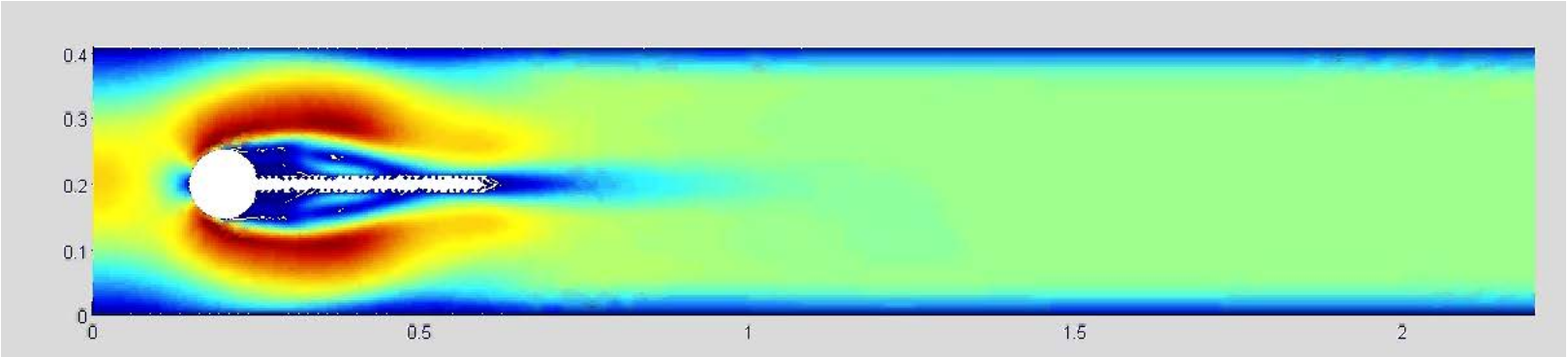
ALE formulations

INTRODUCTION

We want to deal with the numerical simulation of multiphysics problems:

- Fluid Dynamics
- Large deformation solid mechanics



INTRODUCTION

We need to choose the frame of reference in which we write the equations of the continuum mechanics.

Classical approaches:

- Eulerian frame of reference

  The finite element (finite volume, etc…) mesh doesn't move. We write the finite element equations in a **spatial configuration.** Fluid mechanics, allows to deal with large movements of the continuum.

- Lagrangian frame of reference

  The finite element mesh follows the movement of the material particles. We write the finite element equations in a **material configuration.** Solid mechanics, precise interface tracking.

Hybrid approach:

- Arbitrary Lagrangian-Eulerian Formulation

MATERIAL AND SPATIAL COORDINATES

Some definitions:

- Spatial point: A point which is fixed in space (its position doesn't change). We denote spatial coordinates as:

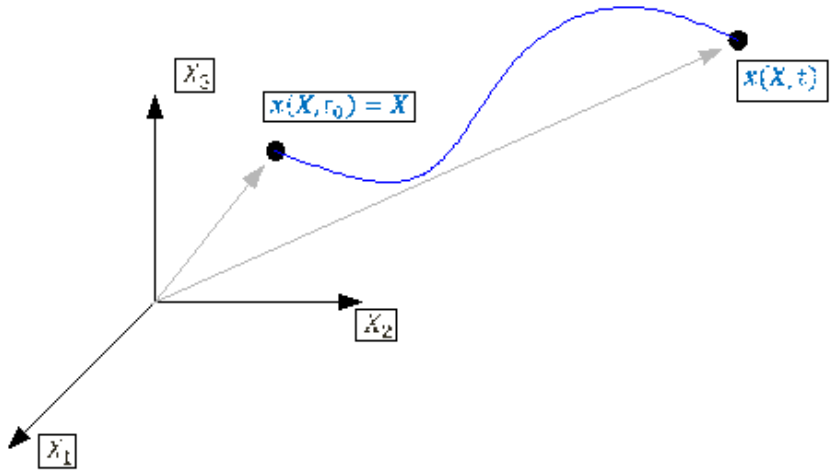
$$\boldsymbol{x} = x_1\hat{\boldsymbol{e}}_1 + x_2\hat{\boldsymbol{e}}_2 + x_3\hat{\boldsymbol{e}}_3$$

- Material point: A particle. It can occupy several positions (spatial points) in time. We identify a particle by its position at the initial configuration t_0:

$$\boldsymbol{X} = X_1\hat{\boldsymbol{e}}_1 + X_2\hat{\boldsymbol{e}}_2 + X_3\hat{\boldsymbol{e}}_3$$

- Equations of movement: The equations of movement allow us to identify, for a given particle $\boldsymbol{X}$, its spatial position $\boldsymbol{x}$ for each time instant t:

$$\boldsymbol{x} = \boldsymbol{\varphi}(\boldsymbol{X}, t) := \boldsymbol{x}(\boldsymbol{X}, t)$$



MATERIAL AND SPATIAL DESCRIPTIONS OF QUANTITIES OF INTEREST

Given a property with values varying in space and time, we can choose to describe it as a function of spatial or material coordinates.

Spatial description:

$$\gamma(\boldsymbol{x}, t)$$

Material description:

$$\Gamma(\boldsymbol{X}, t)$$

Spatial and material descriptions are related through the equations of movement:

$$\gamma(\boldsymbol{x}, t) = \gamma(\boldsymbol{x}(\boldsymbol{X}, t)) = \Gamma(\boldsymbol{X}, t)$$

And the inverse equations of movement:

$$\boldsymbol{X} = \boldsymbol{\varphi}^{-1}(\boldsymbol{x}, t) = \boldsymbol{X}(\boldsymbol{x}, t)$$

$$\Gamma(\boldsymbol{X}, t) = \Gamma\big(\boldsymbol{X}(\boldsymbol{x}, t)\big) = \gamma(\boldsymbol{x}, t)$$

TEMPORAL DERIVATIVES: LOCAL, MATERIAL, CONVECTIVE

Since we have several description of the continuum (material, spatial), there are several definitions for the temporal derivatives:

- **Local time derivative**: Sensitivity of a property with respect to time in a point which is fixed in space. If we have the spatial description of a property, the local time derivative is defined as:

$$local\ derivative := \frac{\partial \gamma(\boldsymbol{x}, t)}{\partial t}$$

- **Material time derivative:** Sensitivity of a property with respect to time following a specific particle (material point) of the continuum. If we have the material description of a property, we can define it as:

$$material\ derivative := \frac{d}{dt}\Gamma = \frac{\partial \Gamma(\mathbf{X}, \mathrm{t})}{\partial t}$$

Note that the two properties are different and have different meanings: in the first one we are focusing in the variation in time of a variable at a fixed point, in the second one, we move around the domain following a particle.

TEMPORAL DERIVATIVES: LOCAL, MATERIAL, CONVECTIVE

How do local and material derivatives relate: the convective derivative

We start by recalling:

$$\gamma(\boldsymbol{x}, t) = \gamma(\boldsymbol{x}(\boldsymbol{X}, t)) = \Gamma(\boldsymbol{X}, t)$$

Then:

$$material\ derivative \coloneqq \frac{d}{dt}\gamma(\boldsymbol{x}(\boldsymbol{X}, t)) = \frac{\partial \Gamma(\mathbf{X}, \mathrm{t})}{\partial t}$$

$$\frac{d}{dt}\gamma(\boldsymbol{x}(\boldsymbol{X}, t)) = \frac{\partial \gamma(\boldsymbol{x}, t)}{\partial t} + \frac{\partial \gamma(\boldsymbol{x}, t)}{\partial x_i}\frac{\partial x_i}{\partial t} = \frac{\partial \gamma(\boldsymbol{x}, t)}{\partial t} + \frac{\partial \gamma}{\partial \boldsymbol{x}}\frac{\partial \boldsymbol{x}}{\partial t} = \frac{\partial \gamma(\boldsymbol{x}, t)}{\partial t} + \boldsymbol{v} \cdot \nabla\gamma$$

Where we have taken into account that the velocity is defined as the derivative of the equations of movement with respect to time:

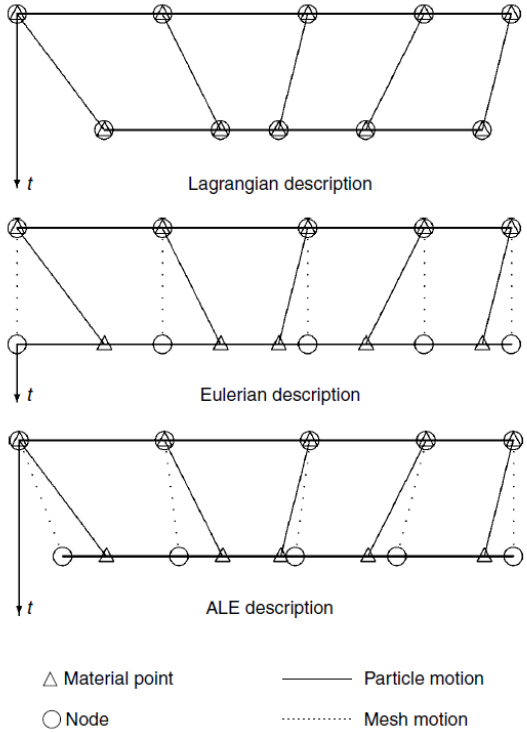
$$v \coloneqq \frac{\partial \boldsymbol{x}(\boldsymbol{X}, t)}{\partial t}$$

These are the material, local and convective derivatives.

In an Eulerian frame of reference, we use local + convective to express the material derivative at a point fixed in space.

In a Lagrangian frame of reference we use the material derivative: we follow a particle.

A HYBRID APPROACH: ARBITRARY LAGRANGIAN-EULERIAN FRAME OF REFERENCE



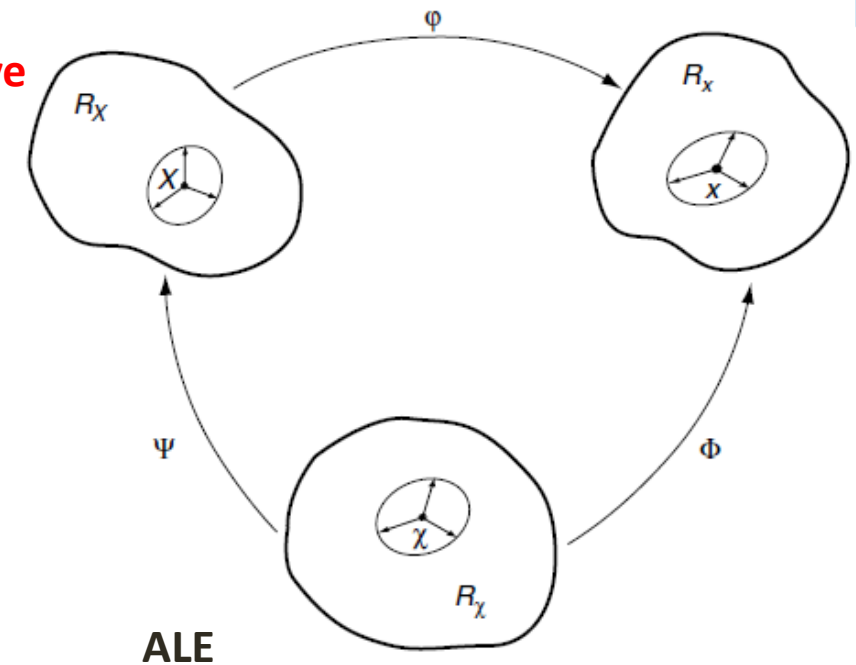
From Donea et al. *Arbitrary Lagrangian-Eulerian methods*, Enciclopedia of Computational Mechanics 2004.

The advantages are the capability for dealing with large domain movements, while keeping a sharp tracking of the interface.

A HYBRID APPROACH: ARBITRARY LAGRANGIAN-EULERIAN FRAME OF REFERENCE

How do we compute the material derivatives in an arbitrary Lagrangian-Eulerian frame of reference

Lagrangian
Material derivative



Eulerian
Local + Convective

ALE
?

From Donea et al. *Arbitrary Lagrangian-Eulerian methods*, Enciclopedia of Computational Mechanics 2004.

A HYBRID APPROACH: ARBITRARY LAGRANGIAN-EULERIAN FRAME OF REFERENCE

The idea is similar to what is done for the Eulerian frame of reference. We start by introducing the mesh movement:

$$\boldsymbol{x} = \boldsymbol{\Phi}(\boldsymbol{\mathcal{X}}, t) = \boldsymbol{x}(\boldsymbol{\mathcal{X}}, t)$$

For each initial position of the mesh nodes $\boldsymbol{\mathcal{X}}$, it gives the position $\boldsymbol{x}$ of the mesh nodes at a given time instant. **It traces the movement of the mesh.** This allows us to define the mesh velocity:

$$\boldsymbol{v}_{MESH} = \frac{\partial \boldsymbol{x}(\boldsymbol{\mathcal{X}}, t)}{\partial t}$$

which is the derivative of the equations of the mesh movement with respect to time.
For a Lagrangian frame of reference, ALE coordinates follow the particles:

$$\boldsymbol{x}(\boldsymbol{\mathcal{X}}, t) = \boldsymbol{x}(\boldsymbol{X}, t) \quad \Rightarrow \quad \boldsymbol{v}_{MESH} = \boldsymbol{v}$$

In an Eulerian frame of reference, ALE coordinates are static in space:

$$\boldsymbol{x}(\boldsymbol{\mathcal{X}}, t) = \boldsymbol{x}(\boldsymbol{x}, t) \Rightarrow \quad \boldsymbol{v}_{MESH} = \boldsymbol{0}$$

A HYBRID APPROACH: ARBITRARY LAGRANGIAN-EULERIAN FRAME OF REFERENCE

On the other hand, we can define the mapping between ALE domain and the material domain as:

$$\boldsymbol{X} = \boldsymbol{\Psi}(\boldsymbol{\mathcal{X}}, t) = \boldsymbol{X}(\boldsymbol{\mathcal{X}}, t)$$

It is convenient, however, to define also the inverse mapping, which transforms material coordinates into coordinates in the ALE reference system:

$$\boldsymbol{\mathcal{X}} = \boldsymbol{\Psi}^{-1}(\boldsymbol{X}, t) = \boldsymbol{\mathcal{X}}(\boldsymbol{X}, t)$$

Referred to this mapping, we define the velocity:

$$\boldsymbol{w} = \frac{\partial \boldsymbol{\mathcal{X}}(\boldsymbol{X}, t)}{\partial t} = \frac{\partial \boldsymbol{\Psi}^{-1}(\boldsymbol{X}, t)}{\partial t}$$

Now, we recall that $\boldsymbol{\varphi} = \boldsymbol{\Phi} \circ \boldsymbol{\Psi}^{-1}$

$$\frac{\partial \boldsymbol{\varphi}(\boldsymbol{X}, t)}{\partial t} = \frac{\partial \boldsymbol{\Phi}(\boldsymbol{\Psi}^{-1}(\boldsymbol{X}, t), t)}{\partial t} = \frac{\partial \boldsymbol{\Phi}(\boldsymbol{\mathcal{X}}, t)}{\partial t} + \frac{\partial \boldsymbol{\Phi}(\boldsymbol{\mathcal{X}}, t)}{\partial \boldsymbol{\mathcal{X}}} \frac{\partial \boldsymbol{\Psi}^{-1}(\boldsymbol{X}, t)}{\partial t} \Rightarrow$$

$$\boldsymbol{v} = \boldsymbol{v}_{MESH} + \frac{\partial \boldsymbol{x}}{\partial \boldsymbol{\mathcal{X}}} \cdot \boldsymbol{w}$$

A HYBRID APPROACH: ARBITRARY LAGRANGIAN-EULERIAN FRAME OF REFERENCE

Let us now consider the description of a property in the ALE frame of reference:

$$\gamma_{ALE}(\boldsymbol{\mathcal{X}}(\boldsymbol{X},t),t)$$

and its material derivative:

$$material\ derivative\ \coloneqq \frac{d}{dt}\gamma_{ALE}(\boldsymbol{\mathcal{X}}(\boldsymbol{X},t)) = \frac{\partial \Gamma(\mathbf{X},\mathrm{t})}{\partial t}$$

$$\frac{d}{dt}\gamma_{ALE}(\boldsymbol{\mathcal{X}}(\boldsymbol{X},t),t) = \frac{\partial \gamma_{ALE}(\boldsymbol{\mathcal{X}},t)}{\partial t} + \frac{\partial \gamma_{ALE}}{\partial \boldsymbol{\mathcal{X}}}\cdot \boldsymbol{w} = \frac{\partial \gamma_{ALE}(\boldsymbol{\mathcal{X}},t)}{\partial t} + \frac{\partial \gamma}{\partial \boldsymbol{x}}\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{\mathcal{X}}}\cdot \boldsymbol{w}$$
$$= \frac{\partial \gamma_{ALE}(\boldsymbol{\mathcal{X}},t)}{\partial t} + (\boldsymbol{v}-\boldsymbol{v}_{MESH})\cdot \nabla\gamma(\boldsymbol{x},t)$$

The first term is evaluated at the mesh points:

$$\frac{\partial \gamma_{ALE}(\boldsymbol{\mathcal{X}},t)}{\partial t}$$

If we discretize in time, we can compute this time derivative as the difference between values of the property at the moving mesh nodes

The second term is evaluated at the spatial coordinates.

$$(\boldsymbol{v}-\boldsymbol{v}_{MESH})\cdot \nabla\gamma(\boldsymbol{x},t) = \boldsymbol{c}\cdot \nabla\gamma(\boldsymbol{x},t)$$

We can integrate it over the deformed mesh.

A HYBRID APPROACH: ARBITRARY LAGRANGIAN-EULERIAN FRAME OF REFERENCE

Conservation equations in ALE form

Mass balance equation:

$$\frac{\partial \rho_{ALE}(\boldsymbol{X}, t)}{\partial t} + \boldsymbol{c} \cdot \nabla \rho(\boldsymbol{x}, t) = -\rho \nabla \cdot \boldsymbol{u}(\boldsymbol{x}, t)$$

Momentum conservation equation:

$$\frac{\partial \boldsymbol{u}_{ALE}(\boldsymbol{X}, t)}{\partial t} + \boldsymbol{c} \cdot \nabla \boldsymbol{u}(\boldsymbol{x}, t) = \nabla \cdot \boldsymbol{\sigma}(\boldsymbol{x}, t) + \rho(\boldsymbol{x}, t)\boldsymbol{b}(\boldsymbol{x}, t)$$

Energy conservation equation:

$$\rho(\boldsymbol{x}, t)\left[\frac{\partial E_{ALE}(\boldsymbol{X}, t)}{\partial t} + \boldsymbol{c} \cdot \nabla E(\boldsymbol{x}, t)\right] = \nabla \cdot \left(\boldsymbol{\sigma}(\boldsymbol{x}, t) \cdot \boldsymbol{u}(\boldsymbol{x}, t)\right) + \boldsymbol{u}(\boldsymbol{x}, t) \cdot \rho(\boldsymbol{x}, t)\boldsymbol{b}(\boldsymbol{x}, t)$$

A HYBRID APPROACH: ARBITRARY LAGRANGIAN-EULERIAN FRAME OF REFERENCE

Integral form of ALE conservation equations

The Reynolds transport theorem applied to an arbitrary volume (not a control volume, nor a material volume), which moves with velocity $\boldsymbol{v}_{MESH}$ is:

$$\frac{\partial}{\partial t}\Big|_x \int_{V_t} f(\boldsymbol{X},t)dV = \int_{V_t} \frac{\partial}{\partial t} f(\boldsymbol{x},t)dV + \int_{\partial V} f(\boldsymbol{x},t)\boldsymbol{v}_{MESH}\cdot \boldsymbol{n}dS$$

Setting $f = \rho$ we get:

$$\frac{\partial}{\partial t}\Big|_x \int_{V_t} \rho(\boldsymbol{X},t)dV = \int_{V_t} \frac{\partial}{\partial t} \rho(\boldsymbol{x},t)dV + \int_{\partial V} \rho(\boldsymbol{x},t)\boldsymbol{v}_{MESH}\cdot \boldsymbol{n}dS =$$

$$= -\int_{V_t} \nabla\cdot\big(\rho(\boldsymbol{x},t)\boldsymbol{u}(\boldsymbol{x},t)\big)dV + \int_{\partial V} \rho(\boldsymbol{x},t)\boldsymbol{v}_{MESH}\cdot \boldsymbol{n}dS =$$

$$\int_{\partial V} \rho(\boldsymbol{x},t)(\boldsymbol{v}_{MESH}-\boldsymbol{v})\cdot \boldsymbol{n}dS = -\int_{\partial V} \rho(\boldsymbol{x},t)\boldsymbol{c}\cdot \boldsymbol{n}dS$$

$$\boxed{\frac{\partial}{\partial t}\Big|_x \int_{V_t} \rho(\boldsymbol{X},t)dV + \int_{\partial V} \rho(\boldsymbol{x},t)\boldsymbol{c}\cdot \boldsymbol{n}dS = 0}$$

A HYBRID APPROACH: ARBITRARY LAGRANGIAN-EULERIAN FRAME OF REFERENCE

Integral form of ALE conservation equations

We can do the same for the momentum and energy balance equations:

Momentum balance equation:

$$\frac{\partial}{\partial t}\Big|_{\chi}\int_{V_t}\rho\boldsymbol{u}(\boldsymbol{\chi},t)dV+\int_{\partial V}\rho(\boldsymbol{x},t)\boldsymbol{u}(\boldsymbol{x},t)\boldsymbol{c}\cdot\boldsymbol{n}dS=\int_{V_t}\left(\nabla\cdot\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{t})+\boldsymbol{\rho}(\boldsymbol{x},t)\boldsymbol{b}(\boldsymbol{x},t)\right)dV$$

Energy balance equation:

$$\frac{\partial}{\partial t}\Big|_{\chi}\int_{V_t}\rho E(\boldsymbol{\chi},t)dV+\int_{\partial V}\rho(\boldsymbol{x},t)E(\boldsymbol{x},t)\boldsymbol{c}\cdot\boldsymbol{n}dS$$
$$=\int_{V_t}\left(\nabla\cdot(\boldsymbol{\sigma}(\boldsymbol{x},\boldsymbol{t})\cdot\boldsymbol{u}(\boldsymbol{x},t)+\cdot\,\boldsymbol{u}(\boldsymbol{x},t)\boldsymbol{\rho}(\boldsymbol{x},t)\boldsymbol{b}(\boldsymbol{x},t)\right)dV$$

MESH MOVEMENT

We do already have a formulation which allows us to write the continuum mechanics equations in a frame of reference which evolves in time (ALE frame of reference.

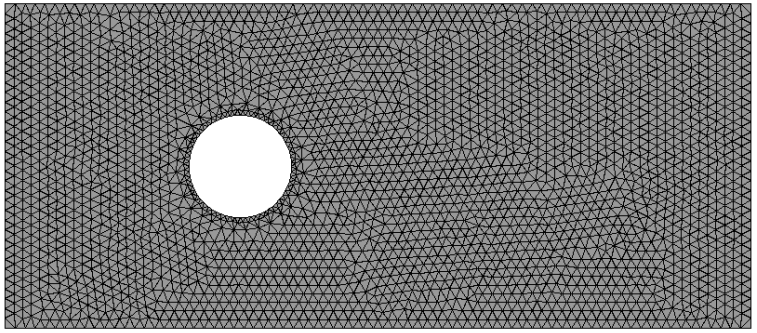
The definition of the mesh movement

The mesh movement must fulfill the following requirements:

- In some boundaries of the domain, it must follow the movement of the particles in the boundaries (Lagrangian boundary)
- In some boundaries of the domain, it must remain static (Eulerian boundary)
- In the interior of the domain, the mesh movement must be such that the shapes of the elements do not get excessively distorted (avoid and increase of the numerical approximation error).

The movement in the Lagrangian boundary can be prescribed a priori, or it can be the result of a couple problem computation (Fluid-structure interaction, free surface flows).

MESH MOVEMENT



MESH MOVEMENT

There are several possibilities for computing the mesh displacements

The boundary conditions are:

$$\boldsymbol{d}_{MESH} = \boldsymbol{d}_L \quad in\ \Gamma_{LAGRANGIAN}$$

$$\boldsymbol{d}_{MESH} = \boldsymbol{0} \quad in\ \Gamma_{EULERIAN}$$

In the interior of the domain, various problems can be solved. For instance:
Poisson problem:

$$-\Delta \boldsymbol{d} = \boldsymbol{0} \quad in\ \Omega$$

An Elasticity problem:

$$\boldsymbol{K}\boldsymbol{d} = \boldsymbol{0} \quad in\ \Omega$$

Different properties can be assigned to different areas of the domain. The objective is always to avoid mesh distortion, because the error of the finite element analysis is related to the shape of the elements.

MESH MOVEMENT

Geometric conservation law

The geometric conservation law responds to the requirement that the ALE formulation must be capable of solving the problem of a uniform flow.

Departing from the mass balance, and assuming uniform velocity and density distribution, we arrive to:

$$\frac{\partial}{\partial t}\Big|_{\boldsymbol{x}} \int_{V_t} dV + \int_{\partial V} \boldsymbol{v}_{MESH} \cdot \boldsymbol{n} dS = 0$$

If we integrate this in time, and we focus in each element in step *n* to step *n+1*:

$$|\Omega_e^{n+1}| - |\Omega_e^n| = \int_{t^n}^{t^{n+1}} \left(\int_{\partial V} \boldsymbol{v}_{MESH} \cdot \boldsymbol{n} dS \right) dt$$

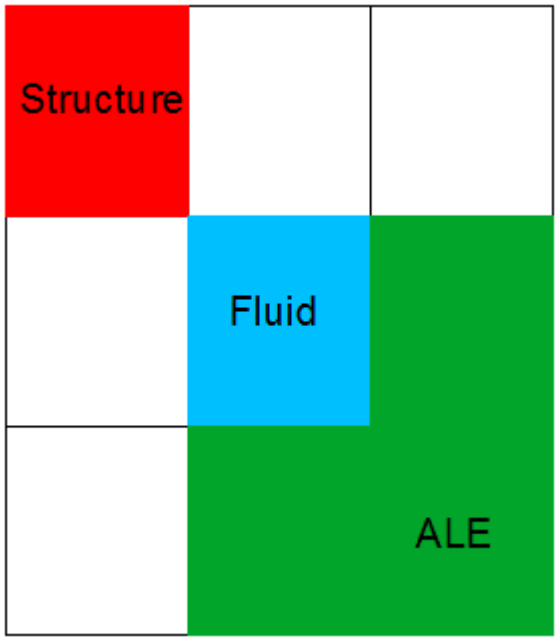
This imposes some restrictions to the update procedure for grid position and velocity. For first order time integrators:

$$\boldsymbol{v}_{MESH}^{n+1/2} = (d_{MESH}^{n+1} - d_{MESH}^{n})/\delta t$$

MESH MOVEMENT

Geometric conservation law

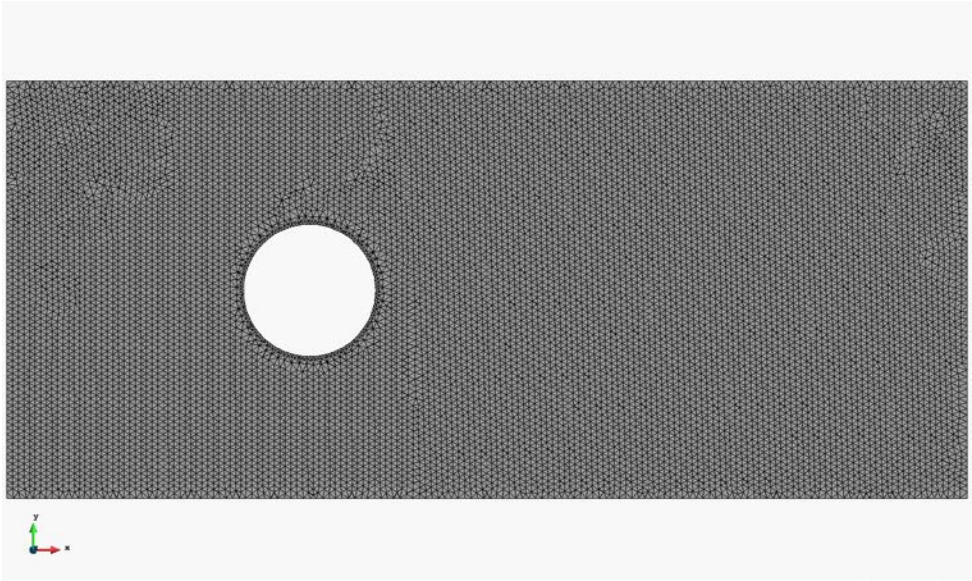
Particularly, for fluid structure interaction, this would mean that a coupled problem with 3 unknowns needs to be solved:



Usually this can be expensive and a semiexplicit partitioned scheme (no geometric conservation law!) is adopted.

MESH MOVEMENT

However, it is not always possible to avoid mesh distorsion, if displacements are too large:



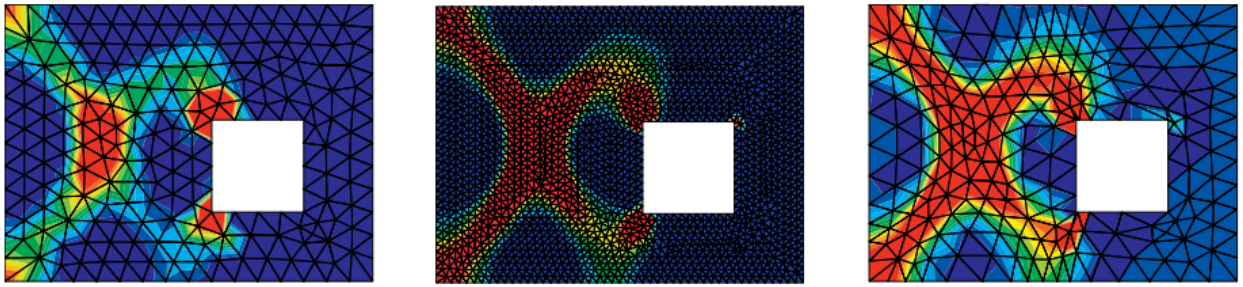
In this case it is necessary to remesh after a number of time steps.

After remeshing, all the results need to be projected onto the new mesh.

MESH ADAPTIVITY

ALE formulations can also be used to obtain mesh adaptivity, even if the physical domain does not evolve in time.

It allows to concentrate more elements in areas where the error is larger (an error estimator is required).



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