Computational Models for the Analysis of positive displacement machines: Real Gas and Dynamic Mesh

4th International seminar on ORC Power Systems

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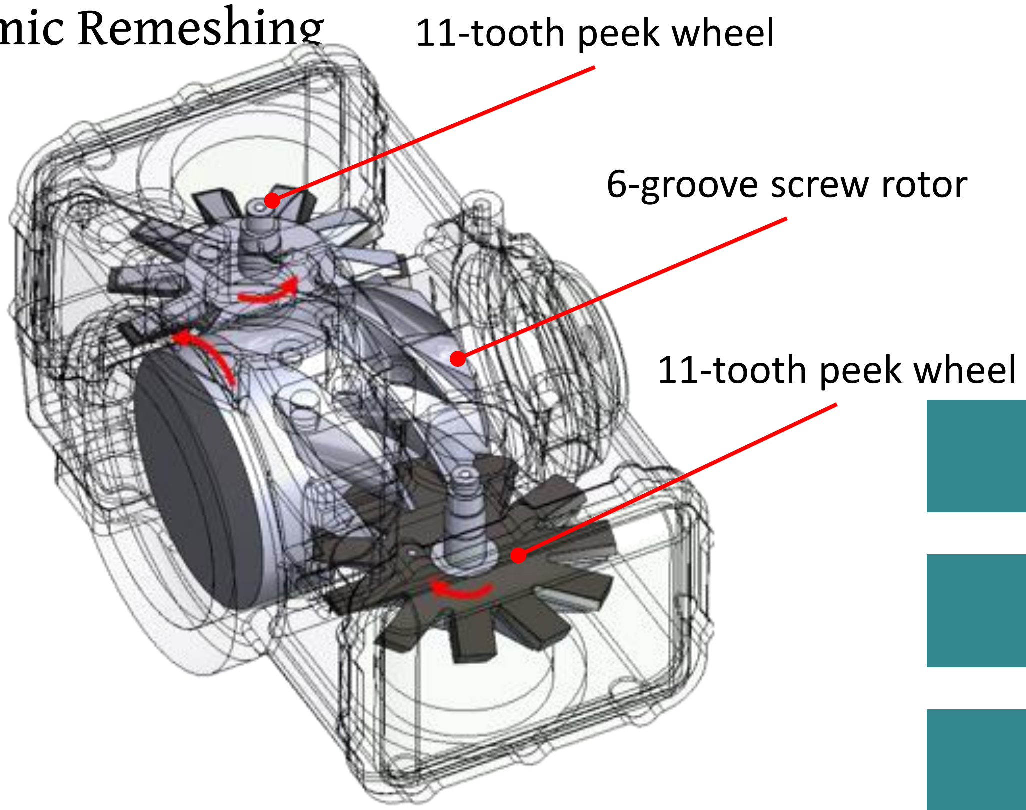
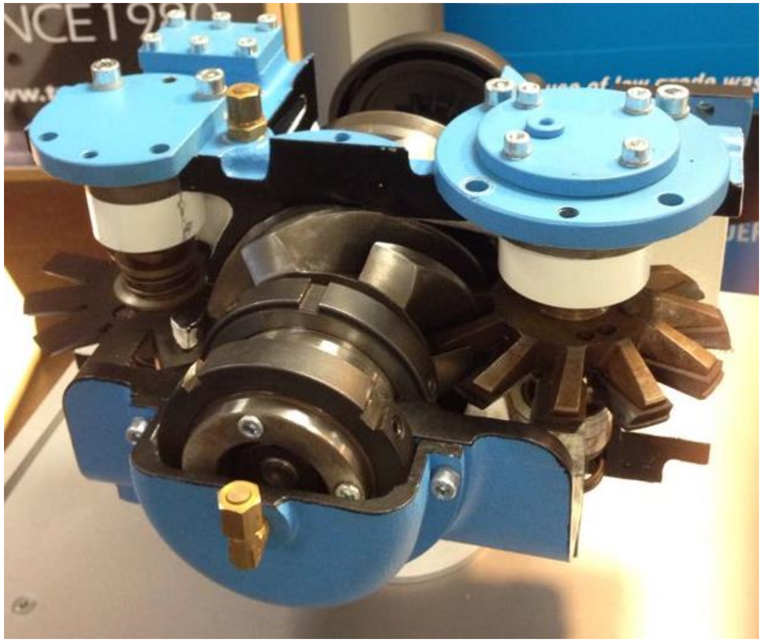
Outline

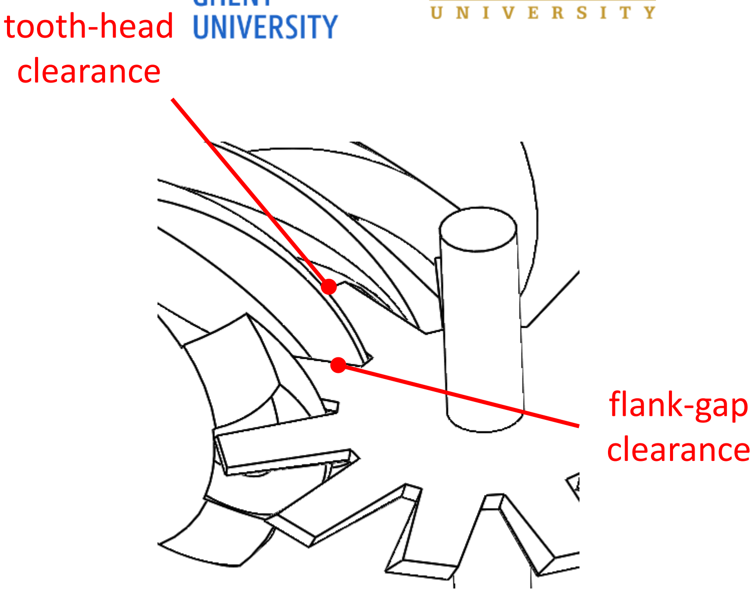
- Introduction
- Available mehtods
  - Immersed Boundary Method
  - Mesh Adaption - Dynamic Remeshing
  - Key Frame Remeshing
- Real Gas model
- Test Case: Results
- Conclusion

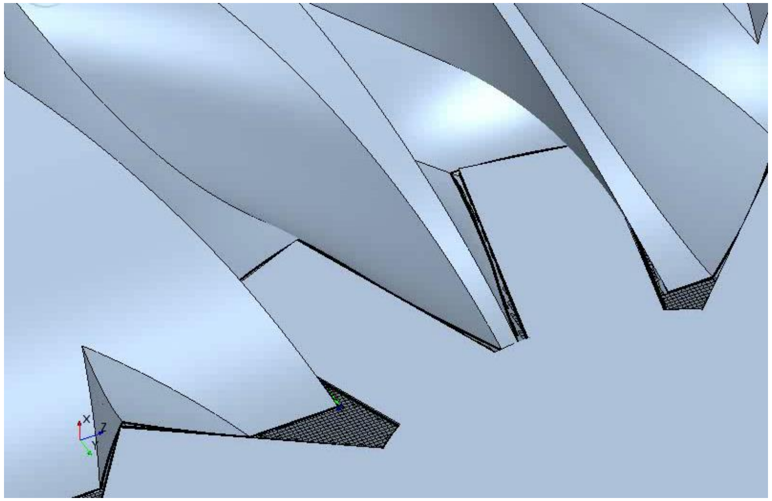


Single Screw Expanders

- Balanced loading on the main rotor
- Wide range of operation







Work aim

- This work is intended to be a review of the available methods in the most used Open source CFD software for the simulation of SSEs
- OpenFOAM: three main branches
  - foam –extend 4.0
  - OpenFOAM-v1606+
  - openfoam - 5

Numerical strategy: Immersed Boundary Method

Numerical strategies: IBM

- Immersed boundary method
  - Available only in the foam-extend suite (3.2 onwards)
  - Features
    - CANNOT be employed for the solution of compressible flows as is

✓ Moving boundaries support

✓ Turbulence support

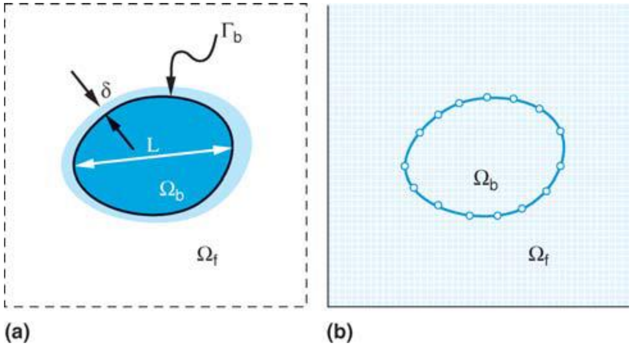
✗ Compressible flows support

IBM: Numerics (1/2)

- **Flow around immersed boundary on a Cartesian grid not conforming to the geometric boundary**
- Grid does not conform to the solid boundary

IMPOSING BC IMPLIES TO MODIFY THE EQUATIONS

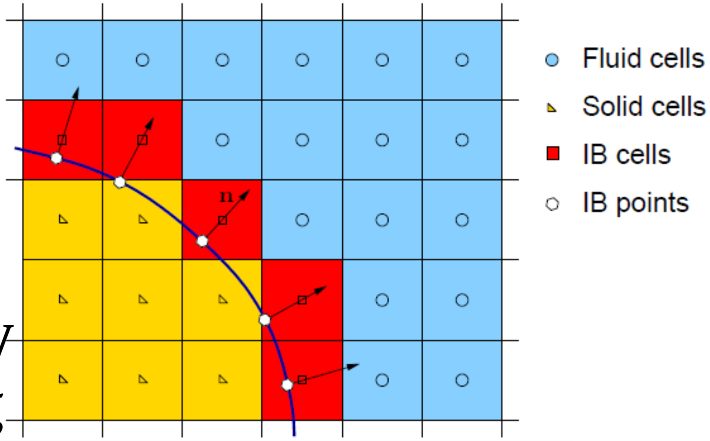
- Two possibilities:
  - **CONTINUOUS FORCING APPROACH** — Force term added before discretization
  - **DISCRETE FORCING APPROACH** — Force term added after discretization



IMMERSED BOUNDARY METHODS
Mittal, R. and Iaccarino, G.

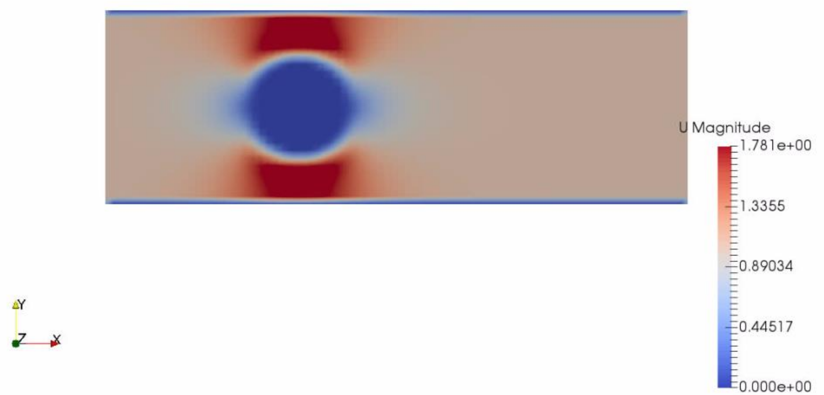
IBM: Numerics (2/2)

- Implementation in foam-extend
  - Discrete forcing approach and direct imposition of boundary conditions
  - Value of dependent variable in the IB cell centres is calculated by interpolation using neighbouring cells values and boundary condition at the corresponding IB point



IMMERSED BOUNDARY METHOD IN FOAM
THEORY, IMPLEMENTATION AND USE
Hrvoje Jasak and Zeljko Tukovic

IBM: Test case



Final remarks on the IBM

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- ✗ Poor resolution of the boundary layer (geometry not aligned with grid lines)
- ✗ Not suitable for detailed fluid dynamics
- ✓ Low computational effort
- ✓ Design phase

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Numerical strategy: Mesh Adaption – Dynamic Remeshing

Numerical Strategy: MADR Mesh Adaption - Dynamic Remeshing

- Comes with the foam-extend suite
- Libraries easily linkable to the other version of OpenFOAM (Less reliable after v 2.3.x)
- Extension of the standard dynamic mesh classes
- **Dynamic mesh & Local re-meshing if the quality falls below a threshold**

MADR: Numerics

- The entire process is divided in three steps:
  1. Mesh Smoothing
  2. Mesh Reconnecting
  3. Solution Remapping

1. Mesh Smoothing

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- Mesh Quality kept as high as possible
- No changes in connectivity
- Local re-meshing requirements delayed
- A wrapper class of the Mesquite optimization library is available

USING THE DYNAMICTOPOFVMESH CLASS IN OPENFOAM
S. Menon
PARALLEL DYNAMIC SIMPLICAL MESHES IN OPENFOAM
D.P. Smith
THE MESQUITE MESH QUALITY IMPROVEMENT TOOLKIT
M. L. Brewer

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2. Mesh Reconnecting

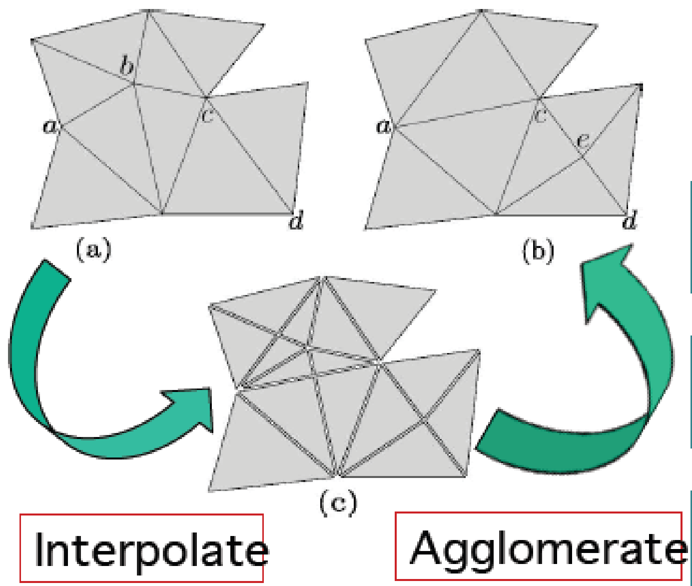
- Handles excessive distortion
- Acts when mesh-deformation mechanisms are insufficient
- Local, in order to reduce interpolation errors
- Refinement based on
  - Mesh quality
  - Length scale
    - Automatic
    - Fixed
  - Field value

3. Solution remapping

- SuperMesh: Old and New mesh are stored on a new mesh

The remapping is comprised of four steps:

- Computation of the intersections between the source and target mesh
- Computation and limitation of the gradients on the source mesh
- Volume and distance weighted Taylor series interpolate to superMesh
- Agglomeration on the target mesh



MADR: Meshing

- Only simplical cells can be handled
- Need for tetrahedral mesh generator
- Our open-source suggestions (all working on both UNIX and Windows OS):
  - CfMesh
  - Salome
  - GMsh

MADR: Test case

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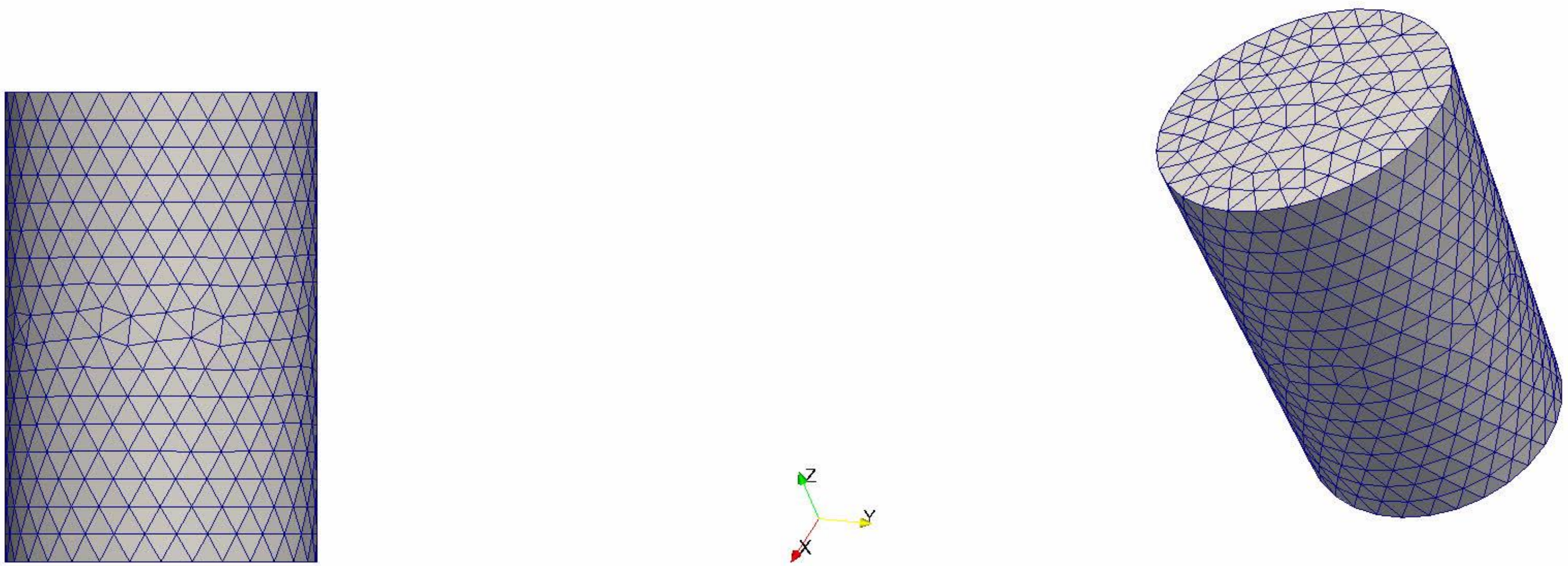
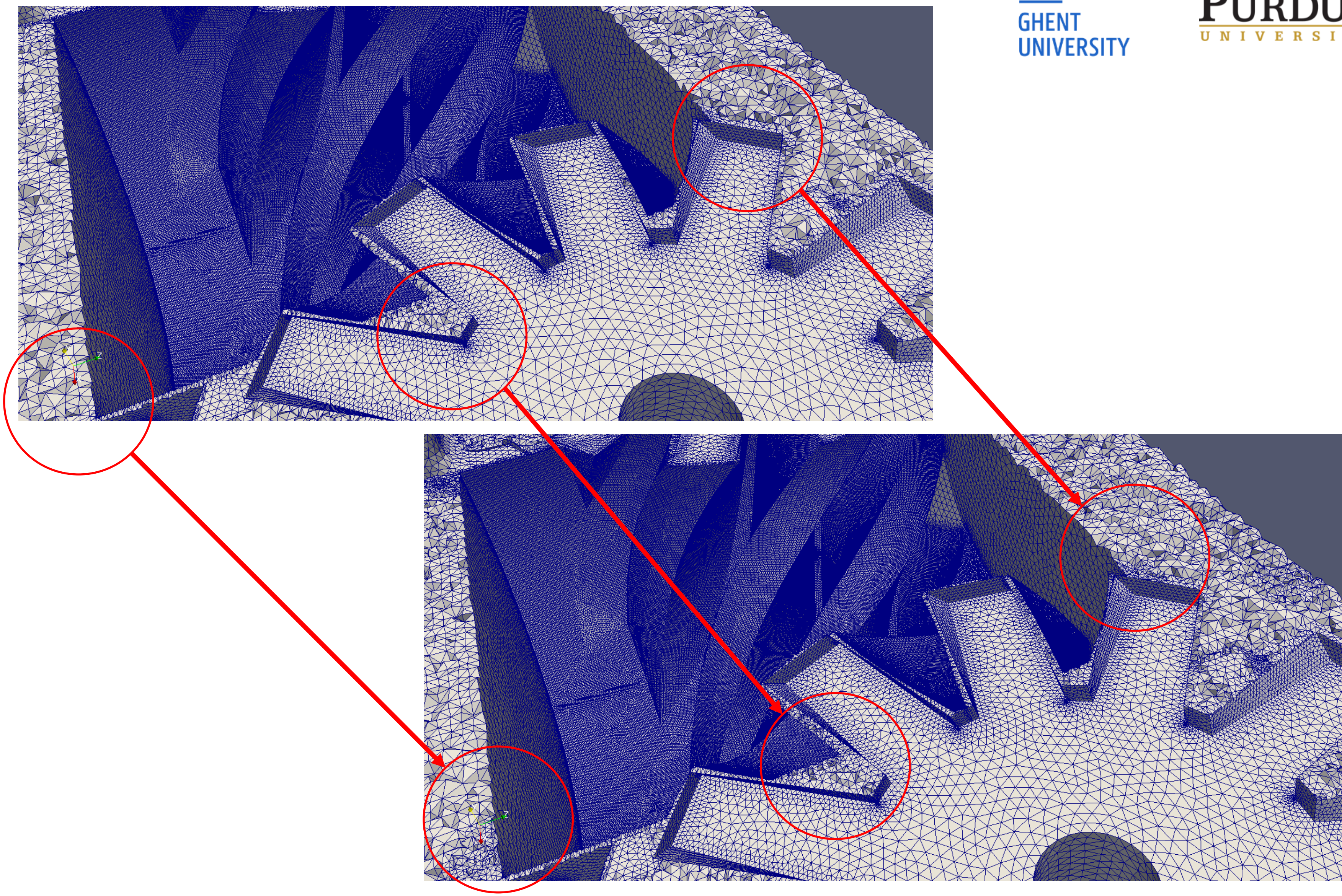


Application to SSE (1/2)



Application to SSE (2/2)

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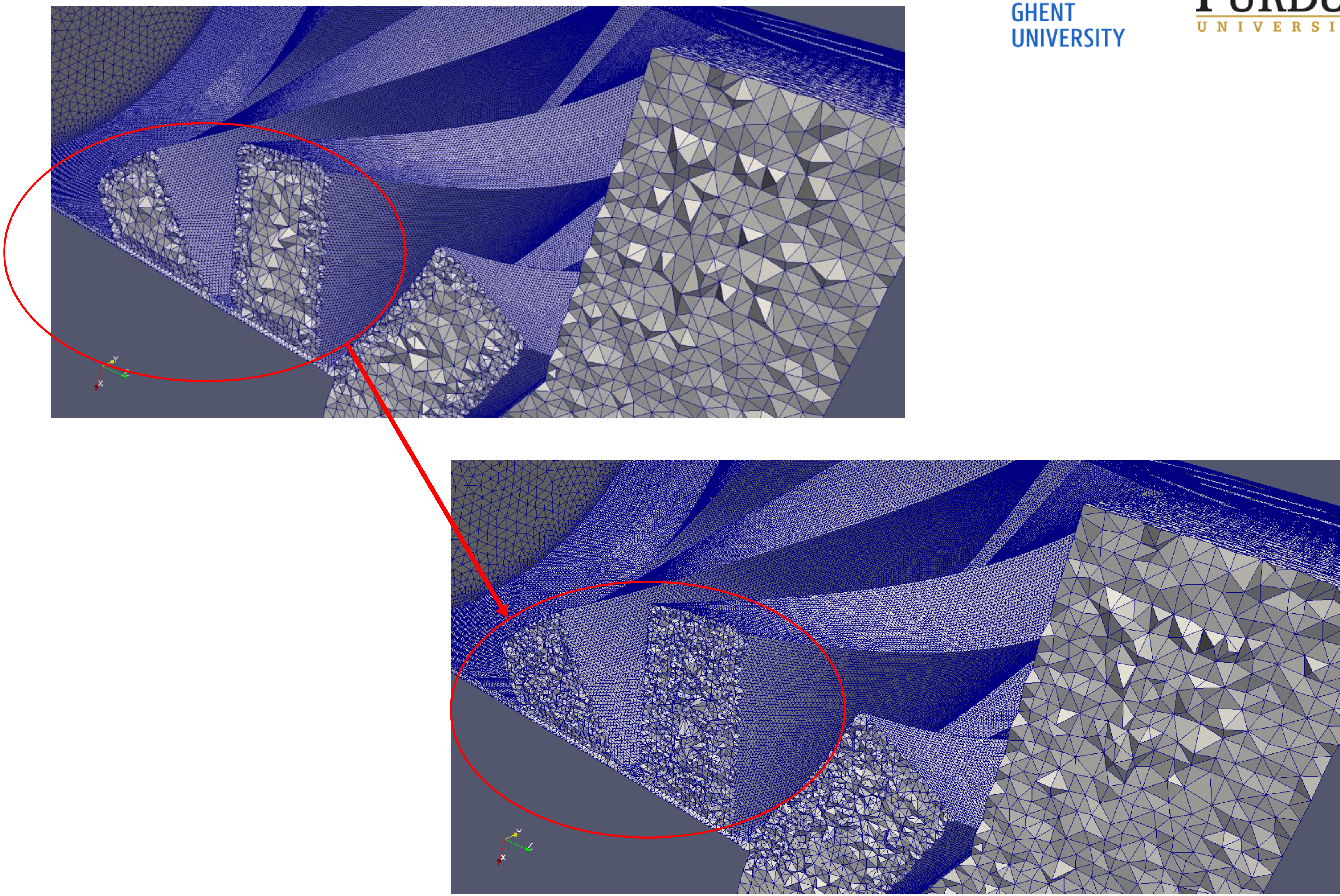


Final Remarks on the MADR

- ✓ Very fast and can handle very big mesh distortion
- ✓ Small error in mass conservation (re-meshing)

Drawbacks:

- ✗ The parallel redistribution is not very robust
- ✗ Simplical cells → no prismatic layers!!!
- ✗ Libraries not maintained any longer

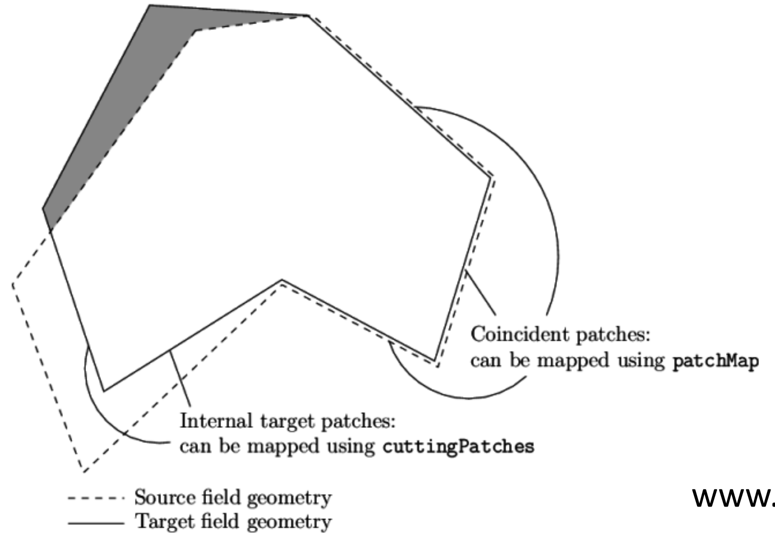
Numerical strategy: Key Frame Remeshing

Numerical strategies: KFR

- Key Frame Remeshing
  - Wrapper of OpenFOAM standard libraries
  - **Complete re-meshing of the geometry every time the quality falls below a threshold**
  - More time consuming than MADR but <u>ROBUST</u>

KFR: Usage

- The set of Meshes for the solution of the problem can be prepared in advance (or in parallel)
- Mesh passed to the solver Just In Time
- Mapping of the old solution
  onto the new "target" mesh



Final Remarks on the KFR

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- ✓ Can handle very big mesh distortion
- ✓ Safe and robust parallel redistribution
- ✓ BL can be solved in detail
- ✓ Mesh: Arbitrary (Cartesian, Tet or Poly)

Drawbacks:

- ✗ Very high computational effort (Mesh generation)
- ✗ Need a little bit of coding
- ✗ May have mass conservation errors

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Thermophysical properties Real Gases

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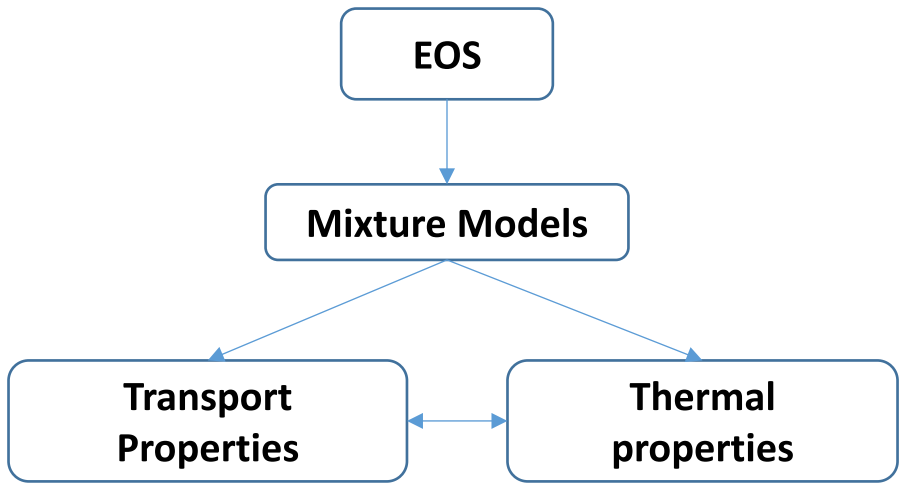
Thermophysical Models

- Required for building the physical properties of compressible flows.
- The first layer is the equation of state → p,T
- The other levels of the thermophysical modeling derive from the previous layer(s)



Section adapted from www.cfd.direct

Thermophysical Properties: EOS

- Close to the critical point molecule size must be taken into account
- Failing to do so (real gas model) can bring about errors in the performance of up to 15%
- Typically, Van der Waals type (cubic) EOS
  - ARK
  - SRK
  - RK
  - PR

Thermophysical Properties: EOS

- Lower level of complexity
  - *Perfect Gas*

$$\rho = \frac{p}{RT}$$

  - *Adiabatic perfect Gas*

$$\rho = \rho_0 \left(\frac{p + B}{p_0 + B} \right)^{1/\gamma}$$

  - *Boussinesq*

$$\rho = \rho_0 [1 - \beta (T - T_0)]$$

Thermophysical Properties: Mixture Models

- Model classes:
  - *psiThermo*
    - Model for fixed composition, based on compressibility $\psi = (RT)^{-1}$
    - Suitable for big pressure variations
    - **To be used for SSEs and positive displacement machines**
    - No multiphase support (no phase transformation allowed)

Thermophysical Properties: Mixture Models

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- Model classes:
  - psiThermo
  - *rhoThermo*
    - Model for fixed composition, based on density
    - Suitable for mild pressure variations
    - **To be used for heat exchangers**
    - No multiphase support (no phase transformation allowed)

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Thermophysical Properties: Mixture Models

- Model classes:
  - psiThermo
  - rhoThermo
  - psiReactionThermo
  - psiuReactionThermo
  - rhoReactionThermo
  - multiphaseMixtureThermo

Thermophysical quantities: Transport Models (μ, κ, α)

- *Constant*

  Constant μ and $Pr = cp\,\mu/\kappa$

- *Sutherland (only for μ)*

  $\mu = f(T)$, known A_s and T_s (Sutherland coefficients)

$$\mu = \frac{A_s\sqrt{T}}{1 + {T_s}/{T}}$$

- *Polynomial*

  $\mu = f(T)$, $\kappa = f(T)$ as polynomial of order N ($N \leq 8$)

$$\mu = \sum_{i=0}^{N-1} a_i T^i$$

- *logPolynomial*

  $\ln(\mu) = f(\ln(T))$, $\ln(\kappa) = f(\ln(T))$ as polynomial of order N ($N \leq 8$)

$$\ln(\mu) = \sum_{i=0}^{N-1} a_i [\ln(T)]^i$$

Thermophysical quantities: Thermodynamic Models ($C_p \rightarrow h, s$)

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- *hConstant*

  Constant c_p and heat of fusion H_f

- *eConstant*

  Constant c_v and heat of fusion H_f

- *janaf*

  $c_p = f(T)$ from a set of coefficient from JANAF tables of thermodynamics.

  Two set of coefficients across above and below a common temperature T_c

$$c_p = R(((a_4 T + a_3)\, T + a_2)\, T + a_1)\, T + a_0$$

- *hPolynomial*

$$c_p = \sum_{i=0}^{N-1} a_i T^i$$

  $\mu = f(T)$, $\kappa = f(T)$ as polynomial of order N ($N \leq 8$)

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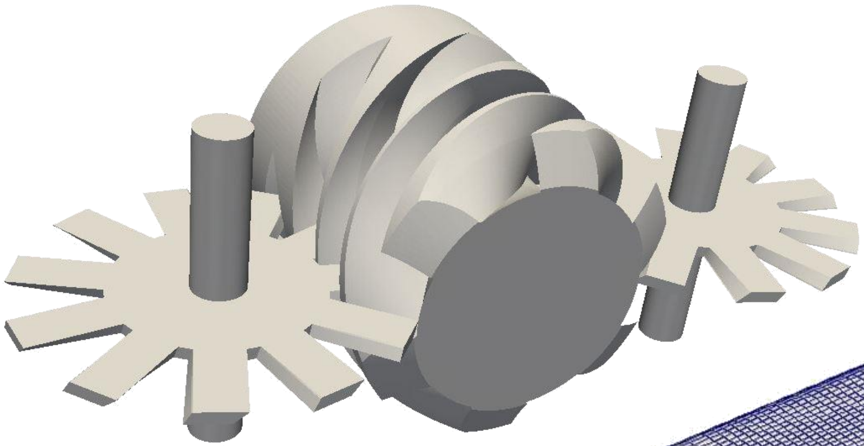
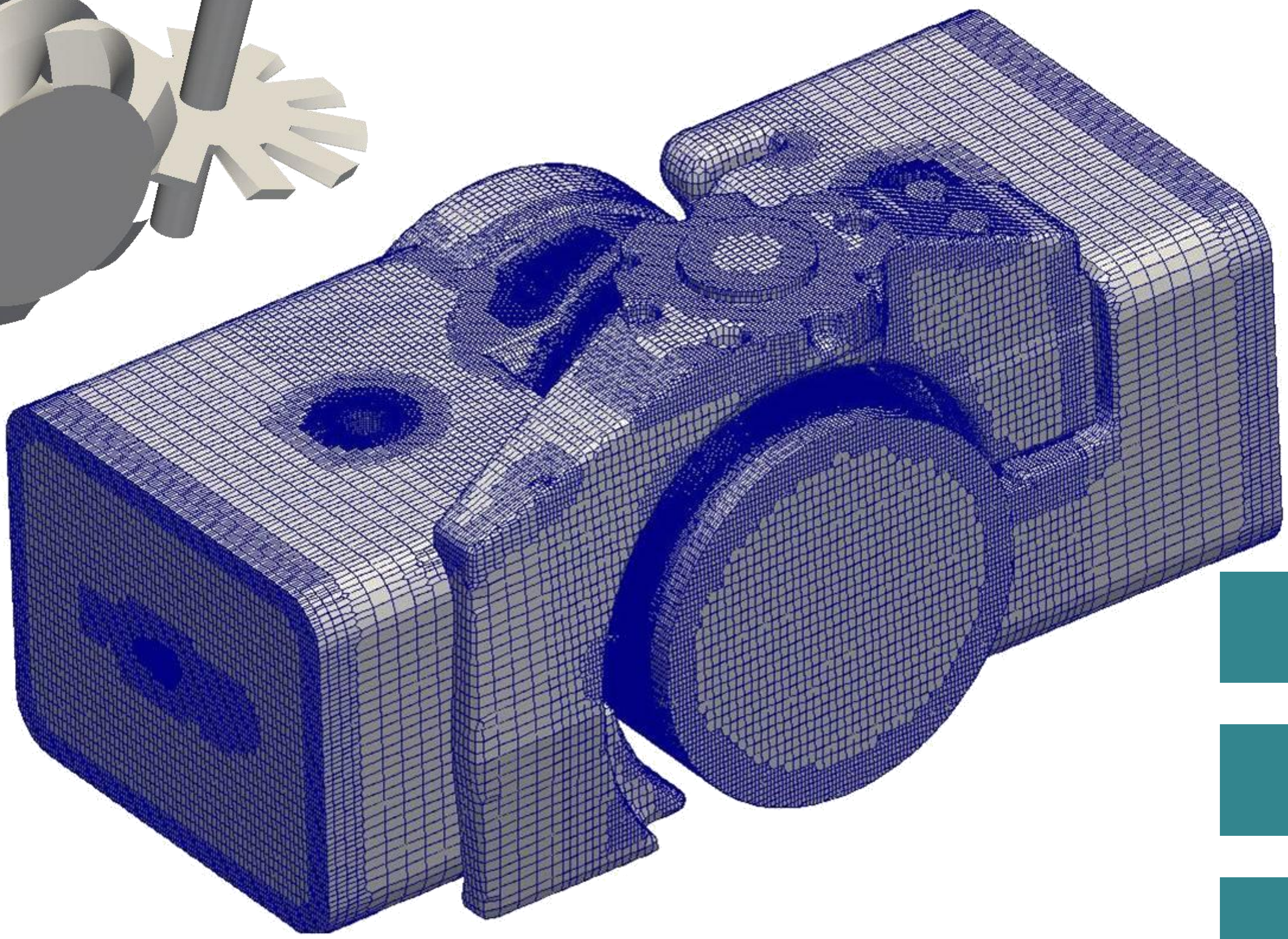
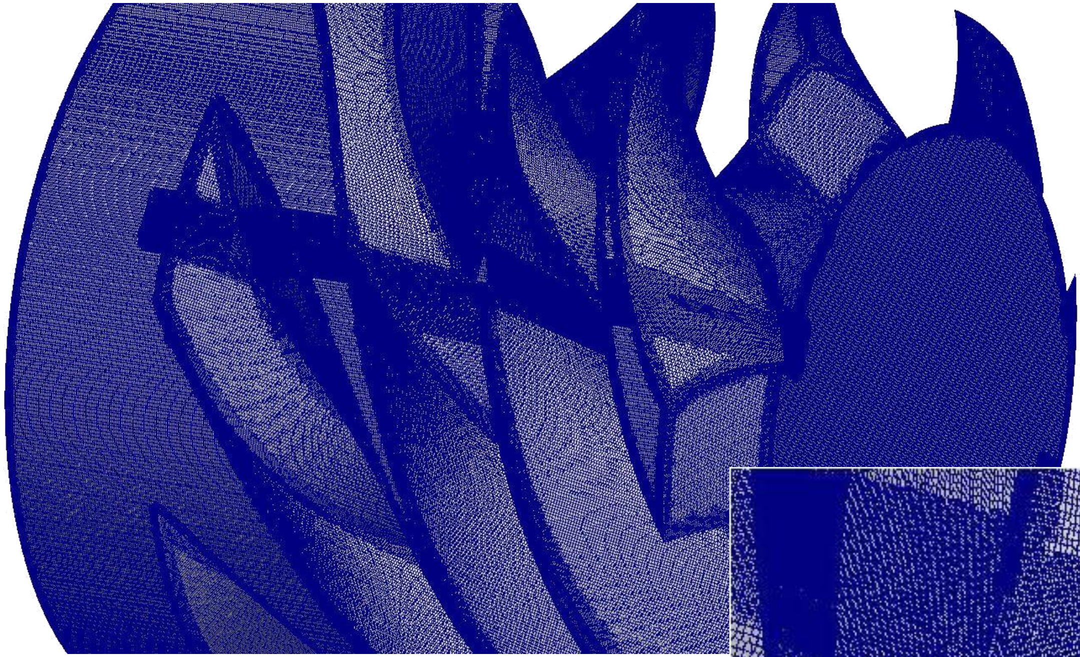
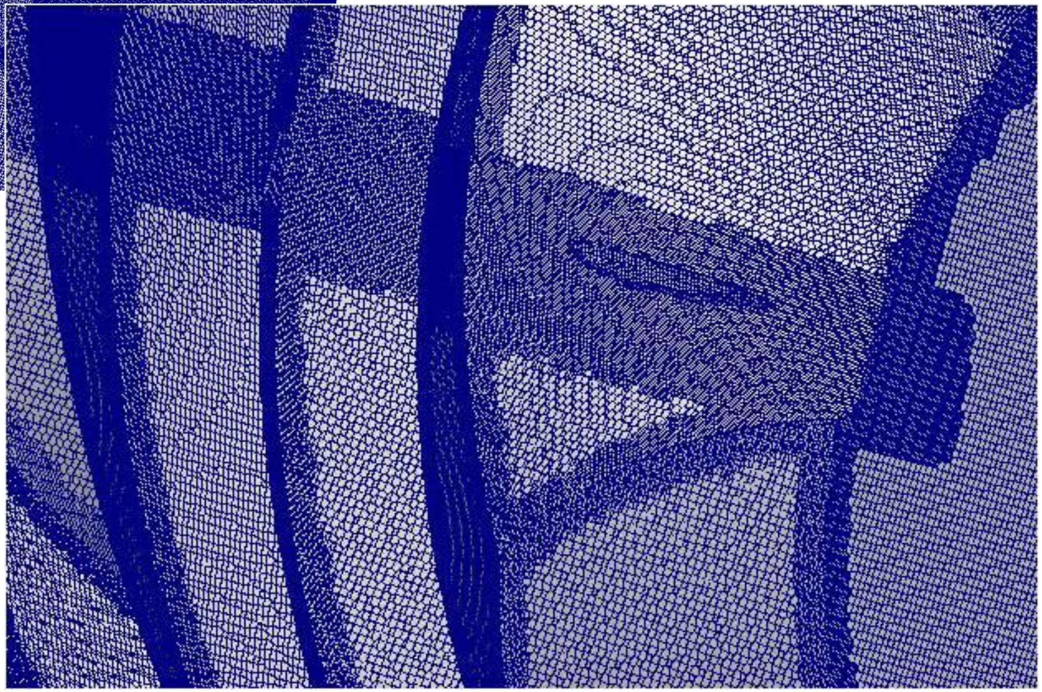
Test Case: Key – Frame remeshing





Test Case: Details





Test Case: Numerical set-up

- Compressible 3D Finite Volume Solver (with Dynamic Mesh support)
- Software: OpenFOAM – v1606+ (ESI get it right®)
- Real Gas model: Peng-Robinson
- $c_p(T)$ and $\mu(T)$ implemented via 8th degree polynomials

Quantity		Inlet	Outlet	Walls
Pressure		11 bar	6 bar	noGradient
Temperature		390 K	noGradient	adiabatic
Turbulent Quanties	k	Turbulent intensity: 10%	noGradient	Standard Wall function
	ε	Mixing length: 2×10^{-4} m	noGradient	Standard Wall function

Test Case: Preliminary Results

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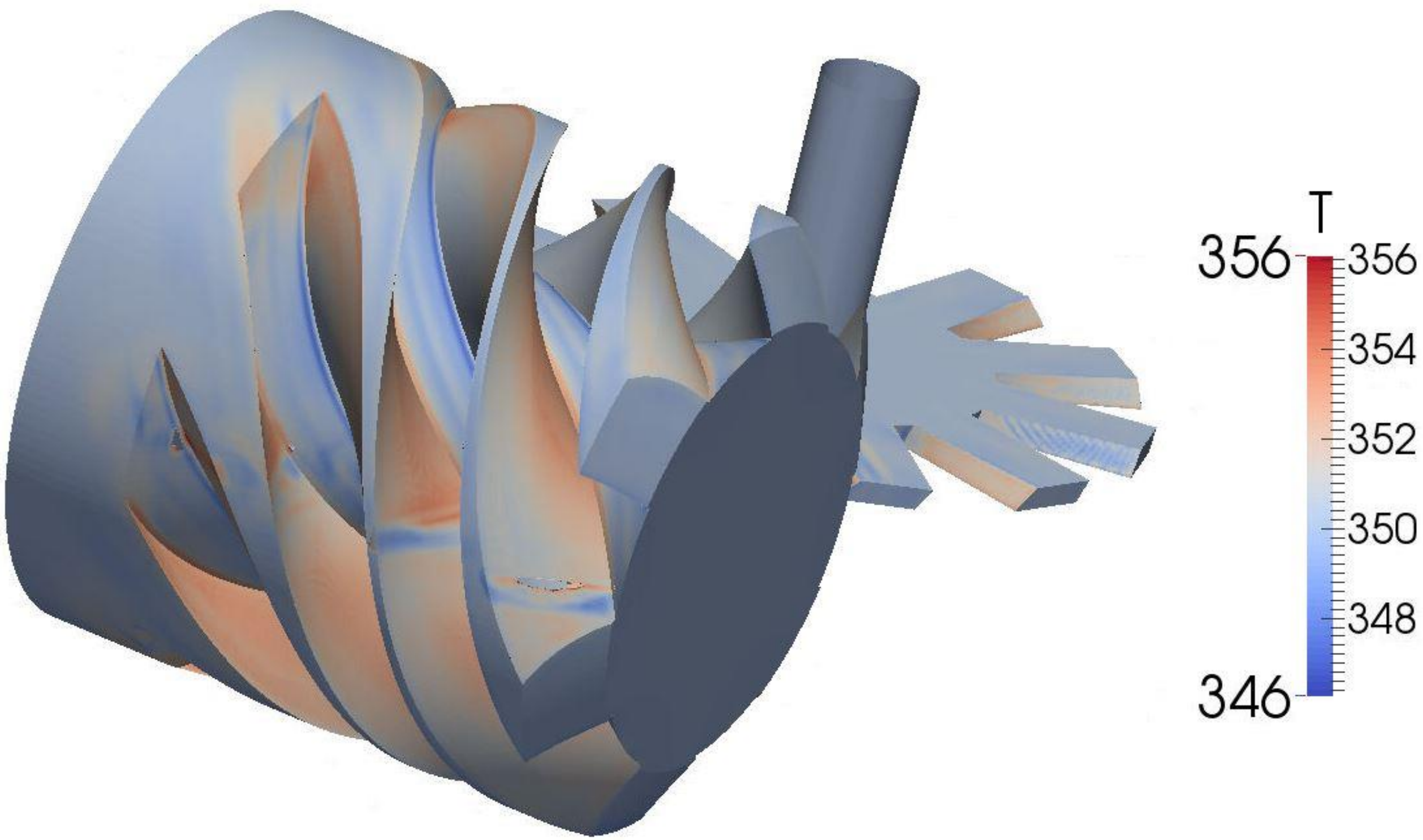

Future works

- Comparison among the results obtained with the other methods presented
- Overset solver
  - released with OpenFOAM – v1706 (July 2017,)
- Implementation of COOLPROP and validation with other real gases
- Experimental Campaign

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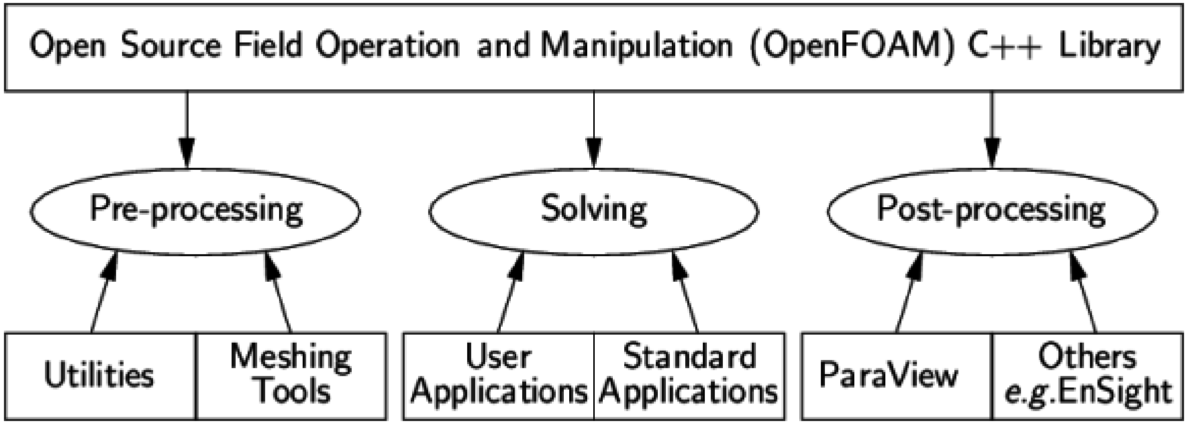
- Open Source Field Operation and Manipulation
- OpenFOAM is first and foremost a *C++ library*, used to create executables (*solvers* and *utilities)* designed to perform tasks that solve a specific problem in continuum mechanics or data manipulation.



Introduction to the software: Timeline