European Project PERFECT
6th Framework Program

Presentation of the Toughness Module

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A Very Few Words about PERFECT

PERFECT is a European Project of the 6th FP

Features:

- Duration: January 2004 – June 2008
- Coordination: EDF (France)
- 12 organisations / 16 universities

Aims of the project:

"The project PERFECT (*Prediction of Irradiation Damage Effects in Reactor Components*) aims at developing and building predictive tools for Reactor Pressure Vessels and Internal structures"

"The main objective of PERFECT is to build 2 'Virtual Reactors' simulating the effect of irradiation respectively on Reactor Pressure Vessel Fracture Toughness and on Internal structure Irradiation Assisted Stress Corrosion Cracking"

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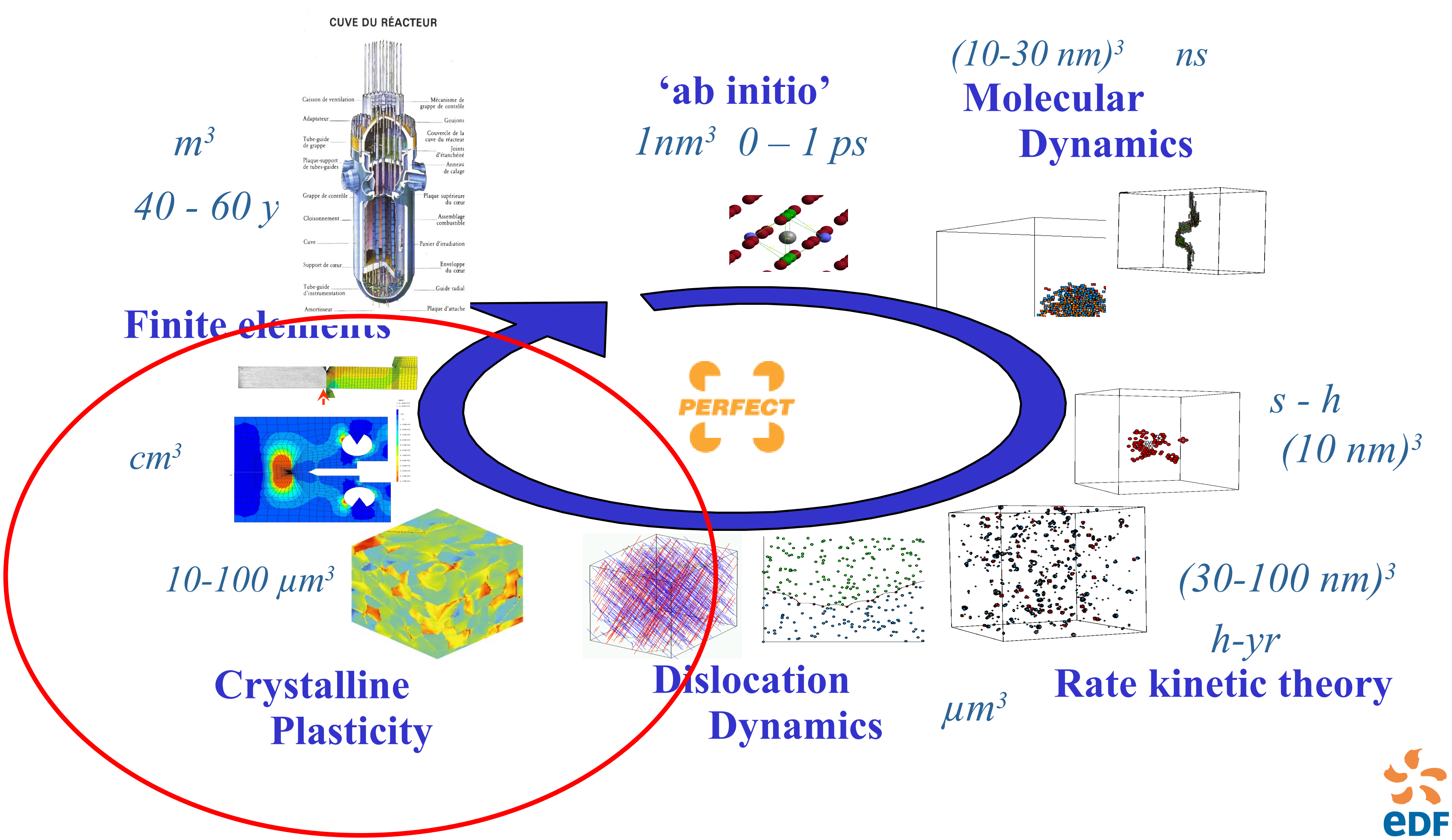
The PERFECT Methodology for multiscale modelling of irradiated RPV steels



OUTLINE

General Background: “integration” in the PERFECT project

Specifications for the Toughness Module

Incoming developments of the Toughness Module

Conclusions & open questions

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General Background
Integration in the PERFECT project

1.1 Aim of the “Integration” sub-project

2 complementary issues are identified:

Collect and condense the scientific and technical advances made within the project into a unique numerical platform

Develop 4 “end-products” aiming to give:

- The prediction of the irradiated microstructure, the mechanical behaviour and the decrease of fracture toughness of RPV steels
- The prediction of the irradiated microstructure, the mechanical behaviour and the irradiation-assisted corrosion cracking of internals

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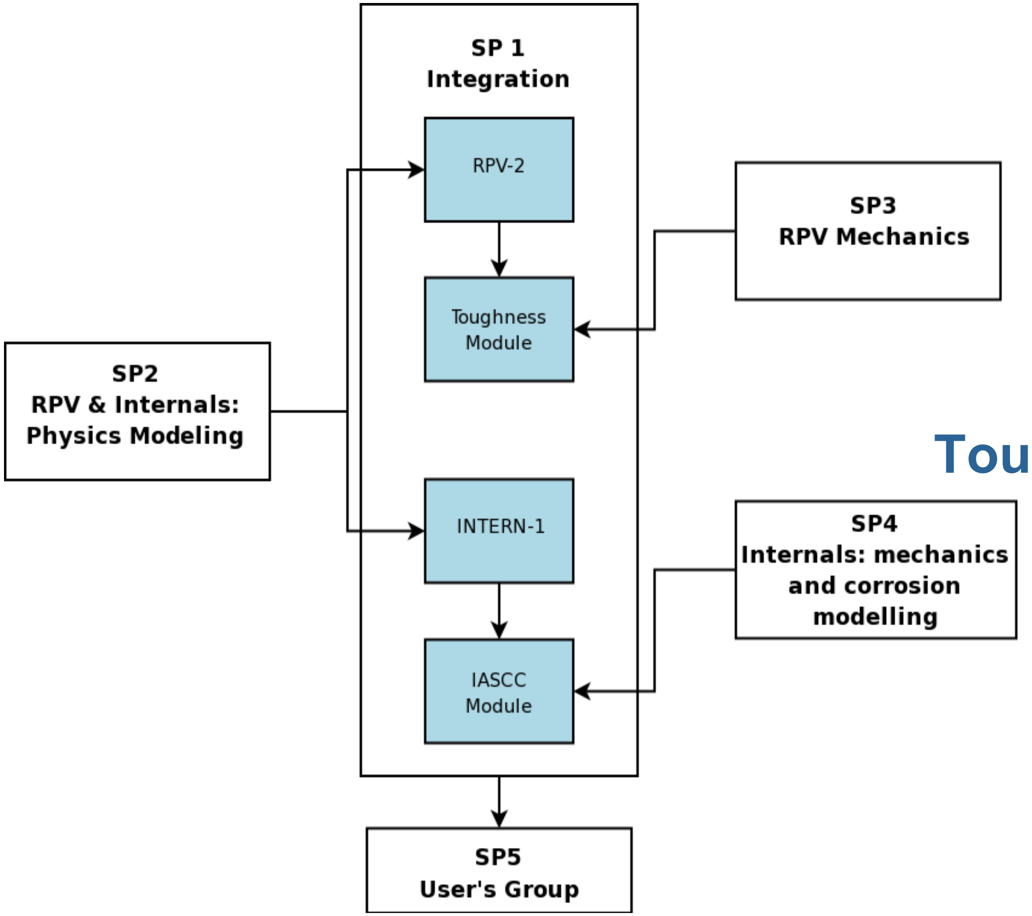
1.2 PERFECT end-products



For RPV steels:

RPV-2 :

- Inputs: irradiation conditions and metallurgical informations about the steel
- Outputs: irradiated microstructure and microstructural hardening

ToughnessModule :

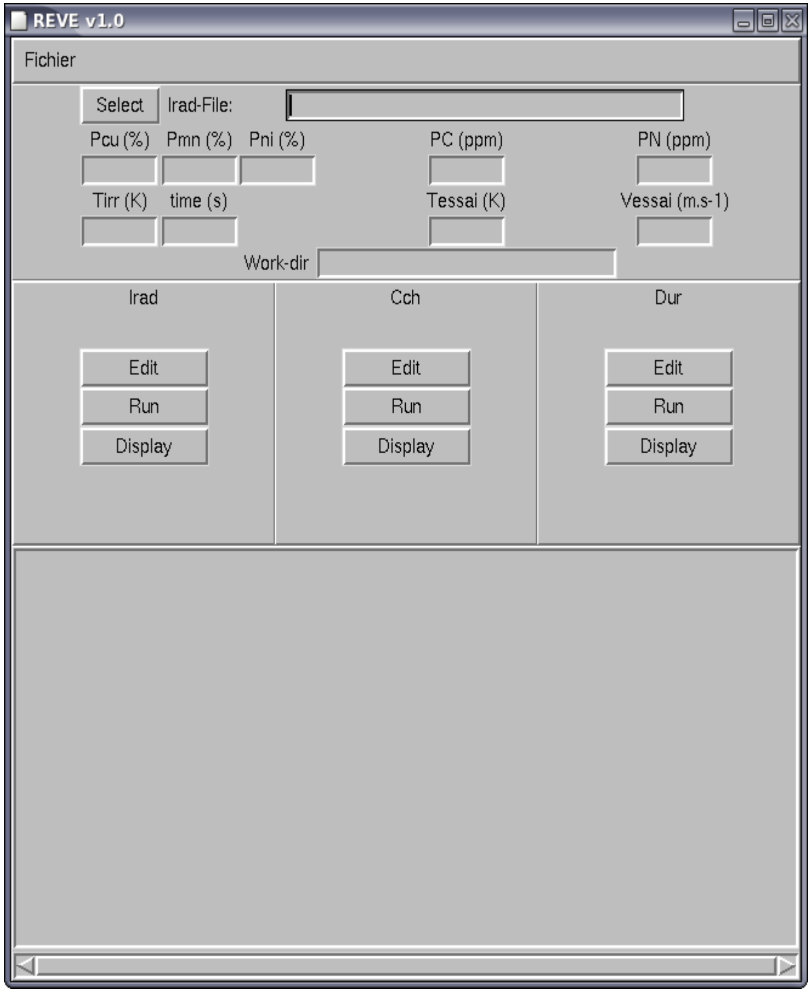
- Inputs: microstructural hardening
- Outputs: macroscopic behaviour of irradiated steel and subsequent decrease of fracture toughness

1.3 A few words about the origin of end-products, and in particular RPV-2

We did not start from scratch!

An RPV-1 tool was already developed:

- Within the frame of the "REVE" initiative (2000-2004)
- Was based on a "chaining" of modules used with databases
- Used codes from diverse origins, launched by shell scripts and chained using a graphical user interface in python-tk



Basic idea: generalise this type of approach to the other end-products

1.4 The integration platform in PERFECT

Specifications for the numerical platform

Architecture:

- Should work on a GNU/Linux type operating system
  - As it is the case for the majority of the scientific codes used
  - As it has to be integrated into a more generic platform SALOME
  - As numerous free and open-source development tools were available for that type of OS
- Choice of a unique development language, *python*
  - Allows a very fast prototyping
  - Is *a priori* multi-platform (MS Windows, Macintosh, Linux)
  - Has a well-furnished library of modules allowing to perform the majority of desired operations
- This choice allows an overall consistency of the platform

1.5 Integration platform in PERFECT (2)

Specifications for the platform

Operation :

- Should allow a "black box" integration of the different codes
  - Specific codes covering a wide range of scientific domains
    - Finite Elements, Kinetic Monte-Carlo, Rate-Theory kinetics, DD, ...
  - Codes developed outside the framework of the PERFECT project
    - No possibility to influence their development
  - Integration of "type-calculations" more than a complete integration of the codes
    - Type calculation = computation that can be easily automated, defining a specific physical operation
- Should allow to use different schemes to get the same results
  - i.e. different type calculations aiming to provide the same output data but using more or less advanced methodologies
  - Should also allow the comparison of the different methods

1.6 Structure of the PERFECT platform

The platform is mainly constituted with:

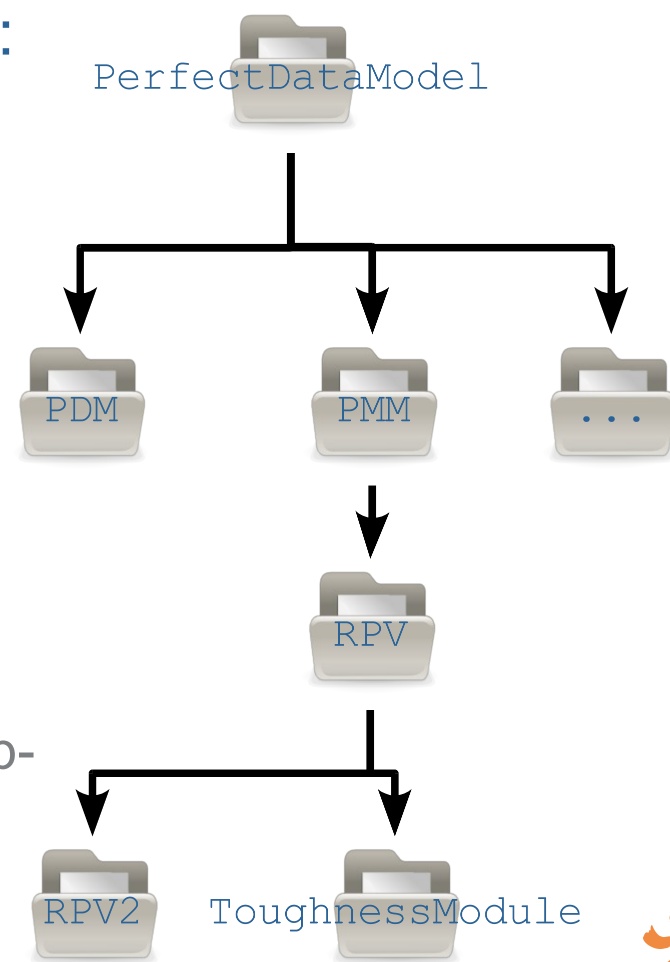
A Data Model
(PDM, for *Python Data Model*)

- Contains class definitions of all possible input/output objects for the different modules

A Module Model
(PMM, for *PERFECT Module Model*)

- Contains the implementation of the different "end-products" (RPV-2, ToughnessModule, etc.) with their sub-modules

"*Orthogonal*" conception



1.7 Structure of the PERFECT platform (2)

Relative roles of PMM and PDM

PDM [*static* part of the platform] :

- Defines all types of input/output data consistent with the different modules that can be chained
- Allow a certain number of verifications on the numerical values entered by the number (validity range, etc.)

PMM [*dynamic* part of the platform] :

- Defines the hierarchy of the modules, and in particular the character (*chained* or *exclusive*) of the sub-modules
- Defines the list of input/output data required by each module to operate
- Defines the operating process (computation) of modules
- Can be easily extended by own user modules !

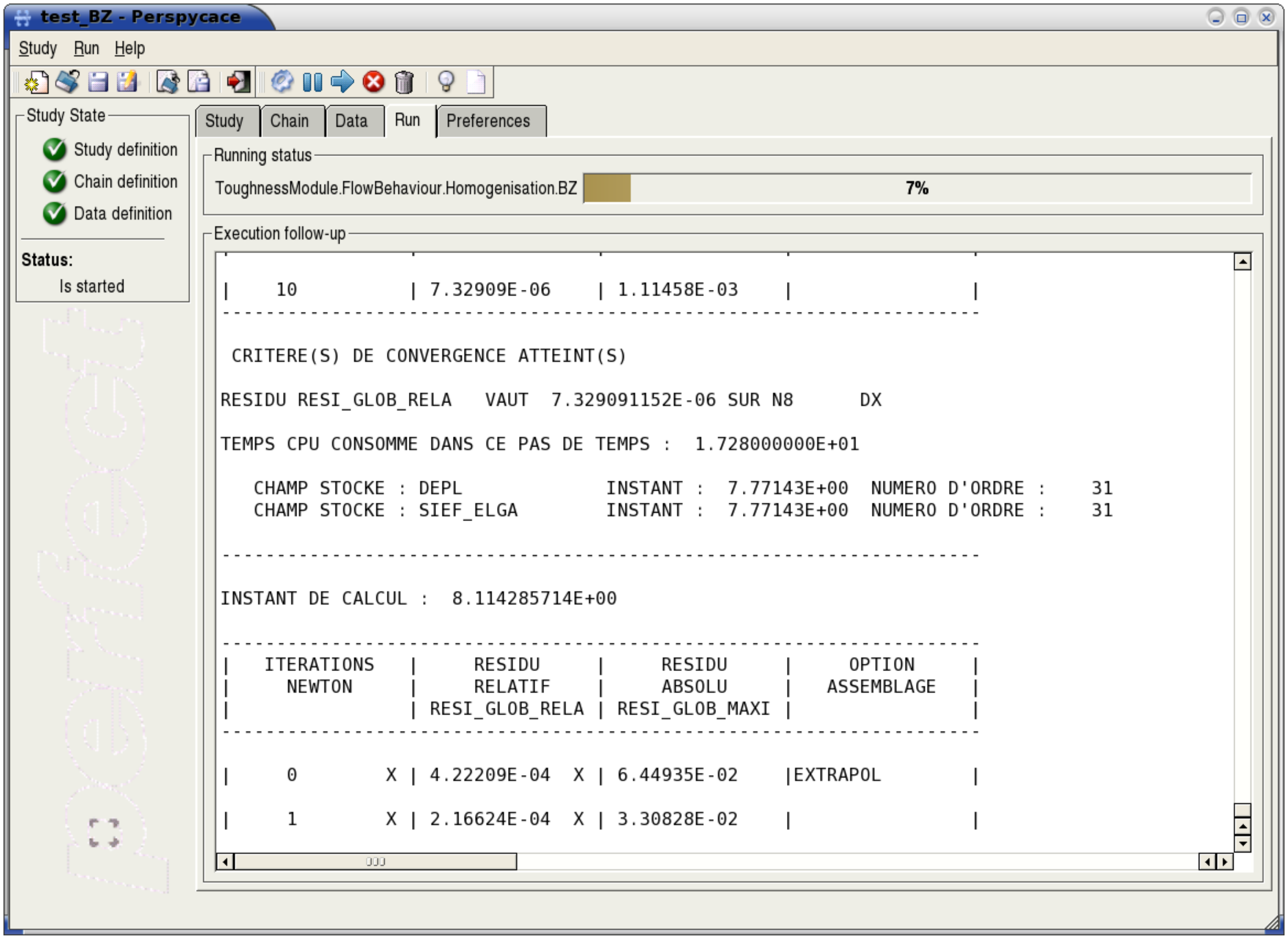
1.8 Launch of PERFECT studies

The Graphical User Interface of PERFECT : **perspycace**

Main characteristics:

- Developed in python-Qt (library compatible with SALOME)
- Allows:
  - The definition of the chaining of the modules
  - The entry of numerical values necessary
  - The launch and the follow-up of the execution of the modules
  - The post-processing of the results (plots of output tables etc.)
- Can be used:
  - As a “standalone” product
    The execution of the modules is held as python processes
  - As a SALOME component
    The execution of the module is held by SALOME

1.9 Perspycace



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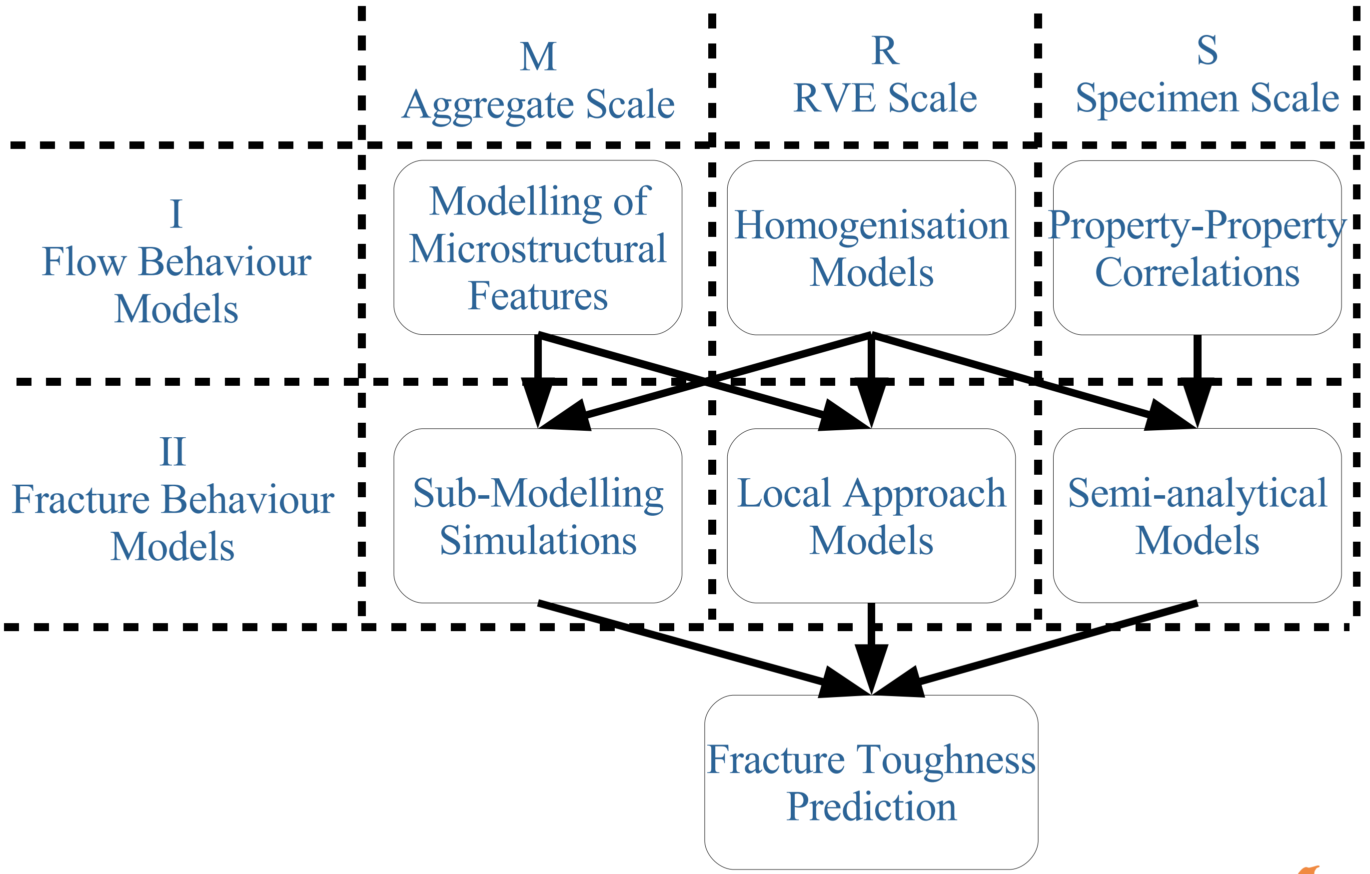
Specifications of the Toughness Module

2.1 Specification Matrix

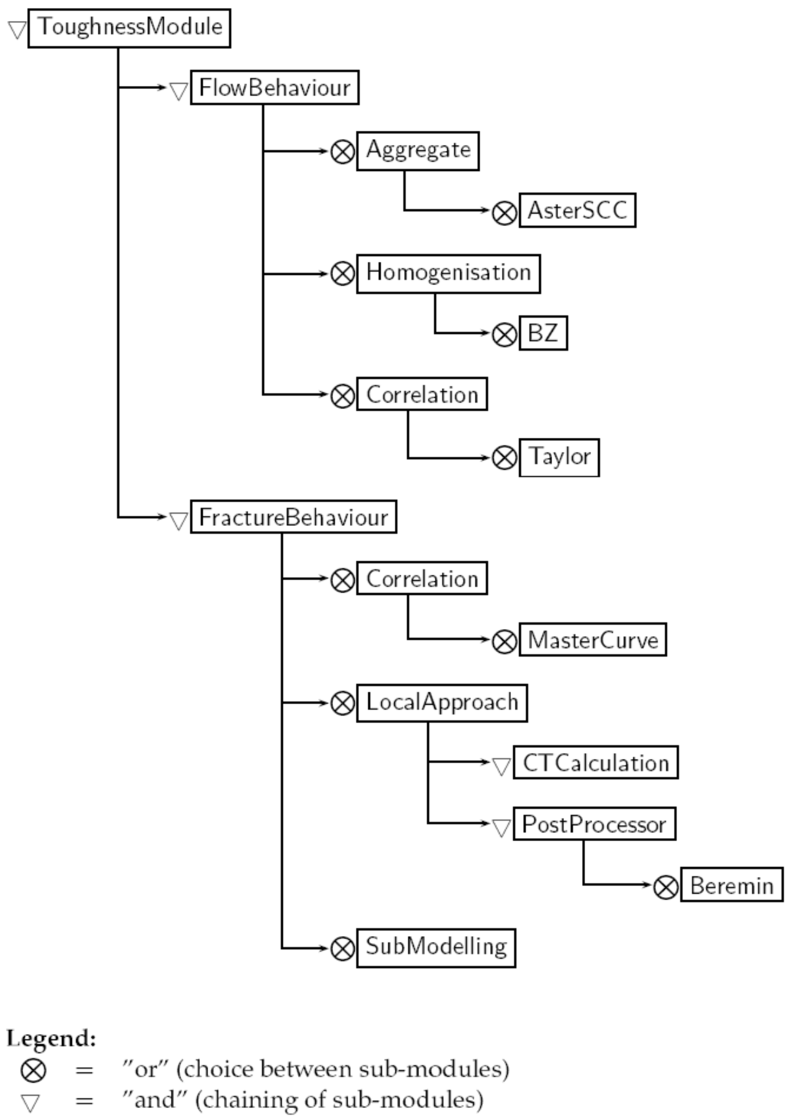
Matrix defined by the SP3 – RPV Mechanics

prediction of the irradiated mechanical behaviour

prediction of the irradiated fracture behaviour



2.2 Subsequent software architecture of the TM

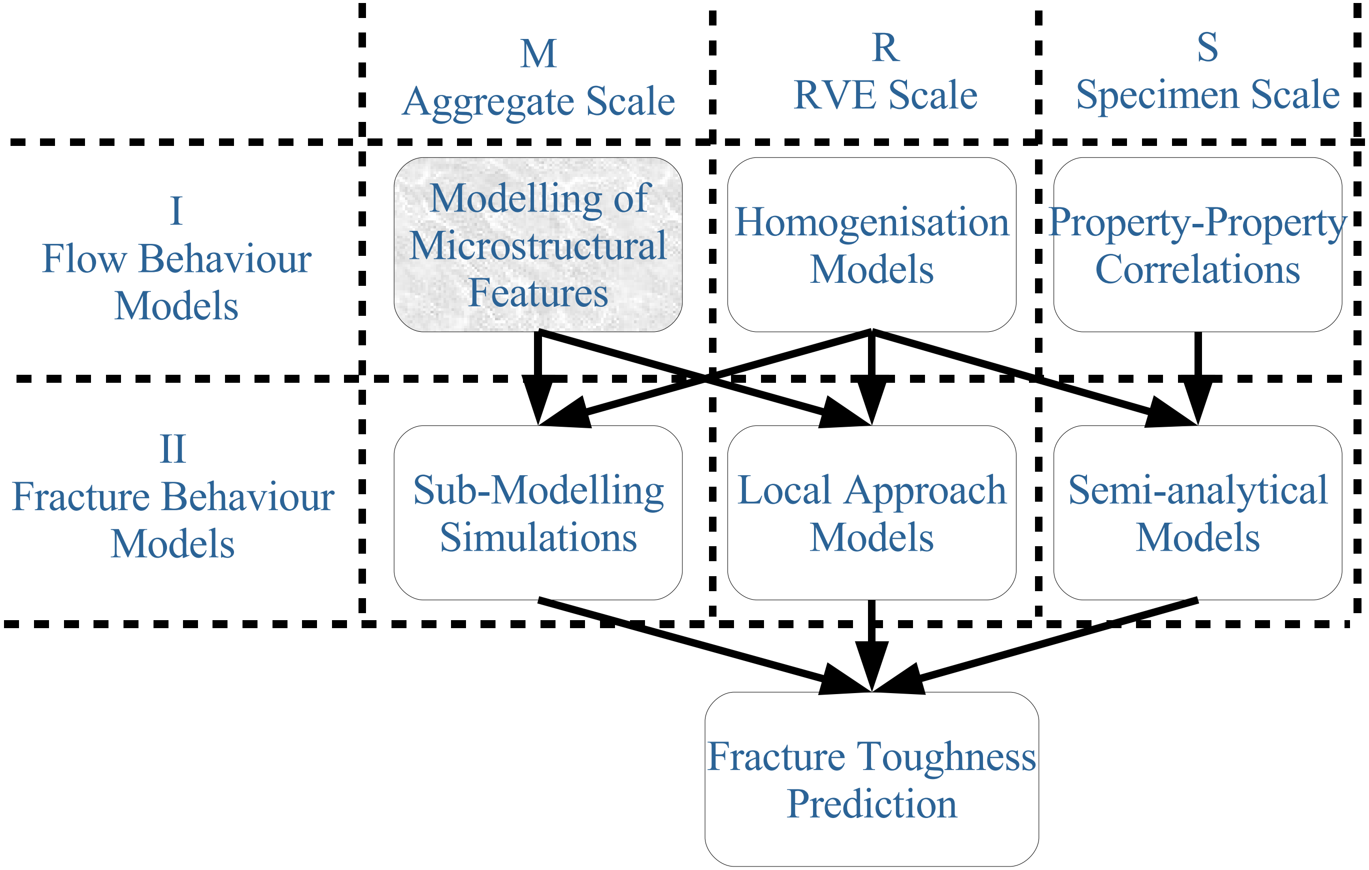


Structure extracted from the documentation of the TM (automatically generated)

Tree view consistent with the specifications

Existence of modules that are *exclusive* or "*chain-able*"

2.3 Description of the different modules of `ToughnessModule.FlowBehaviour`



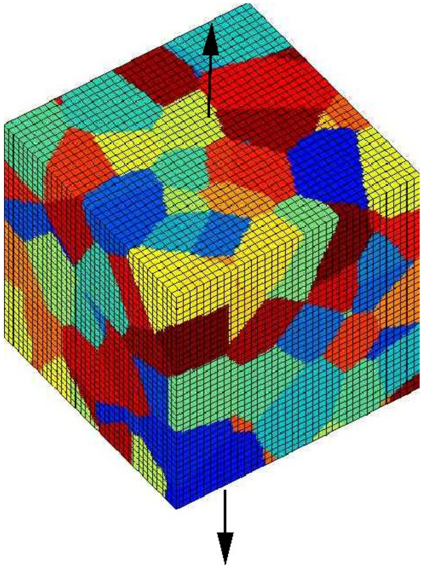
General principle of sub-module **`Aggregate`** :

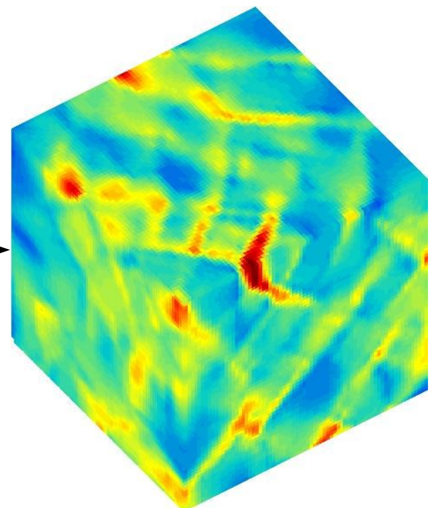
Evaluation of the tensile curve of the irradiated RPV steel by means of a computation of a tensile test on a polycrystalline aggregate

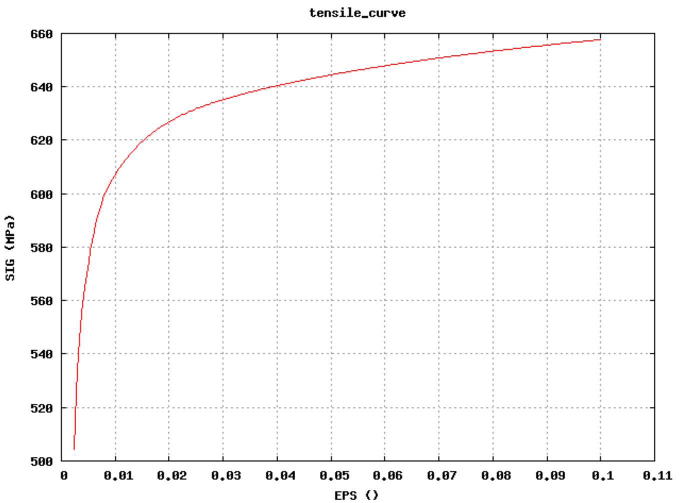
Representative Volume Element

Evaluation of Stress and Strain Fields

Macroscopic mechanical behaviour







Computation of macroscopic stress and strain using the macro-homogeneity hypothesis (averaging on the volume of the RVE)

2.3.2 Description of the modules of `FlowBehaviour` `FlowBehaviour.Aggregate`

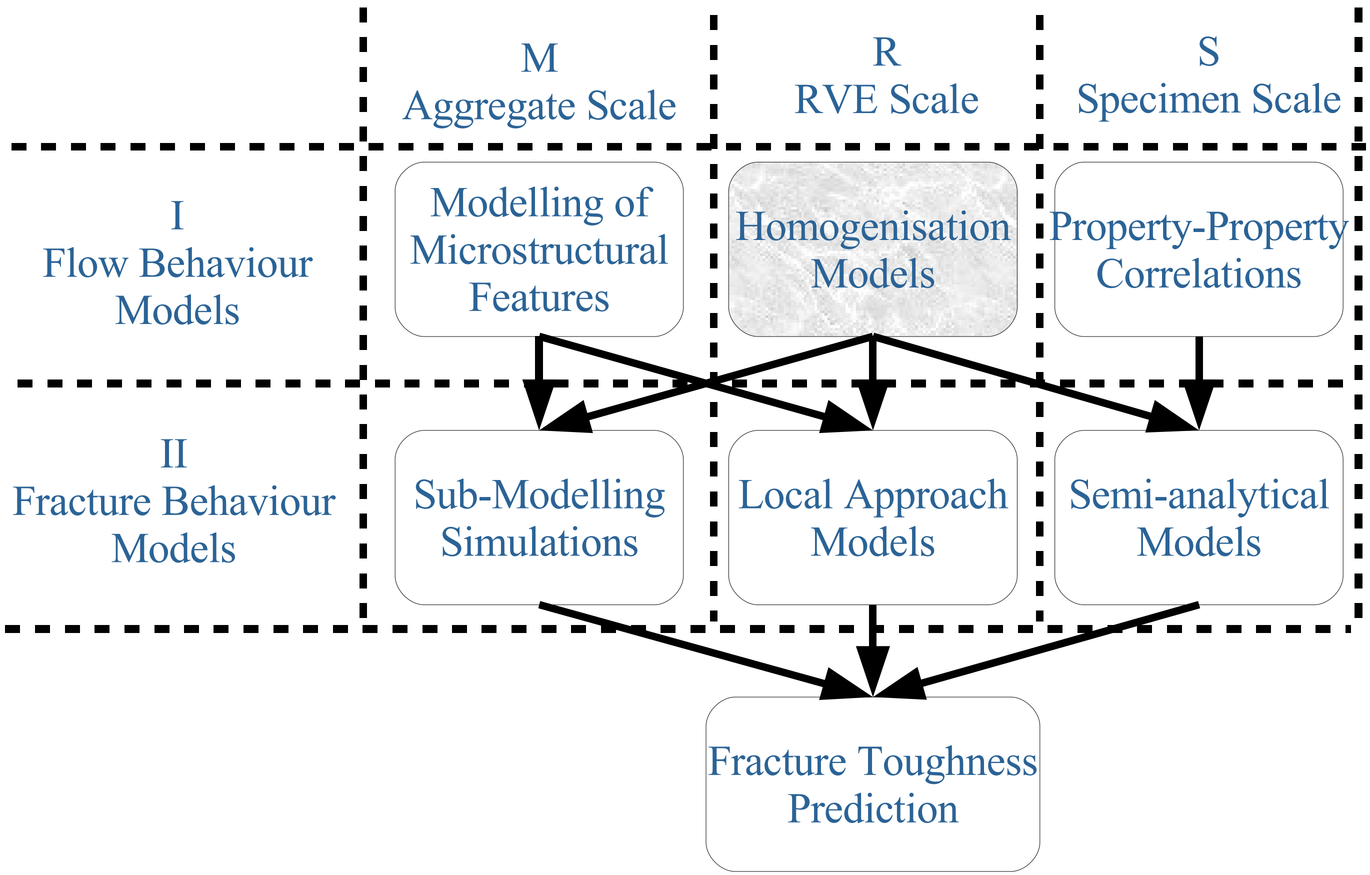
Example of `Aggregate.AsterSCC`

Computation features

- Regular mesh of 18x18x18 elements with 200 grains randomly nucleated (≈ Voronoï cells)
- By default random orientation of the different grains (isotropic texture), but ability to specify an actual polycrystalline texture
- Computation in small deformations (<10%) with the *Code_Aster* F.E. Code
- Crystal Plasticity Model of type Cailletaud-Méric :
  - 2 families of slip systems, $\langle 111 \rangle - \{110\}$ $\langle 111 \rangle - \{112\}$
  - 1 isotropic non—linear hardening (3 parameters)
  - 1 kinematic non—linear hardening (5 parameters)
- **This behaviour law can be parametrised with the output of RPV-2 (in particular the increase of CRSS)**

Very long computation, used mainly to determine $Rp_{0.2}$

2.3.3 Description of the different modules of `ToughnessModule`

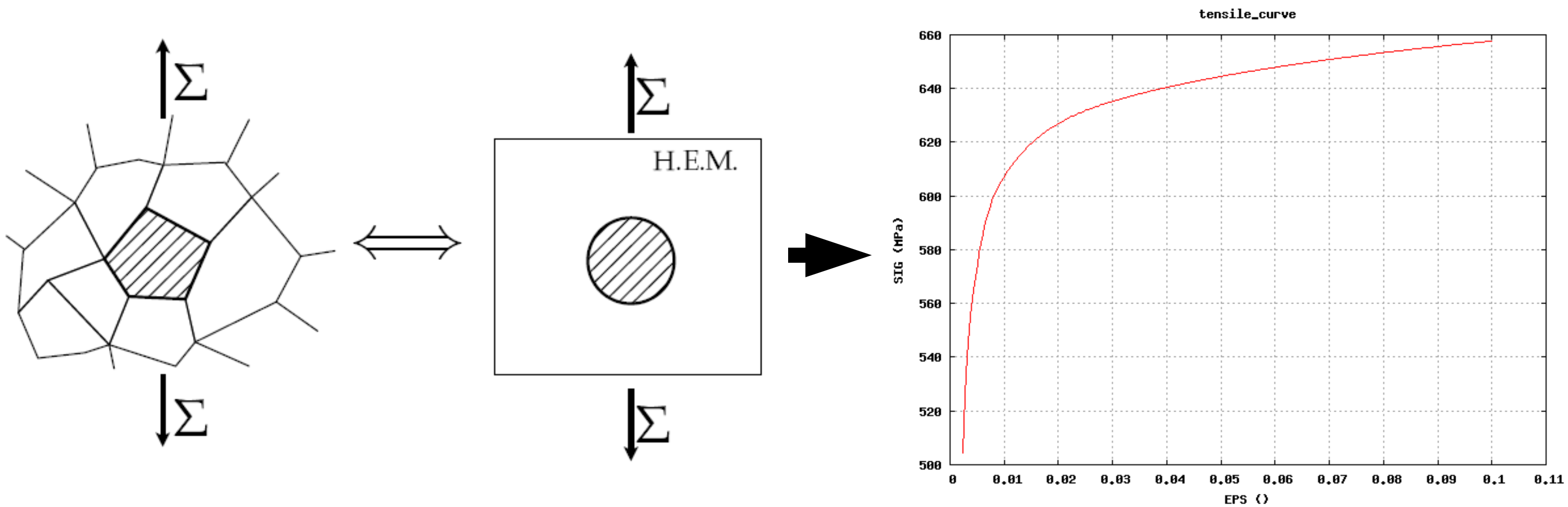


2.3.4 Description of the modules of `FlowBehaviour` Sub-Module `Homogenisation`

General principle of the sub-module **`Homogenisation`** :

Evaluation of the irradiated macroscopic behaviour by means of a computation of a tensile curve on a RVE with a polycrystal interaction law (homogenisation model)

Representative Volume Element   Homogenisation   Macroscopic Tensile Curve



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2.3.5 Description of the `FlowBehaviour` modules `FlowBehaviour.Homogenisation`

Example of `Homogenisation.BZ`

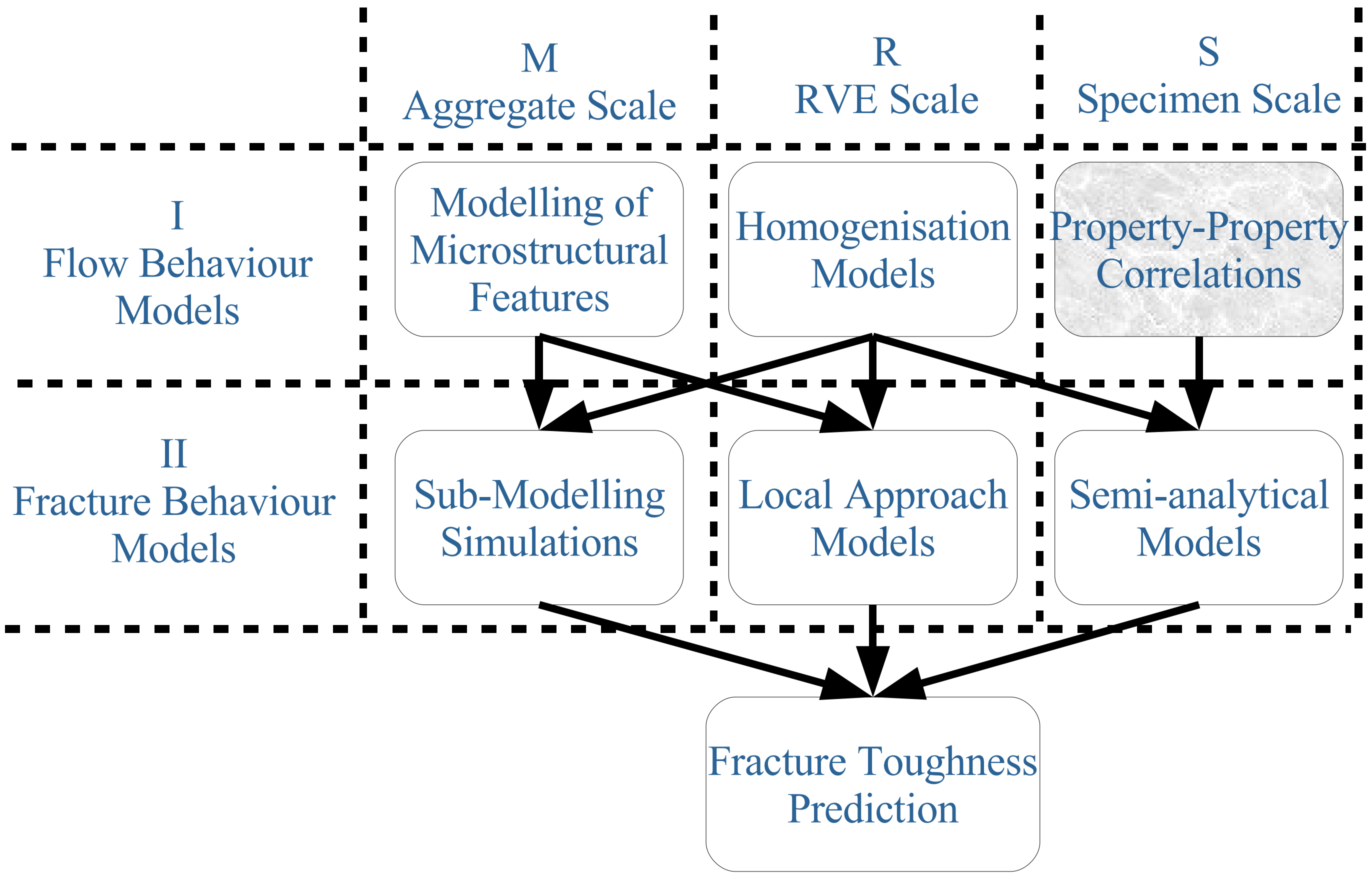
Computation features

- RVE of 30 grains, with a default random orientation of the grains (ability to specify an actual texture)
- Computation in small deformations (<10%) with *Code_Aster*
- Single-crystal behaviour law of Cailletaud-Méric:
  - 2 slip system families, $\langle 111 \rangle - \{110\}$ $\langle 111 \rangle - \{112\}$
  - 1 isotropic non—linear hardening (3 parameters)
  - 1 kinematic non—linear hardening (2 parameters)
- Homogenisation model of Berveiller—Zaoui (no parameter, but valid only for radial-monotonic loadings)

$$\underline{\underline{\sigma}}^{s} = \underline{\underline{\Sigma}} + \frac{\mu}{1 + \frac{3}{2}\mu \frac{E_{eq}}{\Sigma_{eq}}} \left(\underline{\underline{E}}_{p} - \underline{\underline{\varepsilon}}_{p}^{s} \right)$$

Fast computation, used to obtain the stress-strain curve up to 10%

2.3.6 Description of the different modules of `ToughnessModule`



2.3.7 Description of the module of `FlowBehaviour` `FlowBehaviour.Correlation`

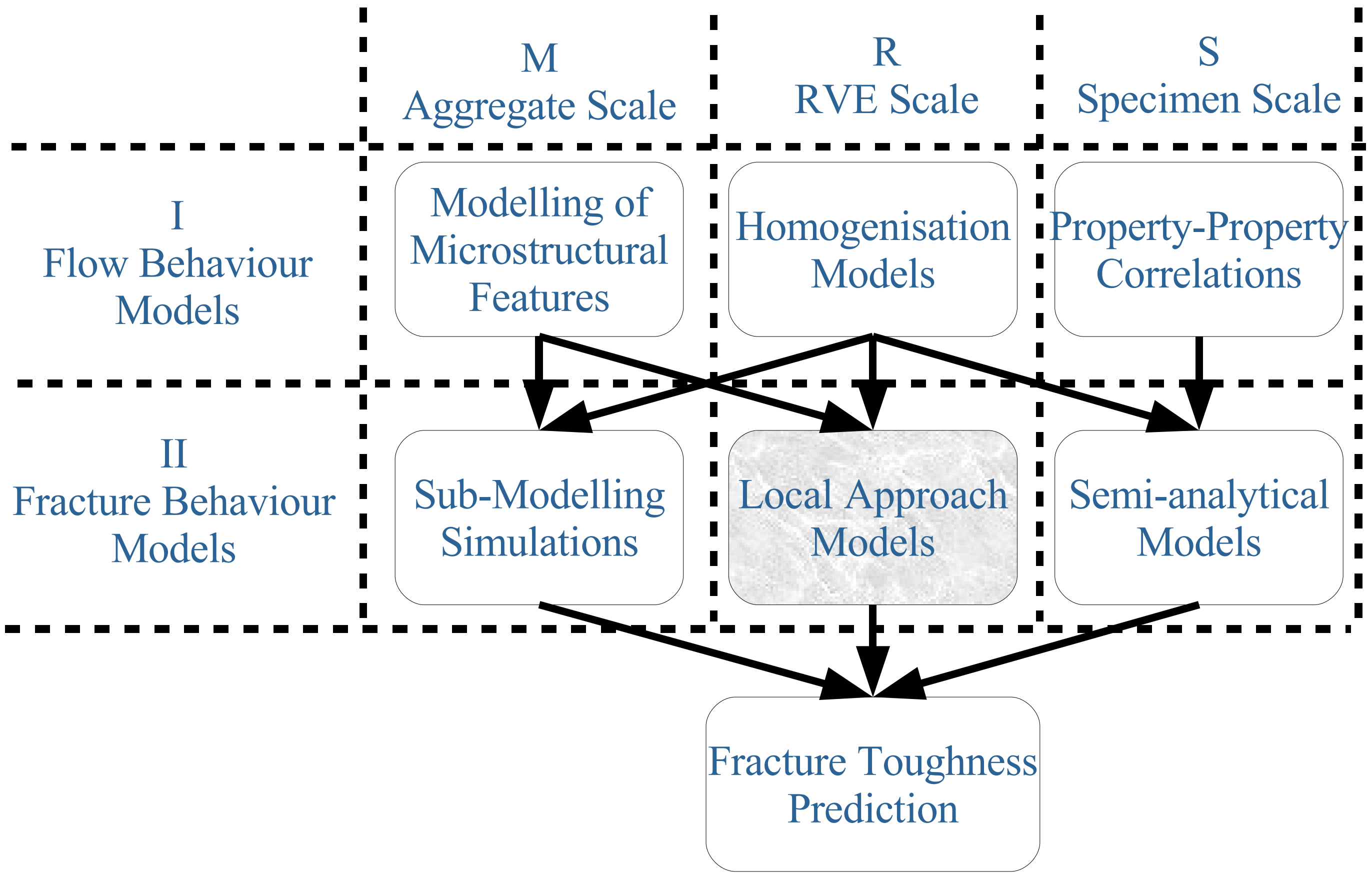
Example of `Correlation.Taylor`

Analytical model that supposes that the increase of yield stress is proportional to the increase of critical resolved shear stress (CRSS) in the bainitic lath:

$$\Delta\sigma_Y = \alpha \times \Delta \mathrm{CRSS}$$

- Coefficient α usually lies between 2 and 3
- The increase of CRSS between the unirradiated and irradiated states is an output of RPV-2
- Coefficient α can also be evaluated from calculations of type `Aggregate` or `Homogenisation` (cf. the work done by O. Diard in PERFECT)
- Very simple model, mainly used with the *Master Curve*, or for comparison of the different methods

2.4 Description of the different modules of `ToughnessModule.FractureBehaviour`



2.4.1 Description of the modules of `FractureBehaviour` Sub-Module `LocalApproach`

General principle of sub-module `LocalApproach` :

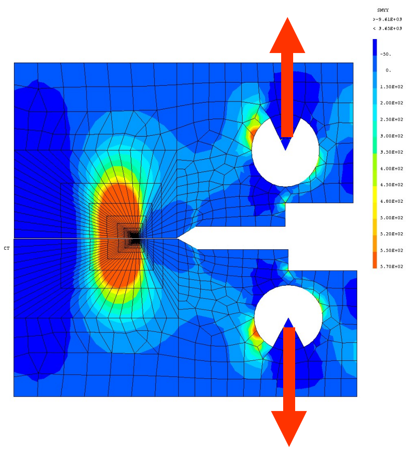
Simulation of a CT specimen with a behaviour law given by a module of FlowBehaviour

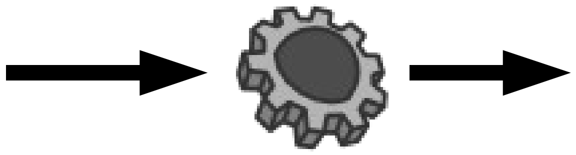
Local approach type post-processor to obtain the failure probability curve as a function of the loading on the CT specimen

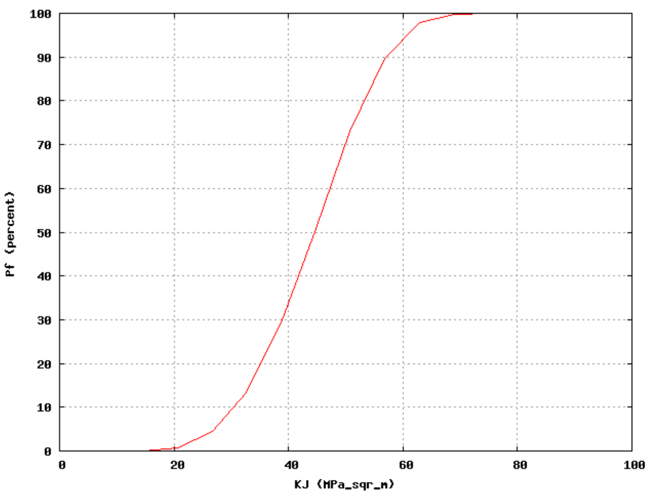
CT Specimen Simulation

Local Approach Post-Processor

Computation of the failure probability as a function of the loading K_J







2.4.2 Description of `FractureBehaviour` modules `FractureBehaviour.LocalApproach`

Example of `PostProcessor.Beremin`

Computation features

- Computation on a standard 1T-CT in 2D-plain strain
- Element size at crack tip: 50µm
- Computation in small deformation with *Code_Aster* F.E. code
- Classical von Mises isotropic elastic—plastic behaviour given by a tensile curve
  - Can be an output of a **`FlowBehaviour`** sub-module
- “Classical” Beremin post-processor, with parameters modifiable by the user:

$$P_f = 1 - \exp\left[-\left\{ \frac{\sigma_w}{\sigma_u} \right\}^m \right] \quad \text{with} \quad \sigma_w = \sqrt[m]{\sum_i (\sigma_I^i)^m \exp\left(\frac{-m\,\varepsilon_I}{k} \right) \frac{V_i}{V_0}}$$

- Computation of KJ with the loading curve according to ASTM-E399

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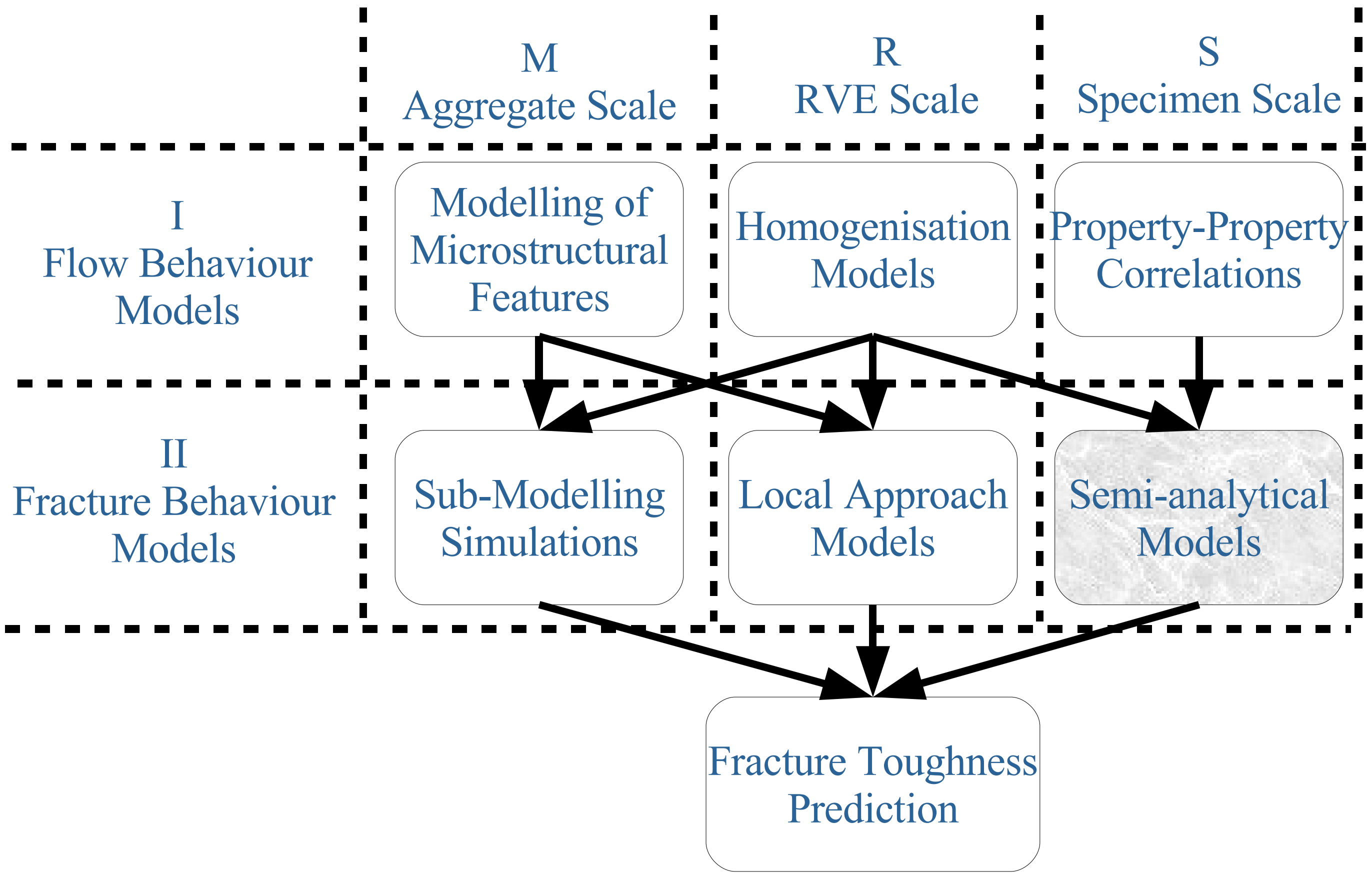
2.4.3 Description of the different modules of `ToughnessModule.FractureBehaviour`



2.4.4 Description of the `FractureBehaviour` modules `FractureBehaviour.Correlation`

Example of `Correlation.MasterCurve`

Evaluation of the shift of reference temperature T0 with a simplified Sokolov model:

$$\Delta T_0 = a \times \Delta \sigma_Y$$

- Coefficient *a* of 0,7 (modifiable by an expert user)
- $\Delta\sigma_Y$ produced by the `FlowBehaviour.Taylor` module for instance

Use of the Master Curve formulation to evaluate toughness curve:

$$P_f = 1 - \exp\left[-\left\{ 0.9124 \left(\frac{K - K_{min}}{K_{med} - K_{min}} \right) \right\}^4 \right]$$

$$\text{with} \quad K_{med} = 30 + 70 \exp\left(0.019 (T - T_0) \right)$$

- Shape factor (0,019) can be modified by an expert user

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3

Future developments of the Toughness Module

3.1 Improvement of existing modules

Improvement of physical modellings

Introduction of advanced single-crystal constitutive equations

- Louchet-Rauch law
  - valid for a wide range of temperatures, starting from the thermal regime to the athermal plateau, for bcc crystals
  - takes into account, as an internal variable, the dislocation density for each slip-system
  - can be fitted on *dislocation dynamics computations*
  - was characterised during the PhD of M. Libert (in PERFECT)

Improvement of numerical schemes

Optimisation of the resolution of homogenisation models in *Code_Aster*

3.2 Development of a new module of `FractureBehaviour`: "sub-modelling"

Principle: based on the PhD of J.-P. Mathieu (in PERFECT)

Basic concept: *the dispersion in failure properties is due to the heterogeneity of the stress field at the scale of the bainitic aggregate, and to the distribution of carbides inside this aggregate*

Scheme:

1. Perform an aggregate computation with an accurate representation of the bainitic morphology and an accurate single-crystal law
2. Make a "realisation" at each GP of 1 or more carbide of a given size from the carbide size distribution
3. Perform a "simple" Griffith post-processor for each loading step with the maximum stress normal to local cleavage planes
4. Stop at the first loading increment when a first carbide breaks (weakest link assumption)
5. Iterate *n* times to step 2 to get a full failure probability curve

3.3 Development of a new module of `FractureBehaviour`: "sub-modelling"

Specification for the sub-modelling module

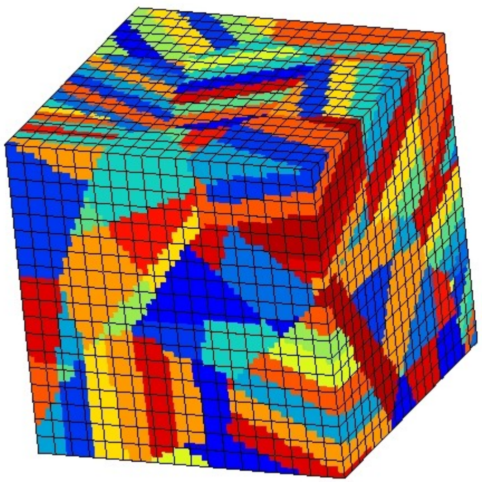
Apply this methodology to a 1T-CT computation

This could allow to:

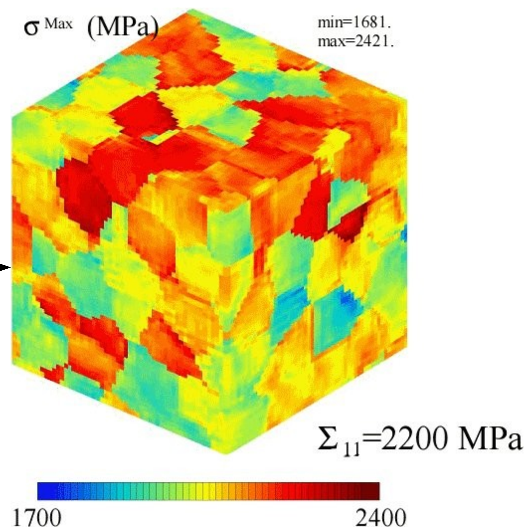
- Identify Beremin parameters from the metallurgical informations of the steel: carbide size distribution, bainitic morphology, lath size, local texture, etc.
- Get a better understanding of the thermal dependency of the parameters of Local Approach models (ex. $\sigma_u(T)$ in Beremin)
- Have a limited number to identify
- Be more predictive on the failure of RPV steels

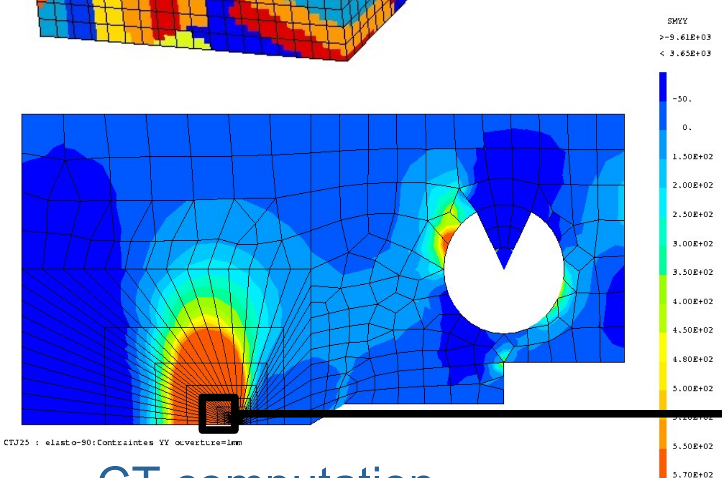
3.4 General scheme for “sub-modelling” module

Creation of a realistic bainitic mesh (PhD of N. Osipov)



Single-crystal behaviour law (PhD of M. Libert)

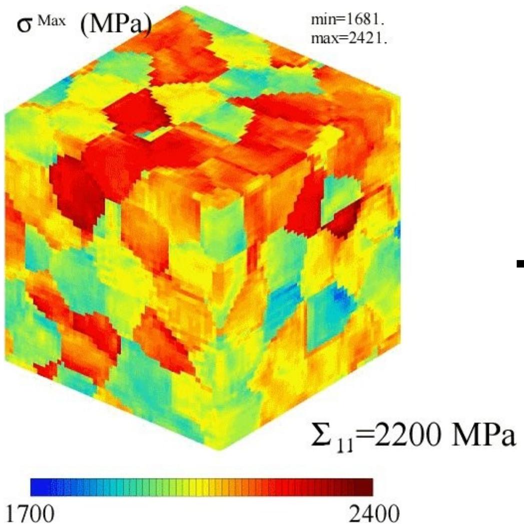




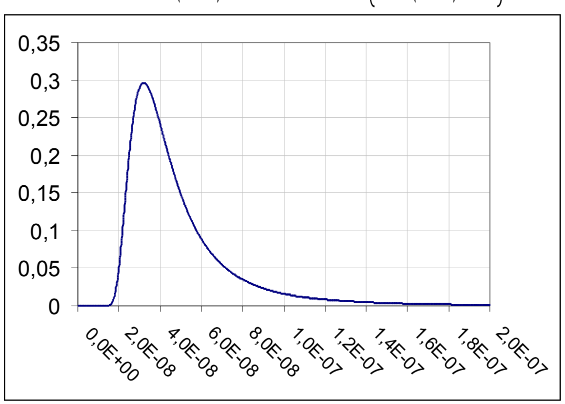
CT computation

Application of the stress tensor of the most loaded area of the CT specimen ahead of the crack-tip as boundary conditions for the aggregate computation

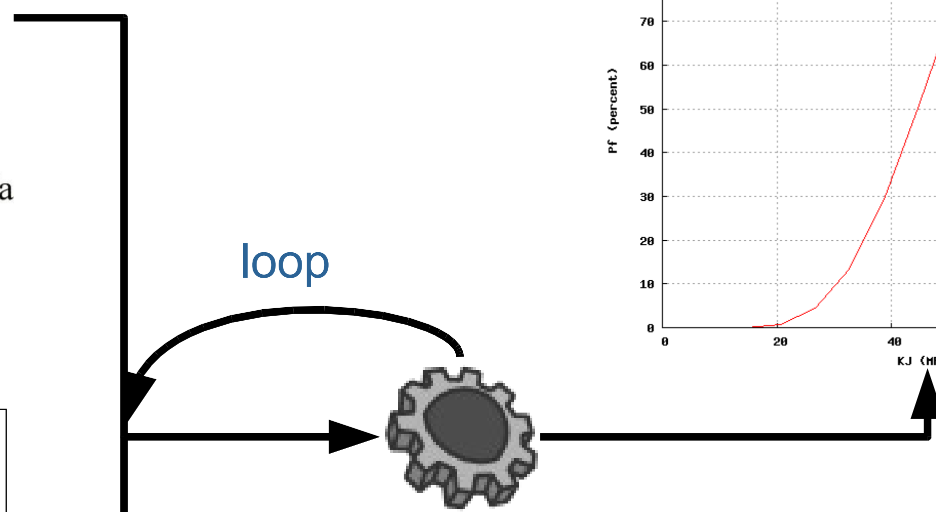
3.4 General scheme for "sub-modelling" module (2)



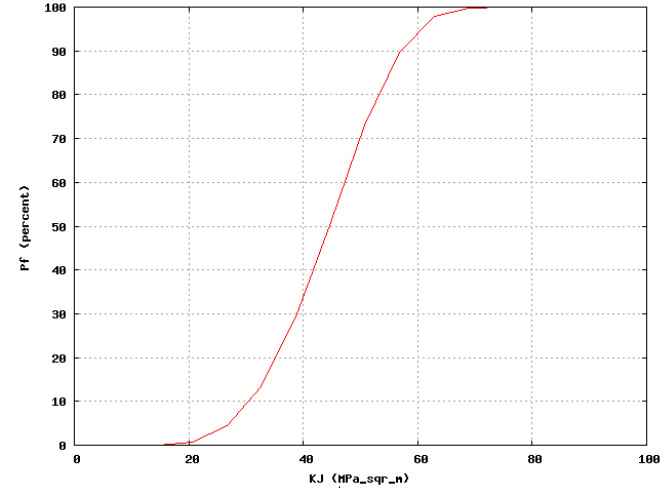
$$f(r)=\frac{\alpha}{\beta}\left(\frac{r}{\beta}\right)^{-\alpha-1}\exp\left\{-\left(\frac{r}{\beta}\right)^{-\alpha}\right\}$$



Carbide size distribution



Failure probability / KJ



Application of the Griffith criterion for each GP and for carbides randomly generated
(PhD of J.-P. Mathieu)

$$\sigma_{\langle 100\rangle} \overset{?}{\geq} \sqrt{\frac{2E\gamma_s(T)}{(1-\nu)\pi r_c}}$$

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4

Conclusions and open questions

4.1 Conclusions

The *Toughness Module* is a convenient tool that aims to provides both:

- the macroscopic curve for irradiated RPV steels, starting from informations on the microstructural hardening,
- the fracture toughness, from either simplified methods, or from more complex methodologies taking into account metallurgical informations of the RPV steel

It is based on the chaining of different modules, and has also different "branches" providing the same output but using more or less complex methodologies

It can be easily extended with new methodologies and is under heavy improvement of the current modules

4.2 Open Questions

Single—crystal behaviour law and irradiation:

- Will the Louchet-Rauch law be able to account for dislocations—irradiation defects interactions?

The "sub-modelling" module works with 2 assumptions:

- the surface energy used in the Griffith criterion has to be temperature dependent to reproduce correctly the dependency of the results on CT specimen with respect to temperature

$$\gamma_s(T)=\gamma_s^0+a\cdot\exp(bT) \quad \text{with} \quad \gamma_s^0\simeq 2\ \text{J.m}^{-2}$$

  - this could be slightly modified if the Louchet-Rauch law is used
  - however some microstructural phenomena have also probably to be taken into account (blunting due to dislocation emission in the cleavage process, microstructural barriers such as bainitic packets, etc.)
- the carbide size distribution has to be cut off for the largest sizes
  - the reason why large carbides cannot initiate cleavage is not very well known and has not been really observed

Appendix: the Louchet-Rauch law

Flow Rule (Kocks)

$$\begin{cases} \dot{\gamma}_s = \dot{\gamma}_0 \exp\left(\dfrac{-\Delta G\left(\tau_s^{\text{eff}}\right)}{kT}\right) \cdot \dfrac{\tau_s}{|\tau_s|} \\ \Delta G\left(\tau_s^{\text{eff}}\right) = \Delta G_0 \left(1 - \left(\dfrac{\langle \tau_s^{\text{eff}} \rangle}{\tau_R}\right)^p\right)^q \end{cases}$$

Effective stress

$$\tau_s^{\text{eff}} = \langle |\tau_s| - \tau_0 - \tau_s^{\mu} \rangle$$

Hardening Law (Rauch)

$$\tau_s^{\mu} = \frac{(\mu b)^2 \sum_u a^{su} \rho^u}{|\tau_s| - \tau_0}$$

Dislocation density evolution

$$\rho^s = \frac{|\dot{\gamma}_s|}{b} \left(\frac{1}{d} + \frac{\sum_{u \neq s} \sqrt{\rho^u}}{K} - g_c \rho^s \right)$$

double kink mechanism

$$T \downarrow \;\Rightarrow\; K \uparrow$$