CIEMAT capabilities related to EoCoE

04 July 2016

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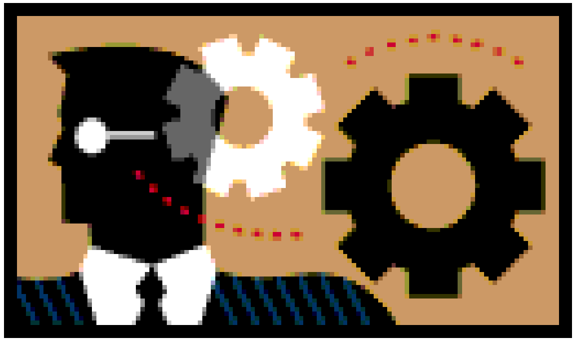
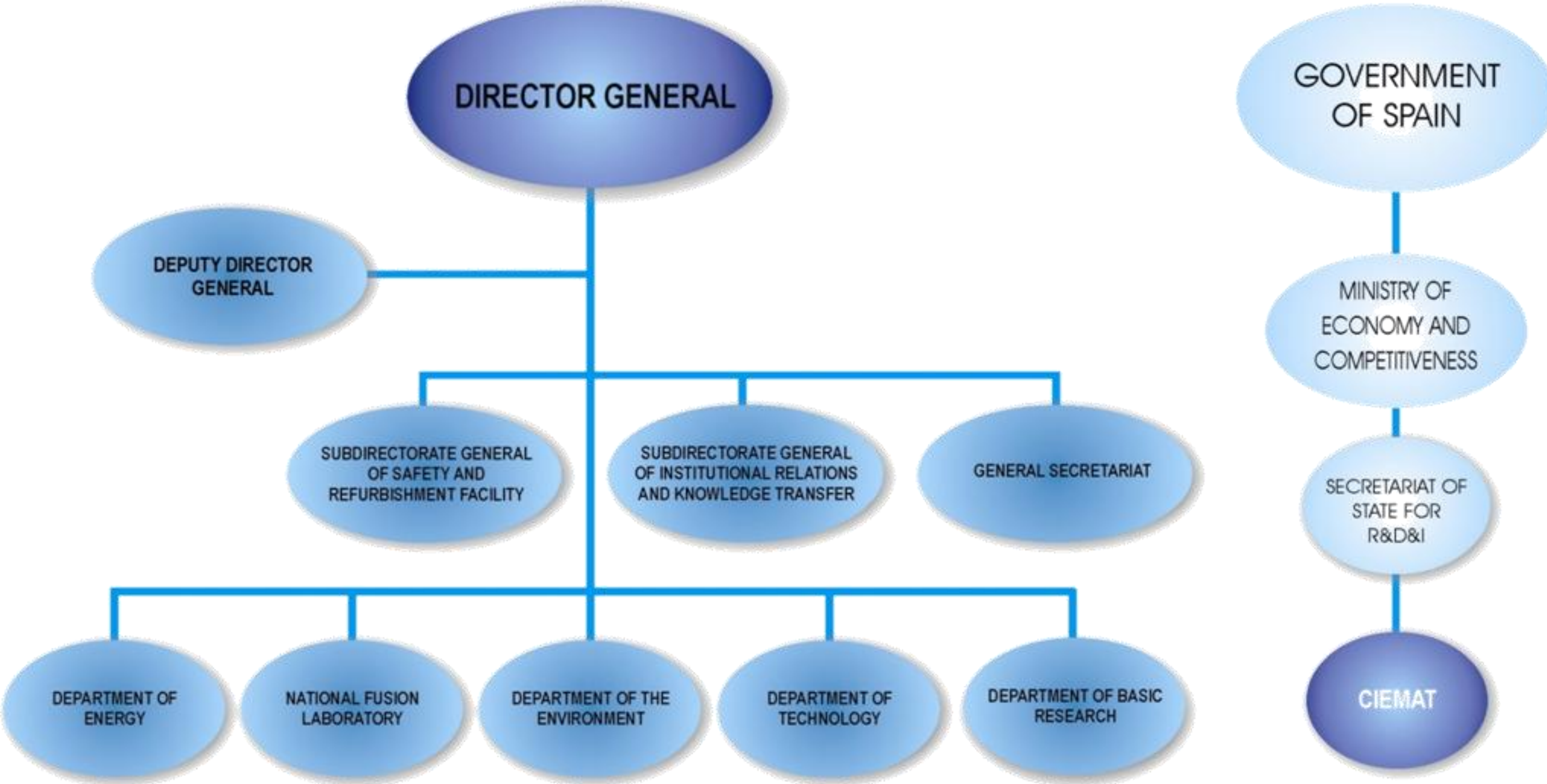


- Some hints about CIEMAT
- Facilities
- Energy+HPC activities at CIEMAT
- Collaborations

- **CIEMAT (http://www.ciemat.es) is the main Spanish public organism devoted to research on energy and its related technologies**

- **It was created in 1951 and was pioneering in supercomputing activities in Spain (1959)**

- **It is structured in 5 technologic Departments**
  - Energy
  - Basic Research
  - Spanish Fusion Lab
  - Environment
  - Technology


DIRECTOR GENERAL
DEPUTY DIRECTOR GENERAL
SUBDIRECTORATE GENERAL OF SAFETY AND REFURBISHMENT FACILITY
SUBDIRECTORATE GENERAL OF INSTITUTIONAL RELATIONS AND KNOWLEDGE TRANSFER
GENERAL SECRETARIAT
DEPARTMENT OF ENERGY
NATIONAL FUSION LABORATORY
DEPARTMENT OF THE ENVIRONMENT
DEPARTMENT OF TECHNOLOGY
DEPARTMENT OF BASIC RESEARCH
GOVERNMENT OF SPAIN
MINISTRY OF ECONOMY AND COMPETITIVENESS
SECRETARIAT OF STATE FOR R&D&I
CIEMAT

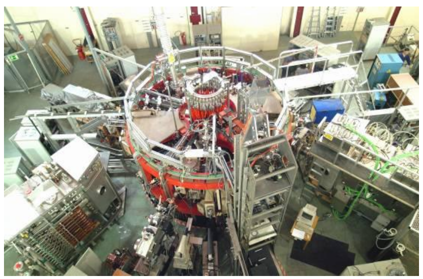
- **Some indicators**
  - Human Resources ~1,350 people
  - Budget (2016) : 89.8 M€
  - R&D income (2015) ~45 M€
  - SCIR 2013
    - Output = 2,588
    - Int. Collaboration (%) = 60.28
    - Normalized Impact = 1.73
    - Q1 (%) = 53.4
    - Excellence (%) = 19

- **Some institutional presence**
  - Fusion for Energy (Governing Board and Technical Advisor Panel)
  - Energy Consultative Committee (Fusion & Fission)
  - ITER Scientific-Technical Advisory Committee
  - Advisory Group on Energy
  - EERA Executive Committee
  - International Energy Agency
  - KIC Innoenergy
  - …
  - ETP4HPC (submitted)

Experimental facilities

	NUMBER
Total scientific-technical facilities	60
Number of laboratories	161
Other facilities (training, protection, medical service, ..)	23

Solar Platform of Almería (PSA)



Heliac Flexible TJ-II

Pilot pelleting plant (300-500 kg/h)

Dosimetric measurements in mannequin

Wind Testing Laboratory

Ionizing Radiation Metrology Laboratory (LMRI)

Safety System Analysis Laboratory (Peca Facility)

Pilot membrane gas separation plant

PET/CT of small animals for biomedical applications

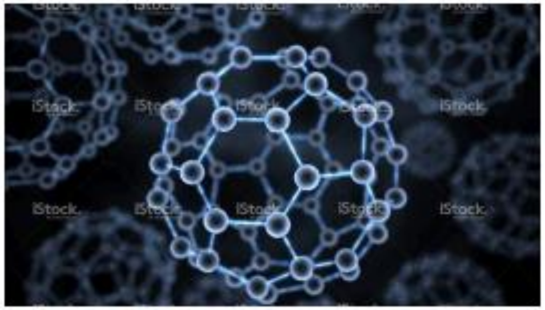
- **ACME (for testing purposes)**
  - 160 Intel Xeon cores ES-2640-V3 (2.6 GHz)
  - 228 Intel Xeon Phi cores
  - DDR4 memory, SSD disks, SAS2 HDD…
  - Additional storage of 72 TB
  - To be doubled through 2016 with Xeon V4 and KNL

- **Euler (in production)**
  - 1920 cores
  - Capable of being configured with new solutions

Potential synergies

Transversal Basis

Meteorology for Energy



Materials for Energy

Water for Energy

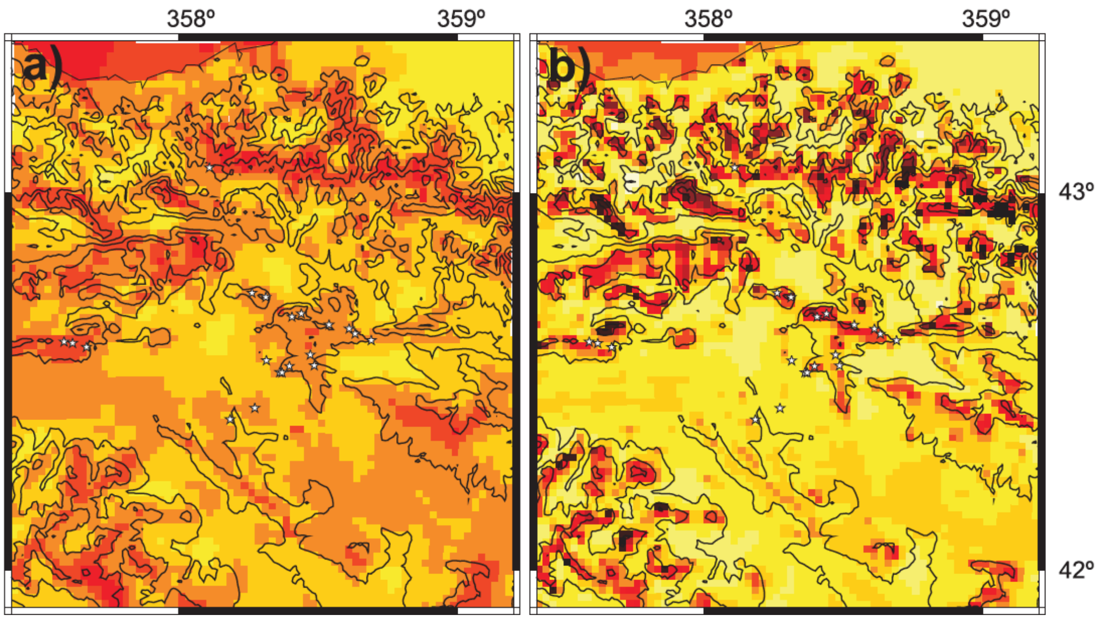
Fusion for Energy

Knowledge management & Networking strategy

Dynamical downscaling: WRF model

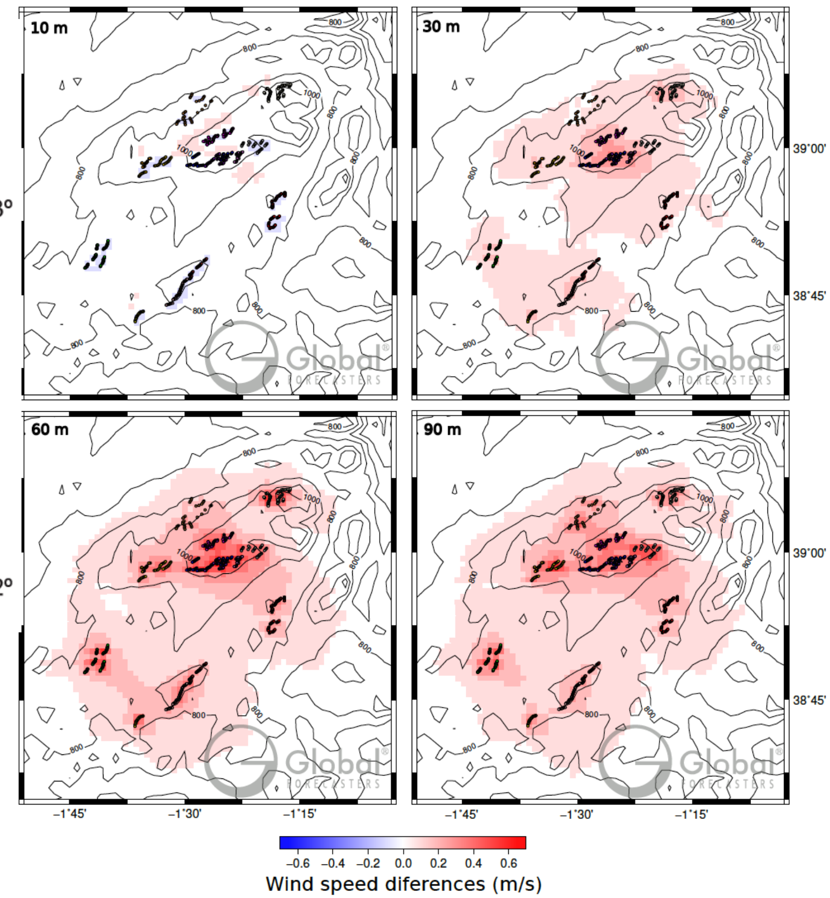
Improvements in the WRF parametrizations

Jiménez *et al., J. Appl. Climatol. Meteorol. 51*, 2012



Improving the Representation of Resolved and Unresolved Topographic Effects on Surface Wind in the WRF Model

Impacts of a Cluster of Wind Farms on Wind Resource Availability and Wind Power Production

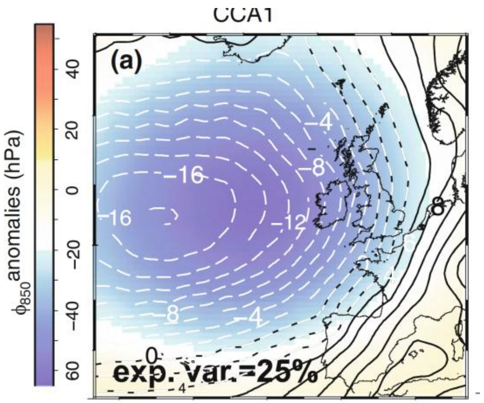


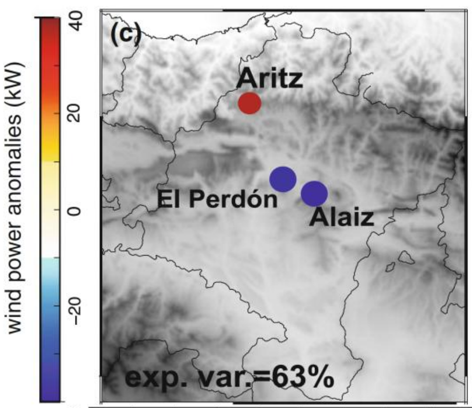
Wind speed as simulated with and without the drag parameterization

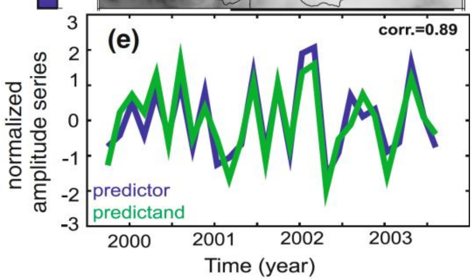
Statistical downscaling

Relationship between wind power production and North Atlantic atmospheric circulation

Garcia-Bustamante *et al., Clim. Dyn. , 40,* 2013

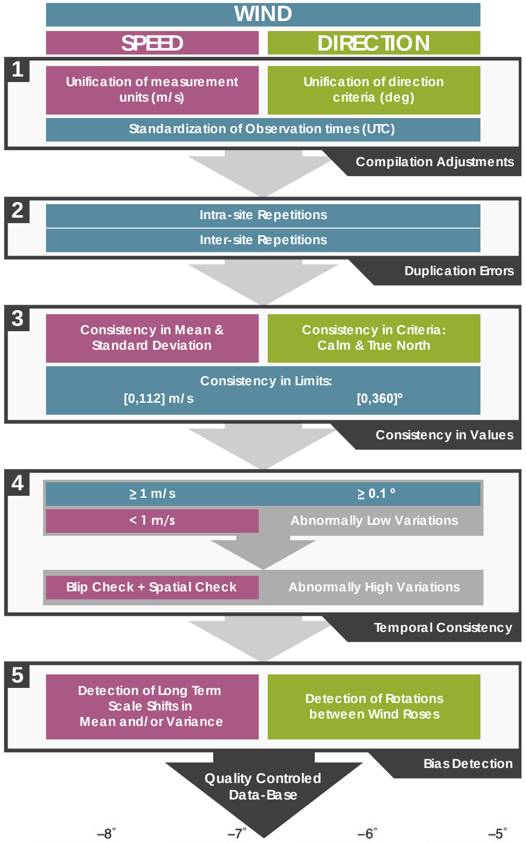






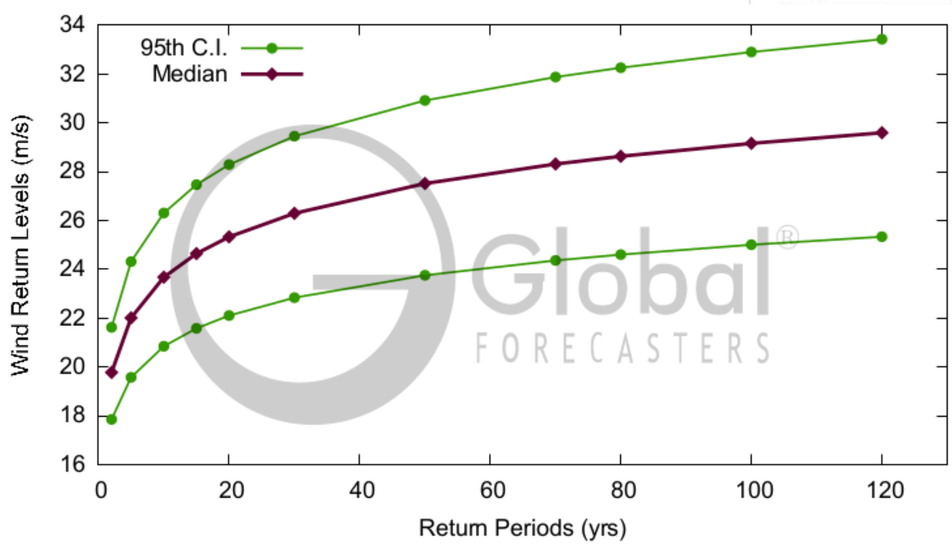
Quality Control of a surface wind observations database

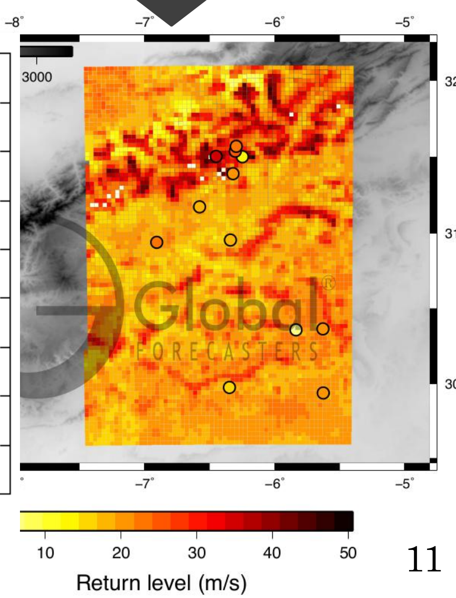
Lucio-Eceiza *et al., (to be submitted)*



Analysis of the extreme winds

Global forecaster Report No. 14gf15a13ou_fase2_3.0, 2016





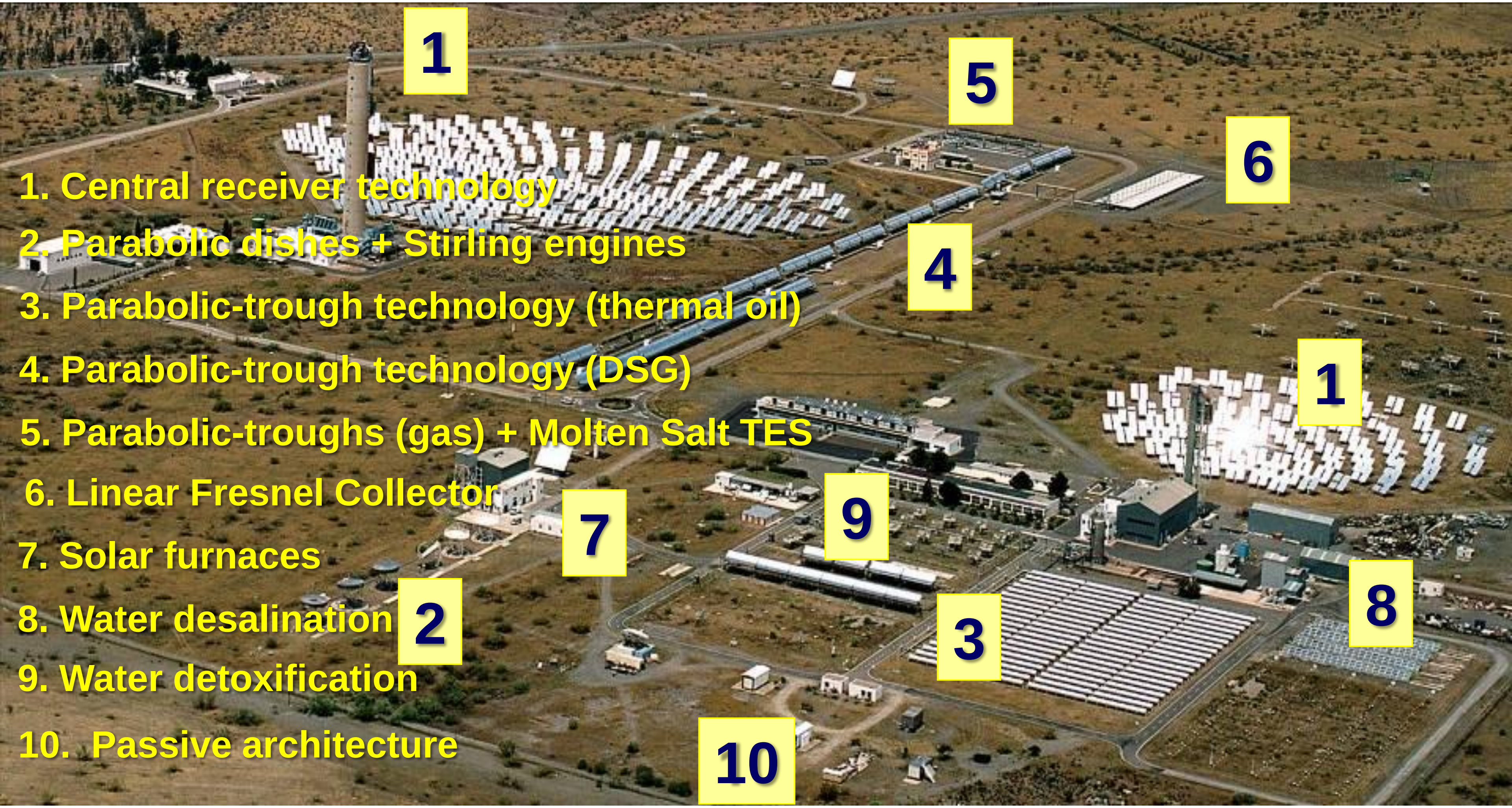
GOBIERNO DE ESPAÑA

MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

Ciemat

Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas

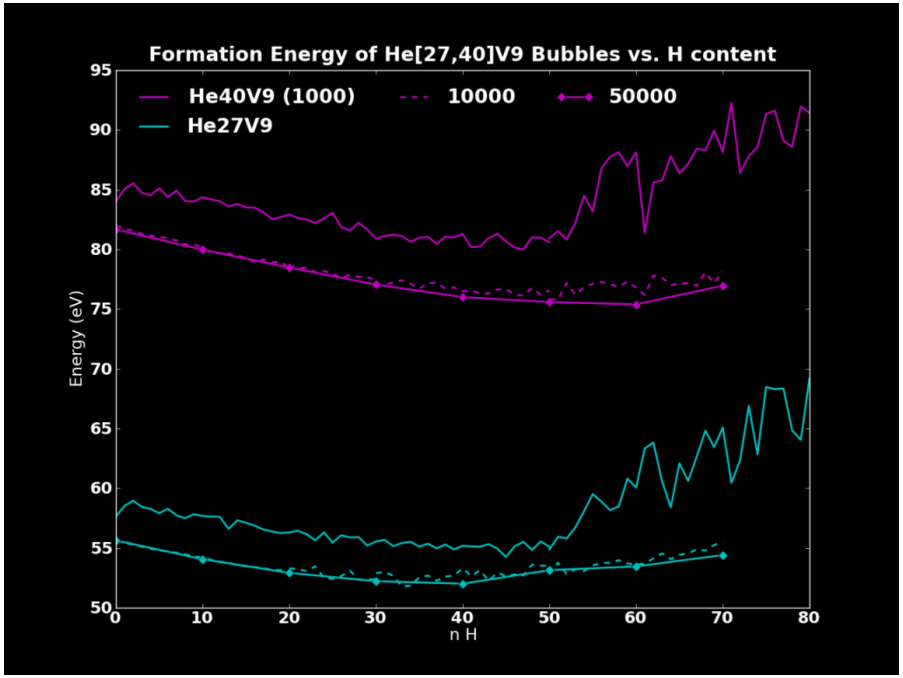
PSA: Main test facilities

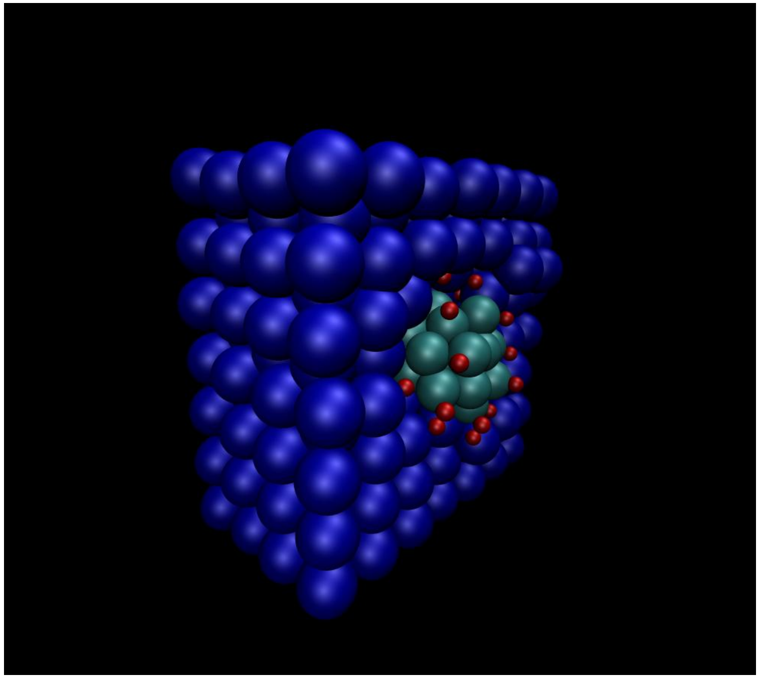


- **Computation Requirements for Solar Concentrating Technologies:**
  - CFD analysis of heat transfer between solar radiation, materials and fluids
  - Fluent & STAR-CCM+
- **Design and simulation of solar thermal power plants, both solar tower and parabolic trough technologies**
  - Detailed simulation, due to size of the plants, consumes time and resources
  - SAM, WINDELSOL & Matlab
- **Measurement and characterization of collectors and components by photogrammetric methods**
  - High resolution required (1mm), intensive memory consumption
  - Matlab

- **Radiation damage in nuclear materials**
  - Energies to form He-H bubbles to be lately used in simulations beyond the atomic scale (Kinetic Monte Carlo, Ray Theory…)
  - Database to be stored for multiscale simulations
    - Bubble size and atoms
  - Not as demanding as ab initio
  - LAMMPS code

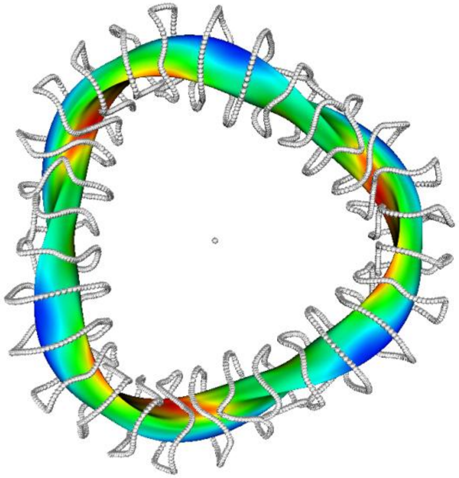
He-H in Fe with 9 vacancies and 27 and 40 He atoms
$5 \cdot 10^4$ iterations to converge in 2 h using 256 cores (Helios)



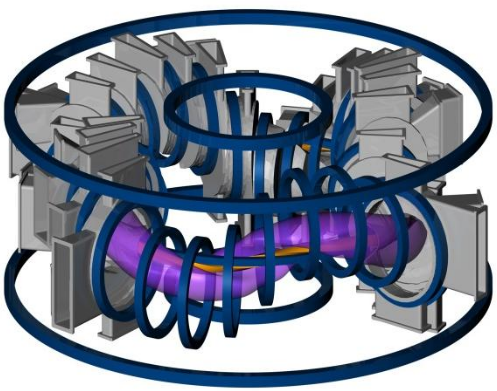


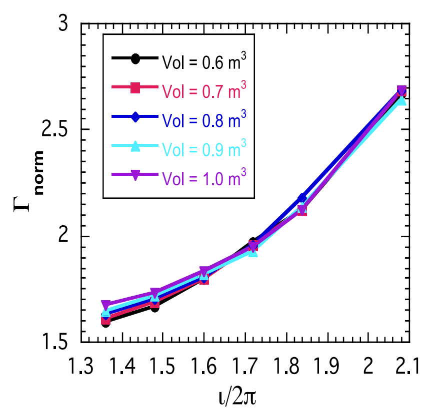
Final bubble geometry
Fe-blue (9 vacancies), 50 He-cyan, 30 H-red

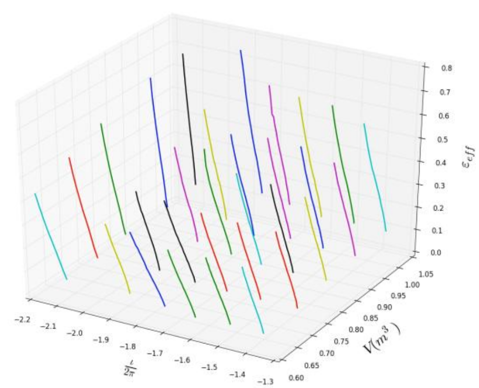
DAB algorithm, based on metaheuristics, is used to optimize stellarators under several criteria: NC, Mercier, ballooning,… [F. Castejón et al. PPCF 2013]



Exploration of the effect of rotational transform on NC transport in stellarators: Extensive estimates of NC transport properties using DKES code (30 configurations x 100 radii).



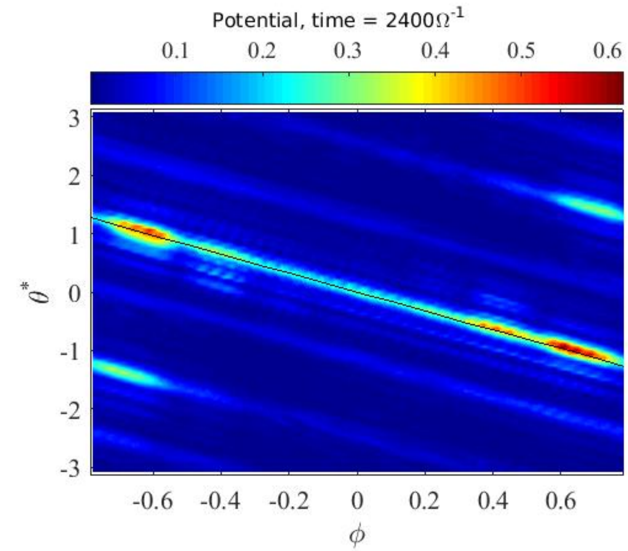




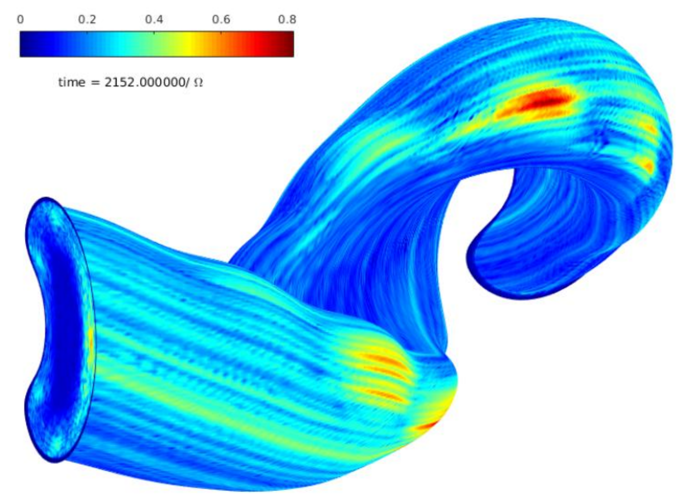
No positive influence of rotational transform on NC, despite the experimental results [F. Castejón et al. FST, 2016]

Turbulence simulations

- Gyrokinetic (GK) simulations of microinstabilities in stellarators with the code EUTERPE
  - Global GK PIC code
  - FE (spline) spatial discretization
  - RK4 time integration
  - PETSc solver
  - VMEC interface for MHD equilibria



- Example: Trapped Eelectron Modes (TEMs) in TJ-II
  - Simulation of TEMs in a TJ-II period with fully kinetic ions and electrons [E. Sánchez et al.]



Monte Carlo reactor & Accelerator Driven Systems calculations:

– Complex 3D designs: high level of detail, large number of materials and isotopes.

– GBs of memory required to accurately describe all materials/isotopes/reactions.

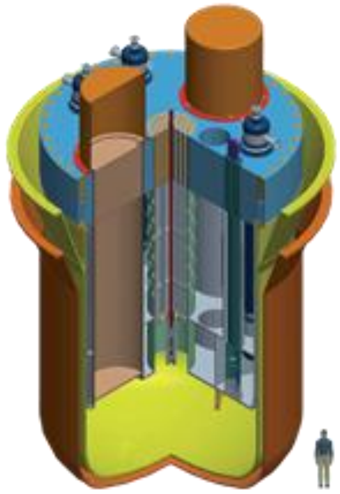
– Large data storage volumes required for nuclear data: different compilations (e.g. ENDF, JEFF, JENDL) and temperatures.

– Large data storage volume for output files (e.g. there are millions of fuel pellets per core).

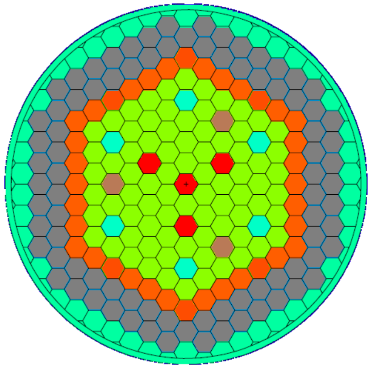
– Large CPU time to accumulate enough statistics ⇒ high processor capability is needed.

– Parallel programming.

MYRRHA: Multi-purpose hybrid research reactor for high-tech applications



XY view of the MYRRHA fuel core layout



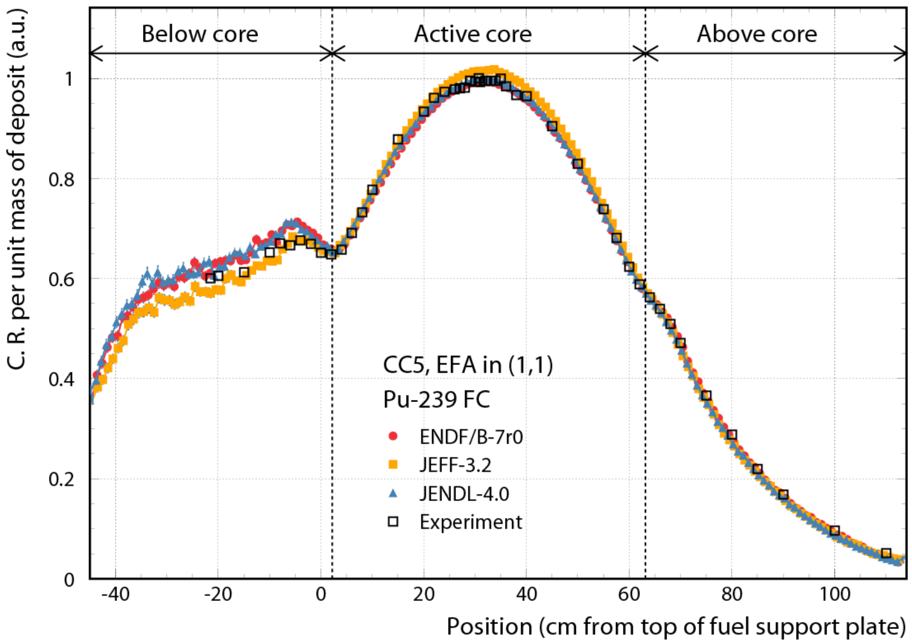
Nuclear data processing:

– Need to process the distributed nuclear data libraries to prepare them for Monte Carlo codes: MCNP, GEANT4…

– Verification of nuclear data libraries is done for more than 400 isotopes, ~5 available major reactions and all the energy range (from meV to MeV).

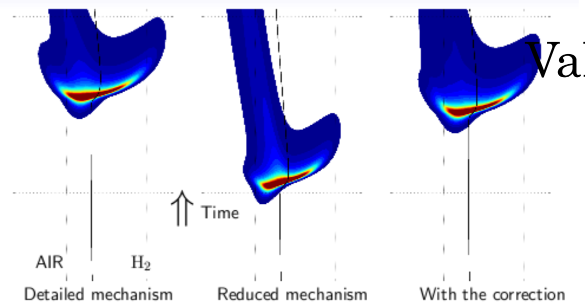
– Large amount of benchmarks required for verification ⇒ large requirements of computer power.

Experiment vs. simulation (MCNP)

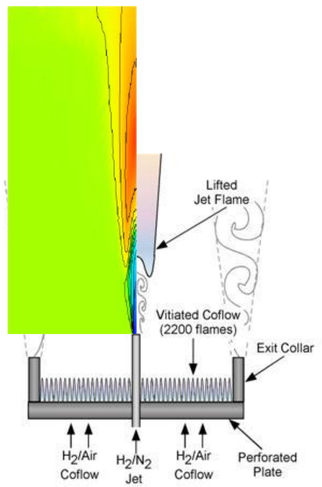


- Neutron flux axial distribution in the reactor VENUS-F.
- Three nuclear data sets investigated (ENDF, JEFF and JENDL).
- CPU time for each set is about 3,000 core-hours in CIEMAT's Euler HPC cluster.
- Taken from FREYA project deliverable No. 3.2, 7th EU Framework Programme.

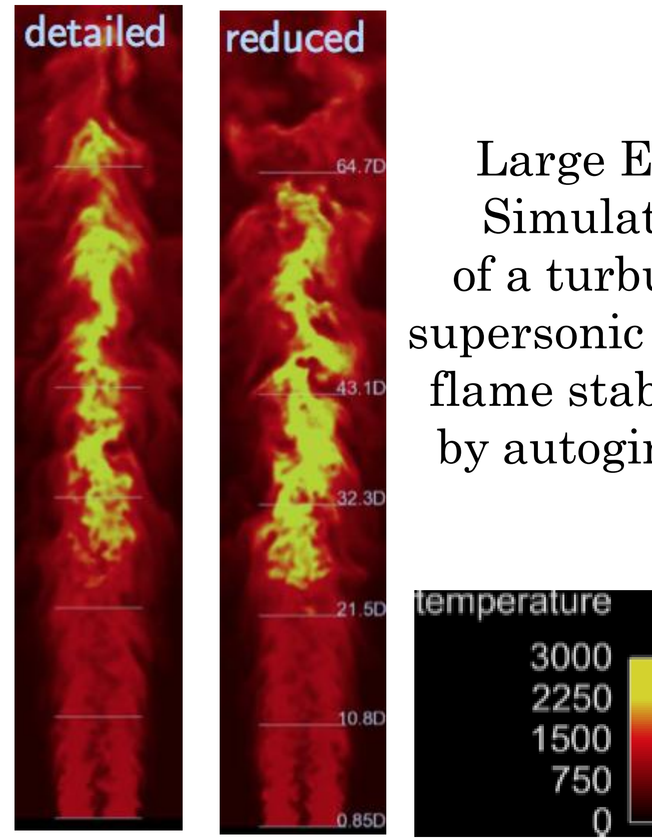
Development and validation of a reduced mechanism for H_2-air combustion: 21 reactions → 3 reactions



Validation in a laminar triple flame configuration.



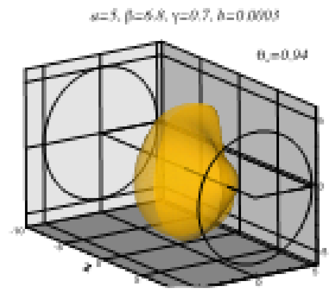
Validation in a turbulent H2-air flame stabilized by autoignition (RANS + transported PDF + reduced chemistry)

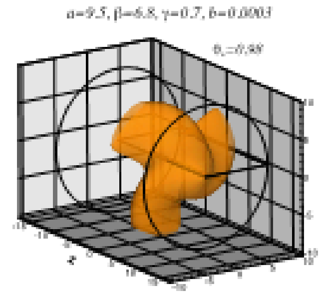


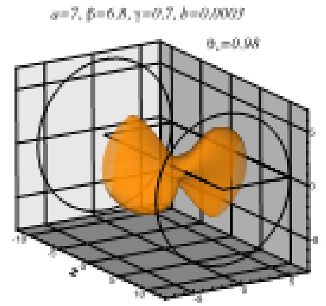
Large Eddy Simulation of a turbulent supersonic H2-air flame stabilized by autoginition

P. Boivin et al. Simulation of a supersonic hydrogen-air autoignition-stabilized flame using reduced chemistry, Comb. Flame 159, 1179-1790 (2012).
P. Boivin et al. A four-step reduced mechanism for syngas combustion, Comb. Flame, 158, 1059- 1063 (2011).
P. Boivin et al. An explicit reduced mechanism for H2– air combustion, Proceedings of the Combustion Institute 33, 517- 523 (2011).

Microcombustion



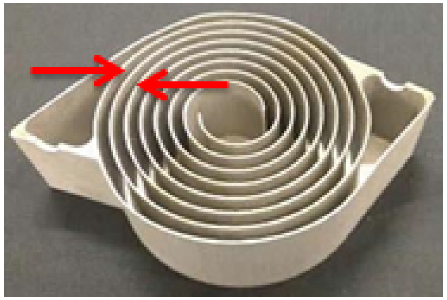


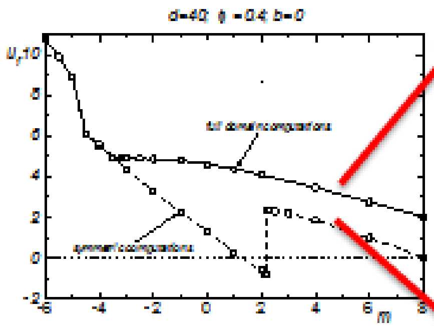


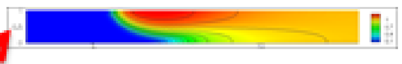
Spinning flame solutions in a solid energetic material (Le → 0)

Portable combustion reformers for hydrogen production from biofuels (HPC4E project H2020)

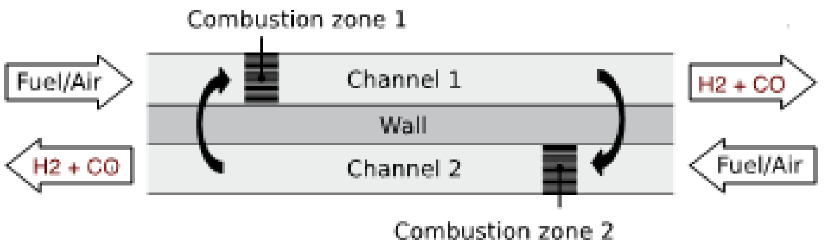
< 1cm







Propagation speeds of symmetric (unstable) and non-symmetric (stable) lean H2 flames (Le < 1)



V. Kurdyumov, A. Kolobov. “Global stability analysis of gasless flames propagating in a cylindrical sample of energetic material: Influence of radiative heat-losses”, Comb. Flame 162 (2015) 1996-2005.

V.N. Kurdyumov, C. Jiménez, “Propagation of symmetric and non-symmetric premixed flames in narrow channels: Influence of conductive heat-losses”, Comb. Flame 161 (2014) 927–936.

C. Jiménez, D. Fernández-Galisteo, V. Kurdyumov, “DNS study of the propagation and flashback conditions of lean hydrogen-air flames in narrow channels: symmetric and non-symmetric solutions”, Int. J. Hyd. Energy 40 (2015), 12541-12549.

- **Dynamic fault tolerance and computational efficiency**
  - Checkpointing
  - Scheduling and migration of tasks
  - Algorithms
  - Homogeneous, heterogeneous and virtualized clusters
- **Current actions tested on the Slurm simulator and computational facilities**
  - Anonymized database with the execution logs of the CIEMAT supercomputer from the latest 6 years
- **Optimization of codes**
  - Wind energy, Fusion, Materials…
- **Partner of the H2020 HPC4E project**

- **Integration of Slurm + FTI + DMTCP**
  - Sequential and parallel jobs
  - Close collaboration with the BSC and the Northeastern University (USA)

- **Model on checkpointing and migration of tasks**
  - Pursuing describing when and how this action is profitable from a performance/energetic point of view
  - Capable of using different libraries (FTI, DMTCP, BLCR, etc.)

- **Model on allocation of tasks**
  - How to feed the facility depending on the load
  - Complementary to the previous

Some collaborations

Conclusion

- **CIEMAT is willing to collaborate with EoCoE in those points of common interest**
  - Simulation
  - Access to experimental facilities and data
  - Inputs for the project deliverables
  - Participation in future events
  - Potential future projects/second phase of EoCoE

THANK YOU!!!

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http://rdgroups.ciemat.es/web/sci-track/