Center of Excellence in Combustion

HPC-enabling technologies for decarbonization of the power and transportation sectors

Daniel Mira (BSC), daniel.mira@bsc.es

Barcelona Supercomputing Center (BSC)

HPC workflows for scientific applications

European Commission | Horizon 2020 European Union funding for Research & Innovation

The CoEC project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 952181.

10/01/2024

Transportation and Energy sectors

Shipping

Aviation

Road transportation

Industrial processes

- ✓ High fossil fuel dependency
- ✓ Pollutant emissions
- ✓ Noise

Responsible for Climate Change

Urgent need of decarbonization

Strategies for decarbonization

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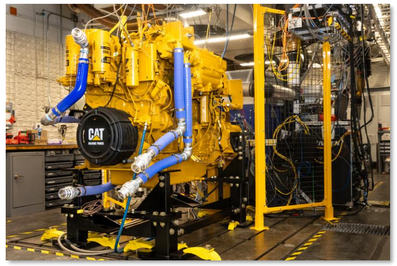
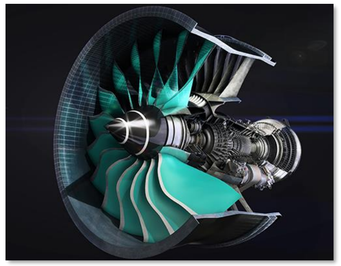
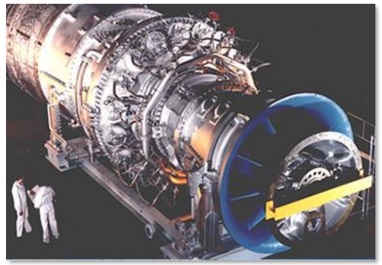
Improving combustion technologies



IC Engines

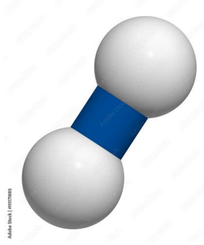


Aeroengines

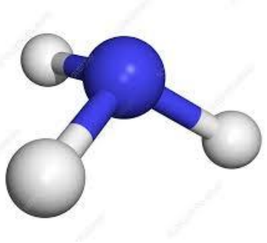


Gas Turbine

Use of synthetic or e-fuels



Hydrogen



Ammonia

SAF

Strategies for decarbonization




New combustion technologies

Use of synthetic (low-carbon) fuels

Combustion plays a central role in **energy conversion systems**

Combustion is a complex multiphysics problem

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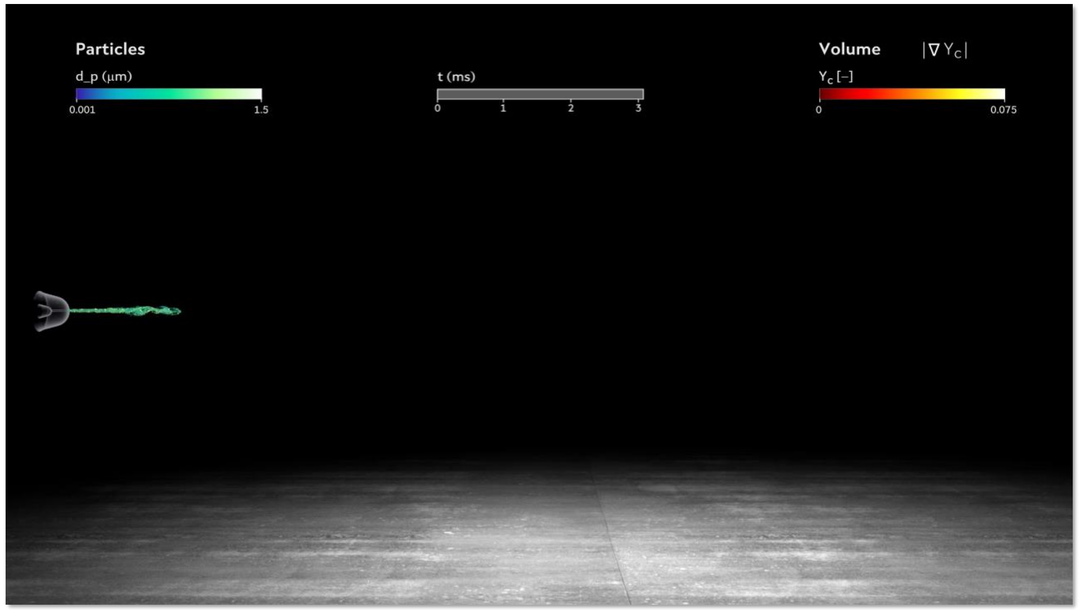

Physics

- ✓ Fuel injection
- ✓ Atomization
- ✓ Evaporation
- ✓ Ignition
- ✓ Combustion
- ✓ Pollutants

Multiscale, multiphase & multiphysics

LES & DNS with HPC

Spray flame simulation of OMEx at ECN Spray A conditions, Mira et al., ICEF2021-67745.

- ❑ Liquid **fuel atomization** and **droplet formation** occurs at smaller scales than turbulence
- ❑ Fuel sensitivity and pollutants require a **high-level description** of chemistry
- ❑ Some pollutants **NOx, PAHs and soot** evolve with **slow time scales**
- ❑ Treatment of **turbulence / chemistry interactions** at conditions of relevance for engines

Combustion simulations will strongly benefit from ***Exascale*** **computers**

What is CoEC?

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Project Information

CoEC

Grant agreement ID: 952181

Start date
1 October 2020

End date
~~30 September 2023~~

31/12/2023

Funded under
H2020-EU.1.4.1.3.

Overall budget
€ 5 644 531,25

EU contribution
€ 5 644 531,25

Coordinated by
BARCELONA SUPERCOMPUTING CENTER-CENTRO NACIONAL DE SUPERCOMPUTACION

Spain

CoEC consortium

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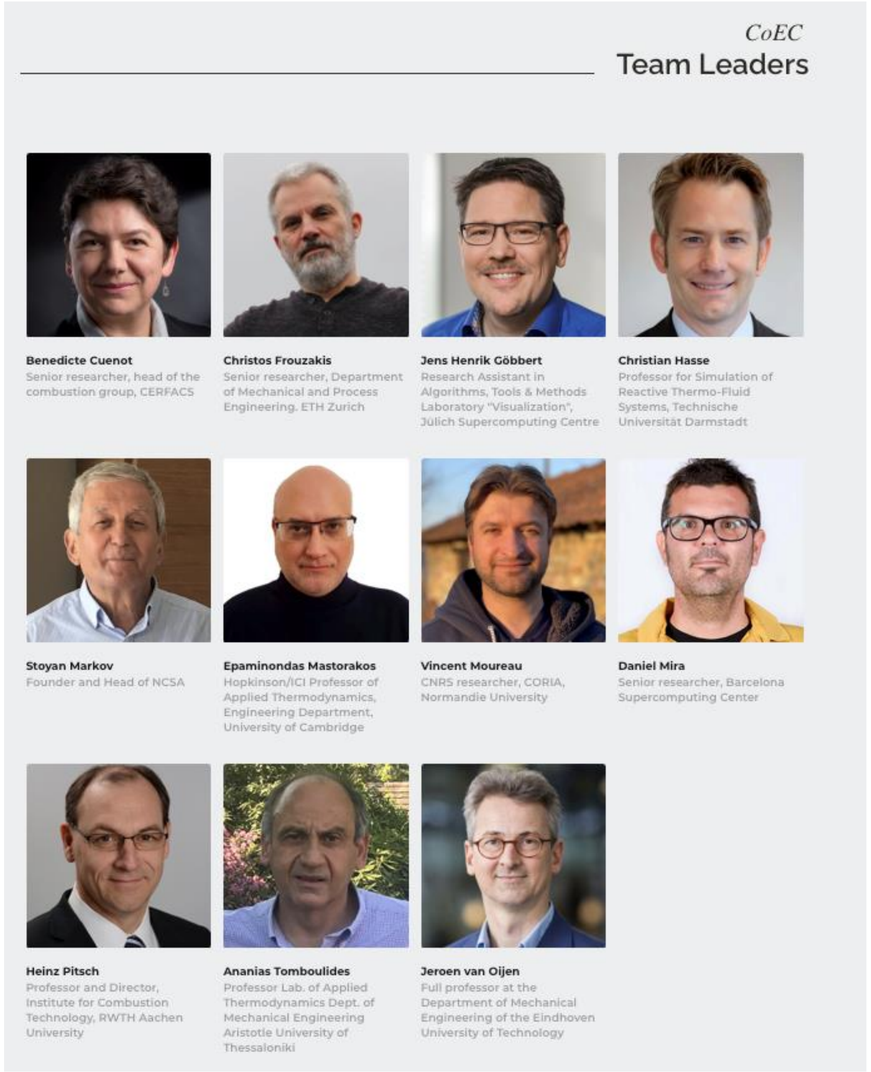

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JÜLICH Forschungszentrum

NCSA
NATIONAL CENTER FOR SUPERCOMPUTING APPLICATIONS

RWTH AACHEN UNIVERSITY

TECHNISCHE UNIVERSITÄT DARMSTADT

UNIVERSITY OF CAMBRIDGE

11 partners from **5 EU member states (with Switzerland & UK)**

- **3 supercomputing centers** (BSC, JSC, NCSA)

CoEC technological pillars

Combustion science

Generation of **advanced simulation methodologies** for turbulent multiphase reacting flows

HPC algorithms for combustion

Exa-enabling combustion simulation codes developed from new **algorithms** and **data processing and analysis** tools

EU HPC combustion codes

Representative **European Combustion Simulation codes** with advanced **users and industry**

From Sectors to Challenges and Demonstrators

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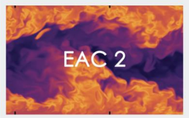
Particulate Matter: Formation, growth, oxidation and transport of soot particles

Sectors: Marine, automotive, power generation, aviation, industrial burners

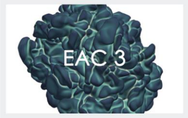
ECD1 ECD2 ECD13



Prediction of gas phase pollutants: NOx and CO

Sectors: Marine, automotive, power generation, aviation, industrial burners

ECD3 ECD4 ECD13



Hydrogen and hydrogen-enriched combustion and related thermo-diffusive instabilities

Sectors: Marine, automotive, power generation, aviation, industrial burners

ECD5 ECD6 ECD13

Fuel atomization and evaporation

Sectors: Marine, automotive, aviation, industrial burners

ECD7

Thermo-acoustic instabilities

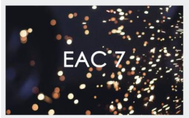
Sectors: Power generation, aviation, industrial burners

ECD4 ECD6

Ignition and plasma assisted combustion

Sectors: Marine, automotive, power generation, aviation, industrial burners

ECD8



Combustion of metal particles

Sectors: Automotive, power generation, industrial burners

ECD10

Flame-wall interactions and near-wall reacting flow modelling

Sectors: Automotive, industrial burners, and aviation

ECD11 ECD12 ECD13

8 x EACs

ECD 1

Large-Scale DNS calculation of formation, growth and transport of particulates

Leading Institution	Collaborating Institutions	Associated EACs	Software involved	ECD type
AUTH	AUTH, RWTH, ETHZ	EAC1	CIAO, Nek5000	Fundamental physics

ECD 5

Detailed chemistry DNS calculation of turbulent hydrogen and hydrogen-blends combustion

Leading Institution	Collaborating Institutions	Associated EACs	Software involved	ECD type
RWTH	RWTH, TUE, ETHZ, AUTH	EAC3 and EAC5	CIAO, DISCO, Nek5000	Fundamental physics

ECD 7

Fuel atomization and evaporation in practical applications

Leading Institution	Collaborating Institutions	Associated EACs	Software involved	ECD type
CNRS	BSC, CNRS, UCAM, TUD	EAC4	Alya, CIAO, YALES2, CLIO, OpenFOAM	Application

13 x ECDs

Application-oriented codes






CoEC includes the flagship codes used by Industry and academia

YALES2
AVIP
JAGUAR
DISCO
Alya
AVBP
PRECISE_UNS
CIAO
Nek5000
CLIO
OpenFOAM

11 Flagship codes

CoEC project structure

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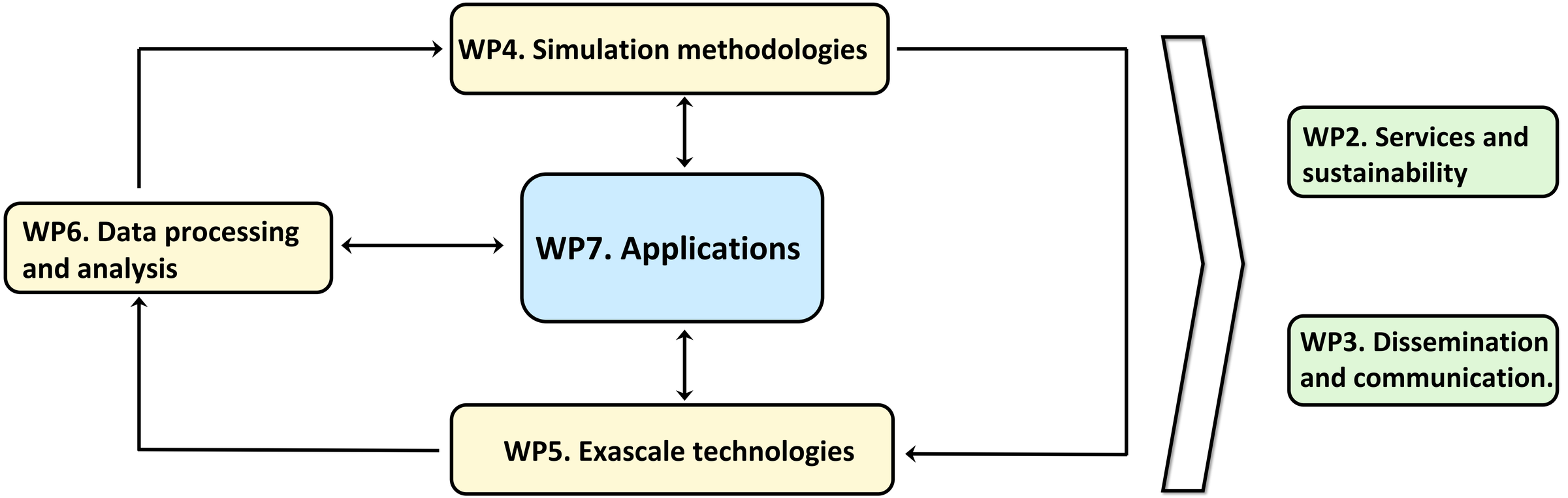

11

Combustion methodologies in CoEC (WP4)

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UMR 6614 CORIA
COMPLEXE DE RECHERCHE INTERPROFESSIONNEL EN AÉROTHERMOCHIMIE

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ETH zürich

UNIVERSITY OF CAMBRIDGE

Tasks 4.1: High-order methods
1. Dynamic grid refinement
2. Overlapping grid
3. Arbitrary Lagrangian-Eulerian framework

Tasks 4.2: Adaptive mesh in EL
1. Dynamic grid refinement
2. Partitioning
3. Quality of the grid discretization

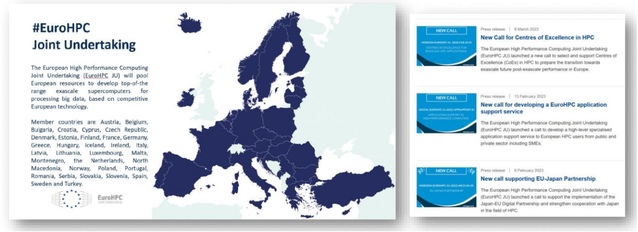
Tasks 4.3: Mechanism reduction
1. Error estimation
2. On-the-fly reduction
3. ODE solver

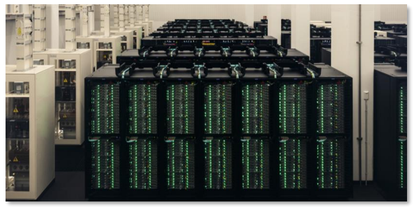
Tasks 4.4: Particle transport
1. Coupling of Lagrangian and Eulerian solvers
2. Modeling of physics
3. Moment-based approach

WP7 ECDs

EuroHPC: Driving EU HPC Progress

The central focus of advanced computing in Europe





2

Combustion methodologies in CoEC (WP4)

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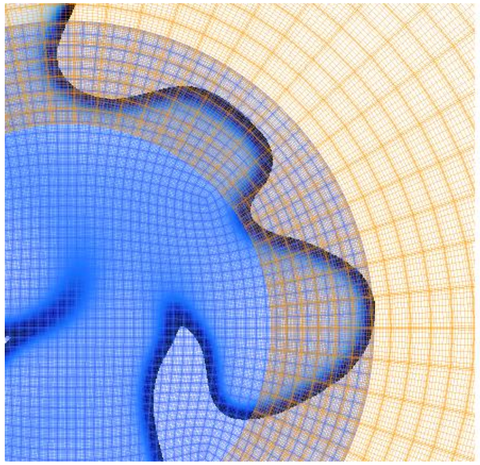
4.1 High-order methods

Nek5000/NekRS: r-adaptativity in Nek5000 and NekRS, and high-order spectral interpolation for arbitrary Lagrangian-Eulerian mesh motion..



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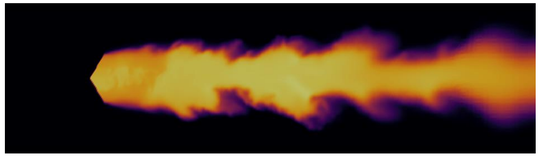
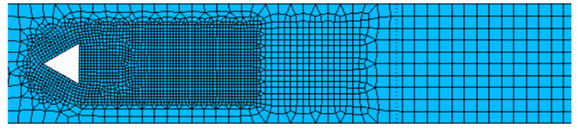
ETH Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich

Jaguar: In-house solver developed by CERFACS and ONERA. It is based on the **Spectral Difference Method** with **unstructured meshes** and **h-p adaptation**. It runs on **both CPU/GPU.**





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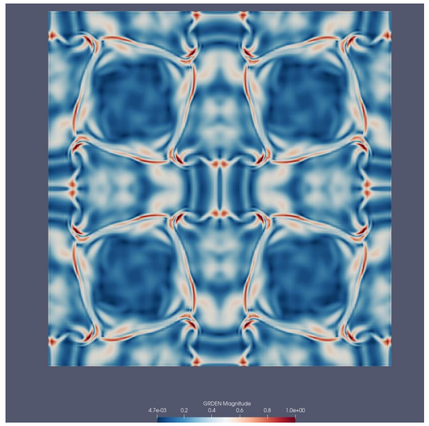
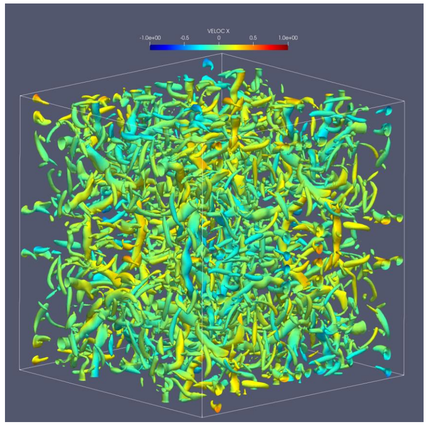
Sod2D: **Spectral Finite Elements (SEM)** with **entropy-stable stabilization** model and **operator splitting to the convective terms** of the compressible Navier-Stokes system.





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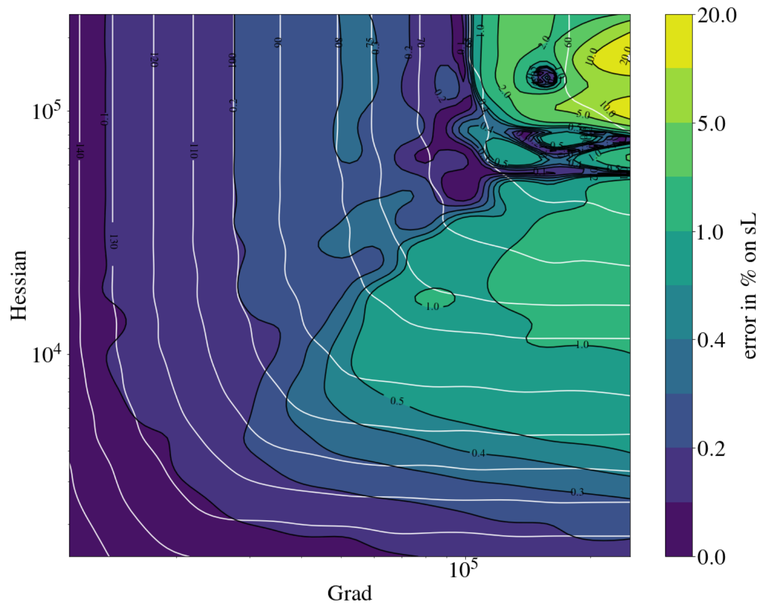
Combustion methodologies in CoEC (WP4)

4.2 Error estimator for dynamic mesh adaption

Error on the laminar flame speed

Gradient and hessian error estimators for mesh parametrization



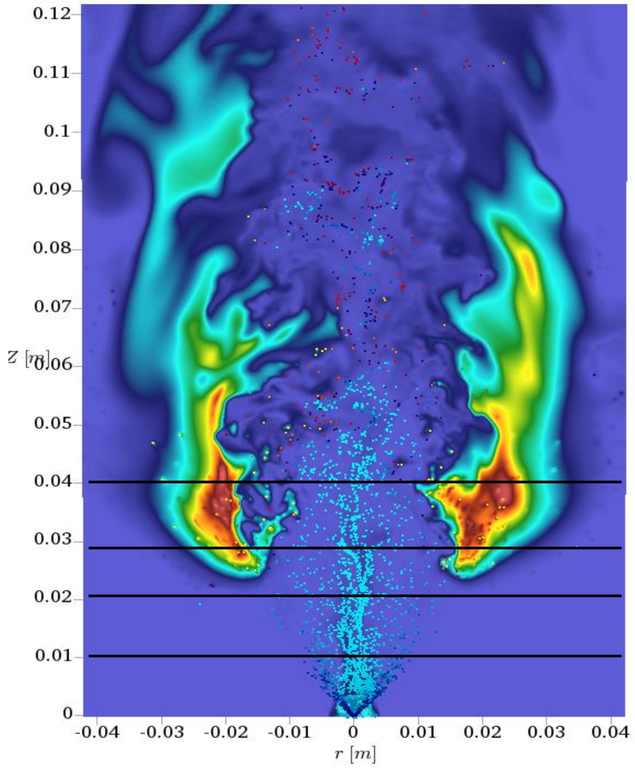
Params

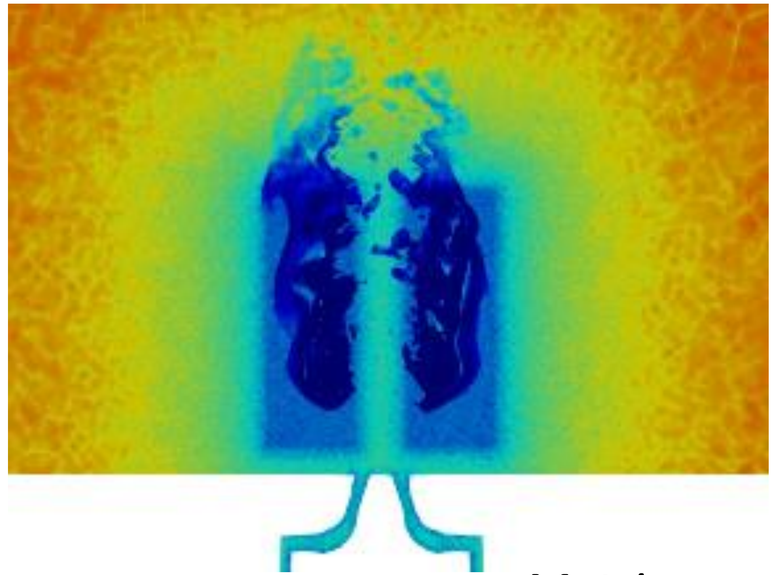
$\Delta x_{min} = 10\ \mu m, \Delta x_{max} = 500\ \mu m$

$h_{grad} = 1$, white iso-lines = constant number of cells

Meetrics and error estimators in a spray flame

CRSB burner with YALES2 Feature detection based on level set of heat release





Metric

Combustion methodologies in CoEC (WP4)

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4.3 Adaptive chemistry and UQ of chemistry reduction

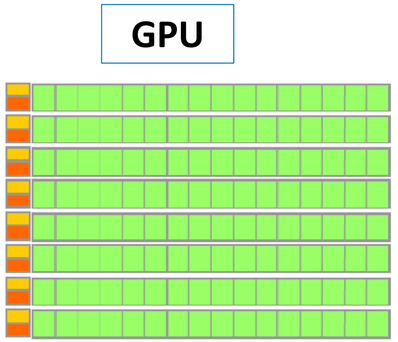
NekRK: Fast kernels for chemistry, thermo and transport for CPU and GPU architectures.

TRAC: Tabulated reactions for Dynamic Adaptive Chemistry for on-the-fly chemistry reduction.

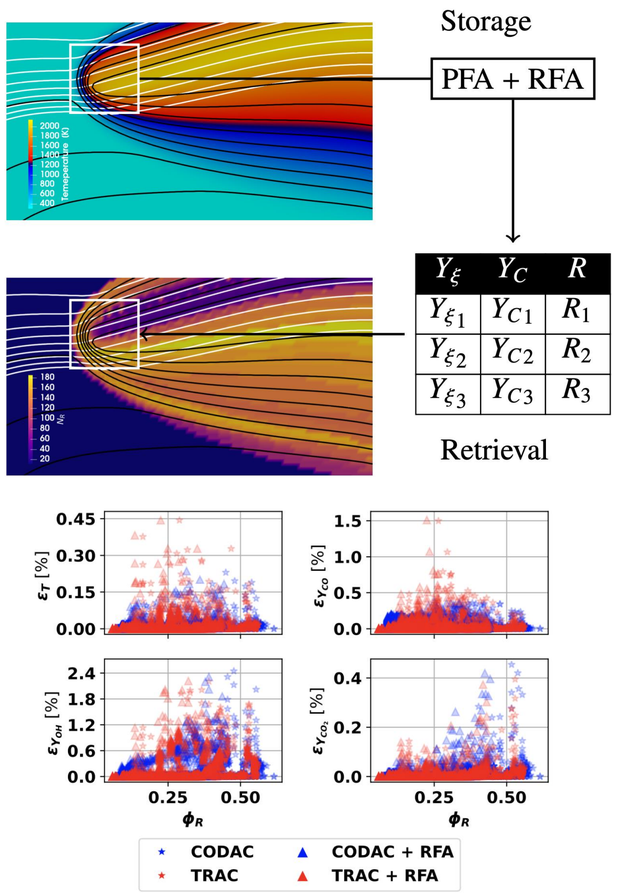
Smaller registers compared to CPU

```
//1: 2 O + M <=> O2 + M
kf = __NEKRK_EXP__(-1.0f*lnT+11.695247021764184f);
Rf = Ci[3]*Ci[3];
k_rev = EXP(-2*gibbs0_RT[2]+gibbs0_RT[3]) * C0;
Rr = k_rev * Ci[4];
cR = kf * (Rf - Rr);
rates[3] += -2*cR;
rates[4] += cR;

//2: O + H + M <=> OH + M
kf = __NEKRK_EXP__(-1.0f*lnT+13.122363377404328f);
Rf = Ci[2]*Ci[3];
k_rev = EXP(-gibbs0_RT[1]-gibbs0_RT[2]+gibbs0_RT[4]) * C0;
Rr = k_rev * Ci[5];
cR = kf * (Rf - Rr);
rates[2] += -cR;
rates[3] += -cR;
rates[5] += cR;
```



Reactions computed individually to avoid storing intermediate results and reduce register pressure



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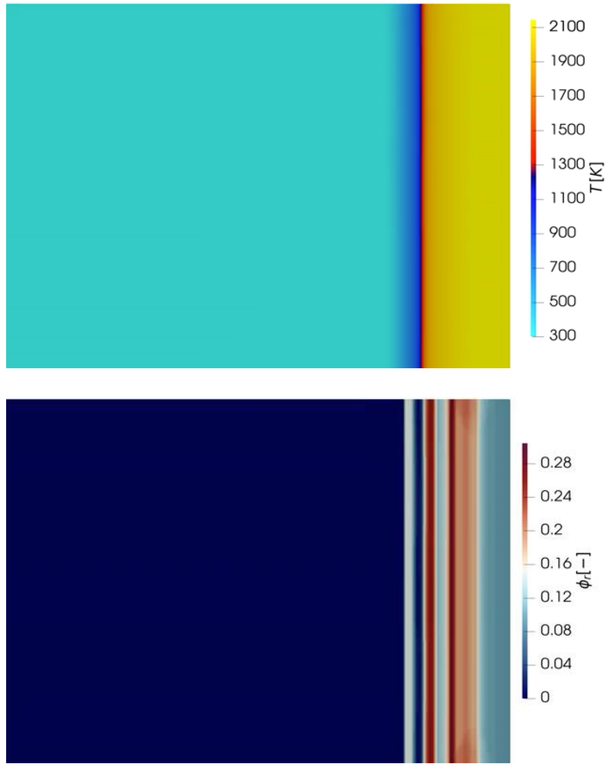

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4.3 Adaptive chemistry and UQ of chemistry reduction

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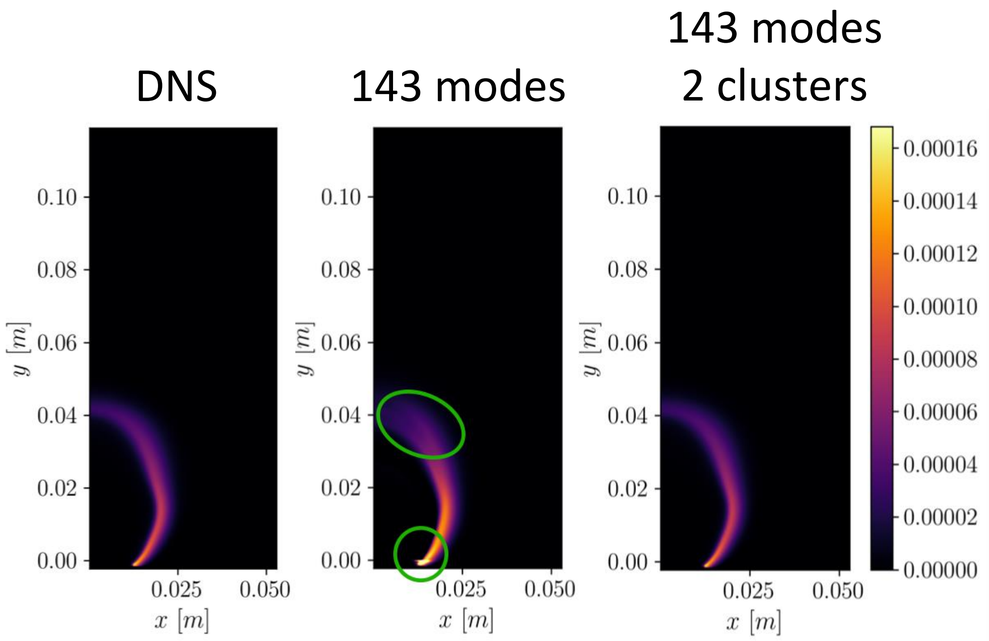
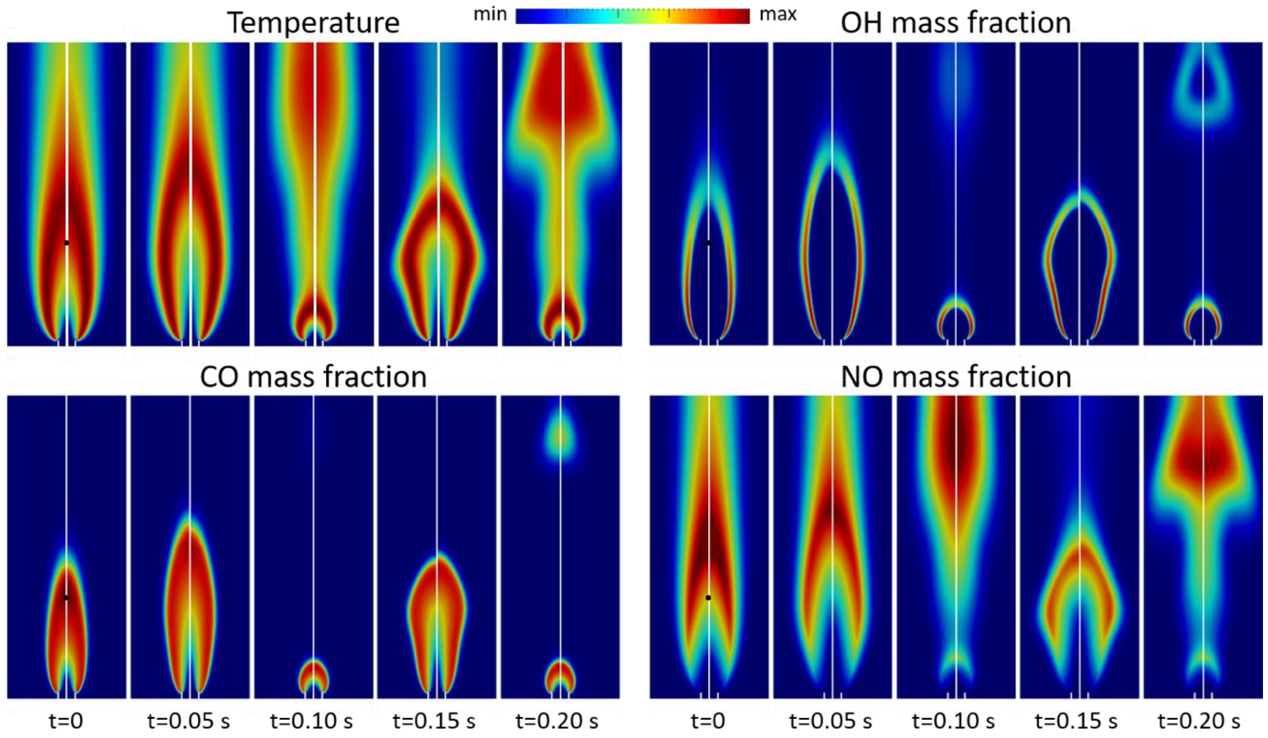
Reduced-order modelling and clustering

- ✓ ROM for chemistry based on DMD
- ✓ Clustering through LPCA
- ✓ PCA-based Cell Agglomeration – P(CA)2





DNS **P(CA)²**

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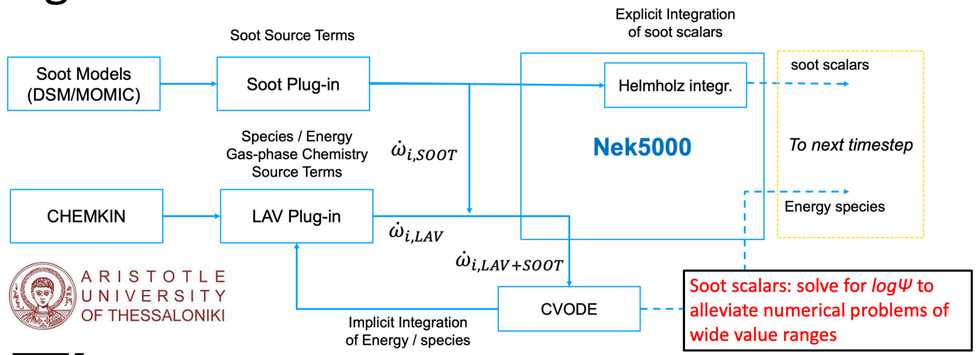
4.4 Eulerian-Eulerian and Eulerian-Lagrangian methods for particle transport

Nek5000: Soot Plugin compatible with LAV plugin for Nek5000



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CIAO: Soot moments library MOMIC and HMOM on C++ stand-alone library

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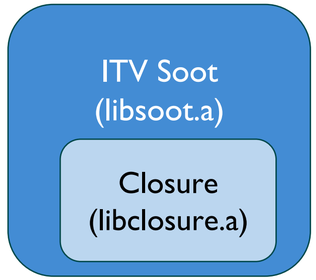
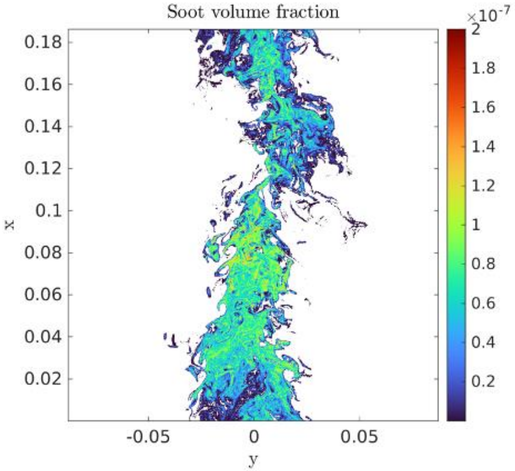
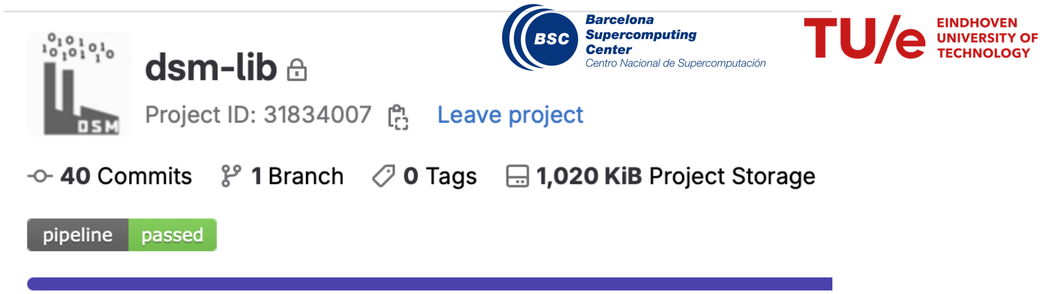




DSMLib: Discrete Sectional Method Library for soot formation using CPU/GPU.



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CLIO: Preferential diffusion model for soot formation in CMC.

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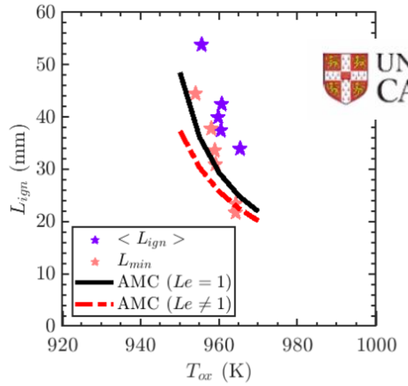

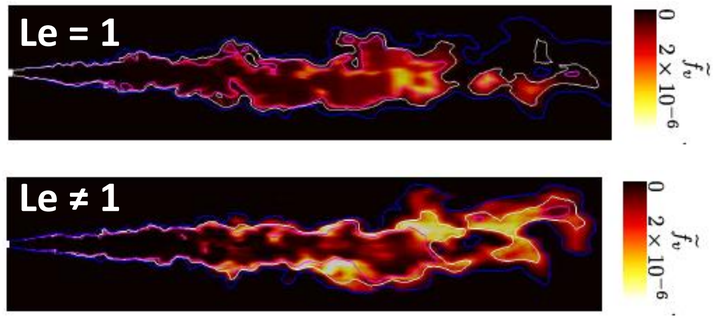

Application cases CoEC (WP7)

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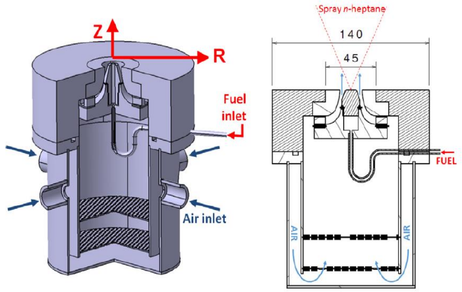
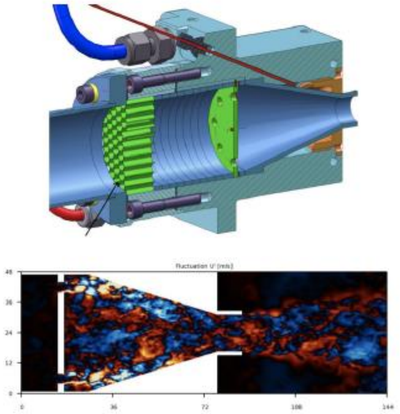
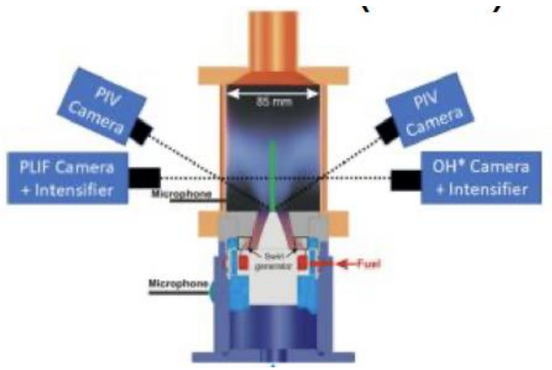


Coria Rouen Spray Burner CRSB (CORIA)





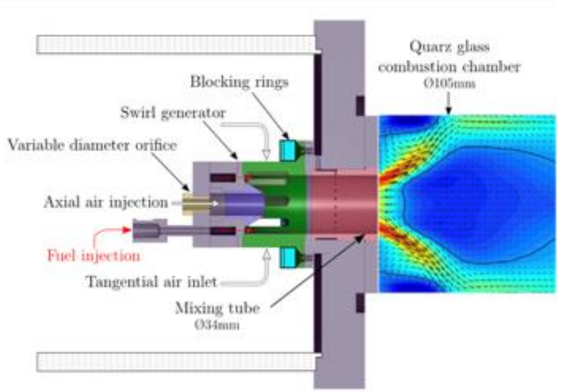
High-pressure h2-enriched natural gas (DLR)

Delft Adelaide Flame III ISF workshop

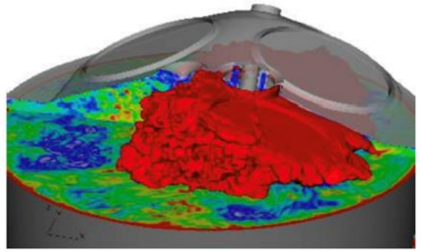
Tornado burner (2 kW)

100kW proof-of-concept

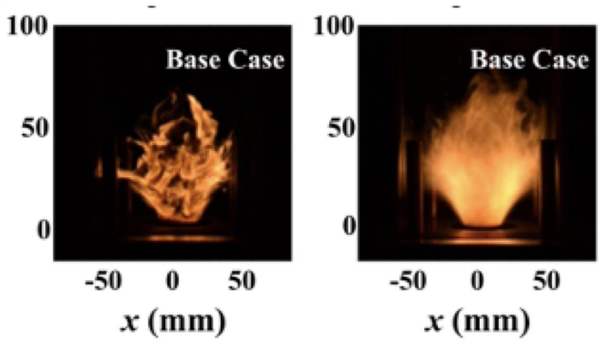
Metal particles (TU/e)



H2-swirl stabilized flames (TU Berlin)



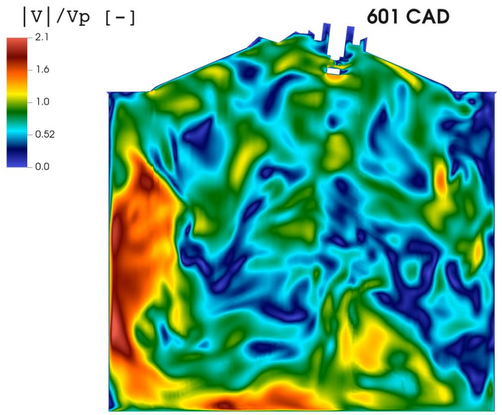
TU Darmstadt IC-engines (TUDa)

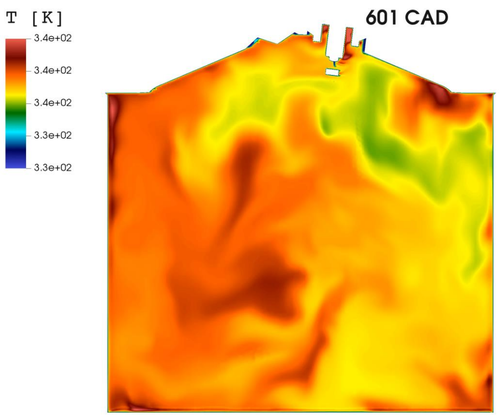


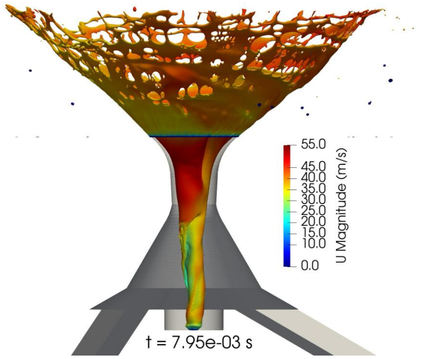
Cambridge RQL (UCAM)

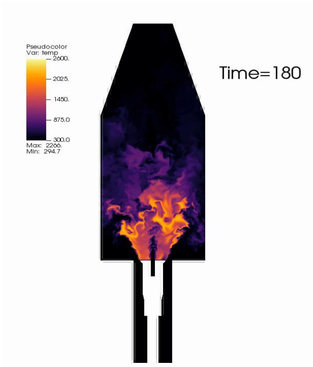
Application cases CoEC (WP7)

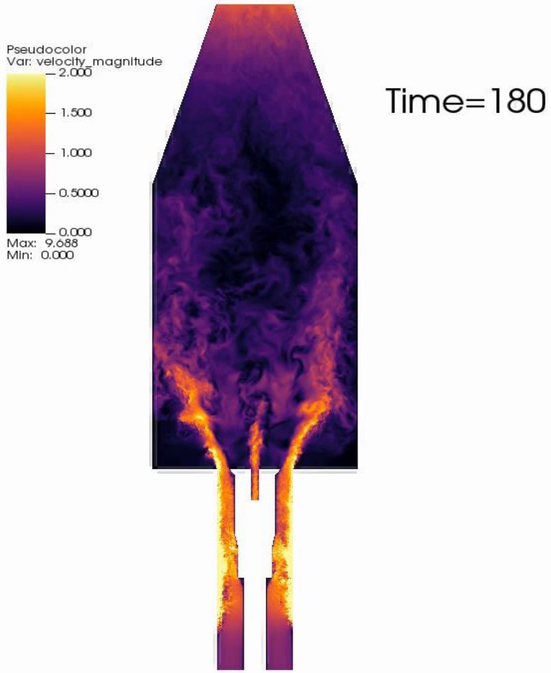
Center of Excellence in Combustion

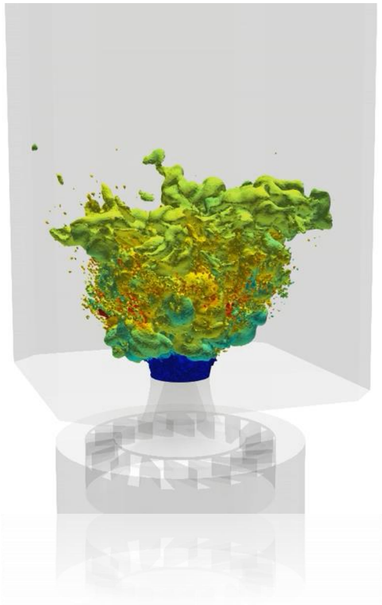


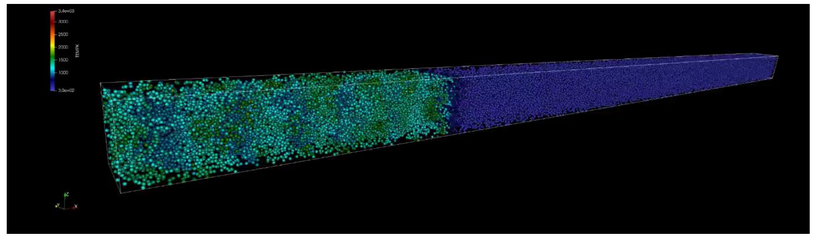


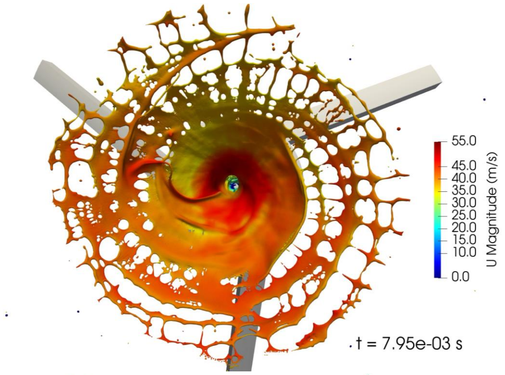


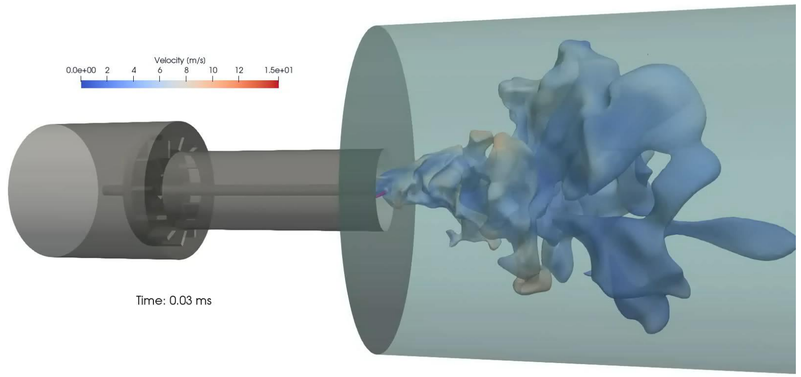


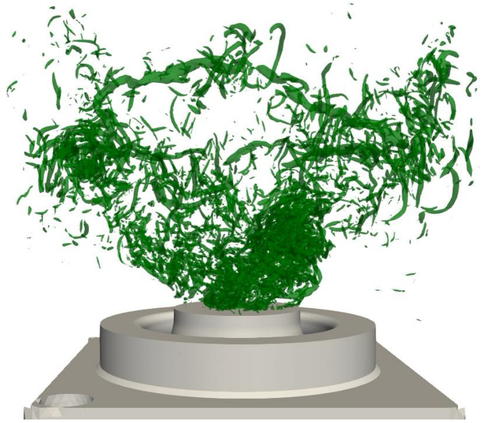


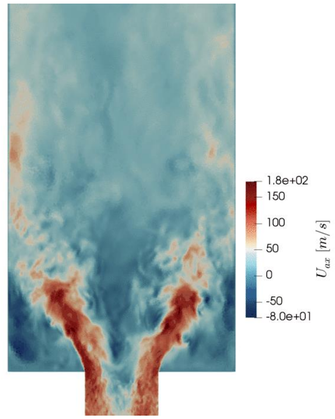


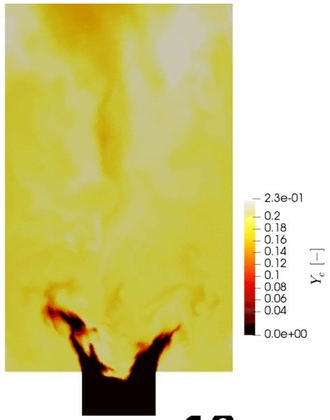












Application cases CoEC (WP7)

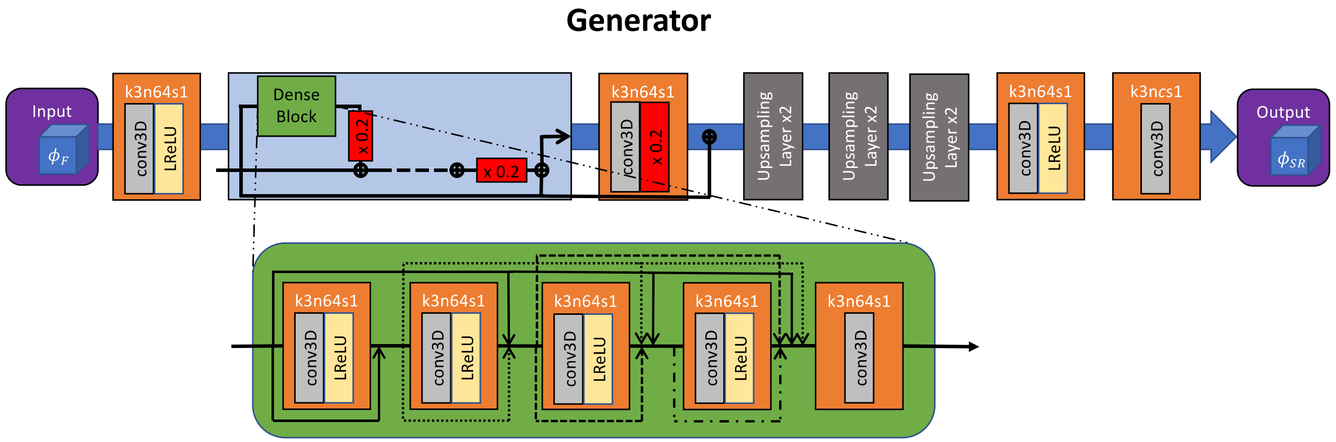
Center of Excellence in Combustion

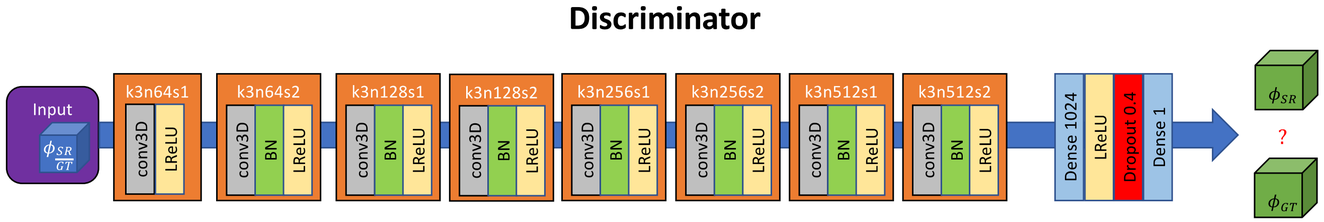
Machine Learning & Data Analytics

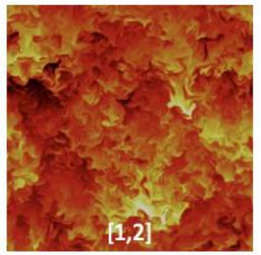
JÜLICH Forschungszentrum

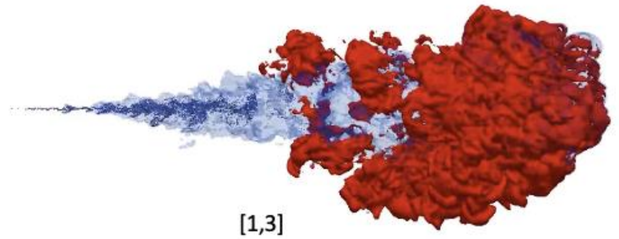
RWTH AACHEN UNIVERSITY

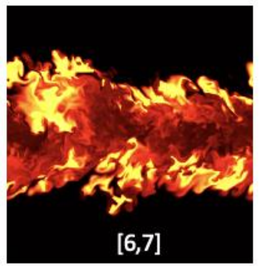
NCSA NATIONAL CENTER FOR SUPERCOMPUTING APPLICATIONS

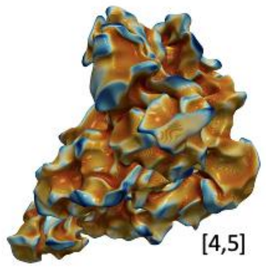


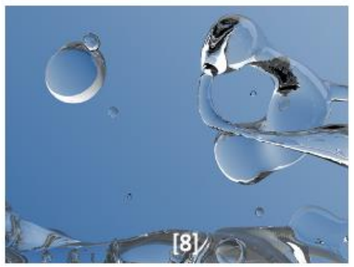












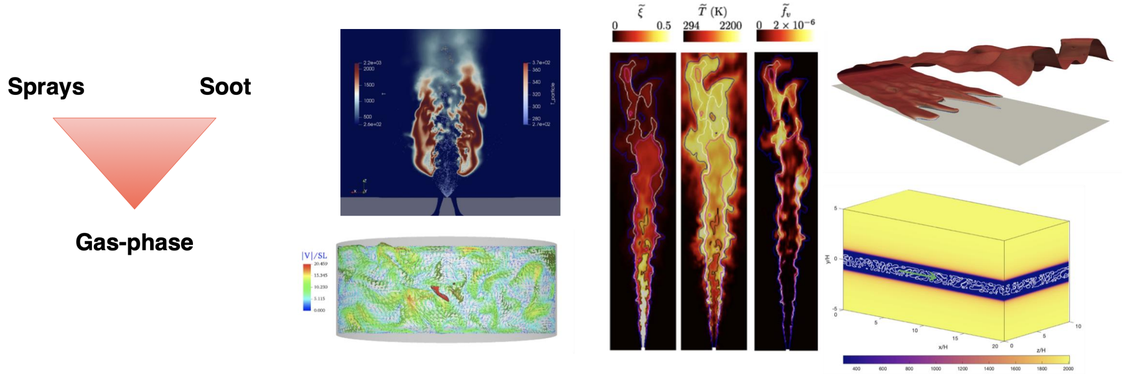
CIAO – SuperLES MLLib: fully parallel and GPU enabled library that calculates the turbulent stress tensor in LES simulations using ML approach (PIERSGAN).

Exa-enabling technologies (WP5)

Center of Excellence in Combustion

- ✓ **Unlock exascale computing** for combustion simulations
- ✓ Develop **advanced algorithms and software implementations** for a **heterogeneous landscape** with coexistence of various architectures
- ✓ Establish **CoEC guidelines** for Exascale methodologies in combustion

POP anlaysis on the Flagship codes



T5.2 Scalable algorithms for combustion

T5.3 Exascale optimizations and performance portability

T5.4 Emerging technologies

T5.1 Analysis and Verification

	512	1024	2048	4096	8192
Global efficiency	96.13	95.54	92.24	90.91	83.78
-- Parallel efficiency	96.13	96.19	95.45	95.97	92.49
-- Load balance	96.50	96.81	95.95	97.58	94.91
-- Communication efficiency	99.62	99.36	99.48	98.35	97.45
-- Serialization efficiency	99.78	99.62	99.77	98.77	97.83
-- Transfer efficiency	99.84	99.73	99.70	99.58	99.61
-- Computation scalability	100.00	99.33	96.63	94.73	90.58
-- IPC scalability	100.00	102.08	103.10	104.90	107.63
-- Instruction scalability	100.00	97.31	93.74	90.32	84.22
-- Frequency scalability	100.00	100.00	99.98	99.98	99.93

Percentage(%) 100 80 60 40 20 0

DISCO

	188	192
Global efficiency	82.67	78.21
-- Parallel efficiency	82.67	76.79
-- Load balance	89.84	89.63
-- Communication efficiency	92.01	85.68
-- Serialization efficiency	92.42	88.19
-- Transfer efficiency	99.56	97.15
-- Computation scalability	100.00	101.86
-- IPC scalability	100.00	99.99
-- Instruction scalability	100.00	102.38
-- Frequency scalability	100.00	99.50

Percentage(%) 100 80 60 40 20 0

Alya

Exa-enabling technologies (WP5)

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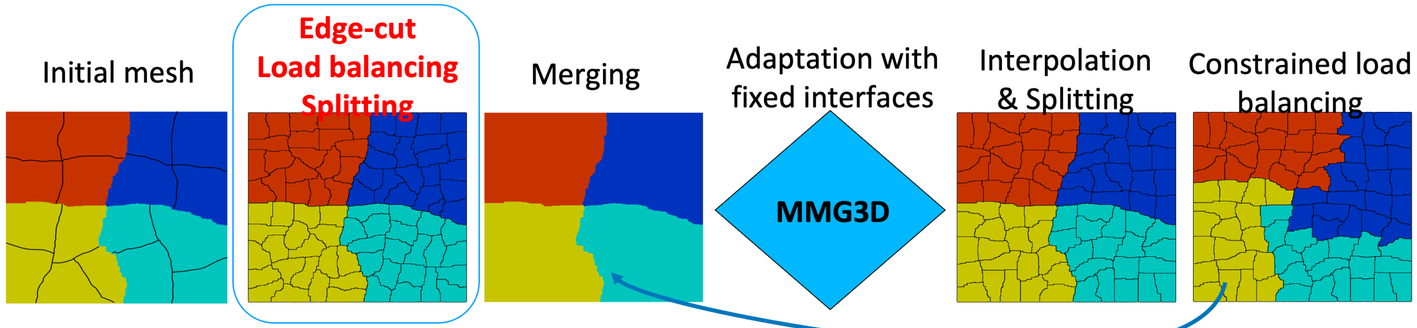
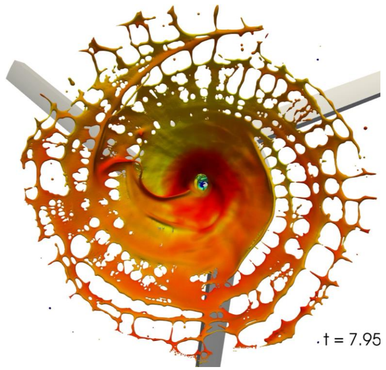
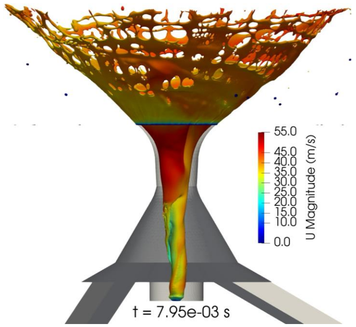
5.2 Scalable algorithms

YALES2: Optimization of massively parallel dynamic mesh adaptation algorithms in YALES2



if $Sk > Sk_{max}$ or $\frac{|\mathcal{M} - \mathcal{M}_{\text{target}}|}{\min(\mathcal{M}, \mathcal{M}_{\text{target}})} > \mathcal{E}_{\mathcal{M}}$





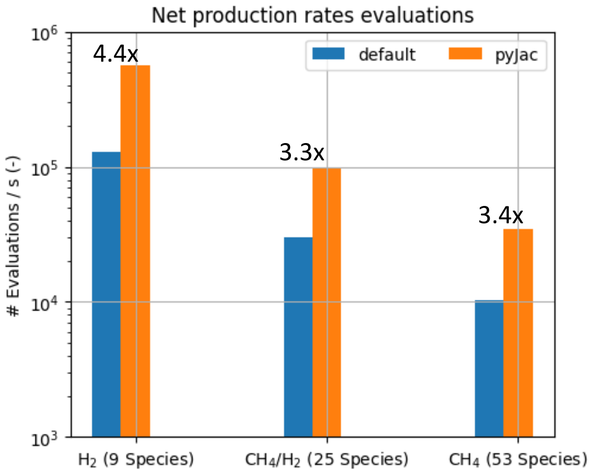
CLIO: adapted for the commercial software CONVERGE CFD to use AMR capabilities in CMC space.

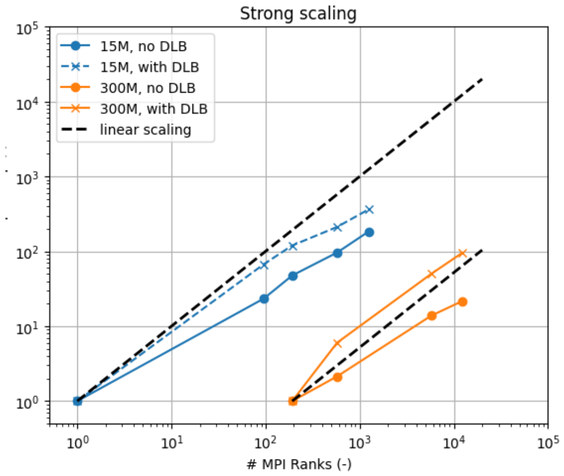
UNIVERSITY OF CAMBRIDGE

OpenFoam: Optimization of chemical integration

- ✓ pyJac-generated functions
- ✓ **DLBFoam-load balancing**

TECHNISCHE UNIVERSITÄT DARMSTADT





Exa-enabling technologies (WP5)

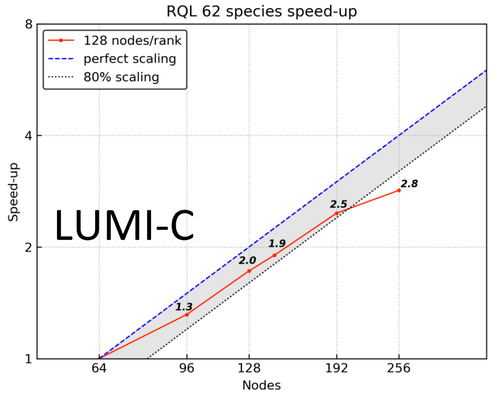
Center of Excellence in Combustion

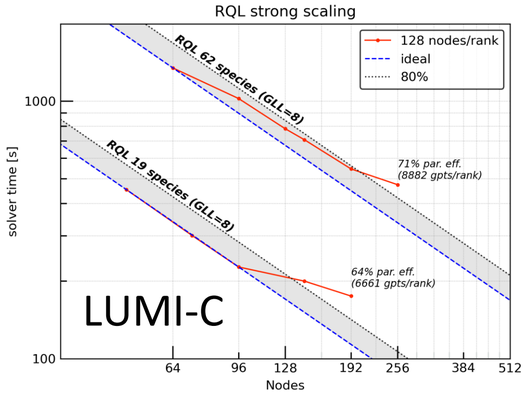
ETH Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich

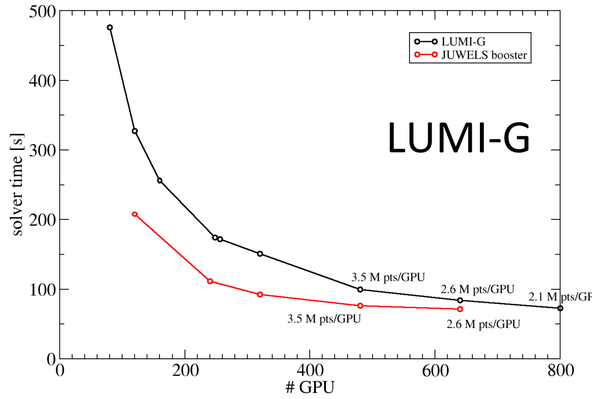
ARISTOTLE UNIVERSITY OF THESSALONIKI

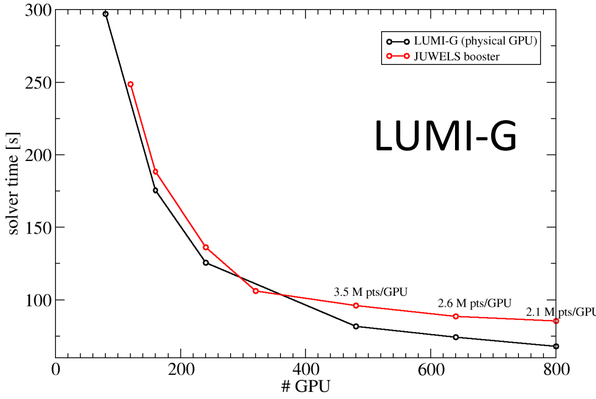
5.3 Exascale optimizations and performance portability

Nek5000: Performance analysis on LUMI-C and LUMI-G



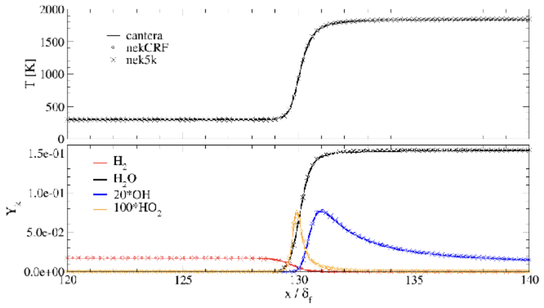


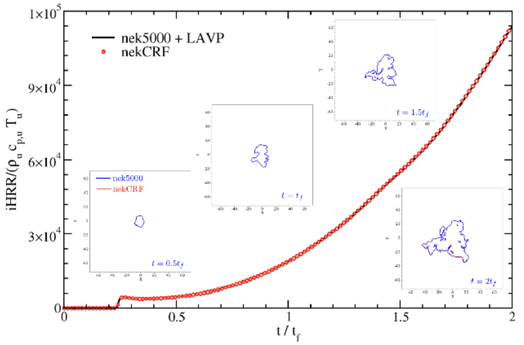




- **nekCRF:** A GPU accelerated high-order reactive flow solver for direct numerical simulations

- implementation of the LAVp plugin in nekRS
- detailed chemistry and transport (nekRK)





Code validation 1-D premixed flame, early flame kernel development (from left to right)

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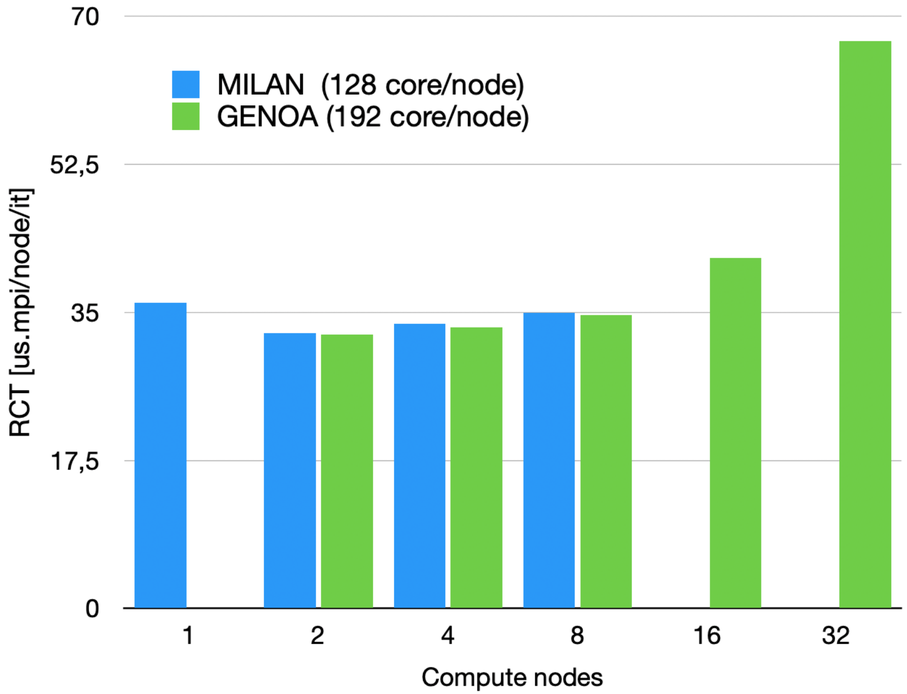
Exa-enabling technologies (WP5)

Center of Excellence in Combustion

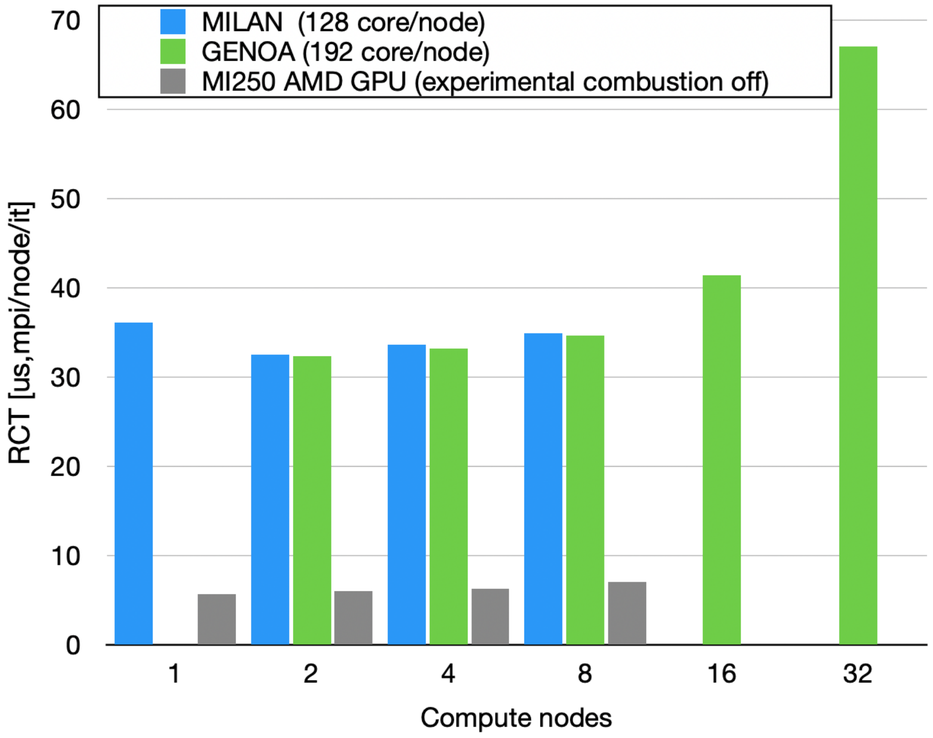
5.3 Exascale optimizations and performance portability

CERFACS
CENTRE EUROPÉEN DE RECHERCHE ET DE FORMATION AVANCÉE EN CALCUL SCIENTIFIQUE

AVBP: Performance of TUB case on MILAN(LUMI C) and GENOA (ADASTRA)



AVBP: performance assessment TUB on AMD GPUs



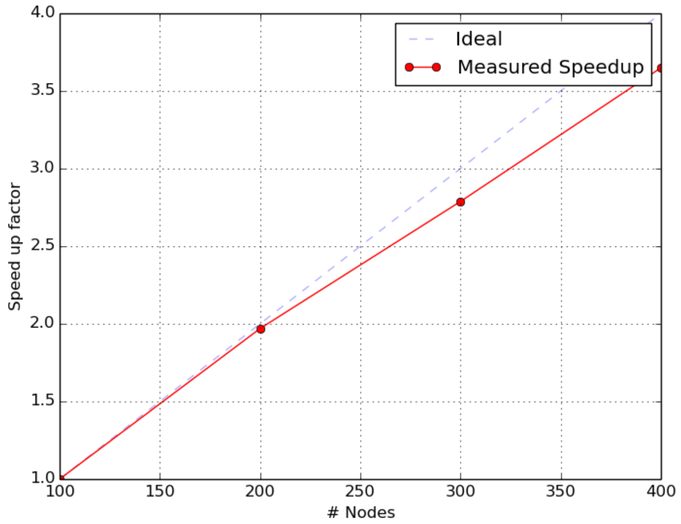
Exa-enabling technologies (WP5)

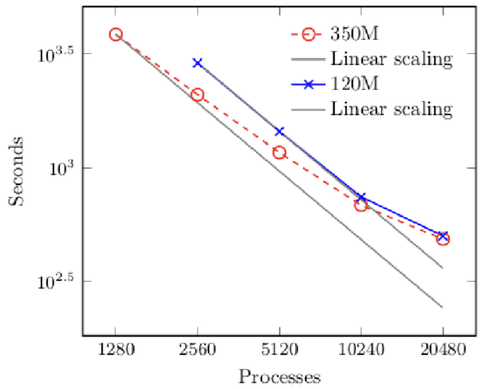
Center of Excellence in Combustion

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

5.3 Exascale optimizations and performance portability

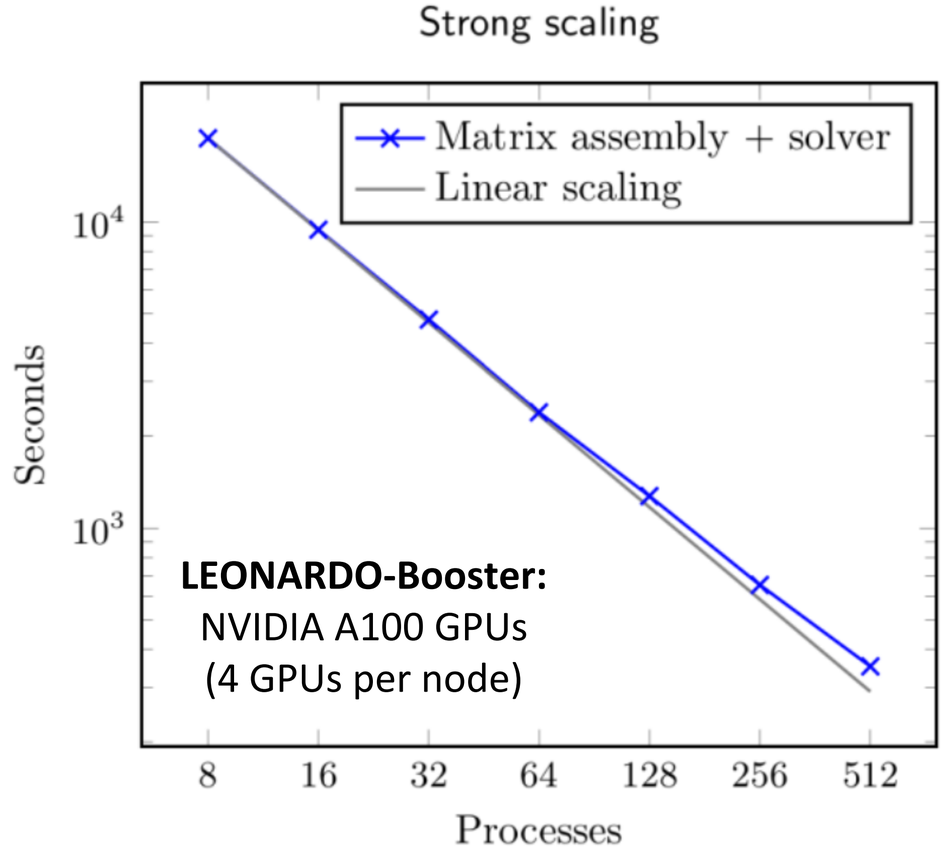
Alya: strong scaling in Hawk, LUMI-C, and VEGA





	350M		120M	
Processes	Seconds	Ideal	Seconds	Ideal
1280	3849.36	3849.36	-	-
2560	2089.18	1924.68	2881.12	2881.12
5120	1162.35	962.34	1439.07	1440.56
10240	681.08	481.17	741.42	720.28
20480	483.44	240.59	499.32	360.14

Alya: combustion solver based on flamelets ported to GPUs



Data processing and analysis (WP6)

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SC23 Denver, CO | i am hpc.

Best Paper Award at ISAV 2023: In Situ Infrastructures for Enabling Extreme-scale Analysis and Visualization

Scaling Computational Fluid Dynamics: In Situ Visualization of NekRS using SENSEI

Victor A. Mateevitsi
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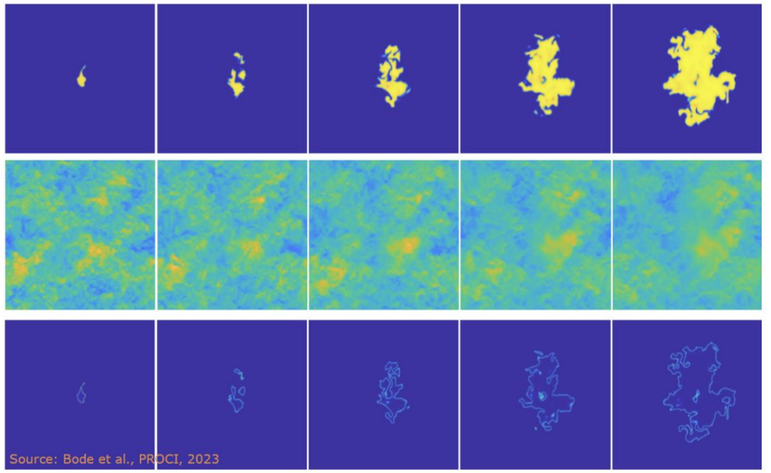


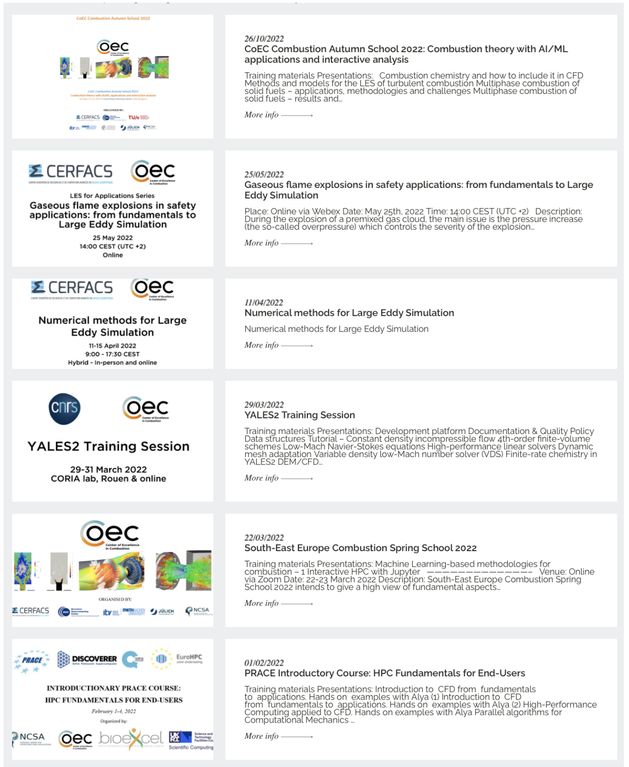
Training activities

Center of Excellence in Combustion

Different events have been achieved:

- ✓ Organization of **internal and external training events.**
- ✓ CoEC involved in **HPC combustion workshops** (PATC, TNF, ISF, …).
- ✓ **South-East Europe Combustion Autumn school in 2022 and 2023**.
- ✓ Successful **ERCOFTAC course on H2 combustion in 2022 and now we repeat in 2023**.

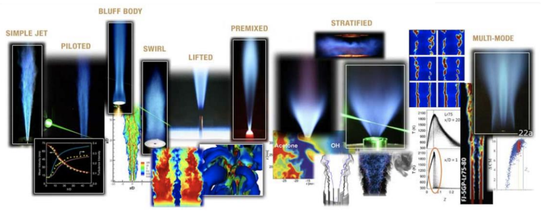
16 training events
+700 participants
34 countries



Final training event:
H2 combustion in December (ERCOFTAC)

TNF Workshop

International Workshop on Measurement and Computation of Turbulent Flames



The ERCOFTAC Knowledge Base Wiki Home Page

ERCOFTAC
European Research Community On Flow, Turbulence And Combustion

Workshop on Turbulent Combustion of Sprays

27

CoEC ambition for aviation

Center of Excellence in Combustion

Rolls-Royce joins Boeing and World Energy for successful 100% Sustainable Aviation Fuel flight

More about: Press release › | Civil Aerospace › | Sustainability › | Sustainable power › | United States › | United Kingdom ›

19 October 2021

Rolls-Royce, working with Boeing and World Energy, has carried out a successful test flight of its 747 Flying Testbed aircraft using 100% Sustainable Aviation Fuel (SAF) on a Trent 1000 engine.

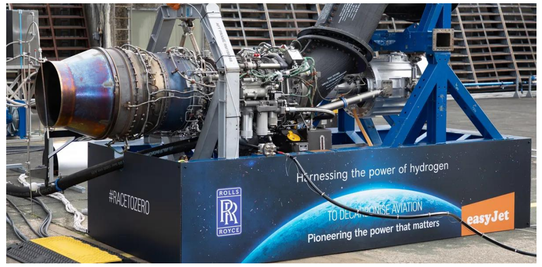
The aircraft flew from Tucson airport in Arizona, passing over New Mexico and Texas, with a Trent 1000 engine running solely on 100% SAF while the remaining three RB211 engines ran on standard jet fuel, arriving back at the airport three hours and 54 minutes later. Initial indications confirm there were no engineering issues, providing further proof of the fuel's suitability for commercial use.

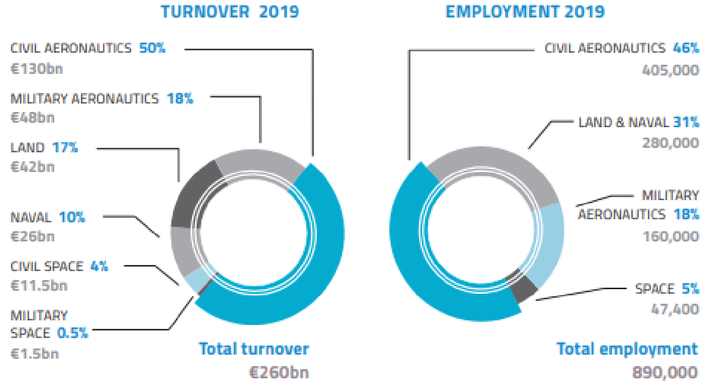
Rolls-Royce has continued to pioneer the adoption of 100% SAF, and

SUSTAINABLE ENERGY

Rolls-Royce uses hydrogen produced with wind and tidal power to test jet engine

PUBLISHED FRI, DEC 2 2022•1:52 AM EST | UPDATED FRI, DEC 2 2022•2:25 AM EST





European aerospace and defence industries - Turnover and Employment, 2019. (2020 Facts & Figures, ASD - Aeronautics, Space, Defence)

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SEP 20, 2021

Shell announces ambition to produce 2 million tonnes of SAF a year

Shell has announced its ambition to produce around 2 million tonnes of sustainable aviation fuel (SAF) a year by 2025.
It also aims to have at least 10% of its global aviation fuel sales as SAF by 2030.
This follows the oil and gas company's revelation that it is to build a 820,000-tonnes-a-year biofuels facility at the Shell Energy and Chemicals Park in Rotterdam.
"Currently, sustainable aviation fuel accounts for less than 0.1% of the world's use of aviation fuel. We want to help our customers use more SAF," said Anna Mascolo, President of Shell Aviation. "With the right policies, investments and collaboration across the sector we can accelerate

REPSOL Global Español Conta

Inicio › Sala de prensa › Notas de prensa

Repsol e Iberia realizan el primer vuelo con biocombustible producido en España con residuos

Otras informaciones · 04/11/2021 · 9 min de lectura

- Repsol e Iberia han completado la ruta Madrid - Bilbao con combustible sostenible producido a partir de residuos en la refinería de Petronor. El vuelo ha sido operado con el Airbus A320neo, uno de los aviones más eficientes de la aerolínea.
- Este vuelo con baja huella de carbono es un paso más hacia la descarbonización del sector de la aviación gracias al uso de biocombustibles y la mejora en la eficiencia energética, y ha supuesto una reducción de emisiones de 1,4 toneladas de CO_2 a la atmósfera.
- Aena, en línea con su papel de impulsor y facilitador del sector en materia de descarbonización del transporte aéreo, apoya esta iniciativa trabajando asimismo en proyectos de colaboración para promover la producción de combustible sostenible para fomentar su uso por parte de las aerolíneas.
- Se trata de la primera iniciativa surgida del convenio de colaboración hacia una movilidad más sostenible firmado por Repsol e Iberia el pasado mes de julio, que contempla en su programa el desarrollo de

Safran sees narrowbodies driving recovery in 2022

By Dominic Perry | 24 February 2022

Safran is hopeful that a recovering civil aviation market in 2022 will see the group deliver an improved financial performance as the industry recovers from its low point in early 2021.

Flightpath 2050
Europe's Vision for Aviation
Maintaining Global Leadership & Serving Society's Needs

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Electrification and Sustainability

GE Aviation CEO Talks Importance of SAF in Future of Aviation

By Kelsey Reichmann | June 24, 2021
Send Feedback

CFM, GE Aviation, John Slattery, RISE, SAF, sustainable aviation

GE Aviation CEO John Slattery was the guest on the latest edition of Eurocontrol's Straight Talk Live on Thursday. (GE Aviation)

GE Aviation and Safran recently unveiled a new development program focused on sustainable technologies for a next-generation CFM engine. During an appearance on EUROCONTROL's Aviation StraightTalk Live, GE Aviation President and CEO John Slattery described why sustainable aviation fuels (SAF) were essential to making a sustainable aviation engine and what obstacles need to be overcome to increase their use.

"We announced RISE, which stands for revolutionary innovation for sustainable engines," Slattery said. "It's a development program that we will look at over 300 different technologies that we will develop. Eventually, that will manifest into an engine that will enter into service sometime in the mid-2030s, but a lot of those technologies...that we will be developing through the RISE program will probably end up feathering a lot of those technologies into our current engines and even engines that we may even introduce before 2030."

September 20, 2021
8:42 AM CEST
Last Updated 3 months ago

Change Suite

Oil giant Shell sets sights on sustainable aviation fuel take-off

3 minute read

By Ron Bousso

final investment decision for a new biofuels plant at our offers certified nature-based carbon credits to offset elp aviation get to net zero, including hydrogen power." reports looking at how the aviation sector can

joint report by Shell and Deloitte, based on the views of experts. It said that the current global industry targets sector should aim to achieve net-zero emissions by ssions between now and 2030 that will help aviation to

Shell's Flight Path outlined how Shell, as one of the icants, could help its aviation customers decarbonise. nieving the new ambition would make Shell a leading nisation of the aviation sector.

Collaboration with industry

Center of Excellence in Combustion

CoEC has a **strong engagement with the European industry** in the power and propulsion sectors

EU Drivers

European Commission

EU STRATEGY for long-term GHG EMISSIONS REDUCTION #EU2050

CLEAN AVIATION

Hydrogen Europe

European HPC ecosystem

EuroHPC Joint Undertaking

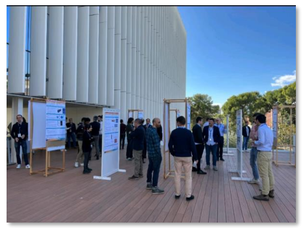
Horizon Europe

THE NEXT EU RESEARCH & INNOVATION PROGRAMME (2021–2027)

Identified HPC Combustion market

Combustion plays a central role in energy conversion for **energy** and **transport.**
Combustion **is a real exascale challenge.**

- ✓ **CoEC flagship codes** are currently used by **industry and technology centers**.
- ✓ **1st Industrial workshop on Aeronautics** (Dec. 2021) with **92 total attendees** from **27 institutions**.
- ✓ **2nd Industrial workshop** (Nov. 2023).



- ✓ **ALL partners** work industry:
- Projects **with SMEs**: > 4
- Projects **with Large Industry**: > 6

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The CoEC project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 952181.

Center of Excellence
in Combustion