Programmes in the European Union (EU) on simulating radiation damage environments

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Outline of the presentation

- **Programmes in EU**
  - PERFECT
  - SINERGY, SMIRN
  - ISMIR, FUSION
- **PERFECT Major Highlights**
- **Material Qualification & Modelling Validation**
  - Materials testing reactor
  - Multiple beam irradiation

- **PERFECT : Integrated Project within the 6th EU Framework Programme 2004- 2007**

  - Develop advanced tools based on the Physics at the relevant scales & experimentally validated at these scales

  - Address the most critical in-service issues for RPV steels and Internals
    - RPV steels : Hardening, Strain Hardening, Fracture Toughness
    - Internals : Hardening, Plastic Localisation, Swelling , IASCC

  - Tools shall be of practical use : (I) integration in a common software environment (“Plat-form”), (ii) prediction capability benchmarked against experimental data (iii) training activities towards potential users

  - Four main deliverables :
    - Microstructure and DDD tools for RPV and Internals (RPV-2 and INT-1)
    - Fracture Toughness of RPV steels (Tough-1)
    - IASCC of Internals (IASCC-1)

EU Multi-scale Modelling Programmes : The French pluri-annual effort for Generation II and III

- **SMIRN** (**S**imulation of **M**aterials for **N**uclear **I**nstallation & PW**R**eactors): 2002-06
  - **Basic Research Programme between CEA, CNRS, and EDF : 6 Post-doc & 6 PhD**
  - **Ab initio :** point defects configuration & energetic in alloys (RPV steel, Zr).
  - **Kinetic pathways prediction of radiation induced microstructure :**
    - Clustering & segregation mechanisms in α Fe model alloys
    - Self Consistent Mean Field (SCMF) tools development for concentrated alloys
  - **Mechanical properties** : Dynamics of Discrete Dislocations (DDD) and Crystalline Plasticity (α Fe and Zr)
- **SINERGY (Simulation for Nuclear EneRGY) 2004-2007: CEA,EDF and FRA**
  - **Development of multi-scale modelling tools to address structural material ageing in the French PWR**
  - **Integration of the development on a common “Plat-form”**

EU Multi-scale Modelling Programmes : Generation IV & Fusion

- **ISMIR** (**I**n**S**ulators **M**odelling of **I**rradiation): 2002-2006
  - **Basic Research Programme between CEA and CNRS : 5 PhD & 5Post-Docs**
    - **SiC, ZrC and Oxides**
  - Ab initio computation : **electronic** and elastic interaction, **defect structure**
  - Diffusion mechanisms under irradiation
  - Microstructure evolution and consequences on mechanical properties

- **Euratom Fusion Materials Multi-Scale Modelling Programme**
  - **Radiation damage in Fusion environment :**
    - **up to high dose**
    - **with high concentration irradiation induced impurities (H and He)**
  - **Ferritic Martensitic Low Activation Steels : Eurofer & F82H**

- **Five Sub-Projects**

- **Sub-Project I** : Integration (EDF)
- **Sub-Project II** : RPV & Internals : Physics Modelling (CEA)
- **Sub-Project III** : RPV : Mechanics modelling (Serco Ltd)
- **Sub-Project IV** : Internals: Mechanics & Corrosion modelling (SCK)
- **Sub-Project V** : Users Group (JRC Petten)

- **Twelve Nuclear Organisations**

EDF, CEA, SCK.CEN, SERCO Ltd, JRC-IE, CIEMAT, VTT, FZR, NRI, AEKI, UKAEA.

- **Seventeen Universities**

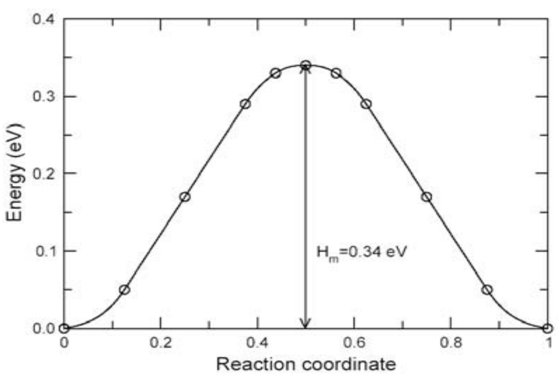
UL Bruxelles (B), Augsburg (D), Liverpool (UK), Edinburgh (UK), Charles U of Prague (CZ), UP Catalunya (SP), Alicante (SP), UP Madrid (SP), SKC (S), Chalmers UT (S),Lille (F), Rouen (F), Saint Etienne (F), INP Grenoble (F), Slovak UT of Bratislava (SI), EPFL (CH), VU Brussel (B), BZF (H)

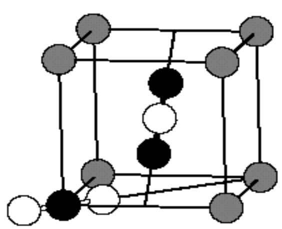
- **Budget : Total 17.75 M€ - EU Contribution of 7.5 M€**

- **Objectives**
  - Provide modelling tools & validation to predict
    - Primary damage
    - Kinetic pathways
    - Dynamics of Discrete Dislocations
- **Work-package structure**
  - WP II-1 RPV & Internals : Ab initio & empirical potentials
  - WP II-2 RPV : Displacement cascades and short term evolution
  - WP II-3 RPV : Long term evolution of radiation induced damage
  - WP II-4 RPV : Discrete Dislocations Dynamics
  - WP II-5 Internals : Displacement cascades and short term evolution
  - WP II-6 Internals : Long term evolution of radiation induced damage
  - WP II- 7 Internals : Discrete Dislocation Dynamics

Ab initio: Reliable Prediction

Exemple of SIESTA results
F. Willaime & C. C. FU
(to be published)





0.34 eV

Experimental $H_{m\sim}$0.3 eV

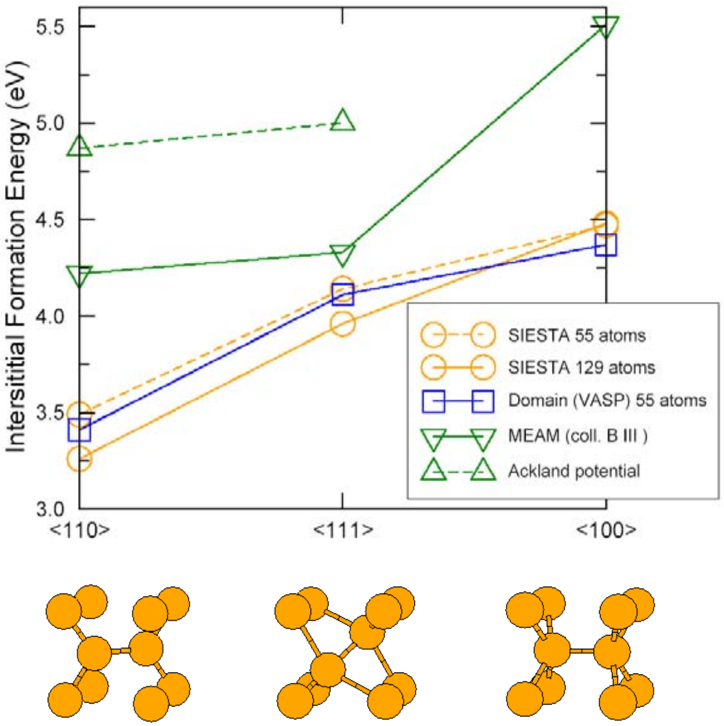
PERFECT

(CEA,EDF)

- ***V, SIA (α Fe and fcc Fe Ni)***
  - ***Formation Energy***
  - ***Diffusion mechanisms & migration Energy***
  - ***Binding Energy with alloying elements:***
    - ***C, Ni, Mn, Cu in α Fe, He in FeNi***
- ***Binding & migration energy of SIA clusters in α Fe alloys***
- ***Data base :***
  - ***Input for kinetics prediction tools***
  - ***Data to fit empirical potentials***

Sixth Framework Programme

Empirical potential:
« limited » predictability



PERFECT

(CEA, EDF, UKAEA, SCK, Edinburgh, Lille)

For RPV : four routes advanced potential

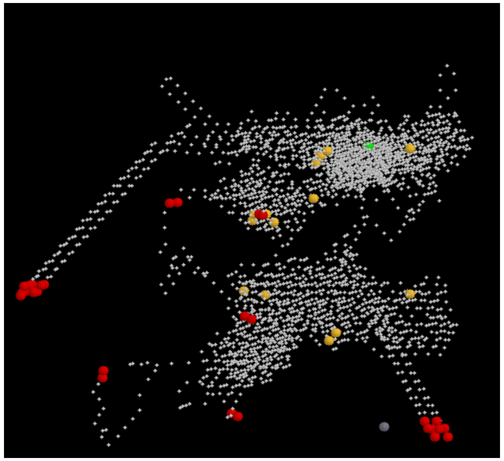
- *Fitting methods based on phase diagram (SCK) & ab initio data (ASSIMPOT dev. by EDF)*
- *Modified Embedded Atom Method (MEAM - (Baskes LANL)) (CEA)*
- *Quantum core inter-atomic for 3d metals (UKAEA Joint work with fusion)*
- *Improved empirical potentials in a two band model (Edinburgh)*

For Internals :

- *EAM potential for fcc Fe Ni model alloys (Lille)*

Data Base :

- *Selection versus exp. data, ab initio results, and, computational performances (MD)*



Cascade with Molecular Dynamics in pure α Fe

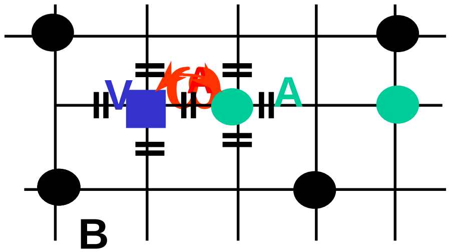
- **Free migrating defects : 20% NRT**
- **Numerous Replacement Sequences**
- **1D motion of interstitials clusters**

Fe + 0.5% Cu: 8 keV PKA– 3ns (After N.V Doan)

PERFECT (EDF, LPOOL, UPC, ULB)

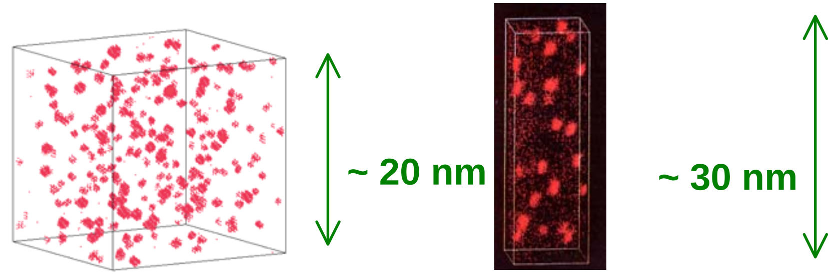
- **Productions of point defect clusters and free migrating defects via MD (LPOOL, UPC)**
  - Effect of improved empirical potentials
  - Effect of alloying elements: C
- **Statistical study of defect production in displacement cascade via Binary Collision Approximation (BCA) (ULB)**
- **Data base**

AB alloy with vacancies



After F. Soisson, G. Martin, A. Barbu (1995)

Fe-1.34%Cu



VAKMC APFIM

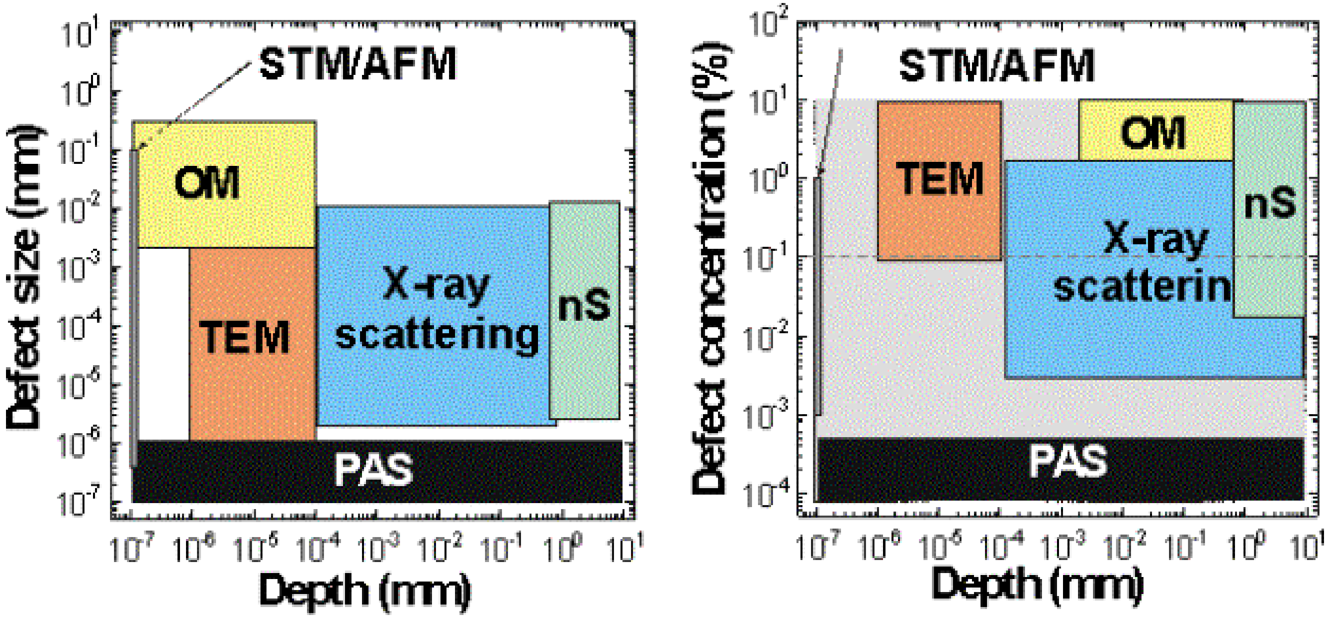
Thermodynamics & Kinetics

PERFECT (EDF, CEA, SCK)

- **Vacancy Atomic Kinetic Monte Carlo (VAKMC) as a first approximation**
  - Better cohesion model, introduction of C and other alloying element Cu, Mn, Ni, Si
  - Application to the formation of Cu, Mn, Ni, Si enriched atmospheres
- **Atomic Kinetic Monte Carlo (AKMC) under irradiation:**
  - Upgrade Atomic Kinetic Monte Carlo to (I) **treat V & I with diffusion mechanisms using ab initio data** (ii) **to introduce sinks**
  - **Application to Fe-Cu and Fe-C-Cu**
- **Hybrid Kinetic Monte Carlo (HKMC)**
  - Attempt to take the best from AKMC and Kinetic Monte Carlo on Objects
  - Application Fe-Cu

PERFECT

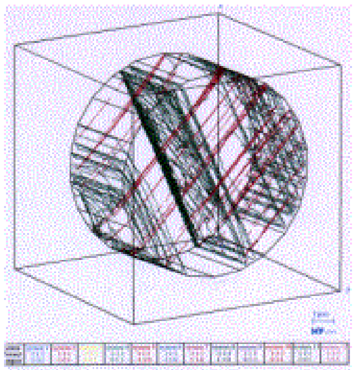
- **Modelling Tools upgrade and validation : EDF,CEA, SCK, CIEMAT, UPM**
  - **Rate Theory (CEA, FZR) : homogeneous alloys – no spatial correlation**
    - Migration & binding energies are **"physically acceptable"** ones **fitted on experimental data**
    - Sensitivity study of the fitted parameters versus microstructure of model alloys and steels
    - Sensitivity study on VVER 1000 steels (NRI, FZR)
  - **Monte Carlo Events & Objects (CEA, EDF, UPM, CIEMAT, SCK)**
    - Upgrade to **treat point defects, alloying elements & diffusion mechanisms from the ab initio data & improved empirical potentials**
    - **Comparison** of the prediction w**ith the microstructure of Fe of various purity, Fe-C and models alloys irradiated with electrons, ions and neutrons**
  - **Inter-comparison of these methods and Rate Theory :selection for RPV-2**
  - **Self Consistent Mean Field (CEA) for segregation application**
    - Upgrade to treat interstitials mechanisms for segregation application

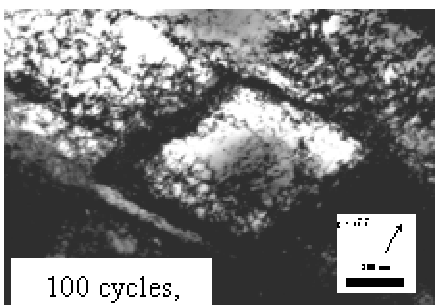


- Microstructure characterisation: CEA, SCK, CIEMAT,VTT, FZR NRI, CUP, Chalmers, SUTB EPFL, GPM
  - TEM, FEGSTEM, APFIM, PAS, SANS
  - TEM image simulation & ab initio calculation of Doppler Broadening in PAS
  - Electron, ion and neutron irradiation on a large temperature (& flux) range
  - Model alloys to actual RPV steels : Western and VVER 1000

WPII-4 RPV: Discrete Dislocations Dynamic

DDD: ability to reproduce dislocation microstructure





100 cycles, T_{max} = 380°C, ΔT=350°C

(316, Low Cycle Fatigue)

C. Robertson, C. Déprés (CEA)

PERFECT (EDF, CEA, SCK, LPOOL)

- **Atom scale simulation (MD & MS) of dislocation dynamics based on best estimate of empirical potential (LPOOL EDF)**
- **bcc code development capable of hardening and strain hardening prediction in irradiated RPV steels (EDF, CEA):**
  - Effect of temperature on dislocation mobility : Peierls & cross slip mechanisms
  - Introduce obstacle forces from atom scale simulation
  - Coupling with Finite Element for use in RPV Mechanics
  - Experimental validation on TEM observation of dislocations structure versus (T and plastic strain)

Sub-Project III : RPV-Mechanics
SERCO Ltd Leader

Physics Modelling

- DDD
- Segregation

WP III-1 Models of micro-cracks nucleation

Selection of representative model(s)

WP III-2 Models of Brittle Fracture Behaviour

Trans-granular Cleavage

Inter-granular failure

RPV-Mechanics

Meso-scale plasticity

WP III-3 Implementation and Application of Preferred Fracture Models

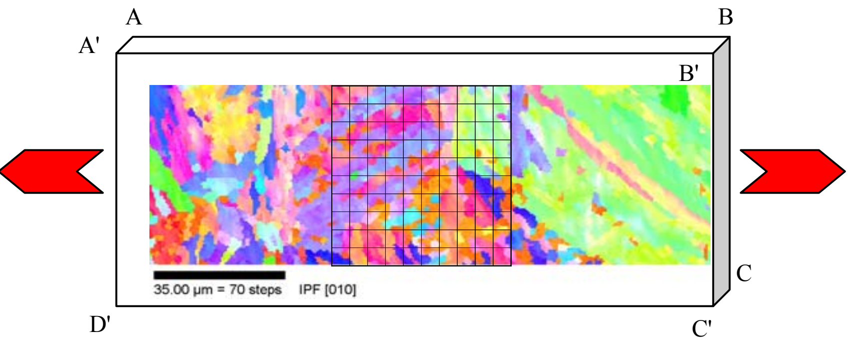
WP III-4 Characterisation of irradiated RPV steels

WP III-5 Fracture Behaviour Modelling of irradiated RPV components : Validation of Models

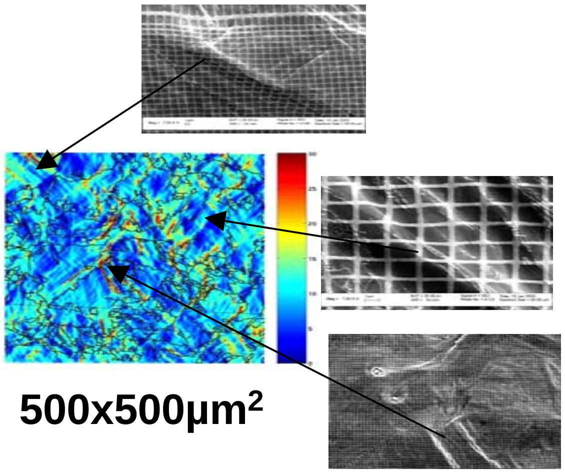
Transferability of specimens data to components with special attention of constraint effect in irradiated materials

Tensile Test on Slab :

- Crystalline orientation : EBSD
- Micro-grid for deformation : mesh 1x1µm²



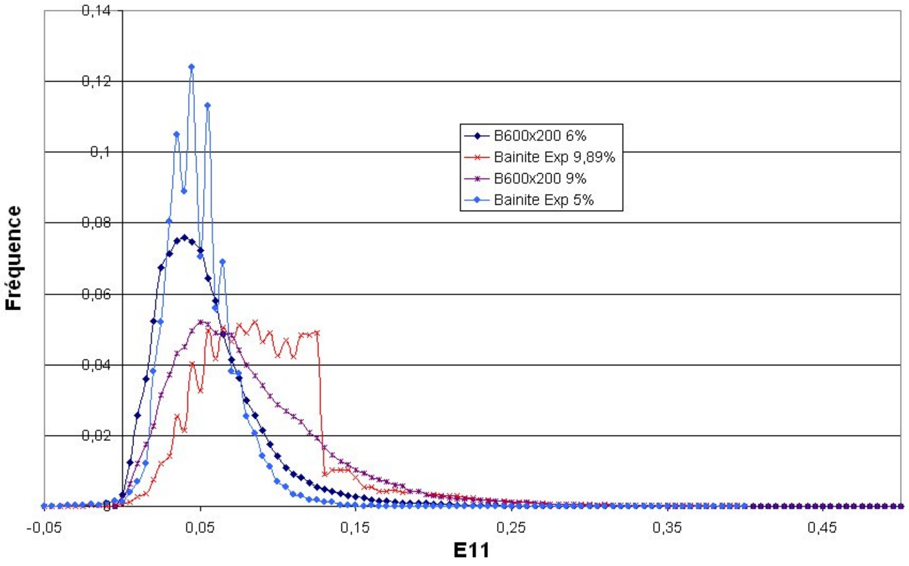
Experimental Strain for <ε> = 9%



500x500µm²

Crystalline FE Modelling

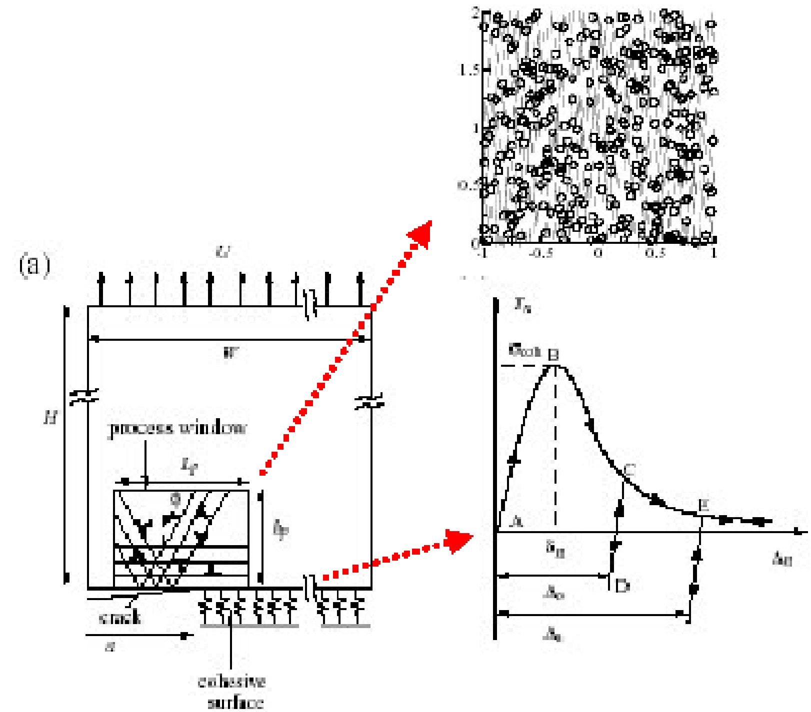
- Large transformation
- 24 slip systems: {110}<111> & {112}<111>
- State Variables : dislocation density on each slip system
- dislocation density evolution : hardening & microstructure (sub-grain boundaries)

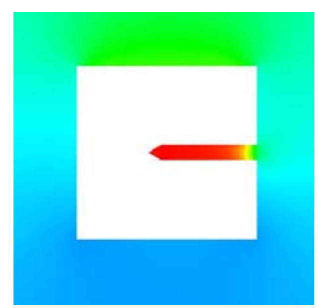


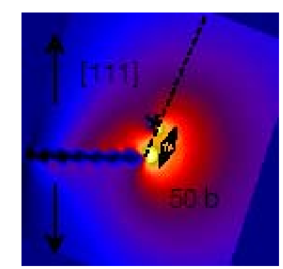
After S.Sekfali, C. Rey & B.Marini – in SMIRN

Internals : Mechanics and Corrosion
Multi-scale Crack growth Modelling

- **Microscopic modelling**
  - Crack tip: dislocation interaction with radiation damage & corrosion induced species (H, V).
- **Mesoscopic modelling**
  - Propagation in multi-grain body.
- **Macroscopic modelling**
  - Continuous mechanics
  - Chemical boundaries and source terms
- **Experimental validation**
  - Post –irradiation crack-growth experiments

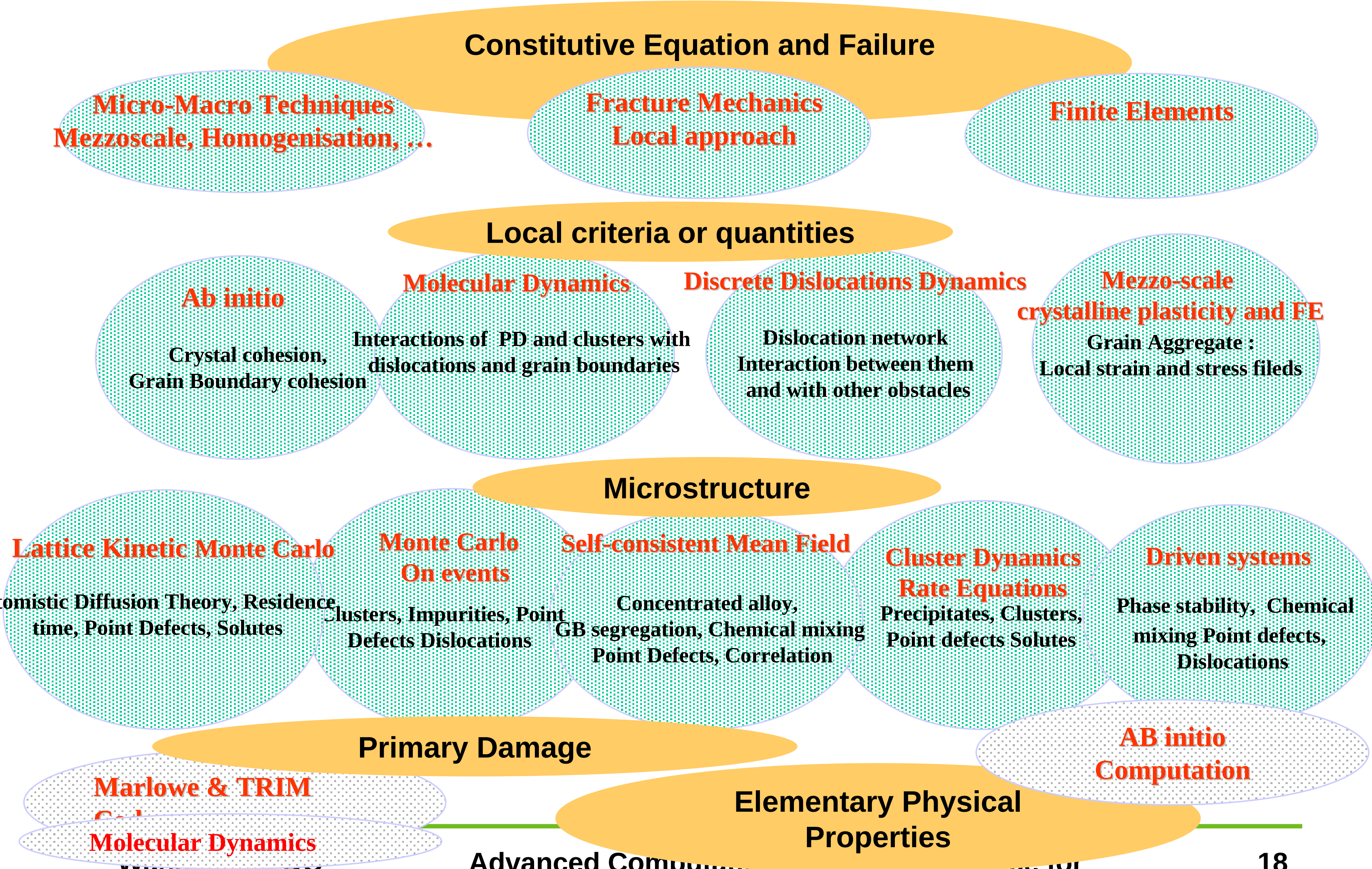






Potential around crack **Stresses at crack tip**

Integration Sub-project: a unique architecture to compare performance & couple tools



Experimental Validation and qualification

- **Multi-beam charged particles irradiation : Jannus Users Facility**
  - Modelling oriented & parametric studies
  - Rapid feedback
  - Point defects dynamics, Long Term Kinetic Pathways
- **Materials Testing Reactor (MTR) experiments : Jules Horowitz Reactor (JHR)**
  - Integrated experiments for fuel and materials qualification
  - Generation I & III: material ageing and fuel performance & safety
  - Generation IV : develop and qualify new materials and fuel

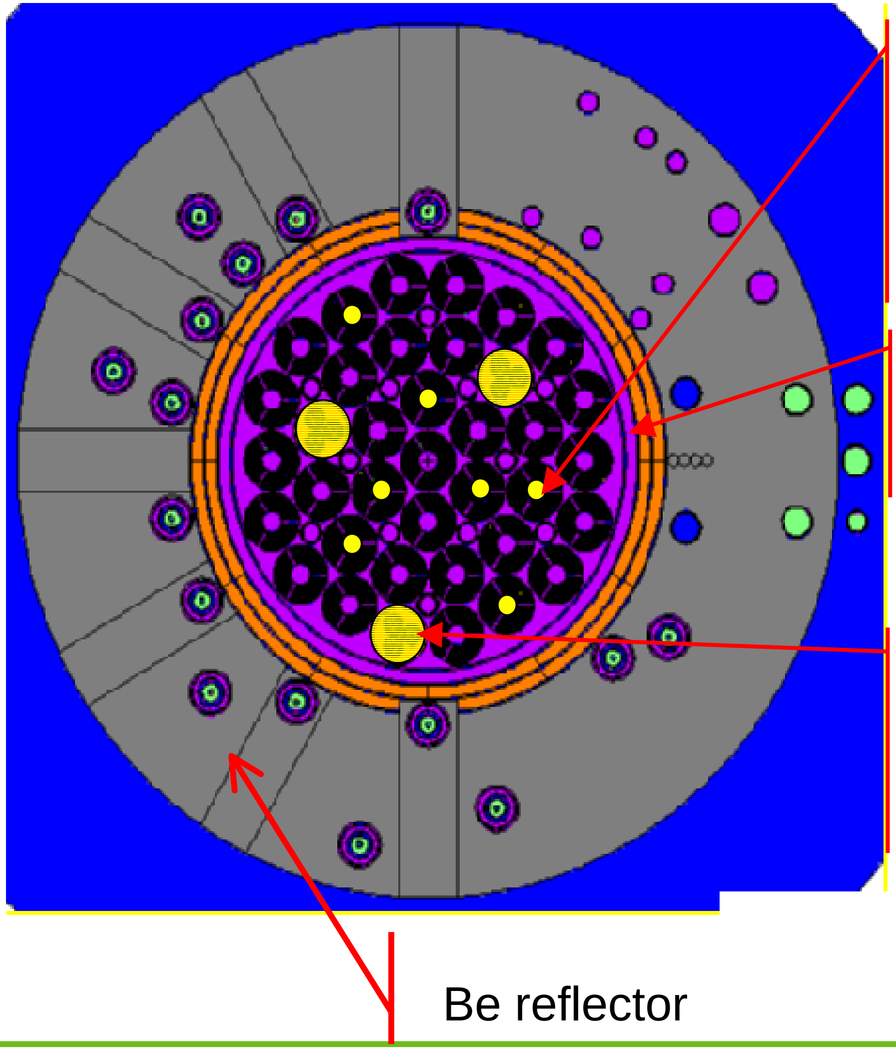
JHR : under design core configuration with experimental locations

In-core material experiment:

Fast flux ≤ 5 10^{14} n/cm²/s

= 16 dpa/year

Ex-core fuel experiment:
Thermal flux ≤ 4 10^{14} n/cm²/s
= 540 W/cm for 1% U5
Fast flux ≤ 7 10^{13} n/cm²/s



In-core elementary location

(Dia. ~30 mm)

Pressure tank

(Dia. ~ 683 mm)

In-core triple location

(Dia. ~90 mm)

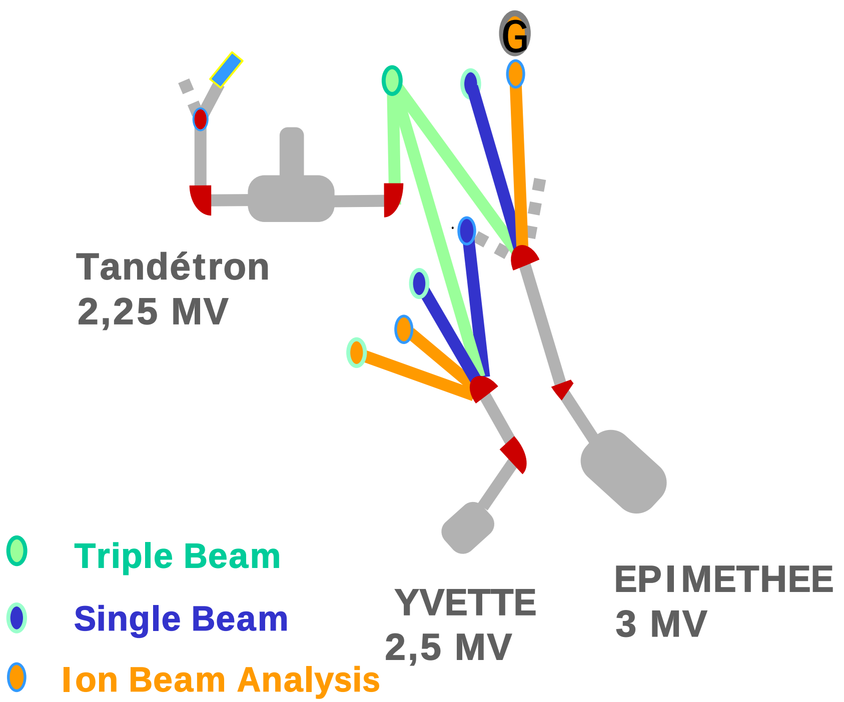
Be reflector

Experimental devices for Materials JHR Coordination Action (6th FP)

	Leader	Main characteristics & Challenges
Materials under high temperature : SiC, ZrC…	NRI	•Pressurized Gas loop : 80 bars, 1000°C •On-line control: T, impurities, pressure, velocity •Post-mortem & Inter-cycle examination: surface, dim. stability, mechanical properties, thermal conductivity, microstructure …
Visco-plasticity: Zr alloys, austenitic steels, SiC, ZrC …	VTT	•Bi-axial loading: pressure/tensile, torsion/tensile •In-pile mechanical testing: T, σ, Δl or $\Delta\alpha$, stress & T jump •Post-mortem : fracture (SEM), microstructure (TEM)
Stress Corrosion under Irradiation: Austenitic steels	CEA	•Pressurized water loop :PWR & BWR chemistry •On-line water control: T, pressure,velocity, chemistry •In-pile mechanical testing: T, σ, Δl, σ & T jump •Post-mortem examination : surface, SEM, TEM

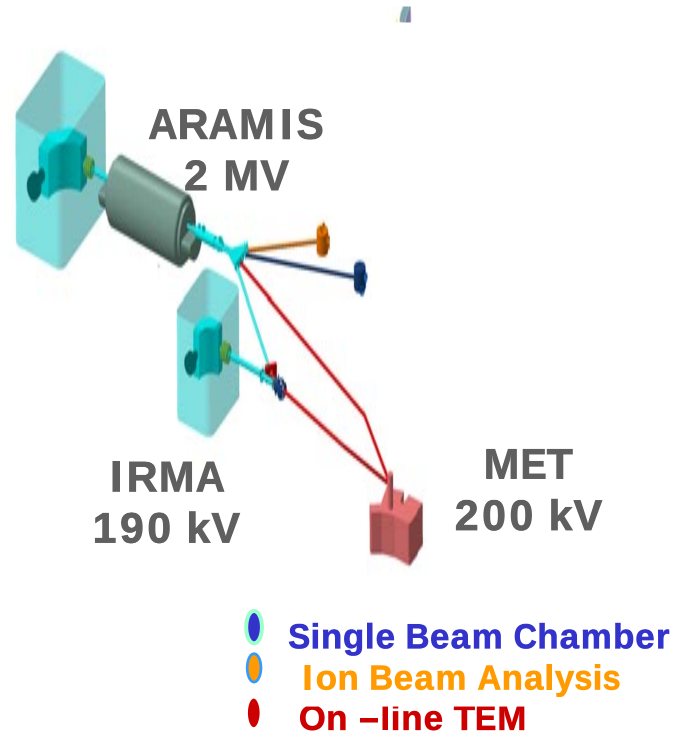
Modelling Oriented Experiments with Rapid Feedback

Triple beam : dpa and 2 implantations



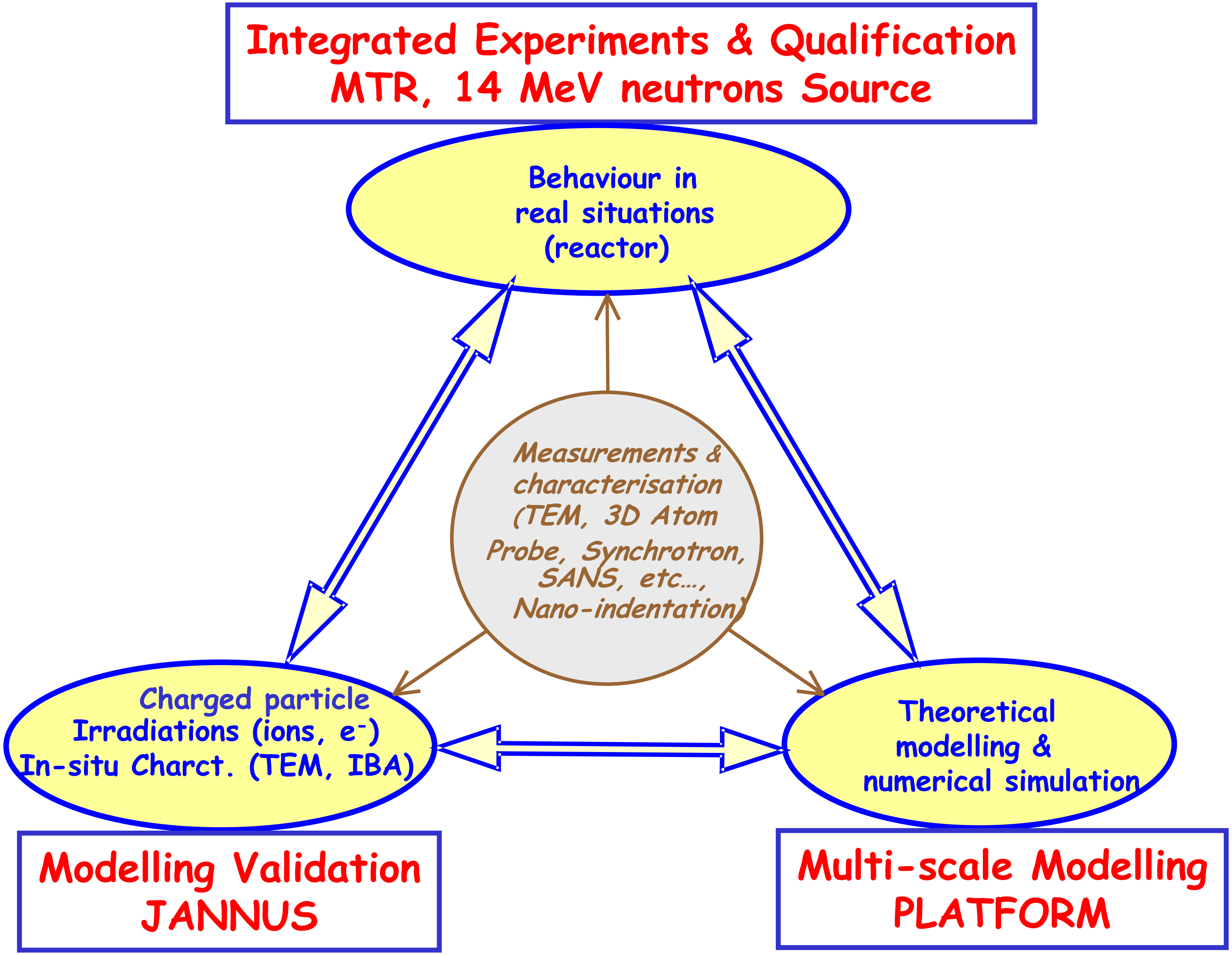
Kinetic Pathway up to ~0.5T_M:
dpa & transmutation

In-Situ TEM : one beam (dpa, implantation)



Point Defect Dynamics (<0.3T_M):
dpa or Implantation

Conclusion: The Virtuous Triangle



PERFECT

- **Cascades (EDF, Lille, ULB)**
  - Creation of a first data-base of cascades for Fe Ni cfc model alloy using MD (with EAM potential developed in WPII-1) and BCA for better statistics

- **Short term prediction (UNIAUG)**
  - Upgrade an AKMC method under irradiation and with possibility of lattice relaxation