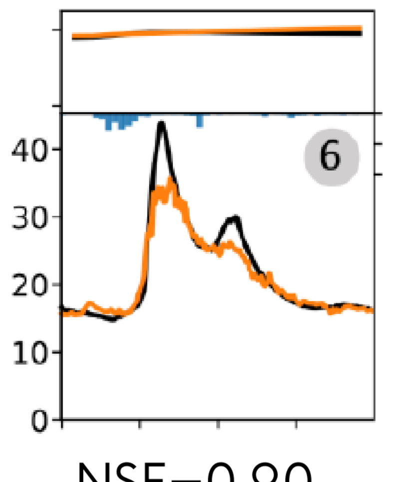


NSE=0.90
180 simulaciones

IBER-PEST: Resultados

García-Alén, G., Hostache, R., Cea, L., & Puertas, J. (2023). Joint assimilation of satellite soil moisture and streamflow data for the hydrological application of a two-dimensional shallow water model. Journal of Hydrology

Anteriormente con Renaud...



NSE=0.90
180 simulaciones

IBER-PEST: Nivel pro

Environmental Modelling and Software 109 (2018) 191–201

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Environmental Modelling & Software

journal homepage: www.elsevier.com/locate/envsoft

pestpp-ies

A model-independent iterative ensemble smoother for efficient history-matching and uncertainty quantification in very high dimensions

Jeremy T. White

GNSScience, Wairakei, New Zealand

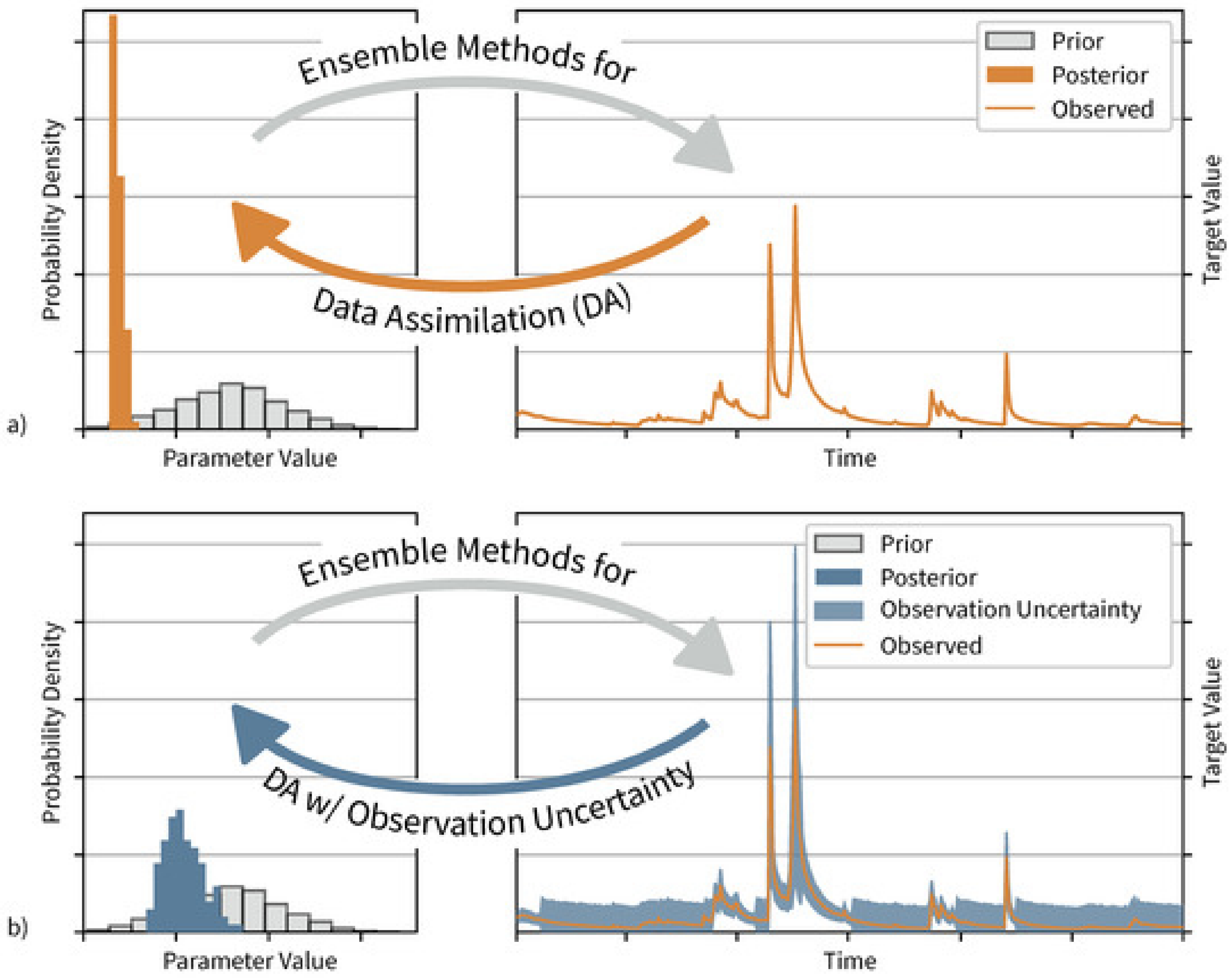
A R T I C L E I N F O

Keywords:
Modeling
Uncertainty
Iterative ensemble smoother
Gauss-Levenberg-Marquardt

A B S T R A C T

An open-source, scalable and model-independent (non-intrusive) implementation of an iterative ensemble smoother has been developed to alleviate the computational burden associated with history-matching and uncertainty quantification of real-world-scale environmental models that have very high dimensional parameter spaces. The tool, named pestpp-ies, implements the ensemble-smoother form of the popular Gauss-Levenberg-Marquardt algorithm, uses the pest model-interface protocols and includes a built-in parallel run manager,

pestpp-ies



Fuente: https://doi.org/10.3390/w15061133

Proceso de cálculo

1. Generación de un conjunto de parámetros iniciales (prior) y simulación del modelo con estos parámetros para obtener un conjunto de resultados (prior predictive ensemble).
2. Comparación de los resultados del modelo con los valores observados para obtener el conjunto de residuos (residual ensemble).
3. Cálculo de una matriz de covarianza de los residuos.
4. Adición de la incertidumbre de medición a la matriz de covarianza para obtener la matriz de covarianza de observación.
5. Aplicación de un algoritmo de filtrado de ensambles (ensemble smoother) que actualiza los parámetros iniciales (prior) para producir un conjunto de parámetros ajustados (posterior) que mejor se ajusten a los datos observados, teniendo en cuenta la matriz de covarianza de observación.
6. Simulación del modelo con el conjunto de parámetros ajustados (posterior predictive ensemble).
7. Comparación de los resultados del modelo con los datos observados y evaluación de la calidad del ajuste.
8. Repetición de los pasos 2 a 7 hasta que se cumpla un criterio de convergencia.

pestpp-ies: caso de estudio

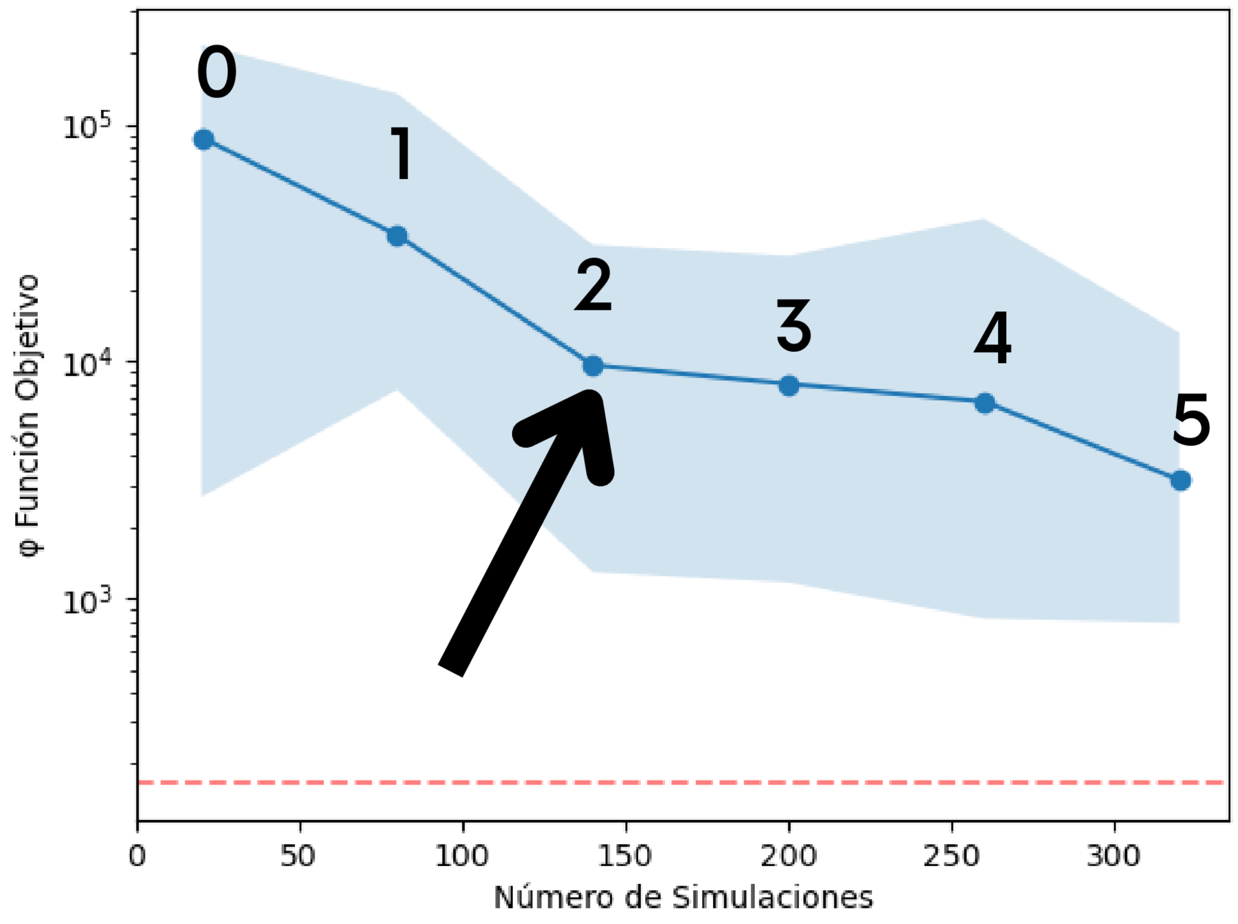
iber_PEST_case.pst | cov.mat | cov.mat | iber_pest_case.rec | iber_pest_case.0.par.csv

```
obs271   16.70056866 1    Obs
obs272   16.77088402 1    Obs
obs273   16.77088402 1    Obs
obs274   16.73571097 1    Obs
obs275   16.63037624 1    Obs
obs276   16.56030677 1    Obs
obs277   16.66545708 1    Obs
obs278   16.52531814 1    Obs
obs279   16.52531814 1    Obs
obs280   16.56030677 1    Obs
obs281   16.42053667 1    Obs
obs282   16.42053667 1    Obs
obs283   16.31603183 1    Obs
obs284   16.49036024 1    Obs
obs285   16.24651562 1    Obs
obs286   16.28125836 1    Obs
obs287   16.21180362 1    Obs
obs288   16.17712236 1    Obs
obs289   16.10785205 1    Obs
* model command line
Iber_PEST_batchfile.bat
* model input/output
Iber_PEST_par2par.tpl    Iber_PEST_par2par.in
Iber_PEST_output.ins     \TimeSeries\Hydrology_Hydrographs.csv
++ ies_num_reals(20)
++ parcov(param.unc)
++ ies_subset_size(5)
++ ies_lambda_mults(0.1,1.0,10.0)
```

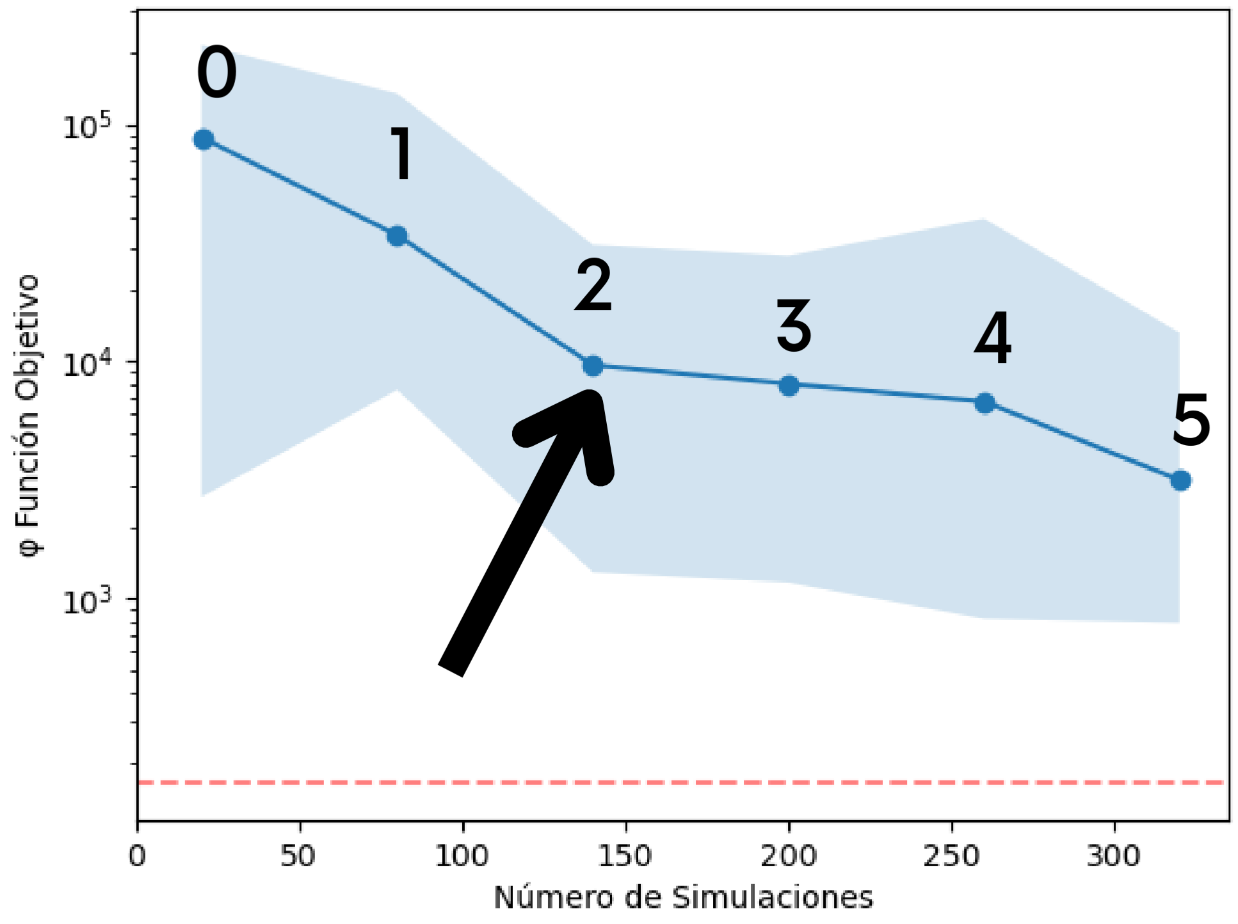
Inputs:

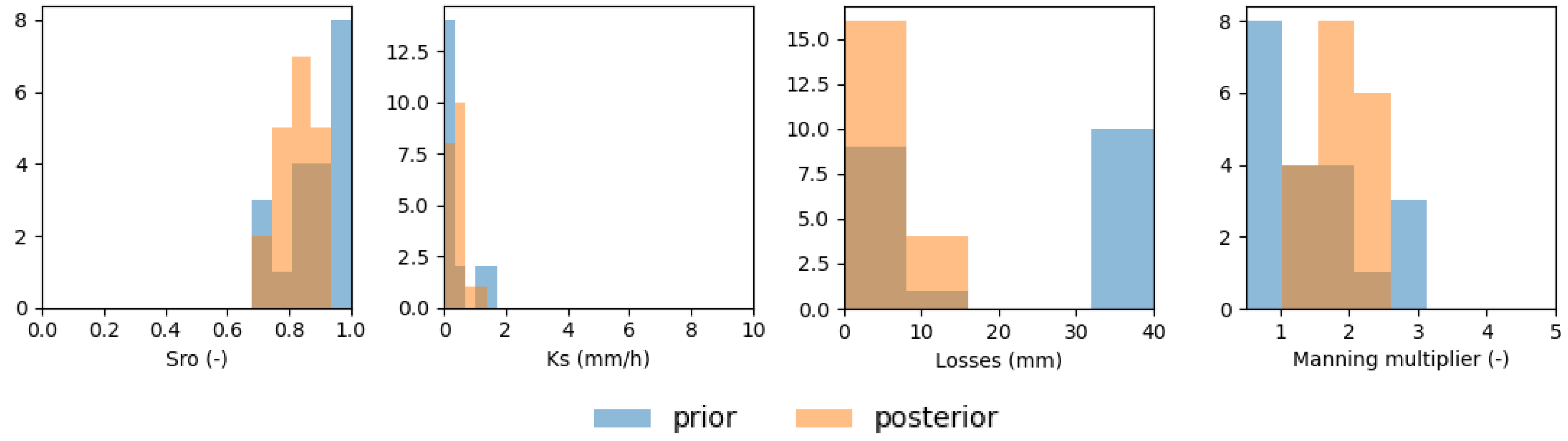
- Ensemble de tamaño 20
- Matrices de covarianza (conocimiento experto)
- Número de miembros del ensemble con los que experimenta con las lambdas
- Número de lambdas que calcula en cada iteración

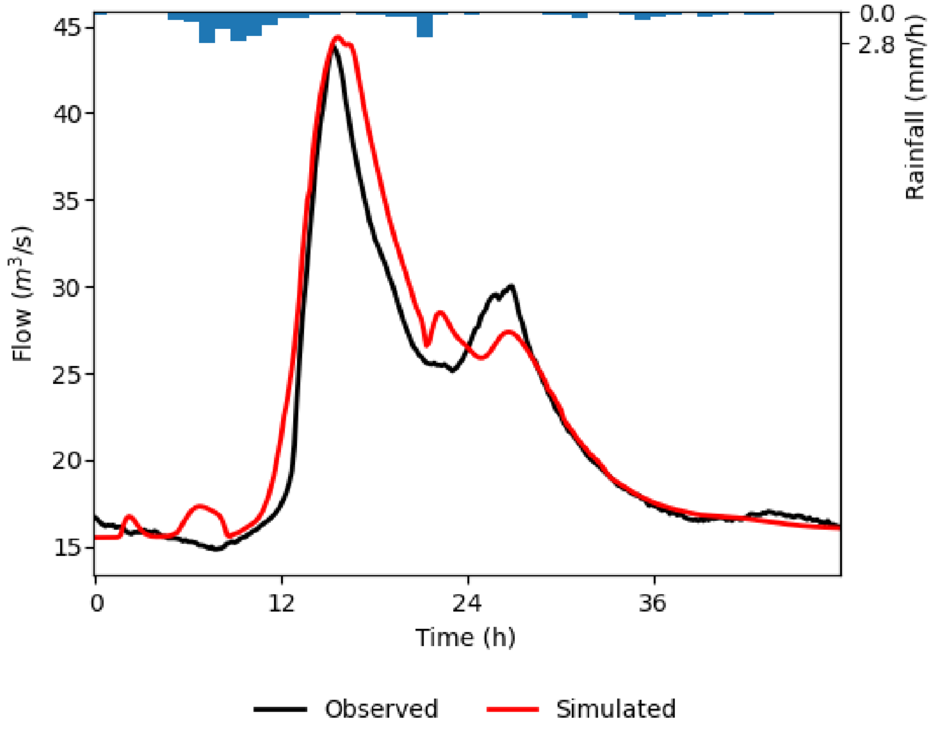
pestpp-ies: Resultados



pestpp-ies: Resultados

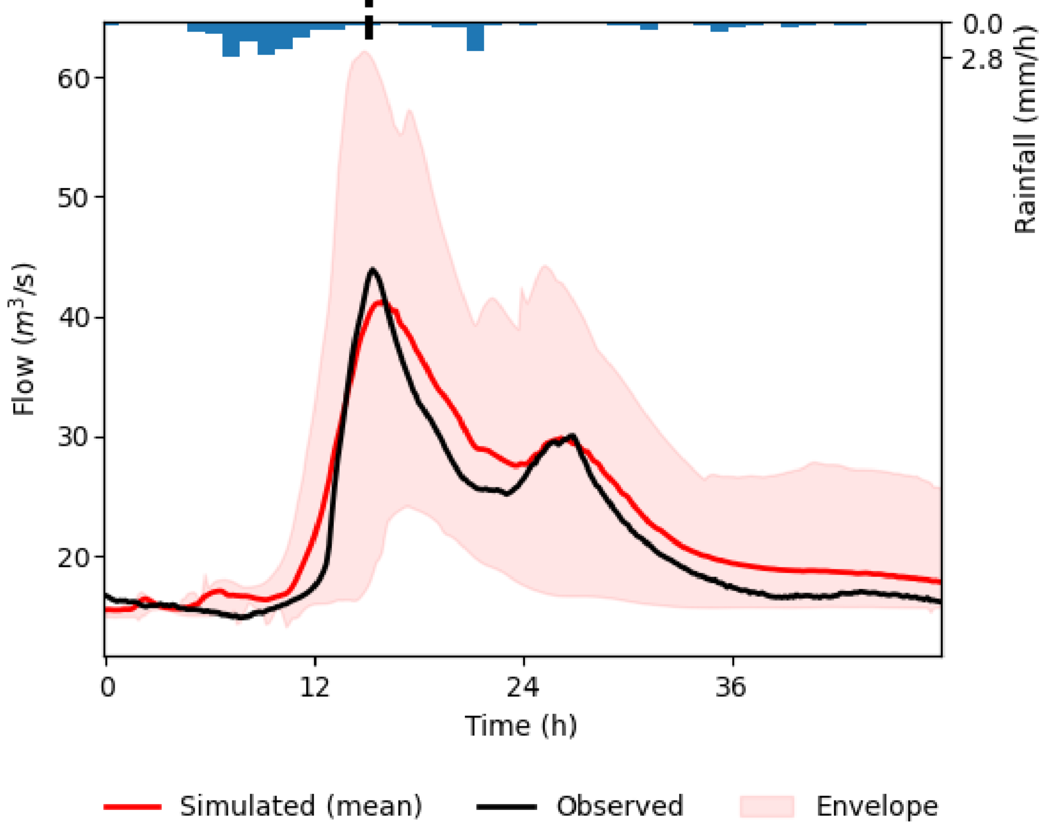




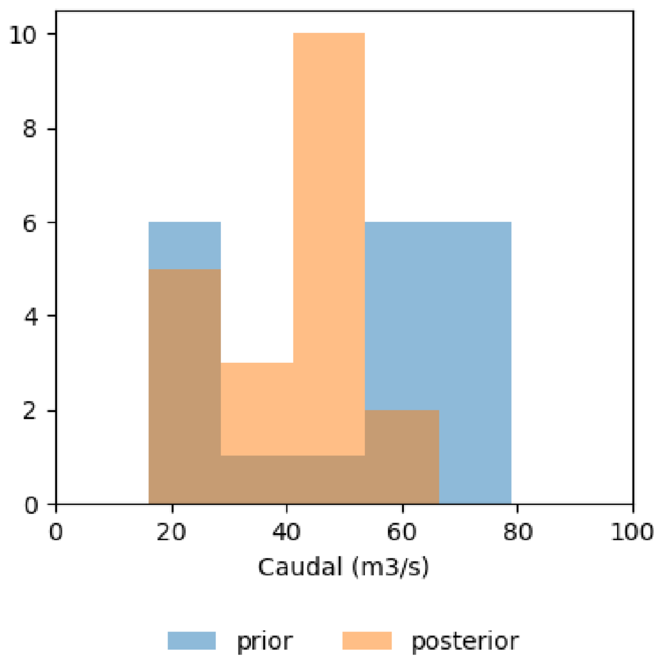


Parámetro	Valor
NSE	0.930
MAE	2.88%
Error rel V	3.58%
KGE	0.931
WNSE	0.889

Parámetro	Valor calibrado
Ks	0.501
Sro	0.876
Initial losses	2.865
Multiplicador Manning	1.984



mean = 41 m3/s
std = 12.1 m3/s
50% de los resultados
están entre 30 y 50 m3/s



pestpp-ies: Data space inversion

Utilizo la función pestpp-ies para crear un modelo subrrogado

↓

Principle Component Analysis (PCA) de la matriz de covarianza entre outputs del modelo

↓

Ejecuto mi modelo de Iber 100 veces y hago todas las pruebas que quiera con mi modelo subrrogado

↓

Futuras líneas de desarrollo?

- Artículo IBER-PEST

Nat Hazards (2018) 91:697–715
https://doi.org/10.1007/s11069-017-3150-6

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Muchas gracias!

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