METHODOLOGIES FOR THE NUMERICAL SIMULATION OF FLUID FLOW IN INTERNAL COMBUSTION ENGINES

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Main characteristics of in-cylinder flow problems in internal combustion (IC) engines

• Turbulent viscous compressible flow.



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- 3D moving domains with complex geometry, high deformation and topological changes.



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Main characteristics of in-cylinder flow problems in internal combustion (IC) engines

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- Low Mach number flow during the major fraction of the cycle.



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Navier-Stokes equations

Using an ALE (Arbitrary Lagrangian Eulerian) strategy, the system of Navier-Stokes equations in its quasi-linear form can be written as

$$\frac{\partial \mathbf{U}}{\partial t} + (\mathbf{A}_i - w_i \mathbf{I}) \frac{\partial \mathbf{U}}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\mathbf{K}_{ij} \frac{\partial \mathbf{U}}{\partial x_j} \right) + \mathbf{S} \quad \text{on } \Omega_t \times (\mathbf{0}, t_{\mathrm{f}})$$

Boundary conditions at solid walls

- Condition on the flow velocity.
- Condition on the temperature or the heat flux.

Boundary conditions at inlet/outlet

• Dynamic absorbing boundary conditions.

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Numerical implementation

- The equations are discretized in space using the Finite Element Method (FEM).
- The method is stabilized by means of the Streamline-Upwind/Petrov-Galerkin (SUPG) technique.
- An isotropic shock-capturing strategy is included in order to stabilize the computations in the presence of sharp gradients.
- The trapezoidal difference scheme is applied for time discretization.
- The absorbing boundary conditions are applied using Lagrange multipliers.

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Numerical implementation

'Mixed' absorbing/wall boundary conditions



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Numerical implementation

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'Mixed' absorbing/wall boundary conditions (cont.)



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Mesh dynamics

Motivation

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Mesh dynamics

Motivation

Remeshing

- A body-conforming mesh has to be regenerated at each time step.
- The projection of solutions from a mesh to another one is needed.
- When implicit schemes are applied in an environment of parallel computing, the matrix profile must be calculated at each remeshing stage.

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Mesh dynamics

Motivation

Remeshing

- A body-conforming mesh has to be regenerated at each time step.
- The projection of solutions from a mesh to another one is needed.
- When implicit schemes are applied in an environment of parallel computing, the matrix profile must be calculated at each remeshing stage.

Mesh movement

• The motion of the grid could cause the deterioration of the mesh quality and, in some situations, generate an invalid mesh.

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The mesh dynamics strategy

The CMD (Computational Mesh Dynamics) strategy developed could be classified as a mesh smoothing method and it is based on an optimization problem, where the functional (F) is defined in terms of some appropriate element quality indicator.

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The mesh dynamics strategy

The CMD (Computational Mesh Dynamics) strategy developed could be classified as a mesh smoothing method and it is based on an optimization problem, where the functional (F) is defined in terms of some appropriate element quality indicator.

Some design conditions for *F* are:

- *F* should be computed from element contributions.
- The minimum of *F* should give the best mesh quality.
- *F* should be well behaved enough in order to solve the minimization problem with Newton-like methods.
- *F* should be convex in order to guarantee uniqueness of the minimum and positivity of the stiffness matrices.

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Functional design

Expression for the element functional proposed

$${m {\sf F}}_e = C_{
m v} \left(rac{V_e}{V_{
m ref}^e} - 1
ight)^m + C_{
m q} q_e^n, \hspace{1em} m \hspace{1em} {
m even}, \hspace{1em} n < 0$$

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Functional design

Expression for the element functional proposed

$$egin{aligned} F_{e} &= C_{\mathrm{v}} \left(rac{V_{e}}{V_{\mathrm{ref}}^{e}} - 1
ight)^{m} + C_{\mathrm{q}} q_{e}^{n}, & m ext{ even}, \ n < 0 \end{aligned}$$

Element quality indicator applied

$$q = C \left[\sum_{i=1}^{N} \left(q_{\mathcal{S},i}
ight)^n
ight]^{1/n}$$

where

$$q_{\mathcal{S}} = rac{V}{S_e}, \quad S_e = \sum_j l_j^{n_{
m d}}$$

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Step 2D



 Imposed displacements on boundary nodes.

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Step 2D



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Step 3D



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Step 3D



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Step 3D



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• $F \rightarrow \infty$ when $q_e \rightarrow 0$ (for simplicial elements, $V_e \rightarrow 0$).

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• $F \rightarrow \infty$ when $q_e \rightarrow 0$ (for simplicial elements, $V_e \rightarrow 0$).



t = 0

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• $F \rightarrow \infty$ when $q_e \rightarrow 0$ (for simplicial elements, $V_e \rightarrow 0$).



t = 0

 $t = \Delta t_{\rm CMD}$ (Valid mesh)

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• $F \rightarrow \infty$ when $q_e \rightarrow 0$ (for simplicial elements, $V_e \rightarrow 0$).



t = 0

 $t = \Delta t_{
m CMD}$ (Valid mesh)

 $t = \Delta t_{
m CFD}$ (Tangled mesh)

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• $F \rightarrow \infty$ when $q_e \rightarrow 0$ (for simplicial elements, $V_e \rightarrow 0$).





 The CMD strategy presented requires valid meshes at the begin of each time step and, thus, conditioning the Δt.

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• The functional is regularized by replacing the volume in the expression of the element quality indicator by the function

$$h(V) = \frac{1}{2} \left(V + \sqrt{V^2 + 4\delta^2} \right)$$

• For
$$V > 0$$
, $h(V) \rightarrow V$ when $\delta \rightarrow 0$.

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Simultaneous mesh untangling and smoothing

- $\delta > 0$ is needed in the untangling stage.
- $\delta \rightarrow 0$ is needed in the smoothing stage.
- Defining a decreasing sequence {δ^k} such that δ^k → 0 when k → ∞, a simultaneous mesh untangling and smoothing technique is obtained.

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Simultaneous mesh untangling and smoothing

- $\delta > 0$ is needed in the untangling stage.
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- Defining a decreasing sequence {δ^k} such that δ^k → 0 when k → ∞, a simultaneous mesh untangling and smoothing technique is obtained.

For the tests, the following convergence criteria is applied:

1. 4

• Valid mesh.

• For the iteration k,
$$\frac{|q_{\text{mesh}}^{k} - q_{\text{mesh}}^{k-1}|}{q_{\text{mesh}}^{k}} < \epsilon_{\text{q}}$$
, being $q_{\text{mesh}} = \min_{e} q_{e}$ and $\epsilon_{\text{q}} > 0$ a prefixed tolerance.

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Results Step 2D

- Imposed displacement on boundary nodes.
- Solved in 1 time step.



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Results Step 2D

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Results Step 2D

- Imposed displacement on boundary nodes.
- Solved in 1 time step.



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% def

% dof

Results Step 3D

- Imposed displacement on boundary nodes.
- Solved in 1 time step.



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Results Step 3D

- Imposed displacement on boundary nodes.
- Solved in 1 time step.





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Results Step 3D

- Imposed displacement on boundary nodes.
- Solved in 1 time step.





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Axisymmetrical flowmeter



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Results Diesel engine with three valves



- Sliding nodes on cylinder walls and valve stems.
- Imposed displacements on remaining nodes.

•
$$\Delta \theta = 1^{\circ}$$
.

• Initial $q_{\text{mesh}} = 0.0211$.

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Diesel engine with three valves



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Diesel engine with three valves



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Resolution of compressible flows with low Mach numbers

Motivation

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Resolution of compressible flows with low Mach numbers

Motivation

Strategies proposed in the bibliography to solve flows in the low Mach number limit:

- The modification of compressible solvers (density based), *e. g.*, preconditioning and asymptotic methods.
- The extension of incompressible solvers (pressure based), *e. g.*, artificial compressibility.
- Unified formulations compressible-incompressible.

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Resolution of compressible flows with low Mach numbers

Motivation

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- The modification of compressible solvers (density based), *e. g.*, preconditioning and asymptotic methods.
- The extension of incompressible solvers (pressure based), *e. g.*, artificial compressibility.
- Unified formulations compressible-incompressible.

It is proposed to use the method of preconditioning due to its ability to work in a wide range of Mach and Reynolds numbers.

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Problem definition

- The preconditioning method in conjunction with the 'dual-time-stepping' technique are applied.
- If Γ denotes the preconditioning matrix, the modified system of equations is written as

$$\Gamma \frac{\partial \mathbf{U}}{\partial \tau} + \frac{\partial \mathbf{U}}{\partial t} + (\mathbf{A}_i - w_i \mathbf{I}) \frac{\partial \mathbf{U}}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\mathbf{K}_{ij} \frac{\partial \mathbf{U}}{\partial x_j} \right) + \mathbf{S}$$

• Physical time: t; pseudo-time: τ .

Two CFL (Courant-Friedrichs-Levy) numbers are considered

$$CFL_c = rac{c\Delta t}{h}$$
 and $CFL_u = rac{\|\mathbf{u}\|\Delta t}{h}$

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Problem definition

The preconditioning matrix used was proposed by Choi and Merkle to solve steady compressible flows with the Finite Volume Method. The 'free' parameters involved in Γ are the following:

- M_r : reference Mach number. It replaces the Mach number and was originally introduced to avoid the singularities that appears when $M \rightarrow 0$.
- β : parameter adjustment for viscous regions.
- δ: coefficient of the time derivative of pressure in the energy equation.

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Preconditioning strategies

The definition of $M_{\rm r}$ allows to choose among different preconditioning matrices:

 'Steady preconditioning' (SP), proposed by Choi and Merkle

 $M_{\rm r} = \min(1, \max(M, M_{\epsilon}))$

• 'Unsteady preconditioning' (UP), proposed by Vigneron *et al.*

$$M_{\rm r} = \min(1, \max(\sqrt{M^2 + CFL_c^{-2}}, M_{\epsilon}))$$

• Non-preconditioned (NP), for $\delta = 1$

$$M_{\rm r} = [\gamma - (\gamma - 1)\delta]^{-1/2}$$

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Condition number of the system



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Condition number of the system



Condition number as a function of CFL_c for several Reynolds numbers with the reference Mach for the inviscid case $(M = 1 \times 10^{-3}).$

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Condition number of the system



Condition number as a function of the Reynolds number for several *CFL_c* numbers for the viscous case. $M = 1 \times 10^{-3}$ and

$$M_{\epsilon}=1 imes 10^{-6}$$

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Numerical implementation

- The equations are discretized in space using FEM.
- The SUPG strategy is applied to stabilize the scheme.
- The matrix of intrinsic time scale is computed with the maximum eigenvalue of the advective jacobian.
- An implicit formulation is applied in time and pseudo-time.
- The derivative with respect to the pseudo-time is discretized using the backward Euler difference scheme.

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Flow in a channel with a moving indentation



- $M = U/c = 2.67 \times 10^{-3}$, $Re = \rho Ub/\mu = 507$.
- Velocity and density imposed on inlet section.
- Isothermal walls.
- No-slip boundary condition on the walls.
- Dynamic absorbing boundary condition on outlet section.



Magnitude of flow velocity [m/s] - NSI

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Flow in a channel with a moving indentation



Flow in a channel with a moving indentation



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Flow in a channel with a moving indentation



Pressure perturbation field ([Pa]) at $t^* = 0.5$ - NP.

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Flow in a channel with a moving indentation



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In-cylinder flow in an opposed-piston engine



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In-cylinder flow in an opposed-piston engine



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In-cylinder flow in an opposed-piston engine



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Coupling of 1D/multi-D domains for compressible flows

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Coupling of 1D/multi-D domains for compressible flows

- Due to the computational cost, CFD-3D models are applied to simulate only a few components of an IC engine at each time.
- Usually, the boundary conditions for these 3D models are imposed by using 0D/1D codes.
- When dimensionally heterogeneous models are used, the need to perform the coupling between sub-domains arises.
- 1D/multi-D coupling will be considered.

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Problem definition

Let an 1D problem discretized by a grid with N elements

$$P \begin{cases} \mathsf{E}_{1}(\mathsf{U}_{1},\mathsf{U}_{2}) = \mathbf{0} \\ \mathsf{E}_{2}(\mathsf{U}_{1},\mathsf{U}_{2},\mathsf{U}_{3}) = \mathbf{0} \\ \vdots \\ \mathsf{E}_{N+1}(\mathsf{U}_{N},\mathsf{U}_{N+1}) = \mathbf{0} \end{cases}$$

Assumptions:

- The equation at node *i* involves only the nodal states at nodes *i* − 1, *i* and *i* + 1.
- The equation at node *i* can be separated in its right and left contributions

$$\mathbf{E}_{i}(\mathbf{U}_{i-1},\mathbf{U}_{i},\mathbf{U}_{i+1}) = \mathbf{E}_{i1}(\mathbf{U}_{i-1},\mathbf{U}_{i}) + \mathbf{E}_{i2}(\mathbf{U}_{i},\mathbf{U}_{i+1}) = \mathbf{0}$$

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Problem definition

1D/1D coupling

The problem P is splitted into two sub-problems (P_1 y P_2)



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Coupling for implicit schemes 'monolithically' solved

$$\begin{cases} \mathbf{E}_{1}(\mathbf{U}_{1},\mathbf{U}_{2}) = \mathbf{0} \\ \mathbf{E}_{2}(\mathbf{U}_{1},\mathbf{U}_{2},\mathbf{U}_{3}) = \mathbf{0} \\ \vdots \\ \mathbf{E}_{i1}(\mathbf{U}_{i-1},\mathbf{U}_{i1}) + \mathbf{U}_{lm} = \mathbf{0} \\ \mathbf{U}_{i1} - \mathbf{U}_{i2} = \mathbf{0} \\ \mathbf{E}_{i2}(\mathbf{U}_{i2},\mathbf{U}_{i+1}) - \mathbf{U}_{lm} = \mathbf{0} \\ \vdots \\ \mathbf{E}_{N+1}(\mathbf{U}_{N},\mathbf{U}_{N+1}) = \mathbf{0} \end{cases}$$

- The constraint U_{i1} = U_{i2} imposes the continuity of the solution and forces the continuity of fluxes through the coupling interface.
- Useful when the contributions to the global residue and the global jacobian matrix from sub-domains are available.

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Coupling for implicit schemes 'monolithically' solved 1D/multi-D coupling

In this case, the conditions at the coupling interface for the multi-D domain are defective.

• One possibility is to impose the constraints

$$\mathbf{U}_{1D} = \mathbf{U}_{MD}^{i} \quad i = 1, \ldots, M$$

• Another option is to impose the constraints

$$\int_{\mathcal{S}} \mathbf{U}_{MD} dS = \int_{\mathcal{S}} \mathbf{U}_{1D} dS = \mathbf{U}_{1D} S$$



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1D/2D coupling: gas discharge from a reservoir



- Inviscid flow.
- Insulated walls and without friction.
- Density, pressure and normal velocity are equalized at coupling sections.

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1D/2D coupling: gas discharge from a reservoir



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1D/2D coupling: gas discharge from a reservoir



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1D/2D coupling: gas discharge from a reservoir



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Results 1D/3D coupling: exhaust manifold branch



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Results 1D/3D coupling: exhaust manifold branch







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Results 1D/3D coupling: exhaust manifold branch



1D/3D coupling: exhaust manifold branch

- *N* = 8000 rpm.
- Boundary conditions for the 3D model:
 - Slip boundary condition on solid walls.
 - Insulated walls.
- Boundary condition at the end of the 1D domains obtained from a 1D/0D simulation of the engine.
- Density, pressure and normal velocity are equalized at coupling sections.
- Tangential components of velocity at coupling sections are constrained to be zero.

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1D/3D coupling: exhaust manifold branch



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1D/3D coupling: exhaust manifold branch



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1D/3D coupling: exhaust manifold branch



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Numerical simulation of the fluid flow in the MRCVC

Description of the geometry



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Numerical simulation of the fluid flow in the MRCVC

Description of the geometry



Main features of the engine:

- The combustion could be performed at constant volume.
- Cycle duration for a MRCVC with *n* vanes:

$$\Delta\theta = 2\pi \left(1 + \frac{2}{n}\right)$$

• There are *n* + 2 operating chambers along a cycle.

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Operation and geometry of the MRCVC

Changes in the flow domain



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Numerical simulation of fluid flow in the MRCVC engine

- The fluid flow problem is solved using a 2D approximation.
- The engine simulated has *n* = 3 vanes.
- Maximum chamber volume: 500 cm³.
- Geometric compression ratio: 9:1.
- Flow under cold conditions (without combustion).

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- The proposed U-S strategy is applied.
- Imposed nodal boundary displacements.
- Triangular elements with h = 0.2 mm on the boundaries and h = 0.5 mm in the interior region of the domain.
- The mesh could be generated for a 'stroke' $(0 \le \theta \le \frac{n+2}{2n}\pi)$ and, then, to flip it around vertical and horizontal symmetry axis.

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Quality of the mesh generated



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Quality of the mesh generated



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Quality of the mesh generated



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The Computational Fluid Dynamics problem



- No-slip boundary condition on solid walls.
- Insulated solid walls.
- Intake and exhaust ports modeled with 'mixed' absorbing/wall boundary conditions.
- *N* = 3000 rpm.

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The Computational Fluid Dynamics problem



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Conclusions

- The main goal of this thesis was the proposition, description and testing of some computational tools to solve in-chamber flows in IC engines.
- An optimization-based simultaneous mesh untangling and smoothing strategy was proposed to solve CMD problems.
 - The technique was successfully applied to solve the mesh movement in IC engines problems.
 - Under certain conditions, this strategy allows to generate conformal meshes in 2D.
- The preconditioning of the governing equations with the dual time stepping method were applied to solve transient compressible flows in the low-Mach number limit.

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Conclusions

- A simple technique to solve the coupling of 1D/multi-D domains was applied in dimensionally heterogeneous computational models.
- A 0D/1D code able to describe IC engine operating characteristics was implemented and validated. This code is useful as a boundary condition generator for the multi-D simulations.
- The proposed techniques were incorporated into the CFD code that is developed at CIMEC (PETSC-FEM).
- The first steps towards the simulation of the fluid flow in the MRCVC engine chambers were done.

Conclusions

During this thesis it has been published/submitted the following articles:

- A minimal element distortion strategy for computational mesh dynamics; López, E.; Nigro, N.; Storti, M. and Toth, J.; Int. J. for Numerical Methods in Engineering 2007, Volume 69, Issue 9 (p 1898-1929).
- Simultaneous untangling and smoothing of moving grids; López, E.; Nigro, N. and Storti, M.; Int. J. for Numerical Methods in Engineering 2008, Volume 76 (p 994-1019).
- Validation of 0D/1D computational code for the design of several kind of internal combustion engines; López, E. and Nigro, N.; Latin American Applied Research. (submitted)
- In search of improvements for the computational simulation of internal combustion engines; López, E.; Toth, J.; Nigro, N. and Storti, M.; chapter book. Nova Science Publishers, Inc.; Frank Columbus Ed. (submitted)

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Future work

A great amount of work remains to be done:

- The effective coupling of the 1D/0D code and the CFD-3D code.
- To incorporate the modeling of the spray dynamics, the mixture formation and the combustion process.
- To implement more accurate boundary conditions.

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Gracias por su Atencion

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