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Numerical Simulation of the Thermal and Fluid-dynamic behaviour of fuel-oil in sunk ships

C.D. Pérez-Segarra, A. Oliva, F.X. Trias, O. Lehmkühl, R. Capdevila,
Heat and Mass Transfer Technological Center (CTTC)
Technical University of Catalonia (UPC)

www.cttc.upc.edu
Presentation:

1. Project objectives and work performed

2. Numerical studies using structured multiblock meshes.
   a. RANS modelling.
   b. Parallelization techniques.

3. Advanced turbulence modelling (DNS & LES models)
   a. Current DNS research at MareNostrum supercomputer.
   b. Conservative Regularization Modelling (CRM) for LES. An overview of the method.
   c. Results for a differentially heated cavity at Ra=$10^{10}$ and Pr=0.71.
   d. Results for a tank cooling problem at very high Pr-number

4. Conclusions and Future research
Basic objective: Development of a code for the numerical simulation of the thermal and fluid-dynamic behaviour of the fuel-oil contained in sunk ships (VEM2003-20046).

Work performed:
1. Main code based on fully-implicit structured multiblock techniques. Turbulence by means of RANS two equation models. Newtonian and non-Newtonian fluids,…
2. Development of a new advanced turbulence model.
Main code based on fully-implicit structured multiblock techniques.
Modelling of the fuel-oil cooling inside the Prestige tanker.

- Case defined by the CIEMAT.
- 2D approach with specular symmetry on the right boundary. Left, top and bottom boundaries with vanishing velocities and constant temperature (2.6 °C). Initial temperature 50 °C.
- Thermophysical properties: \( \rho = 1012 \text{ kg/m}^3; \) 
  \( c_p = 1700 \text{ J/kg K}; \)
  \( \lambda = 0.13 \text{ W/m K}; \beta = 7.40 \cdot 10^{-4} \text{ K}^{-1}. \)
2. Numerical studies using structured multiblock meshes

Mathematical formulation (RANS models). Incompressible flows or gases at low Mach numbers.

\[ \frac{1}{\rho} \frac{D\rho}{Dt} + \nabla \cdot \bar{v} = 0 \]

\[ \rho \frac{D\bar{v}}{Dt} \approx -\nabla \bar{p} + \nabla \cdot \bar{\tau} - \nabla \cdot (\rho \bar{v}'\bar{v}') - \rho \beta (\bar{T} - T_o) \bar{g} \]

\[ \rho c_p \frac{D\bar{T}}{Dt} \approx -\nabla \cdot \bar{q} + \nabla \cdot (\rho \bar{v}'T') \]

Turbulent shear stresses and heat fluxes:

\[ \rho \bar{v}'\bar{v}' = -2 \mu_t \bar{\gamma} + \frac{2}{3} \rho k \delta \]

\[ \rho \bar{v}'T' = -\frac{\lambda_t}{c_p} \nabla \bar{T} = -\frac{\mu_t}{\sigma_T} \nabla \bar{T} \]
2. Numerical studies using structured multiblock meshes

**Numerical method**

- **Finite volume techniques** with semi-implicit differentiation in space and fully implicit in time, using Cartesian staggered grid.
- **Pressure-based method** (SIMPLEC). PLDS and CDS for convective and diffusive terms respectively.
- **Multiblock strategy**
- **Mesh**: \((N_1 + N_2) \times M\). Mesh concentration near the walls. Constant \(\Delta t\).

<table>
<thead>
<tr>
<th>Case</th>
<th>(N_1)</th>
<th>(N_2)</th>
<th>(M)</th>
<th>C.V.</th>
<th>(\Delta t)</th>
<th>Convergence criteria</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ref 1</td>
<td>100</td>
<td>80</td>
<td>200</td>
<td>36800</td>
<td>47.77</td>
<td>2 outer iterations</td>
</tr>
<tr>
<td>mesh</td>
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<td>160</td>
<td>400</td>
<td>145600</td>
<td>47.77</td>
<td>2 outer iterations</td>
</tr>
<tr>
<td>dt</td>
<td>100</td>
<td>80</td>
<td>200</td>
<td>36800</td>
<td>4.777</td>
<td>2 outer iterations</td>
</tr>
<tr>
<td>nº ite</td>
<td>100</td>
<td>80</td>
<td>200</td>
<td>36800</td>
<td>47.77</td>
<td>20 outer iter. or heat imbalance &lt; 1 %</td>
</tr>
<tr>
<td>Ref 2</td>
<td>110</td>
<td>90</td>
<td>210</td>
<td>42840</td>
<td>47.77</td>
<td>2 outer iterations</td>
</tr>
</tbody>
</table>
2. Parallelization techniques

**Computational infrastructure: PC cluster and MareNostrum supercomputer**

Low cost **PC clusters** are loosely coupled parallel computers:
- Good ratio **CPU power / cost**
- Low bandwidth and **high latency** network

Supercomputers:
- Much bigger **number of CPU** and much higher price per CPU
- High bandwidth and **low latency** network
2. Numerical studies using structured multiblock meshes

Some results

• High computational cost. The introduction of subdomain (or multiblock) techniques (as a parallelization strategy) allows much lower computational time. Other techniques to reduce CPU time: variable $\Delta t$ (CFL strategies); semi-explicit methods (solid-fluid); more efficient solvers; variable grid concentration); ... 

• Heat transfer and temperature evolution (ref 2):

![Graphs showing heat transfer and temperature evolution](image)
2. Numerical studies using structured multiblock meshes

Some results:

- The phenomenology at the first 20 days is mainly convective but, once the fluid is cold enough to became very viscous, the velocity decreases and the phenomenology is diffusive predominant.

- The inner tank is almost one degree hotter than the outer (5th day).
More results (ref 2)

- **1st day**: relatively high velocities at the outer tank, specially at the left boundary due to natural convection. The inferior part of the system is the cooler one, with much more vortex (initial Rayleigh = $3.72 \cdot 10^{13}$). Mean temperature around 39 ºC.

- **5th day**: still movement into the tank, but considerably lower. Quite uniform temperature, around 30 ºC.

- From the 20th day velocities are almost null and temperature decrease has the form of an inverse exponential.
Development of a new advanced turbulence model.
Governing equations

Incompressible Navier-Stokes coupled with the energy transport equation:

\[ \nabla \cdot \vec{v} = 0 \]

\[ \frac{\partial \vec{v}}{\partial t} + C(\vec{v}, \vec{v}) = Pr \nabla^2 \vec{v} - \frac{1}{\rho} \nabla p + \vec{f} \]

\[ \frac{\partial T}{\partial t} + C(\vec{v}, T) = \nabla^2 T \]

Where \( \vec{f} = (0,0, Ra Pr T) \) (Boussinesq approximation) and the nonlinear convective term is given by

\[ C(\vec{a}, \vec{b}) = (\vec{a} \cdot \nabla)\vec{b} \]
3. Advanced turbulence modelling (DNS & LES models)

Current DNS research: Differentially heated cavity at 
Ra=10^{11}, Pr=0.71

Some details about DNS simulation:
- *Mesh size*: 128 x 680 x 1280 (111·10^6 nodes)
- *Computing time*: ~3 months using 512 CPUs at MareNostrum supercomputer
- *4th-order symmetry-preserving discretization*

**Complexity of the flow:**
- Boundary layers
- Stratified cavity core
- Internal waves
- Recirculation areas
3. Advanced turbulence modelling (DNS & LES models)

Since the computational cost of a DNS simulation is prohibitive a *dynamically less complex mathematical formulation* is sought. To do so, we consider smooth approximations (regularizations) of the nonlinear terms

\[
\frac{\partial \tilde{v}_\varepsilon}{\partial t} + \tilde{C}(\tilde{v}_\varepsilon, \tilde{v}_\varepsilon) = \text{Pr} \nabla^2 \tilde{v}_\varepsilon - \frac{1}{\rho} \nabla p_\varepsilon + \tilde{f}_\varepsilon
\]

\[
\frac{\partial T_\varepsilon}{\partial t} + \tilde{C}(\tilde{v}_\varepsilon, T_\varepsilon) = \nabla^2 T_\varepsilon
\]

Such approximations may fall in the *Large-Eddy Simulation* (LES) concept,

\[
\frac{\partial \bar{v}_\varepsilon}{\partial t} + C(\bar{v}_\varepsilon, \bar{v}_\varepsilon) = \text{Pr} \nabla^2 \bar{v}_\varepsilon - \frac{1}{\rho} \nabla p_\varepsilon + \bar{f}_\varepsilon + M_1(\bar{v}_\varepsilon, \bar{v}_\varepsilon)
\]

\[
\frac{\partial T_\varepsilon}{\partial t} + C(\bar{v}_\varepsilon, T_\varepsilon) = \nabla^2 T_\varepsilon + M_2(\bar{v}_\varepsilon, T_\varepsilon)
\]

If the model terms were given by

\[
M_1(\bar{v}_\varepsilon, \bar{v}_\varepsilon) = C(\bar{v}_\varepsilon, \bar{v}_\varepsilon) - \tilde{C}(\bar{v}_\varepsilon, \bar{v}_\varepsilon)
\]

\[
M_2(\bar{v}_\varepsilon, T_\varepsilon) = C(\bar{v}_\varepsilon, T_\varepsilon) - \tilde{C}(\bar{v}_\varepsilon, T_\varepsilon)
\]
3. Advanced turbulence modelling (DNS & LES models)

The main idea behind regularization methods is to alter the convective term to restrain the production of small scales of motion by means of vortex-stretching.

However, since now the existing regularization models
- Leray model
- Navier-Stokes-alpha model

Do not conserve some of the inviscid invariants:
- Kinetic energy \[ \int \vec{v} \cdot \vec{v} d\Omega \]
- Enstrophy (in 2D) \[ \int (\nabla \times \vec{v}) \cdot (\nabla \times \vec{v}) d\Omega \]
- Helicity (in 3D) \[ \int (\nabla \times \vec{v}) \cdot \vec{v} d\Omega \]

The approximate convective operator has to be skew-symmetric

\[ (\vec{C}(\vec{a},\vec{b}),\vec{c}) = -(\vec{C}(\vec{a},\vec{c}),\vec{b}) \]
3. Advanced turbulence modelling (DNS & LES models)

This criterion yields the following class of approximations...

\[
\frac{\partial \tilde{v}_\varepsilon}{\partial t} + C_n(\tilde{v}_\varepsilon, \tilde{v}_\varepsilon) = \Pr \nabla^2 \tilde{v}_\varepsilon - \frac{1}{\rho} \nabla p_\varepsilon
\]

In which the convective term is smoothed according to:

\[
C_2(\tilde{a}, \tilde{b}) = C(\tilde{a}, \tilde{b})
\]

\[
C_4(\tilde{a}, \tilde{b}) = C(\tilde{a}, \tilde{b}) + C(\tilde{a}, \tilde{b}') + C(\tilde{a}', \tilde{b})
\]

\[
C_6(\tilde{a}, \tilde{b}) = C(\tilde{a}, \tilde{b}) + C(\tilde{a}, \tilde{b}') + C(\tilde{a}', \tilde{b}) + C(\tilde{a}', \tilde{b}')
\]

Where, \( \tilde{a}' = \tilde{a} - \bar{a} \)

\[
C_n(\tilde{a}, \tilde{b}) = C(\tilde{a}, \tilde{b}) + O(\varepsilon^n)
\]

For any symmetric linear filter
3. Advanced turbulence modelling (DNS & LES models)

Discretization of the convective operator: a symmetry-preserving discretization

The spatially discrete incompressible Navier-Stokes equations can be expressed as

\[
H \frac{du_h}{dt} + C(u_h)u_h + Du_h - M^T \rho_h = 0
\]

\[
Mu_h = 0
\]

It can be shown that the convective matrix \( C(u_h) \) has to be skew-symmetric,

\[
C(u_h) + C^T(u_h) = 0
\]

To preserve the continuous invariants (kinetic energy, enstrophy in 2D and helicity in 3D) in a discrete sense.
3. Advanced turbulence modelling (DNS & LES models)

Results for a differentially heated cavity at Ra=$10^{10}$ and Pr=0.71

- **DNS**: mesh size: 64 x 136 x 324; 4th-order sym.-preserv discret.
- **Regularization model** $C_4$ is tested.
- **Two very coarse meshes are considered**:

<table>
<thead>
<tr>
<th></th>
<th>DNS</th>
<th>RM1</th>
<th>RM2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_x$</td>
<td>64</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>$N_y$</td>
<td>136</td>
<td>17</td>
<td>13</td>
</tr>
<tr>
<td>$N_z$</td>
<td>324</td>
<td>40</td>
<td>30</td>
</tr>
</tbody>
</table>

- Ratio $\frac{\varepsilon}{h}$ (filter length to the average grid width) is kept constant in all three spatial directions.
3. Advanced turbulence modelling (DNS & LES models)

Results for a differentially heated cavity at Ra=10^{10}
Mean fields

\[8 \times 13 \times 30\quad 8 \times 17 \times 40\]

Averaged vertical velocity profile at the horizontal mid-height plane for different $_{\varepsilon/h}$ ratios
3. Advanced turbulence modelling (DNS & LES models)

Results for a differentially heated cavity at Ra=10^{10}
Mean fields

8 x 13 x 30

8 x 17 x 40

Averaged temperature profile at the horizontal mid-height plane for different $\frac{\varepsilon}{h}$ ratios
3. Advanced turbulence modelling (DNS & LES models)

Results for a differentially heated cavity at Ra=$10^{10}$

Convergence studies

The maximum of the averaged vertical velocity at the horizontal mid-height plane and the overall averaged Nusselt number as a function of the $\frac{\varepsilon}{h}$ ratio
Results for a tank cooling problem at very high Pr-number

- Similar to the benchmark case defined by CIEMAT.
- 3D approach.
- Initial temperature: 50°C
- Isothermal boundary conditions at 2.6°C

- $Ra_H = 3.72 \times 10^{13}$
- $Pr = 11115$
3. Advanced turbulence modelling (DNS & LES models)

Results for a tank cooling problem at very high Pr-number

8 x 17 x 20

- Even for very coarse meshes reasonable results has been obtained.
- Temperature evolution is in good agreement with the initial numerical studies.
- Since the time integration is fully explicit we are strongly limited by the $\Delta t$ (CFL condition)
3. Advanced turbulence modelling (DNS & LES models)

Results for a tank cooling problem at very high Pr-number

Evolution of the averaged temperature and the temperature at the centre of the cavity.
3. Advanced turbulence modelling (DNS & LES models)

Results for a tank cooling problem at very high Pr-number

Evolution of the overall Nusselt at the left vertical wall and the temperature stratification at the centre of the cavity.
Conclusions and future actions
4. Conclusions and future actions

- A CFD code for the thermal and fluid dynamic behaviour of fuel-oil in sunk ships has been developed.

- The code is based on structured meshes. Complex geometries are treated using a multiblock strategy. Turbulence is solved by means of RANS models.

- Results of a benchmark case of the cooling process in the sunk tanker Prestige have been presented. High computational effort is required.

- A new LES method has been applied for a tank cooling problem at very high Pr-number

The main advantages with respect the existing LES models can be summerized:

- Robustnest. As the smoothed governing equations preserve the symmetry properties of the original NS equations the solution can not blow-up (in energy-norm; in 2D also enstrophy-norm). Moreover, it seems that even for very coarse meshes reasonably results can be obtained.

- Universality. No ad hoc phenomenological arguments that can not be formally derived from the NS equations are used.

→ Future research should focus on the extension of the overall symmetry-preserving for formulation for CRM-LES to unstructured general meshes….

Moreover, a semi-implicit formulation must be implemented in order to avoid the severe $\Delta t$ restrictions.
4. Final remarks

Turbulence modelling:
- RANS
- CRM-LES
- DNS

Numerical Methods:
- STRUCTURED MULTIBLOCK PARALLELIZATION TECHNIQUES

Numerical simulation of fuel-oil in sunk ships

More basic studies on Turbulence modelling
- DNS & CRM-LES
  (CTTC)

New CFD code development
- Numerical methods (unstructured meshes, stronger couplings, parallelization, …)
- Turbulence modelling (RANS, hybrid RANS-LES, CRM-LES, …)
  (TF)