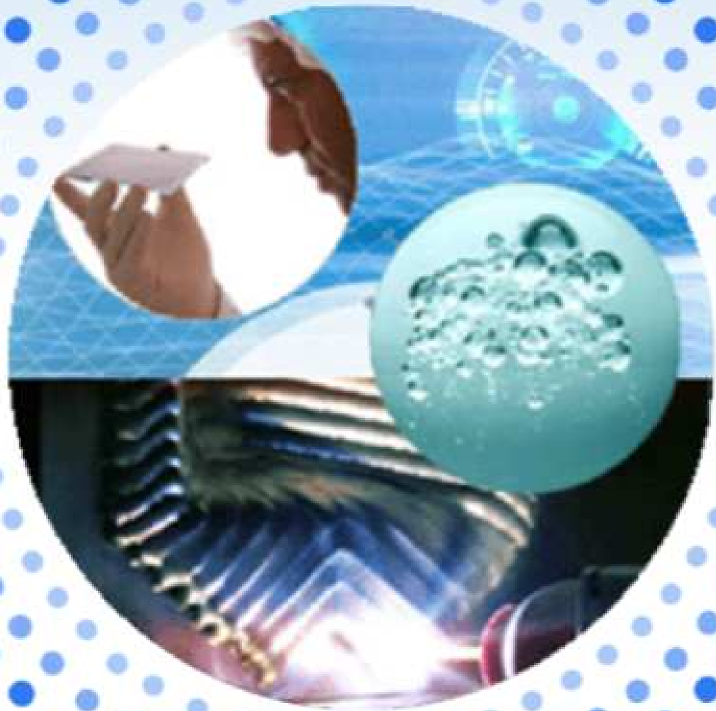
Journées Teratec



Risques, énergie et simulation haute performance : quelques démonstrateurs récents

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HPC and risk computation

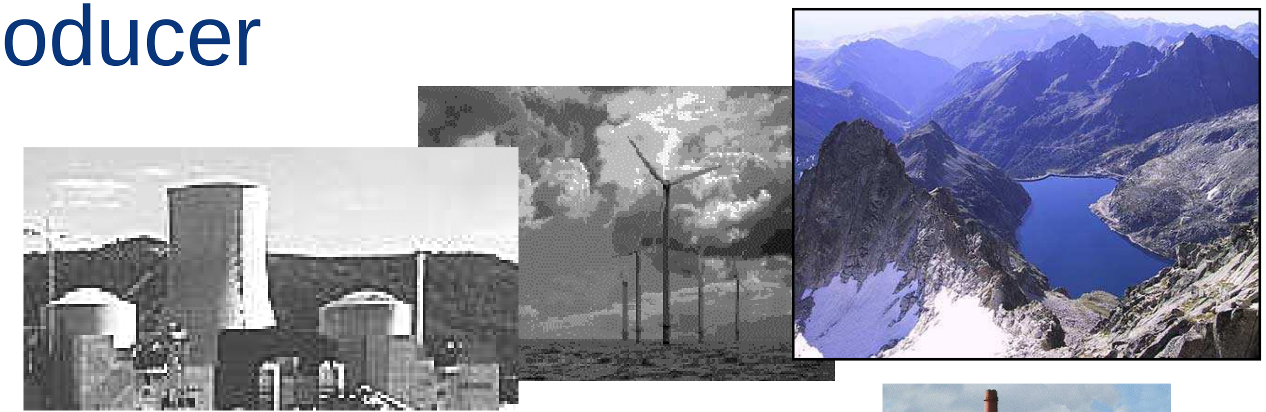
- Stakes for a power producer

- Numerical challenges & recent examples associated to risk quantification
  - Risk computation (or uncertainty propagation)
  - Importance ranking of risk/uncertainty factor (or sensitivity analysis)
  - Stochastic optimisation in high dimension

- Challenges & perspectives ahead for HPC

Disclaimer : subsequent views do not commit EDF R&D in any respect to the actual or recommended practice in the field of risk assessment or environmental control

Major areas for risk quantification for a power producer



The assets

- 58 nuclear power plants on 19 areas (86.6% of production)
- 14 thermal power plants (4.6% of production)
- 440 hydro plants and 220 dams (8.8% of production)
- Solar energy, wind power (< 0.5% of production)

Customers

- Different kind of customers (industry, domestic, …)
- Many kinds of contracts (for example swing where the producer can suspend delivery)

Asset management

Plant safety

Asset management issues

- Manage water stocks, fuel , customers contracts.
- Goal :
  - maximize the expected cash flow
  - minimize risk
-
- Under constraints
  - Satisfy the customer load (no shortage of power)
  - Respect pollution constraints

- Hazards :
  - Demand
  - Hydraulicity (inflows)
  - Weather patterns (cold weather means high demand)
  - Market prices
  - Assets outages (linked to market prices if high demand) ….

→ Stochastic control problem in high dimension

Plant safety issues

- Nuclear safety
  - Internal agressions
    - Conventional accident – Probabilistic CFD & mechanics, gradually multi-scale
    - Mechanical margins – pressurised vessel and other equipment
    - Complex system reliability – Million-branch event or binary trees
  - External agressions : flood & sea levels, temperatures, winds, earthquake …
- Dam safety
  - Flood and external initiators
- Life-cycle (plant asset) management & maintenance issues

→ Deterministic / Probabilistic risk assessment

Scientific computing + stochastics

Probabilistic physics & engineering
Uncertainty & sensitivity modelling

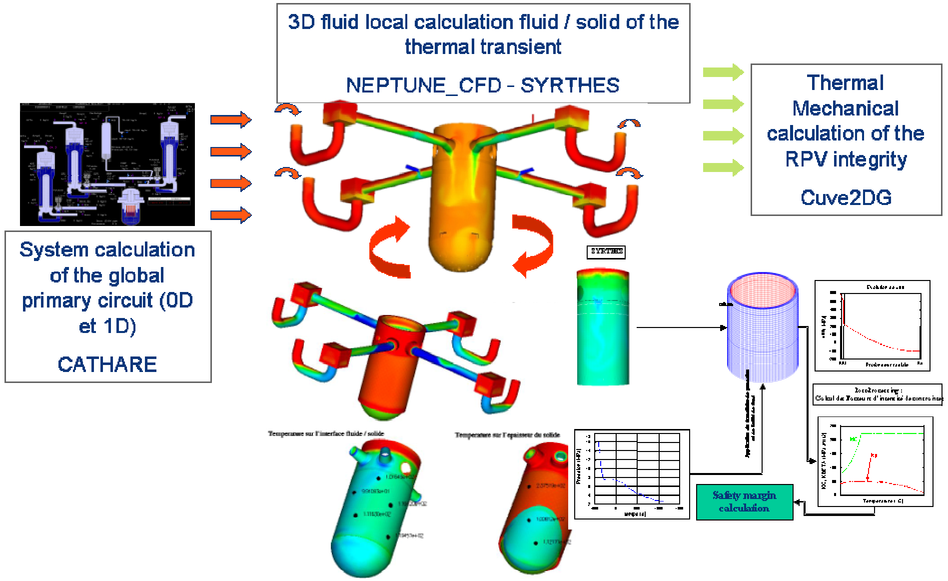
$$\underline{Z} = G(\underline{X}, \underline{d})$$

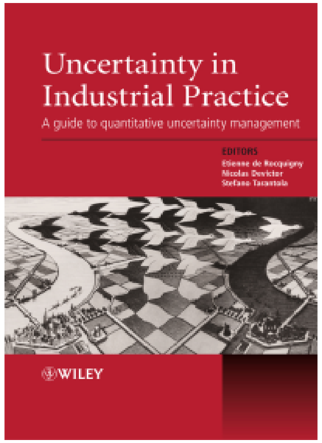
Random vectors, fields or time processes

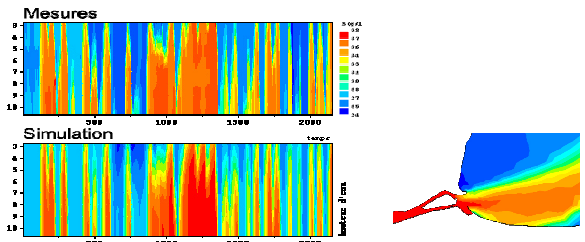
$$\underline{X} \sim f_X(\underline{x} \mid \underline{\theta}_X)$$

Coupled integro-differential operators (ODE, PDEs, …)

G(.) models an industrial or environmental system







Saltelli et al, 2004

de Rocquigny et al, 2008

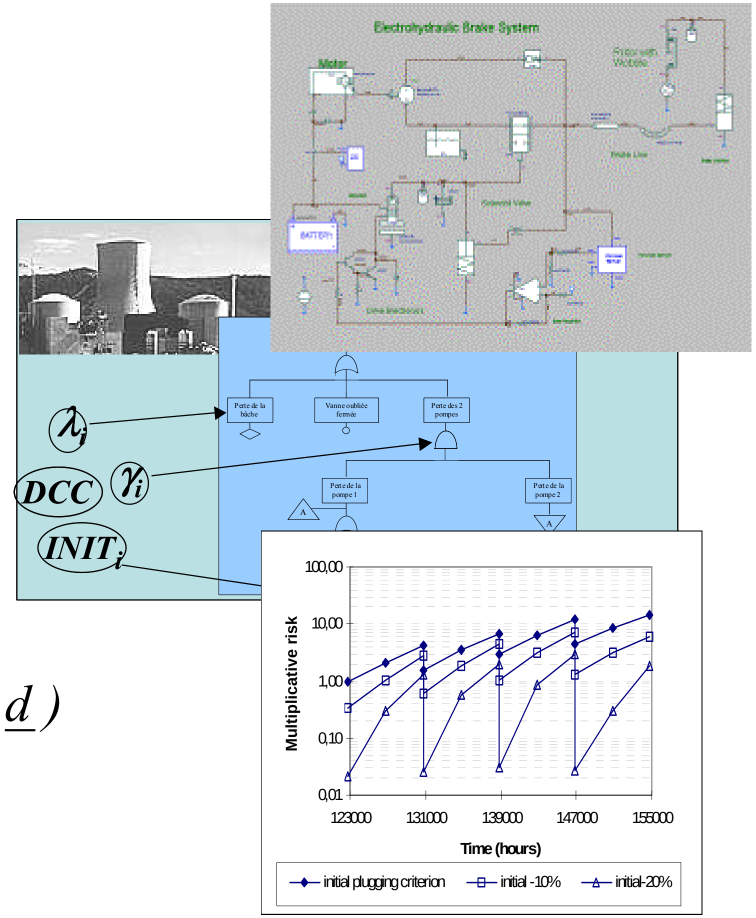
www.openturns.org

Reliability

- Static risk & reliability models
  - Failure/event trees, BDD, BBN etc. + lifetime statistics

$$e = \sum_i \left[e^{in^i} . \prod_{j_i(\underline{d})} e^{sy^{j_i}} \right] = G\left(\underline{e}^{in}, \underline{e}^{sy}, \underline{d}\right)$$

$$E^j = 1_{t=T_j} \quad T_j \sim f_T(t_j | \underline{\theta}_T)$$



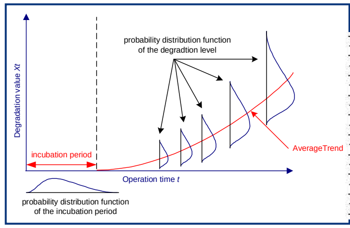
- Dynamic reliability models
  - *« Chained » renewal processes* $Z_t = \sum_j 1_{E^j_t} g_j(\underline{X}_j, \underline{d})$

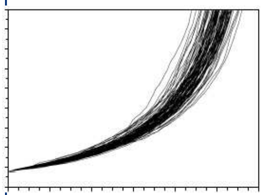
e.g. Probabilistic life cycle management

  - *« Coupled » dynamic processes*

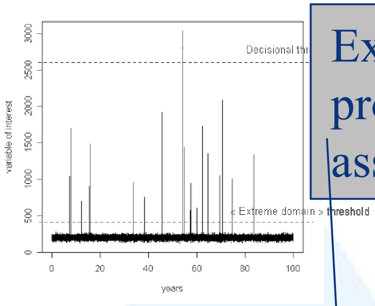
$$\underline{\dot{X}}_t = F\left[\underline{X}_t, \underline{E}_t\right]$$
$$given \quad \underline{E}_t$$
$$or \quad P(\underline{E}_{t+dt} | \underline{E}_t) = h(\underline{E}_t, \underline{E}_{t+dt}, \underline{X}_t) + o(dt)$$

(MP, PDMP …)

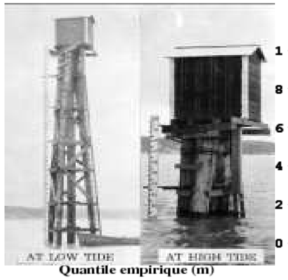


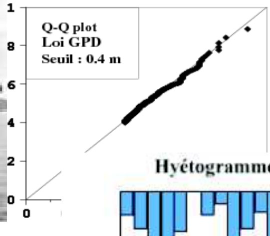


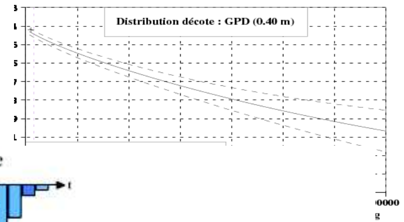
Natural risk / extreme events
(External agressions, …)



Extreme value renewal process (e.g. POT) and associated Pareto cdf



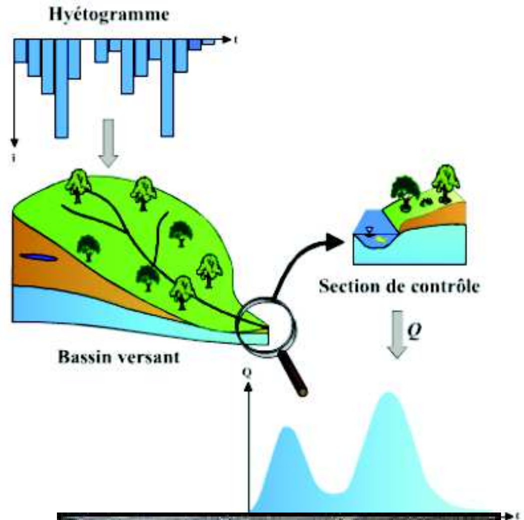




$$X_t = 1_{E^u{}_t} X$$

$$X \sim \boldsymbol{GPD_u}\left(\boldsymbol{x} \middle| \mu_u, \sigma_u, \xi_u\right) = 1 - \left[1 + \xi_u \left(\frac{x - \mu_u}{\sigma_u}\right)\right]^{-\frac{1}{\xi_u}}$$

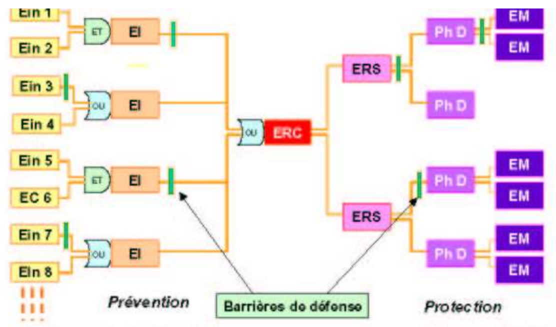
$$z\Big|_{X_t \geq x_\alpha} = G(x_\alpha, x^{en}{}_{pn}, \underline{d})$$



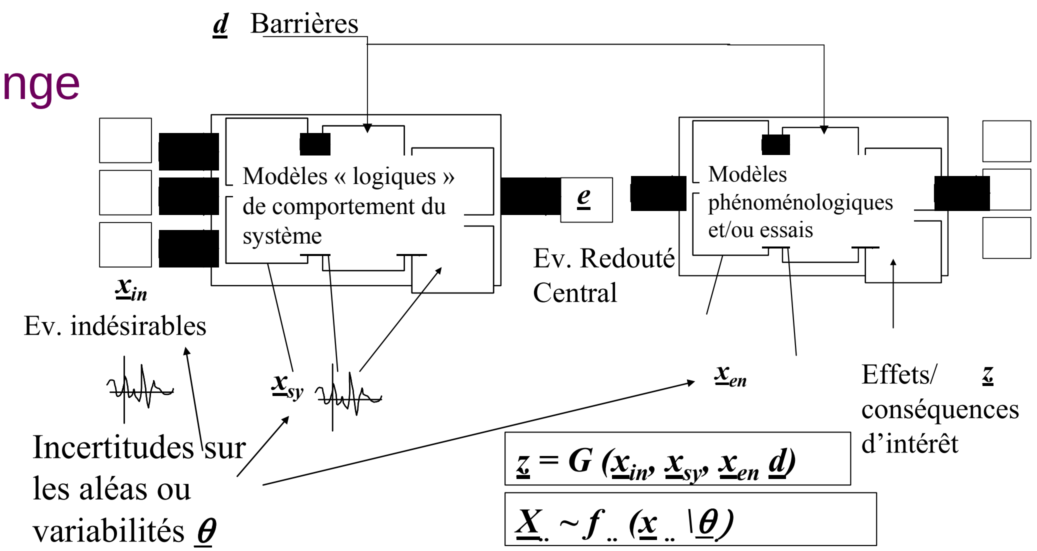
Coupled integro-differential operators (ODE, PDEs, …)

IPRA mixed models
(Integrated Probabilistic Risk Assessment)

- Mixing probabilistic physics, external agressions & reliability
  - Nuclear Level 2 – Probabilistic Safety Analyses
  - (Helton, 1993)
- An enormous computing challenge …



Source: ARAMIS / INERIS



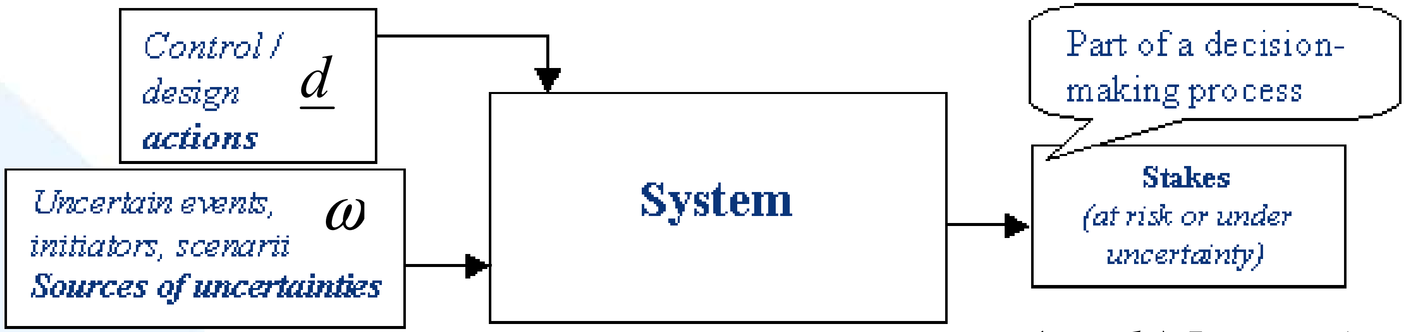
Stakes for a power producer

- Industrial and environmental systems under risk & uncertainty
- Making the best of all information available (statistical data, phenomenological knowledge, expertise …) to
  - optimise the systems at various time scales
  - control safety standards
- … valuing advanced maths & computing
  - Statistical modeling & probabilistic computing
  - Numerical analysis
  - Decision-theory
  - HPC

⦿Numerical challenges & recent examples

⦿Risk computation
(simulation, uncertainty propagation, …)

Risk modeling & the risk measure



$$\underline{z}(\omega,\underline{d})[t,t+\Delta T]$$

- The risk measure, a quantitative tool to property C_z over the period ΔT, in order to
  - *Rank / Optimise risky alternatives* $\quad C_Z : \quad \{c_Z(\underline{d}_A) \leq c_Z(\underline{d}_B)\}$
  - *Control compliance with a risk limit (or budget)* $\quad C_Z : \quad \{c_Z(\underline{d}) \leq c_s\}$

$$c_Z(\underline{d}) = \mathcal{F}\left[\underline{z}(\omega,\underline{d})\right]$$

$$e.g. \quad c_Z(\underline{d}) = EU(z) = \int_\omega U(z(\omega))dP(\omega)$$

$$c_Z(\underline{d}) = EU(z) = E1_{Max_{[t_1,t_1+\Delta T]}Z_t(\omega)\leq z_s} = P\left[Max_{[t_1,t_1+\Delta T]}Z_t \leq z_s \middle| \underline{d}\right]$$

Computing the risk measure

- The key case of threshold exceedance

A key risk measure is

$$c^{(1)}{}_z = E_{\underline{\theta}} P_{X_t|\underline{\theta}}(Z < z_s) = \int_{\underline{\theta}, x_t} 1_{G(x_t, \underline{d}) < z_s} f_{X_t}(x_t|\underline{\theta}) \pi(\underline{\theta}|\varsigma) dx_t d\underline{\theta}$$

enjoying a number of algorithms

- Piecewise closed-form integration
- Accelerated methods
  - Black-box approximation and variance reduction
  - Grey box : value phenomenological regularity (e.g. monotony)
- …

Risk computation : the need for HPC

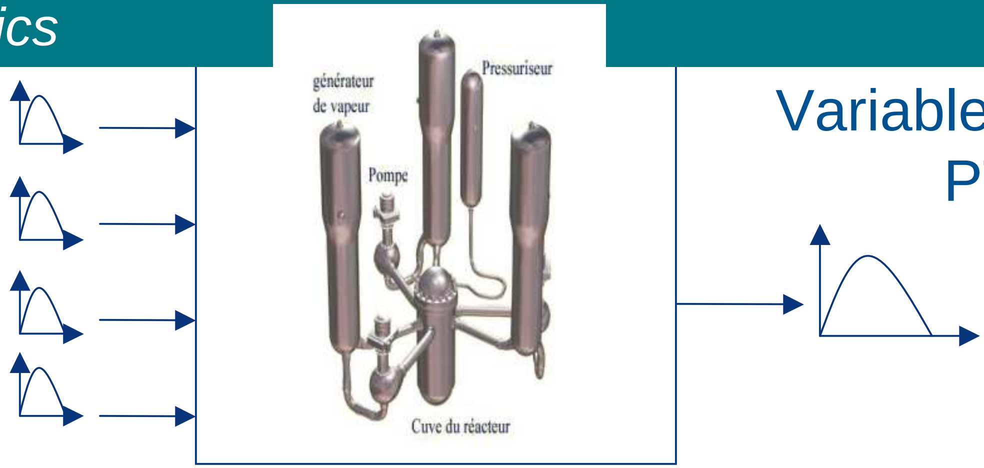
- … or massive distribution

$$c^{(1)}{}_z = E_{\underline{\theta}} P_{X_t|\underline{\theta}}(Z < z_s) = \int_{\theta, x_t} 1_{G(x_t, \underline{d}) < z_s} f_{X_t}(x_t|\underline{\theta}) \pi(\underline{\theta}|\varsigma) dx_t d\underline{\theta}$$

  - Theoretically trivial in the simplest Monte-Carlo/Wilks formulation
    - … but requiring adapting Blue Gene-like operating features
      - see Example APRP hereafter
  - To be done on hybrid accelerated algorithms (such as meta-modeling, adaptive importance sampling …)
    - … some are facially sequential, but could be partially parallelised
      - Either inside each run of G(.) – code parallelism
      - Or on the Monte-Carlo parts – partial distribution

1st risk computation example : Massive Monte-Carlo in Nuclear thermal-hydraulics

Sources d'incertitudes



Variable d'intérêt: PTG

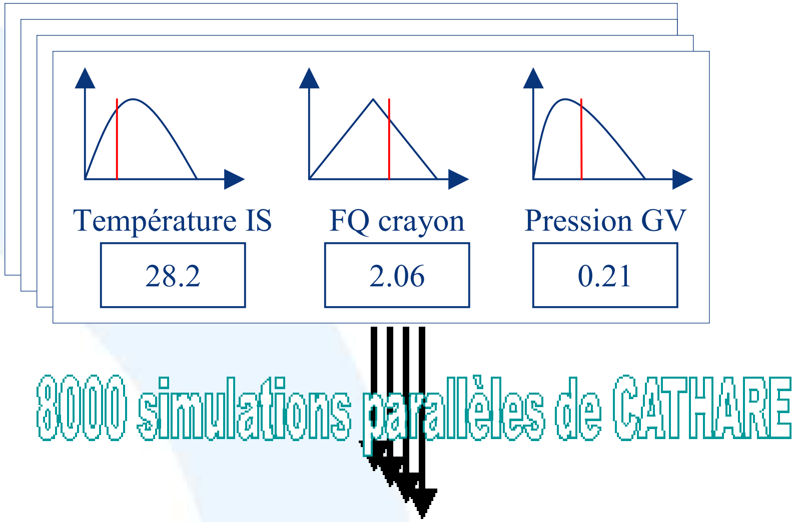
Les sources d'incertitude:

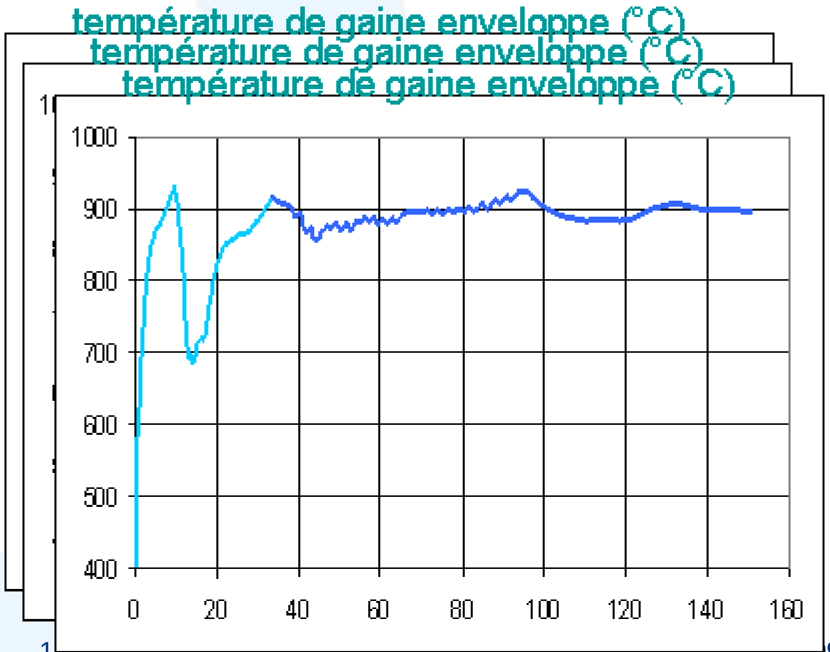
- 74 paramètres physiques incertains parmi 136 paramètres
  - Concernant les crayons de combustible, les GV, les pompes, l'IS, les caractéristiques des fluides…
- Lois de probabilité: Uniforme, Log-Uniforme, Normale et Log-Normale tronquées.

Critère de sûreté: la température maximale des gaines de combustible atteinte durant un APRP GB doit être inférieure à un seuil Tseuil pour un niveau de risque donné: **P (PTG < Tseuil) > 95%**

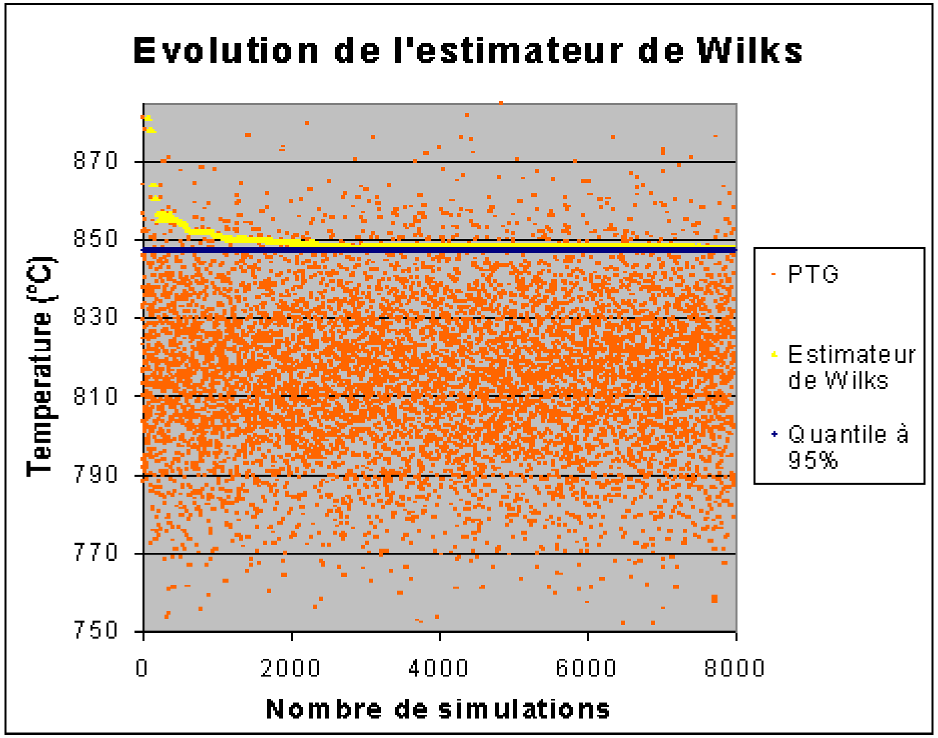
Nombre minimum de tirages tel que le i-ème max. soit un estimateur de Wilks			
Maximum	2^{nd} max.	3^{rd} max.	4^{th} max.
59	**93**	**124**	**153**

8000 simulations de Cathare en parallèle sur Blue Gene…





…et analyse des 8000 températures calculées



NB : résultats sur exemple numérique non-représentatif des installations EDF

Computing features and challenges

- Characteristics (BG/L – 23 Tflops)
  - 8000 (single-core) proc. over 4000 nodes – 0,7 GHz
  - 0.25 Go per proc. but server memory limitations forced a maximum of 1000 nodes

- Performance
  - Each run is x2 to x4 longer than on the equivalent PC
  - Massive distribution achieves a speed-up from 20 yr-CPU down to 40 dy (x200)

- Challenges
  - Significant failure rate, essentially due to physical-numerical instability sensititivies
  - Automatic time step adapting faces limitations due to extensive space-exploring … well beyond traditional code qualification control

Multiple-level probabilistic risk measures

$\underline{X}, \underline{E}, \underline{d}$ → G → $\underline{Z} = G(\underline{X}, \underline{E}, \underline{d})$

$\underline{c_Z} = \mathcal{F}(f_{\underline{Z}}(\underline{z} \backslash \underline{\theta}_{XE}, \underline{d}))$

Aleatory uncertainty is modelled by a random vector joint pdf $\underline{X}, \underline{E} \sim f_{XE}(\underline{x}\ \underline{e} \backslash \underline{\theta}_{XE})$

The specific risk measure relevant to decision-making

$c_Z = P(z > z_s)$, $var\ Z$,

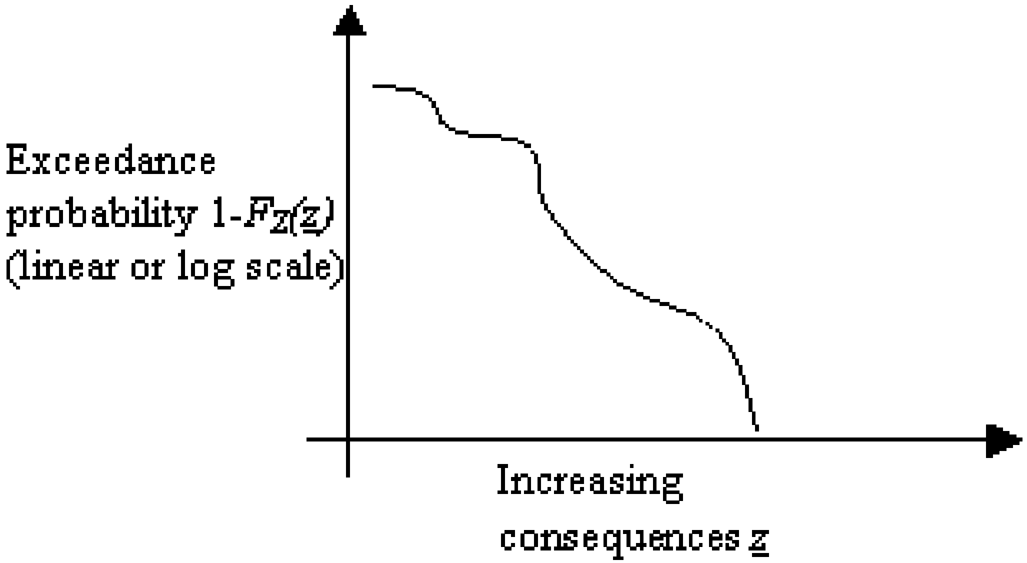
Estimating $\underline{\theta}_{XE}$ with finite data sets => Epistemic uncertainty in $\hat{\theta}_{XE} \sim \pi(\theta_{XE} | \zeta)$

*Even if $\underline{\theta}_X$ was perfectly known, CPU limitations on **propagation** => residual variance on the estimation of* $\hat{C}_z(\theta_{XE})$

Multiple-level (aleatory/epistemic) risk computing

- Single-level setting
  - Mixes all into one pdf

$$f_{XE}(\underline{x}\ \underline{e}\ |\underline{\theta}_{XE})$$



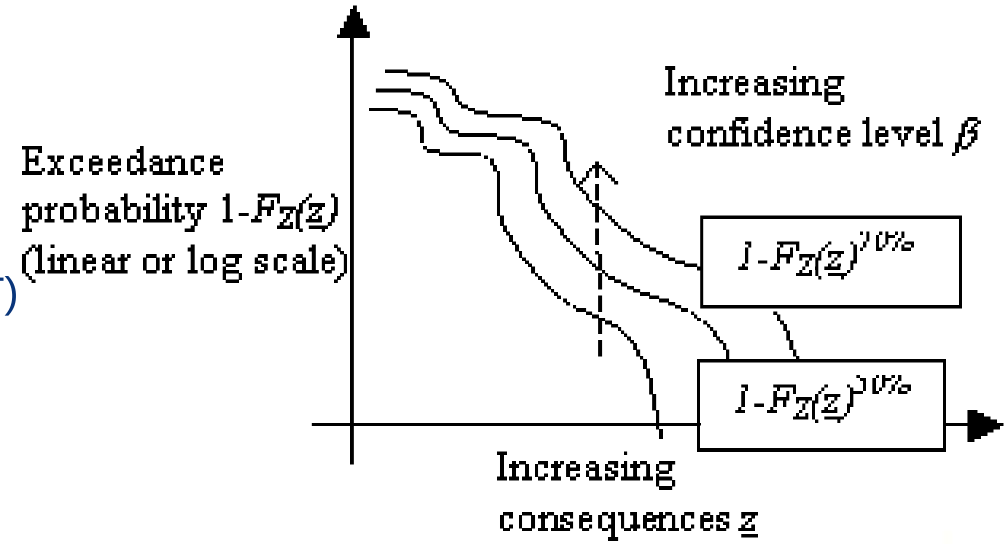
- Two-level settings
  - Separates two layers

  « risk » + « uncertainty »

  - Second one possibly non-probabilistic (deterministic / DST)

(Helton et al, 1996)

$$\{f_{XE}(\underline{x}\ \underline{e}\ |\underline{\theta}_{XE}),\ \pi(\underline{\theta}_{XE}\ |\zeta)\}$$



Risk measure = tougher computational challenges

$$c_Z(\underline{d}) = \mathcal{F}\left[\underline{z}(\omega,\underline{d})\right] = IF\left\langle M(.), f_{XE}(.|\underline{\theta}_{xe})\pi(\underline{\theta}|\varsigma)\right\rangle$$

Two-level sampling

- $\underline{\theta}_{j1} \sim \pi$
- $(\underline{X},\underline{E})_{j2} \sim f_{XE/} \,|\underline{\theta}_{j1}$

$$c_Z(\underline{d}) = P_{\underline{\Theta}}[\,P_{\underline{Z}|\underline{\theta}}(Max_t Z_t \leq z_s|\underline{\Theta},\underline{d}) < \alpha\,]$$

$$= \int_{\theta} 1_{\left[\int 1_{Max_t Z_t \leq z_s} f_{\underline{Z}}(.|\underline{\theta})\right] < \alpha} \pi(\underline{\theta}|\underline{\varsigma})d\underline{\theta}$$

Maximising

- Over time

$$c_Z(\underline{d}) = P\left[Max_{[t_1,t_1+\Delta T]} Z_t \leq z_s|\underline{d}\right]$$

- Over some of the components

$$c_Z(\underline{d}) = Max_{\underline{x}_{pn}\in\Omega_x} c_Z(\underline{d}|\underline{x}_{pn}) = Max_{\underline{x}_{pn}\in\Omega_x} P\left[Max_{[t_1,t_1+\Delta T]} Z_t \leq z_s|\underline{d},\underline{x}_{pn}\right]$$

⦿Importance ranking of risk/uncertainty factors

(sensitivity analysis, design of computer experiments …)

Importance Ranking (sensitivity analysis)

- **Variance-based-ranking : explain contribution of input X_i to variance of output Z**

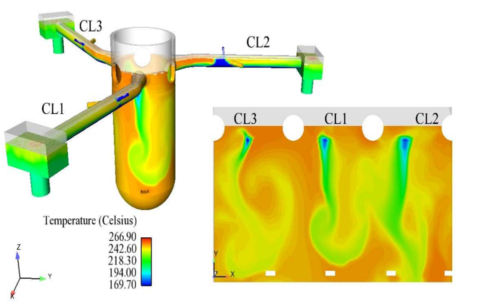
$$\mathrm{Var}(Z) = \sum_{i=1}^{p} V_i(Z) + \sum_{i<j}^{p} V_{ij}(Z) + \cdots + V_{12\cdots p}(Z)$$

$$S_i = \frac{\mathrm{V}[\mathrm{E}(Y \mid X_i)]}{\mathrm{V}(Y)} \quad ; \quad S_{ij} = \frac{\mathrm{V}[\mathrm{E}(Z \mid X_i\, X_j)]}{\mathrm{V}(Z)} - S_i - S_j \ ; \ \ldots \ ; \ S_{Ti} = S_i + \sum_j S_{ij} + \ldots$$

1st order 2nd order Total index

- **Straightforward interpretation in % ranking**
- Algorithms to estimate Sobol indices :
  - **Monte-Carlo > 1000 runs / input for full indices (~30 for additive-dominated rank correlation approximation)**
- FAST (~1000 runs / input) : decompose through Fourier transform of *G(.)*
- Quasi-Monte-Carlo (< 1000 runs / input) : deterministic sampling sequences
- Meta-modeling

A recent example : a double HPC challenge



⦿ Securing lifetime of the Reactor Pressurized Vessel

- **A multi-physics and multi-scale challenge …**
  - **Both thermal hydraulics and rupture mechanics are needed**
  - **TH System and local features are both essential to track margins**

>> chain Cathare + NEPTUNE_CFD-SYRTHES + Cuve2DG

- **… under uncertainty**
  - **moving from deterministic margins to a probabilistic risk**
  - **traditionally only *mechanical* parameters are probabilised**
  - **Yet, how much do the thermal-hydraulic uncertainties contribute to the risk ?**

>> Propagate & rank uncertainty throughout (via Open TURNS)

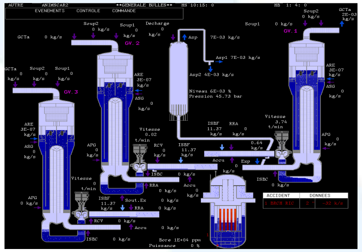
Multi-physics multi-scale coupling

3D fluid local calculation fluid / solid of the thermal transient

NEPTUNE_CFD - SYRTHES

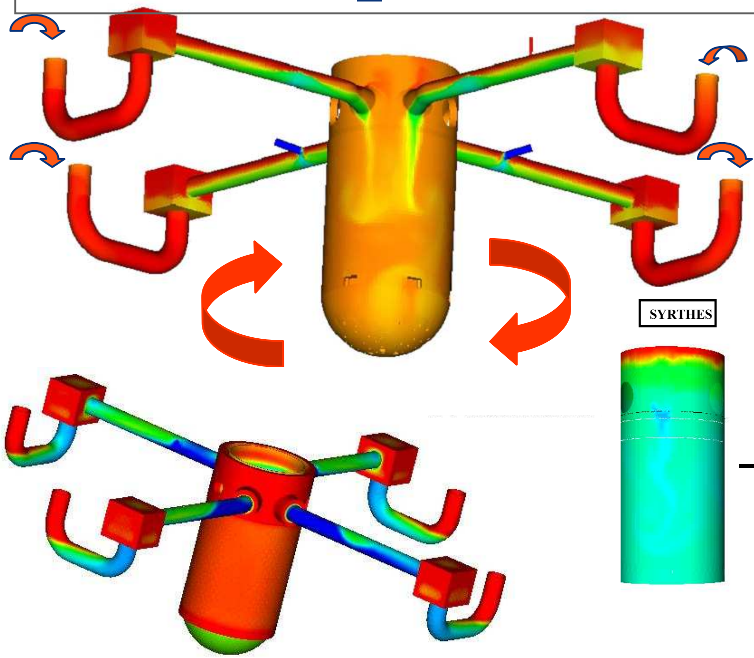
Thermal Mechanical calculation of the RPV integrity

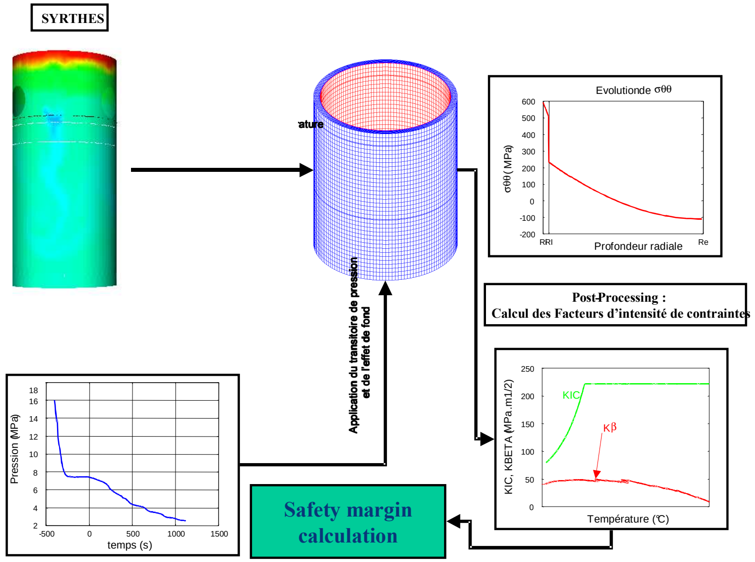
Cuve2DG



System calculation of the global primary circuit (0D et 1D)

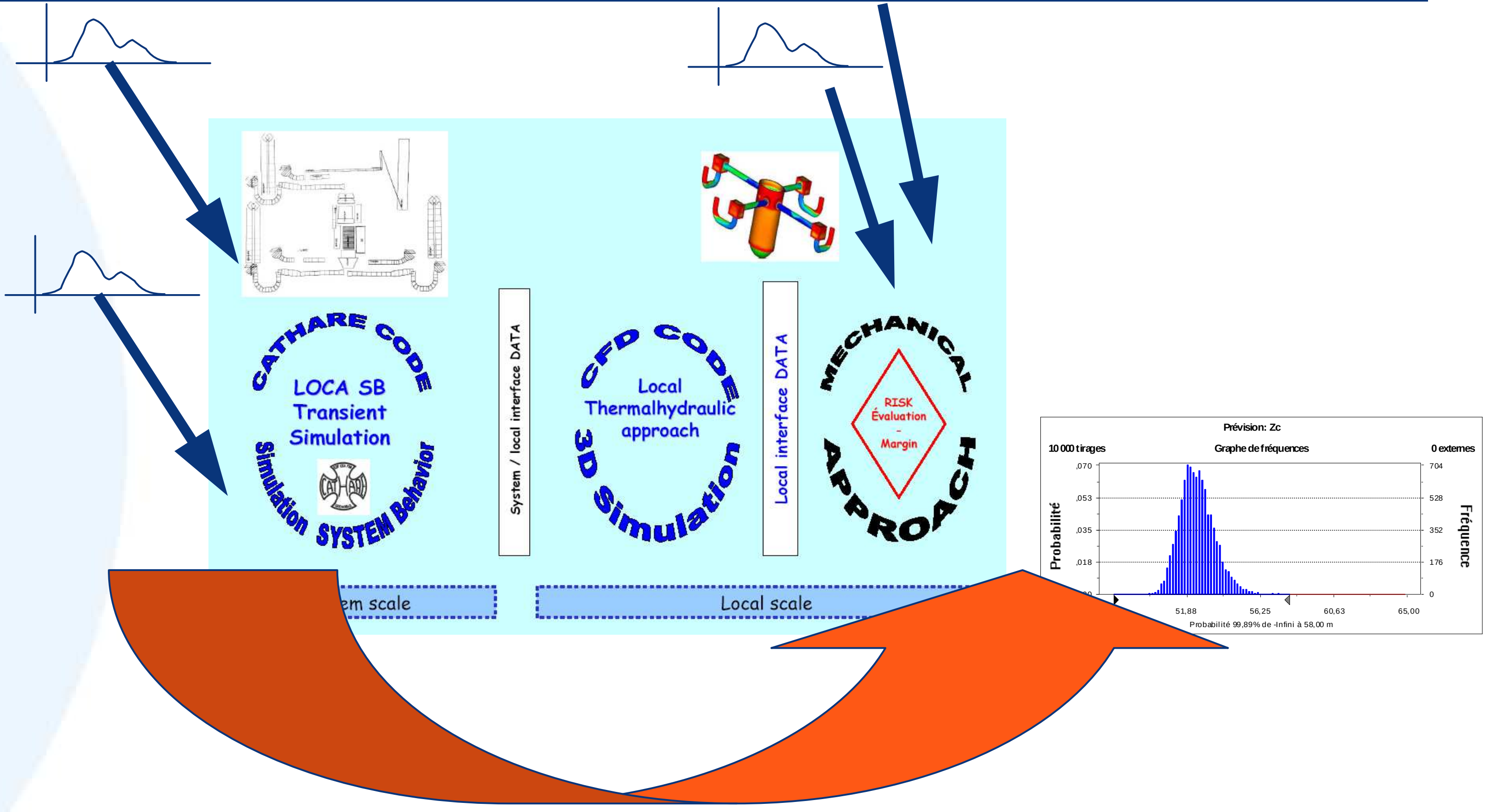
CATHARE





Full uncertainty sampling

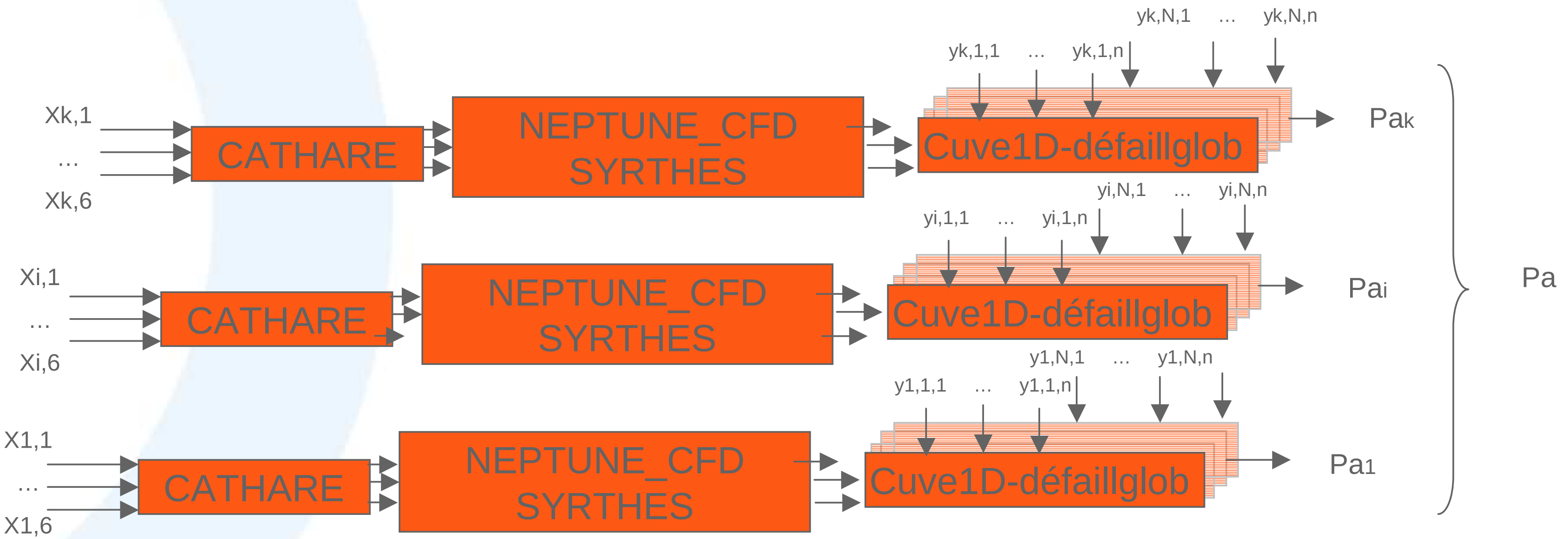
Probabilistic sampling and ranking in two stages
N1 simulations of Cathare-NEPTUNE_CFD-SYRTHES
*N1*N2 (conditional) simulations of the Cuve2DG right-end*



N_1 * N_2 simulations

Probabilising both thermal-hydraulics & mechanical uncertainties

- means computing (flaw initiation) risk under (thermal-hydraulic transient) uncertainty
    - Level-2 Thermal-hydraulic uncertainties xi + level-1 thermal-mechanical uncertainties yi both random
    - A double-level Monte-Carlo is undertaken



Computing features and challenges

- Bottleneck = CFD >> *only step where Blue Gene is mobilised*

- Characteristics (BG/P – 112 Tflops)
  - 32 000 (single-core) proc. grouped over 8 000 nodes – 0,85 GHz
  - 0.50 Go per proc.

- Performance through a mixture of parallel/distributed computing
  - Each unit CFD run was optimised over up to 32-64 nodes (128-256 proc.), improving but far from scalability
  - Planned distribution of up to 100 simultaneous independent Monte-Carlo runs (i.e. 25 600 procs)
  - Anticipated overall computing time for a 200-serie = 2*60 days (instead of 200*40 days on standard cluster)

- Challenges
  - CFD involves the coupling between Neptune_CFD and Syrthès, with highly unbalanced computing power requirement
  - It is uncertain whether Monte-Carlo sampling will lead to qualified/stable parameter ranges
  - Statistical interpretation of two-level ranking is complex

A challenge for importance ranking – double-level sampling

- Scientific Challenge
  - Traditional methods rank $(G(\underline{X}_j))_{j=1\ldots N}$
    - With one-level sampling
    - With respect to output <u>variance</u>
  - In our case $N_1*N_2=200*(100\ 000)$ runs in mixed two-level sampling + look for failure probability instead of variance
- Solutions under way
  - Rank the transformed output $1_{G(X)<0}$
  - Rank conditional probabilities
  - …

⦿Stochastic optimisation

Moving from simulation to optimisation of a risk measure in time

- Step 1 - prior design optimisation w.r.t. risk measure

$$Min_d EU\left[G(X_t,\underline{d})\right] = Min_d \int_{x_t} U[G(x_t,\underline{d})]\, f_{X_t}\, dx_t$$

- Step 2 - prior optimisation of posterior flexibility w.r.t. risk measure

$$\Rightarrow Min_{(D(i))_i} EU\left[\begin{array}{l} C_1[G(\underline{X}(t),\underline{d}(1),t)] \\ +EU\left[\begin{array}{l} C_2[G(\underline{X}(t),\underline{d}(2),t)] \\ +EU\ldots\left[\begin{array}{l} \ldots \\ C_n[G(\underline{X}(t),\underline{d}(n),t)] \mid T_t \end{array}\right] \mid T_2,..T_t \end{array}\right] \end{array} \mid T_1,..T_t\right]$$

Done for Power Asset management

Stochastic control problem in high dimension :

Number of state variable linked to :

- Number of hazards
- Number of stock to be dealt with

Dynamic programming implementation

- Use Monte Carlo for simulations for hazards (flexible, easy to use for risk (thousands of scenarios possible))
- Backward algorithm (Longstaff Schwarz version)

for $t \leftarrow (M-1)\Delta t$ to 0

  for $c \in \{$admissible stock levels$\}$

    for $s \in \{$possible hazard levels$\}$

      $\tilde{J}^*(s,c) = \infty$

      for $nc \in \{$possible commands for stocks$\}$

        $\tilde{J}^*(s,c) = \max\left(\tilde{J}^*(s,c),\ \phi(nc) + \mathrm{E}(J^*(s^*, c+nc) | s) \right);$

  $J^* \leftarrow \tilde{J}^*;$

- At t = 0 interpolate J for current stock c and current uncertainty s

Algorithm problematic

- Sequential in time
- Rather sequential for nc nest
- Parallel for c nest if all J^* are available in memory for all (c,s)
  - N_i number of points discretization in each direction.
  - $\prod_i N_i$ is the number of c to explore
  - IDEA : parallelize the c nest by splitting the hypercube

$$\prod_i N_i$$

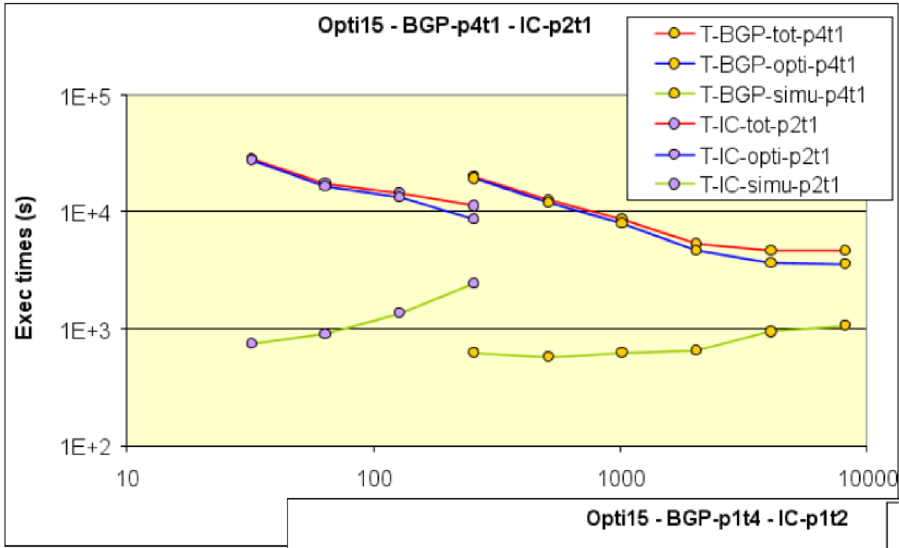
  - Use of communication scheme for optimisation and simulation too (commands spreads with stocks levels on processors)

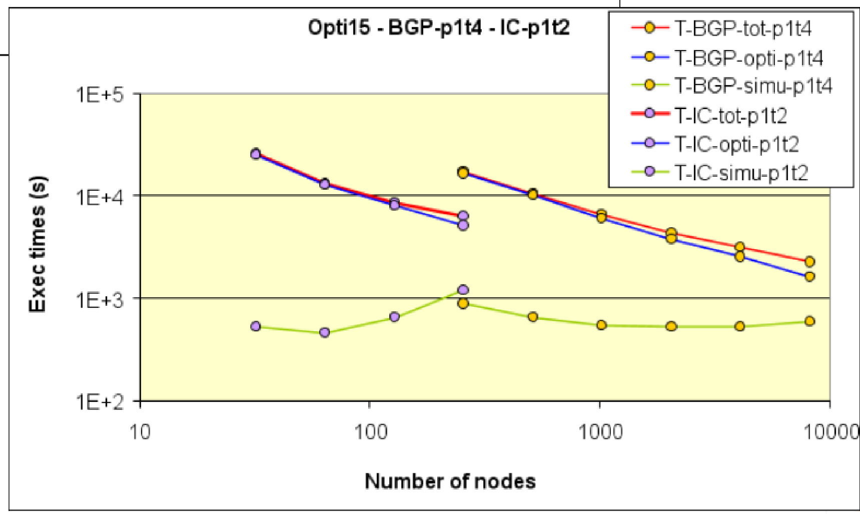
Test case presentation

- Optimization and simulation on 518 days with time step of one day
- One stock of water :
  - 225 points discretizations (c)
  - 5 commands (0 to 5000 MW each day for nc)
- 6 stocks of month future products with delivery of energy (peak and off peak hours)
  - 5 points discretization for each one
  - 5 commands (-2000 MW (sell) to 2000Mw (buy) tested every 2 weeks
- Aggregated view of thermal assets.
- Up to 225*5^6 points discretizations and 5^7 commands to tests

Results Intel 256 *2 cores, BG 8192*4 cores

Comparison BG, cluster without multithreading

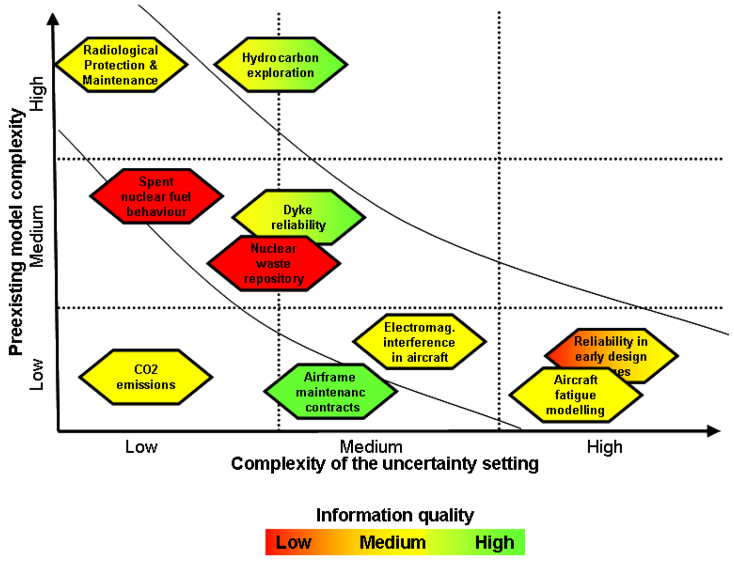




Comparison Blue Gene, Cluster multithreading

⦿Challenges ahead for HPC risk

HPC challenges



- Typically three levels of greediness to optimise
  - Underlying engineering model may require parallel computing (no uncertainty) >> e.g. CFD
  - Handling risk analysis mixes
    - A layer of probabilistic sampling
      - Fully distributed if standard Monte-Carlo, but more generally mixed sequential / parallel >> e.g. adaptive importance sampling
    - A layer of optimisation
      - Because of *mixed deterministic-proba.* risk criteria
      - Because calibrating the uncertainty model requires *inverse techniques*
      - Because the final goal is to *optimise under risk*, not just *compute risk*

How do we efficiently allocate computing power in 3 such layers ?

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