Open TURNS & Random fields

Simulation of synthetic miosrientation maps of alloy 600 specimens

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Open TURNS Users Day #7

Chatou, 20th June 2014

Outline

1. Context : the CORIOLIS project

2. Modelling and simulation of the random field

   a) Parametric approach based on R

   b) Non-parametric approach based on OpenTURNS

3. Induced improvements in OpenTURNS

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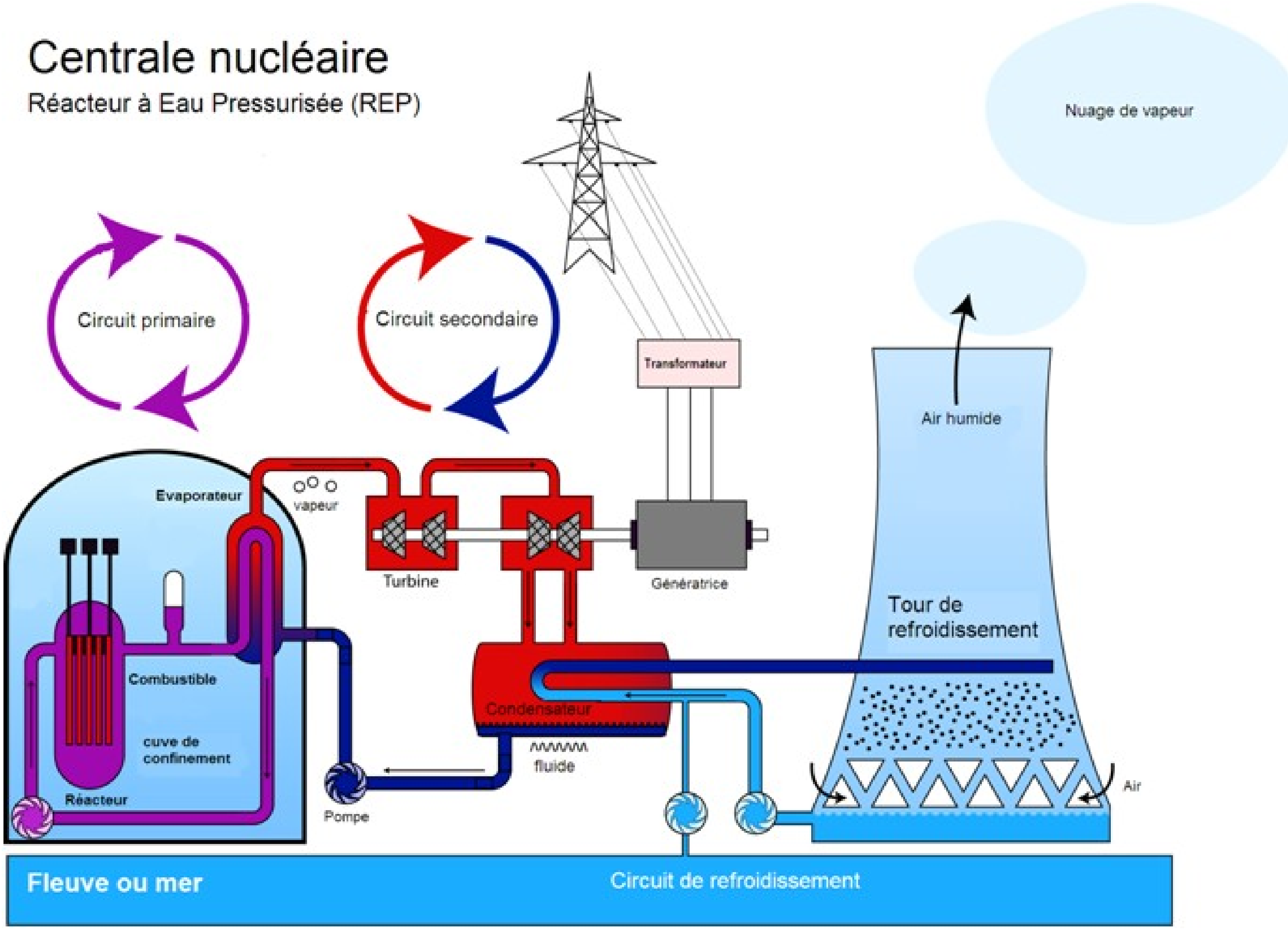
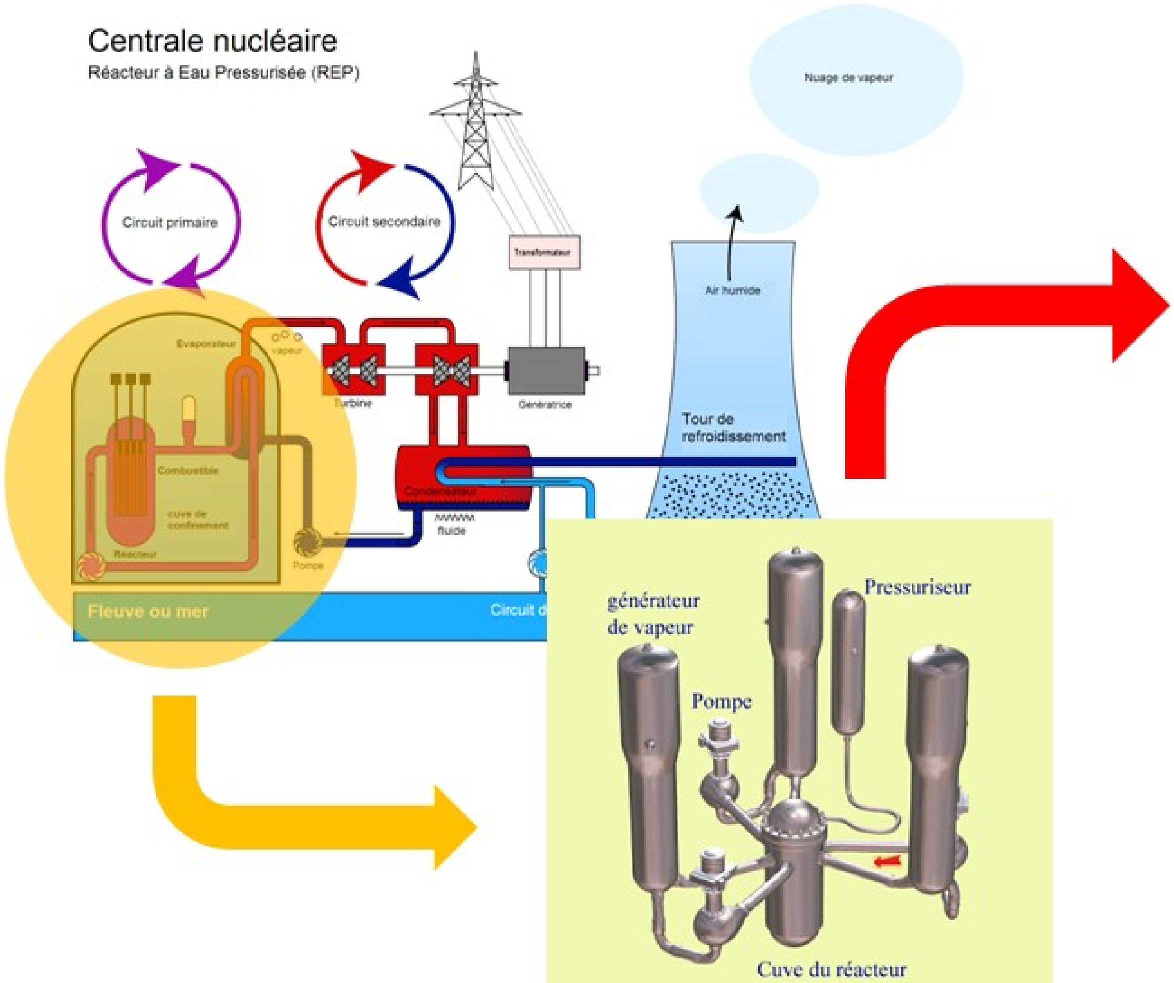
PWR nuclear power plants



PWR nuclear powerplants



Possible susceptibility of alloy 600 components to Stress Corrosion Cracking (SCC)

The Coriolis project

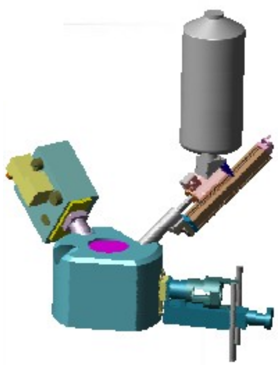
Objective : Develop models predicting SCC initiation & growth

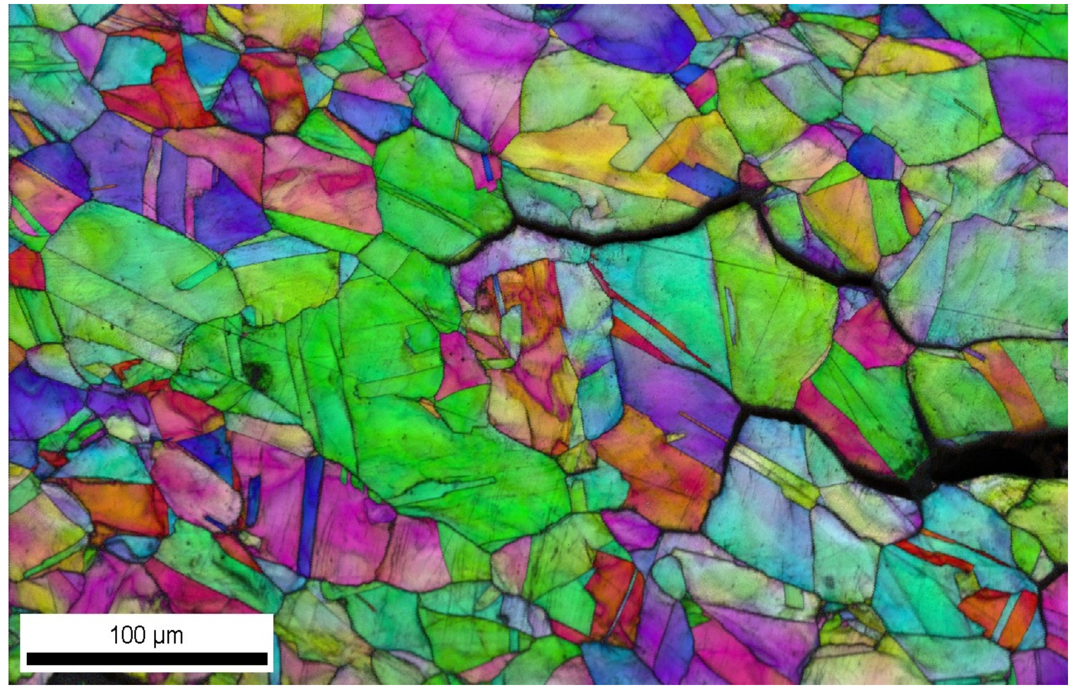
→ Account for significant factors at the microscopic scale : crystal misorientations due to plastic strain

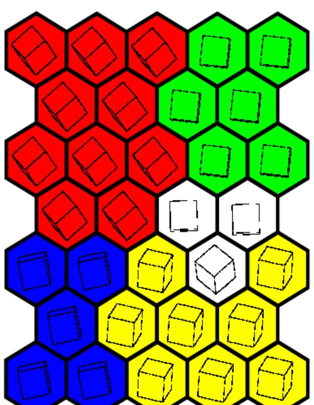
Current work: Model and simulate the morphology of misorientation patterns from A600 tensile specimens

Measurement of crystallographic orientations by EBSD

Scanning Electron Microscope

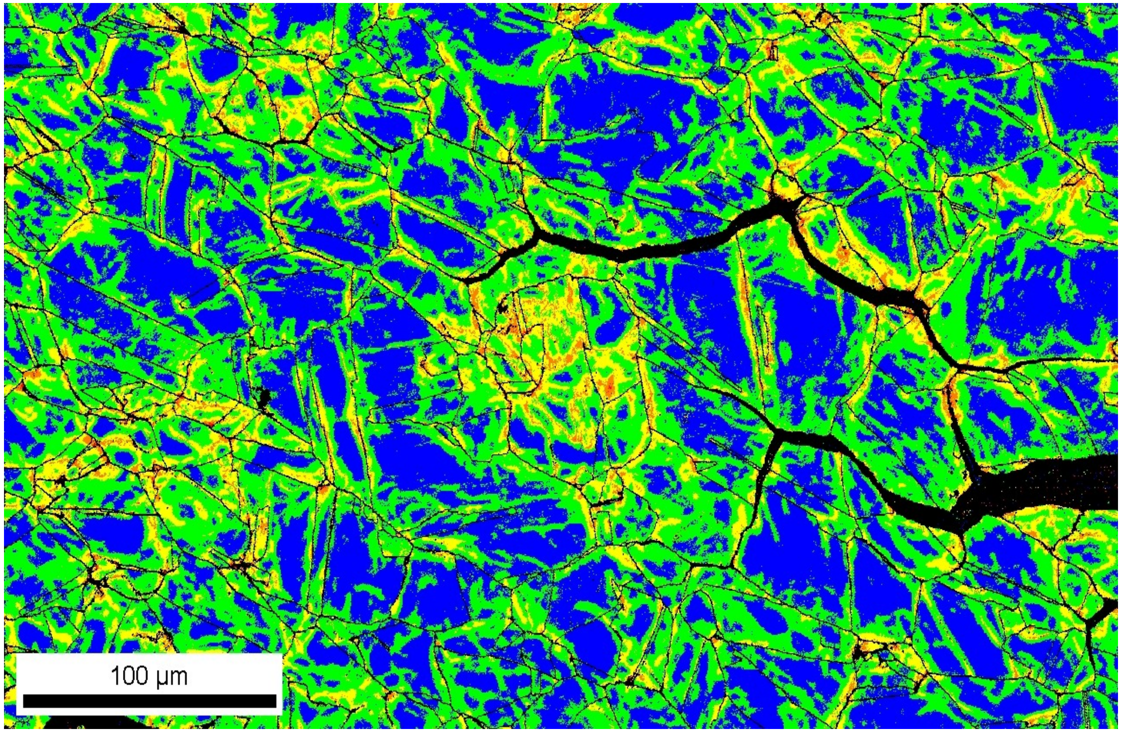




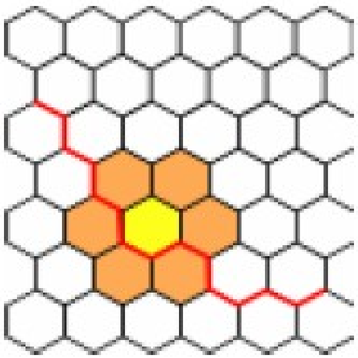


From « Introduction to OIM analysis », TSL

Measurement of misorientations - Kernel Average Misorientation



Mesure the average misorientation among the neighbouring cells



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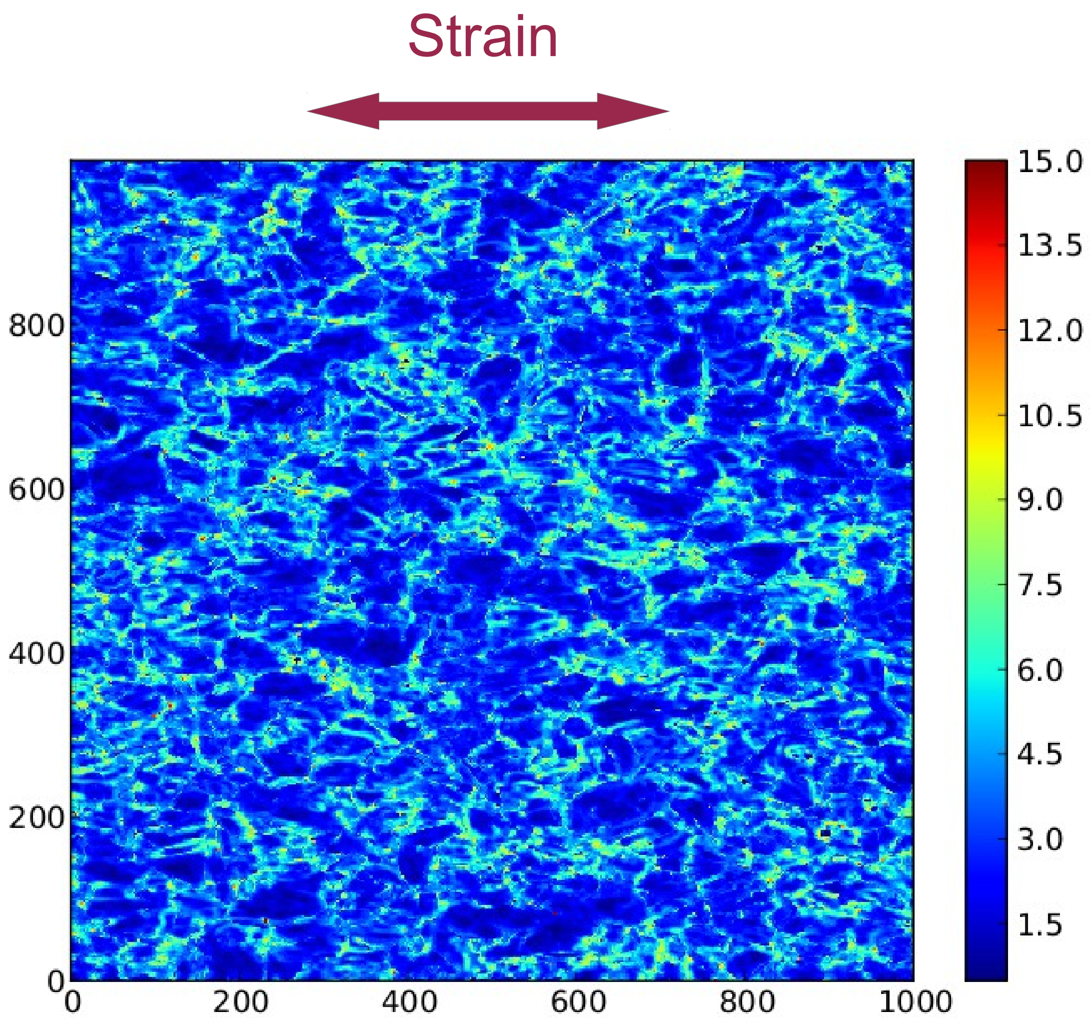
KAM of alloy 600 specimens
Applied microscopic strain = 11,4 %



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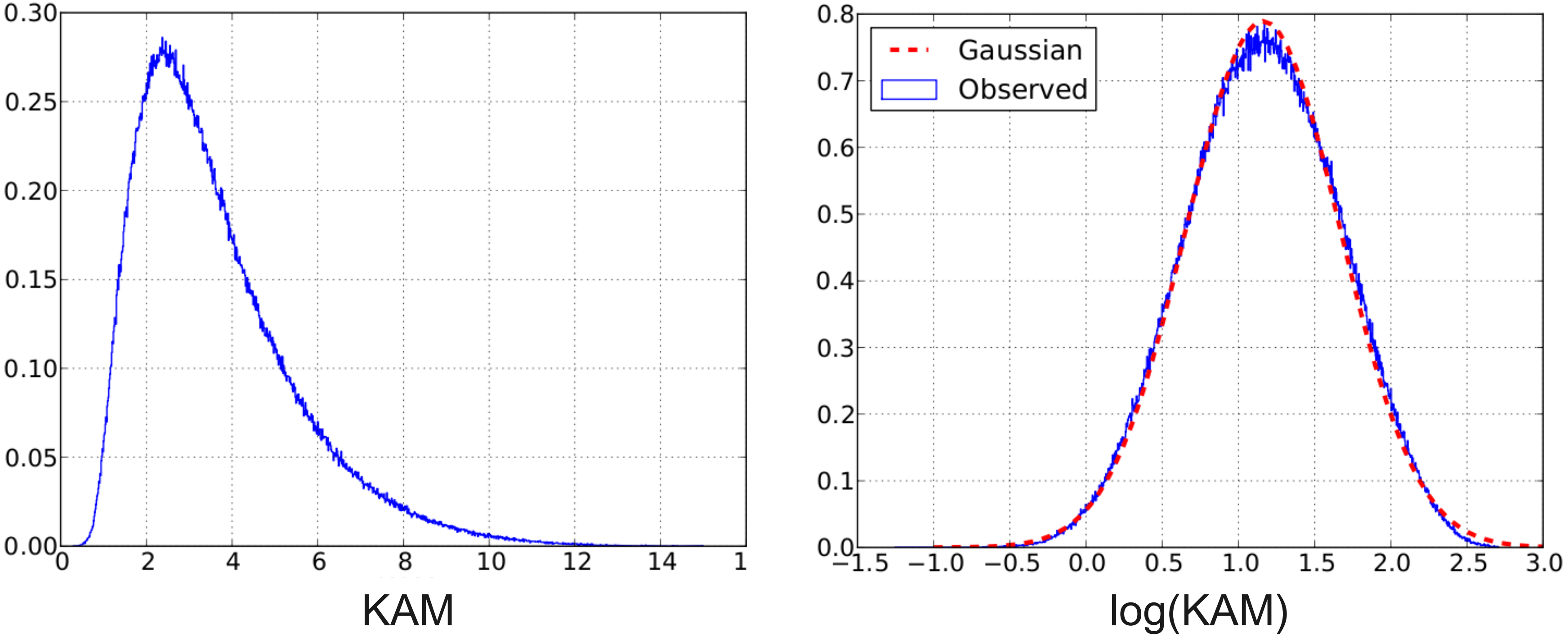
Parametric approach

Tool : R, libraries 'gstat' and 'RandomFields'

Strategy :

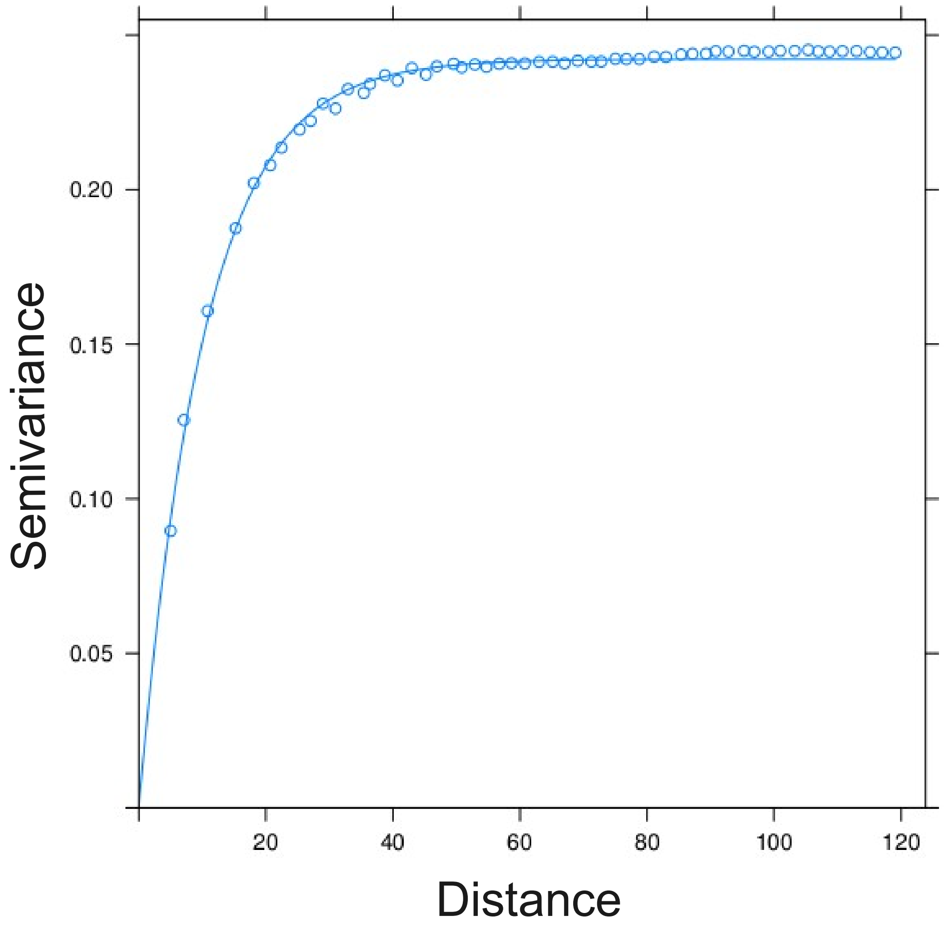
1. « Gaussianize » the random field margin
2. Estimate the mean of the transformed field
3. Estimate its covariance using a parametric variogram model
4. Simulate a Gaussian field with the same moments
5. Create the non-Gaussian field applying the inverse transform

Marginal probability density function



→ Assumption of a lognormal field

Fit of a variogram model



Stationary model (spherical)

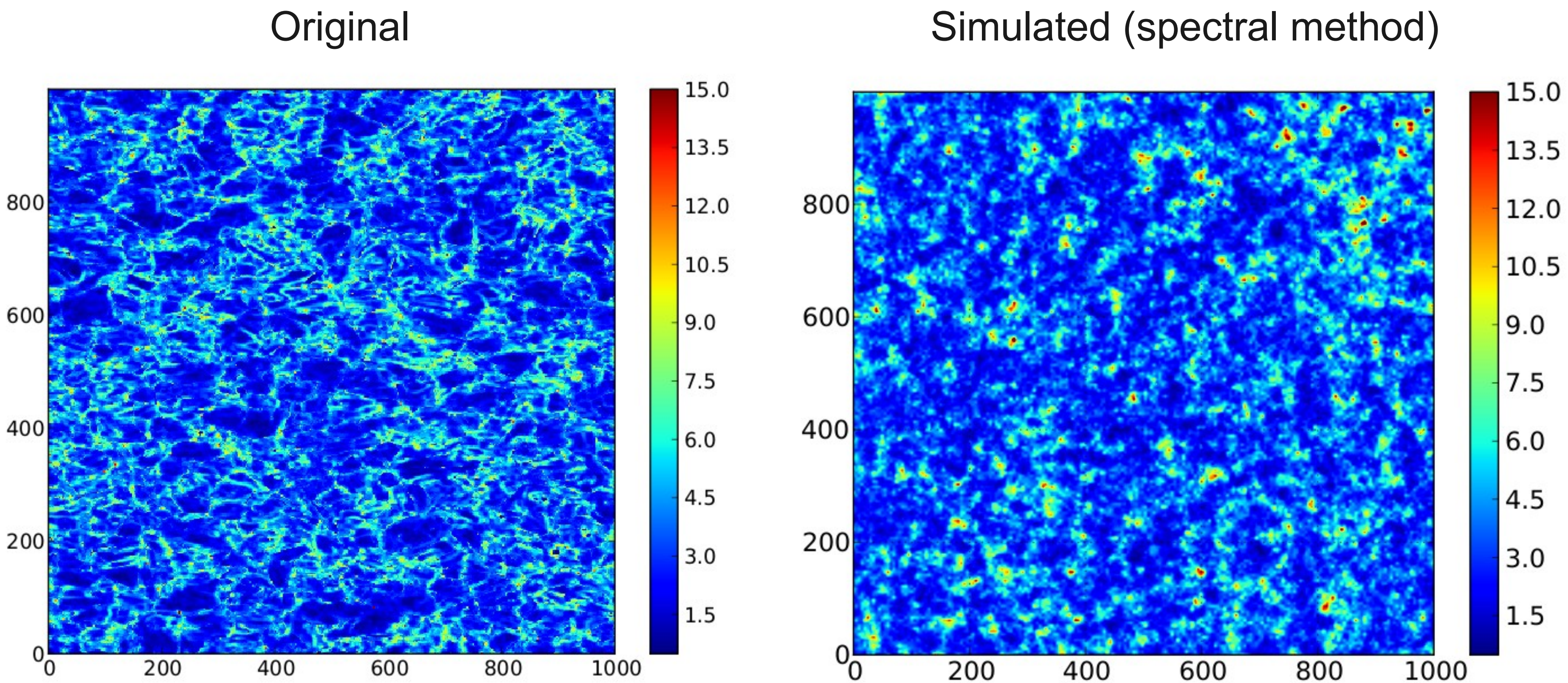
$$\gamma(h) \quad = \boxed{\sigma^2}\left[1 - \exp\left(-\frac{h}{\boxed{a_0}}\right)\right]$$

Variance

Range parameter (Range = 30,9)

→ Good agreement

Original and simulated fields



→ We checked that marginal PDFs and variogram are well reproduced

→ But not the « connectivity » of the high KAM regions

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Non-parametric approach

Tool : Open TURNS version ≥ 1.3

Strategy (Box-Jenkins):

1. Apply optimal Box-Cox transform
   → Field with Gaussian margin
2. Estimate the mean of the transformed field
3. Estimate its covariance
4. Simulate a Gaussian field with the same moments
5. Create the non-Gaussian field applying the inverse Box-Cox transform

Box-Cox transform

Goals :

- Stabilize the variance
- Make the data more Gaussian

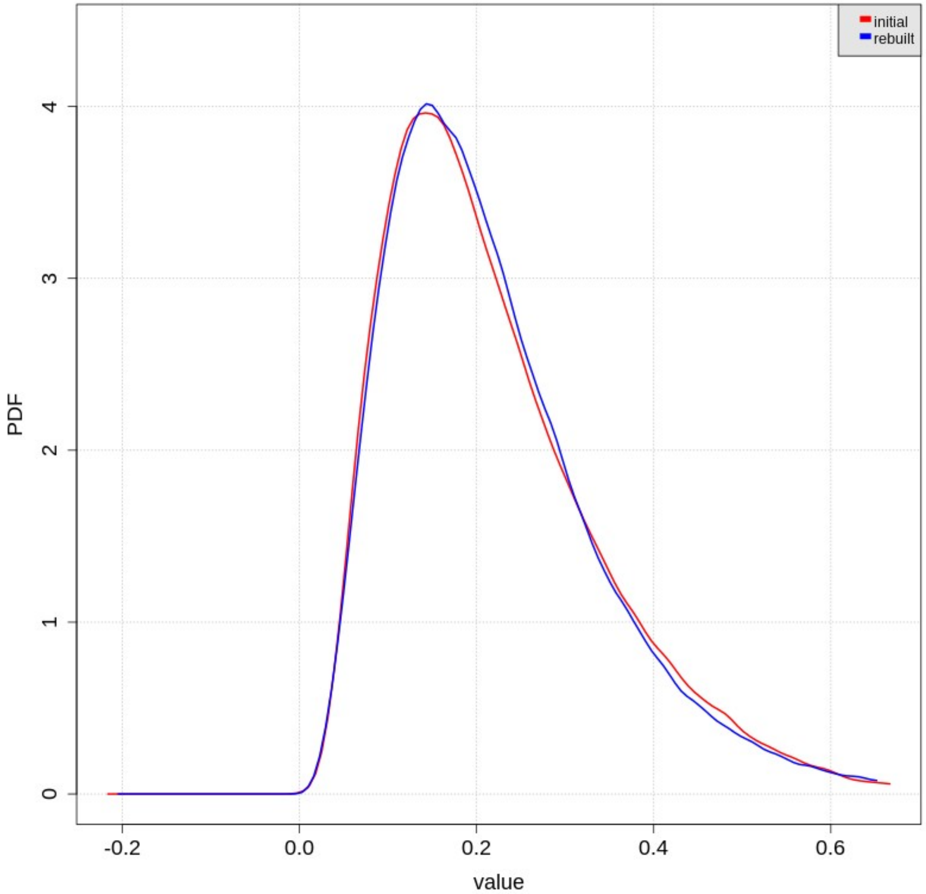
Formula :

$$z_i^{(\lambda)} = \begin{cases} \frac{z_i^\lambda - 1}{\lambda} & \text{if} \quad \lambda \neq 0 \\ \log(z_i) & \text{else} \end{cases}$$

Choice of λ by maximum likelihood

Comparison of marginal PDFs

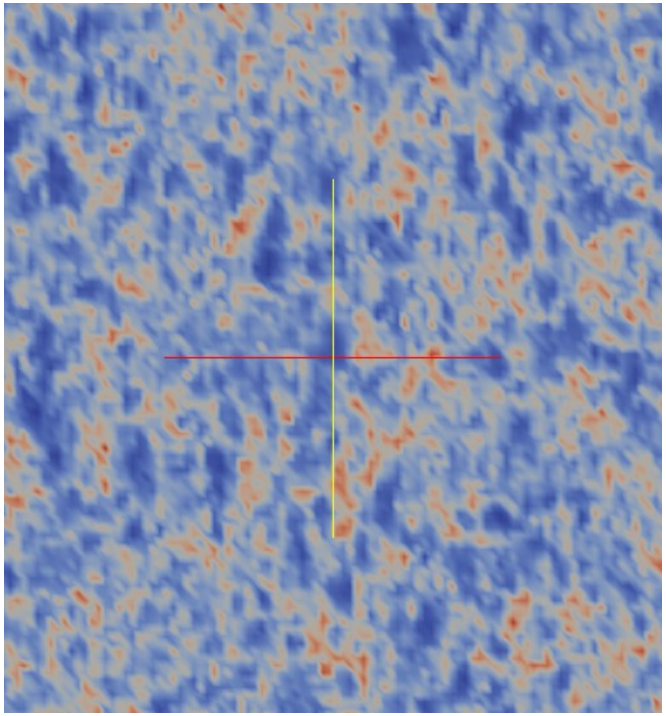
λ_{opt}=0.2 → Consistent with the previous lognormal hypothesis



Mean estimation

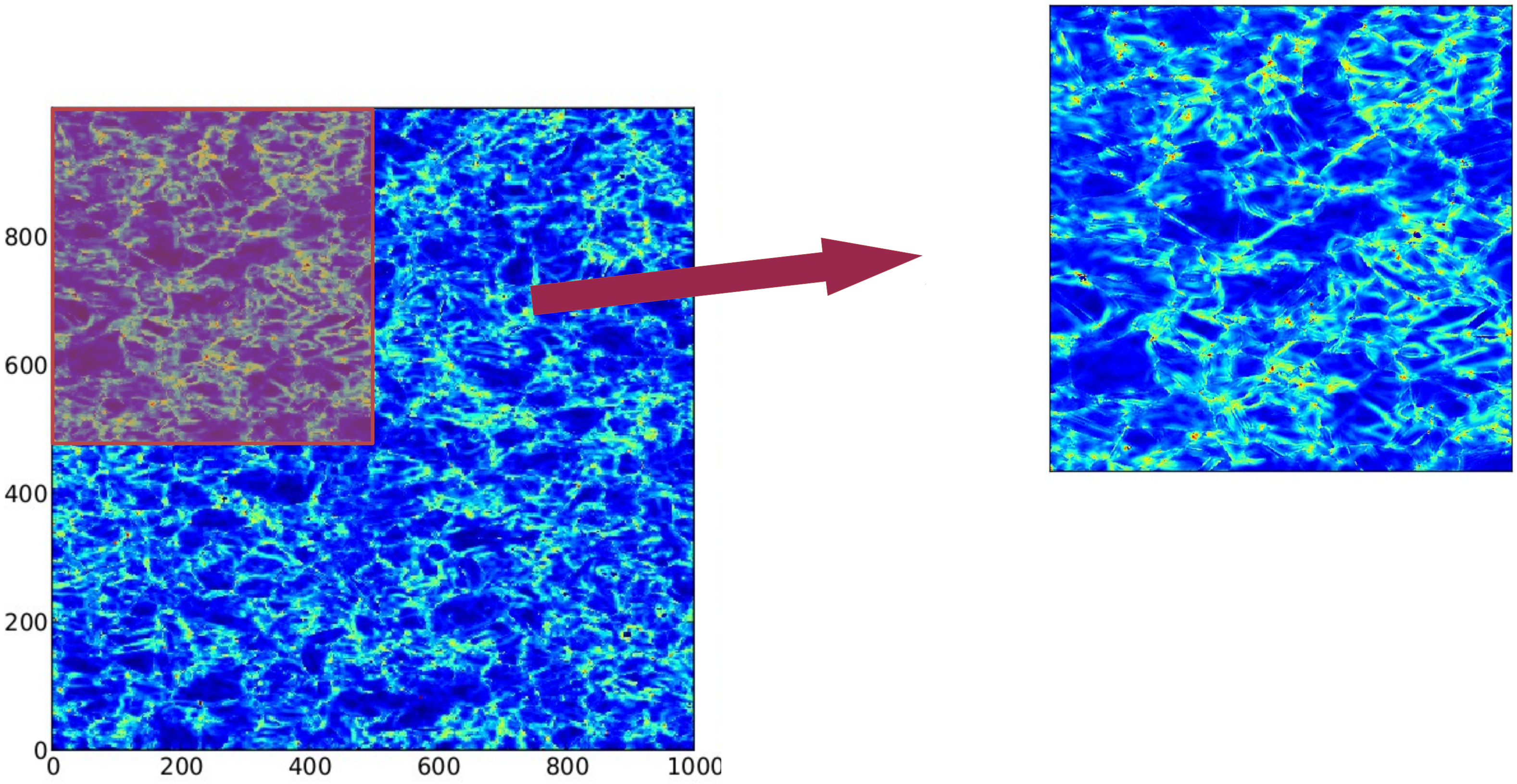
Assumed trend : bilinear

+ Fourier basis

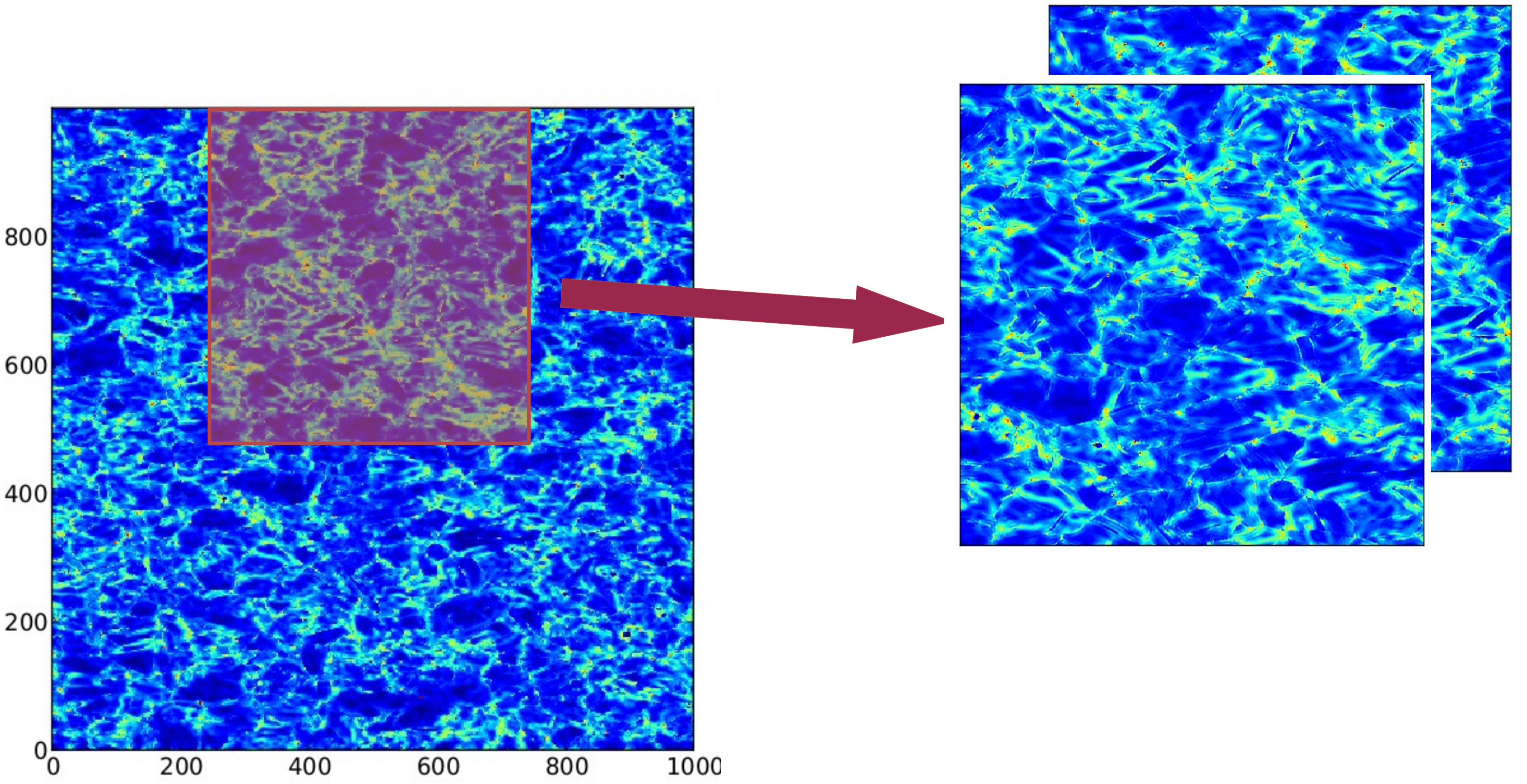


Coefficients estimated
by least squares

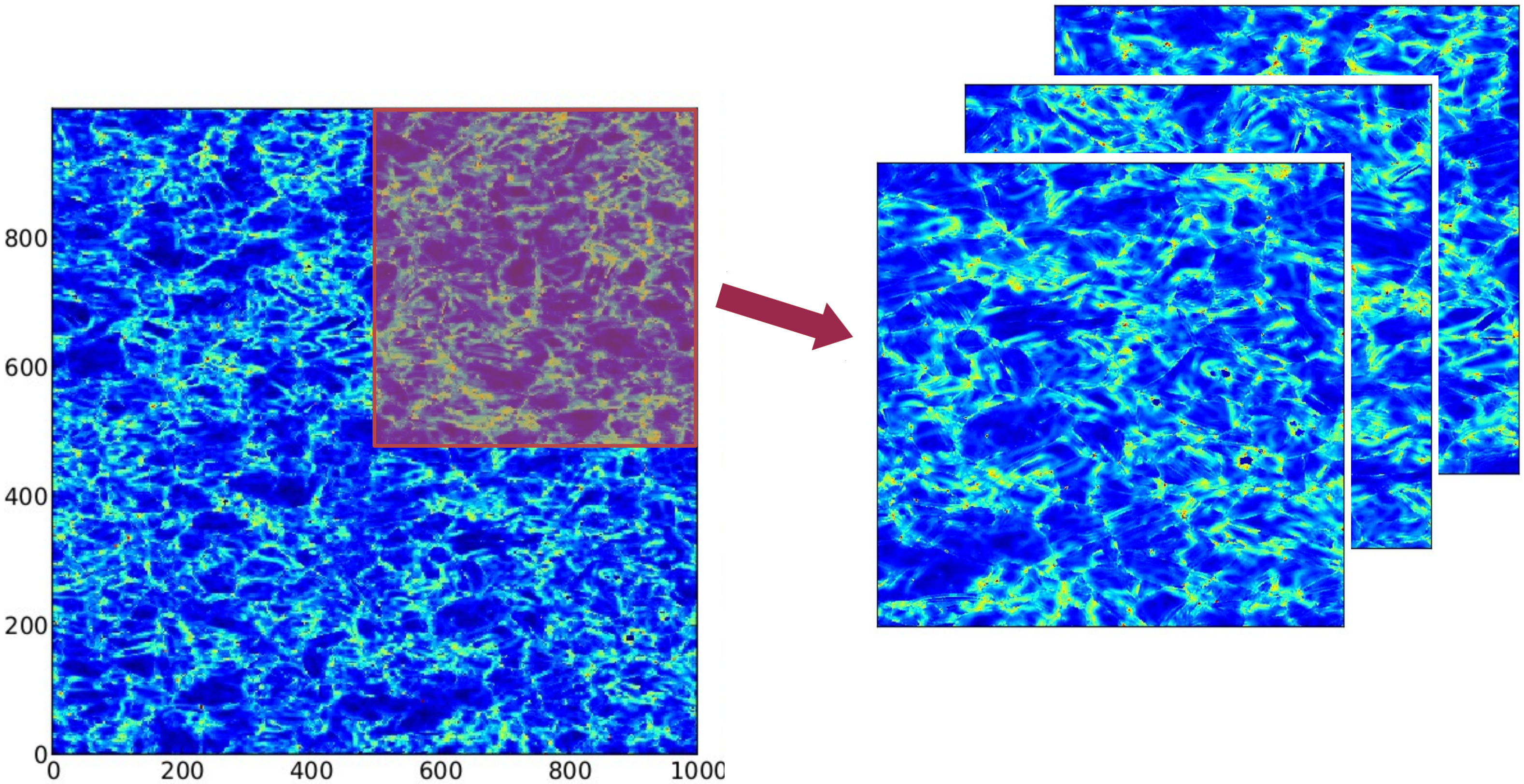
Non-parametric covariance estimation



Non-parametric covariance estimation



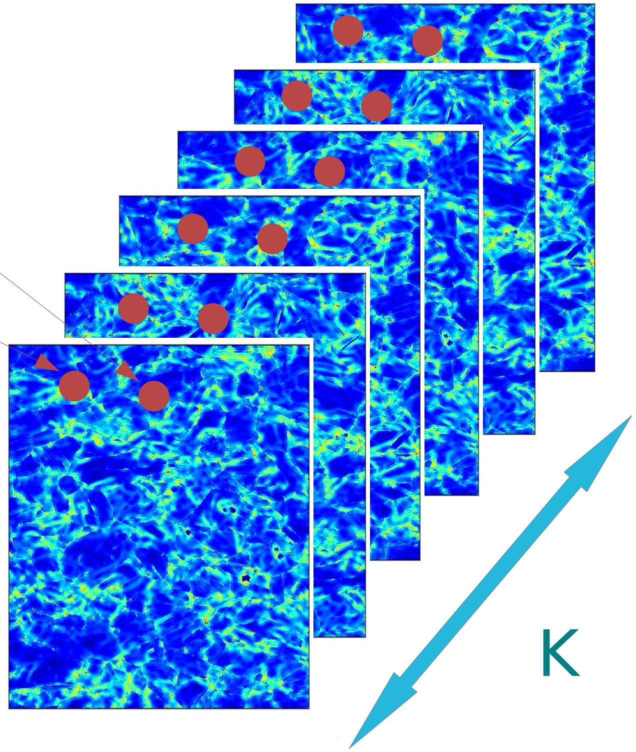
Non-parametric covariance estimation



Non parametric covariance estimation

Covariance estimate (non stationary model)

$$\hat{C}(Z_i, Z_j) = \frac{1}{K}\sum_{k=1}^{K} \left(z_i^{(k)} - m_i\right)\left(z_j^{(k)} - m_j\right)$$

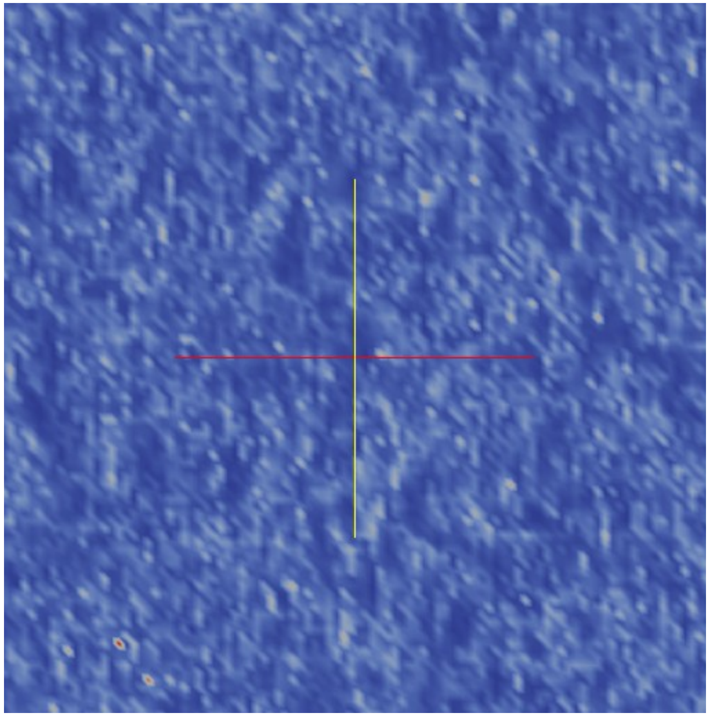


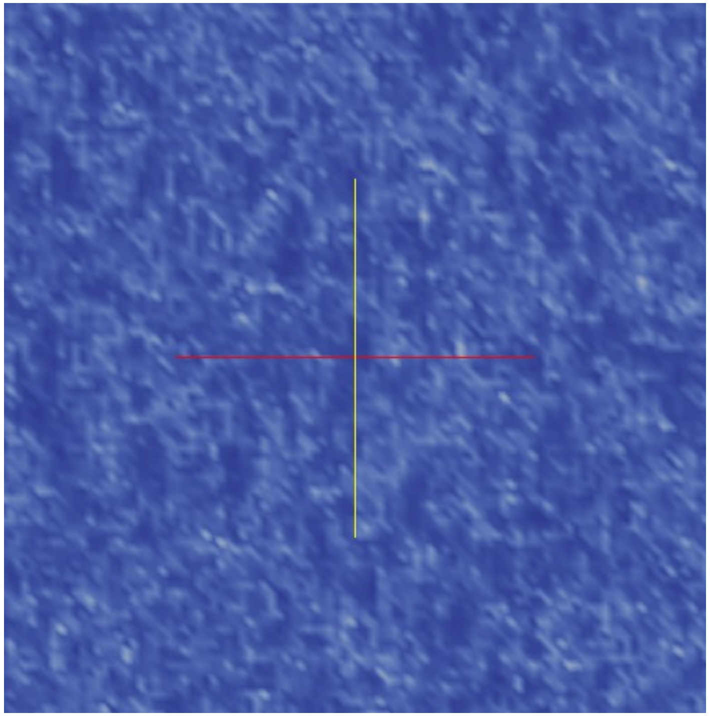
- Find a compromise number of subsquares vs overlapping rate

  → 50% overlapping
  K=50 subsquares

Random fields realizations (new results)

(Cholesky method)





Discussion

Possible reasons for not properly representing the fine dependences :

- Optical illusion due to a lack of data ?
  → Work with the full image

- Use of too small subsquares when estimating the covariance ?

- The random field is not Gaussian
  → Need to account for higher-order correlations

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Improvements & creation of OT classes

Parallelization of several OT classes

- BoxCoxFactory : maximum likelihood, direct & inverse transforms
- NonStationaryCovarianceModelFactory : non-parametric estimation of the covariance

Creation of a new class

- IntervalMesher : creates spatial mesh grids

Efficient Gaussian field simulation

Method	Cholesky	Gibbs sampler
Availability in OT	Already available	In the next release
Memory	$O(n^2)$	$O(n)$
Initialization	$O(n^3)$	$O(1)$
Simulation	$O(n^2)$ Small constant (~0.5)	$O(n^2)$ Large constant (~20-100)

Conclusion

- The feasability of the Box-Jenkins procedure with 2D spatial data in OT has been shown

- The Coriolis application has motivated several improvements in OT

  → Great reactivity of the OT development team

- Further developments in OT :

  - Simulation of Gaussian random fields :

    → h-matrix

    → Spectral method (for spatial data)