

# Multiphysic

## A short introduction

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## Objectives of this talk

- 1 Provide an overview of current coupled problem solving strategies
- 2 Give some example of formulations of multiphysics problems
- 3 Discuss about some key points for the implementation of multifield/multiphysic problems

**What is a multiphysic problem ?**

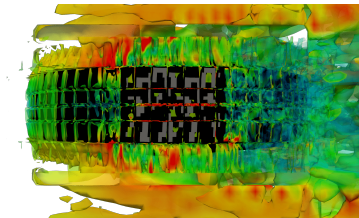
## What is a multiphysic problem ?

Can be represented by a system of equations with **more than one conservation equation** which can be **strongly or weakly** coupled together.

$$\left\{ \begin{array}{l} F_1(u_1, u_2) = 0 \\ F_2(u_1, u_2) = 0 \\ + \text{ boundary and initial conditions} \end{array} \right.$$

## Type of multiphysics problems

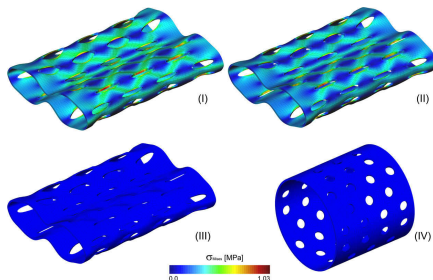
- Different physics coupled with a common **interface**,  
example : FSI



Tire aerodynamics coupled to tire contact with the road. From *Kuraishi et al, Comp. Mech. 2019*

## Type of multiphysics problems

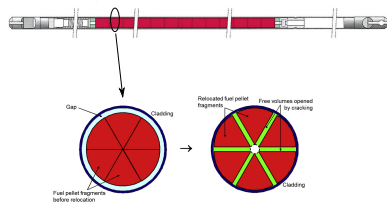
- Different physics coupled with a common **interface**,  
example : FSI
- Physics coupled in the **bulk** at the macroscopic scale,  
example : thermo-mechanics



Thermo-mechanical cycle for a shape memory polymer stents. From *Reese et al, CMAME, 2010*

## Type of multiphysics problems

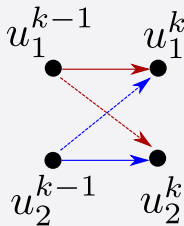
- Different physics coupled with a common **interface**, example : FSI
- Physics coupled in the **bulk** at the macroscopic scale, example : thermo-mechanics
- Physics **coupled across scales**, example : modeling thermo-mechanical behavior of fuel pin in nuclear reactor



Chemo-physical phenomena in fuel pellets  
From *Lainet et al, J. Nucl. Mat., 2019*

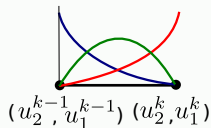
## Time stepping methods

Considering (semi-)discrete methods for the time



## Space-time methods

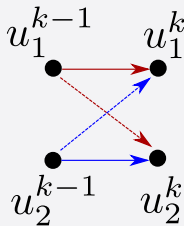
Considering continuous approximation for the time





## Time stepping methods

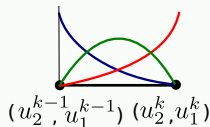
Considering (semi-)discrete methods for the time



- **Monolithic**

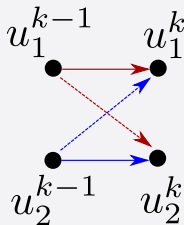
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## Time stepping methods

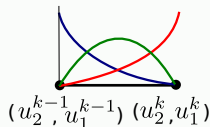
Considering (semi-)discrete methods for the time



- **Monolithic**
- **Operator splitting**  
(staggered)

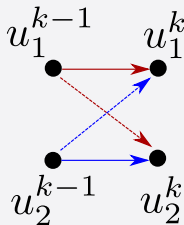
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## Time stepping methods

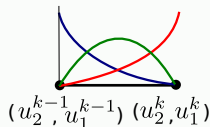
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## Space-time methods

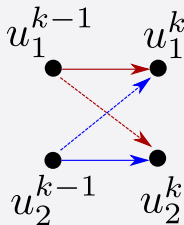
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- **Continuous or discontinuous** over elements in time

## Time stepping methods

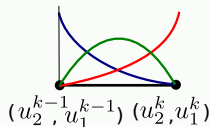
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- **Monolithic**
- **Operator splitting** (staggered)

## Space-time methods

Considering continuous approximation for the time



- **Continuous or discontinuous** over elements in time
- **Mono or Multi-grids**

## Constraints

- Existing code architectures
- Transient phenomena
- Precision and stability (robustness)
- Global/local integration of the system of equations (ex : internal variables for time dependant materials)

## Opportunities

- Separation of the different physics in terms of time scale
- Variational principles (e.g. Incremental Variational Principles : *Ortiz & Stainier, 99, Miehe 02, ...*)

## Time stepping methods

## Idealized coupled problem

Let  $\mathbf{u} = (u_1, u_2, \dots)$  the vector of physical variables,  $\mathbf{A}$  a linear operator

Assuming the following form :

$$\begin{cases} \mathbf{R}(\mathbf{u}) = \mathbf{A}\dot{\mathbf{u}} - \mathbf{F}(\mathbf{u}) = 0 \\ \mathbf{u}(t = 0) = \mathbf{u}_0 \\ + BC \end{cases}$$

### Time stepping

Let  $[t_{n-1}, t_n]$  an interval of time, knowing  $\mathbf{u}^{n-1} = \mathbf{u}(t_{n-1})$  we consider a discrete approximation for  $\dot{\mathbf{u}}$ . If :

$$\dot{\mathbf{u}} = \frac{\mathbf{u}^n - \mathbf{u}^{n-1}}{\Delta t}$$

we can use :

$$\text{Forward Euler} \rightarrow \mathbf{A}\mathbf{u}^n = \Delta t \mathbf{F}(\mathbf{u}^{n-1}) + \mathbf{A}\mathbf{u}^{n-1}$$

Easy to implement but can pose stability and precision problems



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Easy to implement but can pose stability and precision problems

or :

$$\text{Backward Euler} \rightarrow \mathbf{A}\mathbf{u}^n - \Delta t \mathbf{F}(\mathbf{u}^n) = \mathbf{A}\mathbf{u}^{n-1}$$

Depending on intrinsic times : monolithic or operator splitting

### Monolithic approach (tight coupling)

Set  $\mathbf{u}_0 = \mathbf{u}^{n-1}$ , linearize the system and iterate :

$$\text{solve : } \mathbf{K}\Delta\mathbf{u}_k = \mathbf{f}$$

$$\text{update until convergence : } \mathbf{u}_k = \mathbf{u}_{k-1} + \Delta\mathbf{u}_k$$

$$\text{set : } \mathbf{u}^n = \mathbf{u}_k$$

## Time stepping methods

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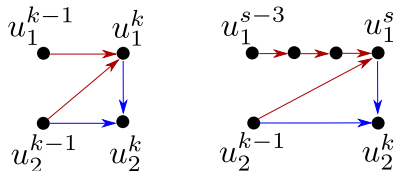
update until convergence :  $\mathbf{u}_k = \mathbf{u}_{k-1} + \Delta\mathbf{u}_k$

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### Operator splitting (loose coupling)

Additive splitting such  $\mathbf{F}(\mathbf{u}) = \mathbf{F}_I(\mathbf{u}) + \mathbf{F}_{II}(\mathbf{u})$ . An example :

$$\mathbf{F} = \begin{pmatrix} F_1(u_1^n, u_2^{n-1}) \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ F_2(u_1^n, u_2^n) \end{pmatrix}$$



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Robustness of the Newton methods but costly

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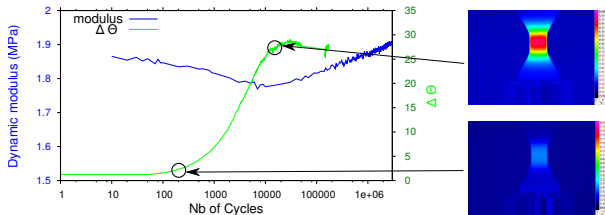
$$\mathbf{F} = \begin{pmatrix} F_1(u_1^n, u_2^{n-1}) \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ F_2(u_1^n, u_2^n) \end{pmatrix}$$

Interesting if  $\tau_1 \ll \tau_2$

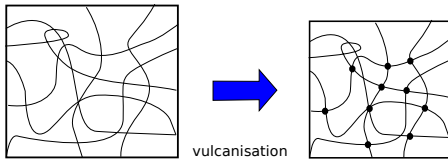
Well chosen splitting allows to build stable and efficient schemes

### Modelling the evolution of chemical crosslinks

- 1 thermal ageing phenomena (concomitant or not to mechanical loads)

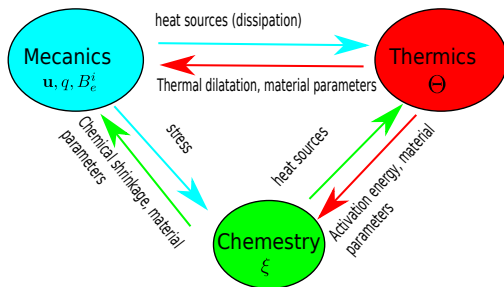


- 2 Modelling rubber processing (vulcanisation)



### Modeling material behavior, main ingredients :

- 1 Finite strain and nearly-incompressible behavior
- 2 Non linear viscoelasticity (with  $N$  internal variables)
- 3 Phenomenological modelling of chemical reactions without diffusion (chemical conversion  $\xi(\mathbf{X}, t) \in [0, 1]$ )
- 4 Thermal expansion and chemical shrinkage



### Material Behavior

- Constitutive equations (mechanics)

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_{hyp}^D(\bar{\mathbf{B}}, \xi, \Theta) + \sum_{i=1} \boldsymbol{\sigma}_v^{iD}(\bar{\mathbf{B}}_e^i, \Theta, \xi) + \frac{q}{J_\Theta} \mathbf{1}$$

$$g(q) = \frac{(1 - JJ_\Theta^{-1})}{\rho_0}$$

- Evolution laws for viscosity (mechanics)

$$\bar{\mathbf{D}}_v^i = \frac{1}{\eta_i(\xi, \Theta)} \boldsymbol{\sigma}_v^i \quad i = 1..N$$

- Evolution law (chemistry)

$$\dot{\xi} = A \exp\left(\frac{-E_a}{R\Theta}\right) \langle \mathcal{A}_\xi(\bar{\mathbf{B}}, \bar{\mathbf{B}}_e, \xi, q, \Theta) \rangle$$

### Weak form

Find  $(\mathbf{u}, \Theta, \xi, q)$  such that  $\forall(\delta \mathbf{u}, \delta \Theta, \delta \xi, \delta q)$

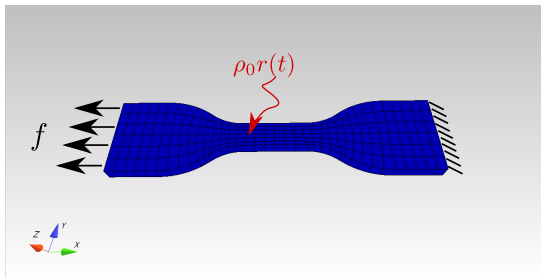
$$\left\{ \begin{array}{l} \int_{\Omega_0} (\boldsymbol{\Pi}^D + q \frac{J}{J_\Theta} \mathbf{F}^{-T}) : \mathbf{F}(\delta \mathbf{u}) d\Omega_0 - \mathcal{P}_{ext}(\mathbf{u}, \delta \mathbf{u}) = 0 \\ \int_{\Omega_0} \rho_0 C_p \dot{\Theta} \delta \Theta d\Omega_0 - \int_{\Omega_0} (J \phi_m + J \phi_\xi + J l_m + J l_\xi + \rho_0 r) \delta \Theta d\Omega_0 \\ \quad - \int_{\Omega_0} J \mathbf{Q} \cdot \text{GRAD}_x \delta \Theta d\Omega_0 + \int_{\partial \Omega_{q_0}} \mathbf{Q} \cdot \mathbf{N} \delta \Theta dS = 0 \\ \int_{\Omega_0} \left( \frac{J}{J_\Theta} - 1 + g(q) \right) \delta q d\Omega_0 = 0 \\ \int_{\Omega_0} \left( \dot{\xi} - \kappa(\Theta) < A_\xi > \right) \delta \xi d\Omega_0 = 0 \end{array} \right.$$



### Numerical implementation :

- Time discretization of heat and chemical equation with **Backward-Euler** scheme and **Monolithic** (tight coupling) resolution (non-symmetric operator)
- Local, at Gauss point level, integration of mechanical flow rules with a **BDF integrator** (chemical and thermal state are freeze)
- Implementation done in FEMJava (in-house code) : advanced platform for multiphysics simulations with **FE or IGA**
- Fields approximation for FE : quadratic interpolation for  $\mathbf{u}$ ,  $\Theta$ ,  $\xi$  and linear for  $\mathbf{q}$  (for stability)

### Thermal aging of a tensile specimen under creep



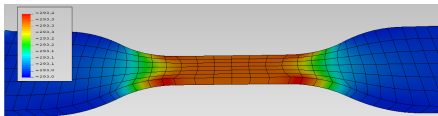
*adiabatic boundary conditions*

Loadings :

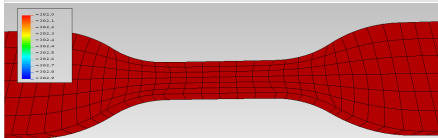
- Step 1 : stretching of the specimen up to the constant force  $f$  at initial temperature
- Step 2 : uniform heating with volumetric term  $\rho_0 r(t)$

## Thermal aging of a tensile specimen under creep

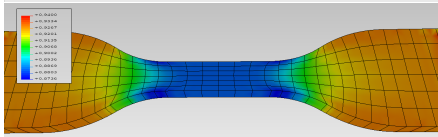
Equivalent stress at  
the end of step 2



Temperature field at  
the end of step 2



New crosslinks  
density at the end  
of step 2



## Space-Time methods

### Idealized coupled problem

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### Space-time formulations

Let  $Q = \Omega \times [T_0, T_1]$  the space time cylinder and  $P$  its boundary, we can consider the weak form (among others) :

$$\int_Q \mathbf{A}\dot{\mathbf{u}}\delta\mathbf{u}dQ - \int_Q \mathbf{F}(\mathbf{u})\delta\mathbf{u}dQ = 0$$

$BC$  and  $IC$  can be taken into account as Dirichlet condition or in the weak form

## Separate approximations (semi-discrete form)

Example of piecewise linear functions in time :

$$\mathbf{u}^e(\mathbf{x}, t) = \frac{(t - T_0)}{\Delta t} \mathbf{N}_1^e(\mathbf{x}) \mathbf{d}_1^u + \frac{(T_1 - t)}{\Delta t} \mathbf{N}_0^e(\mathbf{x}) \mathbf{d}_0^u$$
$$\dot{\mathbf{u}}^e(\mathbf{x}, t) = \frac{1}{\Delta t} (\mathbf{N}_1^e(\mathbf{x}) \mathbf{d}_1^u - \mathbf{N}_0^e(\mathbf{x}) \mathbf{d}_0^u) = \frac{1}{\Delta t} (\mathbf{u}_1^e(\mathbf{x}) - \mathbf{u}_0^e(\mathbf{x}))$$

with constant integration for the time ( $\int_Q dQ = \int_{T_0}^{T_1} \int_{\mathbf{x}} dT d\mathbf{x}$ ) :

- Left Riemann sum  $\rightarrow \mathbf{A}\mathbf{u}^1 = \Delta t \mathbf{F}(\mathbf{u}^0) + \mathbf{A}\mathbf{u}^0$
- Right Riemann sum  $\rightarrow \mathbf{A}\mathbf{u}^1 = \Delta t \mathbf{F}(\mathbf{u}^1) + \mathbf{A}\mathbf{u}^0$

Allows more general definitions of semi-discrete integration schemes

### Arbitrary approximations

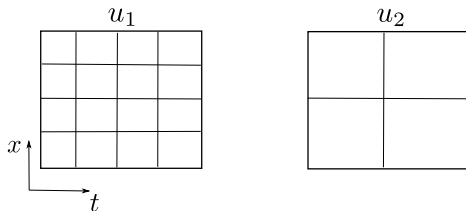
Discretizing the space and time with a mesh, constructing approximations over elements :

$$\mathbf{u}^e(\mathbf{x}, t) = \mathbf{N}^e \mathbf{d}^u \quad \rightarrow \quad \dot{\mathbf{u}}^e(\mathbf{x}, t) = \mathbf{B}_t^e \mathbf{d}^u$$

leads to the resolution of a "larger" linear or non-linear system

$$\mathbf{K} \Delta \mathbf{d}^u = \mathbf{f}$$

Allows to use multi-grids formulations (in space and time) in an easy way and higher order integrators (especially with IGA)





## Example : Impact of a thermoelastic bar

### Strong form of the problem

Momentum conservation

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} - \operatorname{div}_x \boldsymbol{\sigma} - \mathbf{f} = 0$$

Heat transfer (with linearized coupling)

$$\rho C \frac{\partial \Theta}{\partial t} - \Theta_0 \left( \frac{\partial \boldsymbol{\sigma}}{\partial \Theta} \right) : \dot{\boldsymbol{\varepsilon}} + \operatorname{div}_x \mathbf{q} - \mathbf{r} = 0$$

Constitutive laws

$$\begin{aligned} \boldsymbol{\sigma} &= 2\mu \boldsymbol{\varepsilon} + \lambda \operatorname{tr}(\boldsymbol{\varepsilon}) \mathbf{I} - \alpha k (\Theta - \Theta_0) \mathbf{I} \\ \mathbf{q} &= -k_t \operatorname{grad}_x \Theta \end{aligned}$$

+Boundary and Initial conditions

## Example : Impact of a thermoelastic bar

### Weak form (3 fields)

Find  $(\mathbf{u}, \mathbf{v}, \Theta)$  such  $\forall(\delta\dot{\mathbf{u}}, \delta\dot{\mathbf{v}}, \delta\Theta)$

$$\int_Q \rho \dot{\mathbf{v}} \delta \dot{\mathbf{u}} dQ + \int_Q \boldsymbol{\sigma} : \boldsymbol{\varepsilon}(\delta \dot{\mathbf{u}}) dQ - \int_P \mathbf{T} \delta \dot{\mathbf{u}} dP - \int_Q \mathbf{f} \delta \dot{\mathbf{u}} dQ +$$
$$\int_Q \rho (\mathbf{v} - \dot{\mathbf{u}}) \delta \dot{\mathbf{v}} dQ + \int_Q \rho C \dot{\Theta} \delta \Theta dQ + \int_Q k_t \nabla \Theta \nabla \delta \Theta dQ - \int_p \mathbf{q} \mathbf{n} \delta \Theta dP -$$
$$\int_Q r \delta \Theta dQ - \int_Q \Theta_0 \left( \frac{\partial \boldsymbol{\sigma}}{\partial \Theta} : \dot{\boldsymbol{\varepsilon}} \right) \delta \Theta dQ + \sum_e \int_{Q_e} \rho (\ddot{\mathbf{u}} - \dot{\mathbf{v}}) \tau (\delta \ddot{\mathbf{u}} - \delta \dot{\mathbf{v}}) = 0$$

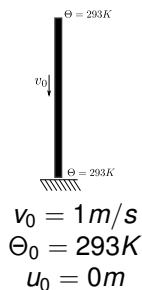
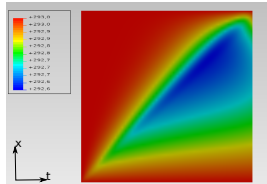
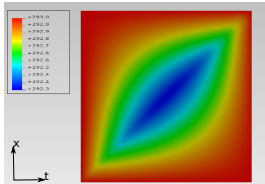
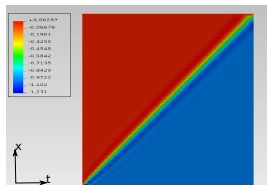
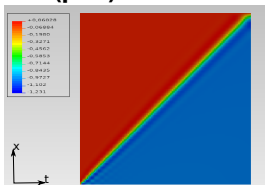
### Discrete form

Introduction of (NURBS or FE) approximations :  $\mathbf{u}^e = \mathbf{N}_u^e \mathbf{d}^u$ ,  
 $\mathbf{v}^e = \mathbf{N}_v^e \mathbf{d}^v$ ,  $\Theta^e = \mathbf{N}_\Theta^e \mathbf{d}^\Theta$

$$\begin{bmatrix} k_{uu} & k_{uv} & k_{u\Theta} \\ k_{vu} & k_{vv} & 0 \\ k_{\Theta u} & 0 & k_{\Theta\Theta} \end{bmatrix} \begin{Bmatrix} \mathbf{d}^u \\ \mathbf{d}^v \\ \mathbf{d}^\Theta \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}^u \\ \mathbf{f}^v \\ \mathbf{f}^\Theta \end{Bmatrix}$$

# Example : Impact of a thermoelastic bar

## Results with ST-IGA ( $p=2$ )

 $\sigma$  $\Theta$ 

$$\rho Cl^2/k_t = 0.1s,$$
$$\sqrt{E/\rho} = 1m/s$$

$$\rho Cl^2/k_t = 5.1s,$$
$$\sqrt{E/\rho} = 1m/s$$

## To sum-up

### Time stepping methods

#### pros

- Allows to couple existing codes

#### cons

- Full linearization not always easy to obtain
- High order implicit schemes in time are difficult to express

### Space-time methods

#### pros

- Very general formalisms
- Ease the obtention of the linearized form and high order schemes in time

#### cons

- Needs to rewrite code (at least partially)

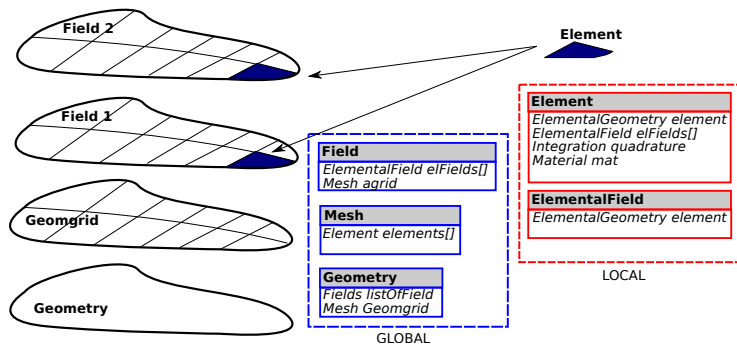
## Some aspects about code architecture

### **Multifields management : good practices**

- Separate conceptual entities into simple objects : geometry, formulation, fields, material, ...

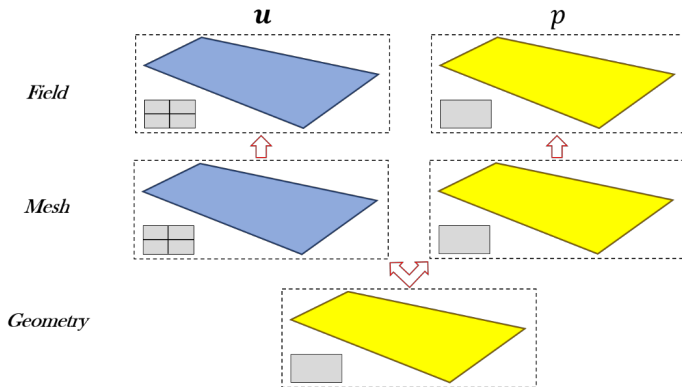
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### Multifields management : good practices

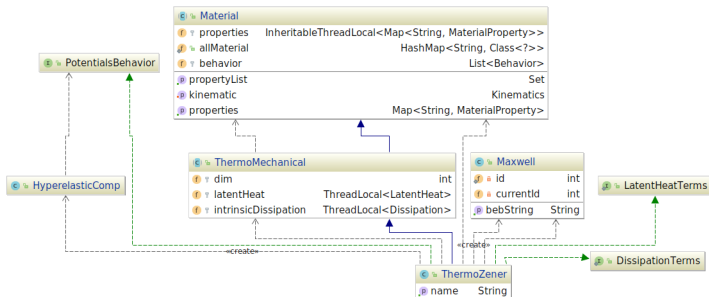
- Separate conceptual entities into simple objects : geometry, formulation, fields, material, ...
- Have global/local management of fields
- Natively integrate multigrids situation





## Materials

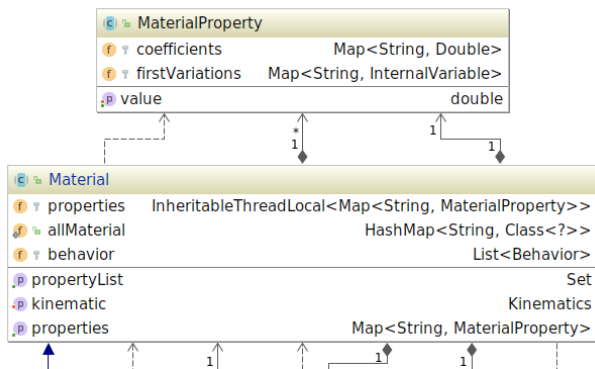
- Do not rewrite the existing code if possible, ex :  
thermomechanical=thermo+mechanical



Powered by yFiles

### Materials

- Do not rewrite the existing code if possible, ex : thermomechanical=thermo+mechanical
- Take into account the dependency of material parameters on fields in a general manner → have a mechanisms to compute the derivatives of the material parameters



Thank you for listening !