Summer School CEA-EDF-INRIA 2011 of Numerical Analysis

Uncertainty quantification for numerical model validation

Introduction – Concepts - Organization

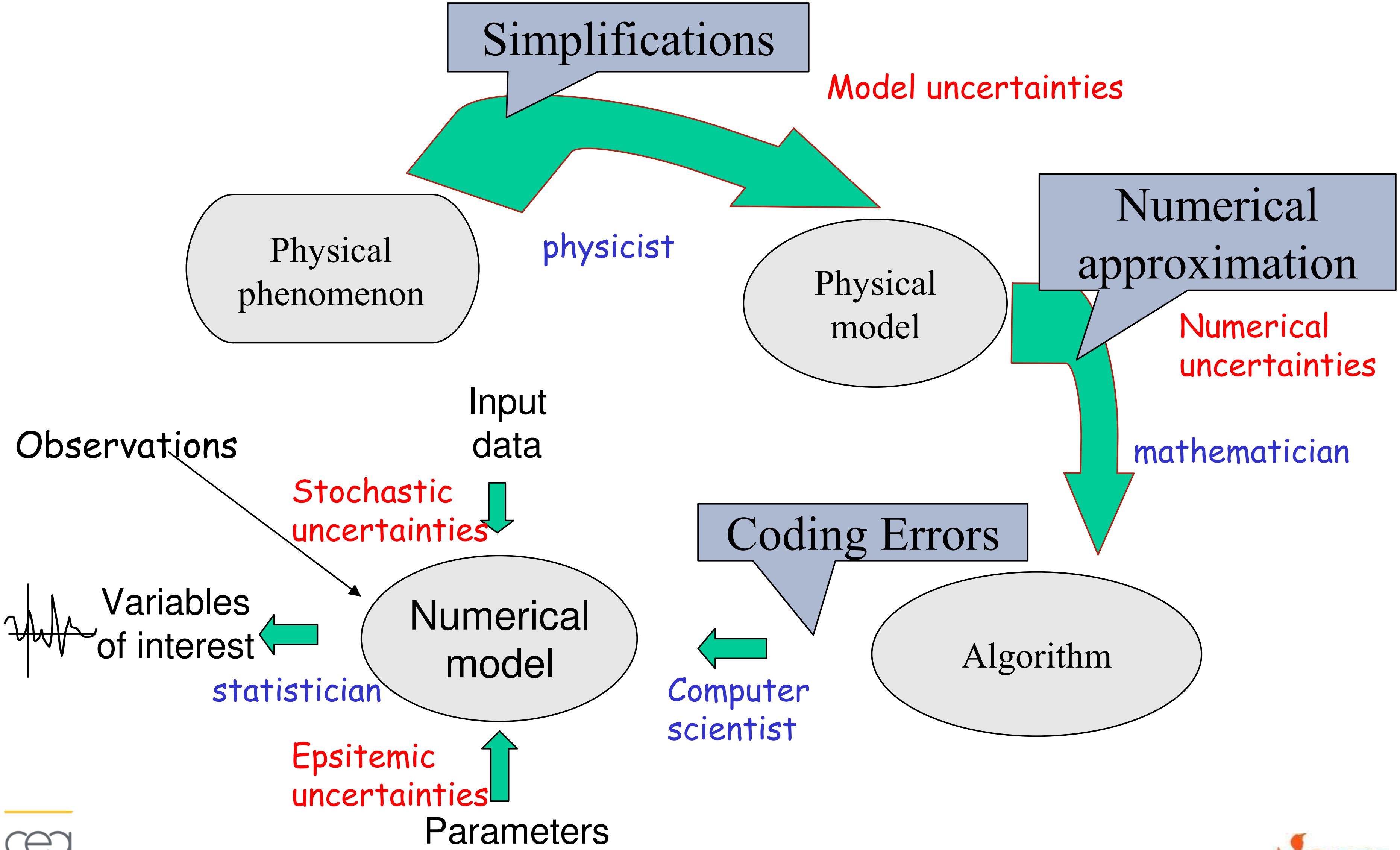
Bertrand Iooss
EDF R&D Chatou
Département Management des Risques Industriels

Marc Sancandi
CEA CESTA

28/06/2011

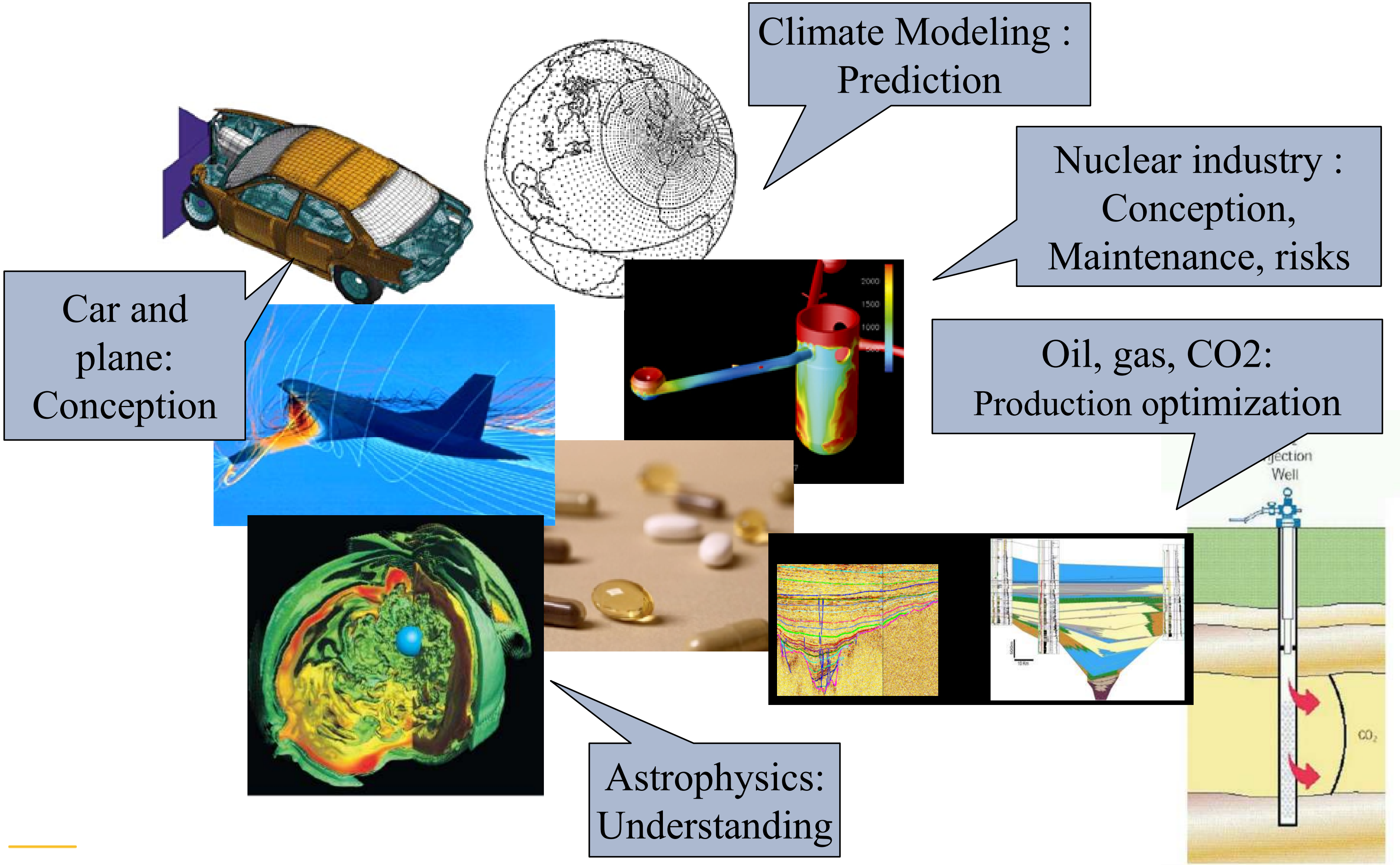
Starting point: uncertainties everywhere in the modeling chain !

Main problem: credibility of predictions



Similar safety and uncertainty issues in CS&E and Nature sciences

CS&E : Computational Science & Engineering



Main stakes of uncertainty management

- **Modeling phase:**
  - Improve the model
  - Explore the best as possible different input combinations
  - Identify the predominant inputs and phenomena in order to priorize R&D
- **Validation phase:**
  - Reduce prediction uncertainties
  - Calibrate the model parameters
- **Practical use of a model:**
  - **Safety studies:** assess a risk of failure (rare events)
  - **Conception studies:** optimize system performances and robustness

Uncertainties in simulation experiments

Two kinds of uncertainties

1. Epistemic
   aka "reducible" (with sufficient learning)
2. Stochastic (aleatoric)
   aka "irreducible" (excepted huge extra expense, ie meas. devices)

An open problem : What is the best way to model such uncertainties ?

Hints :

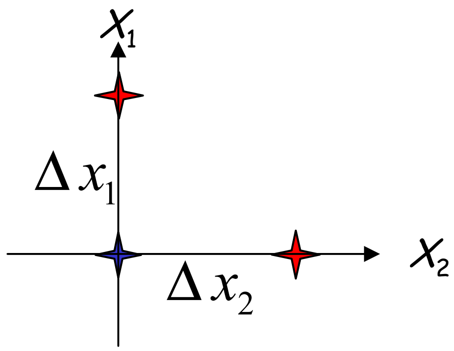
1. Stochastic → Probability Theory
   aka "reducible" (with sufficient learning)
2. Epistemic → idem … but many other ways :
   - Possibility Th., Evidence Th., Fuzzy Sets, Dempster-Schaffer, …

Only Probability Th. used in the framework of this Summer School

Uncertainties in simulation experiments $Y = a_1 x_1 + a_2 x_2$

Ancient way

$$\Delta Y = a_1 \Delta x_1 + a_2 \Delta x_2$$



Still learned in Schools

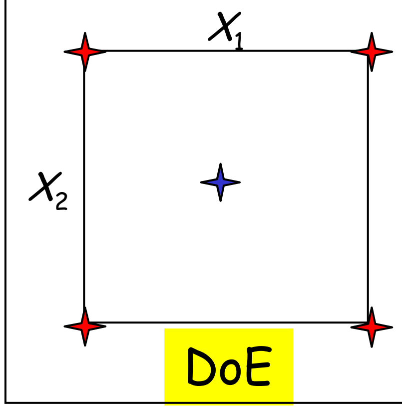
Pre-modern way

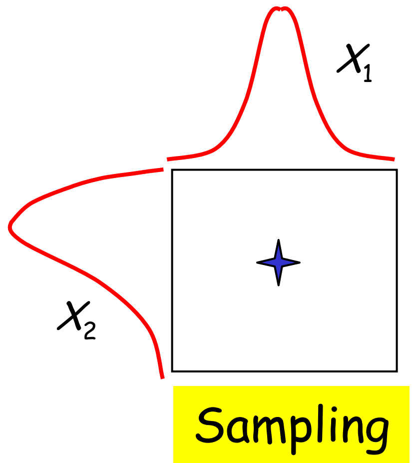
x's identified to R.V.
… but same algebra

$$\sigma_Y = \sqrt{a_1^2 \sigma_1^2 + a_2^2 \sigma_2^2}$$

Still used in metrology (GUM)

Really Modern way

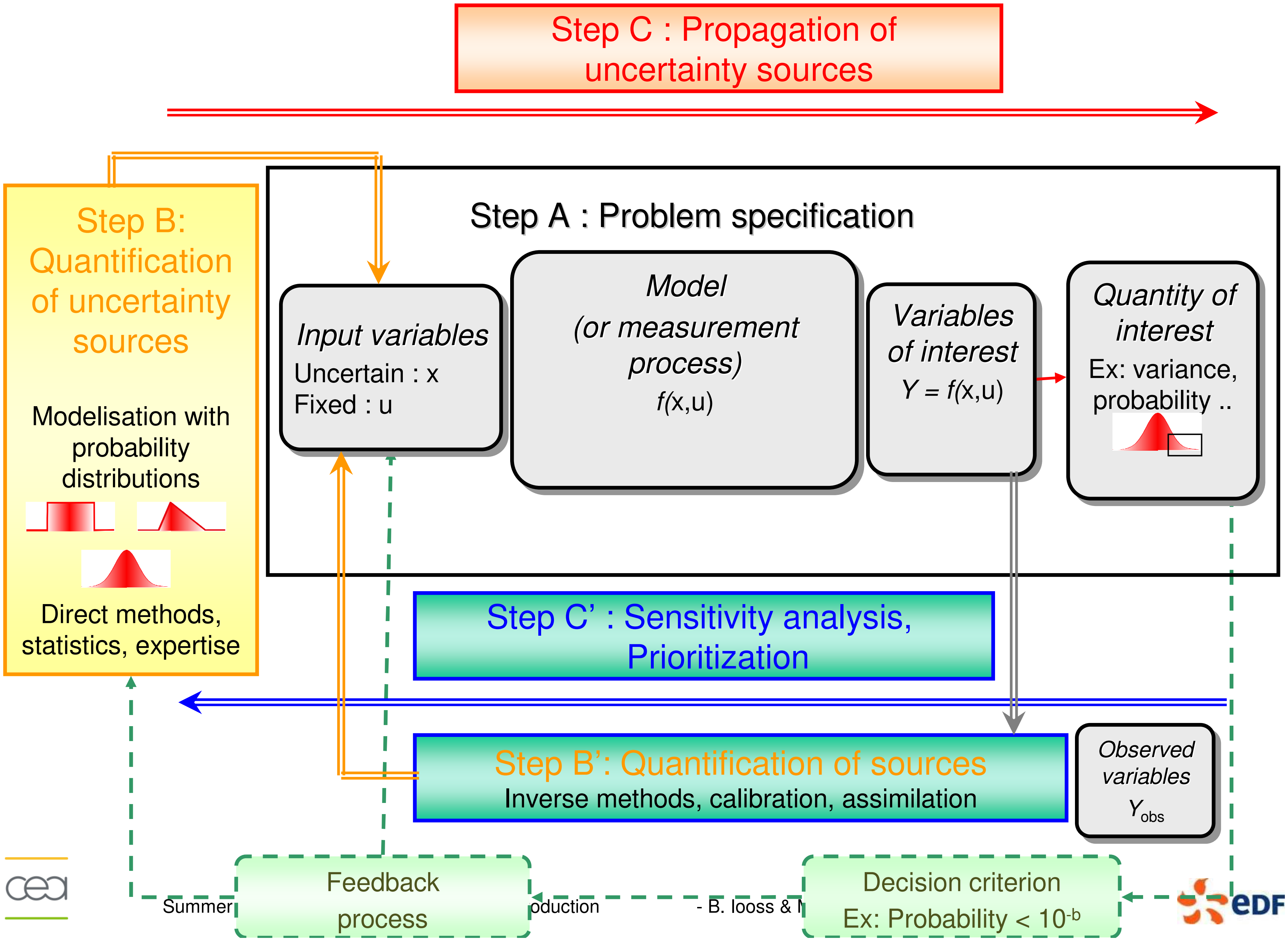




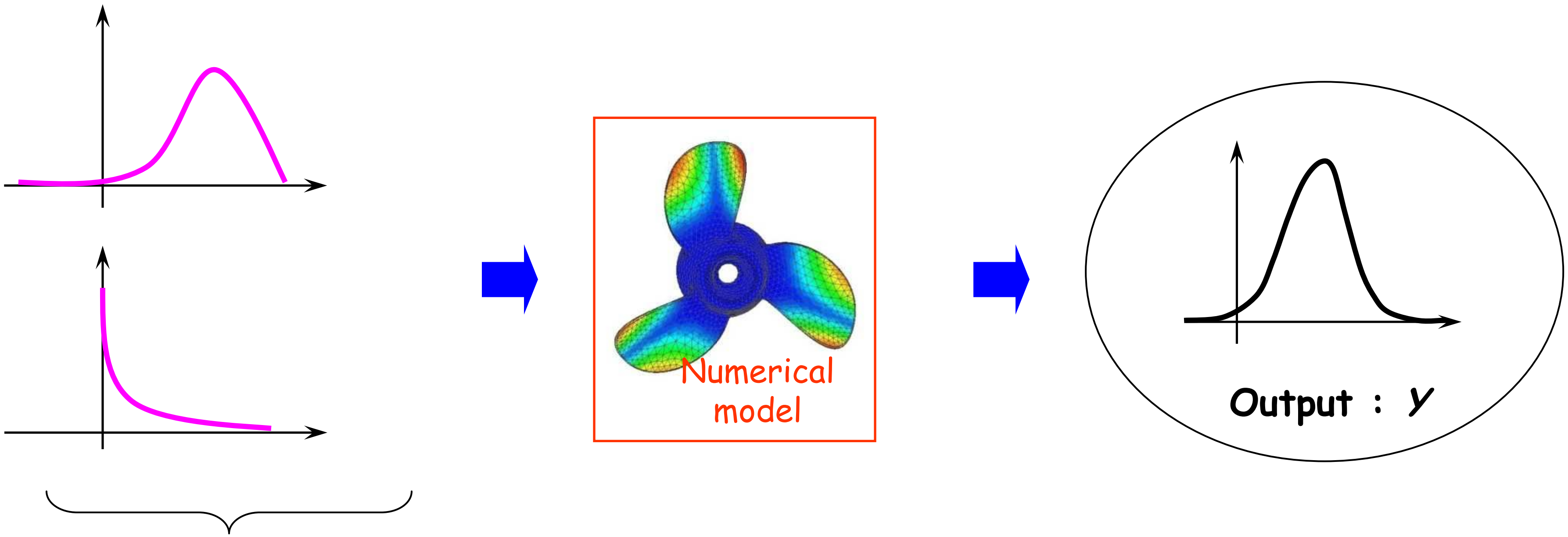
x's fully treated as R.V.

Can give moments, quantiles, and even pdf of Y …
…if fair waiting time

Uncertainty management - The generic methodology



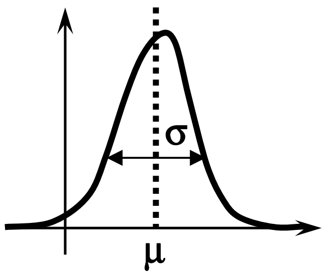
Step A – Focus on the quantity of interest



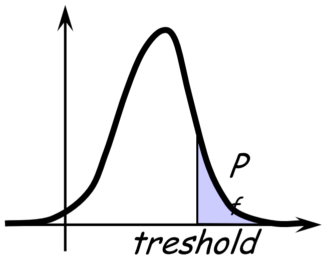
Inputs : X

What is really interesting in our study?

Sometimes a cost/information compromise



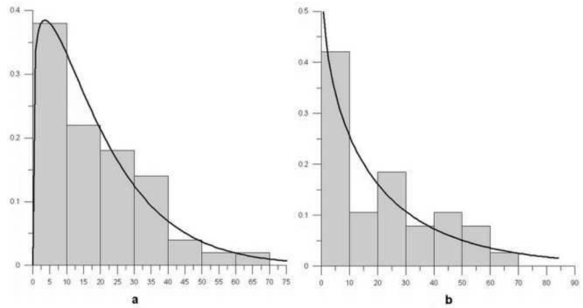
Mean, median, variance, (moments) of *Y*



Quantiles (extrems), probability of treshold exceedence

Step B - Quantification of uncertainty sources

Different cases



1. A lot of data
   - Fitting of probability distributions
   - Statistical hypothesis test (often parametric tests)

2. Few data (n < 10)
   - Use of probabilistic inequalities to obtain the mean and some bounds
   - Hypothesis on parametric probability distribution
   - Non-parametric tests : less powerfull, wide bounds
   - Expert judgement, then Bayesian inference

3. No data
   - Maximum entropy principle
   - Expert judgment techniques
   - Cristal Ball ?

Step B' - Calibration issues: use of indirect observations of the outputs in order to retrieve the model inputs

Step C - Uncertainty propagation: main principles

Propagate uncertainties from X to *Y*, via the deterministic function f(•)

- Conceptually simple problem, but with sometimes a complex implementation
- Choice of method strongly depends on the quantity of interest

=> importance of step A

this quantity of interest is linked to decisional issues

<u>Two kinds of problems :</u>

- Central tendancy (ex. mean) or dispersion (variance)
  - Metrology

➡ Analytical methods sometimes applicable

- High quantile, « probability of failure »
  - → justification of a safety criterion

➡ Numerical methods (optimization, Monte Carlo sampling)

Step C' - Sensitivity analysis: main objectives

- **Reduction of the uncertainty of the model outputs by prioritization of the sources**
  - Variables to be fixed in order to obtain the **largest reduction** (or a fixed reduction) **of the output uncertainty**

    A purely mathematical variable ordering

  - Most influent variables in a given output domain

    - if reducibles, then R&D prioritization

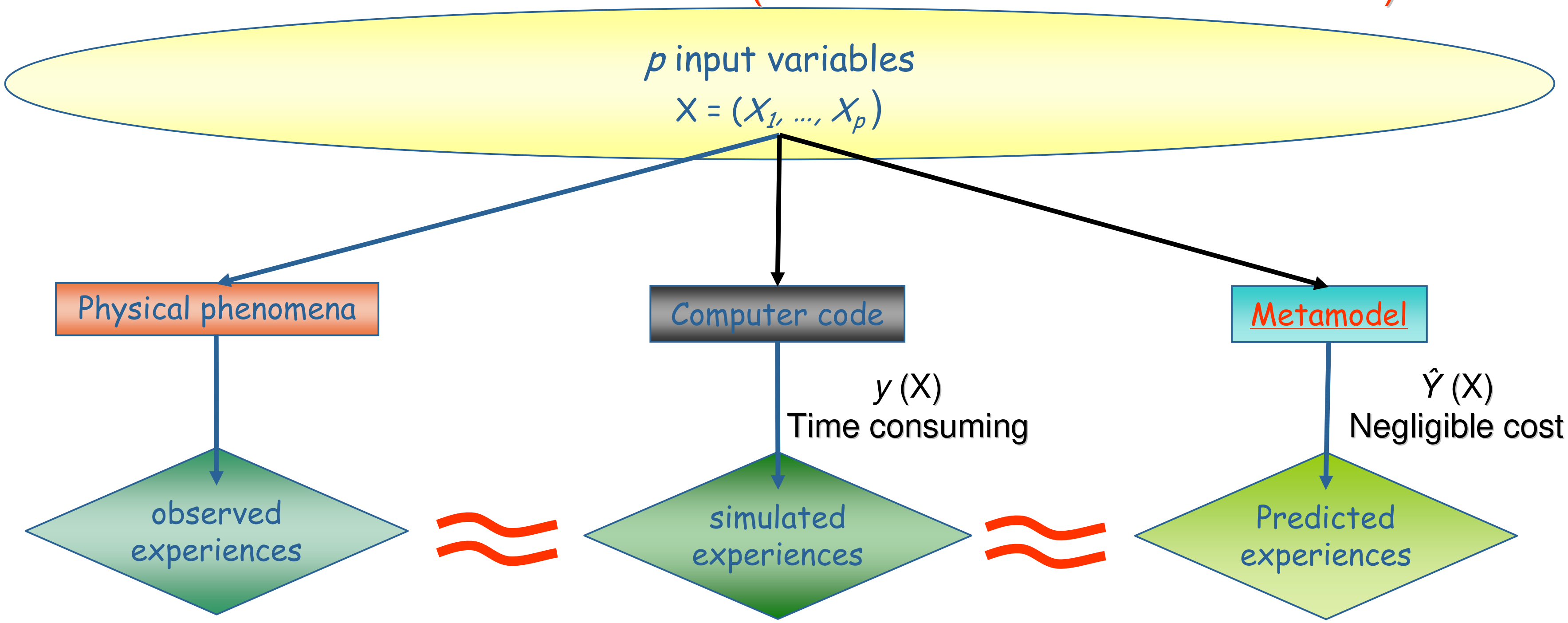
    - else, modification of the system

    The individual cost of the reduction may change the previous variable ordering

- **Simplification of a model**
  - **determination of the non-influent variables,** that can be fixed without consequences on the output uncertainty
  - building a simplified model, a metamodel

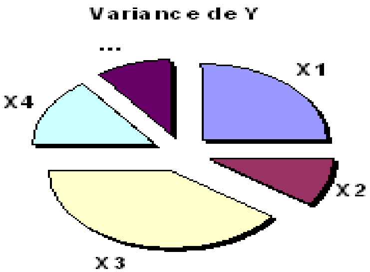
Uncertainties management for cpu time consuming models

A useful solution : the metamodel (model of the numerical model)

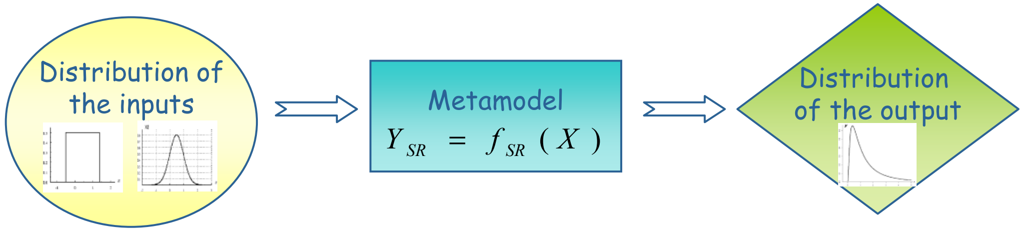


Use of the metamodel :

- C':Sensitivity analysis



- C:Uncertainty propagation (via Monte Carlo methods)



- B':Calibration

Identification of input parameters values

Adequation between observed and simulated experiences

V&V Verification and Validation

To sum up :

Verification : do I solve the equations right ?

Validation : do I solve the right equations ?
(at least for the intended application)

Two levels for Verification :

1. Code Verification : some kind of "*internal*" correctness of the code

   may be assessed by formal methods from Software Engineering

2. Calculation Verification : concerns the calculations themselves

   Convergence, grid adaptation, solution algorithms, …

   Is the solution closed to the exact one ?

We'll talk later on subtilties between Code and Model(s)

V&V Verification and Validation

Validation

1. Should occur AFTER Verification

2. Here the goal is to test the Code against Reality ….

   Roughly speaking : code (C) gives information I(R|C) on Reality ; so does Experiment (I(R|E)) ; the couple (C,E) is valid if I(R|C) and I(R|E) agree (statistically)

   (need to validate also experiments !!!)

3. Must not be confused with calibration ; schematically :
   1. Validation : just test for the agreement between I(R|C) and I(R|E) and then decide if (C, E) is valid or not
   2. Calibration : tune C in order to improve the agreement between I(R|C) and I(R|E)

V&V : a first step to assess the credibility of the code

Don't forget that the true objective is to gain confidence in our simulations

So ask the questions :

1. Is the code able to simulate the system/phenomena of interest ?

   that is the Accreditation (Expert-like decision) step

2. What is the strategy if I(R|C) and I(R|E) disagree ?

3. And if I(R|C) and I(R|E) agree : can I assess a confidence interval for future predictions ?

And always remember that

All models are wrong but some are useful
G.E.P. Box

Motivations for this summer school

- **We are convinced that, at the present time, each simulation result should be associated with an uncertainty (as in the measurement science)**

- **High Performance Computing becomes accessible to many scientists**

- However, statistical tools are not so easy to use ; there are also some cultural barriers in the engineering world

- This subject has recently received a lot of attention (software development, interdisciplinary working groups, many research works, etc.)

For us, this summer school is an occasion to:

1. Disseminate the uncertainty culture in our research institutes and companies

2. Offer in an educational way recent advances about the topics of uncertainty quantification and simulation model validation

3. Create a strong event on this subject (in reference to the last CEA-EDF-INRIA summer school in 2005)

Organization of this summer school

Three main lectures from international experts:

1. François Hemez (Los Alamos) - Introductive course
2. Rui Paulo (Univ. Tech. Lisboa) – Bayesian view
3. Emmanuel Vazquez (SUPELEC) – Rare events evaluation

showing the scientific diversity of the problems

Computer practical works in various programming languages:

1. Matlab
2. R

Two software demonstrations:

1. OpenTURNS (from EDF-EADS-Phimeca)
2. URANIE (from CEA/DEN)

Several seminars on connected subjects:

- Remainder of statistics
- Calibration
- Chaos polynomials
- Model validation
- Multidisciplinary and robust optimization
- High Performance Computing

First week – 27 june to 1 july

Each lecture and each practical work goes on 1h30. Morning : 8h30-12h – Afternoon : 14h-17h30

- 27 june
  - Morning (beginning 11h) : Iooss & Sancandi (45mn) – Presentation/organization of the school
  - 11h45-12h30 : Seminar 1 Part 1 (45mn) Marrel
  - Afternoon : Course 1.1 Hemez & Seminar 1' (1h) Pasanisi
  - End of afternoon : Seminar 1 Part 2 (1h) Marrel
- 28 june
  - Morning : Course 1.2 Hemez – Course 1.3 Hemez
  - Beginning of afternoon (14h-15h30) : visit of Iter construction site
  - Afternoon : Optional TD to be chosen between TD A and TD B
  - End of afternoon : TD 1.1
- 29 june
  - Morning : Course 2.1 Paulo – Course 2.2 Paulo
  - Afternoon : TDs 1.2 et 2.1
- 30 june
  - Morning : Course 1.4 Hemez – Course 2.3 Paulo
  - Afternoon : TDs 1.3 et 2.2
  - End of afternoon : Seminar 2 (1h30) de Crécy & Couplet
- 1er july
  - Morning : Course 1.5 Hemez – Course 2.4 Paulo
  - Afternoon (end 15h30) : TD 2.3

Second week – 4 july to 8 july

Each lecture and each practical work goes on 1h30. Morning : 8h30-12h – Afternoon : 14h-17h30

- 4 july
  - Morning (beginning 11h) : Course 3.1 Vazquez
  - Afternoon : TDs C et 3.1
  - End of afternoon : Social event
- 5 july
  - Morning : Course 3.2 Vazquez – Seminar 3 (1h30) Le Riche
  - Afternoon : TD 3.2 – Seminar 4' (45') Blatman - ??course on sensitivity analysis?? (45')
- 6 july
  - Morning : Course 3.3 Vazquez – Seminar 5 (1h30) Sancandi
  - Afternoon : Atelier logiciel OpenTURNS (3h)
  - End of afternoon : Seminar 4 (45') Martinez
- 7 july
  - Morning : Cours 3.4 Vazquez – Seminar 6 (1h30) Prud'homme
  - Afternoon : Atelier logiciel URANIE (3h)
  - Gala dinner
- 8 july
  - Morning : Course 3.5 Vazquez – TD 3.3 – Conclusion/Information (1h)
  - End at 13h00

The entire team wishes you a happy summer school !

Your private assistants …

Amandine

Vincent

Claire

Géraud

Nadia

Mathieu

… and your major assistants

Marc

Bertrand