Simulation of gas exchange and combustion processes in SI and Diesel engines: current state of models and examples of applications

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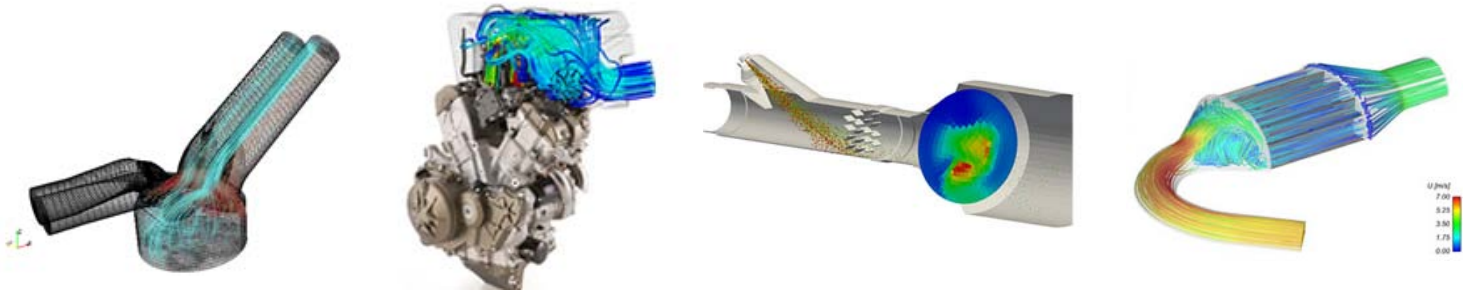
http://www.engines.polimi.it

Topics

- In-cylinder flow and combustion modeling using the OpenFOAM® technology.
  - Lib-ICE code
  - Available models to simulate:
    - Gas exchange
    - Fuel air/mixing
    - Combustion
  - Examples of use, experimental validation.

Lib-ICE

- Set of libraries and solvers for IC engine modeling using OpenFOAM technology:
  - Mesh motion for complex geometries
  - Combustion
  - Lagrangian sprays + liquid film
  - Unsteady flows in intake and exhaust systems: plenums, silencers, 1D-3D coupling.
  - Reacting flows in after-treatment devices: DPF, catalyst, SCR.



Lib-ICE

- **Simulation of in-cylinder flows and combustion.**

  What is needed?

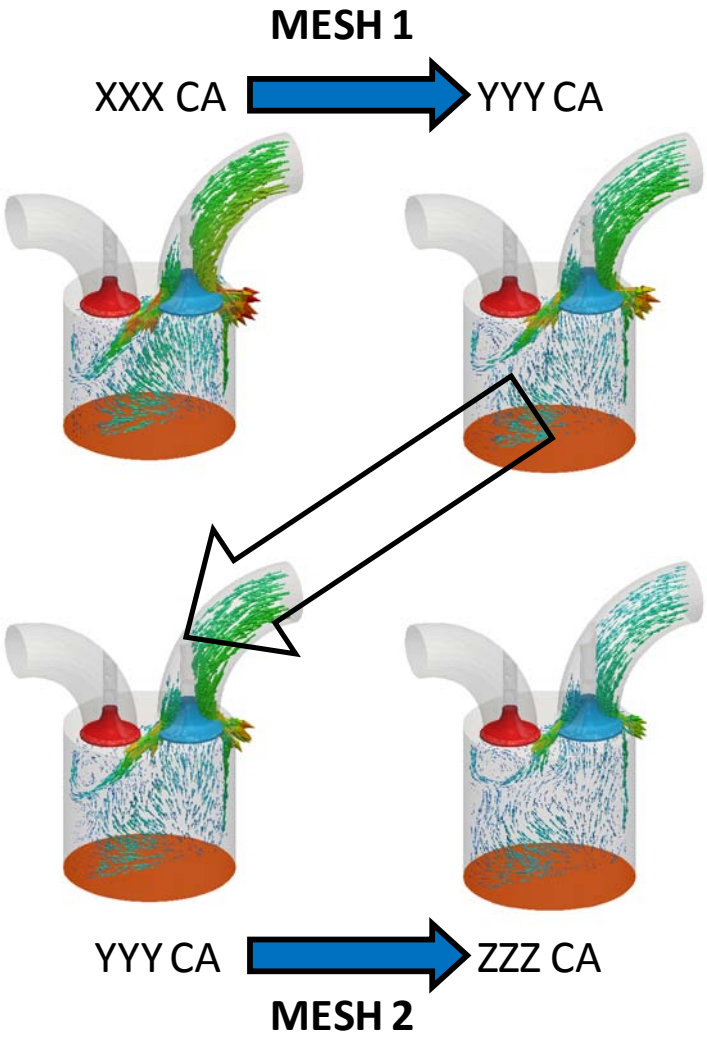
  1) Reliable, consolidated algorithms for mesh management.
  2) A complete set of models to predict fuel-air mixing process in both Diesel and SI engines:
     - Spray sub-models: atomization, injection, breakup, wall-impingement.
     - Liquid film models.
  3) Models for both conventional and advanced combustion modes.

Mesh management

Mesh management

- Bottleneck for CFD modeling of IC engines: geometry is complex and boundaries are moving. Requirements:
  - Flexibility with respect to the mesh structure and the grid generators adopted.
  - Grid quality should be preserved during motion.
  - Limited amount of pre-processing required for mesh generation and case set-up.
  - Topology modifiers should operate automatically according to prescribed and easy-to-be-defined settings.

Mesh management



1) Multiple meshes cover the entire cycle simulation.
2) Each mesh is valid in a user-specified interval.
3) During each time-step:
   - ✓ Grid points are moved using automatic mesh motion and/or pre-defined points motion.
   - ✓ Mesh topology can be eventually changed
4) Mesh-to-mesh interpolation.

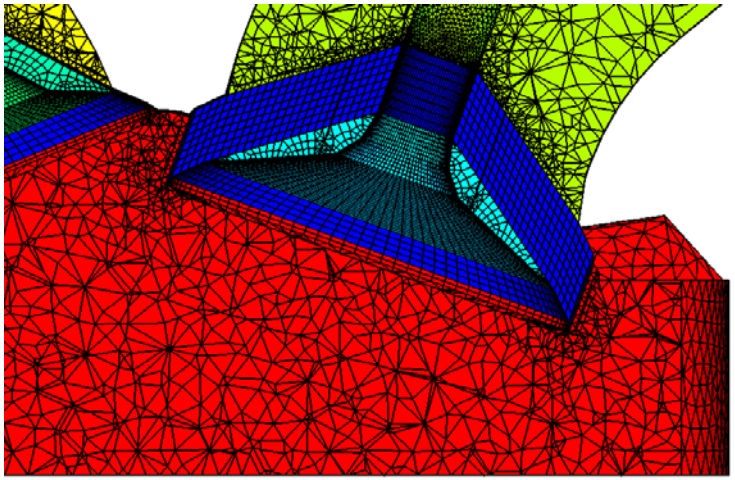
Mesh management

Mesh motion

- Grid points motion computed by an automatic mesh motion solver, based on the Laplace equation.

$$\begin{cases} \nabla^2(\gamma \cdot \mathbf{u}) = 0 \\ \mathbf{x}_{new} = \mathbf{x}_{old} + \mathbf{u} \cdot \Delta t \end{cases}$$

- Grid quality during motion improved by the possibility to pre-define the point velocity field in regions of interest.



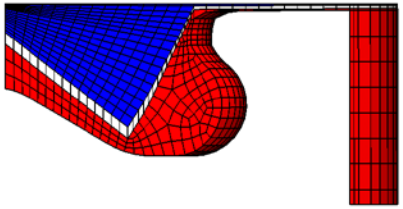
Algorithms developed in collaboration with Dr. Z. Tukovic (FSB, University of Zagreb) and Dr. F. Brusiani (DIEM, University of Bologna)

Mesh management

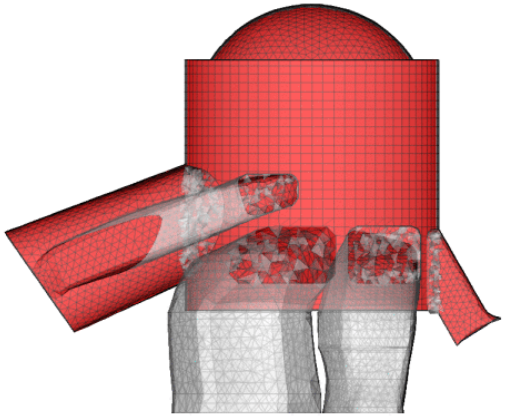
Topological changes

- Reduction of the overall number of meshes.
- Mesh is modified according to user-defined parameters, no need to specify exactly when a specific event should take place.

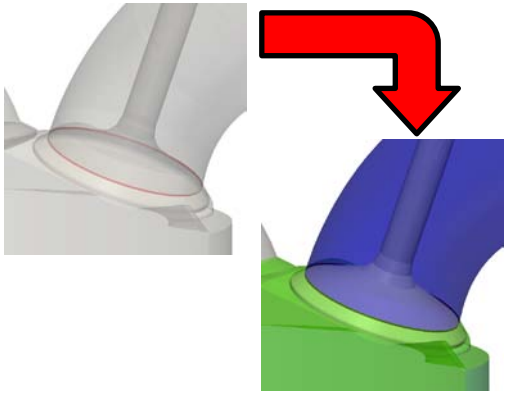
Dynamic mesh layering



Sliding interface



Attach/detach boundary



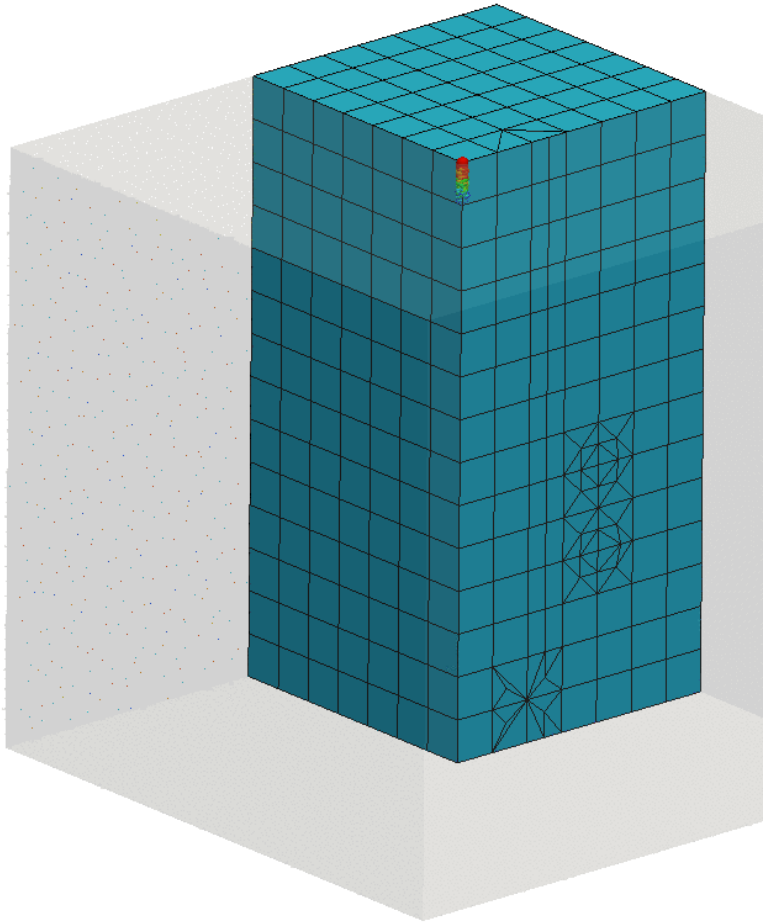
Work developed in collaboration with Dr. H. Jasak (Wikki Ltd.)

Mesh management

Topological changes

➢ Adaptive local mesh refinement

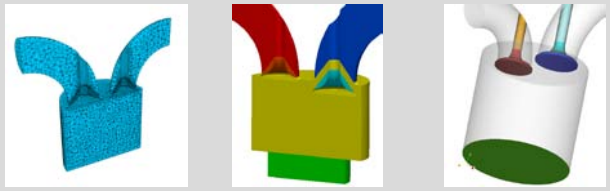
- Mesh is refined only where the most important processes takes place:
  - ➢ Fuel-air mixing in a direct-injection engine
  - ➢ Flame propagation in a SI engine
  - ➢ Main charge motions during gas exchange.
- Works with polyhedral meshes.
- Consistency of the methodology extensively verified.



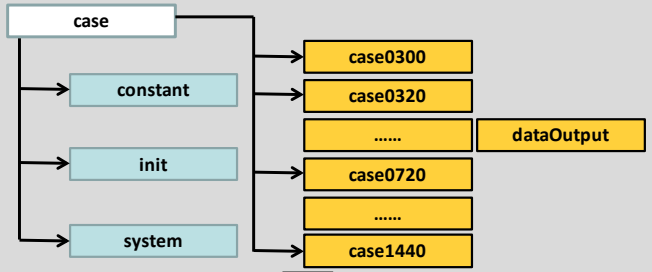
Mesh management

Specific utilities for case set-up

1) Generation of multiple meshes
2) Definition of a template case



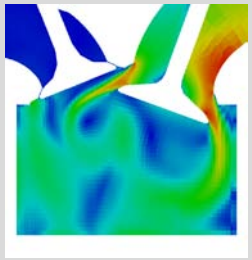
3) `engineCaseSetUp` utility

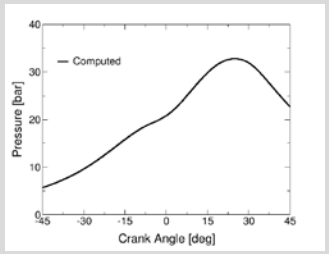


4) `runMultiCycleCase`

```
solverName simpleColdSpeciesEngineDyMFoam;

startTimes
(/* list of startTime for each mesh */);

endTimes
(/* list of endTimes for each mesh */);

writeInterval
(/* list of writeInterval for each mesh */);

parallelRun on;
```

5) Post-processing





Mesh management

Gas exchange process simulation: solvers

- Based on PIMPLE algorithm (PISO + SIMPLE): improved stability. Possibility to run cases with high Courant Numbers (> 10) and time-steps (> 0.1 CA)

1) `simpleColdSpeciesEngineDyMFoam`: solver for cold-flow in IC engines with chemical species tracking and spray. Parallel.

2) `simpleFilmSpeciesEngineDyMFoam`: includes also the wall-film dynamics. Parallel.

Mesh management

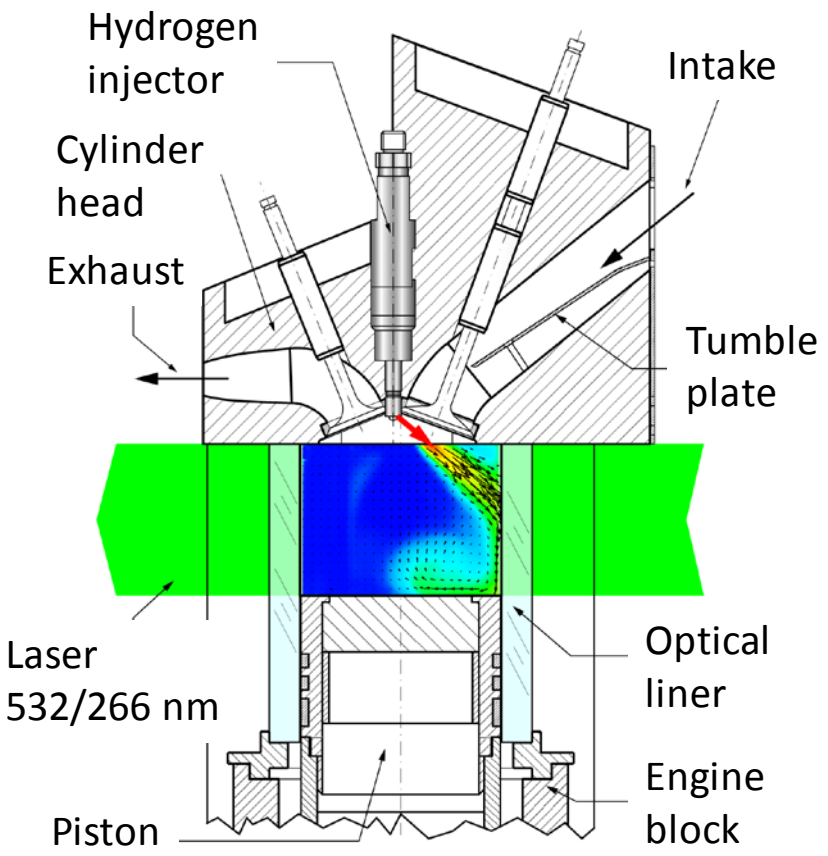
Gas exchange process simulation: SANDIA engine

- The Engine Combustion Network, coordinated by SANDIA (www.ca.sandia.gov/ecn), is an open-forum for international collaboration among experimental and computational researchers in engine combustion:
  1) Internet library of well-documented experiments that are appropriate for model validation and the advancement of scientific understanding of combustion at conditions specific to engines.
  2) Framework for collaborative comparisons of measured and modeled results.
  3) Identify priorities for further experimental and computational research.
- 1st ECN workshop: Ventura, May 2011. 2nd ECN workshop: Europe, september 2012.

Mesh management

SANDIA Engine details

Displaced volume	560 cm^3
Stroke	85 mm
Bore	92 mm
Compression ratio	11
Intake valve timing (IVO/IVC)	346°/-140° CA
Exhaust valve timing (IVO/IVC)	130°/356° CA
Injection timing (SOI/EOI)	-137°/-119° CA
Intake pressure/temperature	1 bar / 36 °C
Engine speed	1500 rpm



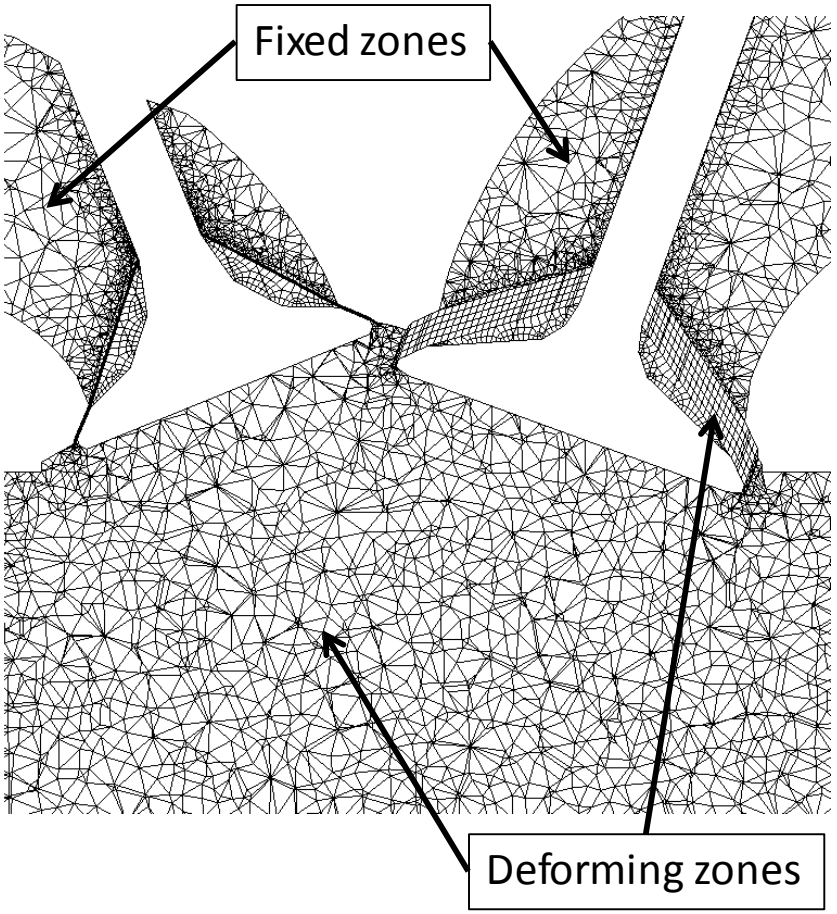
Mesh management

SANDIA Engine: mesh layout and boundary conditions

- Motored conditions. Experimental pressure and temperature profiles imposed at intake and exhaust ports.

- Mesh structure:

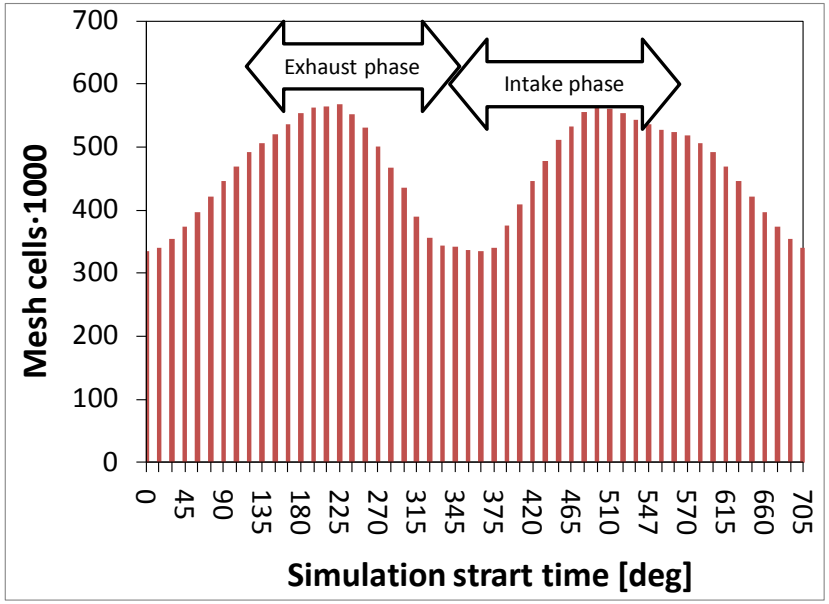
1) hexahedra in the valve region
2) tetrahedra in the remainder of the cylinder.



Mesh management

SANDIA Engine: mesh layout and boundary conditions

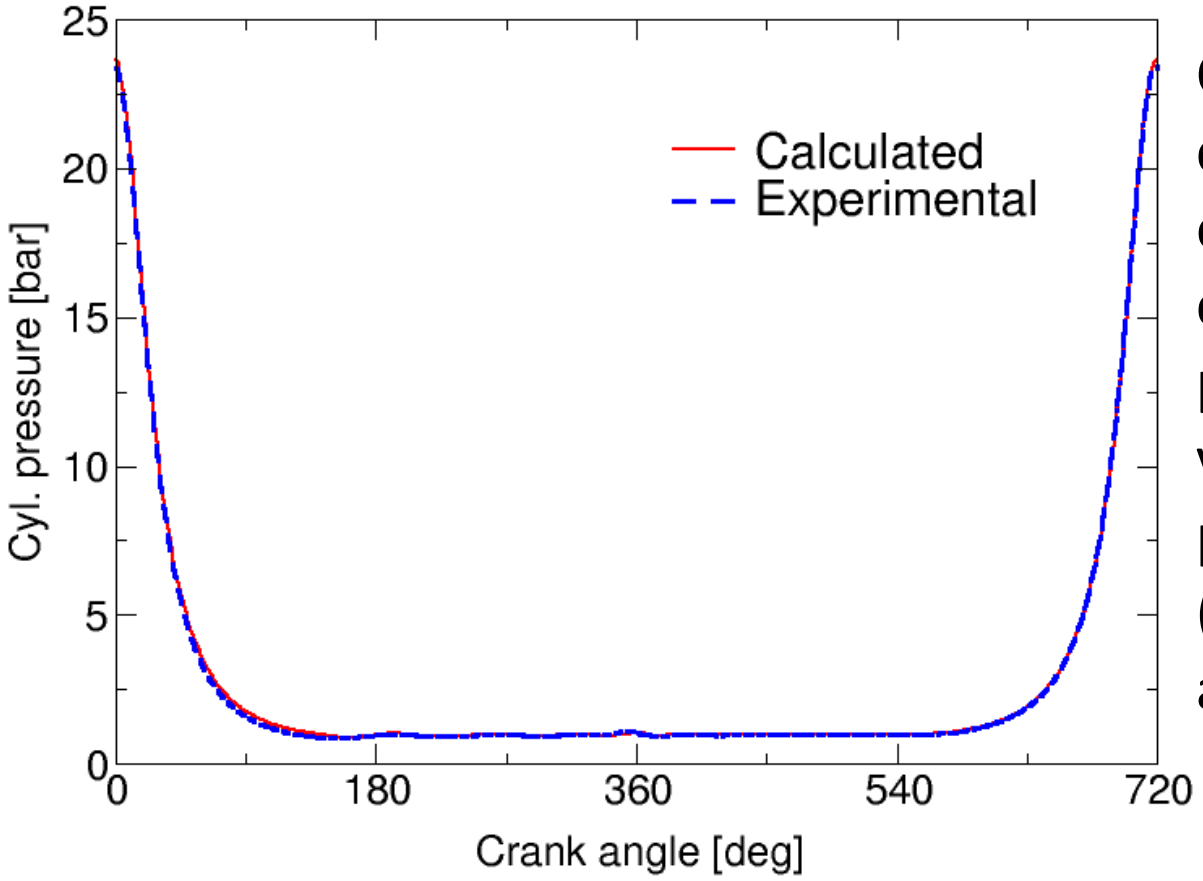
- Mesh validity: 15 deg each. Average cell size ranging from 300 to 600 thousand.
- Mesh size:
  - Cylinder: 2.5 mm
  - Valve region: 0.75 mm
  - Ducts: 2.5 – 5 mm
- Turbulence model: standard k-ε.



Acknowledgement: Dr. Riccardo Scarcelli, Argonne National Labs.

Mesh management

SANDIA Engine: cylinder pressure validation



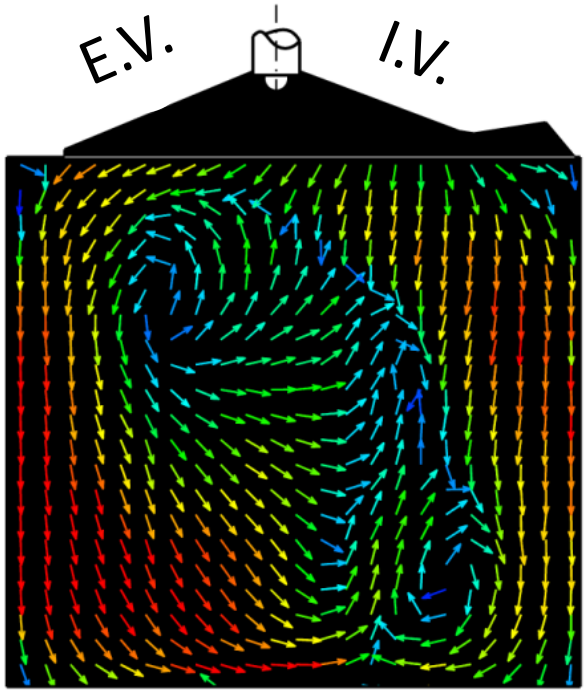
Comparison between computed and experimental in-cylinder pressure profiles to verify the validity of the proposed set-up (boundary conditions and meshes).

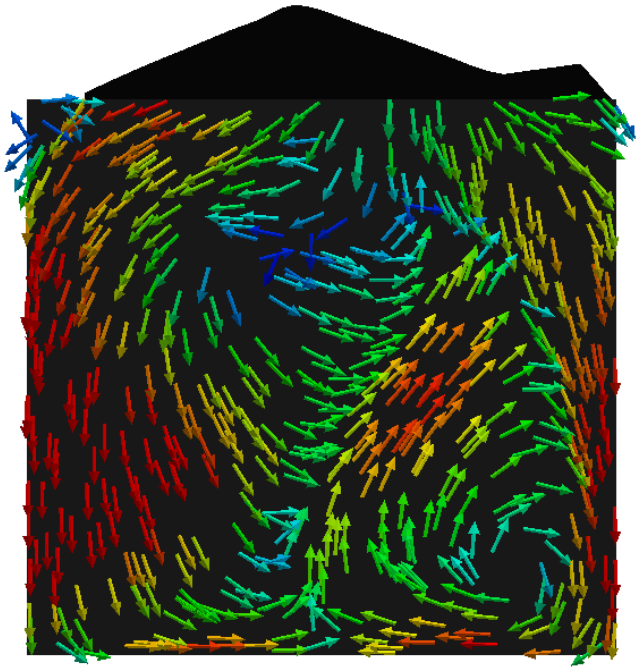
Mesh management

SANDIA Engine: flow-field validation

Comparison between experimental and computed velocity field on the cylinder symmetry plane during compression

-180 CA





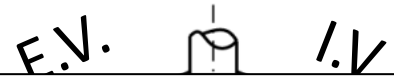
EXPERIMENTAL **COMPUTED**

Mesh management

SANDIA Engine: flow-field validation

Comparison between experimental and computed velocity field on the cylinder symmetry plane during compression

-180 CA



1) Presence of two main streams due to the flow coming from the intake valve.
2) Formation of two vortexes
3) Collision between the two main jets induces the air to move from the piston to the cylinder head.
4) Model correctly describes the main features of in-cylinder flows at BDC.

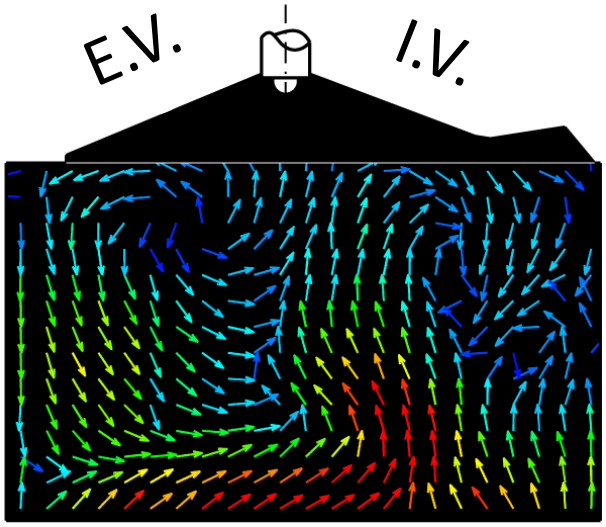
EXPERIMENTAL **COMPUTED**

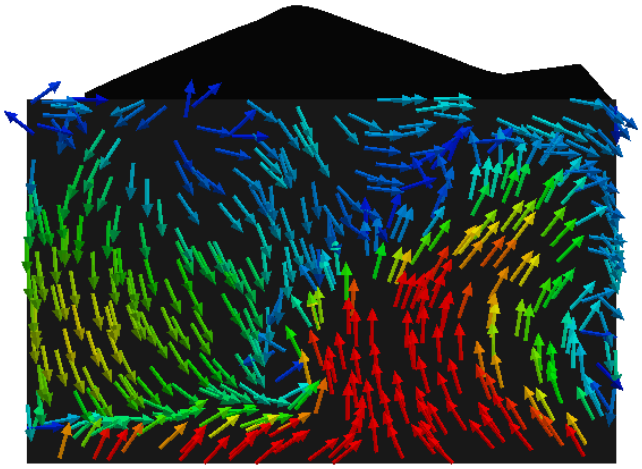
Mesh management

SANDIA Engine: flow-field validation

Comparison between experimental and computed velocity field on the cylinder symmetry plane during compression

-100 CA





EXPERIMENTAL **COMPUTED**

Mesh management

SANDIA Engine: flow-field validation

Comparison between experimental and computed velocity field on the cylinder symmetry plane during compression

-100 CA

1) The two main vortexes reduces their size and move towards the cylinder head.
2) Significant establishment of a gas motion from the piston towards the head.
3) The left stream remain significant.
4) Rather good agreement between experiments and models.

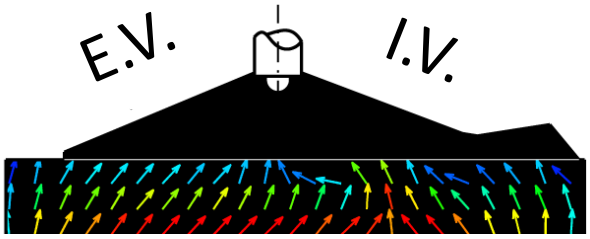
EXPERIMENTAL **COMPUTED**

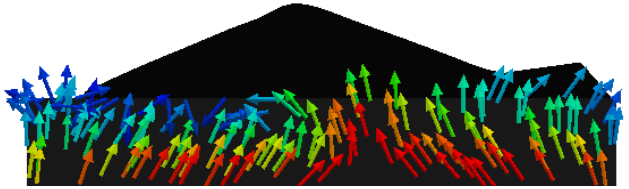
Mesh management

SANDIA Engine: flow-field validation

Comparison between experimental and computed velocity field on the cylinder symmetry plane during compression

-40 CA





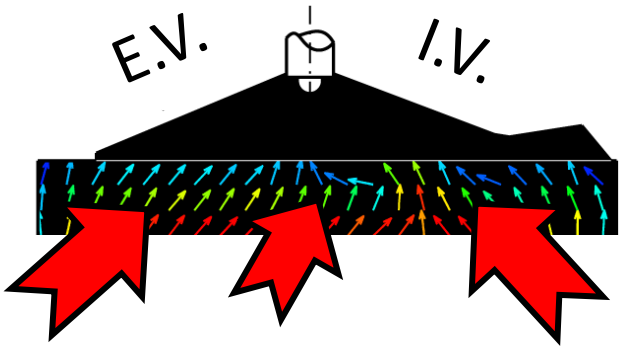
EXPERIMENTAL **COMPUTED**

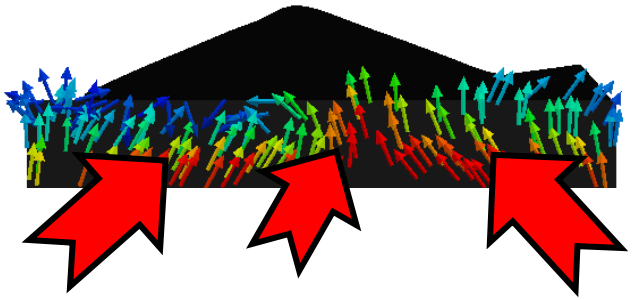
Mesh management

SANDIA Engine: flow-field validation

Comparison between experimental and computed velocity field on the cylinder symmetry plane during compression

-40 CA





1) Flow mostly aligned with piston velocity.

EXPERIMENTAL **COMPUTED**

Mesh management

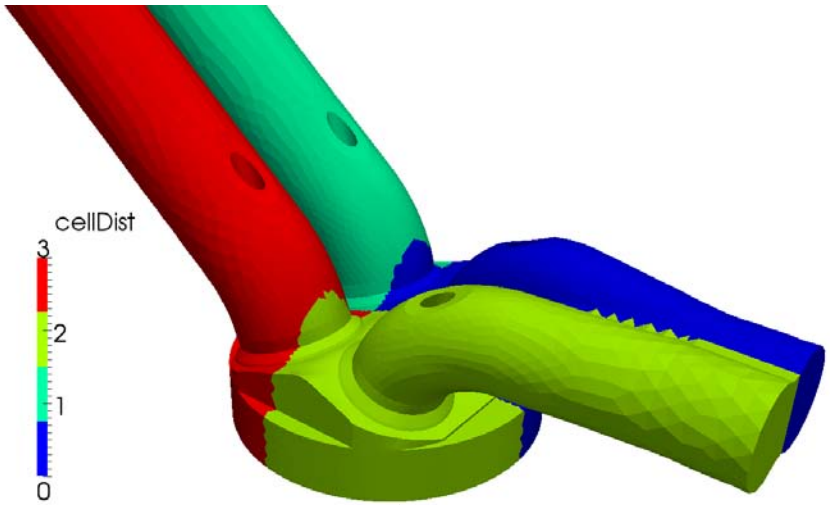
Parallel calculations

- Automatic mesh motion and topological changes works now in parallel.
- **Deforming mesh simulations**: any decomposition can be used:
  - `simple, hierarchical, scotch, …`
- **Meshes with topological changes**: decompositions is not straightforward (manual + preserve patches) or use the advanced decomposition method called `engineScotch` (developed by Wikki Ltd.)

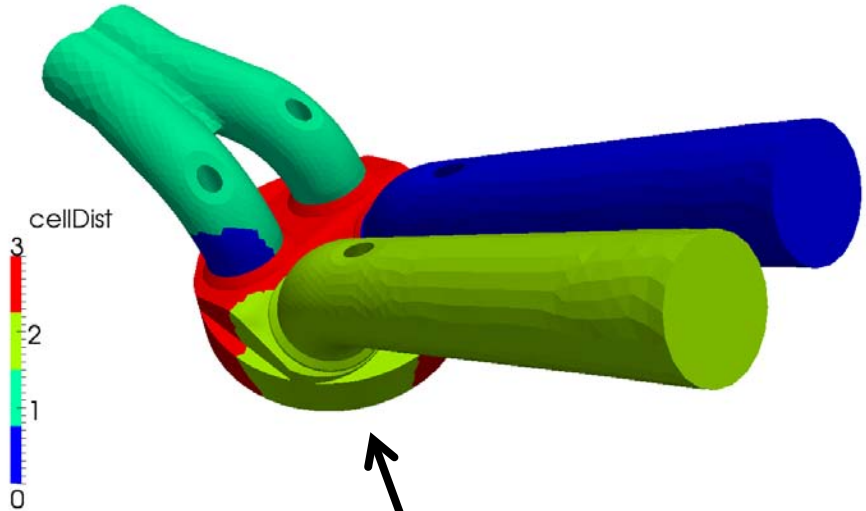
Mesh management

Parallel calculations: example of decompositions

- Grid decomposed into four domains



simple

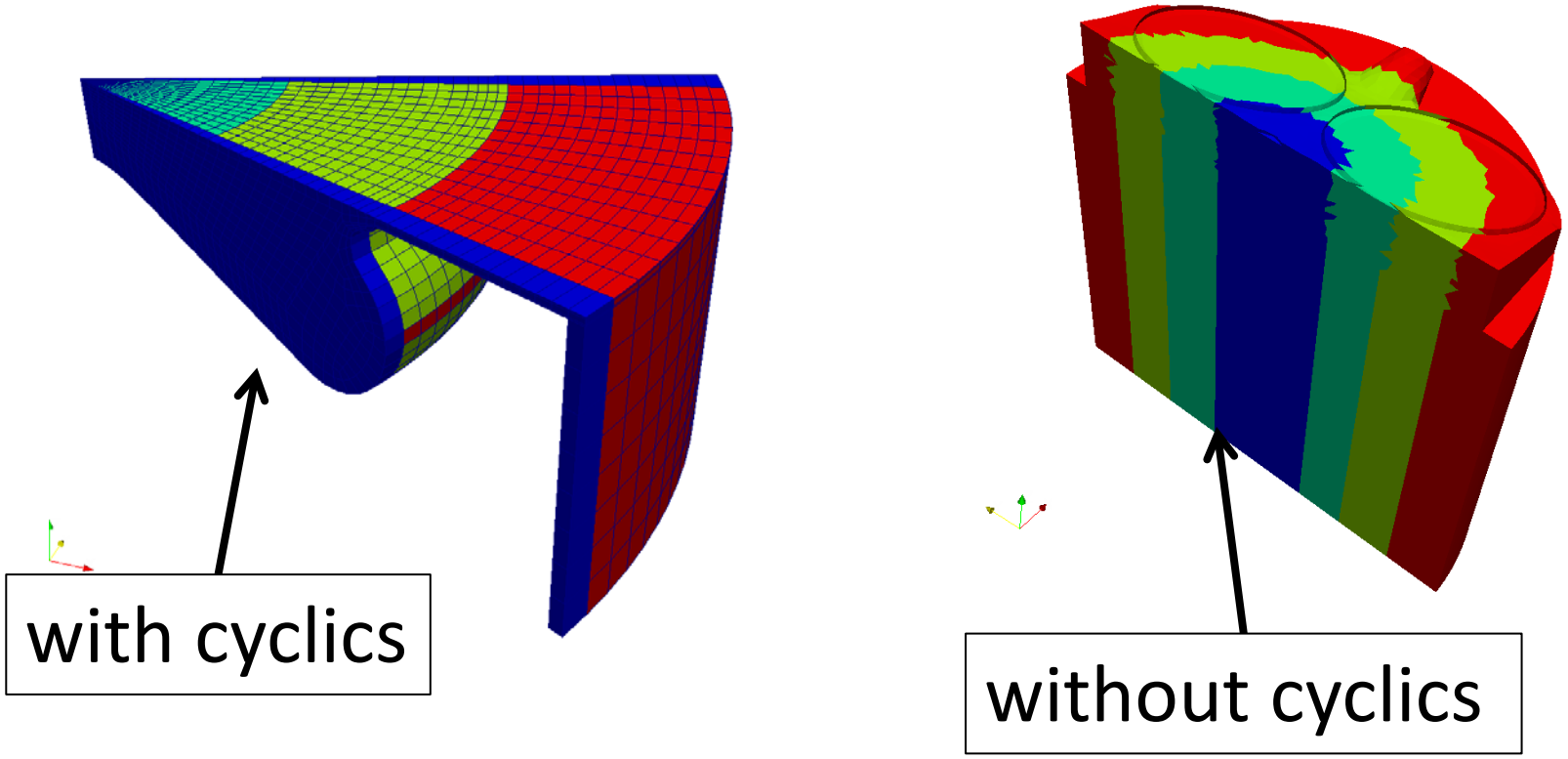


scotch

Mesh management

Parallel calculations: example of decompositions

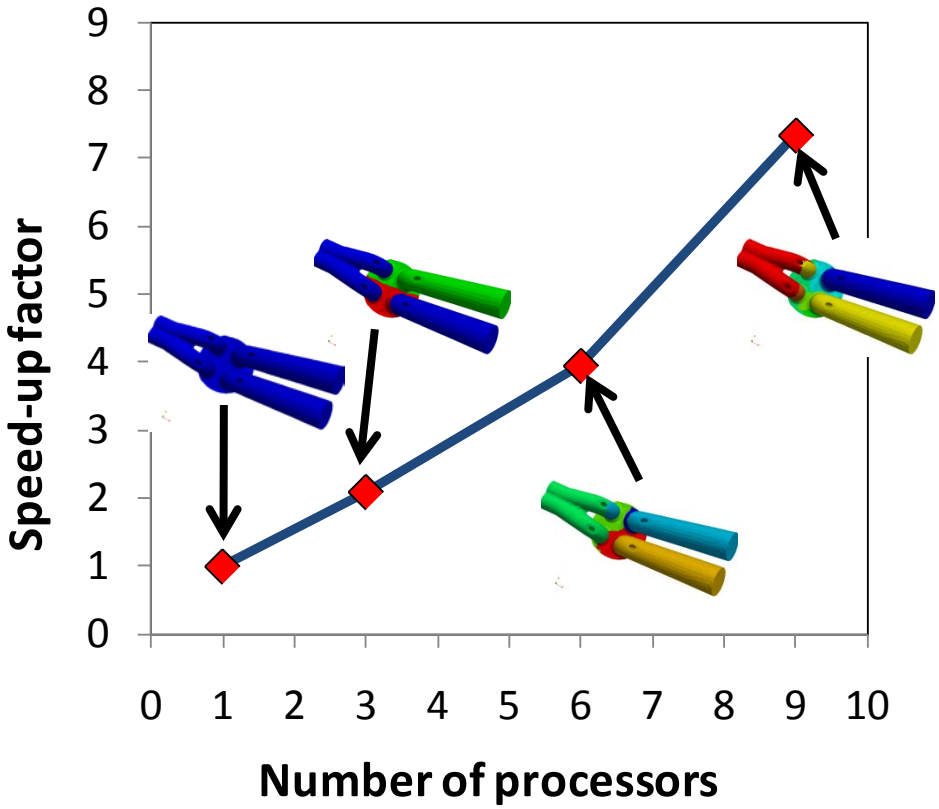
- Meshes for compression-combustion using layering



Mesh management

SANDIA Engine: parallel performance

- Full cycle simulation with deforming mesh.
- Decomposition method: **SCOTCH**
- Test performed on 1, 3, 6 and 9 processors
- Average mesh size: 500 thousand cells.
- Significant speed-up achieved.



Mesh management

Current state

- Proposed approach is reliable and provides results in rather good agreement with experimental data.
- Tested with different engine geometries without problems.
- Parallelization significantly reduce the CPU time.

Future work

- Integration of snappyHexMesh (OpenFOAM-2.0) into the proposed approach for fully-automatic mesh generation.

Spray models

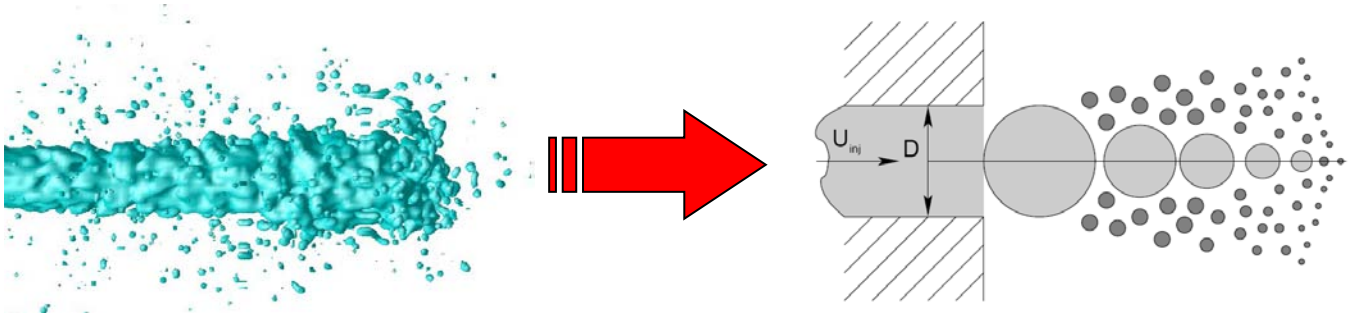
Spray models

- Extending the capabilities of the standard OpenFOAM spray library, by introducing new models for:
  - High pressure injection
  - Liquid fuel atomization
  - Droplet-wall interaction
- Reducing the grid-dependency and CPU time of spray simulations:
  - Easy development of new models.
  - Fast tuning of existing models.

Spray models

Modified Huh-Gosman model (Diesel spray)

- **Blob injection**: parcels are injected with the same nozzle diameter and injection velocity.
- Turbulent quantities (L_t, τ_t) initialized for each parcel according to the nozzle flow conditions.

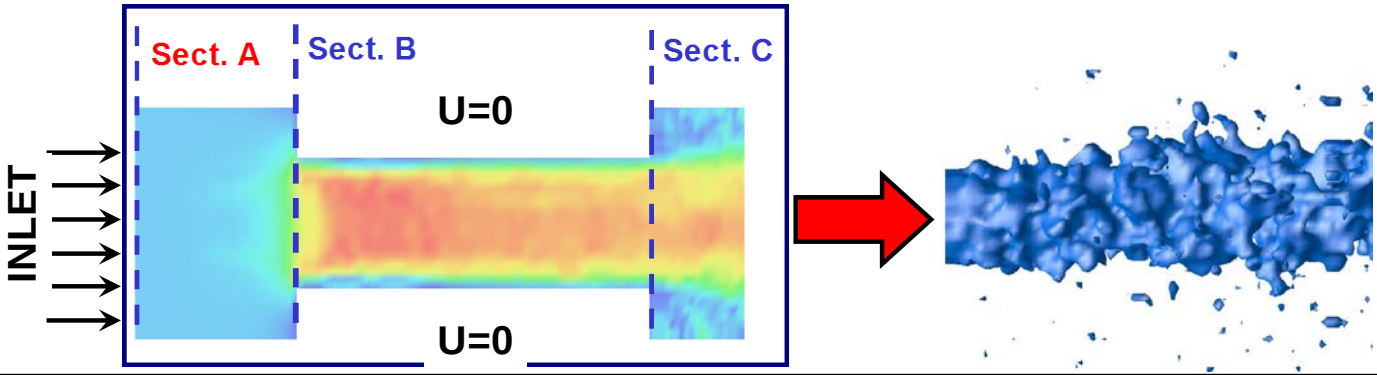


- Liquid jet atomization is modeled as:
  - Diameter reduction of the injected droplets
  - Stripping of secondary droplets from the liquid jet

Spray models

Modified Huh-Gosman model (Diesel spray)

- LES calculations of liquid-jet breakup to:
  - Verify the model assumptions on turbulence length and time scales.
  - Derive the value of the main model tuning constants.
  - Compute the diameter of the atomized droplets and the corresponding distribution.

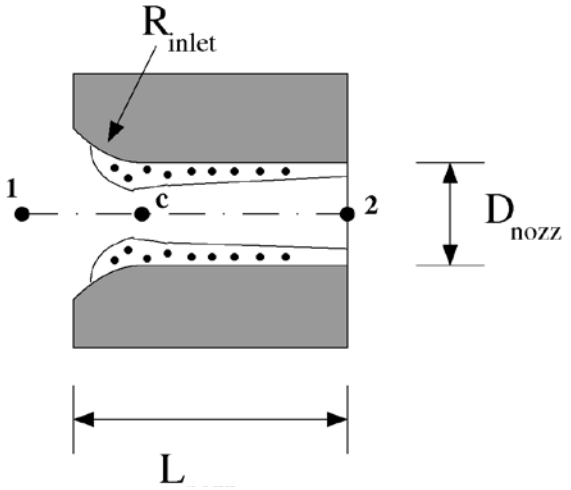


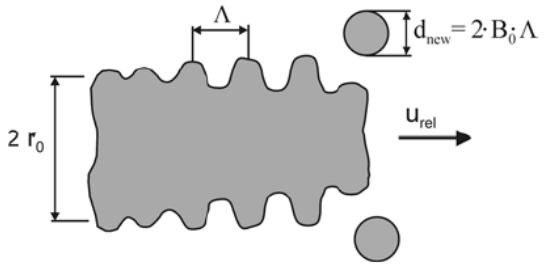
Atomization model developed in collaboration with Prof. G. Bianchi and Dr. F. Brusiani (DIEM, University of Bologna). LES calculations performed by Dr. Minelli, Dr. Scardovelli, Dr. Zaleski (DIEM, University of Bologna).

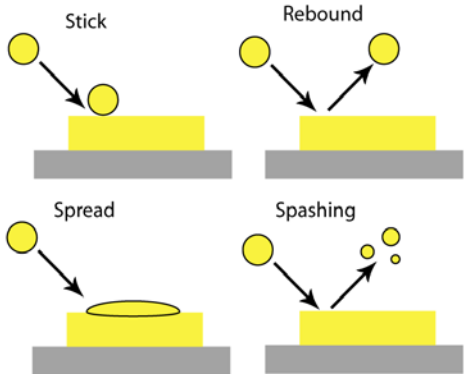
Spray models

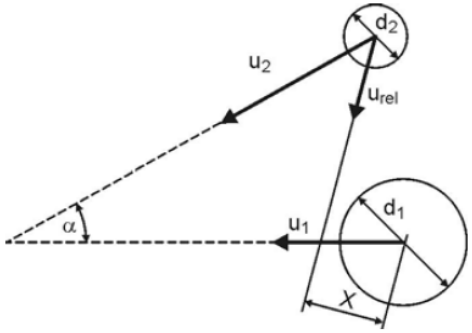
Gasoline sprays from multi-hole nozzles

- **Injection**: Huh-Gosman + Nurick models to account for the effects of cavitation on the fuel jet velocity and cone angle.
- **Breakup**: Kelvin-Helmholtz
- **Collision**: Nordin model (reduced grid-dependency)
- **Wall-impingement**: Stanton et al.





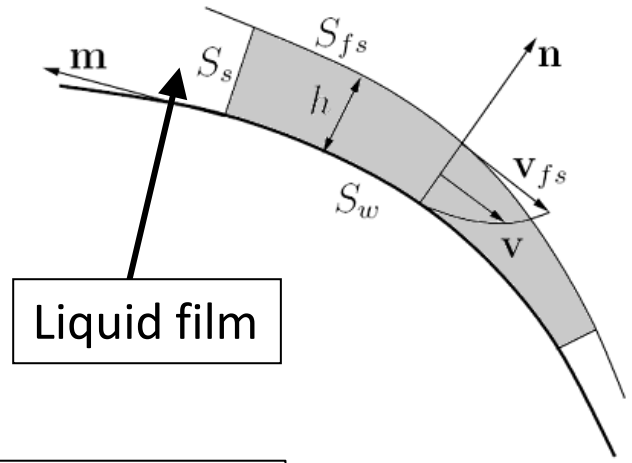




Spray models

Liquid film model

- Approach originally proposed by Bai and Gosman (SAE-960626). Thin film approximation.
- Mass, momentum and energy equation for the liquid film solved on the mesh boundary, using the finite area method.
- Droplet formation from the liquid film taken also into account.
  - Curved wall surface: **S_w**
  - Free liquid surface: **S_{fs}**
  - Liquid film thickness: **h**
  - Velocity profile



Algorithms developed in collaboration with Dr. Z. Tukovic (FSB, University of Zagreb) and Dr. H. Jasak (Wikki Ltd.)

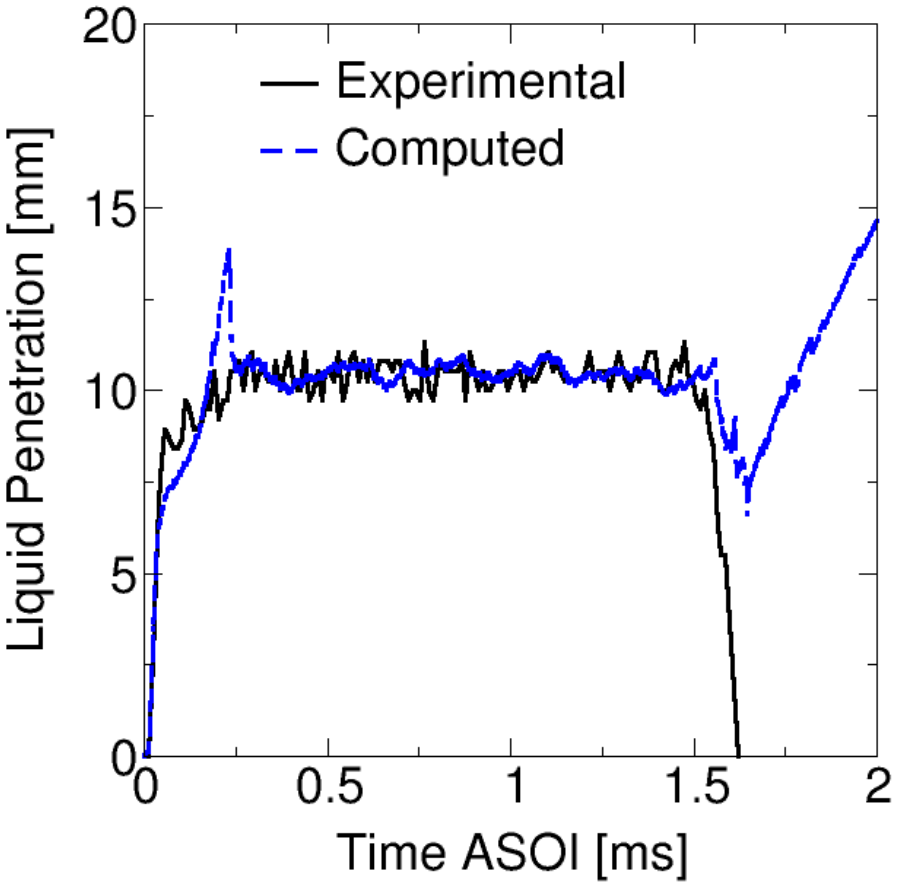
Spray models

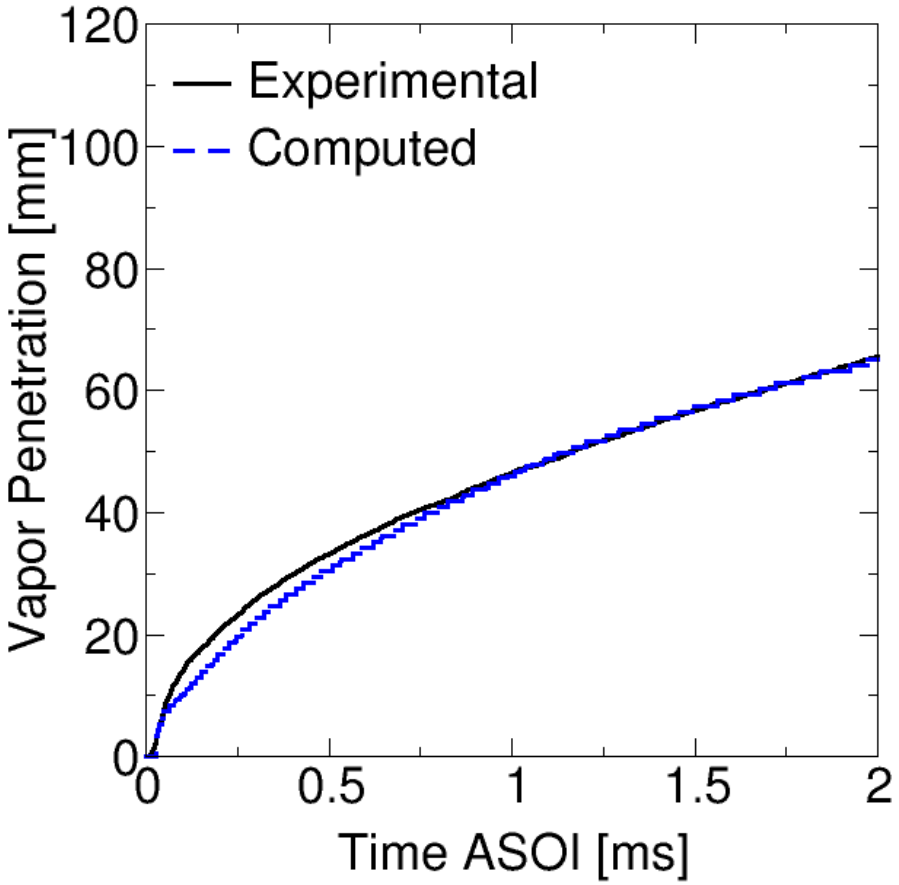
Validation: evaporating spray at Diesel conditions

Operating conditions ("Spray A" – ECN)	
Fuel	n-dodecane
Injection pressure	150 Mpa
Ambient density	22.8 kg/m^3
Ambient temperature	900 K
Oxygen volume fraction	0%
Injector properties	
Diameter	0.09 mm; k-factor: 1.5
Discharge coeff.	0.86

Spray models

Validation: evaporating spray at Diesel conditions





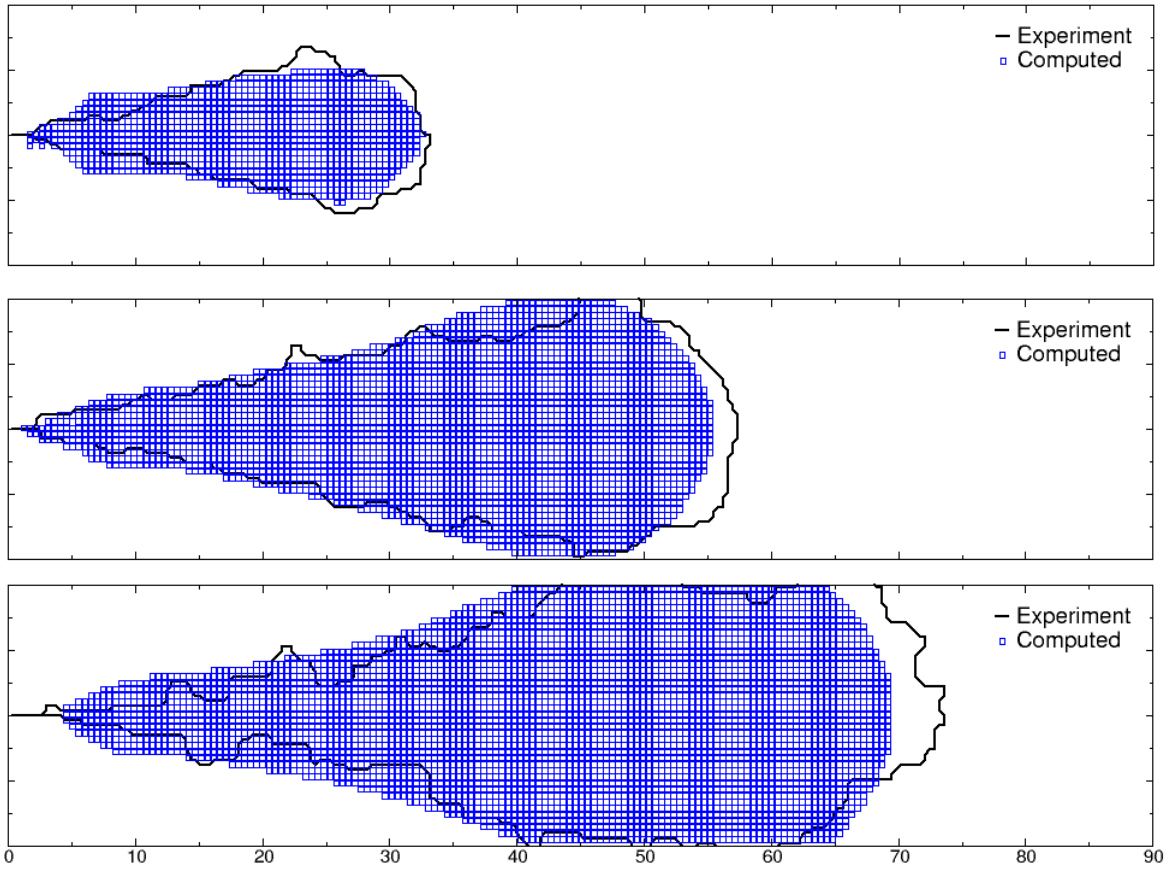
Spray models

Validation: evaporating spray at Diesel conditions

0.5 ms ASOI

1.5 ms ASOI

2.5 ms ASOI

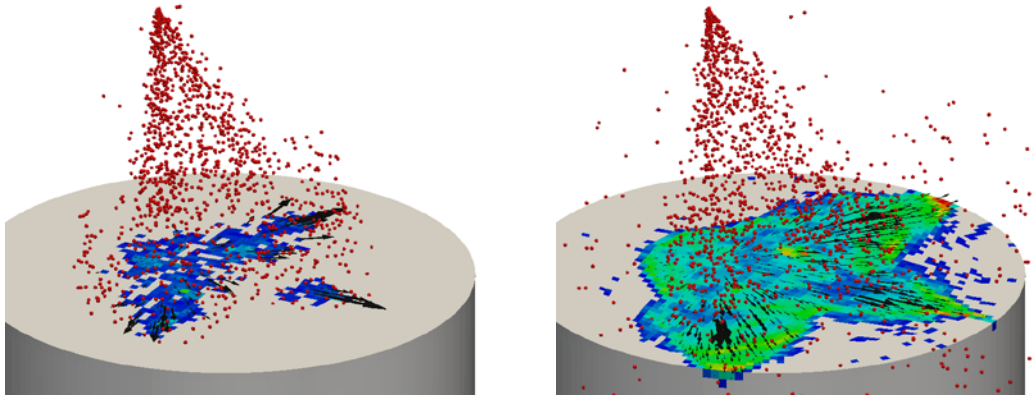


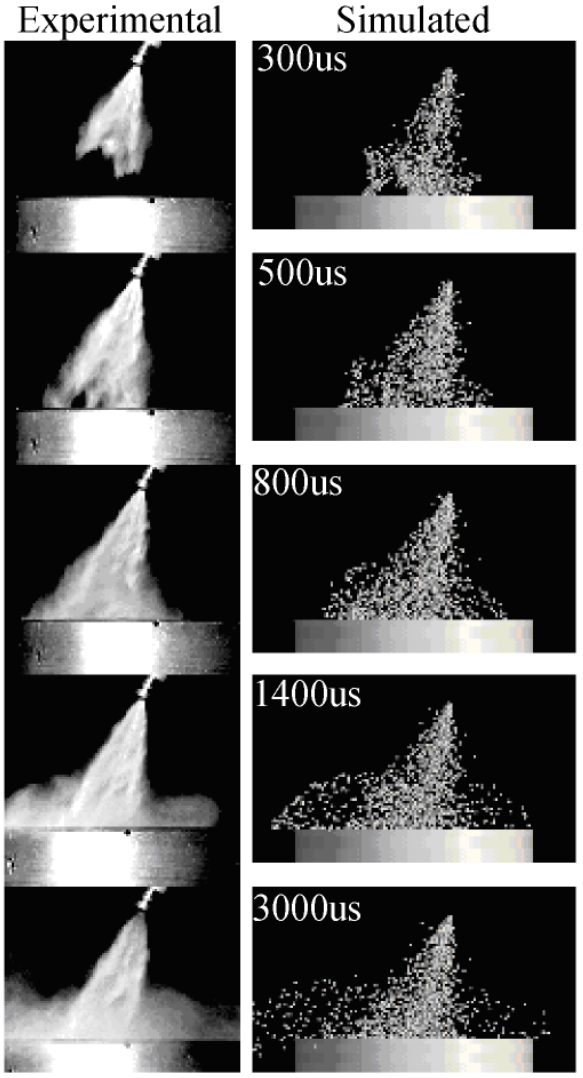
Spray models

Validation: impinging spray

Liquid film formation on the plate

(a) t = 400 µs **(b) t = 2300 µs**

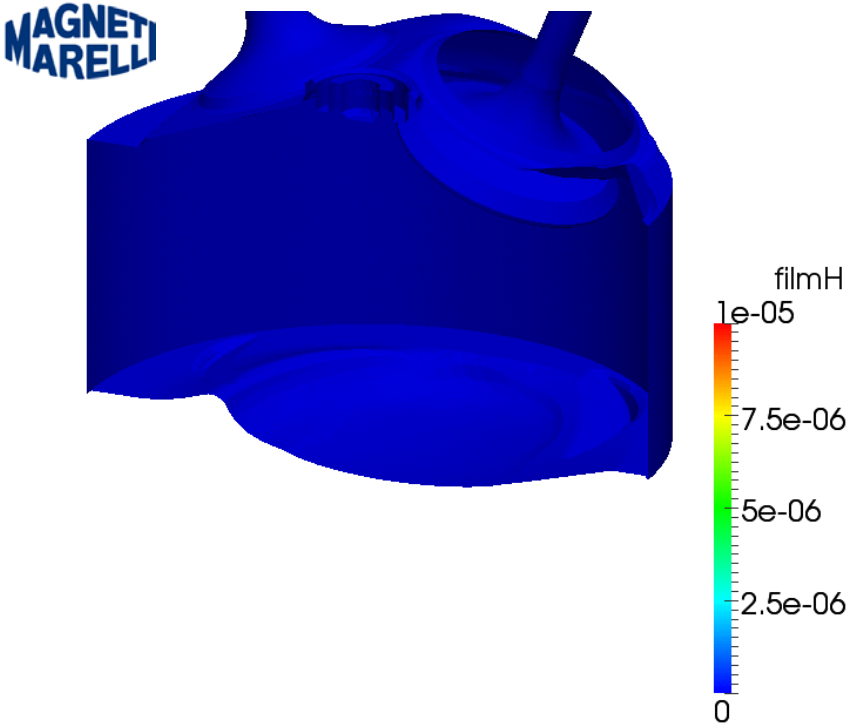




Experimental data provided by Dr. Alessandro Montanaro and Dr. Luigi Allocca, CNR, Istituto Motori, Naples.

Spray models

Application: fuel-air mixing in a GDI engine



Time: -285 CA

Simulation includes:

- Exhaust + intake + compression phases
- Fuel emerging from a multi-hole injector
- Wall film dynamics
- Film atomization due to the interaction between air and film on the valve

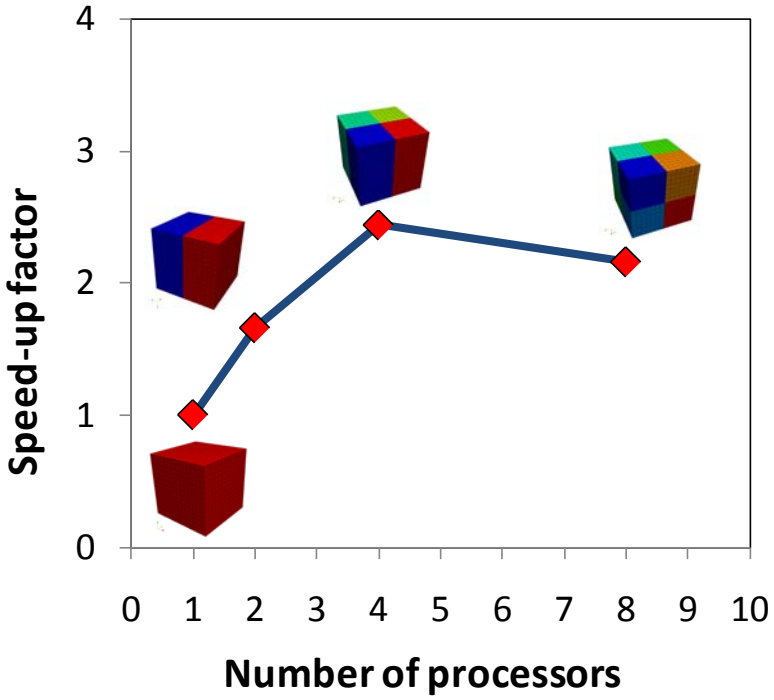
Work performed in collaboration with Ing. Rita Di Gioia, Dr. Giovanni Bonandrini, Ing. Luca Venturoli, Magneti Marelli, Bologna.

Spray models

Parallelization

- Spray library and wall film now works in parallel, including also ALMR. Decomposition methods currently used: scotch and simple.
- Scalability test performed on a constant-volume, evaporating and non-reacting case with ALMR.

- ➢ Decomposition method: **simple**
- ➢ Test performed on 1, 2, 4 and 8 processors
- ➢ ALMR scalability: very good until 4 processors are used.
- ➢ Parallel spray simulations: manual decomposition for load balancing.



Spray models

Current state

- Consolidated library to simulate IC engine sprays.
- Parallelized.

Future work

- Inclusion of new wall impingement models, to better account for Leidenfrost effect.
- PhD project on atomisation models for advanced Diesel fuel injection systems.

Combustion models

Combustion models

- A reliable and fast set of models has been developed for industrial calculations:
  - CTC for Diesel combustion
  - CFM for SI combustion (including GDI)
- Advanced combustion models under development:
  - To perform fundamental studies
  - Improving the capabilities of the existing models
  - Study of new combustion modes

Combustion models: Diesel

Diesel combustion models

Modified CTC (Characteristic Time-Scale) model

- 11 chemical species (fuel, O_2, N_2, CO, CO_2, H_2O, O, OH, NO, H, H_2)

- Auto-ignition computed by the Shell auto-ignition model; turbulent combustion simulated accounting for both laminar and turbulent time scales:

$$\dot{Y}_i = \alpha \cdot \dot{Y}_{i,Shell} + (1-\alpha) \cdot \dot{Y}_{i,CTC}$$

- Temperature threshold to switch between auto-ignition ($\alpha=1$) and turbulent combustion ($\alpha=0$).

Diesel combustion models

Modified CTC (Characteristic Time-Scale) model

New formulation to compute the characteristic time-scale:

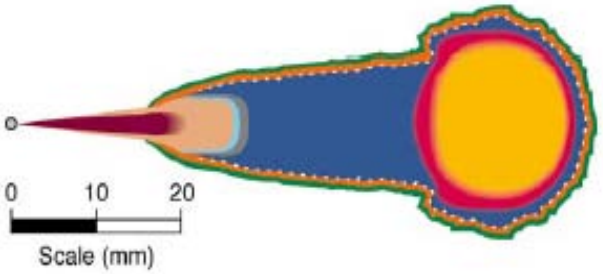
$$\dot{Y}_{i,CTC} = -\frac{Y_i - Y_i^*}{\tau_{CTC}} \quad \text{, where} \quad \tau_C = (1-f)\cdot\tau_l + f\tau_t$$

- Fuel oxidation rate under rich conditions and during the expansion stroke correctly described.
- **The multi-scale approach** was also included, to account for the different oxidation mechanisms of fuel and CO.
- Pollutant emission sub-models: Zeldovich for NO_x, Hiroyasu for soot.

Diesel combustion models

Direct integration of complex chemistry

- Detailed chemistry is necessary to describe the main features of the flame structure under advanced combustion modes:
  - Auto-ignition
  - Pollutant formation (soot, NO_x)
  - Diffusion flame



- Proposed approach: direct integration of complex chemistry in each computational cell. Each cell is an homogeneous reactor and species reaction rates are computed by means of an ODE stiff solver:

$$Y_i^*(t+\Delta t) = Y_i(t) + \int_t^{t+\Delta t} \dot{\omega}_i \frac{W_i}{\rho} dt' \quad \Rightarrow \quad \dot{Y}_i = \frac{Y_i^*(t+\Delta t) - Y_i(t)}{\Delta t}$$

- Detailed approach but very time-consuming.

Diesel combustion models

Direct integration of complex chemistry

- **Reduction of CPU time**

- **ISAT: In-situ adaptive tabulation** of the reaction mapping for a species array. The complete ISAT implementation is used including the mapping gradient matrix.

- **DAC (dynamic adaptive chemistry)**
  - Reduction of a detailed chemical mechanism in each computational cell before every call to the stiff solver using the DRG (direct relation graph) method.
  - Only the significant reactions and species are involved.

Work performed in collaboration with Dr. Francesco Contino, Prof. Herve Jeanmart, University of Leouvain. Belgium.

Diesel combustion models

Diesel combustion process simulation: solvers

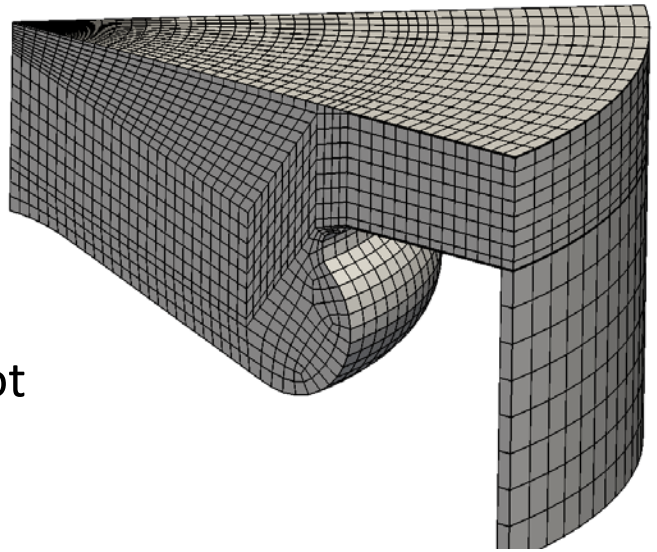
1) `CTCEngineDyMFoamSootNOx`: solver for diesel spray combustion in engines, including mesh motion and topological changes. **Combustion model**: characteristic-timescale combustion model. Prediction of NO_x and soot emissions.

2) `dieselEngineDyMFoam`: solver for diesel spray combustion in engines, including mesh motion and topological changes. **Combustion model**: direct integration of detailed chemistry with TDAC.

Diesel combustion models

Case study: passenger-car, common-rail engine

Bore	85 mm
Stroke	88 mm
Compression ratio	~15



Operating conditions:

- Full load with post-injection to reduce soot
- Medium high load with:
  - Variable EGR rate
  - Three injection events (pre, main, post)

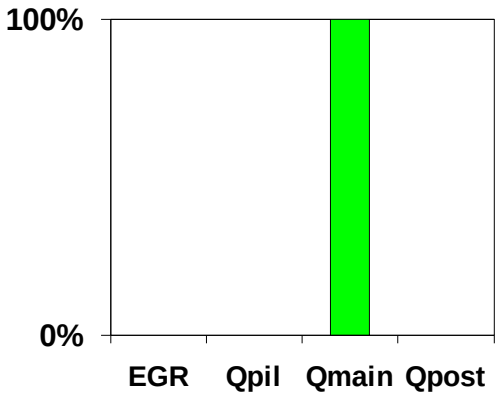
Models:

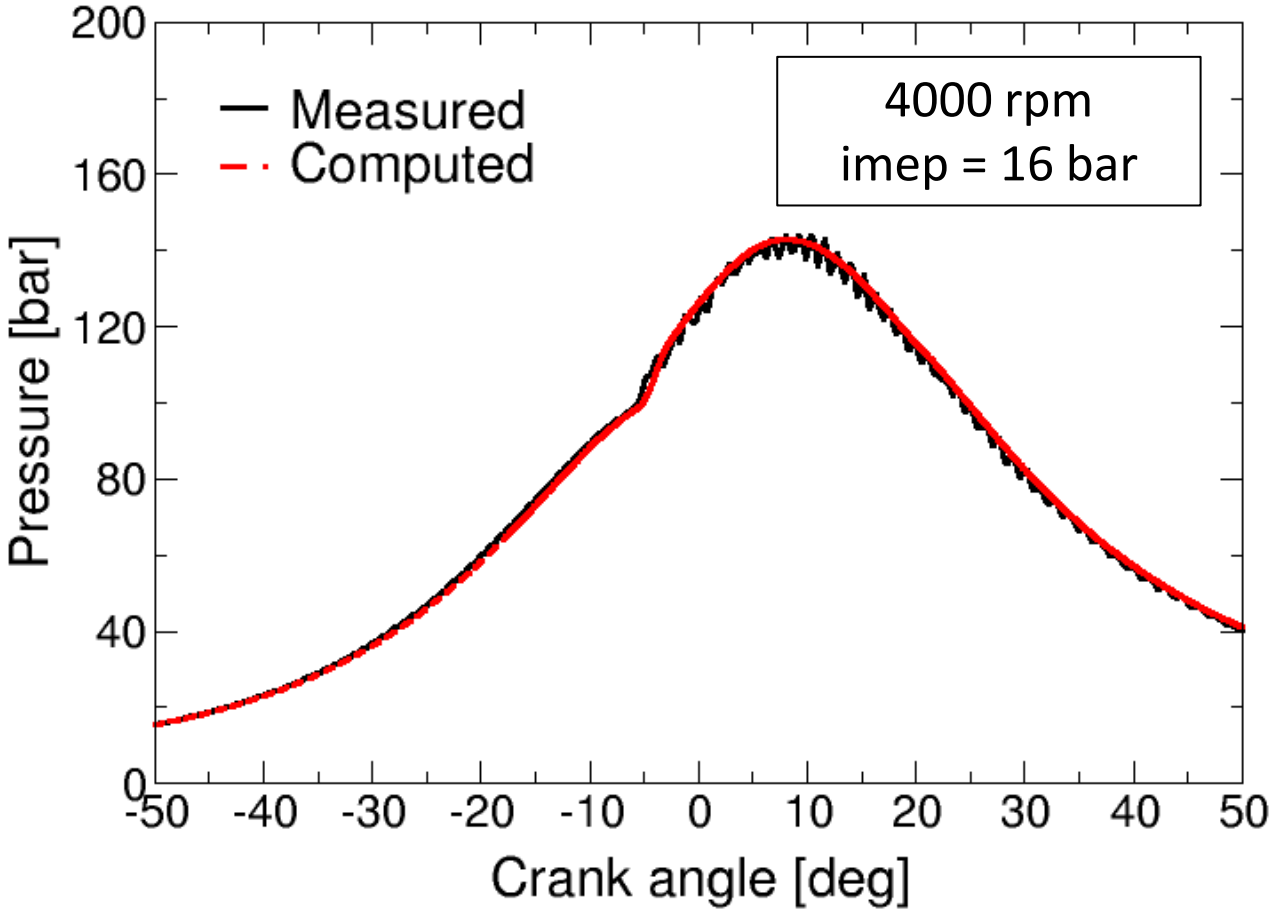
- Modified Huh-Gosman for atomization. Diesel fuel approximated as $C_{12}H_{26}$
- CTC+Shell for combustion. $C_{12}H_{26}$ Shell-model constants proposed by Reitz.

Diesel combustion models

Case study: cylinder pressure validation at full load

Full load, single injection, No EGR

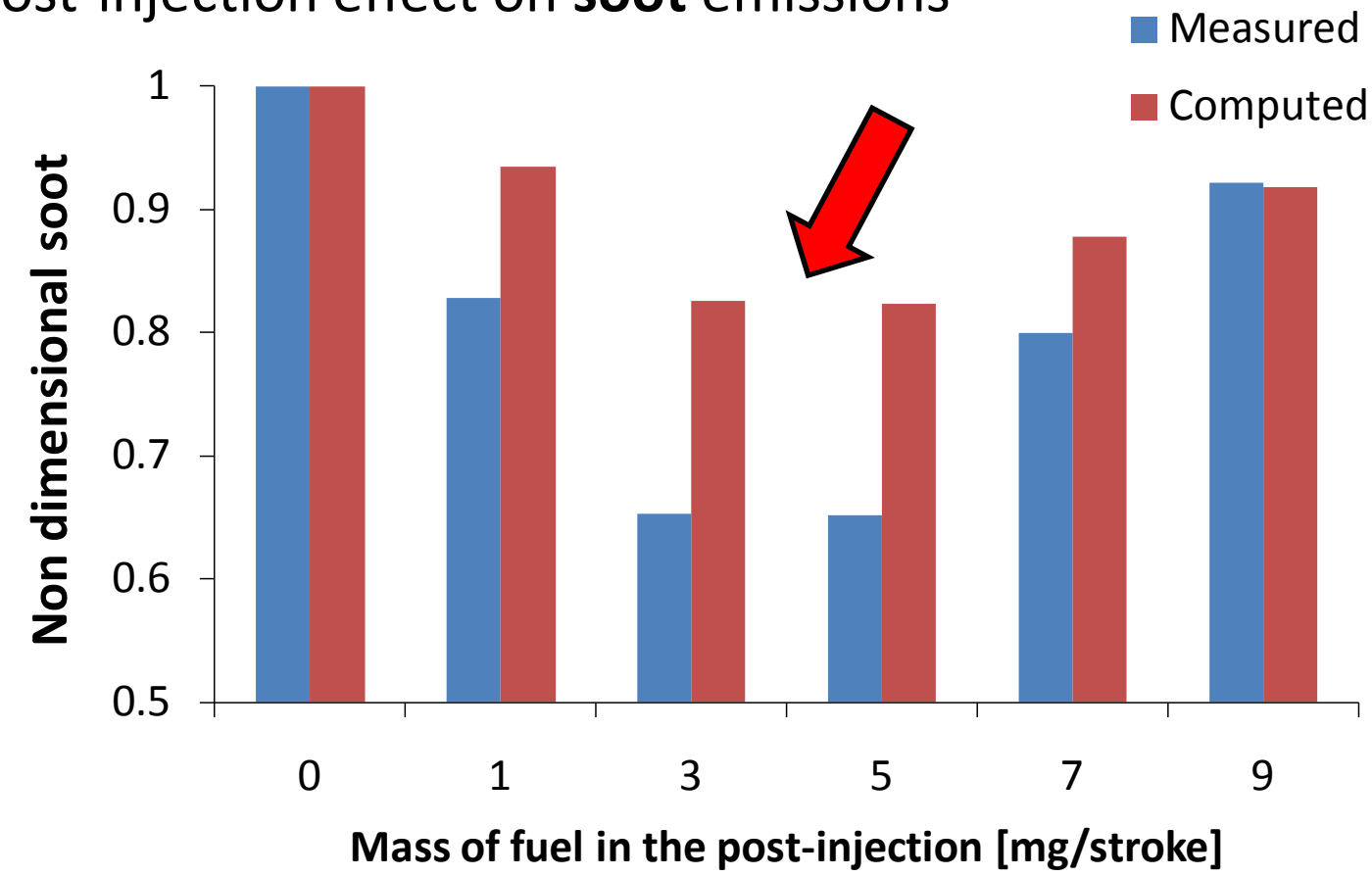




Diesel combustion models

Case study: soot emissions, full load

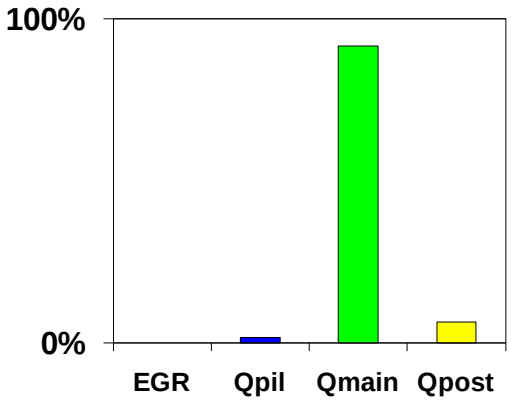
- Post-injection effect on **soot** emissions

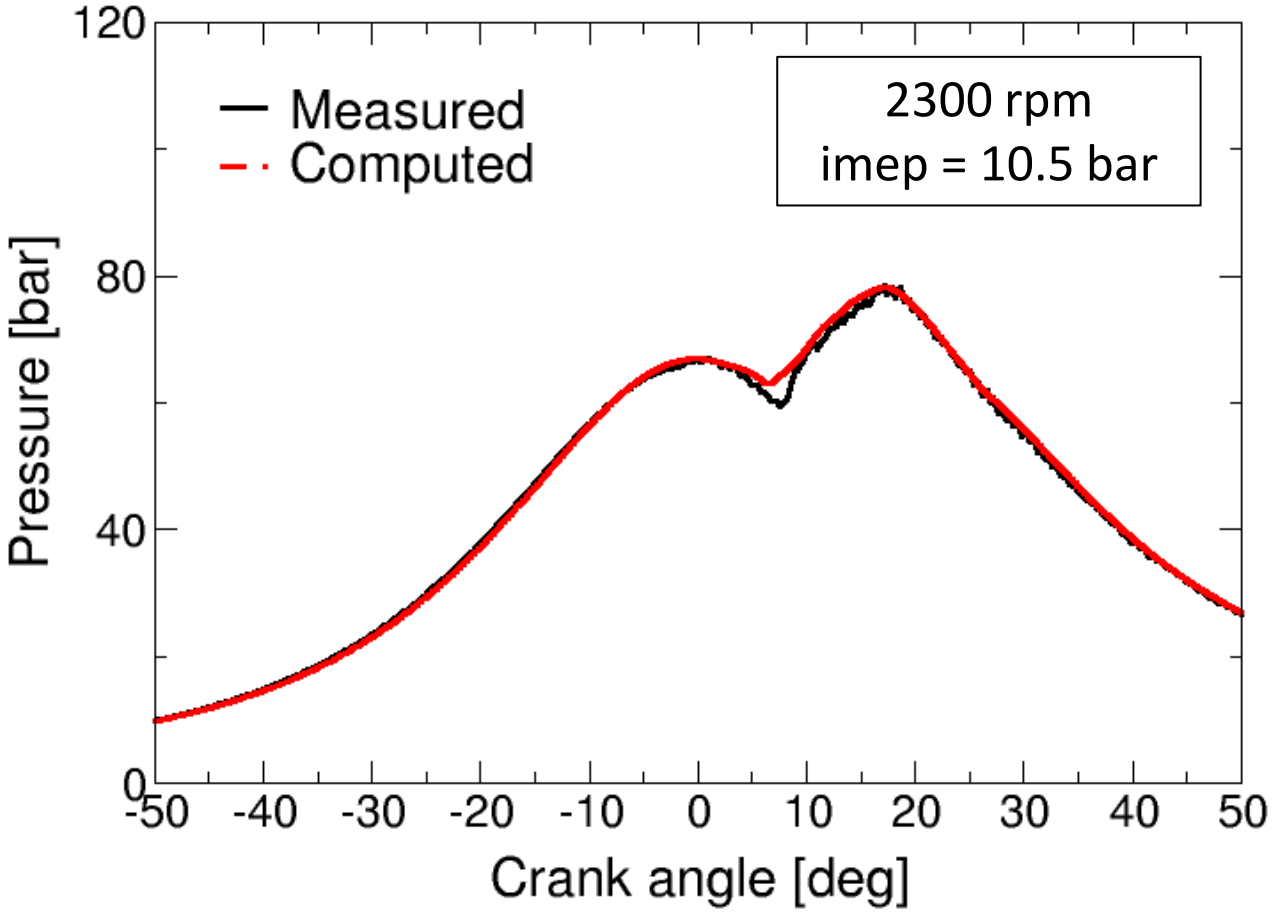


Diesel combustion models

Case study: cylinder pressure validation at mid-load

Medium-high load,
0% EGR
3 injections

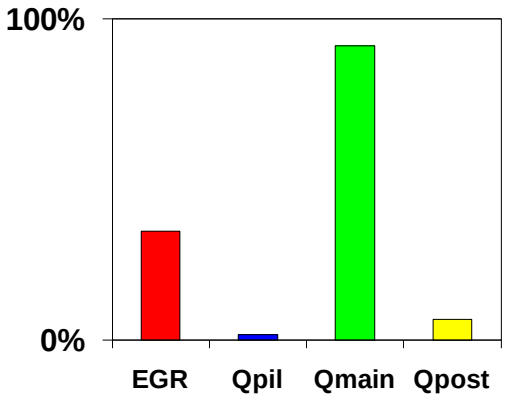


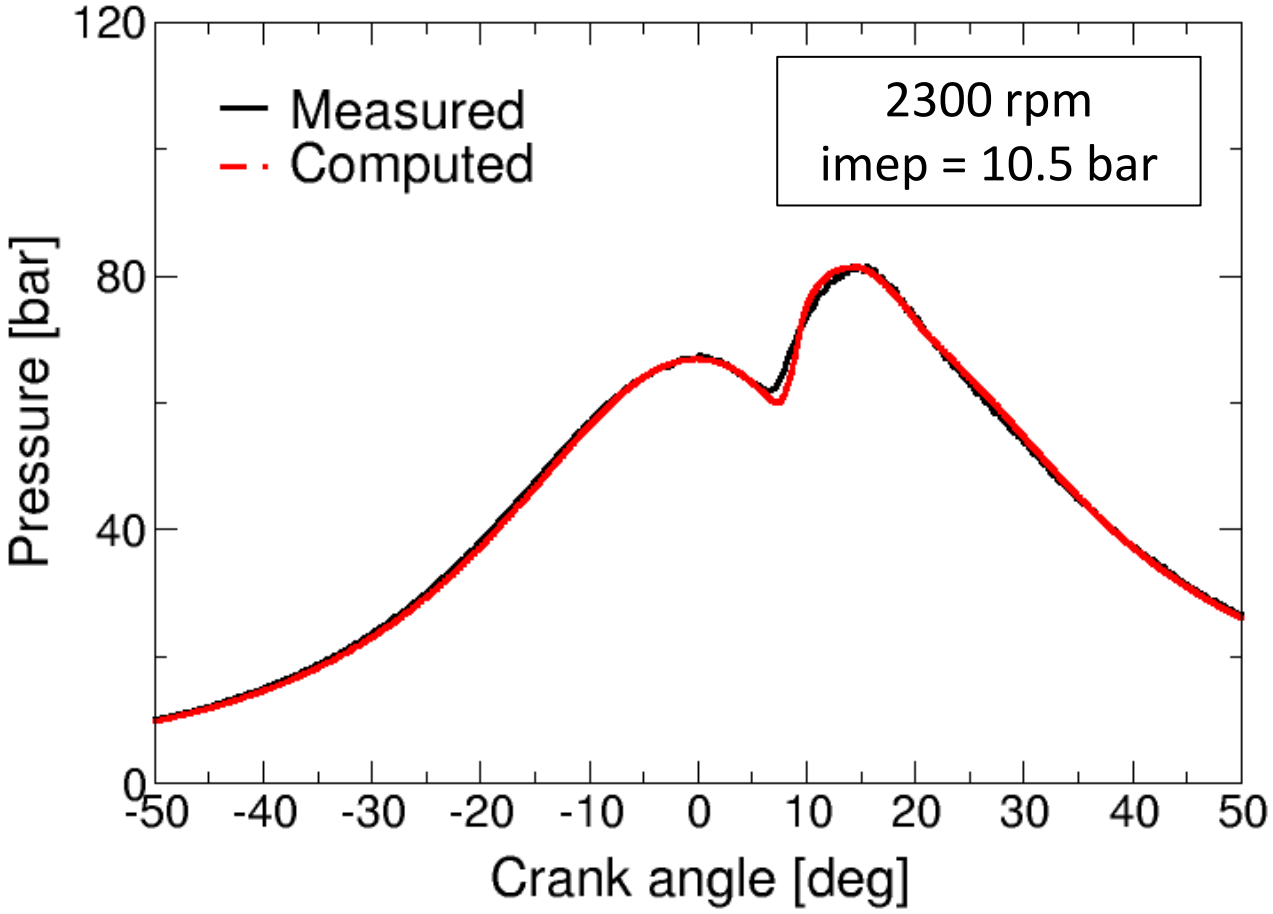


Diesel combustion models

Case study: cylinder pressure validation at mid-load

Medium-high load,
34% EGR
3 injections

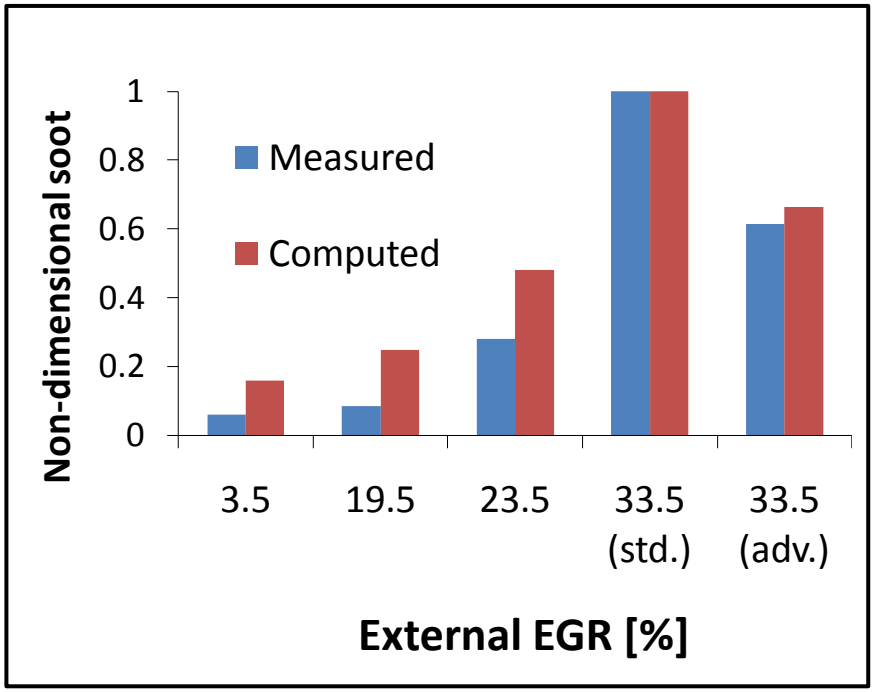


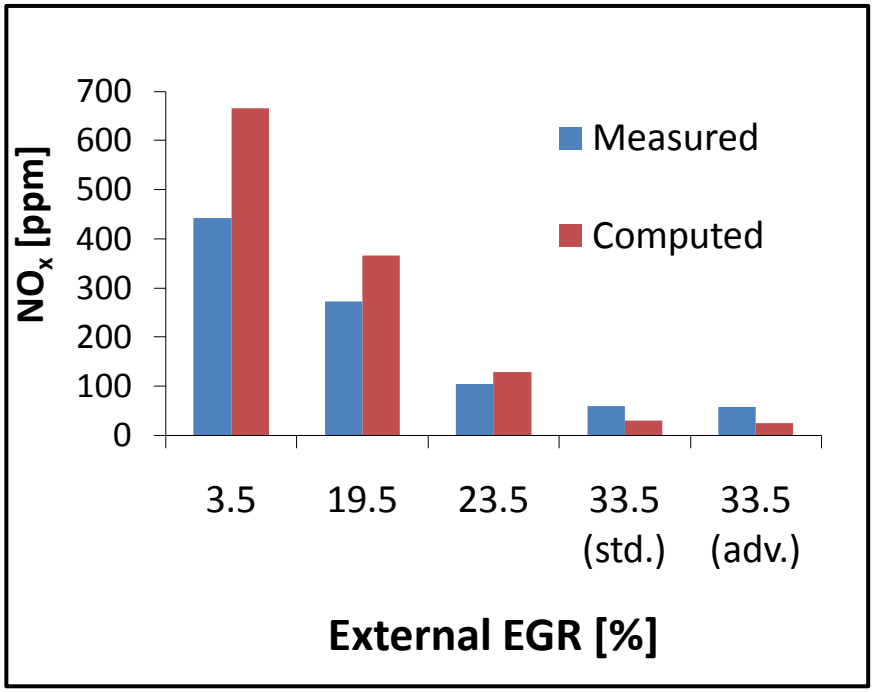


Diesel combustion models

Case study: soot emissions, medium-high load

- Injection strategy and external EGR effects on **soot** and **NO_x** emissions

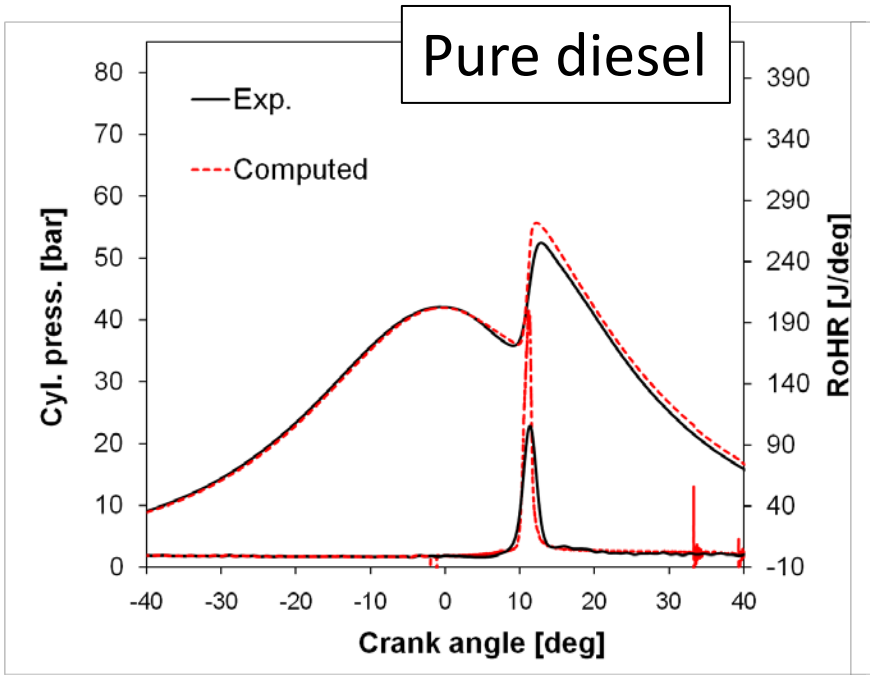


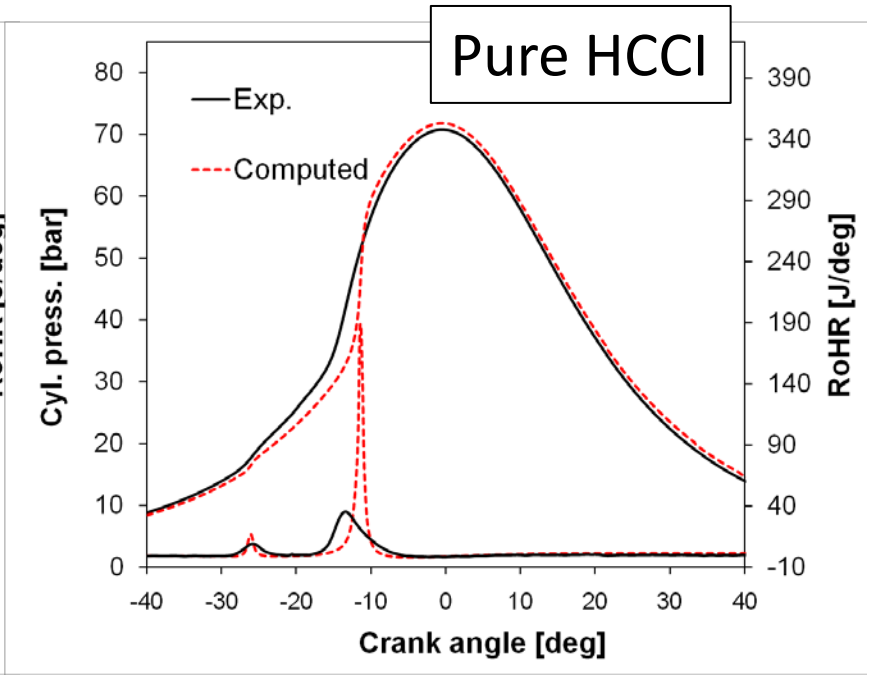


Diesel combustion models

Study of mixed mode HCCI/Diesel combustion

- **Lean condition: ϕ = 0.28, fuel: n-heptane**





- Chemical mechanism by Golovichev et al. (56 species, 290 reactions).

Work performed in collaboration with Dr. Maya Briani, Dr. Valentina Fraioli, Dr. Marianna Migliaccio, CNR-Istituto Motori, Naples.

Diesel combustion models

Current state

- **Modified CTC:** extensively tested and reliable for diesel combustion simulations, also with multiple injections. Limitations: multi-component fuels, advanced combustion modes. Parallel.

- **Direct integration of complex chemistry:** study of advanced combustion modes (dual-fuel, HCCI, PCCI..) possible with a limited amount of CPU time. Limitations: turbulence-chemistry interaction is not taken into account. Parallel.

Future work

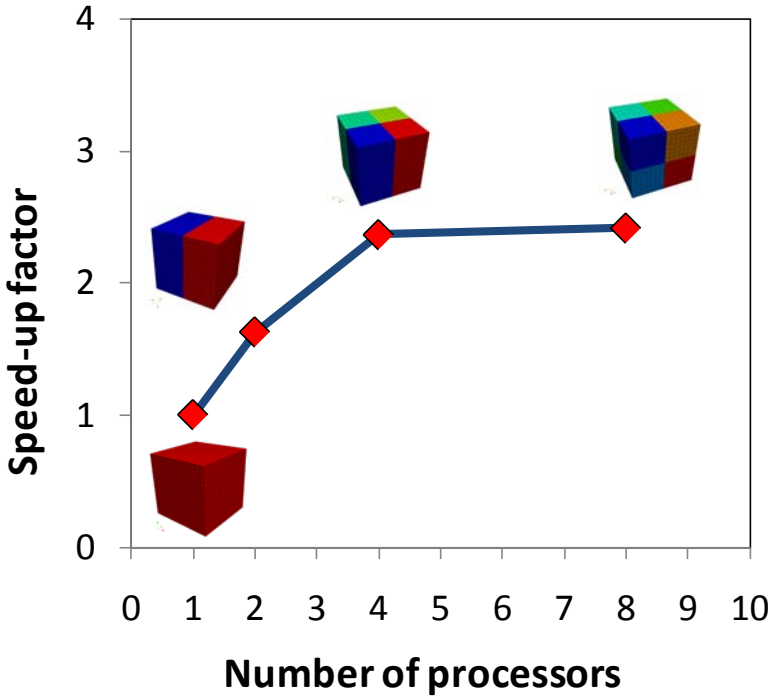
- Development of combustion models accounting for turbulence/chemistry interaction: multi-zone chemistry, FGM, CMC, …

Diesel combustion models

Parallelization

- Chemistry library now works in parallel. Decomposition methods currently used: scotch and simple. Scalability test performed on a constant-volume, evaporating and reacting case with ALMR and TDAC.

- Decomposition method: **simple**
- Test performed on 1, 2, 4 and 8 processors
- ALMR scalability: very good until 4 processors are used.
- Scalability depending on decomposition.



Combustion models: Spark-ignition and GDI

Spark-ignition combustion models

Coherent flamelet model (CFM)

- Model available for simulating SI and GDI engines.
- 12 chemical species (fuel, O_2, N_2, CO, CO_2, H_2O, O, OH, NO, H, H_2, unburned fuel).
- Burned gas composition computed at equilibrium. Unburned fuel taken also into account for very rich mixtures.
- Modified version of the Eulerian AKTIM model to compute flame kernel growth. Flame surface computed from intersection between a spherical STL surface and the combustion chamber.
- Transport equation solved for the flame surface density Σ.

Spark-ignition combustion models

Diesel combustion process simulation: solvers

1) `simpleCFMEngineDyMFoam`: solver for combustion in SI engines with mesh motion and topological changes.

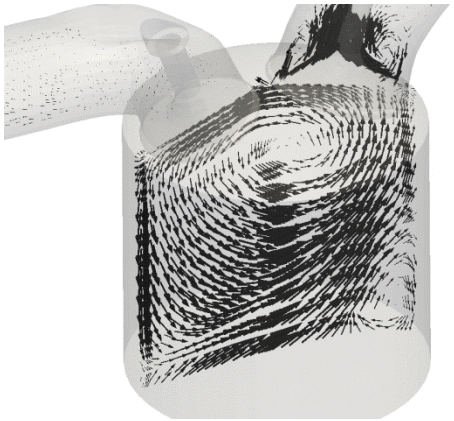
   Combustion model: Coherent Flamelet Model. Prediction of NO_x emissions and soot. It accounts for unburned fuel in burned gases during stratified combustion.

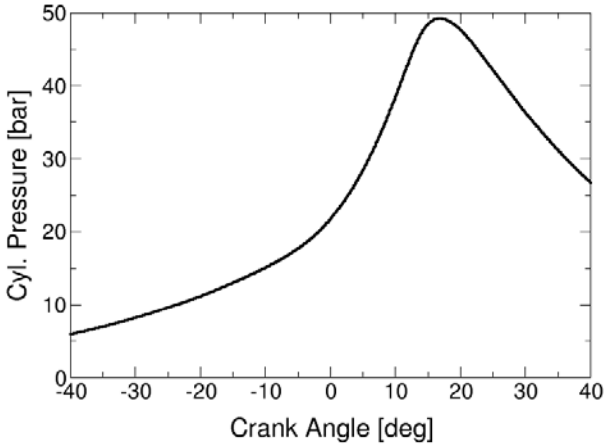
   Pollutant prediction: NO_x (Zeldovich) and soot (Hyroyasu + NSC)

Spark-ignition combustion models

Coherent flamelet model (CFM): application

- Example of application: two-valve engine, homogeneous
- Compression stroke (after intake) and combustion





Computational mesh provided by Dr. Marco Chiodi, Prof. Dietmar Schmidt, Msc. Benjamin Boose, FKFS, Stuttgart.

Spark-ignition combustion models

Current state

- **CFM:** reliable model, validation almost finished. Drawbacks:
  - Flame kernel growth
  - Highly stratified combustion

Future work

- Introduction of a new flame kernel model, based on the Lagrangian approach.
- Development of a flameled-based combustion model, to correctly account for stratified combustion.

Collaborative research projects

Past research projects

- **University of Leouvain (2009):**
  - **Dr. Francesco Contino:** *simulation of HCCI combustion using detailed chemistry and advanced tabulation and mechanism reduction techniques*. Supervisors: Prof. H. Jeanmart, Prof. G. D'Errico, Dr. T. Lucchini.

- **Malaysian Campus of the Nottingham University (2010)**:
  - **Phd student Harun Ismail**: *combustion simulation using biodiesel and detailed chemistry*. Supervisors: prof. Ng, Dr. T. Lucchini.

New research projects

Starting from September 2011:

- **Aalto University, Helsinki:**
  - Phd student **Jukka Pekka:** LES simulation of in-cylinder flows. Supervisors: Prof. M. Larmi, Prof. O. Kaario, Dr. F. Piscaglia, Dr. A. Montorfano

- **University of New South Wales, Sidney**:
  - Phd student **S.Pasunurthi**, *Combustion modeling of Dual Fuel SI engines using LES.*
  - Phd student **J. Behzadi Aghaei**, LES of stratified engines.
  - Phd student **F. Salehi,** Modelling efficient engines with large-eddy simulation.

  Supervisors: Prof. E. Hawkes, Prof. G. D'Errico, Dr. T. Lucchini

Conclusions

Conclusions

Lib-ICE, library for IC engine simulations based on OpenFOAM® technology:

- Reliable, validated and parallel tool for massive calculations of gas exchange, fuel-air mixing and combustion.

- Consolidated set of libraries that can be further developed to include more complex spray and combustion models.