Workshop *"HPC enabling of OpenFOAM® for CFD applications"*
Cineca SuperComputing Applications and Innovation, Bologna (Italy) - April 6th-8th, 2016

Parallel Simulations of Compressible Flows in Moving Boundary Problems using a Scale-adaptive Turbulence Model

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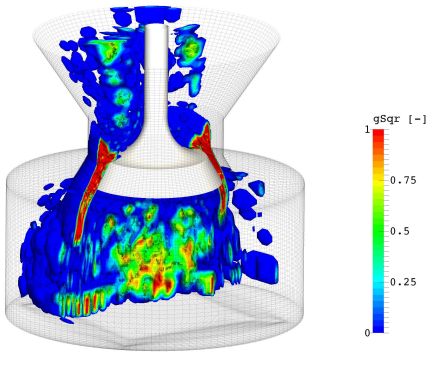
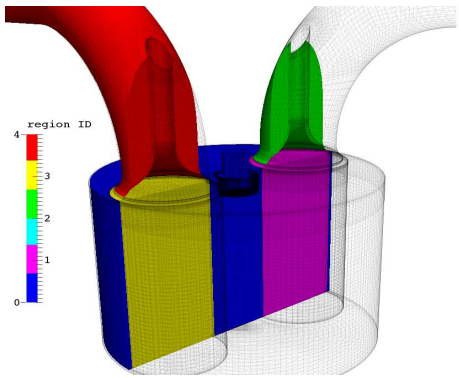
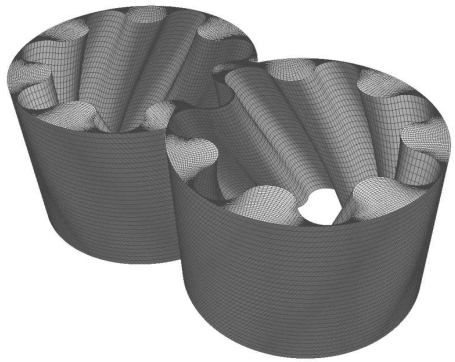
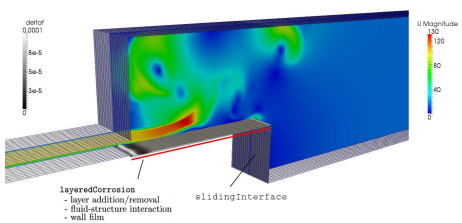
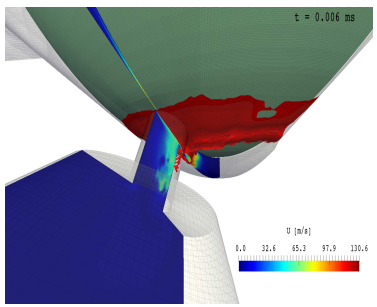
Motivation

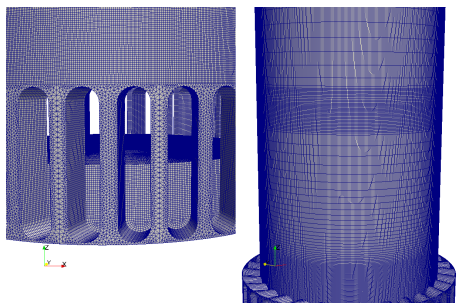












OBJECTIVE: *time-resolved simulation of turbulent flows with moving grids*

To begin with...

- **Parallel Automatic Mesh Motion with Topological Changes**
  - → SAE 2013-24-0027, LES4ICE-2012, IMEM 2013, IMEM 2014
    - implementation of `slidingInterface`, `attachDetach` into the releases of the software by the OpenFOAM® Foundation
  - → SAE 2015-01-0384
    - Improvements and extensions of the dynamic mesh class
    - run-time addition of user-defined moving components to existing motion solvers
  - → IMEM 2015 (`https://imem.cray.com/2015/agenda-2015.html`)
    - combined operation of topology modifiers with Arbitrary Mesh Interface (AMI)
    - novel compressible dynamic solver: `topoEngineFoam`
    - automatic decomposition with topological changes: `$SRC/parallel`
- **Time resolved turbulence modeling of wall-bounded flows**
  - → Computers&Fluids Vol. 93, Computers&Fluids Vol. 117, FTC-2015 Vol. 95(2)
    - LES of IC engines
  - → SAE Int. J. Engines 8 (2), pp. 426-436
    - Scale-adaptive hybrid RANS/LES turbulence modeling (DLRM model)

`dynamicMesh` class

Dynamic mesh handling is available and well established in the official version of OpenFOAM®:

- Grid points moved by means of an automatic mesh motion solver
- Mesh to mesh interpolation
- `AMI` (Arbitrary Mesh Interpolation)
- `layerAdditionRemoval` (basic features)

Implementation and operation of **dynamic mesh handling BASED ON TOPOLOGICAL CHANGES** is strictly dependent on the mesh handling strategy of the code:

- **foam-extend-3.1** (released by the *Extend Community*): *mesh definition contains all the topological changes performed during the simulation* as a set of faces, cells and points labeled as "inactive".

- **OpenFOAM** (released by the *OpenFOAM Foundation*): *mesh definition contains the topology of the current calculation only*. Additional information about the topological changes is stored separately $\rightarrow$ official releases by OpenCFD are not configured to allow for the decoupling of the mesh through an interface.

`dynamicMesh` class

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- Mesh to mesh interpolation
- `AMI` (Arbitrary Mesh Interpolation)
- `layerAdditionRemoval` (basic features)

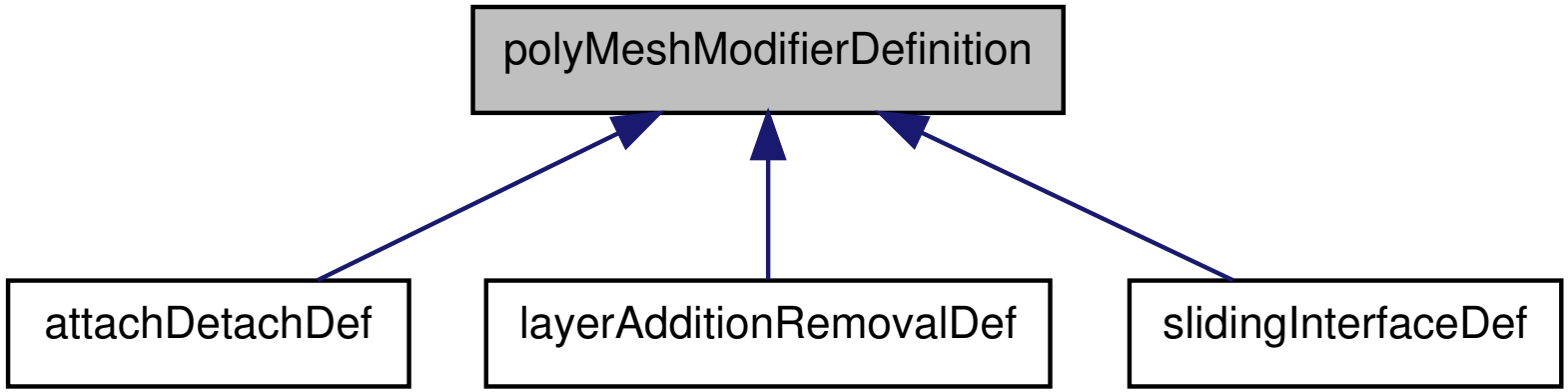
Author's choice: implementation compatible with OpenFOAM® by OpenCFD®

REQUESTED FEATURES:

- very general implementation → must be compatible:
  - to any distribution of OpenFOAM® (released by the Foundation) also for non-engine applications (spray nozzles, extAero, renewable energy, etc);
  - with any solver/application/utility (VOF, multiphase,...) already available in OpenFOAM®, without modifications.

NOTE: a *similar* theory (but completely different technology, implementation and operation) is available in *foam-extend-3.1*; **porting is not possible**.

`dynamicMesh` class: novel development



Topology modifiers

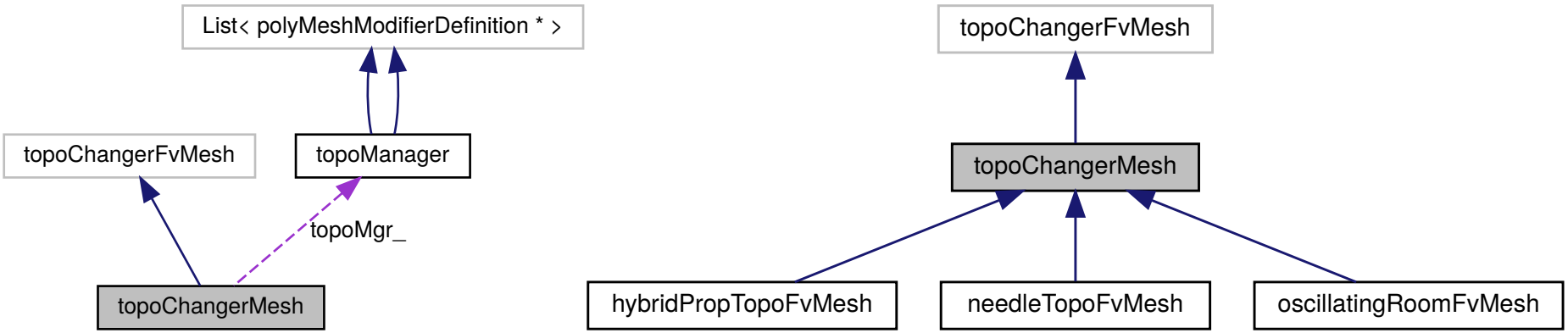
1. sliding interface
2. layer addition/removal
3. attach/detach boundary

Revised structure of the dynamic mesh class

- topological changes completely transparent to the mesh motion solver
- automatic *case setup* with topological changes
- `topoManager` class: very flexible and fully object-oriented implementation

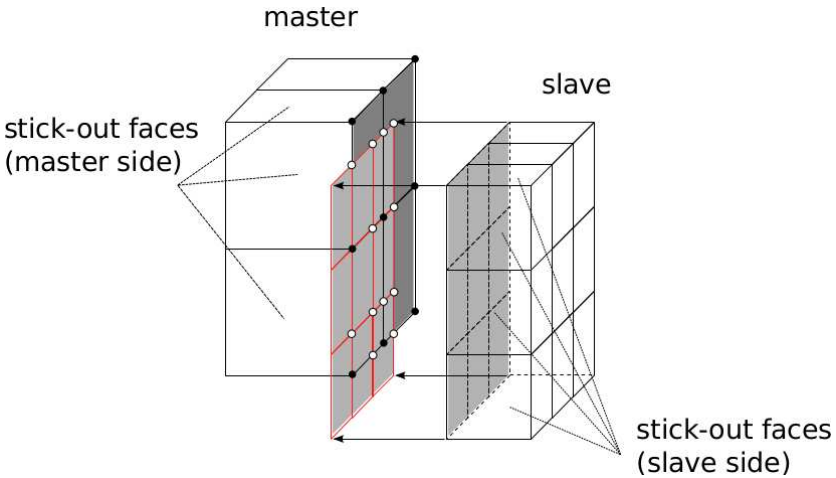
dynamicMesh class

INHERITANCE AND COLLABORATION



- management of topoChanges (definition, parallelization/synchronization, variables interpolation) implemented at low-level (class `topoManager`)
- `topoChangerMesh` class: any extension can be easily done by adding new physical components (needle)
- implementation of new 'components' requires only the **point motion law**
- mesh motion functionality supported by ALL the solvers of the code

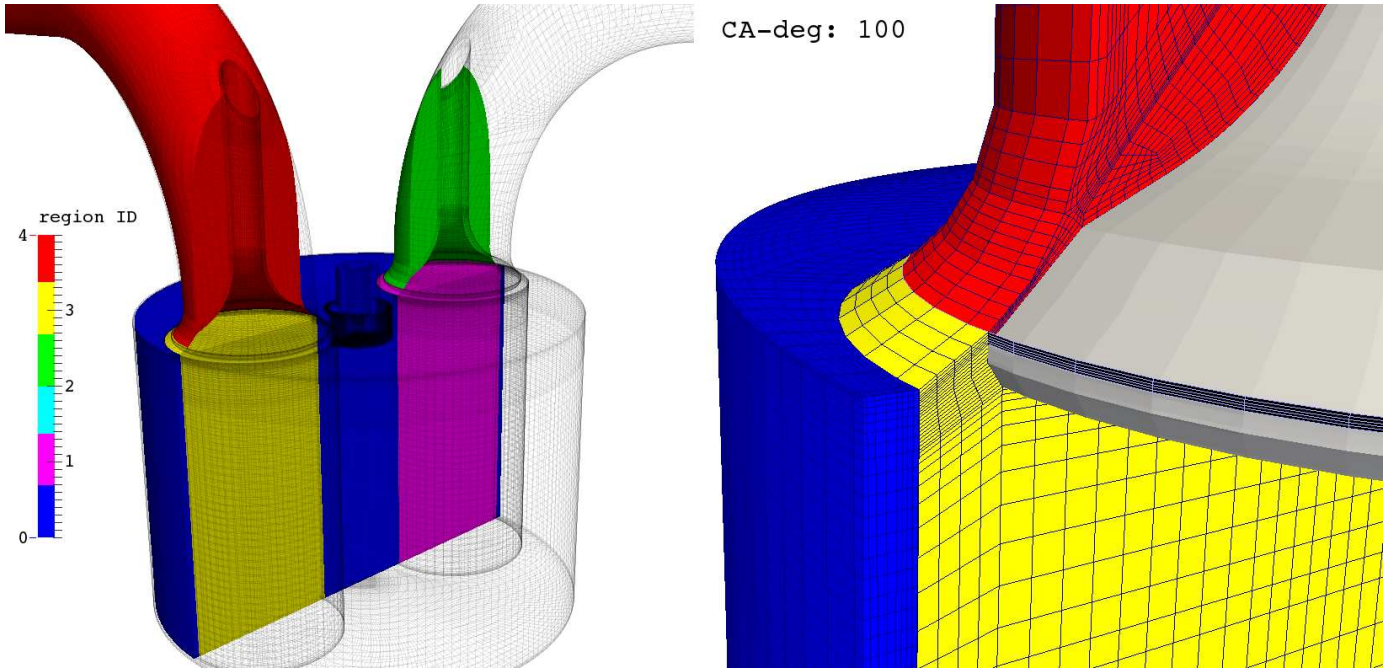
`dynamicMesh` class: extensions



- **TARGET MESH APPROACH** (`slidingInterface` → SAE 2015-01-0384[1]): coupling/decoupling of mesh regions based on polyhedral cells support.
  - updating the mesh topology updated anytime the algorithm operates;
  - no specific treatment for interpolation of fluid-dynamic quantities over the supermesh.
- **SUPERMESH APPROACH** (`AMI`): vertex-based solution using a bounded Galerkin projection over a virtual triangulated surface mesh
  - allows to avoid updates in mesh change every time step;
  - optimized solution with full overlap of fluid regions;

[1] Montorfano, A., Piscaglia, F., and Onorati, A., "An Extension of the Dynamic Mesh Handling with Topological Changes for LES of ICE in OpenFOAM®," **SAE Technical Paper 2015-01-0384**, 2015, doi:10.4271/2015-01-0384.

`dynamicMesh` class: example of application



- Combination of different methods to handle non-conformal interfaces (IMEM 2015) (significant increase of speed of the mesh motion):
  - valve opening closure $\rightarrow$ target-mesh approach (`attachDetach` based on `slidingInterface`)
  - sliding valve $\rightarrow$ supermesh approach (`AMI`)
- Integration of the two methodologies together with `layerAdditionRemoval` in one single fluid-dynamic solver (**consistent handling of face fluxes in a single solver not trivial!**)

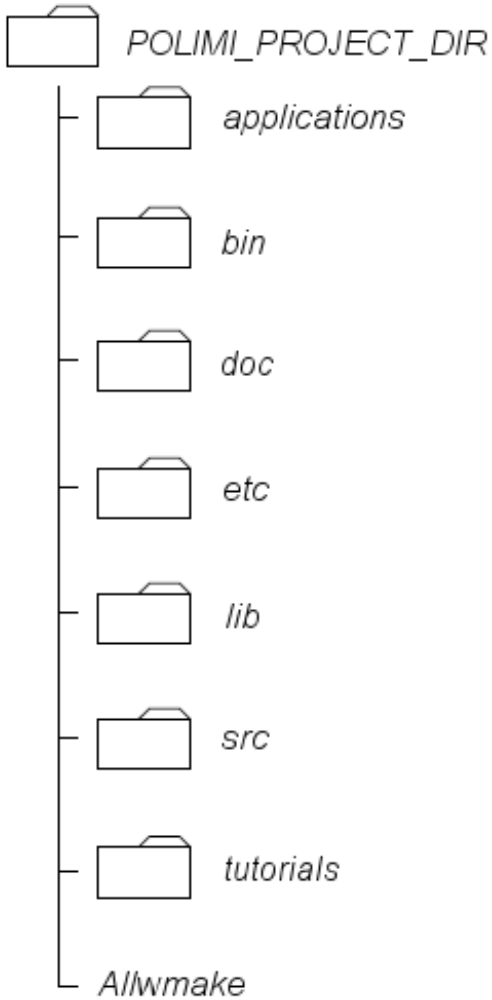
[1] A. Montorfano, F. Piscaglia et al. **SAE Technical Paper 2015-01-0384.**
[2] F. Piscaglia, A. Montorfano et al. **Int. Multidim. Engine Modeling Meeting 2015.** Downloadable at `https://imem.cray.com/`

Code development (April 2015-present)

- *Dynamic mesh with topological changes*
  - `layerAdditionRemoval`: conservation of intensive quantities with 2nd order discretization *in time*
  - `attachDetach`, `slidingInterface`: improved efficiency
  - simulation of gear pumps: ACMI with multiple interfaces
- `TopoDyM` *dynamic solver family (compressible/incompressible/VOF)*
  - enhanced formulation of momentum interpolation for solution-independence on under-relaxation factors and time-step advancement
  - consistent pressure-velocity coupling algorithm in inner iteration
  - enhanced formulation of flux correction after topological changes
- *Enhanced domain* `decompositionMethods` for faster simulations on parallel machines:
  - semi-automatic decomposition for full load balancing with topological changes
- *Turbulence modeling*: DLRM hybrid RANS/LES scale-adaptive model - extended to work with any RANS model

All the presented work is compatible with the technology released by the OpenFOAM® Foundation. The presented development is therefore fully compatible and tested with the **new releases** `3.0.x` **and** `-dev` of the software.

Library implementation



The library structure replicates the original code structure:

- code development is organized in dynamic libraries in the OpenFOAM® Technology;
- *mainstream development for the base classes* (`dynamicMesh`, `engine`, `turbulence`) *is cross-compiled with the original software libraries*;
  - ALL the original applications/solvers/utilities of the software are implicitly enabled and see the extensions
  - source files of the OpenFOAM® distribution are not changed
- sub-models are linked dynamically at run-time in OpenFOAM® accordingly to the standard procedure
- the library is *DAILY* maintained to work with OpenFOAM®-dev release by the Foundation.

Models theory and details about implementation available on authors' publications

Library implementation

Programming:

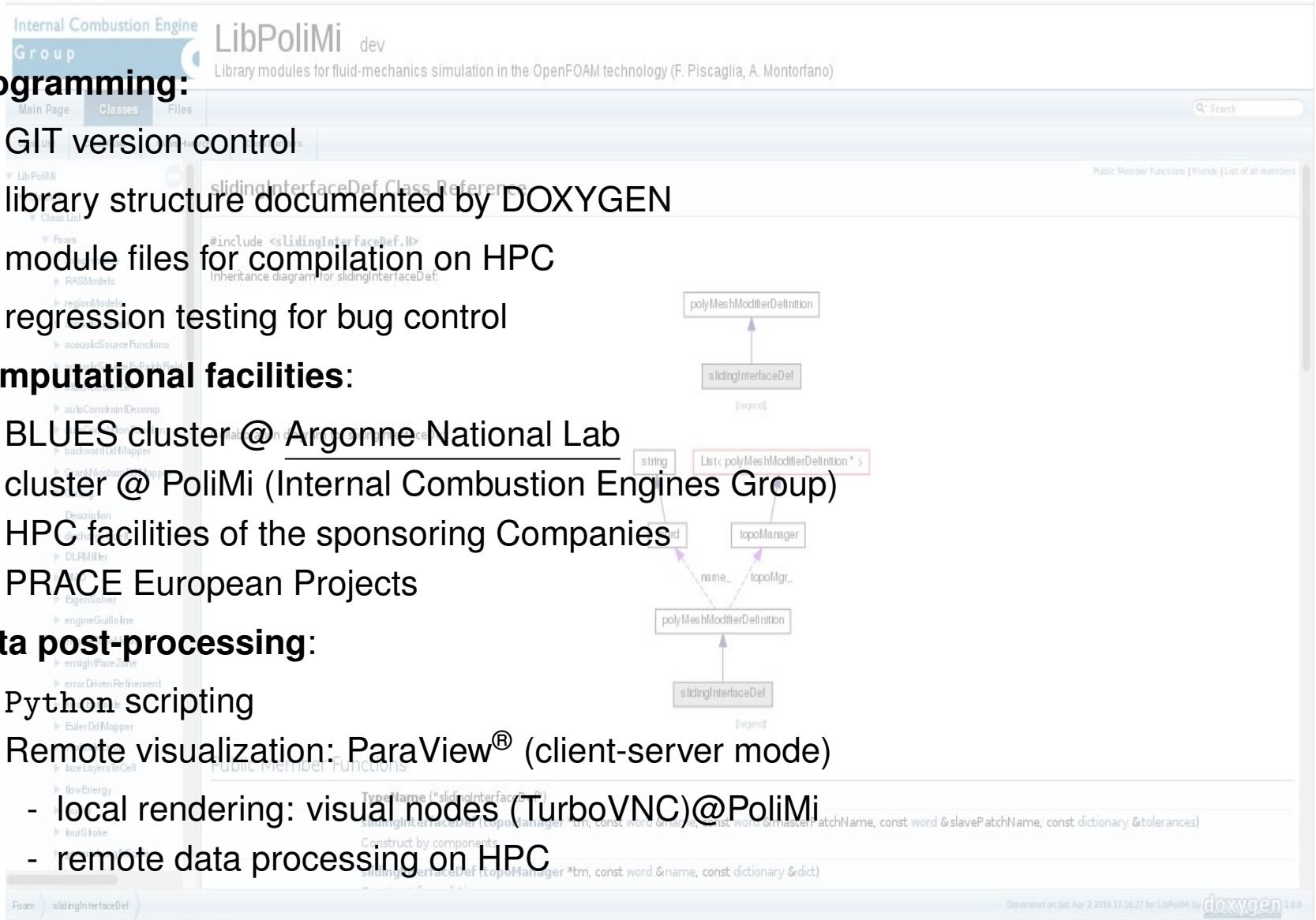
- GIT version control
- library structure documented by DOXYGEN
- module files for compilation on HPC
- regression testing for bug control

Computational facilities:

- BLUES cluster @ Argonne National Lab
- cluster @ PoliMi (Internal Combustion Engines Group)
- HPC facilities of the sponsoring Companies
- PRACE European Projects

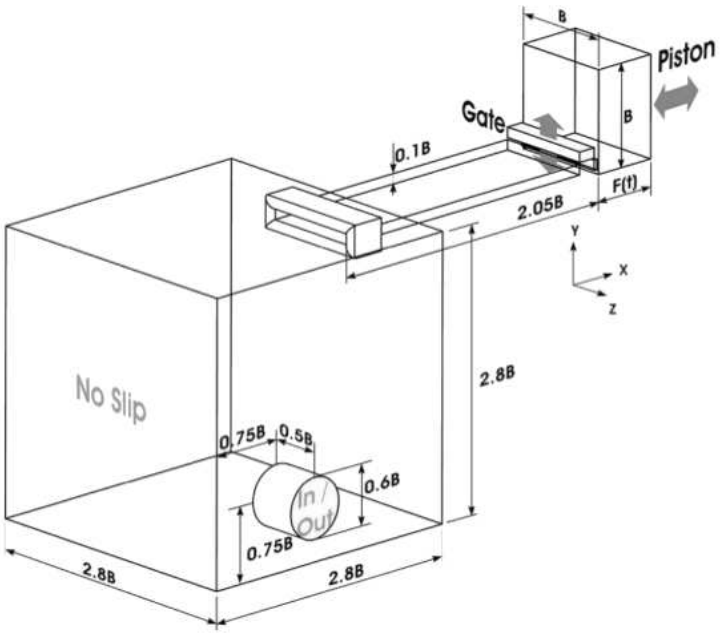
Data post-processing:

- `Python` scripting
- Remote visualization: ParaView® (client-server mode)
  - local rendering: visual nodes (TurboVNC)@PoliMi
  - remote data processing on HPC

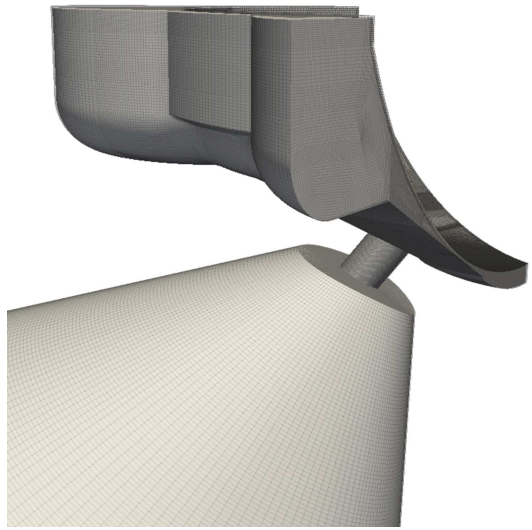


Test cases

a)



b)



Detailed 2-d PIV measurements provided by

ISAE Institut Supérieur de l'Aéronautique et de l'Espace ENSMA

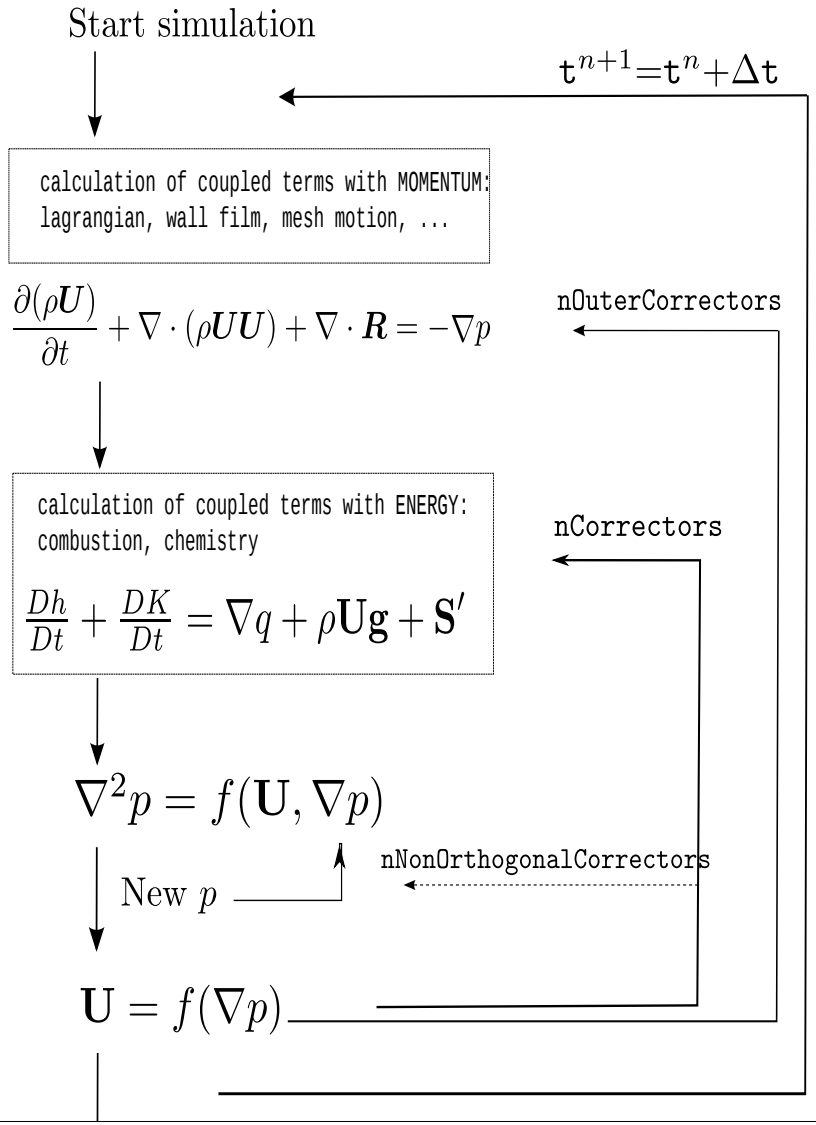
- Moving valve mode, 720 CA/cycle
- Open valve mode, 360 CA/cycle

Multi-hole GDI injector geometry: MAGIE by

Continental

- Real geometry
- Real needle lift (X Ray in ANL)
- Atomization visualization
- Large spray visualization
- PDA

Integration solver-dynamic mesh



NOVEL DEVELOPMENT:

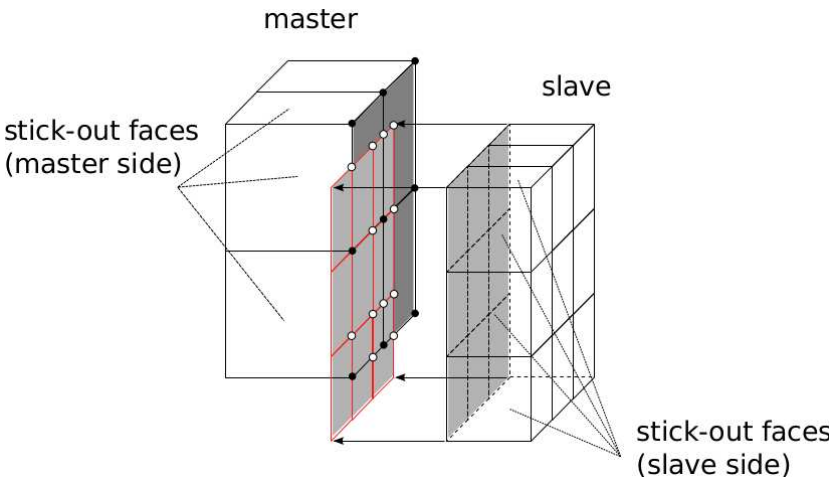
- 2nd order time discretization
- Grid Conservation Law (GCL)
- enhanced flux correction after topoChanges
- strict coupling between pressure and energy
- enhanced momentum interpolation method

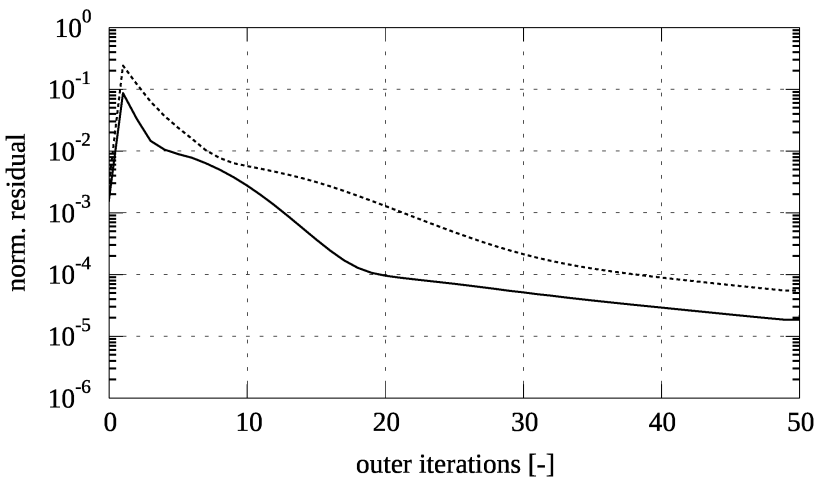
[1] Piscaglia, F. and Montorfano, A. et al. "Hybrid RANS/LES of Moving Boundary Problems: Application to Cavitating Sprays and In-Cylinder Flows". Available for download at: `https://imem.cray.com/2016/agenda-2016.html`

Integration solver-dynamic mesh

ENHANCED FLUX CORRECTION for faster convergence

Dynamic solvers (compressible/incompressible/VOF) with topological changes may be **SLOW TO CONVERGE**: as topological changes are triggered and solution is re-sampled onto the new mesh, old face fluxes might not be fully compliant with the continuity equation.





- Modified form of Poisson equation for a pressure corrector p_{corr}:

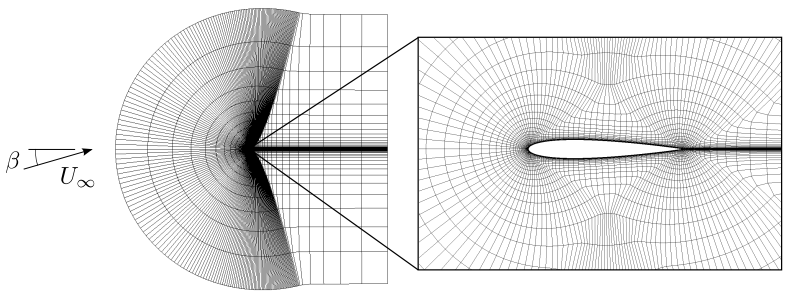
$$\nabla^2 p_{\text{corr}} + \frac{1}{\Delta t} \nabla \cdot \left[\rho(\mathbf{x}, t^{n+1}) \mathbf{u}(\mathbf{x}, t^{n+1}) \right] = 0$$

[1] Montorfano, A., Piscaglia, F., and Onorati, A., "An Extension of the Dynamic Mesh Handling with Topological Changes for LES of ICE in OpenFOAM®," **SAE Technical Paper 2015-01-0384**, 2015, doi:10.4271/2015-01-0384.

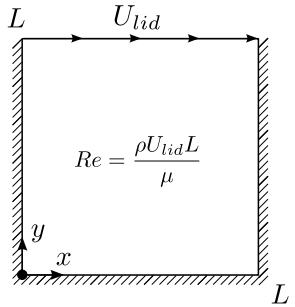
Rhie-Chow Momentum Interpolation Method

The Rhie-Chow momentum interpolation method presents some (well known) inherent limits:

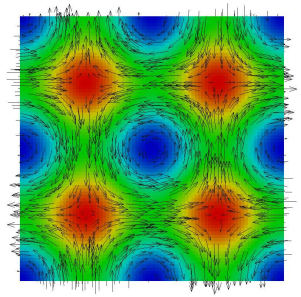
1. UNDER-RELAXATION FACTOR DEPENDENCY in the p-v coupling algorithm
2. TIME-STEP DEPENDENCY of the solution



a) NACA-012 airfoil



b) lid cavity flow

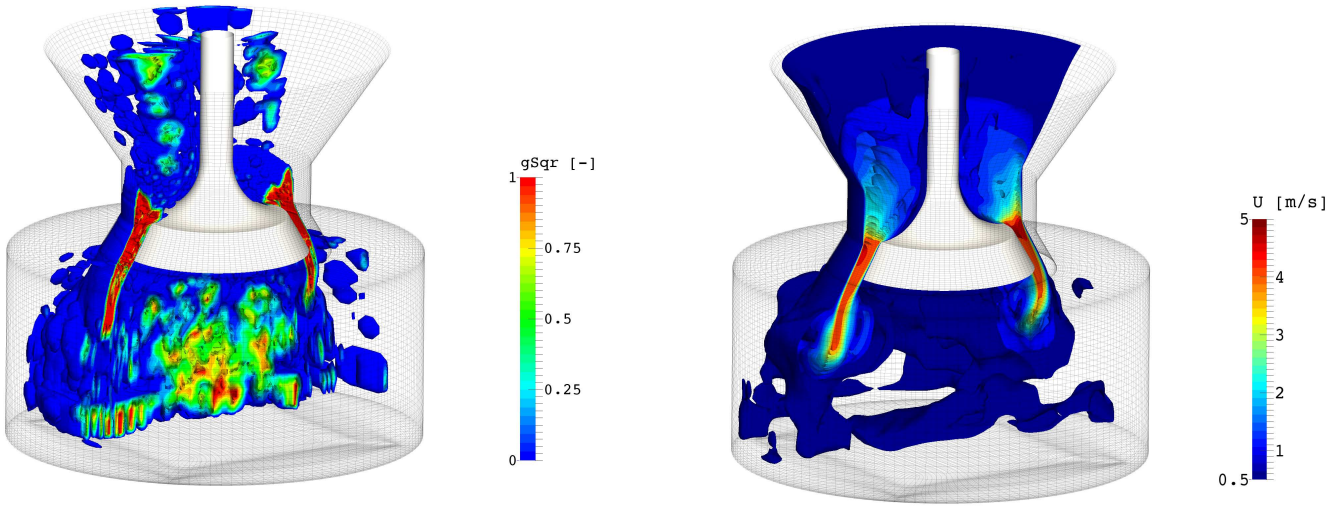


c) Taylor-Green vortex

1. **Flow field evolving <u>towards a STEADY solution</u>**:
   a) NACA-012 airfoil (`simpleFoam`);
   b) lid-cavity flow (`pimpleFoam` $\rightarrow$ steady solution)
2. **<u>UNSTEADY flow field</u>**:
   c) Taylor-Green vortex (`pimpleFoam` transient mode)

J. Martìnez, F. Piscaglia, A. Montorfano, A. Onorati, S. M. Aithal. “Influence of momentum interpolation methods on the accuracy and convergence of pressure-velocity coupling algorithms in OpenFOAM”. Accepted *Journal of Computational and Applied Mathematics.*

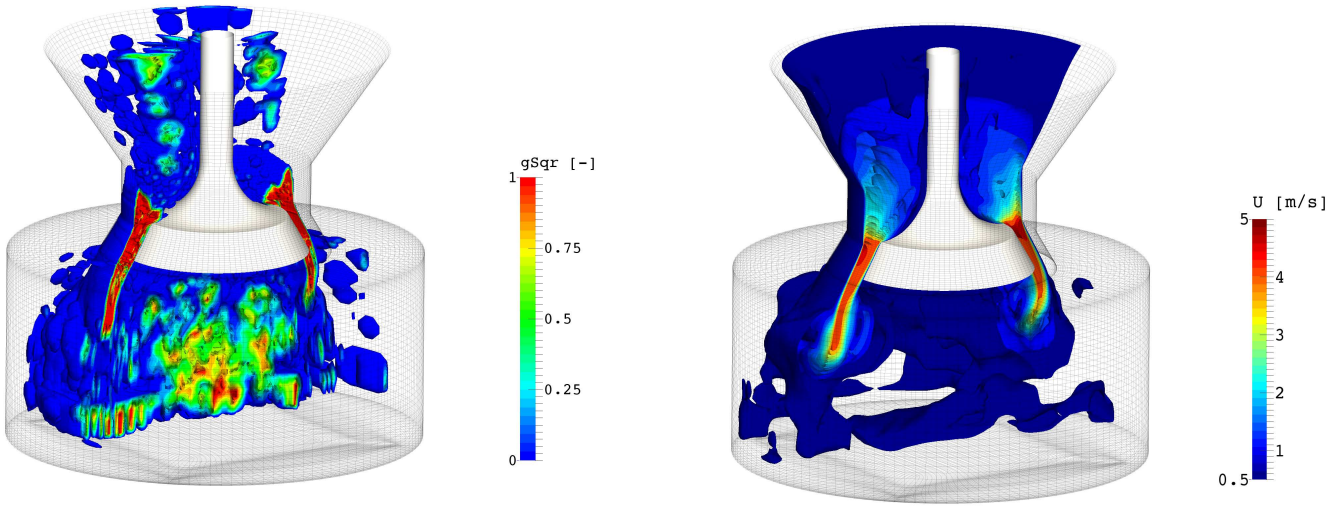
Hybrid RANS/LES



- **Hybrid RANS/LES $\rightarrow$ Scale-Adaptive Dynamic Filtering**:
  - can distinguish between what can be resolved and what cannot;
  - produces an accurate estimate of the wall shear stress;
  - allows for an easy case-setup (mesh requirements, boundary and initial conditions);
  - produces results in a reasonable computational time;
  - is able to automatically switch between LES and URANS.

Piscaglia, F., Montorfano, A., and Onorati, A., "A Scale Adaptive Filtering Technique for Turbulence Modeling of Unsteady Flows in IC Engines". *SAE Int. J. Engines 8(2):426-436*, 2015, doi:10.4271/**2015-01-0395**.

Hybrid RANS/LES



In a scale-adaptive filtered model:

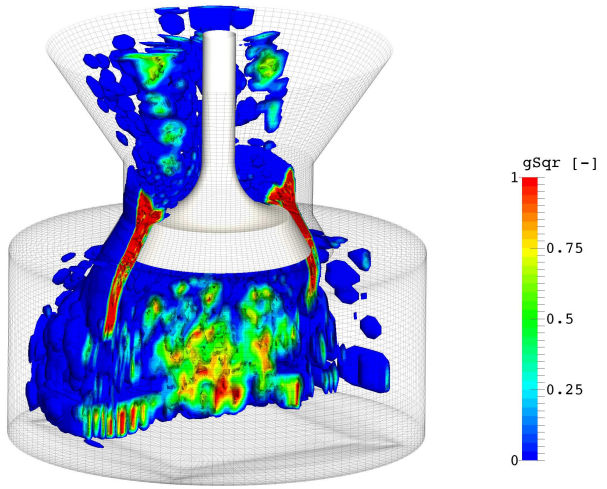
- a RANS turbulence model is used to model turbulent scales (kω-SST in this paper);
- a filter function g is applied **locally** and **dynamically** to the MODELED length scales:

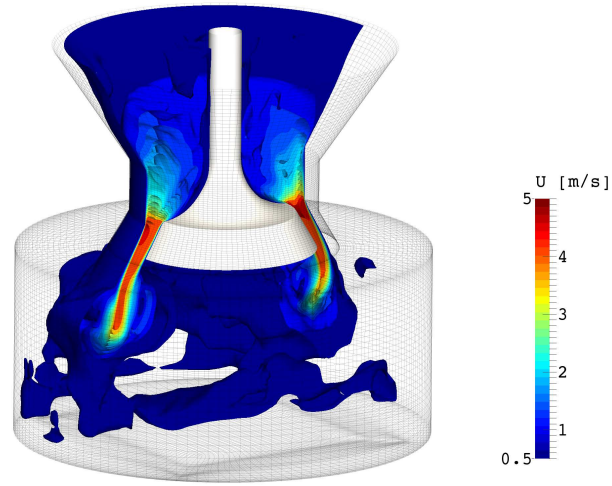
$$\mu_t = g^2 \rho \frac{k}{\omega}$$

The method is converse to the filtering approach that is used in LES.

Piscaglia, F., Montorfano, A., and Onorati, A., "A Scale Adaptive Filtering Technique for Turbulence Modeling of Unsteady Flows in IC Engines". *SAE Int. J. Engines 8(2):426-436*, 2015, doi:10.4271/**2015-01-0395**.

VALIDATION WITH EXPERIMENTS





STATIC MESH (SAE 2005-01-0395):

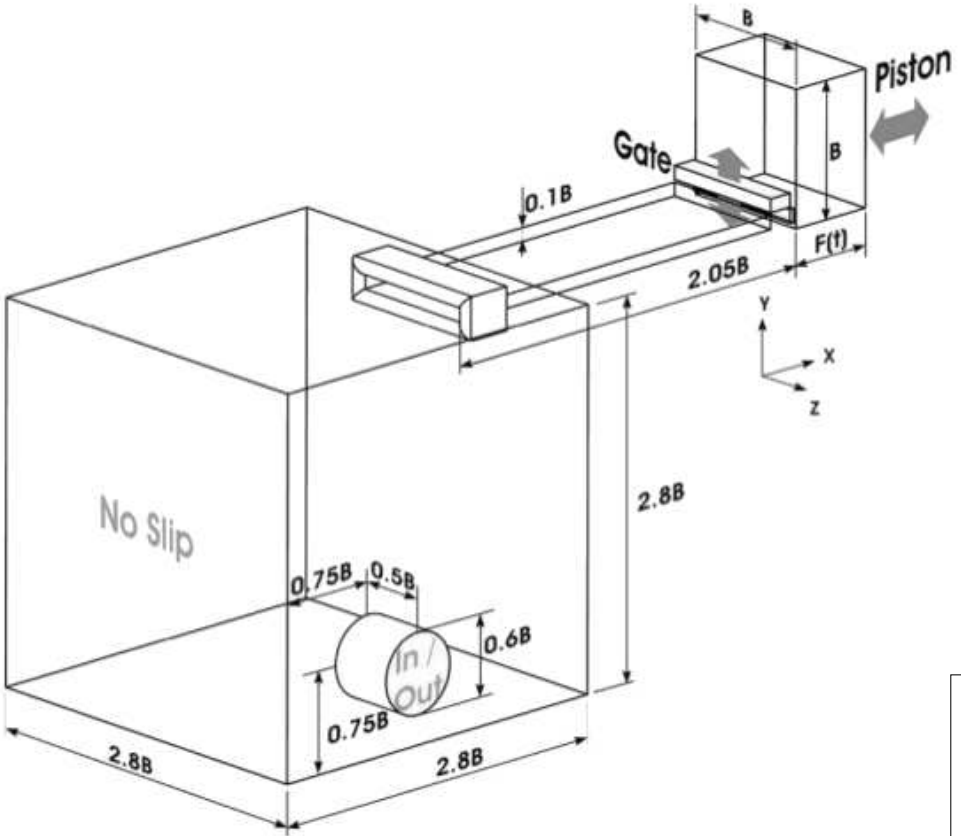
- Swirling flow in a abrupt expansion
- Flow around a poppet valve

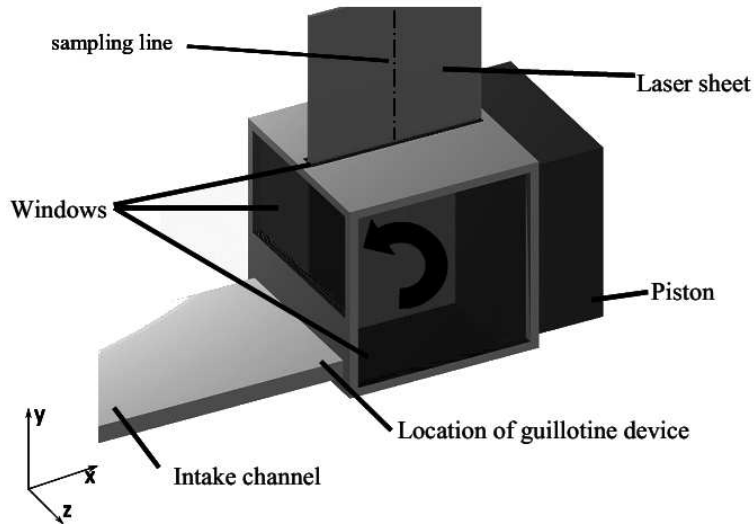
DYNAMIC MESH WITH TOPOLOGICAL CHANGES:

- An engine-like geometry → (https://imem.cray.com/2015/agenda-2015.html)
- A square piston engine with a guillotine valve → (https://imem.cray.com/2016/agenda-2016.h

Test case: Square Piston Engine

Cold Optical Engine with **Square Piston & Straight Intake Port**



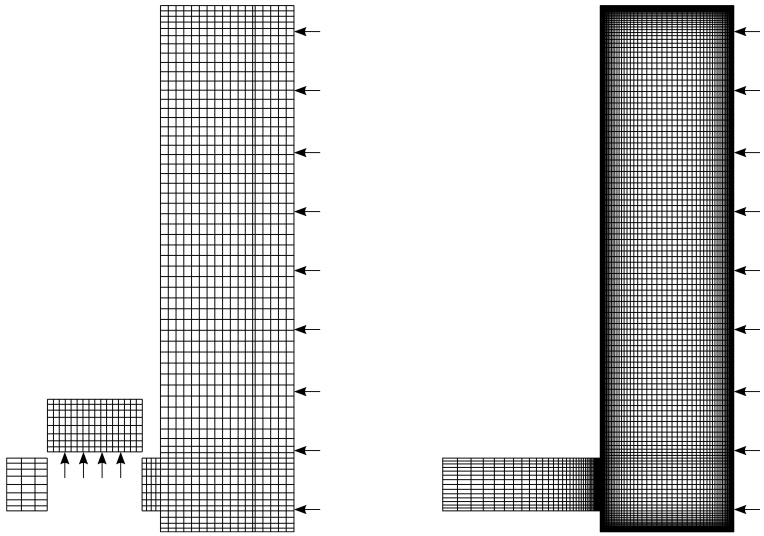


Detailed 2-d PIV measurements provided by

- Moving valve mode, 720 CA/cycle
- Open valve mode, 360 CA/cycle

Test case: Square Piston Engine

Cold Optical Engine with **Square Piston & Straight Intake Port**



"moving valve" mode "open valve" mode

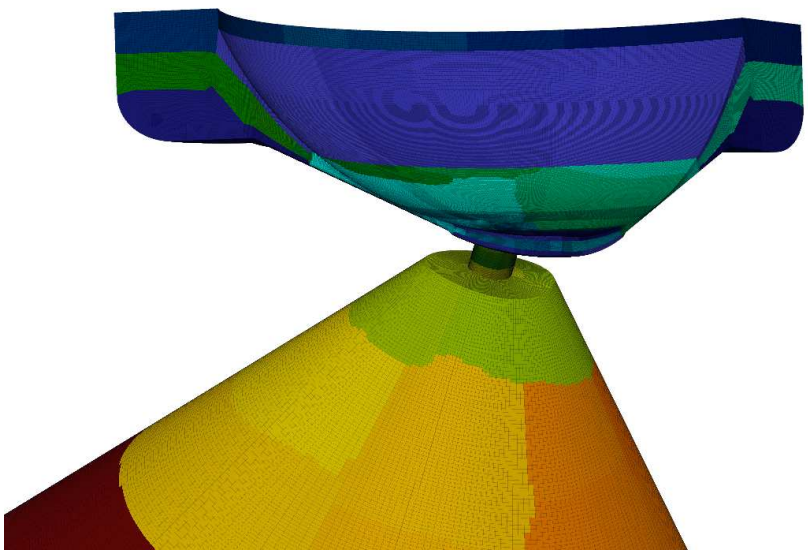
- a “**compressed**” or “**moving valve**” mode, where the guillotine moves up and down to mimic the stages of a four-stroke engine;
- an “**uncompressed**” or “**open valve**” mode, in which the guillotine is constantly open

[1] Wu, Y. and Piscaglia, F. and Montorfano, A. , "*A Study of Organized Motions of in-Cylinder Flow with Hybrid RANS/LES Modeling*", submitted for publication.

Internal Nozzle Flow: VOF

SIMULATION OF NEEDLE OPENING/CLOSURE - WHAT IS NEEDED:

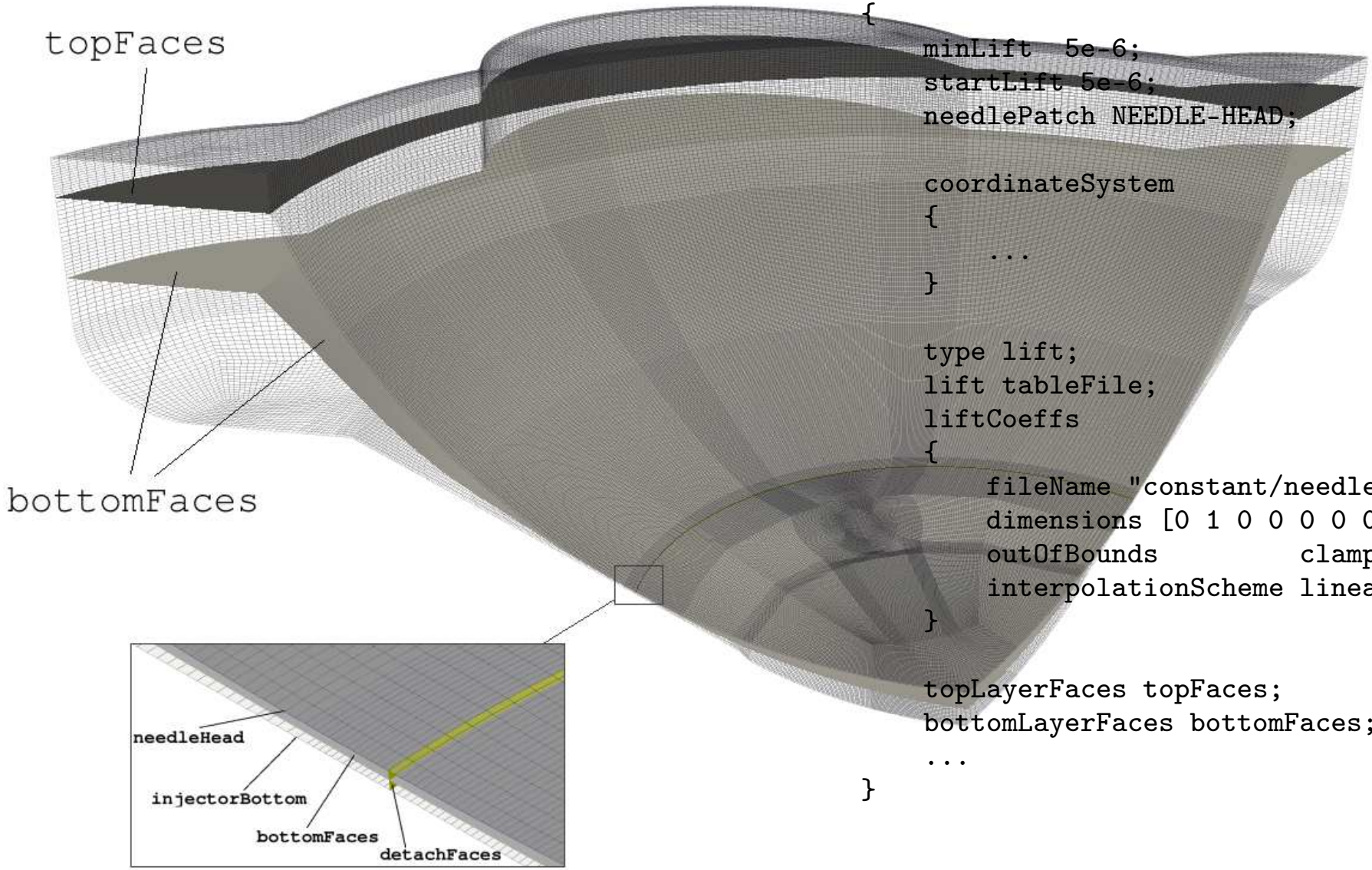
- complex **mesh motion strategy based on topological changes** to ensure high grid quality
- compressible VOF **transient dynamic solver** (fast, accurate, stable)
- domain decomposition and **strong parallelization**
- **time-resolved turbulence modeling** (LES, hybrid RANS/LES)
- complex **cavitation sub-models**



Multi-hole GDI injector geometry: MAGIE by Continental

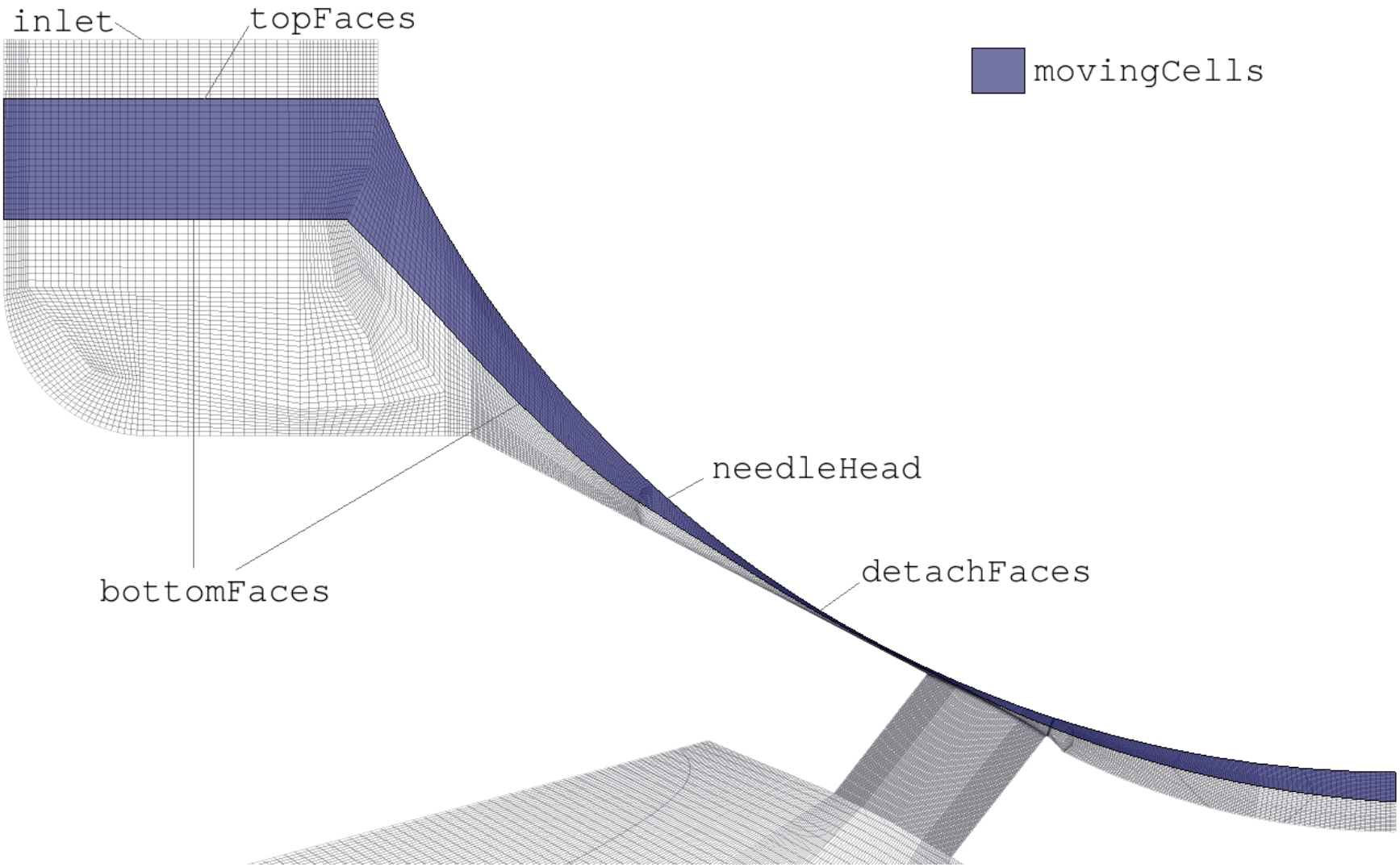
- Real geometry
- Real needle lift (X Ray in ANL)
- Atomization visualization
- Large spray visualization
- PDA

Dynamic mesh with `topoChanges`



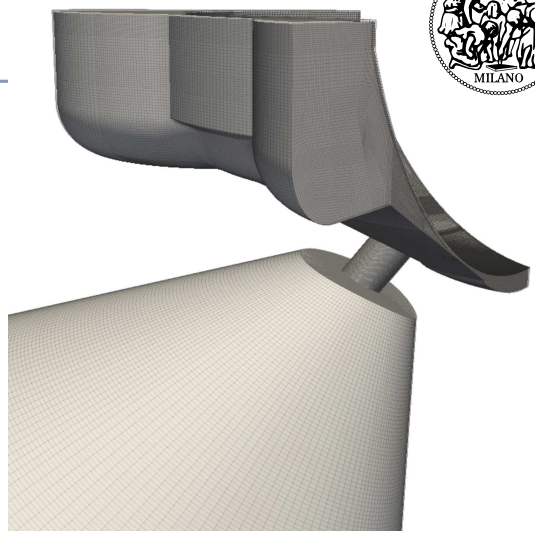

```
needleTopoFvMeshCoeffs
{
    minLift  5e-6;
    startLift 5e-6;
    needlePatch NEEDLE-HEAD;

    coordinateSystem
    {
        ...
    }

    type lift;
    lift tableFile;
    liftCoeffs
    {
        fileName "constant/needleLift";
        dimensions [0 1 0 0 0 0 0 ];
        outOfBounds         clamp;
        interpolationScheme linear;
    }

    topLayerFaces topFaces;
    bottomLayerFaces bottomFaces;
    ...
}
```

Mesh motion: class `needleTopoFvMesh`



A. Montorfano, F. Piscaglia, A. Onorati. *An extension of the dynamic mesh handling with topological changes for LES of ICE in OpenFOAM®*. **SAE Technical Paper 2015-01-0384.**

Gasoline Injector: opening event



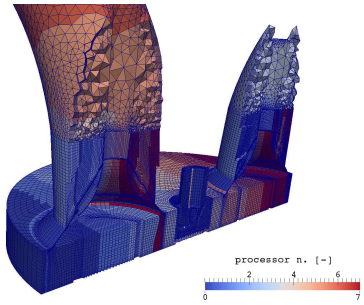
- **COMPUTATIONAL MESH**:
  - Fully-hex multi-block grid $\approx$ 11 M cells
  - Mesh motion based on `topologicalChanges`:
    - prescribed needle motion from tabulated data
    - two `layerAdditionRemoval` zones
    - `attachDetach` to simulate needle opening/closure
- **SOLVER**
  - compressible **Volume-of-Fluid** (VoF) phase-fraction based interface capturing approach;
    - 2 compressible, non-isothermal immiscible fluids with cavitation
  - Discretization:
    - backward differencing in time (2nd order)
    - `LUST` on momentum convection
    - limited schemes for scalar transport
- **TURBULENCE MODELING**: DLRM (scale-adaptive) RANS/LES

Decomposition with topoChanges

FULLY AUTOMATIC (class `autoDecomp`)

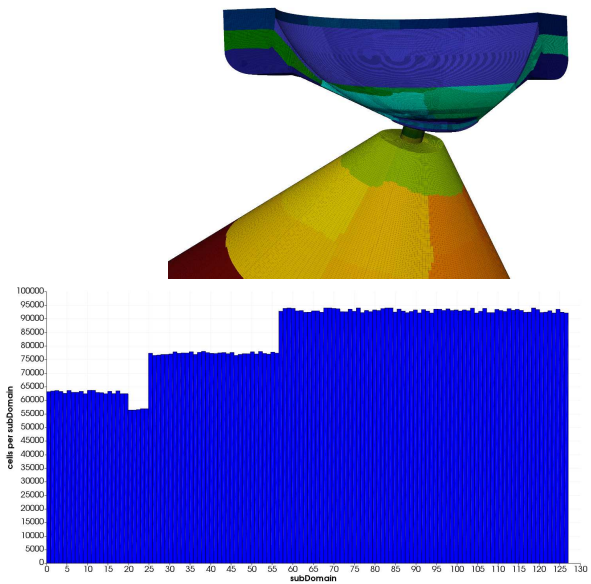
- extension to the `meshTools` class to extend the functionalities of the decomposition tools

→ **SAE 2013-24-0027 &2015-01-0384**
IMEM 2013 & 2014



CONSTRAINED (class `structuredSetDecomp`)

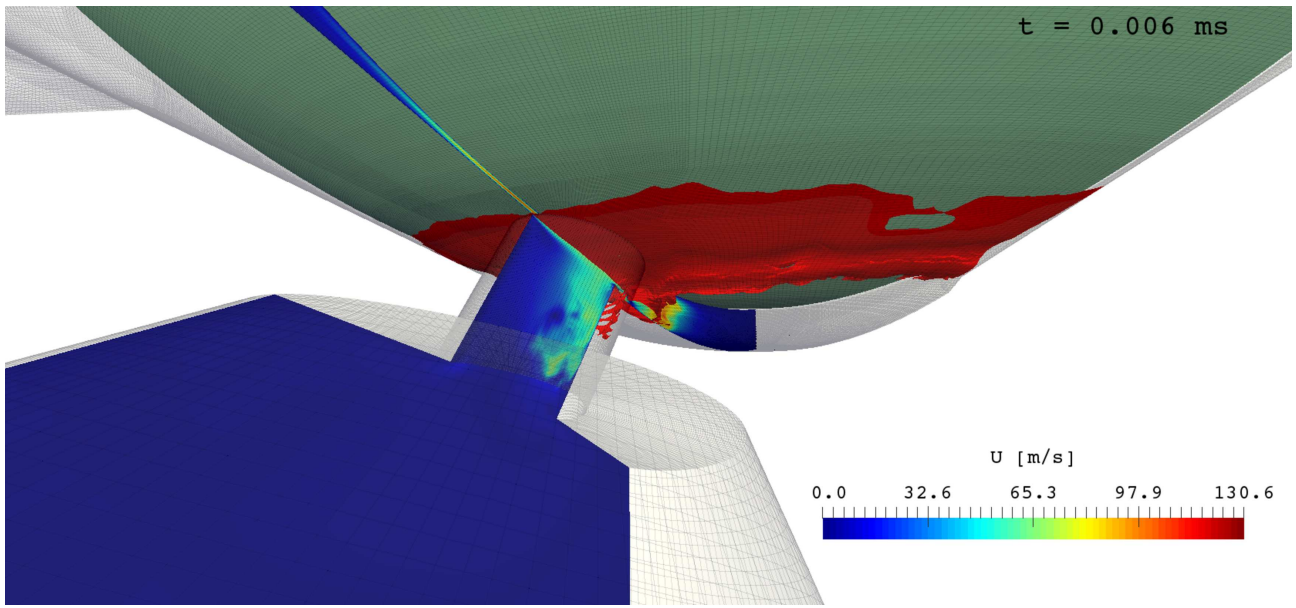
- mesh is splitted into regions on the basis of layering zones;
- decomposition of topology modifiers is computed (new class `structuredSetDecomp`);
- the remaining zones of the mesh are decomposed;
- cell-processor assignment is stored and the decomposition of the mesh is performed.



The above steps are fully automated and included in shell scripting.

GDI Injector: opening event - dynamic VOF

MAGIE injector: injector opening. Simulation ran on 128 cores on Blues (machine operating at Argonne National Lab).



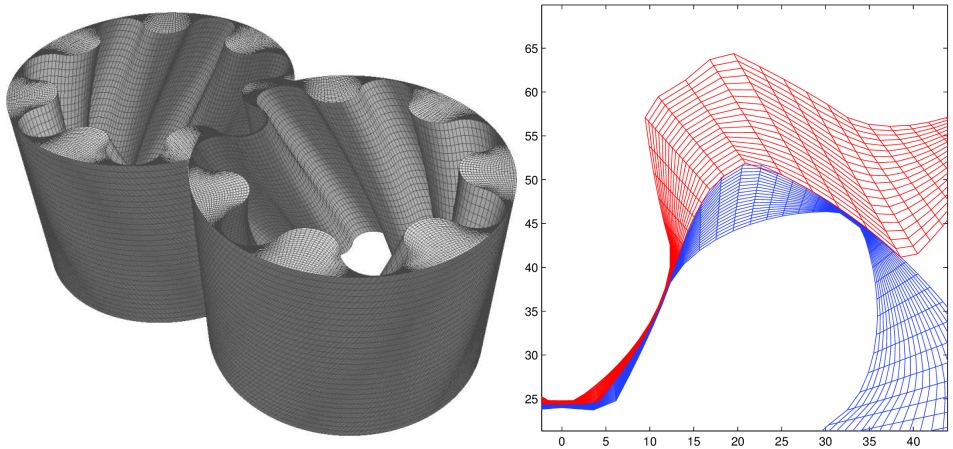
Conclusions and Future Work

Class `dynamicMesh`:

- fully general, it is completely transparent to OpenFOAM® solvers;
- `topoManager` class handles topological changes at low level ($\rightarrow$ strongly favors usage for non-expert users/developers)
- fully compatible with OpenFOAM®-dev family branches
- very easy to extend

`Turbulence`:

- dynamic filtering is not a zonal approach $\rightarrow$ automatic switch between RANS and LES
- possible to combine *ANY* RANS and LES model
- allows to a significant speed up in time-resolved simulations



`CURRENT/FUTURE WORK`:

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Computational resources

Simulations were carried out by the computing resources provided on BLUES, a high-performance computing cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory (IL, USA).

- Compute – 310 nodes, Each with two Sandy Bridge 2.6 GHz Pentium Xeon (hyper threading disabled.) 4960 available compute cores
- Memory – 64GB of memory
- Storage – 110TB of clusterwide space provided by GPFS (shared with Fusion) 15GB on node Ramdisk
- Network – Infiniband Qlogic QDR

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Thank you for your attention!

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