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Batch Submission with URANIE

F. Gaudier

fabrice.gaudier@cea.fr

HPC and Uncertainty Treatment
Examples with OPEN TURNS and URANIE

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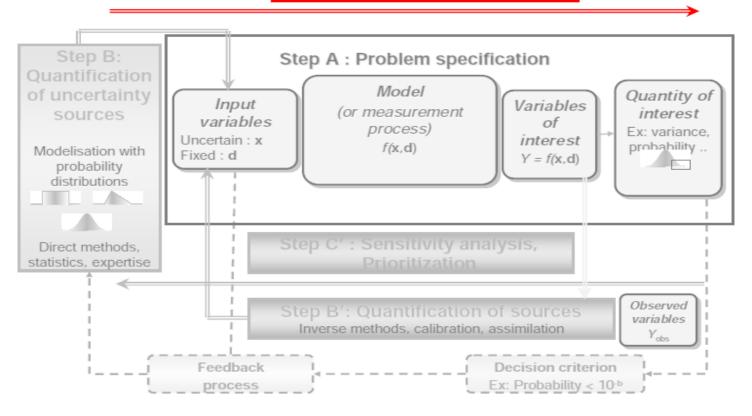


Uncertainties Flowchart



[De Rocquigny et al., 2008]

Step C : Propagation of uncertainty sources





Outline



- External code for the Use Case **Beam**
- Submitting **Sequential** job
- ullet Submitting ${\it Parallel}$ job



Use Case Beam - "external code"



• A "external code" simulates the "beam" problem (if beam ∉ \$PATH; source ...)

```
beam -h

** Usage: ./beam [-v] [-h|-?] [-x [file]]

-v: Pass to the verbose mode

-h|-?: Print the usage message

-x: Set the input file with XML format [beam_input_with_xml.in]
```

- The parameters of the study, with their deterministic values, are:
 - \mathbf{E} (3.0 e^7): the Young modulus
 - \mathbf{F} (300): the ponctual load
 - L (2.5): the length of the beam
 - \mathbf{I} (4.0 e^{-6}): the flexion inerty
- The values of these parameters are stored in the "XML" input file "beam.xml":



Use Case Beam - "Evaluation"



• Evaluate the external code on the "XML" input file "beam.xml":

```
beam -x beam.xml
```

• The same in "verbose" mode (-v option)

```
beam -v -x beam.xml
********
** The Beam use case
** Nb Argument [4]
** verbose mode
** XML Input File[beam.xml]
************
** writeXMLOutputs in the XML file [ _beam_outputs_.xml] ...
** End Of writeXMLOutputs with XML file
***********
*************
** beam::printLog
** sFile[beam.xml]
** Inputs : E[3e+07] F[300] L[2.5] I[4e-06] *********
** Output :
** Deviation[13.0208]
```



<u>Use Case Beam</u> - "Output File"



• The target variable is stored in the "XML" output file _beam_outputs_.xml

```
<?xml version="1.0"?>
<beam>
<description name="beam" title="UseCase beam with XML input file" version="1.0" date="2014-04-</pre>
07">
    <tool name="beam exe" version="1.0"/>
</description>
<inputs F="300.0" E="3.0e7" L="2.5" I="4.0e-6"/>
<computation>
    <derivate activate="on"/>
    <hessian activate="off"/>
</computation>
<outputs deviation="1.3020e+01">
  <derivates partialE="-4.340e-07" partialF="4.340e-02" partialL="1.562e+01" partialI="-</pre>
3.255e+06"/>
  <hessian><partialE partialE="2.893518519e-14" partialF="-1.446759259e-09" partialL="-</pre>
5.208333333e-07" partialI="1.08506944e-01"/><partialF partialF="0.000000000e+00" partialL="5.208333333e-
02" partialI="-1.085069444e+04"/><partialL partialL="1.250000000e+01" partialI="-3.906250000e+06"/>
<partialI partialI="1.627604167e+12"/></hessian></outputs></beam>
```



Use Case Beam - XPATH



• XPATH for the inputs attributes in the "XML" file "beam.xml"

- type : Attribute, Field
- E :: //inputs/@E
- F :: //inputs/@F
- L :: //inputs/@L
- I :: //inputs/@I
- XPATH for the output attribute deviation in the "XML" file "_beam_outputs_.xml"

```
<outputs deviation="1.3020e+01">
     <derivates partialE="-4.340e-07" partialF="4.340e-02" partialL="1.562e+01" partialI="-3.255e+06"/>
```

- type : Attribute, Field
- deviation :: //outputs/@deviation



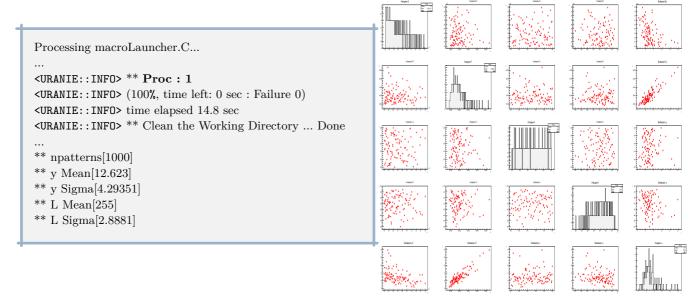
Sequential Job



• Evaluate a LHS DoE of nS=100 patterns with the Uranie macro "macroLauncher.C"

root -l macroLauncher.C

• which gives





Parallel Job



- Cluster: Poincarre (92 nodes, 2 processors/nodes and 8 cores/processors)
- Use the **LoadLeveler** (IBM) as Job Submission
 - List the tools in your environment

module list

- List the tools available

module avail

Load a tool in your environment

module load tool/version

Unload a tool from your environment

module unload tool/version



Parallel Job - "LoadLeveler"



- Useful commands of LoadLeveler
 - Get the number of free ressources



- Submit the job file "batch.sh" (describe in a next slide)

```
llsubmit batch.sh
```

List LoadLeveler jobs in the cluster

```
llq <-u user>
```

Delete a LoadLeveler job

```
llcancel JobID
```

• Help on the Poincare cluster



• Job submission file "batch.sh"

```
#!/bin/bash
#@ job_name
                     = BeamLauncher
                                           # Request name
                                           # Number of tasks to use
#@ total tasks
                      = 64
#@ node
                      = 4
#@ node_usage
                     = not\_shared
#0 wall_clock_limit = 00:30:00
                                           # Elapsed time limit in seconds of the job (default: 1800 = .5h)
#@ output
                                           # Standard output with the job id
                     = run_$(jobid).o
                     = run_$(jobid).e
                                           # Error output with the job id
#@ error
                                           # Choosing standard nodes
                     = clallmds
#0 class
#@ job type
                     = mpich
#@ environment
                      = COPY_ALL
#@ queue
# Load the modules if necessary
# module load intel intelmpi
# Source the environment variables if necessary
# source /gpfslocal/pub/training/uncertainty_may2017/URANIE/root5.34.36/URANIE3.10.0/uranie.bashrc
# Remove all old files
rm -f _launcher_code_.* run_*.o run_*.e
# Execute the Uranie macro with the -q option to quit ROOT
root -l -q macroLauncher.C
# End Of File
```





Command to submit the job file "batch.sh"

llsubmit batch.sh



Conclusions



- It is the same macro to launch in the sequential mode than in the parallel mode
- Operational for other Job Submission systems as SGE, LSF and SLURM (Cu-rie/TGCC)
- Don't forget the **-q** option in the ROOT command to quit ROOT when the computation is finished and free the core
- Exists also Parallel computing in a personnal desktop with several cores:

launcher->run("localhost=5");