LES of the lean-premixed PRECCINSTA burner with wall heat loss using finite-rate chemistry

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Motivation

- Topology of swirling flows
 - Recirculation zones [1,2]
 - Advantages
 - ✓ Improved flame stabilization
 - ✓ Improved compactness



Objectives

Better understand **lean-premixed combustion** in **swirl** burners Study the impact of **wall heat loss** using **finite-rate chemistry LES**

- VVall heat transfer [3]
 - May influence the ORZ
 - Affects the stabilization process
 - May lead to local flame extinction

Chemistry models

- Tabulated chemistry (limited parametrization) [4]
- Global chemistry (good reproduction of global parameters only) [5]
- Finite-rate chemistry [6,7]





Syred, Beer, Combust. Flame, 1974
 Poinsot, Veynante, RT Edwards, 2005
 Mercier et al., Combust. Flame, 2016





[4] Moureau et al., Combust. Flame, 2011
[5] Franzelli et al., Combust. Flame, 2012
[6] Franzelli et al., C.R. Mecanique, 2013
[7] Lourier et al., Combust. Flame, 2017

Application PRECCINSTA burner

Experimental set-up

- Aeronautical swirl burner
- Detailed experimental database [1,2]
- Numerous numerical studies [3-6] (adiabatic)

Operating condition

- 'quiet' case at P=30kW

Numerical set-up & models

Mesh name	1	2	3	4
#cells [million]	1.7	14	110	877
Cell size [mm]	1.2	0.6	0.3	0.15

- Chemistry: Lu17 (17 species, 73 reactions) [7]
- Turbulence: Localized Dynamic Smagorinsky model
- Flame-turbulence interaction: DTFLES model





Air flow rate [g/min]	734.2
Methane flow rate [g/min]	35.9
Inlet temperature [K]	300.0
Thermal power [kW]	30.0
Equivalence ratio	0.83





Meier et al., Combust. Flame, 2007
 Lartigue et al., Appl. Therm. Eng., 2004
 Moureau et al., Combust. Flame, 2011
 Franzelli et al., Combust. Flame, 2012

[5] Franzelli et al., C.R. Mecanique, 2013[6] Lourier et al., Combust. Flame, 2017[7] Sankaran et al., PCI, 2007

Numerical method

LES solver

- Developed at CORIA and distributed in the SUCCESS scientific group [1,2]
- 220 users in labs and in the industry
- 3 PRACE projects
- Features
 - Unstructured meshes (complex geometries) and adaptive grid refinement
 - Low-Mach number Navier-Stokes equations (incompressible and variable density)
 - Double-domain decomposition [3]

ΞS

- Highly efficient solvers for linear system inversion (PCG, DPCG)
- 4th-order central finite-volume method and 4th-order time integration
- Combustion modeling (tabulated or finite-rate chemistry, NOx prediction model, ...)
- Two-phase flows (Lagrangian particles), spray and atomization (Levelset)
- Suited for massively parallel computing (>32 000 procs)









[1] YALES2 web site, <u>http://www.coria-cfd.fr</u>[2] SUCCESS web site, <u>http://success.coria-cfd.fr</u>

[3] Moureau et. al., CR Mecanique, 2011



Numerical method High-performance strategy for finite-rate chemistry

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot \rho Y_k \mathbf{u} = \nabla \cdot (-\rho \mathbf{V}_k Y_k) + \dot{\omega}_k$$

Key ingredients

Operator splitting	 Each phenomenon is advanced at its own characteristic time
CVODE stiff integrator	

- Validated with schemes up to 91 species, 700+ reactions
- Very good parallel performances up to 32'000 cores



Mesh nameAD1AD2AD3Adiabatic cases#cells [million]1.714110Cell size [mm]1.20.60.3

- Flame structure
 - Isocontour c=0.7





M-shape flame instead of V-shape

Non-adiabatic condition Determination of the wall thermal condition

- Trial and error process
 - 1. Modification of wall thermal condition
 - 2. Convergence of LES results
 - 3. Comparison of temperature profile to experimental data
 - 4. Back to 1.
- On 14M and 110M meshes
- Resulting Dirichlet condition
 - External injector wall
 - + chamber base
 - + chamber windows
 - Start at T=300K
 - Slight rise of temperature in injector
 - T=500K on chamber base
 - High rise up to 1800K on windows
 - No heat loss in the CRZ







Mesochallenge Myria 2017 @ CRIANN FIRELES PRACE project of the 15th call

Mesh #4, 877M cells



Mesh name 1 2 3 4 Results #cells [million] 1.7 14 110 877 **Non-adiabatic cases** Cell size [mm] 1.2 0.6 0.3 0.15 Flame structure • Heat loss/Total HR [%] 6.5 6.0 3.4 6.1 Isocontour c=0.7 _ T[K]1600.0 1475.0 1350.0 1225.0 NAD4 NAD1 NAD2 NAD3 1100.0

Extinction of external flame => V-shape flame

NAD4

OH field







Mean and RMS temperature











Mean and RMS CO2 mass fraction













Results Analysis of external flame extinction process

• Enthalpy defect on NAD4 case

$$\Delta H = H - H_{ad}$$

local total enthalpy

total enthalpy of the adiabatic mixture



Enthalpy defect is promoted by the high residence time in the ORZ => Higher sensitivity to stretch



Impact of heat loss on 1D stretched flames





Results Analysis of external flame extinction process

• Scatter plot of points with 0.75<c<0.8 for case NAD4





High heat release and adiabatic → Internal flame front

ZONE 2

ZONE 1

- Moderate heat release, high enthalpy defect
- \rightarrow Reactive outer flame

ZONE 3

- High enthalpy defect and no reaction
- \rightarrow Quenched outer branch



The enthalpy defect decreases the resistance of premixed flame front to high stretch rates.



When can we expect DNS of lab-scale burners?



ling

 Y_{CH}

- 150 microns
- 878M tets, 4M CPUh
- 4'000 cores, 4 weeks

Can we reach DNS faster ?



www.mmgtools.org

Dynamic h-adaptation of a premixed flame

- F-TACLES combustion model [1], refinement ratio = 6
- H-adaptation performed with the MMG library from INRIA
- More details in Bénard et al., IJNMF, 2015







[1] Fiorina et al., C&F, 2009

Application: Ignition in a SAFRAN HE combustor

- SAFRAN Tech simulation (R. Mercier)
- F-TACLES model with variable filter width
- Iso-temperature at 1300K colored by vorticity
- Parameters
 - Refinement ratio = 5
 - 41M to 75M tets
 - Physical duration = 0.3 ms
 - 5h on 512 Cobalt cores
 - 1 adaptation every 15 iter.
 - 1 adaptation = 4 minutes
 - Adaptation cost = 50%



On-going simulations with periodic dynamic remeshing by G. Vaudor



Application: primary atomization of a jet-in-cross-flow

• Kerosene jet in air at 10 bar

10 microns at the interface Up to 600M cells Up to 10k Broadwell cores

Ragucci et al. 2007 Atomization & Sprays







Injector diameter: D=0.5 mm
Flow section: 25 mm x 25 mm
Pressure: 10 bars

$$\begin{split} \textbf{V}_{air} = 37 \text{ m/s} & \text{and} \quad \textbf{V}_{kerosene} = 17 \text{ m/s} \\ \textbf{\cdot} \textbf{R}e_{air} = 590 \ 287 \text{ and} \quad \textbf{R}e_{kerosene} = 4477 \\ \textbf{\cdot} \textbf{W}e_{aero} = \rho_{air} V^2_{k\acute{e}ro} D/\sigma = 63.5 \\ \textbf{\cdot} \textbf{q} = \rho_{kero} V^2_{kero} / \rho_{air} V^2_{air} = 14.2 \end{split}$$

Dynamic mesh adaptation of a kerosene jet in cross flow. J. Leparoux, H. Musaefendic, R. Mercier, V. Moureau, accepted to ICLASS 2018, Chicago.





Primary atomization in a SAFRAN Aircraft Engines injector

- Pressure-swirl atomizer
- Simulation includes the full injector geometry

YALES2





Parameters

Kerosene/Air @ P₀

 $\Delta \mathbf{x}_{min}$ = 4.4 to 15 μ m

180h on 1120 cores

Adaptation cost: 50%

Cobalt @ TGCC

33 to 390 Mcells

Conclusions

- Finite-rate chemistry at high-res is now feasible in complex burners
- PRECCINSTA simulations are the closest to experiments to date
- FIRELES PRACE project
 - 23.5 million of CPU hours on Curie and Irene at TGCC, CEA
 - Dynamic mesh adaptation with finite-rate chemistry (GRIMech)
 - Up to 50 microns in flame front
 - More detailed analysis of external flame extinction process

Dynamic mesh adaptation is an option to reach higher resolutions

- Surface adaptation is in the work





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- R. Mercier SAFRAN Tech
- C. Dobrzynski, A. Froehly INRIA Bordeaux
- A. Pushkarev, G. Balarac LEGI







BACK-UP

Outline

- Motivation
- Flow solver
- Modeling of turbulent premixed combustion with finite-rate chemistry
 - The PRECCINSTA burner
 - Results for the adiabatic case
 - Results for the non-adiabatic case
- Towards DNS of the PRECCINSTA burner
 - Dynamic mesh adaptation for propagating fronts and interfaces



Towards optimal and user-independent LES of aeronautical burners

• Courtesy R. Mercier, SAFRAN TECH



Motivation

- Turbulent combustion modeling in realistic devices is highly challenging
 - Unsteady, multi-scale and multi-physics flow
 - Complex geometry
- Large-Eddy Simulation (LES) is a powerful tool for the modeling of the physics in aeronautical engines



Goal: better prediction of pollutant emissions



Results	Mesh name	NAD1	NAD2	NAD3
Non-adiabatic cases	#cells [million]	1.7	14	110
	Cell size [mm]	1.2	0.6	0.3





Lifted external flame Lower temperature in flame front

Mesochallenge Myria 2017 @ CRIANN

- Objective
 - Get a reference solution for the non-adiabatic case => NAD4

Increased grid resolution

- To have a better description of flame-turbulence interaction
- To reduce the influence of sub-grid scale models on CO production

M	esochallenge Myria 2017 – July 2017	Mesh name	1	2	3	4
•	9.2 ms physical time	#cells [million]	1.7	14	110	877
•	900'000 hCPU (8 days on 4992 cores)	Cell size [mm]	1.2	0.6	0.3	0.15

Performances

Portion du solveur	Part de la boucle temporelle [%]	RCT $[\mu s/noeud/iteration * N_{proc}]$	
Advection	0.78	6.5	
Implicit diffusion	3.41	28.7	
Pressure correction	8.48	71.2	ly 17% of computational
Scalar advection	9.26	77.8	
Scalar diffusivity	10.29	86.4 tin	ne in species source term !
Scalar source term	16.62	139.6	
Scalar diffusion	47.09	395.7	
GLOBAL	100.0	840.2	



LES of a partially premixed academic burner

- Dynamic mesh adaptation of a turbulent flame
- Collaboration with R. Mercier, SAFRAN TECH
- 1.8B tets, 8400 cores of Cobalt
- 18 min to adapt the mesh
- $\Delta x = 20$ microns in the flame



Longitudinal cut of the Cambridge burner (Mercier, 2015)

Case	ϕ_i	ϕ_o	ϕ_{cf}	$\overline{U_i}\left[m/s\right]$	$\overline{U_o}\left[m/s\right]$	$\overline{U_{cf}}\left[m/s\right]$
SwB5	1.0	0.5	0	8.31	18.7	0.4







Results plane Y=0























Numerical method An important feature of YALES2

- Two-level domain decomposition (Moureau et al., CRM, 2011)
 - Cache aware
 - Additional concurrency level







Driving mechanism: Moore's law

The power of super-computers almost doubles every 18 months •









Driving mechanism: Moore's law (revisited)

•



Erich Strohmaier, ISC 2017, Frankfurt

The end of Moore's law has a strong impact on the new architectures •



Mitigation of Moore's law weakening in YALES2

Optimization

- Improvement of memory accesses
- Vectorization: all the finite-rate chemistry is fully vectorized
- Low-latency communications: PhD of F. Gava, ICARUS project
 - Hybrid OpenMP/MPI model
 - Partitioned Global Address Space (PGAS)

Increased asynchronism

- Non-blocking collective communications (MPI3) in pipelined CG
- Dynamic scheduling of source terms

• Porting on new architectures

- GPU with ROMEO and in GENCI novel technology group
- KNL with INTEL/UVSQ
- NEC vector coprocessor (AURORA)
- Other alternative?



H-adaptation

- Mesh adaptation consists in the use of numerical techniques to refine or unrefine the mesh locally
 - Node insertion in Delaunay triangulations
 - Edge or face swapping
 - Element collapsing
- Several sequential libraries exist
 - MMG3D, C. Dobrzynski, http://www.math.ubordeaux1.fr/~dobrzyns/logiciels/mmg3d.php
 - MADLIB, http://sites.uclouvain.be/madlib/
 - NETGEN, http://www.hpfem.jku.at/netgen/
 - TETGEN, http://wias-berlin.de/software/tetgen/
 - CGAL, http://www.cgal.org/
 - MeshAdapt, http://www.scorec.rpi.edu/~xli/MeshAdapt.html
- Very few libraries are (massively) parallel





Challenge

- Can we imagine a parallel algorithm based on sequential adaptation?
- If mesh adaptation is performed on each processor, problems will arise at the proc interface. The choice made in YALES2 is to leave the proc interface and the boundaries untouched





Parallel h-adaptation strategy

- Designed for massively distributed meshes [1]
- Quality of the mesh is ensured during adaptation
- Tetrahedral elements only
- Example for 4 processors





Application: Turbulent flame kernel propagation

- CH4/air BFER scheme, DTFLES model, phi = 1.0, u'/S_L = 22.5
- Refinement ratios = 1, 3, 6



Jet-in-cross-flow

• Kerosene jet in air at 10 bar



Ragucci et al. 2007 Atomization & Sprays





Injector diameter: D=0.5 mm
Flow section: 25 mm x 25 mm
Pressure: 10 bars

 $\begin{array}{ll} \bullet V_{air} = 37 \text{ m/s} & \text{and} & V_{kerosene} = 17 \text{ m/s} \\ \bullet Re_{air} = 590 \ 287 \ and & Re_{kerosene} = 4477 \\ \bullet We_{aero} = \rho_{air} V^2_{kéro} D/\sigma = 63.5 \\ \bullet q = \rho_{kero} V^2_{kero} / \rho_{air} V^2_{air} = 14.2 \\ \bullet Dx = 20 \ microns \end{array}$

Dynamic mesh adaptation of a kerosene jet in cross flow. J. Leparoux, H. Musaefendic, R. Mercier, V. Moureau, submitted to ICLASS 2018, Chicago.



Jet-in-cross-flow

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Application to primary atomization with R. Mercier, J. Leparoux, H. Musaefendic, SAFRAN

- High-pressure kerosene jet in cross-flow
- Relevant for multi-point injection systems
- Ragucci et al., Atomization & Sprays, 2007
- Reference operating conditions
 - Injector diameter: D=0.5 mm
 - Flow section: 25 mm x 25 mm
 - Pressure: 10 bars
 - V_{air} = 37 m/s and $V_{kerosene}$ = 17 m/s
 - Re_{air}= 590 287 and Re_{kerosene}= 4477
 - We_{aero}= $\rho_{air}V^{2}_{k\acute{e}ro}D/\sigma = 63.5$
 - . Momentum ratio $q = \rho_{kero} V_{kero}^2 / \rho_{air} V_{air}^2 = 14.2$
- Numerics
 - Ghost-Fluid Method [Fedkiw et al., 2000]
 - Accurate Conservative Levelset [Desjardins et al., 2009]
- Paper accepted to ICLASS 2018, Chicago







Application to primary atomization with R. Mercier, J. Leparoux, H. Musaefendic, SAFRAN

Quantitative comparisons



Spray modeling with finite-rate chemistry PhD of H. Larabi



Picture of the jet spray flame



- KIAI spray flame [1]
- Finite-rate chemistry model
 - n-heptane/air scheme from Analytically Reduced Chemistry (ARC) [2]
 - built from Jerzembeck et al. [3]
 - 24 transported species, 32 QSS species and 217 reactions.
- Spray model
 - Point force approach
 - Droplet assumed to be fully atomised at injection
 - Rosin-Rammler distribution with a SMD of 32 µm and dispersion q of 2.3 (at Z = 10 mm)
 - LISA (Liquid Injection for Swirl Atomizers) model to obtain the hollow cone
- Evaporation model
 - Spalding (1953) / Abramzon & Sirignano (1989)
- Mesh
 - 520 million tetrahedra, 120 microns in the flame front region
 - [1] A. Verdier et al., 2016, Proceedings of the Combustion Institute.
 - [2] P. Pepiot-Desjardins and H. Pitsch. (2008). Combustion and Flame, 154(1):67-81
 - [3] S. Jerzembeck, N. Peters, P. Pepiot-Desjardins, and H. Pitsch. (2009). Comb. Flame, 156:292–301.



Spray modeling with finite-rate chemistry PhD of H. Larabi

• Flame topology





Spray modeling with finite-rate chemistry PhD of H. Larabi

• Flame lift-off





Spray modeling with finite-rate chemistry

- Lagrangian spray models are not well-suited for distributed computing
- They lead to strong imbalance between the processors
- Solution: double-constraint dynamic load balancing





Conjugate and radiative heat transfer

• Conjugate heat transfer can be modeled by solving the heat equation in the solid and coupling it with the fluid solver



• If radiative heat transfer is involved



Radiative heat transfer in CHT PhD of L. Boulet

Additional term in the energy transport equation •

$$\frac{\partial \rho h_s}{\partial t} + \frac{\partial \rho u_i h_s}{\partial x_i} = \frac{DP}{Dt} + \frac{\partial q_i}{\partial x_i} + \tau_{ij} \frac{\partial u_i}{\partial x_j} + \dot{\omega}_T + \frac{\partial q_i}{\partial x_i}$$

Radiative heat transfer solved by the RTE •





Spectral quadrature: FS-SNB-Ck Angular quadrature: Discrete Ordinate Method (Modest, 2013)

Modeling strategy

•

- **Spatial discretization: Finite-Volume** •
- Linear solver: BICGSTAB2
- **HPC: vectorization + distributed memory** •



Stabilization of a flame behind a metallic cylinder PhD of L. Boulet

1915

1508

1101 695 288

- 2 types of flame stabilisation
 - $\varepsilon = 1$: downstream stabilized
 - Low T & little recirculation zone
 - $\varepsilon = 0$: upstream stabilized
 - High T & large recirculation zone
- Angle profile
 - Gap between $\varepsilon = 0.15$ and $\varepsilon = 0.1$
 - Good comparison with [1]









Conjugate and radiative heat transfer PhD of L. Boulet

- Fire resistance tests
 - Manufacturers need to certify equipments in terms of fire resistance (housing, fastening engine, ...)
 - Certification: the apparatus needs to be submitted [1]
 - to a kerosene / air burner
 - during a fixed time (5 to 15 minutes)
 - with a standardized flame: 1100°C (${\approx}2010^{\circ}F)$ and 116 kW/m^2
- Objectives
 - Model fire resistance tests with Large-Eddy Simulation (LES)
 - Improve comprehension of phenomena involved in tests
 - Characterize inhomogeneities inside the torch (burnt gases, droplets)
 - Progress on test modeling
 - Reach a good confidence level for certification
- Difficulties
 - Very different time and space scales
 - Multi-physics and complex geometry
 - Very few studies



Liquid-fuel burner





Results for a complex CHT case PhD of L. Boulet

- Instantaneous temperature fields
 - Seems to be lower with participative gases
- Mean temperature at the outlet
 - Adiabatic: too high values
 - Transparent: same level as adiab. case
 - Participative: ≈200 K lower -> almost at ISO values
- Limitations

- Simple chemistry (2 reactions)
- No model for soot





