Turbulent Combustion Modelling and Simulation

Eugenio Giacomazzi

TER-ENE-IMP, ENEA – C. R. Casaccia, Rome, ITALY

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Overview of Presentation

• Physical and Theoretical Aspects

• Physical Modelling

• Numerical Aspects

• Structure of a Numerical Code and Supercomputing

• Some Applications
Turbulent Combustion
- Physical and Theoretical Aspects -

Combustion Physics Scenario

Fluid dynamics – Turbulence
Chemical kinetics
Radiant transfer of energy
Acoustics
Multi-phase flows
Turbulent combustion is an intrinsically unsteady multi-physics and multi-scale phenomenon.

Modelling this physics and the multi-scale interaction is the key to capture the complex dynamics of turbulent flames, in terms of localized extinctions and reignitions, flame pulsations, lift-off and blowout, noise emissions and to test control strategies.

MOST PHYSICS IS HIDDEN IN THE UNSTEADINESS

Accurate knowledge of phenomena is the only key to achieve new steps in the progress. Synergic investigation based on Observation, Measurements and Numerical Analysis is critical.

A stable flame anchoring is provided by H₂ preferential diffusion and preheating, even though the heat release time is much slower than convective time. [Giacomazzi et al., Combustion Theory and Modelling, 2008]
What is Turbulence?

- Turbulence may be visualized as a loosely tangled “spaghetti” of line vortices, which continuously advect each other in complex ways. As L.F. Richardson wrote in 1922:
  
  Big whorls have little whorls
  That feed on their velocity
  And little whorls have lesser whorls
  And so on to viscosity.

- Some vortices are created via rollup resulting in vorticity concentration “lines” whose rotation rate increases to conserve angular momentum when stretched by the surrounding flow. Some vortices are also created by this vortex stretching and some other are decaying due to viscosity that dissipates vorticity and fluxes it away from strongly rotational regions.

\[
\frac{D\omega}{Dt} = \omega \cdot \nabla u + \nu \nabla^2 \omega + \frac{1}{\rho} \nabla p \times \nabla \omega - \omega \nabla \cdot u - \frac{1}{\rho} \nabla \cdot (E \nabla \mu)
\]

- Many, however, are in a state of approximate equilibrium among these processes, so that they appear as longlived, coherent features of the flow.

- Mixing is not accomplished within the vortices themselves that, in fact, are relatively stable.

- Mixing occurs mainly in regions of intense strain that exist between any two nearby vortices that rotate in the same direction.
What is Turbulence?

- **Mixing enhanced by turbulence**
  The initial state includes a circular region of dyed fluid in a white background.
  Two possible evolutions are shown: one in which the fluid is motionless (save for random molecular motions), and one in which the fluid is in a state of fully developed, two-dimensional turbulence. The mixed region (yellow-green) expands much more rapidly in the turbulent case.

- Cross-section of the temperature field in Kelvin-Helmholtz billows before (a) and after (b) the transition to turbulence. **The whole spectrum of scales contributes to mixing.**

- Large scales mix via **convective transport** by enlarging contact surfaces.
- Small scales mix via **molecular diffusion**.

Turbulent Kinetic Energy Spectrum

\[ \frac{\partial E}{\partial t} = W(k, t) - 2\nu k^2 E \]

- **Anisotropic Scales**
- **Isotropic Scales**

- **Reactive**
- **Nonreactive**

- **Boundary conditions effect**
- **Integral macroscale**
- **Dissipative scale**

- **Kolmogorov**
- **Höenengberg**

- **Dissipative subrange**

- **Chemical reactions**

- **Controlled by chemical reactions**
- **Controlled by molecular diffusion**
- **Controlled by boundary conditions**
- **Controlled by macroscale**
Towards Instability Analysis

Spectra averaged by using 60 spectra, each sampled in 1 s, when a flame is stable and when is close to extinction.

When the flame is unstable, small scales fluctuations cause large scale fluctuations (opposite when the flame is stable).

Non local (in wave numbers and not in space) scale interaction!

Control

Dynamics of the three ranges when the flame is close to extinction.

Flame Radiative Emission

ODC System [Giacomazzi E., Troiani G. et al., Exp. in Fluids, 2007]

Turbulence: Spatio-Temporal Ordered Chaos ...

• Chaos: popular meaning of disorder.

• Introducing the idea of sensitivity to initial conditions, chaotic phenomena have spatio-temporal correlations of fluctuations tending toward zero as the time interval tends to infinity and the spatial displacement tends either toward infinity or toward the maximum dimension of the domain.

  • Disordered chaos: correlations vanish for all intervals of time or spatial displacements different from zero.

  • Ordered chaos: correlations do not all vanish for finite intervals of time and spatial displacements.
... but Deterministic Chaos

Turbulence is also deterministic, i.e.,

- it is a chaotic situation that can be described by a closed system of equations with initial, boundary and external conditions;
- it is replicable.

Determinism is the expression of causality.

Concept of causality in modern terms:

“Nothing occurs without a cause or, at least, without a determining reason, which is to say, something that may provide an a priori reason why it should exist rather than not exist and why it should have this form rather than another.”

[Leibniz]

The Equations of Flow Motion

The flow motion is ruled by a system of equations, that for a reacting flow is

\[
\frac{\partial p}{\partial t} + \nabla \cdot (\rho u) = 0
\]

\[
\frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u u) = \nabla \cdot S + \rho \sum_{i=1}^{N_a} Y_i f_i
\]

\[
\frac{\partial (E + k)}{\partial t} + \nabla \cdot [\rho u (E + k)] = \nabla \cdot (S u) - \nabla \cdot q + \rho \sum_{i=1}^{N_a} Y_i f_i \cdot (u + V_i)
\]

\[
\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho u Y_i) = -\nabla \cdot J_i + \rho \omega_i
\]

\[
p = \rho \sum_{i=1}^{N_a} \frac{Y_i}{W_i} \mathcal{R}_w T
\]

Therefore, a turbulent flow can be predicted by accurately solving the Navier-Stokes equations, but ...
Why is Modelling Needed?

The Cost of Solving the Whole Spectrum of Scales

- Turbulence ⇒ spectrum of scales, from $L$ down to $\eta$
- Dissipation takes place for $0.1 < k \eta < 1$, i.e., $6 \eta < l < 60 \eta$

Hence, to resolve the whole spectrum of scales

- Spatial resolution required:
  \[(L/\eta)^3 \sim \left(Re_L^{3/4}\right)^3 = Re_L^{9/4}\]
- Time resolution required:
  \[\tau_L/\tau_\eta \sim Re_L^{1/2}\]
- CPU time required:
  \[\propto N_{\text{nodes}} \times N_{\Delta t} \sim Re_L^{11/4}\]

Note that this simple estimate is valid for a free flow. Near walls spatial resolution increases (the mixing length decreases).

Today DNS is feasible only for relatively simple flows, even using supercomputing!
**DNS, LES and RANS**

**DNS**
- Energy injection
- Forward cascade
- Dissipation
- Subgrid scales

**Direct Numerical Simulation:**
Navier-Stokes equations are solved **without modelling** (the error is only numerical).

**Large Eddy Simulation:**
Navier-Stokes equations are spatially **filtered**, hence, scales larger than the filter size $\Delta$ are resolved, while the smaller ones are modelled (thanks to their universal features).

**Reynolds Averaged Navier-Stokes:**
Navier-Stokes are **filtered in time**, hence, the spectrum of scales is reduced just to one scale, i.e., the average scale.

**LES**
- with respect to **DNS**, the description of small scales is **lost**;
- with respect to **RANS**, the dynamics of large scales is **gained**.

**RANS**
- still needed in design due to the **much lower** computational time. **LES** can be used for unsteady analysis of the **selected geometries**.
LES in Turbulent Combustion

Computing large scales and modelling small scales is the key of success of LES upon RANS/FANS technique.

For reactive problems (turbulent combustion) this success could not be so clear because

• chemical reactions take place at small scales (close to molecular mixing);

• in both RANS/FANS and LES the reacting scales are not solved, hence, the whole turbulent subgrid combustion physics must be modelled.

This is the reason why many turbulent combustion models can formally work in both formulations.

However, large structures are explicitly computed and instantaneous fresh and burnt gases zones, with different turbulence characteristics, are clearly identified.

An important application of LES is the analysis of combustion instabilities, that exhibit large scale coherent structures due to coupling between heat release, hydrodynamic flow field and acoustic waves.

DNS for Model Validation

J.CHEN: “Direct numerical simulation is our numerical probe to measure, understand, or see things in great detail at the finest scales where chemical reactions occur.”

CO/H2 nonpremixed flames extinction/reignition Varying Re 500M grid points

Lifted H2/Air flames in Vitiated Coflow 1B grid points CrayXT3 at ORNL on ~10,000 cores 3,5 million cpu-hrs , 35 TB data

Ethylene non-premixed sooting flames, varying Damköhler no. 350M grid points

Lean premixed CH4/air flames (2006) 200M grid points
LES of the Ignition of a Full Helicopter Combustor
- Combustion Instabilities in Annular Combustion Chambers -

G. Staffelbach: “The complexity of this chamber and the high wave length of such modes render laboratory tests very difficult or even impossible. One solution to study these modes and their effects on realistic cases is the use of Large Eddy Simulation.”

Date: 2007
Author(s): M. Boileau and G. Staffelbach
Credit: CERFACS and Turbomeca (SAFRAN group)

40 millions cells - 5120 IBM BlueGene processors
Collaboration between CERFACS and IBM

Turbulent Combustion
- Commonly Simplified Physics in Modelling and Simulation -
Commonly Simplified Physics in Turbulent Combustion

- **Chemical kinetics**: consider not only the main products but also some radicals.
  ⇒ Some level of “detail” is important to capture ignition and extinctions.

- **Compressibility**: acoustic-thermo-fluid-dynamic coupling is critical in instabilities.
  ⇒ The “low Mach number” approximation must be avoided even though $M \ll 1$.
  This increases computational time in unsteady simulations.

Mach 1.92 supersonic jet
[Freund, 2001 – APS Gallery of Fluid Motion]

Combustion Noise

Commonly Simplified Physics in Turbulent Combustion

- **Preferential diffusion**: close to injection, turbulent stirring is not so strong to make the effective individual diffusivities nearly equal.
  This results into thermo-diffusive mechanisms and thus additional wrinkling in turbulent flames.

- **$L_e < 1$**: diffusion of reactants (“R”) towards flame front is favoured, thus increasing flame surface area and enhancing flame wrinkling.

- **$L_e > 1$**: heat (“H”) diffusion towards reactants is favoured, thus decreasing flame surface up to a planar flame front.
Simplifying Individual Species Diffusion Coefficients Calculation

In multicomponent gaseous diffusion, at least the zeroth-order model of Hirschfelder and Curtiss should be applied:

\[ D_{ij}^{[0]} = D_i = \frac{1 - Y_i}{\sum_{j=1, j \neq i}^N Y_j D_{ji}} \]

This model still involves the calculation of binary mass diffusion coefficients from kinetic theory expressions. This is still expensive in a CFD computation.

A very simple and economic way to obtain individual species diffusion coefficients consists in deriving them from assumed Lewis or Schmidt numbers [Smooke and Giovangigli, 1991]:

\[ L_i = \frac{\alpha}{D_i} = S c_i / P r \Rightarrow D_i = \alpha / L_i \]

\[ S c_i = \nu / D_i \Rightarrow D_i = \nu / S c_i \]

where \( \alpha = k / (\rho C_p) \) is the mixture thermal diffusivity, and \( P r = \mu C_p / k \) is the Prandtl number.

As a matter of fact, the constant Lewis and Schmidt number assumptions have never been justified nor verified in practical flames.

Lewis and Schmidt Number vs Temperature Distributions

- Nonpremixed flames experience more thermochemical states than premixed ones.
  ⇒ Thus, Lewis or Schmidt numbers against temperature distributions are expected to be broader.

- The Schmidt number distributions are tighter than the Lewis distributions.
Effect of Localized Extinctions on Lewis Against Temperature Distributions

Five regions can be identified, related to different mixture conditions:
1. lean; 2. stoichiometric; 3. rich; 4. nonreacting; 5. quenched.

Mass Diffusivities via Individual Lewis or Schmidt Numbers?

Final Receipt

- Since Schmidt number against temperature distributions for individual species are less broad than those of Lewis number, in both premixed and non-premixed flames, the constant Schmidt number assumption seems more correct.
- Since non-premixed flames, and in particular those experiencing localized extinctions, involve many thermo-chemical states, distributions derived from non-premixed flames are more meaningful than those of premixed ones.
- Since these distributions are generally skewed or unbalanced, the median describes their central tendency better than the mean.

Thus,

\[ D_{i,\text{mix}} = \frac{\alpha}{L_i} \]
\[ D_{i,\text{mix}} = \frac{\nu}{S_{ci}} \]

where \( S_{ci} \) is the median of the non-premixed flame \( S_{ci} \) against T distributions.

[Giacomazzi E. et al., Combustion Theory and Modelling, 12(1):557-564, 2008]
Summary and Computational Efficiency

<table>
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<tr>
<th>Diffusion Model</th>
<th>Most Diffusion Flux</th>
<th>Diffusion Coefficient</th>
<th>Included Phases</th>
<th>Application</th>
<th>$N_p$ Operations</th>
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<tbody>
<tr>
<td>Multi-component</td>
<td>Eqn. (1) and (5)</td>
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<td>compress., shear., thermal-diff.</td>
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The last column reports the time required to compute molecular properties with respect to the time needed to integrate the 3D reactive, compressible Navier-Stokes equations for a complete time-step.

The solver is explicit (3rd order Runge-Kutta time scheme and 2nd order centered spatial scheme, with an explicit filtering); NSCBCs are applied at boundaries; 10 species are transported; a six-steps reduced mechanism (skeletal mechanism of 70 reactions with 5 species assumed in partial equilibrium) is implemented; computational grid has ~5.3x10^6 nodes.

Commonly Simplified Physics in Turbulent Combustion

- Mixture transport properties: most simplifications strongly affect flame dynamics.
  - E.g., the nonpremixed syngas-air SANDIA “Flame A” is stably anchored in experiments.
  - In numerical simulations, the anchoring changes depending on the modelling of the mixture thermal conductivity, $K_{mix}$.
    - if $K_{mix}$ is modelled with the more accurate Mathur’s empirical law, the flame is more stably anchored.
    - if $K_{mix}$ is modelled as $\sum_{i=1}^{N_s} Y_i K_i$, the flame shows more localized extinctions.
Commonly Simplified Physics in Turbulent Combustion

• **Thermal radiation**: cannot be neglected in sooting flames, or when there is a strong dilution due to CO\textsubscript{2} and H\textsubscript{2}O (as in MILD combustion).

• **Small scale phenomena**:
  - **Dilatation** due to heat release
    - non-equilibrium of small scales
    - nonnegligible reverse energy cascade expected
  - **intermittency**
  - **Interaction** between eddies and flame structures → effects on turbulent spectra
  - **Pressure and temperature gradient diffusion** (Soret effect): important in mixing
  - **Viscous heating**
  - **Bulk viscosity**: cannot be neglected when flows experience “rapid” compressions, such as across shock waves, or expansions, as in supersonic expansion from holes in vacuo
  - **Dufour effect**: commonly negligible even though Soret effect is not

These effects should be included in SGS modelling of turbulent combustion.

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**Example: Small Scale Helicity Injection Close to Flame Fronts**

**Helicity transport equation (inviscid flows)**

\[
\frac{\partial H}{\partial t} = \mathbf{u} \cdot \frac{\partial \omega}{\partial t} - \omega \cdot \nabla \mathcal{G} - \nabla \left( \frac{\mathbf{u} \cdot \mathbf{u}}{2} \right)
\]

• Found by working out the scalar product of Crocco’s equation (inviscid)

\[
T \nabla S + \mathbf{u} \times \omega = \nabla H + \nabla \left( \frac{\mathbf{u} \cdot \mathbf{u}}{2} \right) + \frac{\partial u}{\partial t}
\]

with vorticity and by using the thermodynamic relation between Gibb’s free energy, enthalpy and entropy \( d\mathcal{G} = dH - T dS \).

• Although valid only for inviscid flows, this form of helicity transport equation shows the effect of combustion by means of \( \omega \cdot \nabla \mathcal{G} \) that is a strong source close to flame fronts.

• Nondimensionalizing the helicity equation, all terms have order 1 except the combustion term that scales as \( M^{-2}/(\gamma - 1) \).

In burnt zones \( M \) decreases by \( \sim \)3 times, thus the combustion term increases by \( \sim \)7 times.
Variable Decomposition in LES

- Field variables are decomposed into resolved and subgrid-scale (or residual) parts.

  For reacting flows
  - a Reynolds decomposition is used for quantities per unit volume: \( \rho = \bar{\rho} + \rho' \)
  - a Favre (density-weighted) decomposition is used for quantities per unit mass:
    \[ u = \bar{u} + u'' \] with \( \bar{u} = \bar{\rho} \bar{u}/\bar{\rho} \)

  For nonreacting flows
  - only the Reynolds decomposition is used (sometimes also for reacting flows).

- The resolved, large-scale fields are related to the instantaneous full-scale fields through a grid filtering operation (applied to the Navier-Stokes equations) that removes scales too small to be resolved by the simulation.
A spatial filter operator \( G_\Delta \) separates large resolved scales from small modelled scales.

Filtering is mathematically expressed by means of a convolution integral

\[
\tilde{f}(x) = \int_D f(x') G_\Delta (x - x') \, dx'
\]

or

\[
\tilde{\sigma f}(x) = \int_D \rho f(x') G_\Delta (x - x') \, dx'
\]

where \( D \) is the whole domain and \( G_\Delta \) is the filter of scale \( \Delta \) with these properties:

\[
\int_D G_\Delta (x, x') \, dx' = 1 \quad (1)
\]

\[
G_\Delta (x) \rightarrow 0 \quad \text{for} \ x > \Delta \quad (2)
\]

The size of the filter has not to be necessarily uniform, i.e., \( \Delta \) can vary over the grid.

Furthermore:

- \( \tilde{f} \neq \bar{f} \) and \( \tilde{f} \neq \zeta \) (= only when a cut-off filter in the spectral space is used);
- commutation is assumed for derivative and filter operations, i.e., \( \frac{\partial \tilde{f}}{\partial x} = \frac{\partial f}{\partial x}, \frac{\partial \tilde{f}}{\partial x'} = \frac{\partial f}{\partial x'} \),

  **Commutation error** for symmetric filters does not depend on their shape and is \( O(\Delta^2) \).

Some filters are not affected by this error. However, it is generally neglected and assumed to be incorporated in the SGS model.
Spatial Filters in LES

- **Sharp (spectral) Cut-Off** (in the spectral space):
  \[ G(k) = \begin{cases} 
 1 & \text{if } k \leq \pi/\Delta \\
 0 & \text{otherwise}
\end{cases} \]
  where \( k \) is the spatial wave number and the cut-off length scale is \( 2\Delta \).
  corresponding to \( G(|x|, \Delta) = 1/\Delta \sin [\pi |x| / \Delta] / (\pi |x| / \Delta) \).

- **Top-hat or box** (in the physical space, corresponding to averaging over a box of size \( \Delta \)):
  \[ G(x) = \begin{cases} 
 1/\Delta & \text{if } |x| \leq \Delta/2, i = 1, 2, 3 \\
 0 & \text{otherwise}
\end{cases} \]
  corresponding to \( \bar{G}(k) = \sin [k\Delta/2] / (k\Delta/2) \) that filter scales with \( k \leq \pi/\Delta \).

- **Gaussian** (in the physical space):
  \[ G(x) = \left( \frac{6}{\pi \Delta^2} \right)^{1/2} \exp \left( -\frac{6}{\Delta^2} |x| \right) \]
  corresponding to \( \bar{G}(k) = e^{-k^2\Delta^2/2\Delta^2} \).

- **Implicitly defined** by the computational grid and directly used in the SGS model (corresponds to top-hat or grid filtering):
  \[ \Delta = \sqrt{Vol_{cell}} \]
Implementation of Gaussian Spatial Filtering

\[ \tilde{f}(x) = \int_D f(x') G(x - x') \, dx' \]

\[ G(x) = \left( \frac{6}{\pi \Delta^2} \right)^{1/2} \exp \left[ -\frac{6}{\Delta^2} |x|^2 \right] \]

- In LES, equations are filtered in space to remove non-resolved subgrid turbulence.
- Spatial filtering has also numerical effects: it removes high frequency oscillations due to spatial discretization (centered schemes).

LES Filtered Navier-Stokes Equations

LES equations for the resolved fields are formally derived by substituting the field variables decomposition into the governing equations, and then subjecting the equations to the grid filter.

\[ \frac{\partial \bar{p}}{\partial t} + \frac{\partial \bar{u}_i}{\partial x_i} = 0 \]

\[ \frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_j}{\partial x_j} \left[ \bar{p} \delta_{ij} + \bar{u}_j + \sum_{k=1}^{Ns} \bar{T}_{ik}^{SGS} - \tau_{ij}^{SGS} \right] = 0 \]

\[ \frac{\partial \bar{E}}{\partial t} + \frac{\partial \bar{u}_i}{\partial x_i} \left[ (\bar{p} + p) \bar{u}_i + \bar{q}_i + \sum_{k=1}^{Ns} \bar{T}_{ik}^{SGS} - \tau_{ij}^{SGS} \right] + H_i^{SGS} + \sigma_i^{SGS} = 0 \]

\[ \frac{\partial \bar{v}}{\partial t} + \frac{\partial \bar{v}_i}{\partial x_i} = \bar{p} R_T \]

Statistical effects of the instantaneous small-scale fluctuations are in unclosed terms representing the influence of the subgrid scales on the resolved scales:

\[ \tau_{ij}^{SGS} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j \]

\[ H_i^{SGS} = \bar{p} \bar{u}_i - \bar{p} \bar{u}_i \]

\[ \sigma_i^{SGS} = \tau_{ij} \bar{u}_i - \tau_{ij} \bar{u}_i \]

\[ \Theta_{ik}^{SGS} = \bar{q}_{ik} \bar{Y}_k - \bar{q}_{ik} \bar{Y}_k \]

These unclosed terms contain SubGrid Scale (SGS) effects and have to be modelled.
Large Eddy Simulation
- Subgrid Scale Models -

Type of SGS Modelling

The **dissipative effect of subgrid scales** can be

- explicitly modelled by means of an SGS model, i.e., by introducing a subgrid eddy viscosity (**Eddy Viscosity Models**);

- implicitly taken into account by using the diffusive effect of the numerical error associated to the particular scheme implemented (**MILES**, Monotone Integrated LES). This procedure is difficult to use because
  - only a posteriori analysis is possible;
  - it is difficult to understand the links and interactions between numerics and physics.

The **LES requirements** for engineering problems are

- **spatial** (and not frequency) domain formulation;
- no **external constants** to the model;
- correct **behaviour** close to walls;
- the SGS model should be able to automatically turn off in the laminar region of the flow to capture laminar – turbulence transition.
### The Eddy Viscosity in LES and RANS/FANS Modelling

- Eddy Viscosity (viscous stress analogy) models link subgrid stresses $\tau_{ij}^{SGS}$ to strain rate $\varepsilon_{ij}$

$$\tau_{ij}^{SGS} = \frac{\delta_{ij}}{3} \tau_{kk}^{SGS} = -2\nu_{l}\varepsilon_{ij}$$

- Usually the SGS eddy viscosity is defined via algebraic models.
  - Easy and low cost.
  - Describe physics of small scales, that are more homogeneous and isotropic than large scales.
  - SGS stresses are a small fraction of the total, thus errors of the model should not decrease global accuracy.

Eddy viscosity is distributed differently in RANS and LES and it has different order of magnitudes.

Example: eddy viscosity distribution in the recirculation zone downstream of a bluff-body.

<table>
<thead>
<tr>
<th>RANS: $k-\varepsilon$ EDC</th>
<th>LES: FM (averaged)</th>
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### The Smagorinsky Model (1/3)

- The oldest model (1963) and very popular because of its simple formulation.

- **Equilibrium of small scales** is assumed (their lifetime is shorter than that of large scales)

  ⇒ At small scales, the energy source due to the energy transfer from large scales to small scales is balanced by dissipation ($\varepsilon_v$)

  $$-\tau_{ij}^{SGS}\varepsilon_{ij} = \varepsilon_v$$

  Then

  $$\begin{align*}
  \varepsilon_v &= 2\nu_{l}\varepsilon_{ij} \varepsilon_{ij} = \nu_l |E|^2 \\
  u_{SGS} &= C_S \Delta |E|
  \end{align*}$$

  Finally

  $$\nu_l = (C_S \Delta)^2 |E|$$

- Energy “subtracted” to large scales: $\varepsilon_{SGS} = \tau_{ij}^{SGS} \varepsilon_{ij} = -(C_S \Delta)^2 |E|^3 < 0$

  ⇒ Energy backscatter cannot be predicted!
The Smagorinsky Model (2/3)

- In 1967, Lilly worked out the Smagorinsky constant by assuming the cut-off wave-number in the Fourier space \( k_c = \pi/\Delta \) be inside the Kolmogorov inertial range

\[ E(k) = K_K \varepsilon^{2/3} k^{-5/3} \quad \text{with} \quad K_K = 1.4 - 1.5 \]

The strain rate module can be estimated by integrating the dissipation spectrum \( \varepsilon_r \) over the whole range of resolved wave-numbers \( \sim 2\pi \int_0^{k_c} k^2 E(k) \, dk \):

\[
\overline{E}^2 \sim 2 \int_0^{\pi/\Delta} k^2 E(k) \, dk = 2K_K \varepsilon^{2/3} \int_0^{3/\Delta} k^{1/3} \, dk = \frac{3}{2} K_K \varepsilon^{2/3} \frac{\pi^{4/3}}{\Delta} \quad (1)
\]

Assuming the ensemble average of the dissipation of subgrid kinetic energy equal to the kinetic energy flux along the Kolmogorov cascade, i.e.,

\[ \varepsilon = |\varepsilon_{SGS}| \quad \Rightarrow \quad \varepsilon = (C_S \Delta)^2 |\overline{E}|^5 \]

and substituting \( \overline{E} \) from Eqn. (1), it is found

\[ C_S = \frac{1}{\pi} \left( \frac{2}{3K_K} \right)^{3/4} \]

Assuming \( K_K = 1.41 \) it follows \( C_S = 0.18 \).
When there is shear, \( C_S = 0.065 + 0.1 \) is used [Deardorff and McMillan].

The Smagorinsky Model (3/3)

- In the Smagorinsky model the constant has the same value everywhere.

- The Smagorinsky eddy viscosity does not tend to zero at wall.

  - The Van Driest damping function is assumed close to walls to take into account the length scale decrease:

\[ \nu_t = \left[ C_S \Delta \left( 1 - e^{-y^+/25} \right) \right]^2 |\overline{E}| \]

- Some tricks are needed to simulate laminar – turbulence transition, such as

  - the introduction of an intermittency factor to decrease the SGS stresses;

  - the use of the dynamic model of Germano to estimate locally the \( C_S \).
**Models Based on Transported SGS Kinetic Energy**

- The turbulence closure for compressible flows

\[
\tau_{ij}^{SGS} = -2\nu P_k \left( S_{ij} - \frac{1}{3} S_{kk} \delta_{ij} \right) + \frac{2}{3} \rho k \delta_{ij}
\]

is based on a subgrid kinetic energy transport equation

\[
\frac{\partial \rho k^{SGS}}{\partial t} + \frac{\partial \left( \rho u_i k^{SGS} \right)}{\partial x_i} = \frac{\rho}{Pr} \frac{\partial}{\partial x_i} \left( \rho \nu_i \frac{\partial k^{SGS}}{\partial x_i} \right) - \frac{\partial}{\partial x_i} \left( \rho u_i \delta_{SGS} \right)
\]

with \( P^{SGS} = -\tau_{ij}^{SGS} \frac{\partial u_i}{\partial x_j} \) and \( k^{SGS} = \frac{\epsilon}{\Delta} \) as sole source/sink terms.

Note that in this equation no subgrid combustion effects are explicitly taken into account, apart from density changes. The complete energy (mechanical and thermal) equation shows links with combustion.

The local subgrid kinetic energy is finally used to estimate local velocity fluctuations and then the eddy viscosity, e.g.,

\[ v_{ij} = 0.067 \sqrt{k^{SGS}} \Delta \]

---

**Kinetic Energy in Turbulent Combustion**

In subsonic flows local destruction/production rate of kinetic energy may be altered by forcing acoustic waves, as in "synthetic jets".

Depending on how fast chemical kinetics is inside a reacting "fine structure", this term may produce local laminarization or increase of turbulence in subsonic flows. Instead, in supersonic flows it tends to laminarize the flow locally, since combustion in reacting "fine structures" tends to be isochoric.

Diffusive heat fluxes cannot be neglected at small scales. Thus, reacting small scales cannot be considered closed adiabatic reactors.

Heat release tends to increase local turbulence. This is amplified in fast kinetics case, thus eventually resulting into peaks at high frequency.

TIP: writing this equation at subgrid level, the term \( \partial K_{SGS}/\partial t \) would be strongly coupled to combustion and it might be interpreted as an intermittency factor in SGS models.
The Fractal Model (FM)

• FM is an algebraic *eddy-viscosity* subgrid model
  - generating a vortex cascade in each cell of a CFD domain
    from the cell scale $\Delta$ down to the dissipative scale $\eta \rightarrow N_\eta$ dissipative scales
  - using the *Eddy Dissipation Concept* idea to model combustion:
    “chemical reactions take place in the fine structures close to $\eta$”

• FM “feels” the local turbulent Reynolds number $\rightarrow$ turns off automatically in laminar regions

• FM includes the effect of *increasing temperature* on the dissipative scale $\eta$

  \[ \eta = \chi^{1/4}_\eta \left( \frac{V_\eta}{V}\right)^{3/4} \frac{\Delta}{\text{Re}_{\lambda}^{3/2}} = \pi^{-1/6} \left( \frac{V_k}{V_\lambda} \right)^{1/2} \frac{\Delta}{\text{Re}_{\lambda}^{3/2}} \]

  \[ \mu_s \approx \sigma N_\eta \mu \approx \sigma \pi^{-1} \left[ \left( \frac{\Delta}{\eta} \right)^2 - 1 \right] \mu_\lambda \]

• FM treats the reactive “fine structures” as a local PSR (Perfectly Stirred Reactor), its volume fraction $\gamma$ (cell volume %) depends on the local Reynolds number and the local fractal dimension $D_3$

  \[ \gamma = \left( \frac{\Delta}{\eta} \right)^{D_3-3} \]

• The *heat released* is naturally modeled as a subgrid effect

  \[ \tilde{\omega}_i = \gamma^* \omega_i^* \]

  \[ \tilde{Q} = \sum_{i=1}^N \gamma^* \omega_i^* \Delta h_i^* \]

The Closure of Subgrid Scalar Fluxes

\[ \frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial \tilde{\rho} \tilde{u}_i}{\partial x_i} = 0 \]
\[ \frac{\partial \tilde{\rho} \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left[ \tilde{p} \tilde{u}_j \tilde{u}_i + \tilde{p} \delta_{ij} - \tau_{ij} + \tau_{ij}^{SGS} \right] = 0 \]
\[ \frac{\partial \tilde{E}}{\partial t} + \frac{\partial}{\partial x_i} \left[ \left( \tilde{p} \tilde{E} + \tilde{p} \right) \tilde{u}_i + \tilde{q}_i + \sum_{k=1}^N q_{i,k}^{SGS} - \tau_{ij} \tilde{u}_i + H_i^{SGS} + \tau_{ij}^{SGS} \right] = \mathcal{C} \]
\[ \frac{\partial \tilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_i} \left[ \tilde{p} \tilde{Y}_k \tilde{u}_i - \tilde{p} \tilde{Y}_k \tilde{v}_i + Y_i^{SGS} + \Theta_{i,k}^{SGS} \right] = \tilde{\rho} \omega_k \]
\[ \tilde{p} = \rho \tilde{R}_p \tilde{T} \approx \tilde{p} \tilde{R}_p \tilde{T} + \tilde{T}^{SGS} \]

• $\tau_{ij}^{SGS}$, $q_{i,k}^{SGS}$, $\Theta_{i,k}^{SGS}$ are usually neglected.

• $T^{SGS}$ is the temperature – species correlation term, defined as $\tilde{Y}_k \tilde{T} - \tilde{Y}_k \tilde{T}$. For low heat release can be expected to be negligible, but this may not be true for high heat release. However, it is difficult to model and therefore it is generally neglected.

• A *gradient closure*, together with turbulent Prandtl and Schmidt numbers, are commonly assumed to model subgrid scalar fluxes:

  \[ H_i^{SGS} = -\frac{\mu_s}{P_{\text{Pr}_i}} \frac{\partial \tilde{H}_k}{\partial x_i} \]

  \[ Y_{i,k}^{SGS} = -\frac{\mu_s}{S_{\text{Cl}_i}} \frac{\partial \tilde{Y}_k}{\partial x_i} \]
This procedure is a method for calculating dimensionless scaling coefficients in SGS models for filtered nonlinear terms.

Filtering the nonlinear term \( t(u) \)

\[
\tilde{t}(u) = t(\tilde{u}) + m(\tilde{u})
\]

(1)

\( m(u) \) being an algebraic SGS model.

Dynamic procedure: how do \( t(u) \) and \( m(u) \) vary with the filter width?

Considering a test filter \( \Delta > \Delta \) (usually \( \Delta = 2\Delta \))

\[
\tilde{t}(u) = t(\tilde{u}) + m(\tilde{u})
\]

(2)

Subtracting Eqn. (2) from the \( \hat{\Delta} \) filtered (1)

\[
\tilde{t}(\tilde{u}) - \tilde{t}(\tilde{u}) = m(\tilde{u}) - m(\tilde{u})
\]

This identity (of Germano) is computable from the known resolved field.

The Dynamic Model of Germano

The identity of Germano represents the “band-pass filtered” contribution to the nonlinear term in the scale range between the grid and test filter levels. The subgrid scales should behave as the smallest resolved scales (grid - test filters band). The identity can be used as a constrain for calibration of SGS models.

Application of the Dynamic Model

- The dynamic model is useful to calculate locally constants of SGS algebraic models.
  ⇒ The SGS models work differently in flow regions with different turbulence levels.

- **EXAMPLE**: calculation of the Smagorinsky constant \( C_s \)

- At the grid filter level \( \Delta \):
  \[
  \tau_{ij}^{SGS} = \bar{u}_i\bar{u}_j - \bar{u}_i\bar{u}_j
  \]

- At the test filter level \( \hat{\Delta} \):
  \[
  \tau_{ij}^{SGS} = \bar{u}_i\bar{u}_j - \bar{u}_i\bar{u}_j
  \]

- Work out the resolved turbulent stress: \( L_{ij} := \tau_{ij}^{SGS} - \tilde{\tau}_{ij}^{SGS} = \bar{u}_i\bar{u}_j - \bar{u}_i\bar{u}_j \)

- According to the Smagorinsky model

  \[
  \tau_{ij}^{SGS} - \frac{\delta_{ij}}{3} T_{kk}^{SGS} = -2\nu \bar{e}_{ij} = -2\left(C_s \hat{\Delta}\right)^2 \bar{E} \bar{e}_{ij}
  \]

\[
\Rightarrow \bar{z}_{ij}^{SGS} - \frac{\delta_{ij}}{3} T_{kk}^{SGS} = -2\left(C_s \hat{\Delta}\right)^2 \bar{E} \bar{e}_{ij}
\]

\[
\Rightarrow L_{ij} - \frac{\delta_{ij}}{3} L_{kk}^{SGS} = \left(\tau_{ij}^{SGS} - \frac{\delta_{ij}}{3} T_{kk}^{SGS}\right) - \left(\tilde{\tau}_{ij}^{SGS} - \frac{\delta_{ij}}{3} \tilde{T}_{kk}^{SGS}\right) =
\]

\[
-2C_s^2 \Delta^2 \bar{E} \bar{e}_{ij} - \Delta^2 \bar{E} \bar{e}_{ij} = -2C_s^2 M_{ij} \Rightarrow C_s
\]

**NOTE**: Stabilization is required and often this is obtained by averaging \( C_s \) in homogeneous directions (e.g., parallel to walls) or locally.
Large Eddy Simulation
- Numerical Aspects -

importance of spatial resolution

- Motions with scales comparable to the grid-spacing may have significant energy at high Re.
  - Coarse meshes cause aliasing errors (from nonlinear terms of equations): the energy of high wavenumbers not represented on the grid is aliased onto the resolved wavenumbers.
  - The resulting grid-to-grid oscillations (wiggles) can become locally dominant and cause numerical instability when using high-order central difference schemes.
  - The presence of spurious waves is an indication of poor resolution of relevant lengthscale. In linear, constant coefficients problems, smoothing of spurious waves is only cosmetic, as it simply changes the nature of the error from dispersive to dissipative. For nonlinear problems smoothing is necessary to avoid failure of the solution.
  - These spurious oscillations are reduced by:
    - explicit filtering of field variables;
    - rewriting the convective terms to reduce aliasing errors;
    - adding artificial selective (for short spatial scales) damping;
    - higher-order schemes, WENO schemes, upwind schemes (with large stencil).

BUT it is preferable to use mesh refinement, higher-quality grids and higher quality BCs.
Numerical Errors

- **Dispersive Error**
  If a numerical scheme gives a solution whose all Fourier components travel at the same constant phase speed, waveforms comprised of a superposition of modes retain their shape as they propagate. Such a scheme is called non-dispersive.

  When the discrete wavenumber differs from the actual one, different Fourier components travel with different phase speed. The numerical error causing this solution behaviour is called dispersive error.

  This error is typically associated to odd derivatives in the leading term of the truncation error of Taylor expansion.

- **Diffusive Error**
  When a numerical scheme attenuates the amplitude of the Fourier components of the solution, the error is called diffusive.

  This error is usually associated to even derivatives in the leading term of the truncation error of Taylor expansion.

Importance of Numerical Accuracy

- In a periodic domain with \( N \) uniformly spaced points on \( x \in [0, L) \), with \( h = L / N \), the discrete Fourier transform (DFT) of the function \( f \) is

\[
\tilde{f}_j = \frac{1}{N} \sum_{m=1}^{N} f_m e^{-i k_j x_m} \quad j = -N/2, \ldots, N/2 - 1
\]

where \( k_j = 2 \pi j / L \) is the wavenumber and \( x_m = (m - 1) h \).

- The \( j\)-th component of the DFT of \( \partial f / \partial x \), denoted \( \tilde{f}_j' \), is simply \( i k_j \tilde{f}_j \).

  Taking the DFT of a finite difference numerical scheme

\[
\langle \tilde{f}_j' \rangle_{fd} = i K(k_j h) \tilde{f}_j
\]

where \( K(k, h) \) is the so called modified wavenumber.

- For \( k_j h = \pi \), the period \( (L / j) \) of the wave is \( 2h \). Hence, \( k h \) is usually normalized by \( \pi \).

- The number of points per wavelength, \( N_\lambda \), needed depends on the scheme.
  
  \[ \Rightarrow \text{The energy of higher wavenumbers that cannot be represented on the grid is aliased onto the resolved wavenumbers.} \]
Importance of Numerical Accuracy

- The wave propagation characteristics of finite difference (FD) schemes give information about all the Fourier components that are supported on the grid.
- The $j$-th component of the DFT of $\partial f / \partial x$, denoted $\tilde{f}_j$, is simply $i k_j \tilde{f}_j$ ($k_j = 2 \pi j / L$).
- A numerical spatial scheme modifies the real wavenumber of the solution:
  \[ \left( \tilde{f}_j \right)_{fd} = i K(k_j h) \tilde{f}_j \]
  - The range of wavenumbers over which the modified wavenumber approximates the exact differentiation within a specified error tolerance defines the set of well-resolved waves (the compact FD schemes have superior modified wavenumbers to explicit schemes).
  - As the maximum tolerable error is reduced, the low-order schemes require large numbers of grid points $N_h$ per wavelength. The computational efficiency of higher-order schemes must be tempered with their additional computational cost.

Dispersion of Finite Difference Schemes

- The dispersion and dissipation of Fourier components depends on the particular PDE. A simple example is the one dimensional advection equation
  \[ u_t + c u_x = 0 \]
  that represents the advection of $u$ at a constant speed $c$. The exact solution is $u = u(x - c t)$.
- If all Fourier components of the solution travel with the same constant phase speed $\omega / k = c$ (dispersion relation), waveforms comprised of a superposition of modes retain their shape as they propagate, and are therefore called non-dispersive ($\omega$ is the angular frequency, $k$ the wave number).
- When the spatial derivative is approximated with a FD scheme (the time derivative is treated continuously for now), the dispersion relation for the semi-discrete numerical scheme is $\omega h / c = K(k h)$ where $K(k h)$ is the modified wavenumber.
- The phase speed is now given by $c_p = \omega / k = c K(k h) / (k h)$ and therefore different Fourier components travel with different phase speed. Such a system is said to be dispersive, as waveforms comprised of a superposition of modes do not retain their identity as they propagate.
**Dispersion of Finite Difference Schemes**

- A group velocity can be defined:
  \[ c_g = \frac{\partial \omega}{\partial k} = \frac{c}{h} \frac{\partial K (kh)}{\partial k} \]

  The group velocity of a wave is the velocity with which the overall shape of the wave's amplitudes - known as the modulation or envelope of the wave - propagates through space. If \( \omega \) is directly proportional to \( k \), then the group velocity is exactly equal to the phase velocity. Otherwise, the envelope of the wave will become distorted as it propagates.

- **Example**: frequency dispersion in groups of gravity waves on the surface of deep water. The red dot moves with the phase velocity, and the green dots propagate with the group velocity. In this deep-water case, the phase velocity is twice the group velocity. The red dot overtakes two green dots, when moving from the left to the right of the figure.

- The above definition of group velocity is only useful for wavepackets. Since waves at different frequencies propagate at differing phase velocities in dispersive media, for a large frequency range the wavepacket would change its shape while travelling, making group velocity an unclear or useless quantity.

**Dispersion of Finite Difference Schemes**

- For a given frequency, centered schemes have two solutions to the dispersion relation:
  \[ c_g = \frac{\partial \omega}{\partial k} = \frac{c}{h} \frac{\partial K (kh)}{\partial k} \]

  - for long wavelength solution, the group velocity is positive
    \( \Rightarrow \) these are the so called smooth waves, i.e., the well-resolved components of the solution and they approach the real solution as the grid is refined;

  - for short wavelength solution, the group velocity is negative
    \( \Rightarrow \) these are the so called spurious waves, that are poorly-resolved.

- For the \( H \) order centered FD scheme, the group velocity of spurious waves is equal (in module) to the smooth waves.

- As the order of the scheme is increased, the speed of spurious waves increases.
Still on Dispersion … and Dissipation

- **Centered FD formulas with** $K(kh)$ **real** for real wavenumbers, have dispersion of waveforms **but** the amplitude of each Fourier component **remains constant.**
- **When asymmetric stencils** are used, $K(kh)$ becomes complex.
  $\Rightarrow$ Disturbances will be **exponentially attenuated** when the imaginary part is positive, and will **grow exponentially** when the imaginary part is negative.
  It is therefore necessary for stability that the scheme be dissipative for all $kh$.

Spatial Discretization: Compact Schemes

A centered compact approximation for the first derivative $f'$, on a uniform mesh is:

$$
\sum_{j=1}^{N_\alpha} \alpha_j \left( f'_{i+j} + f'_{i-j} \right) + f' = \frac{1}{h} \left( \sum_{j=1}^{N_\alpha} \alpha_j \left( f_{i+j} - f_{i-j} \right) \right) + O(h^n)
$$

- If $N_\alpha = 0$ the scheme is explicit.
- If $N_\alpha \neq 0$ the scheme is implicit (Padé or compact).

The coefficients $\alpha_j$ and $\alpha$ are chosen to give the largest possible exponent $n$ in the truncation error, for a given stencil width, i.e., chosen $N_\alpha$ and $N_\alpha$.

The maximum possible exponent is $n_{\text{max}} = 2 \left( N_\alpha + N_\alpha \right)$.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>$\alpha_1$</th>
<th>$\alpha_2$</th>
<th>$\alpha_3$</th>
<th>$\alpha_4$</th>
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</tr>
<tr>
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<td>-</td>
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<td>-</td>
<td>4</td>
</tr>
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<td>-</td>
<td>3/4</td>
<td>-</td>
<td>-</td>
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</tr>
<tr>
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<td>1/4</td>
<td>-</td>
<td>-</td>
<td>-</td>
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</tr>
<tr>
<td>C6</td>
<td>1/3</td>
<td>-</td>
<td>7/9</td>
<td>-</td>
<td>6</td>
</tr>
<tr>
<td>DRP</td>
<td>-</td>
<td>(996 - 153\pi)/42\pi</td>
<td>(1725 - 5632\pi)/34\pi</td>
<td>(272 - 85\pi)/14\pi</td>
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<tr>
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</table>

Coefficients for conventional explicit (E2,E4,E6) and implicit (C4,C6) centered FD schemes, as well as the optimized schemes of Tam and Webb (DRP; where $c = 45 \pi - 128$) and Lui and Lele (L1; where the constants are: $a_0 = 0.5381301488732363; a_1 = 0.0666331012388123; a_2 = 1.16757724399269; a_3 = 0.8234281701082790; a_4 = 0.01852078348686639 / 6$).
Spatial Discretization: Compact Schemes

- Central formulation both in left and right-hand-side.
- Up to 10th order.
- Much better dispersive behaviour than "classical" central type schemes (even if same formal order!).
- Require tri- or penta- diagonal solver.

Effect of Staggering the Variables on Numerical Accuracy

Modified wavenumber spectrum of various first derivative operators.

Note that the transfer function of interpolators reduces accuracy.

Modified wavenumber spectrum of various second derivative operators. Curves for the collocated scheme (dotted line) and two first derivative evaluations with the staggered scheme (dashed line) lie almost on each other.

**Effects of Numerical Accuracy on Results - LES of a Channel Flow -**

- \( \text{Re}_\tau = 180 \) and \( \text{Re}_{\text{t}} = 590 \)
- Mesh: \( 32 \times 64 \times 32 \) and \( 16 \times 32 \times 16 \)
- Control volume formulation
- **Compressible** flow equations
- Smagorinsky model
  - No dynamic procedure
  - Van Driest damping at walls
- Schemes:
  - **Standard central** scheme
  - 4th and 6th order compact schemes
- Temporal solver:
  - Explicit multi-stage **Runge-Kutta**

- Homogeneous directions are those parallel to the walls

---

**LES of a Channel Flow: Re = 590 on a 32*64*32 mesh**

Averaged velocity distribution
LES of a Channel Flow: Re = 590 on a 32*64*32 mesh

Turbulence intensities

Streamwise spectra at y+=20 (DNS: y+=19.39)

Spanwise spectra at y+=20 (DNS: y+=19.39)
Computational Efficiency

- High-order FD schemes provide lower error than low-order methods.
- Their increased accuracy must be weighed against the increased number of computations per node.
- The impact of the spatial discretization on the time step that can be used must also be considered. Thus, here a Courant constraint is assumed as limit:
  \[
  \Delta t \sim \frac{\Delta x}{K_{\text{MAX}}} = \frac{\lambda/N^2}{K_{\text{MAX}}}
  \]

Cost data for several FD schemes

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Nodes</th>
<th>Multipoles</th>
<th>Nop</th>
<th>Measured CPU</th>
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</tr>
</tbody>
</table>

The measured CPU times are normalized with the E2 CPU time.

NOTE. Penalty associated to compact schemes run in parallel codes is not considered here.

Which numerical scheme is computationally more efficient in reactive flow problems?
Some Tips

- In LES, it is better that the error of the numerical scheme used for convective terms be dispersive than diffusive, in order to reduce the interaction with SGS model, whose effect is diffusive.

  ⇒ Centered finite difference schemes are preferable.
  - Centered first derivative schemes do not dissipate (when used in hyperbolic systems of linear first-order PDE). This is important in turbulence and aeroacoustics.
  - Instead, centered second derivative schemes do not cause any dispersion. It is suggested not to compute viscous terms by two applications of a first derivative scheme, since this provide no diffusion for the highest wavenumbers. Furthermore, the second derivative operator generally have better modified wavenumber characteristics than two applications of first derivatives (Not true in staggering).

- The order of accuracy near the boundaries is not as important as stability and related conservation properties.

- When focusing on acoustics: acoustic waves are very weak compared to near-field fluctuations and they must propagate with little attenuation over long distances.

  ⇒ This dictates the use of high-order-accurate numerical methods (compact and optimized finite difference and Runge-Kutta time marching schemes) and close attention to boundary conditions.

Conclusions About Numerical Schemes to Be Used

- In fact, compact schemes are efficient but difficult to manage in parallel computing.

- To reduce dispersion error, optimized finite difference schemes seem to be a better choice than compact schemes, since they are explicit. However, since they have better dispersive properties only at high wave numbers and not at small ones, they are not very accurate for turbulent flows.

- Hence, centered high order (from 2nd up to 8th) explicit schemes are more practical and implemented in many LES codes (eventually coupled with fine grids).
Large Eddy Simulation
- Initial and Boundary Conditions -

Initial Conditions: Perturbing the Flow

- Overimposing some disturbing signal on initial field is *commonly* used to destabilize a flow, e.g.,

\[ A' = I \cdot \exp \left( -K_z (R_o - r)^2 \right) \frac{1}{2} \left\{ 1 - \tanh[K_z(z - Z_o)] \right\} \cdot \sin \theta \]

- *Is it really necessary to force the flow destabilization?*
  - The equations simulate *deterministic chaos*: if the flow must be turbulent, transition to turbulence is *spontaneous after a characteristic time!*
  - … but for non-periodic boundary problems, the *effect of inlet turbulence is strong!*
    - **Bluff-bodies** and **edges** helps flow destabilization.

- Initial condition in practical flows: *no flow motion* inside the domain.
Waves leaving (outgoing waves) and entering (incoming waves) the computational domain through an inlet and outlet plane for a subsonic flow.

**Inlet and Outlet Boundary Conditions**

- According to characteristics analysis, information flows in terms of waves $L_c$.
- These waves propagate at characteristic velocities, $U$, $U+a$, $U-a$, being $a$ the sound speed.
- Thus, for a subsonic flow four information enter the domain at the inlet and just one at the exit.
- We need to specify:
  - Four BCs at inlet
  - One BC at outlet among physical and numerical BCs.
- What to do when no explicit BC fixes one of the dependent variables required by the numerical implementation?
  - Extrapolation
  - Integration of conservation equations

**What Variables at Subsonic Inlet and Outlet?**

**INLET**

- Distribution for $T$, $Y_i$, $U_z$, $U_r$ and $U_\theta$ are typically assumed.
- What about inlet turbulence? Random fluctuation or inflow turbulence generation.
  
  No experimental velocity profile is usually available at the inlet. To simulate jets:
  
  ⇒ three choices to have injection conditions closer to experiment
  
  • solve the flow along the whole injector;
  
  • assuming the inlet of domain calculation at the first experimental section;
  
  • trial and error strategy to obtain the first experimental profile.
  
  Sometimes mass flow rate could be a better choice.

**OUTLET**

- Pressure must be specified, but …
- Numerical P waves reflection
  
  Incident Physical Wave, $P$
  
  Reflecting Inlet Speed $U$
  
  Reflecting Outlet Speed $U$
  
  Incident Physical Wave, $P$
  
  Reflecting Inlet Speed $U$
  
  Reflecting Outlet Speed $U$
  
  When $N$ waves reach another boundary
  
  ⇒ reflection in the form of physical waves
  
  ⇒ Numerical feedback between inlet and outlet
Effects of Reflecting and Non-Reflecting Boundary Conditions

3-D axisymmetric jet: wrong Strohual number (St ≠ 0.24) using reflecting inlet BC! Partially non-reflecting inlet BC solves the problem.

- Downstream outflow is purely non-reflecting.
- Outflow coaxial to the jet is partially non-reflecting.
- If inlet is reflecting it forces shedding at \( f = U/L \) ⇒ Expansion waves moving upstream are reflected at the inlet, resulting in a phenomenon that seems physical, but in fact it is numerical.

NSCBC-LODI Boundary Conditions

To reduce numerical wave reflections
⇒ Navier-Stokes Characteristic Boundary Conditions - Local One Dimensional Inviscid

- Conservation equations solved at boundaries.
- All incoming waves amplitude expressed in terms of outgoing waves amplitude.
- Waves identified as for Euler equations, neglecting waves associated to diffusion processes.
- Theoretical problem: Navier-Stokes equations are not hyperbolic due to viscous terms.
- However, Navier-Stokes equations propagate waves like Euler equations do.
- For DNS of high Reynolds number flows this approximation is probably well justified.
- But, what is the effect of subgrid viscosity in LES? (This problem seems only theoretical).

Procedure
- LODI (Local One Dimensional Inviscid) system at each point of the boundary:
  - Compatibility conditions between the physical boundary conditions chosen and the amplitude of waves crossing the boundary.
  - Approximate incoming waves amplitude variation.
- Recast the hyperbolic terms in Navier-Stokes equations specialized at the boundary to show directly the amplitudes \( L_i \) of (inviscid) characteristic waves associated to each characteristic velocity \( \lambda_i \).
- And solve them.
**NSCBC-LODI Boundary Conditions**

\[ r \frac{\partial \rho}{\partial t} + d_1 + \frac{\partial \rho U_t}{\partial r} + \frac{\partial \rho U_r}{\partial \theta} = \ell \]

\[ r \frac{\partial \rho U_t}{\partial t} + r U_t d_1 + r \rho d_2 + \frac{\partial \rho U_t^2}{\partial r} + \frac{\partial \rho U_r}{\partial r} + \frac{\partial \rho U_r}{\partial \theta} = -\frac{\partial \rho}{\partial r} + \frac{\partial \rho U_r}{\partial r} + \frac{\partial \rho_{\theta \theta}}{\partial \theta} + \frac{\partial \tau_{r r}}{\partial r} + \frac{\partial \tau_{r \theta}}{\partial \theta} + \frac{\partial \tau_{\theta \theta}}{\partial \theta} + r \rho B_t \]

\[ r \frac{\partial \rho U_r}{\partial t} + r U_r d_1 + r \rho d_3 + \frac{\partial \rho U_t}{\partial r} + \frac{\partial \rho U_r}{\partial r} = \frac{\partial \tau_{r r}}{\partial r} + \frac{\partial \tau_{r \theta}}{\partial \theta} + \frac{\partial \tau_{\theta \theta}}{\partial \theta} + r \rho B_r \]

\[ r \frac{\partial \rho U_\theta}{\partial t} + r U_\theta d_1 + r \rho d_5 + \frac{\partial \rho U_t}{\partial r} + \frac{\partial \rho U_r}{\partial r} + \frac{\partial \rho U_\theta}{\partial \theta} = -\frac{\partial \rho}{\rho \theta} + \frac{1}{2} \rho \frac{\partial U_r}{\partial r} + \frac{r \rho B_\theta}{\rho \theta} \]

\[ r \rho C_v \left[ \frac{\partial Y_t}{\partial t} + \frac{d_2}{C_p} \frac{\rho C_v (\gamma - 1)}{C_p} + U_t \frac{\partial Y_t}{\partial r} + \frac{1}{r} \frac{\partial Y_r}{\partial \theta} \right] = -p \left( \frac{\partial U_r}{\partial r} + \frac{\partial U_\theta}{\partial \theta} \right) - \left[ \frac{\partial \phi_t}{\partial r} + \frac{\partial \phi_r}{\partial \theta} + \frac{\partial \phi_\theta}{\partial \theta} \right] - r \sum_{k=1}^{N_k} Y_k \omega_k + r \sum_{k=1}^{N_k} Y_k B \cdot V + r \tau_{r r} \frac{\partial U_r}{\partial r} + r \tau_{r \theta} \frac{\partial U_\theta}{\partial \theta} + \tau_{r \phi} \left( \frac{\partial U_r}{\partial r} + \frac{\partial U_\theta}{\partial \theta} \right) + \tau_{r \phi} \left( \frac{\partial U_r}{\partial r} + \frac{\partial U_\phi}{\partial \phi} \right) \]

Having assumed \( \frac{\partial \rho \theta}{\partial z} \) and \( \frac{\partial \phi}{\partial z} = 0 \).

**LODI Equations**

\[ d_1 = \frac{1}{a^2} \left( L_2 + L_1 + L_5 \right) \]
\[ d_2 = \frac{L_1 + L_5}{2} \]
\[ d_3 = \frac{L_5 - L_1}{2 \rho a} \]
\[ d_4 = L_3 \]
\[ d_5 = L_4 \]

\[ L_1 = (U_z - a) \left( \frac{\partial U_z}{\partial z} - \rho a \frac{\partial U_z}{\partial z} \right) \]
\[ L_2 = U_z \left( a \frac{\partial \rho}{\partial z} + \frac{\partial \phi}{\partial z} \right) \]
\[ L_3 = U_z \frac{\partial U_r}{\partial z} \]
\[ L_4 = U_z \frac{\partial U_\theta}{\partial z} \]
\[ L_5 = (U_z + a) \left( \frac{\partial \rho \theta}{\partial z} + \rho a \frac{\partial U_z}{\partial z} \right) \]

\[ \frac{\partial \rho}{\partial t} + d_1 = 0 \]
\[ \frac{\partial \rho}{\partial t} + d_2 = 0 \]
\[ \frac{\partial U_t}{\partial t} + d_3 = 0 \]
\[ \frac{\partial U_r}{\partial t} + d_4 = 0 \]
\[ \frac{\partial U_\theta}{\partial t} + d_5 = 0 \]
Outflow NSCBC-LODI Boundary Conditions

- **Completely non-reflecting**: $L_1 = 0$, for the incoming wave, while the outgoing waves $L_2, L_5$ are calculated from the computational domain by means of asymmetric stencils. Note that $p$ must be imposed somewhere, otherwise it will drift.

- **Partially non-reflecting**: $L_1$ is modelled relaxing pressure to an external pressure $p_\infty$.

$$L_1 = \sigma \left( 1 - M^2 \right) \frac{\nu - \nu_\infty}{L}$$

$L$ is the domain length relevant to the wave motion considered.

$M$ is the Mach number.

$\sigma$ is a constant (typically $0.1 - 0.5$ depending on the problem).

- This partially non-reflecting boundary reacts to incident waves by changing the boundary variables’ values to reduce reflection.

- The boundary relaxes to the desired pressure $p_\infty$ in a characteristic time $\tau$.

Substituting the modelled $L_1$ and $L_5 = 0$ in $\tau = 2L / (\sigma a)$.

- Waves having frequencies lower than $1/\tau$ are reflected inside the domain.

- $\sigma$ not too low to avoid $p$ drift, and not too high to reduce spurious reflections.

Inflow NSCBC-LODI Boundary Conditions

- Lele and Poinsot suggest:
  - impose velocity and temperature profiles $\Rightarrow$ incoming waves $L_2, L_5$ from LODI eqns.:

$$L_2 = \frac{\gamma - 1}{2} (L_1 + L_5) + \frac{\rho a^2}{T} \frac{\partial T}{\partial t} \quad (1)$$  

$$L_5 = L_1 - 2\rho a \frac{\partial U_z}{\partial t}$$

- work out $\rho$ by solving NSCBC continuity equation;

- work out $U_z(y,t)$ by solving LODI momentum eqn.

This method does not work. In fact, at steady state $L_5 = L_1$ and reflection takes place.

- **Partially non-reflecting inflow**:
  - $L_5$ is modelled relaxing velocity profile to an external velocity profile $U_z(y,t)$

$$L_5 = \sigma \rho a^2 \frac{U_z - U_z^\infty}{L}$$

- the other velocity components and temperature are imposed $\Rightarrow L_2$ from LODI eqn. (1);

- work out $\rho$ by solving NSCBC continuity equation;

- work out $U_z(y,t)$ by solving LODI $U_z$ momentum eqn., $\frac{\partial U_z}{\partial t} = \frac{L_1 - L_5}{2\rho a}$.

This method works. Only frequencies lower than $1/\tau$ are reflected inside the domain.
NSCBC-LODI Relaxing Method

**Non-reflecting outflow**

Incoming wave

\[ L_1 = (U_z - a) \left( \frac{\partial p}{\partial z} - \rho \frac{\partial U_z}{\partial z} \right) \]

Outgoing wave

\[ L_5 = (U_z + a) \left( \frac{\partial p}{\partial z} + \rho \frac{\partial U_z}{\partial z} \right) \]

Model incoming pressure wave

\[ L_1 = \sigma \left( 1 - M^2 \right) a \frac{p - p_\infty}{l}. \]

From inner field

**Non-reflecting inflow**

Incoming wave

\[ L_1 = (U_z - a) \left( \frac{\partial p}{\partial t} - \rho \frac{\partial U_z}{\partial t} \right) \]

Outgoing wave

\[ L_5 = (U_z + a) \left( \frac{\partial p}{\partial t} + \rho \frac{\partial U_z}{\partial t} \right) \]

Model incoming “velocity” wave

\[ L_5 = \sigma \rho a^2 \frac{U_z - U_\infty}{l}. \]

From inner field

The **incoming wave** is

\[ L_1 = \sigma \left( 1 - M^2 \right) a \frac{p - p_\infty}{l}. \]

When it will be \( p = p_\infty \Rightarrow L_1 = 0. \)

The LODI equation

\[ \frac{\partial p}{\partial t} + L_1 + L_5 = 0 \]

modelled, and at **target conditions** is

\[ \Delta p \approx \frac{\sigma \left( 1 - M^2 \right) a}{\Delta t} \frac{p - p_\infty}{l}. \]

This state is reached after a time

\[ \Delta t \approx \frac{2L}{\sigma \left( 1 - M^2 \right) a} \]

That is roughly equal for subsonic flows.

**NSCBC-LODI Relaxing Method**

**Non-reflecting inflow**

The **incoming wave** is

\[ L_2 = \sigma \rho a^2 \frac{U_z - U_\infty}{l} \]

When it will be \( U = U_\infty \Rightarrow L_1 = 0. \)

The LODI equation

\[ \frac{\partial U_z}{\partial t} + L_5 - L_1 = 0 \]

modelled, and at **target conditions** is

\[ \Delta U_z \approx \frac{\sigma a U_z - U_\infty}{\Delta t} \frac{U_z - U_\infty}{l}. \]

This state is reached after a time

\[ \Delta t \approx \frac{2L}{\sigma a} \]
Effect of $\sigma$ on a Partially Non-Reflecting Outflow

Time evolution of pressure at partially non-reflecting boundary

- **Overcritical:** unstable
  - $\sigma = 10$
- **Subcritical:** stable
  - $\sigma \leq 0.3$
- **Critical:** stable
  - $\sigma = 3$

Effects of Reflecting, Partially and Fully Non-Reflecting BCs

- **Inflow** is treated according to NSCBC.
- **Reflecting outlet** (assumed $p$ and nil gradient for other variables) ⇒ **WRONG** dynamics.
- **Partially non-reflecting** ⇒ **SLIGHTLY WRONG** dynamics, but $p$ is constrained.
- **Fully non-reflecting** ⇒ **EXACT** dynamics, but $p$ could drift over long time and large domains.
Synthetic Turbulent Inlet Boundary Conditions

- **Random numbers** do not necessarily develop into turbulence with the desired statistics. Furthermore, they require a costly development section.

- **Unsteady inflow** conditions can be generated by simulating a spatially periodic, fully developed, parallel duct flow and constraining it using corrective forcing technique.
  - The inflow generator code saves a cross section of velocity data to the inflow database at every few time steps, until sufficient inflow data have been accumulated to provide converged turbulence statistics.
  - At each time step, the streamwise averaged velocity and fluctuation variance are calculated
    \[
    \bar{u}(y, z, t) = \langle u(x, y, z, t) \rangle_x \quad \bar{u}^2(y, z, t) = \langle u(x, y, z, t)^2 \rangle_x - \bar{u}(y, z, t)^2
    \]
    - If the desired mean velocity profile is \(U(y, z)\), and the fluctuation is \(U'(y, z)\),
      the instantaneous velocity field must be rescaled and shifted to have the specified mean and fluctuating velocity profiles:
      \[
      u(x, y, z, t) \rightarrow \frac{U'(y, z)}{\sqrt{\bar{u}^2(y, z, t)}} \left[ u(x, y, z, t) - \bar{u}(y, z, t) \right] + U(y, z)
      \]
      If only the mean is constrained: \(u(x, y, z, t) \rightarrow u(x, y, z, t) - \bar{u}(y, z, t) + U(y, z)\).

- The main code will read velocity data from the inflow database as inlet BCs (cyclically). The main simulation must contain time scales longer than the inflow recycling interval.


The inner position of the coflow peak in the Sommerfeld test case is captured only with turbulent inflow conditions.
Large Eddy Simulation
- Structure of a Numerical Code and SuperComputing -

HeaRT: Implementation Characteristics

- **Modularity**
  
  **Libraries:** chemical kinetics, boundary conditions, solvers.

- **Porting**
  
  **Language:** Fortran 95, MPI (parallelization paradigm).
  
  **Operating Systems:** Unix, Linux, AIX.
  
  **Supercomputing platforms:**
  
  - Distributed Memory – MIMD
  - Shared Memory – MIMD
  - Symmetric MultiProcessors (e.g. IBM-SP4, ES40, ...)
  - Cluster di PC/SMP (FERONIX, FERONIA, IBM-SP3, PROMETEO, TURAN)

- **Codes for simulation**
  
  **Pre-processing:** generation of initial field, inlet profiles, case configuration;
  
  **Post-processing:** statistics, turbulent structures identification ($\lambda_2$, helicity, vorticity), pollutant emissions (thermal NO, Prompt, via NO2)
Description of the Numerical Code: HeaRT

- **Numerics**
  - compressible, density based, formulation;
  - 2nd order centred finite difference (non-uniform) scheme in space with staggered approach (large accuracy enhancement with respect to collocated scheme, J.C.P., 191:392-419, 2003);
  - 6th order compact scheme with staggered approach in phase of validation;
  - 5th-3rd order WENO scheme for supersonic flows;
  - 3rd order Runge-Kutta (Shu-Osher) scheme in time;
  - NSCBC technique at boundaries.

- **Molecular Transports**
  - Heat: Fourier, species enthalpy transport due to species diffusion;

- **Molecular Properties**
  - kinetic theory calculation and tabulation (200-5000 K, ΔT=100 K) of single species Cp, μ, κ;
  - Wilke’s law for μmix (mass-weighted mixing law slightly less accurate);
  - Mathur’s law for κmix (mass-weighted mixing law much more less accurate);
  - Hirschfelder and Curtiss’ law for Dmix from single species tabulated Sc, or direct use of kinetic theory.

- **Complex Geometries**
  - Immersed Boundary method (2nd order for the time being) rearranged in Finite Volume formulation in the staggered compressible approach (Cut Cell Method).

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Description of the Numerical Code

- **Physical Models**
  - transport equations for mass, momentum, temperature, mass fractions, and perfect gas law;
  - transport equations for mass, momentum, internal + chemical energy, temperature, progress variable and its variance, and perfect gas law.
  - The Flamelet-Progress/Variable approach is the best compromise between detailed description and computational costs when realistic chemical kinetic mechanisms are used.

- **SGS models**
  - subgrid stresses: eddy viscosity Fractal Model (FM);
  - subgrid scalar fluxes: gradient laws;
  - subgrid reactions: idea of PSR taken from Eddy Dissipation Concept revisited in FM;
  - when the flamelet - progress variable - flame surface density approach is used
    - subgrid fluxes in progress variable and its variance equations are based on Pr and Sc;
    - laminar combustion chemistry is implemented in the form of premixed steady-state flamelet library;
    - the progress variable, Yc = YCO + YCO2, is used to characterize the amount of fuel that has been consumed, or the degree of progress in the reaction;
    - flamelets, in terms of all flame quantities (species mass fractions, temperature, source terms, …) are tabulated as function of the progress variable, its variance, enthalpy and filter size;
    - flamelets are precomputed by simulating burner stabilized flames at different mass flow rates in order to take into account heat losses by decreasing the enthalpy level h0 in the library from adiabatic to quenching.
• Enstrophy
  \[ \Rightarrow \text{seems to give a better representation} \]

• \( \lambda_2 \) method
  \[ \Rightarrow \text{seems to work only in the nonreactive zones, where dilatation is less important} \]

**Coherent Structures Visualization**

Three-dimensional vortices shown by using:

- Enstrophy
- Helicity
- \( \lambda_2 < 0 \) (eigenvalues of \( \mathbf{E}^2 + \mathbf{\Omega}^2 \))

**Sydney Nonreactive HM1 Case**

Sections: \( Y = 0 \) and \( Z = 41 \text{ mm} \)

Cross-Section \( Z = 41 \text{ mm} \)
Hythane Flame Sydney HM1

Instantaneous iso-temperatures and streamlines.

Tomography of temperature field at another time.
Syngas flames anchor easily:
- H2 preferential diffusion
- heat diffusion
- vortex shedding
Attention should be payed when converting old plants!

Mild Combustion


Very weak gradients of temperature are present in the combustion chamber.

![ROTA H2](image2)

Strong recirculation region, that favours the preheating of the mixture and its dilution, is evidenced in the near nozzle region.

MILD COMBUSTION

\[ T_{\text{inlet}} > T_{\text{SI}} \text{ and } \Delta T < T_{\text{SI}} \text{ [K]} \]

Laboratory Scale Bluff-Body Premixed Flame

DG-15-CON premixed CH4/Air burner in ENEA’s laboratory.

Effects of Forced Acoustic Waves onto Jet Shear Layers

- **Nonreacting shear layer without and with coaxial sound waves (coarse DNS).**
- Numerical simulation (1330000 nodes) of a jet with Re~10000 shows that acoustic excitation favours vortex roll-up in the shear layer and reduces the stable laminar length of the jet (same experimental trend).

Jets at Re = 13000 [Van Dyke]

In particular: the instability point moves from 5.5 cm to 4 cm from the inlet.
Exotic Theme: Effect of Helicity on Turbulent Spectrum

Considering the incompressible vorticity equation,

$$\frac{\partial \omega}{\partial t} + \nabla \times (\omega \times u) = \nu \nabla^2 \omega$$

if helicity $< \omega \cdot u > = 0$, the vector product, and therefore the energy transfer, reaches a maximum $\Rightarrow$ the $E_k$ slope increases [k $^{-4}$ is typical of 2D mixing layers]

Non-Reactive Multi-Phase Sommerfeld Test Case

- Dump combustor configuration with two coaxial injections.
- Glass spheres (45 micron diameter) are injected from the central jet.
- Central jet: $U_{z_{max}} = 12.4$ m/s
- Coaxial jet: $U_{z_{max}} = 18$ m/s, Swirl num. $= 0.5$, $U_t = 23$ m/s
- Global inlet $Re = 52400$. 

Re$_g$ = (mass flow of liquid phase coloured by its own velocity)
HeaRT: Domain Decomposition

• Execution of code is split into $N_p$ processes.
• The calculation domain is also split into $N_p$ sub-domains (genetic algorithm).
• Each processor of the parallel machine executes just one of the $N_p$ processes.
• The calculation sub-domains have boundary nodes (ghost frame) used to exchange data between processors of adjacent sub-domains or used for physical boundary conditions.

Top 500 Ranking (June 2009)
The relative speed-up $S$ is the ratio between the time needed with one processor, $T_1$, and the time needed with $N$ processors, $T_N$.

The linear (ideal) speed-up is a straight line:

$$S = \frac{T_1}{T_N} = \frac{T_1}{(T_1/N)} = N$$

**Case**: 15M grid nodes, 3D, 10 species, reactive, cresco2

**Dynamic Domain Decomposition**

**Instantaneous computational cost** for the chemical mechanism in a CH$_4$/H$_2$/Air flame.

**Domain decomposition** based on the number of computational nodes and communications between processors.

**Details of computational grid**

CH$_4$-H$_2$ finite chemistry with 19 species e 15 global steps

Dynamic decomposition: Load balancing between CPUs during computation.
Dynamic Domain Decomposition

Numerical simulation with 20 CPUs: 10 (z) x 1 (r) x 2(θ).

Average time per time-step:

- dynamic decomposition OFF: 17.5 s
- dynamic decomposition ON: 12 s

Gain: 30%
(communication time included)

Imposed tolerance: 10% of average time per time-step.

Hea.R.T

Development Team

E. Giacomazzi
F.R. Picchia
N. Arcidiacono
D. Cecere
F. Donato

Thanks for your attention