IES08

Napoli 27-29 Maggio 2008

ENEA GRID a supporto della ricerca e dell'industria

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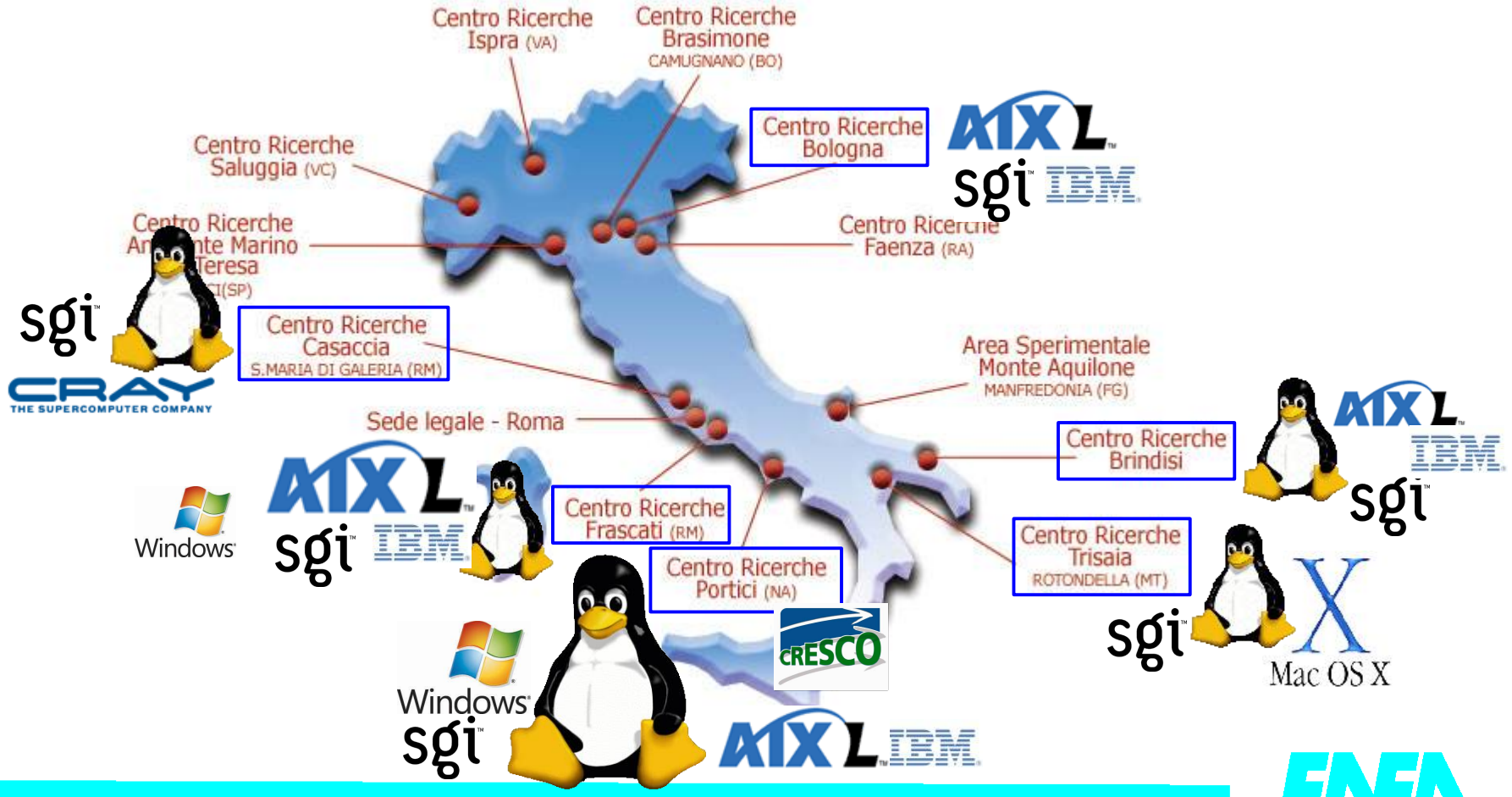
- Architettura e risorse di ENEA-GRID prima di CRESCO
- ENEA-GRID e la ricerca in ENEA
  - Il progetto MINNI (dispersione e chimica degli inquinanti)
  - Simulazioni nell'ambito della fusione nucleare controllata
  - Simulazioni accoppiate oceano/atmosfera
  - Simulazioni di chimica computazionale
- ENEA-GRID e l'industria
  - AVIO
  - AnsaldoRicerche/AnsaldoEnergia
  - CETMA
- Il progetto CRESCO in ENEA-GRID: un salto di qualità delle risorse disponibili

ENEA e le risorse per il calcolo scientifico

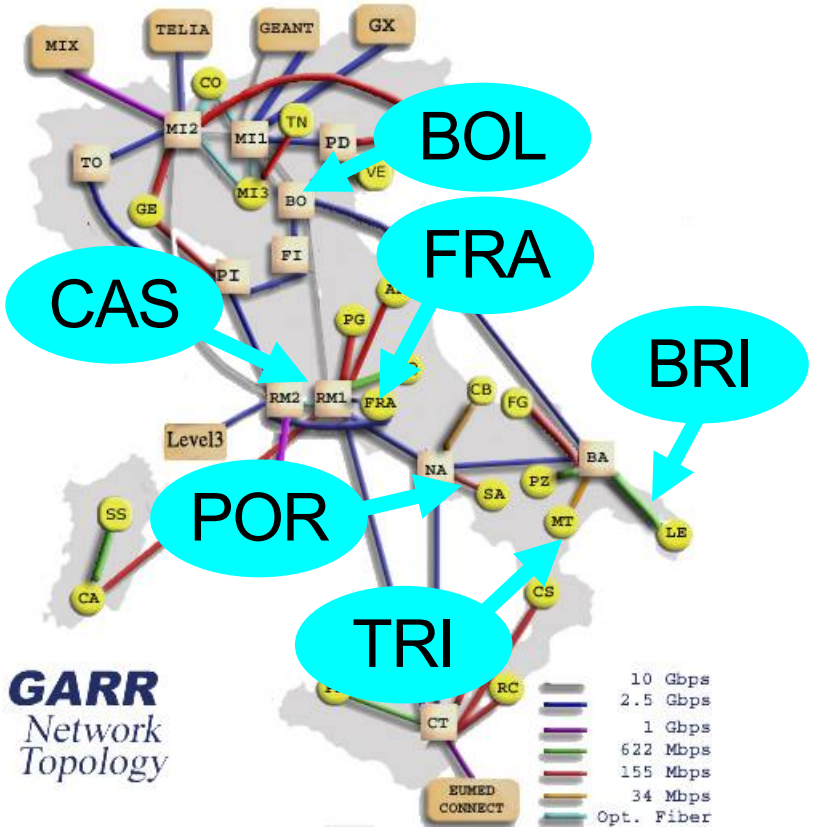
12 Centri di Ricerca e una struttura dedicata al calcolo all'interno del dipartimento ENEA-FIM con 6 centri che gestiscono sistemi multipiattaforma per il calcolo seriale e parallelo e strumenti per la visualizzazione 3D inseriti in una unica infrastruttura: ENEA-GRID



ENEA GRID e la rete GARR

ENEA-GARR
9 PoP, 18-1000 Mbps

Brindisi 150 Mb/s
Bologna 30 Mb/s
Casaccia 100 Mb/s
Frascati 155 Mb/s
Portici 1000 Mb/s
Trisaia 18 Mb/s
Palermo
Pisa
Roma Sede



Nell'ultimo anno la banda disponibile è aumentata di fattore da 3 a 60 per l maggioranza dei siti

risorse di ENEA-GRID prima di CRESCO

Le risorse di calcolo in ENEA-GRID:

- Hardware: ~100 hosts e ~650 cpu : IBM SP; SGI Altix & Onyx; Linux clusters 32/ia64/x86_64; Apple cluster; Windows servers. Risorsa più rilevante: IBM SP5 256 cpu (12 p575 1.5GHz, 16 cpu + 1 p595 1.9 Ghz, 64 cpu, 1.5 TFlops)
- software: codici commerciali (fluent, ansys, abaqus..); ambienti di elaborazione (Matlab, IDL,..), codici di ricerca (CPMD, MCNP,..)

la missione di ENEA-GRID [iniziata nel 1998]:

- fornire un "unified user environment" e una modalità omogenea di accesso a tutti i ricercatori ENEA e ai loro collaboratori esterni, indipendentemente dalla loro sede.
- ottimizzare l'uso delle risorse

Architettura di ENEA-GRID

Le funzionalità GRID (autenticazione, autorizzazione, gestione delle risorse) sono fornite da componenti “maturi” e multipiattaforma:

File System distribuito: OpenAFS

Gestore di risorse: LSF Multicluster [www.platform.com]

Interfaccia utente: Java & Citrix Technologies

Nel loro insieme costituiscono l' ENEA-GRID Middleware. che negli anni ha permesso di inserire senza problemi risorse allo stato dell'arte della tecnologia.

Openafs: home degli utenti, distribuzione di dati e del software

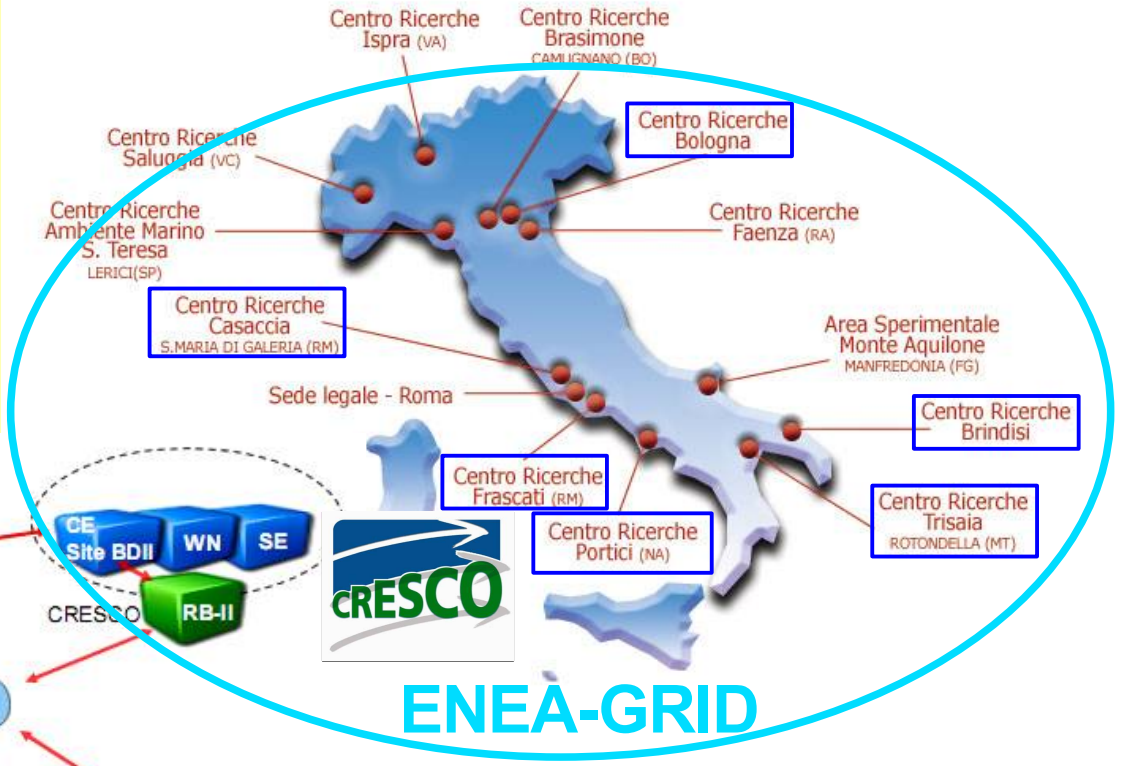
integrato con LSF

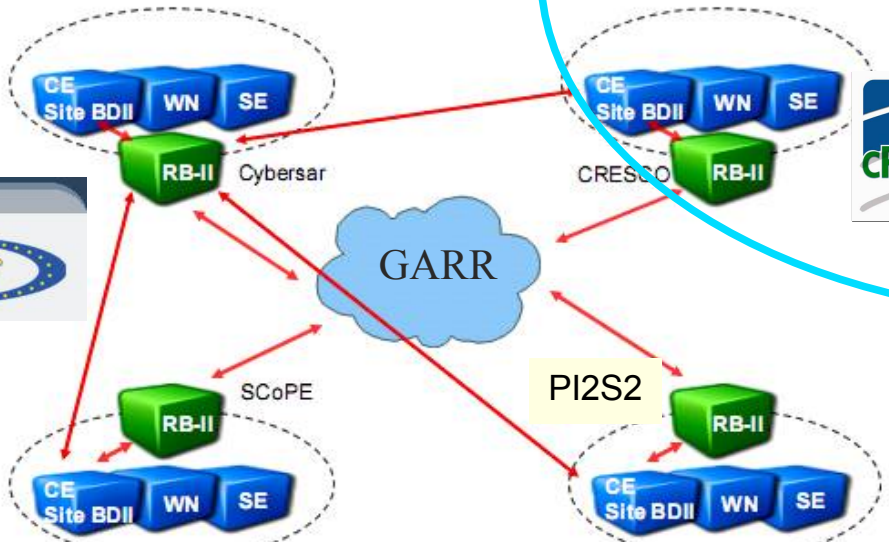
insieme a Kerberos 5 fornisce autenticazione/autorizzazione

Nell'ambito dei progetti GRID (Datagrid, EGEE,EGEE-II & III, Interoperabilità PON, BEINGRID) ENEA ha sviluppato soluzioni di interoperabilità verso altri middleware (gLite, Unicore)

ENEA-GRID: Interoperabilità

L'interoperabiltà con gLite: realizzata col metodo **SPAGO** (Shared Proxy Approach for Grid Objects): una o piu' macchine proxy gLite che condividono lo spazio disco con i worker node ENEA-GRID



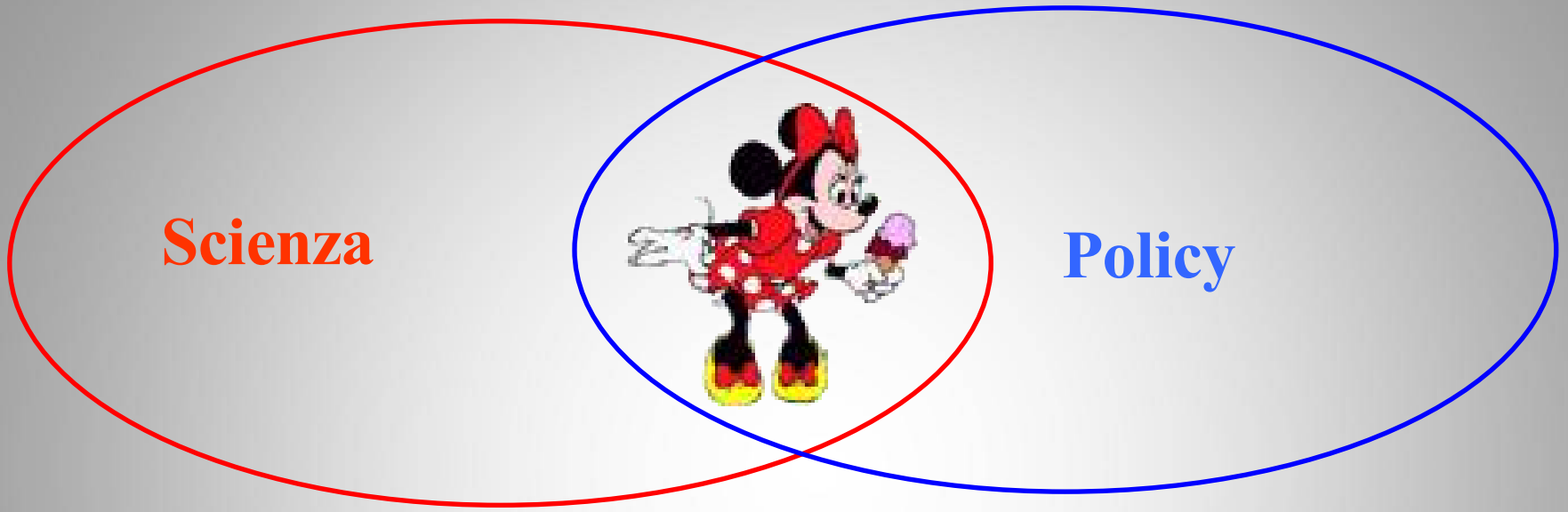


ENEA-GRID e la Ricerca

- ENEA-GRID e la ricerca in ENEA: alcuni esempi
  - Il progetto MINNI per la dispersione degli inquinanti
  - Simulazioni nel campo della Fusione Nucleare controllata
  - Simulazioni Climatologiche
  - Simulazione di chimica computazionale
- Le esigenze
  - Risorse per High Performance / High Throughput Computing
  - Sistemi allo stato dell'arte in quanto a prestazioni
  - Ambiente utente affidabile
  - Supporto di sistema
  - Supporto all'integrazione/ottimizzazione in grid
  - Supporto algoritmico

ENEA-GRID
&
il progetto MINNI per la simulazione della dispersione e la trasformazione chimica degli inquinanti atmosferici

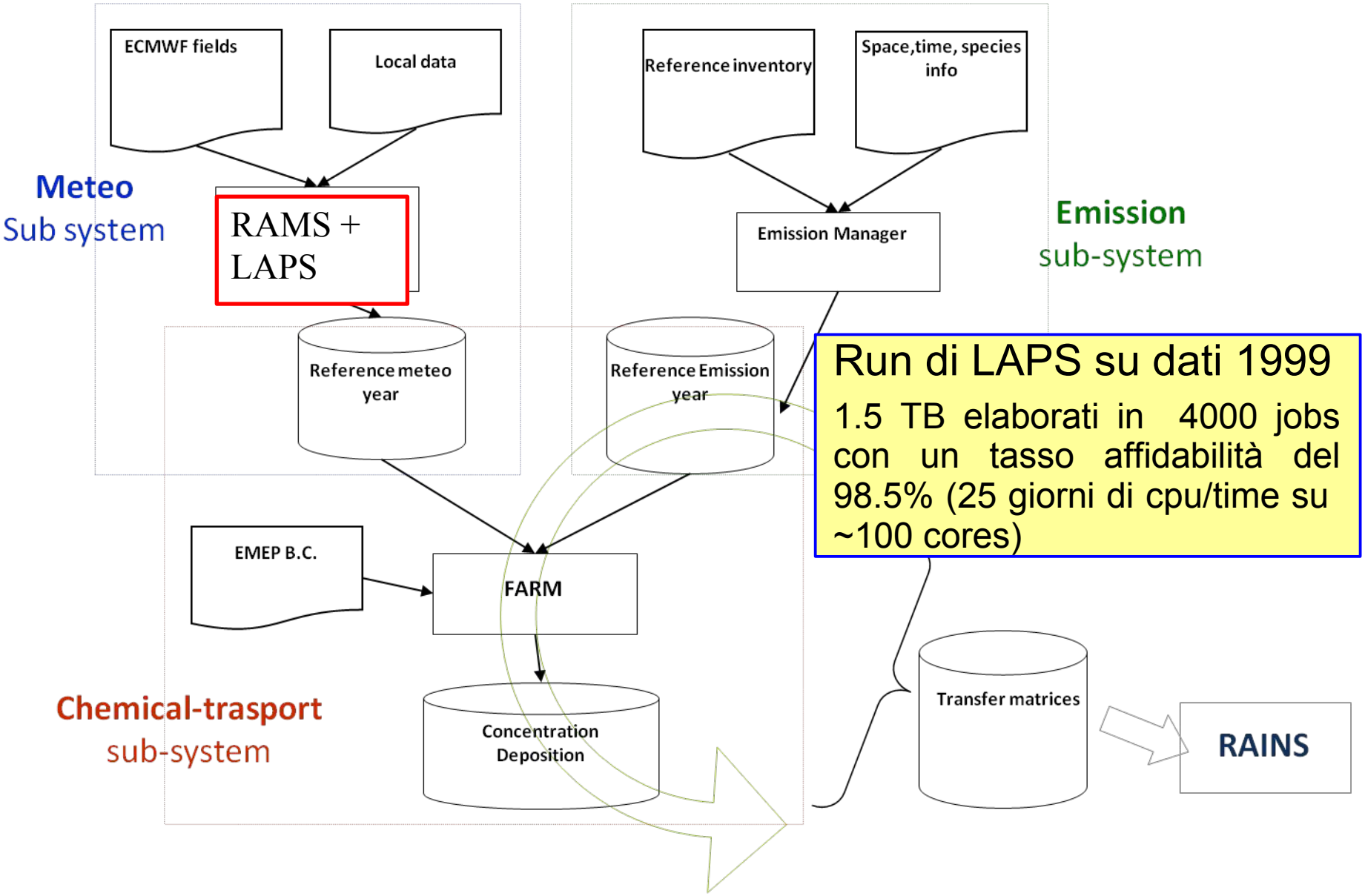
G. Zanini (ENEA-ACS)



MINNI

Modello Integrato Nazionale a supporto della Negoziazione Internazionale

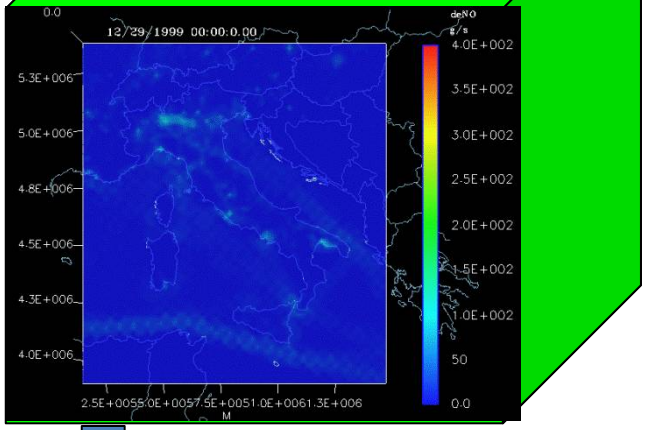
MINNI – Atmospheric modelling system



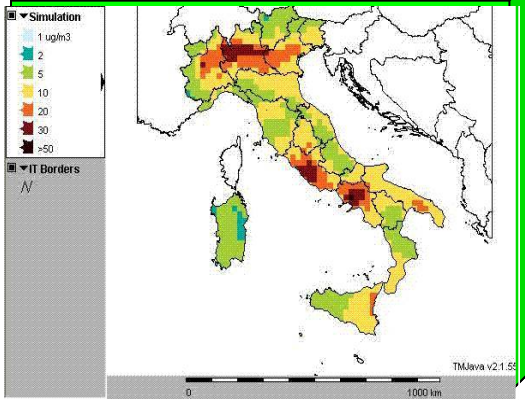
Il Sistema Modellistico MINNI

Proiezioni delle emissioni

AMS-Italia



RAINS-Italia



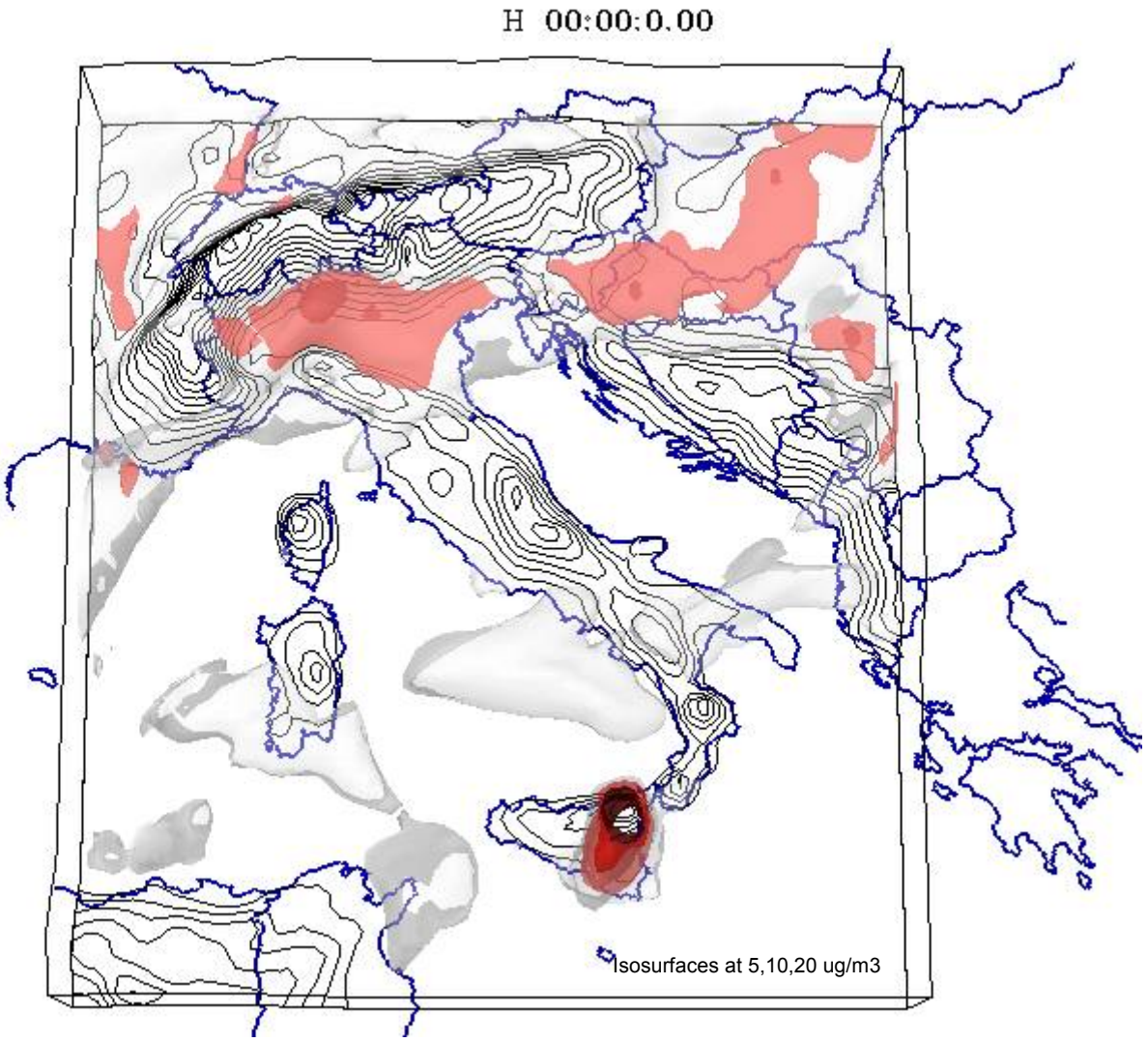
Matrici di Trasferimento Atmosferico

AMS: *Atmospheric Modelling System*

RAINS: *Regional Acidification INformation Simulation*

concentrazioni PM_{10}

ciclo giornaliero 2 Feb anno di riferimento, risoluz. 20 km



ENEA-GRID
&
Simulazione degli effetti delle instabilità di plasma dovute alle particelle veloci

S. Briguglio (ENEA FPN)

Controlled nuclear fusion

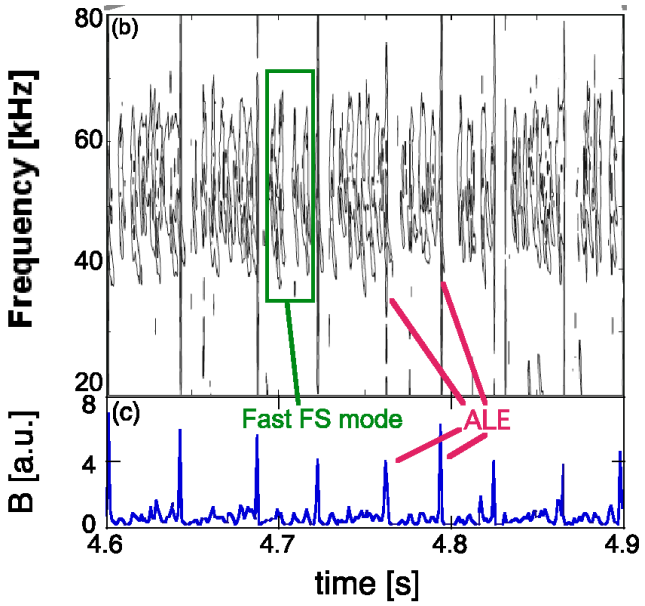
- Crucial issue for reaching reactor conditions in controlled nuclear fusion experiments: good confinement of fast ions (additional heating /fusion reactions)
- Basic problem: fast ions can excite electromagnetic modes; the resulting turbulence can affect fast-ion transport, degrading their confinement

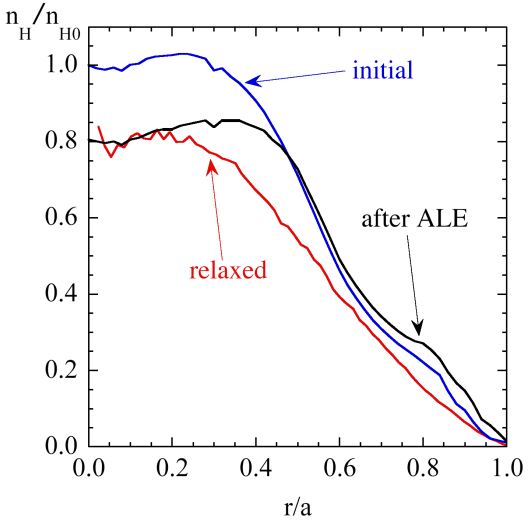
Simulation approach (S. Briguglio, G. Fogaccia, G. Vlad)

- The relevance of kinetic effects (wave-particle resonances) and nonlinear dynamics (effects on fast-ion transport) motivates a particle-simulation approach
- Hybrid MHD-Gyrokinetic Code (HMGC): at each time step
- electromagnetic fields computed on a spatial grid by solving MHD equations
- fast ions are pushed according to such fields (particle-in-cell techniques)
- fast-ion pressure is computed on the mesh and given back to field solver
- MPI+OpenMP parallel portable version (AIX, Linux systems)

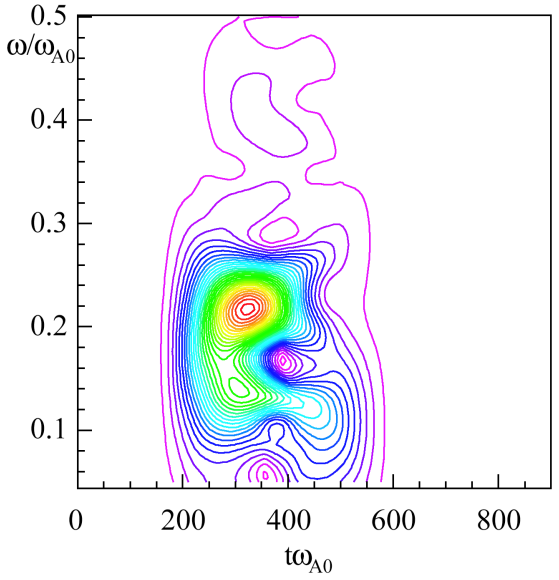
Application: JT-60U experiments

- Explosive modes, called Abrupt Large amplitude Events (ALEs), observed in neutral-beam heated JT-60U discharges
- Each of these events causes a relaxation of the fast ions density profile ("after ALE" profile)
- Particle simulation reproduces such effect ("relaxed" profile) and the magnetic-field burst features





$|\delta B_\theta(t,\omega)|$



Today simulation size and perspectives

- A relevant parameter for determining the size of such simulations is the typical wave-number n of the electromagnetic mode spectrum the simulation is able to investigate:

$$\text{Size} \propto n^3$$

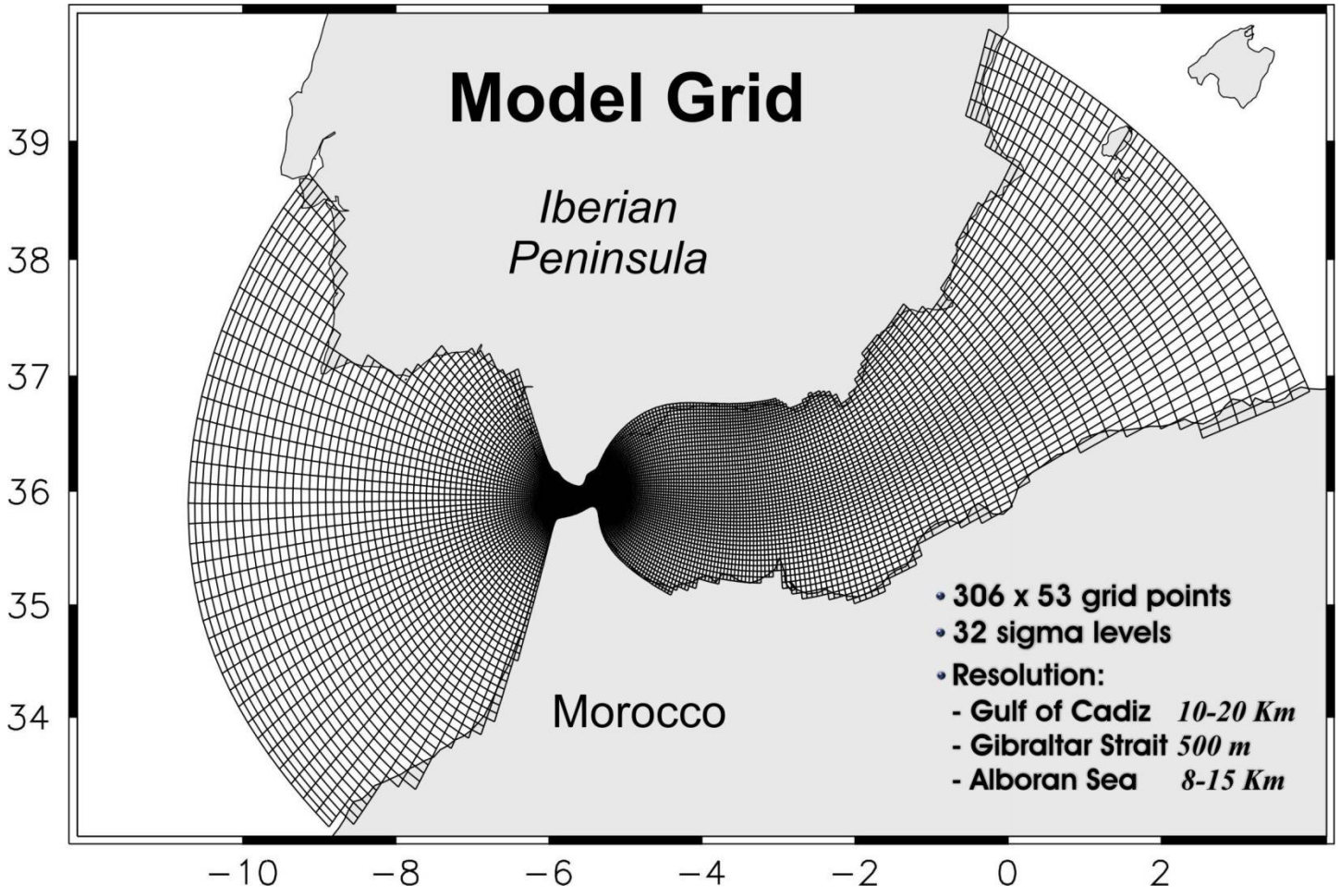
- Today simulations (on cluster of IBM SP5 nodes at ENEA Frascati) allow to investigate up to $n \sim 10$
- Values of interest for ITER experiment simulations: $n \sim 30$

ENEA-GRID
&
Simulazioni numeriche del flusso mareale attraverso lo stretto di Gibilterra e modelli accoppiati oceano atmosfera

G. Sannino (ENEA, ACS)

Numerical Model - Grid & Bathimetry

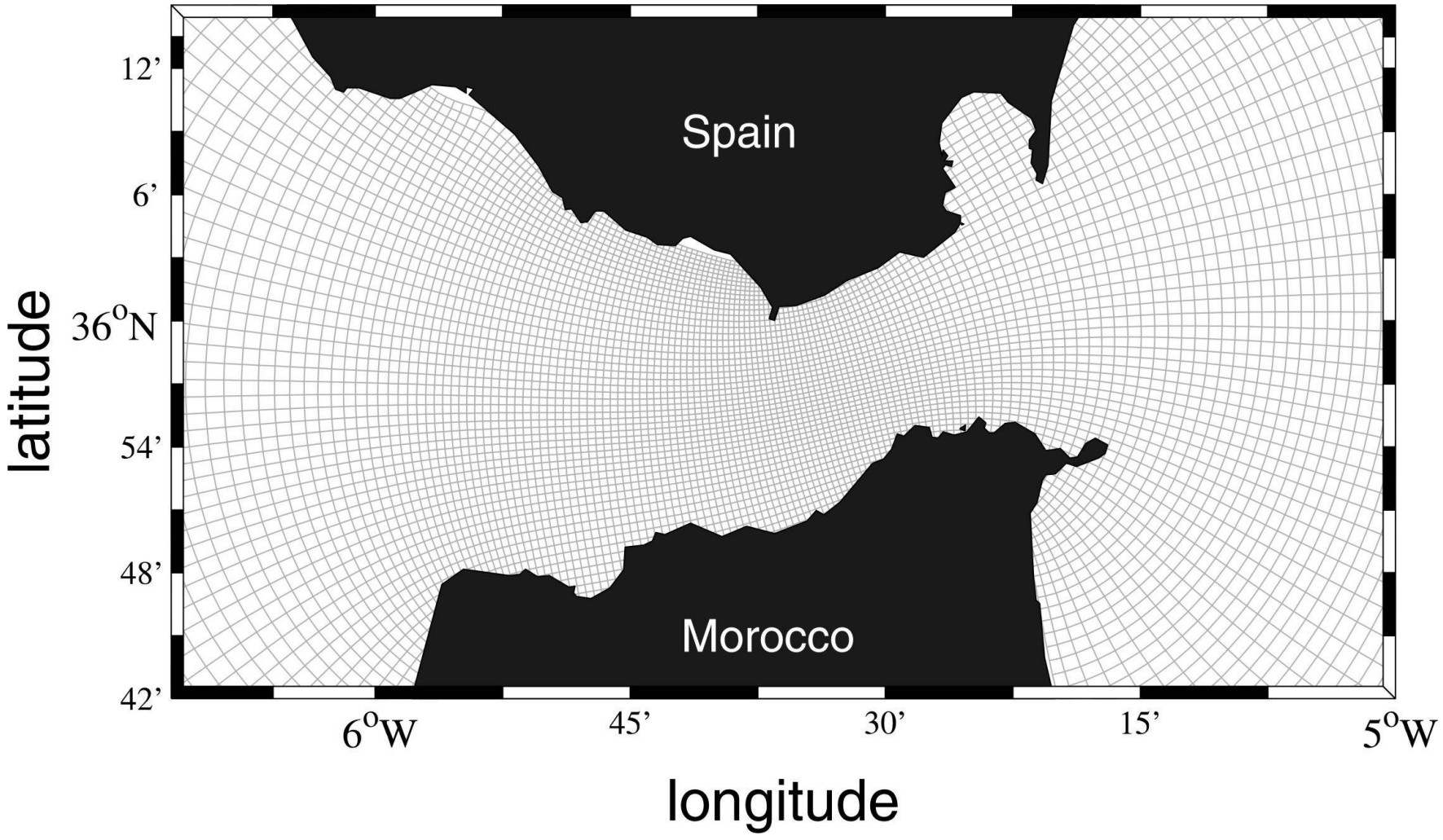
Orthogonal curvilinear model grid



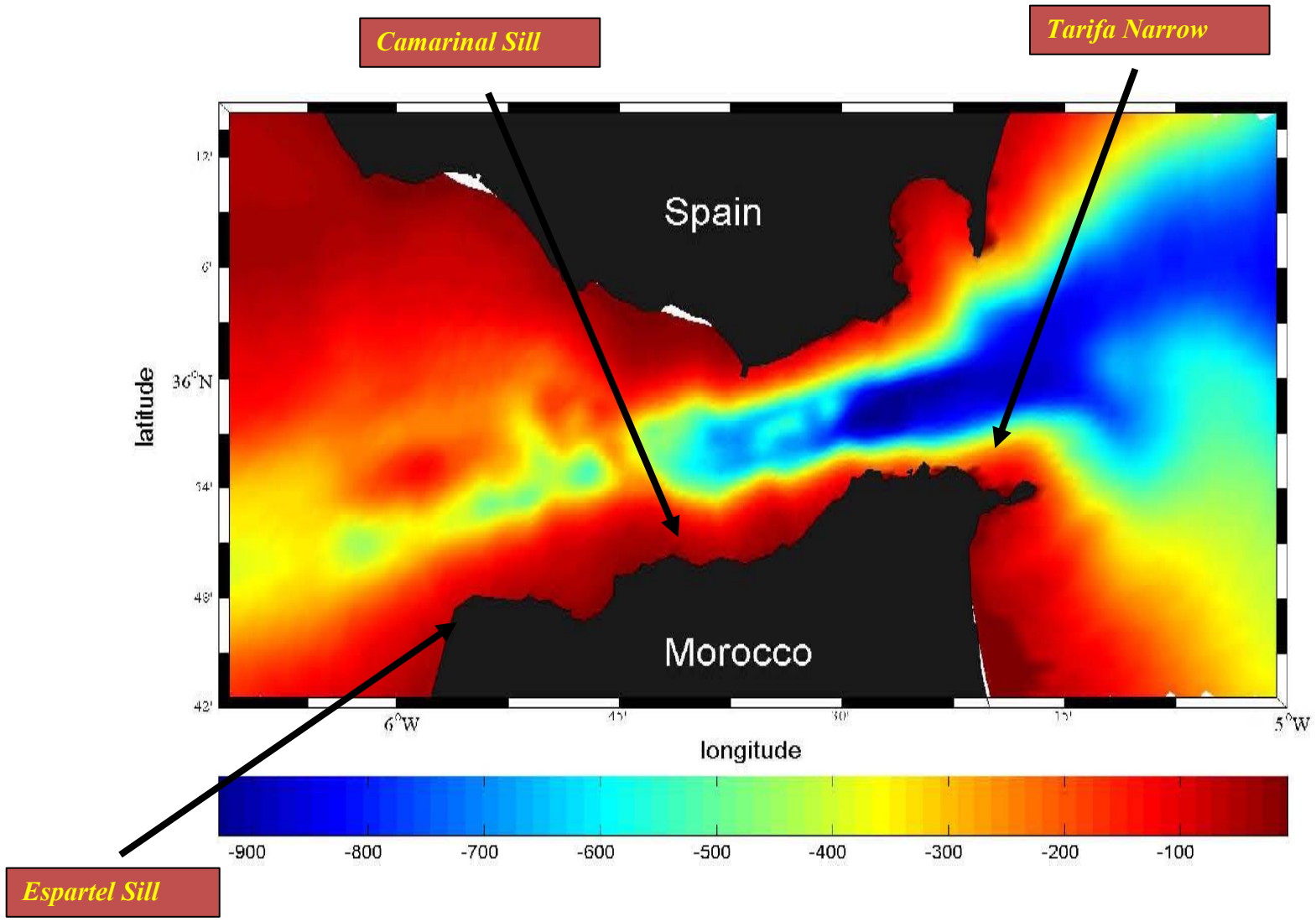
Numerical Model - Grid & Bathimetry

zoom

Orthogonal curvilinear model grid within the strait



Numerical Model - Grid & Bathimetry

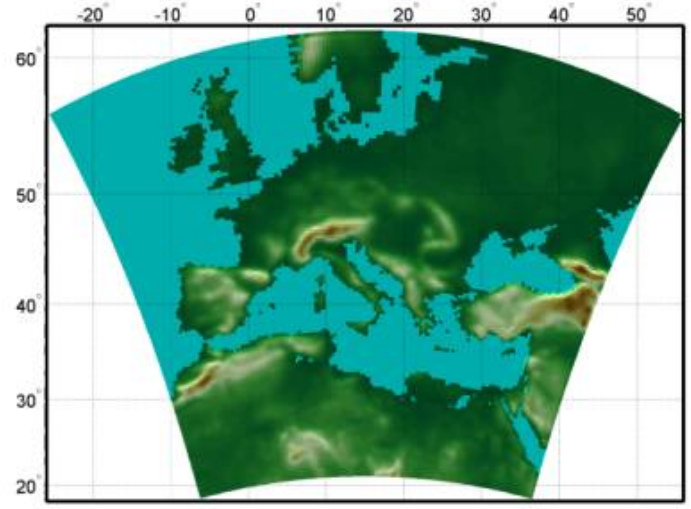


c'e' un filmato su youtube.com cercando “Tidal Simulation Gibraltar”

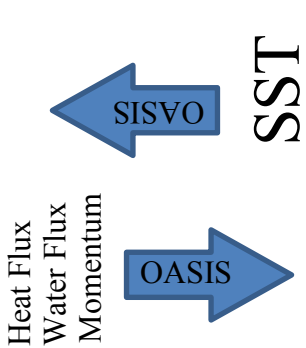
Regional coupled climate system

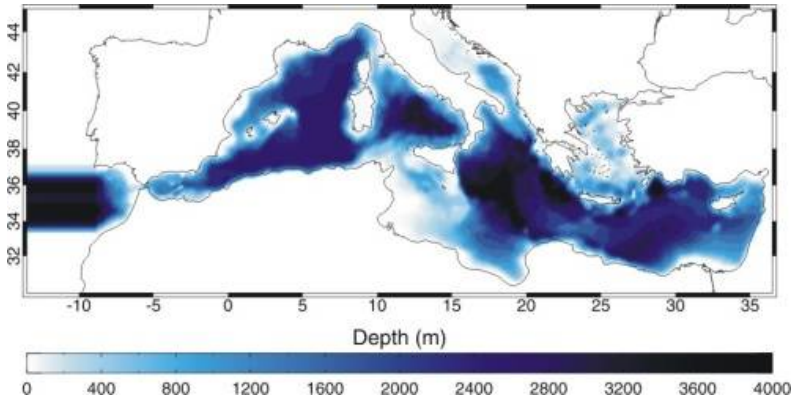
RegCM
Resolution:30 Km, 18 sigma levels
Validation with ECMWF-ERA40 data

MITgcm
Resolution: 1/8°, 42vert. Levels
Validation with ECMWF-ERA40 data



Coupled every 6 hours





ENEA-GRID
&
Simulazioni di chimica computazionale: interfaccia Mg-Mg-H2 con il codice CPMD

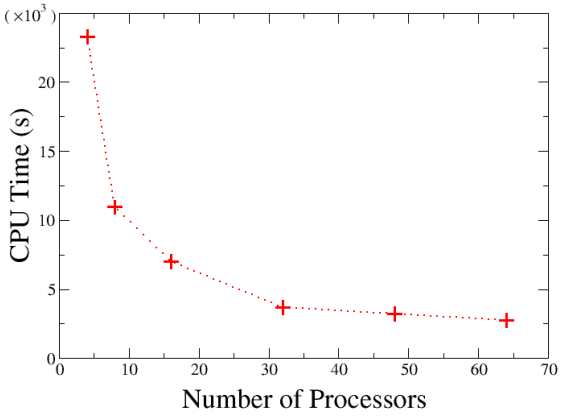
M. Celino, S. Giusepponi
(ENEA MAT)

Hydrogen storage in MgH_2 matrices: a study of Mg-MgH_2 interface using Car-Parrinello molecular dynamics code on ENEA-GRID.

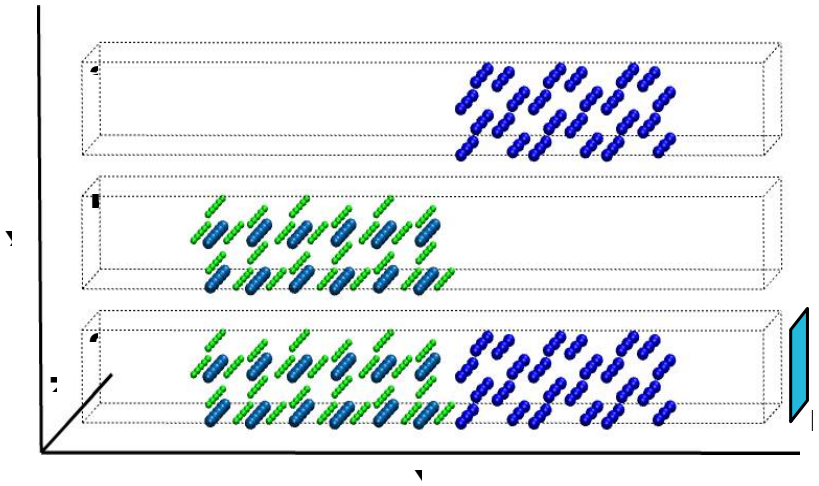
- Remarkable ability of magnesium to store significant quantities of hydrogen;
- Intense research efforts in the last years in view of Mg future applications where light and safe hydrogen-storage media are needed;
- Magnesium material, characterized by light weight and low cost of production, can reversibly store about 7.7 wt% hydrogen (MgH_2);
- Further research is needed since Mg has a high operation temperature and slow absorption kinetics that prevent for the moment the use in practical applications.

For these reasons a detailed study of the interface between Mg and MgH2 is needed.

Problem: intensive use of computational resource



We test the CPMD code for the system showed in this poster that represent a Mg-MgH_2 interface costituited by **132 atoms of magnesium and 120 atoms of hydrogen**. We use a CPMD (version 3.11.1) code compiled on IBM architecture with MPI parallelization, and exploit the Power5 IBM CPUs (1.5 GHz). In the figure in side we show the total time required by the code to perform 300 molecular dynamics time steps using increasing number of processors (from 4 up to 64). Every nodes is set up by 16 CPUs. The benchmark results demonstrate the high performance of the parallelization on Power5 CPUs for floating point intensive applications and the good scalability up 64 processors.



a) Mg surface: 72 Mg atoms;

b) MgH_2 surface: 60 Mg and 120 H atoms;

c) Mg-MgH_2 interface: 132 Mg and 120 H

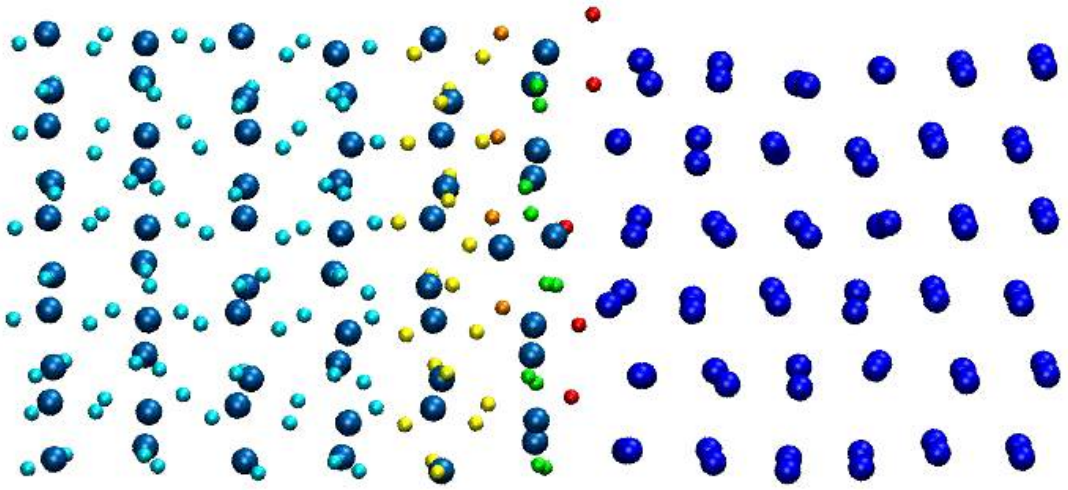
Periodic boundary conditions
are kept in the x and y direction.

The interface was characterized in terms of total energy calculations, and an estimate of work of adhesion was given

$$E_{inter} = E_{MgH2} + E - E_{tot} = 310 \text{ mJ/m}^2$$

To understand the atomic level dynamics of hydrogen diffusion at the interface, we performed MD simulations at volume and constant temperature in the range 300 K – 900 K.

MD simulation at 700 K ⇨



At this temperature there is a clear tendency of hydrogen atoms near the interface to perform bigger displacement. Good agreement with experimental studies.

ENEA-GRID e l'Industria

- ENEA-GRID e l'industria: alcuni esempi
  - AVIO
  - AnsaldoEnergia/AnsaldoRicerche
  - CETMA

- Le esigenze aggiuntive
  - Accesso a codici proprietari “Certificati” (gestione delle licenze)
  - Riduzione dei tempi di simulazione anche a prezzo di modesta scalabilità
  - Sinergia di utilizzo tra codici commerciali e codici opensource (OpenFoam)
  - Sicurezza e tracciabilità
  - Garanzia della proprietà intellettuale

ENEA-GRID
&
AVIO

Ing. E. Lambiase (Avio Spa)

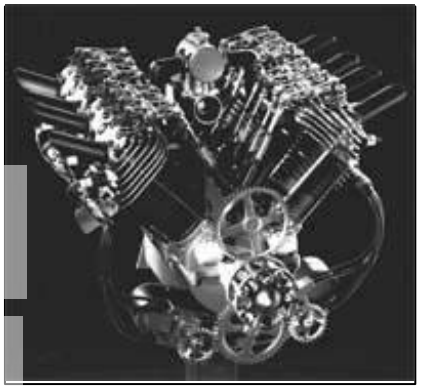
Un po' di storia…

1908 Avio inizia le proprie attività in Fiat

1915 Dalla prima guerra mondiale, Fiat progetta e produce velivoli completi

1969 Fiat si focalizza sui motori lasciando l'aspetto velivolistico ad Aeritalia

1976 Fiat Aviazione nasce come azienda autonoma



1994 FiatAvio acquisisce le attività spaziali dal gruppo Fiat

1996 FiatAvio nelle revisioni civili con l'acquisizione di Alfa Romeo Avio

Luglio 2003 FiatAvio diviene Avio aerospace propulsion

Avio S.p.A. in Italia

Sangone (Torino)

Area m² 12.200

Test e sviluppo:
motori e componenti

Rivalta di Torino (Torino)

Area m² 163.000

Trasmissioni meccaniche
Parti rotanti

Colleferro (Roma)

Area m² 157.918

Propulsione spaziale a solido

Brindisi

Area m² 48.403

Montaggio motori militari
Revisioni militari, Package navali

Pomigliano d'Arco (Napoli)

Area m² 84.418

Combustori, parti strutturali
Revisioni civili

Acerra (Napoli)

Area m² 36.309

pale

16 sedi, circa 4,800 dipendenti

7 in Italia: Torino (2), Colleferro (Roma), Brindisi, Pomigliano d'Arco (Napoli), Acerra (Napoli), AvioFix (Lecco)

2 in Sud America: (Guyana francese)

1 in nord America: (New Jersey)

1 in Olanda: (Eindhoven)

1 in Polonia: (Bielsko-Biala)

4 uffici rappresentanza: Roma (Italia), Beijing (Cina), Varsavia (Polonia), Bruxelles (Belgio)

Propulsione spaziale

Ariane 5

Vega

Ariane 5

Propulsione criogenica

Propulsione tattica

Aster

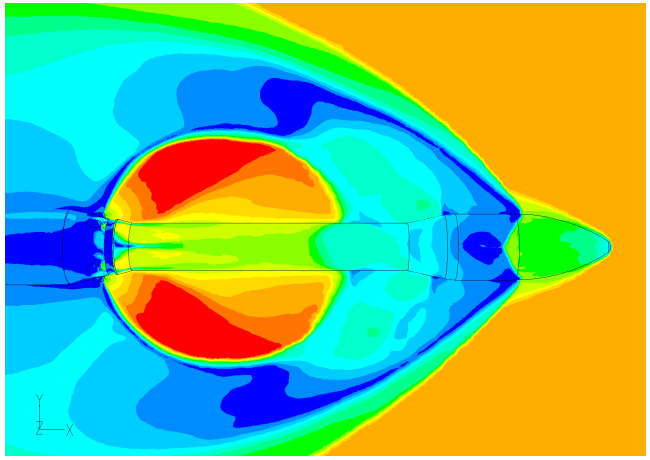
Unico fornitore in Europa, anche attraverso le sue joint venture di “complete solid rocket motor” per lanciatori

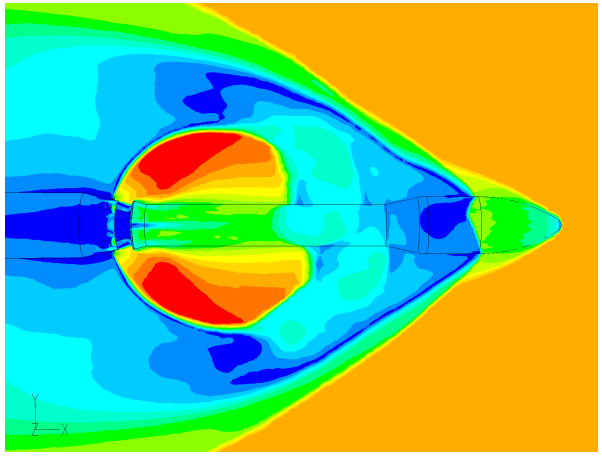
Attività CFD sul GRID ENEA (1)

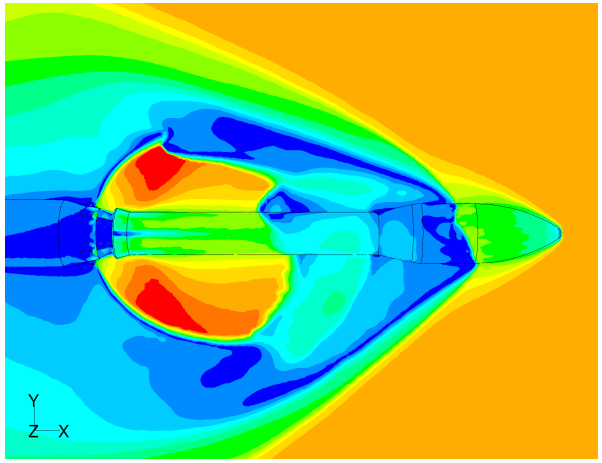
La separazione del 1° stadio del lanciatore Vega è stata oggetto di una vasta campagna di analisi CFD.

Complessivamente sono state realizzate 10 simulazioni 3D con flusso turbolento, utilizzando il codice Fluent sul GRID ENEA.

	Tempo macchina per 1 CFD [gg]		Guadagno tempo [%]
Celle di calcolo	AVIO hardware (4CPU)	ENEA Grid (16CPU)	
2,000,000	55	30	45%





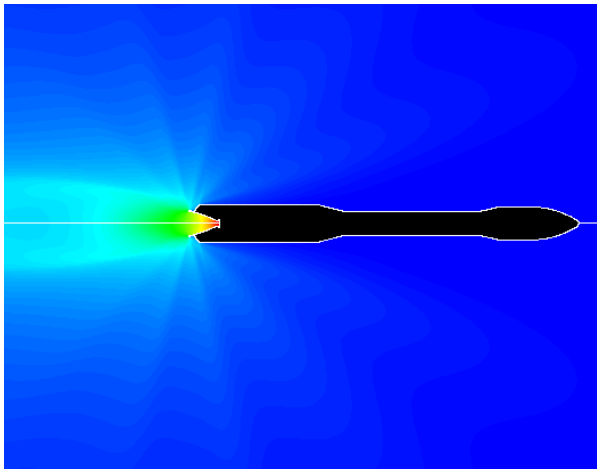


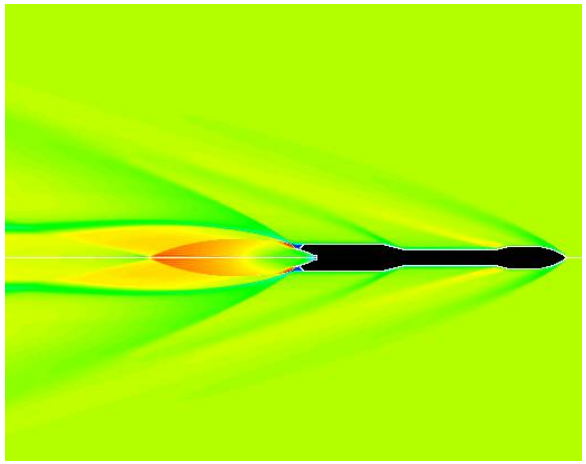
Attività CFD sul GRID ENEA (2)

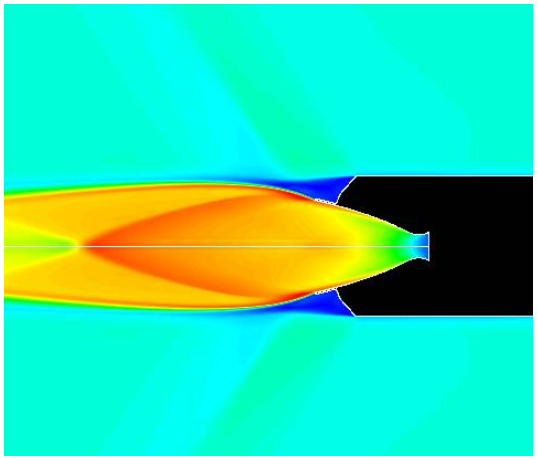
Un set di 3 analisi CFD è stato dedicato al calcolo del carico radiativo sulla base del 1° stadio del Vega in diverse condizioni di volo.

E' stato adottato un approccio bi-fase (fase gassosa + particelle solide di allumina) con il modello radiativo.

	Tempo macchina per 1 CFD [gg]		Guadagno tempo [%]
Celle di calcolo	AVIO hardware (4CPU)	ENEA Grid (8CPU)	
400,000	15	7	53%



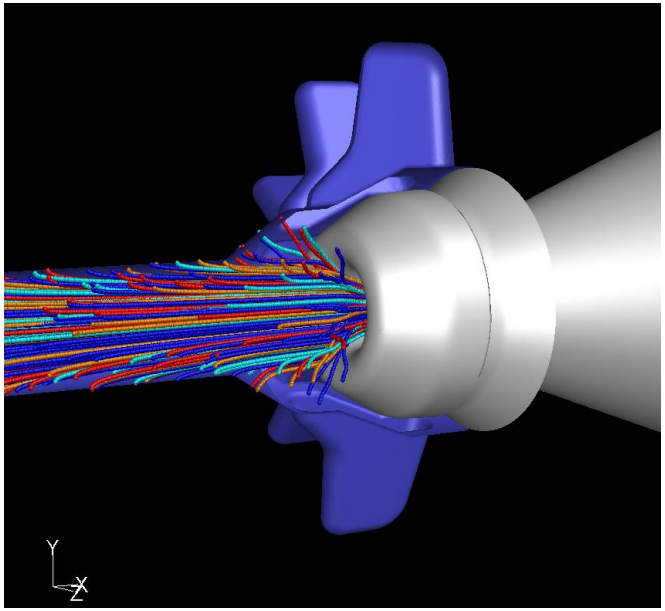


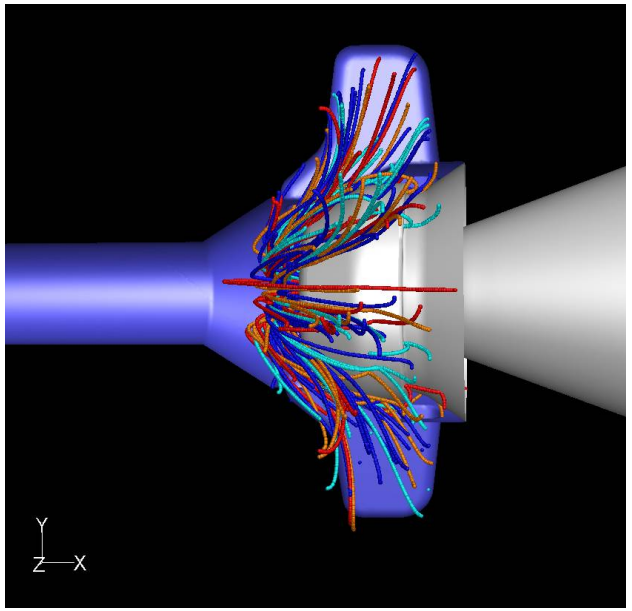


Attività CFD sul GRID ENEA(3)

E’ stata realizzata un’analisi CFD per valutare l’interazione meccanica tra le particelle di allumina e la parte di sommergenza dell’ugello all’interno del motore del 3° stadio del lanciatore Vega.

	Tempo macchina per 1 CFD [gg]		Guadagno tempo [%]
Celle di calcolo	AVIO hardware (4CPU)	ENEA Grid (8CPU)	
1,500,000	25	10	60%





ENEA-GRID
&
AnsaldoRicerche/AnsaldoEnergia

Ing. M. Cioffi (CRIS Napoli)

HPC AND GAS TURBINES DEVELOPMENT TOOLS

AnsaldoRicerche
Una Società Finmeccanica

AnsaldoEnergia
A Finmeccanica Company

Gas Turbines Development

FINMECCANICA

MARKET REQUIREMENTS:

- Decrease emissions.
- Increase Major Overhaul Interval.
- Increase fuel flexibility.

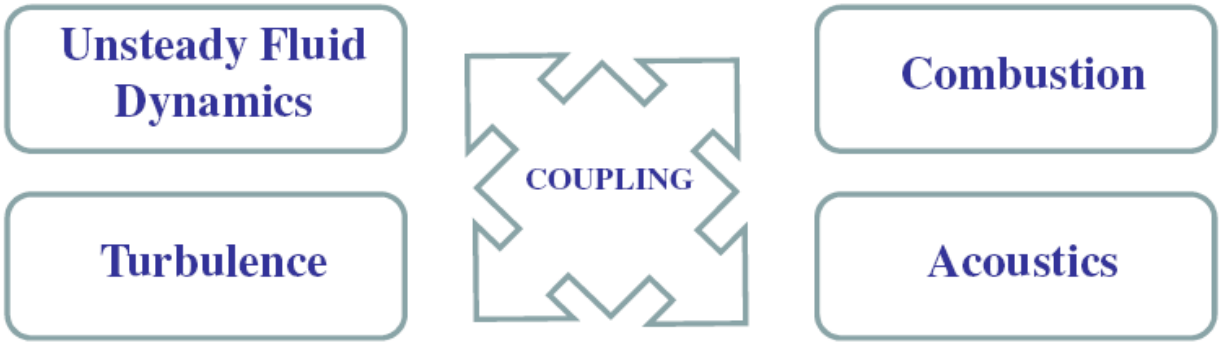
PRODUCERS STRATEGIES:

Combustion Dynamics modelling has become the major issue in power systems R&D.

Technical Issues

FINMECCANICA

Combustion chamber instabilities (i.e. humming phenomena) numerical simulation.



TURBULENCE:

Large Eddy Simulation (LES) numerical technique has become the most reliable numerical method to understand humming phenomena.

LES is quite computer expensive: 100÷1000 more classical RANS (Reynolds Averaged Navier Stokes).

LES Modelling and HPC Numerical Approaches

FINMECCANICA

Due to the Gas Turbines combustion chamber geometrical characteristics and to the main azimuthal acoustic mode it is necessary to simulate the overall 3D combustion system (computational grid with O(1E6) ÷ O(1E7) cells).

PRESENT GOAL:

- Execution of LES 3D model of a complete combustion chamber by decreasing the run time by a factor of 100.
- Smart use of HPC HW and SW solutions.

Preliminary tests are in progress on CRESCO ENEA machine by an Ansaldo-ENEA research agreement.

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A Finmeccanica Company

ENEA-GRID
&
CETMA

D. Bardaro CETMA, Brindisi

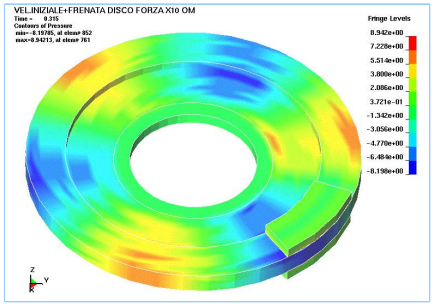
CETMA is a private and non-profit research center specialized in development of innovative products and processes, through the integration of specific competences in materials engineering, industrial design and computer science engineering.

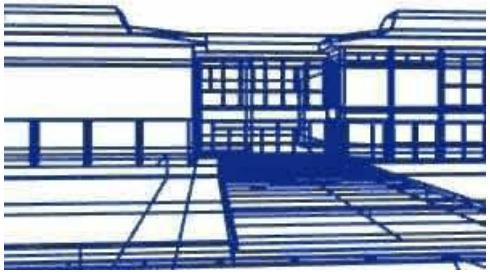
The shareholders are:

ENEA
Università del Salento
D'Appolonia
Infobyte
Telcom
Alfa Edile
Cemit
Igeam

CETMA DEPARTMENTS

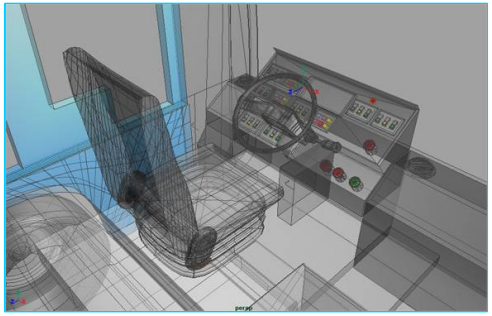
Materials and structures engineering





Information Technologies

Industrial & Communication Design



CETMA – ENEA GRID Activities

PROCETMA Project - Potenziamento delle attività di Ricerca e delle Opere infrastrutturali per il Supercalcolo, la Simulazione e Visualizzazione del consorzio CETMA

CETMA / ENEA Activities – CFD (Computational Fluid Dynamic Analyses) and Grid Computing

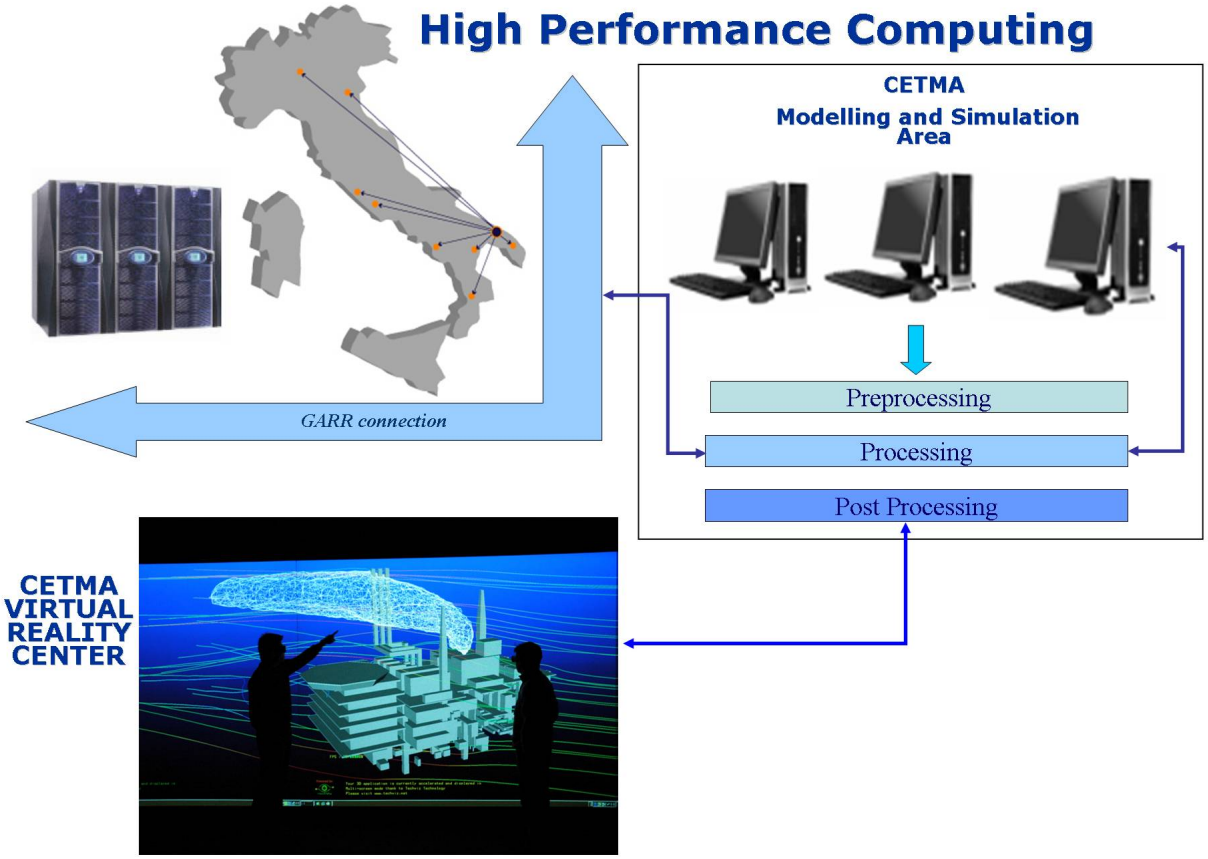
CRESCO Project – Computational Research Center for Complex Systems

CETMA Activities – Development of numerical modelling strategies to perform complex structural analyses and to simulate sintering processes

Design CETMA - The present document is CETMA property. Can't be copied and handout to others without permission - All rights are reserved

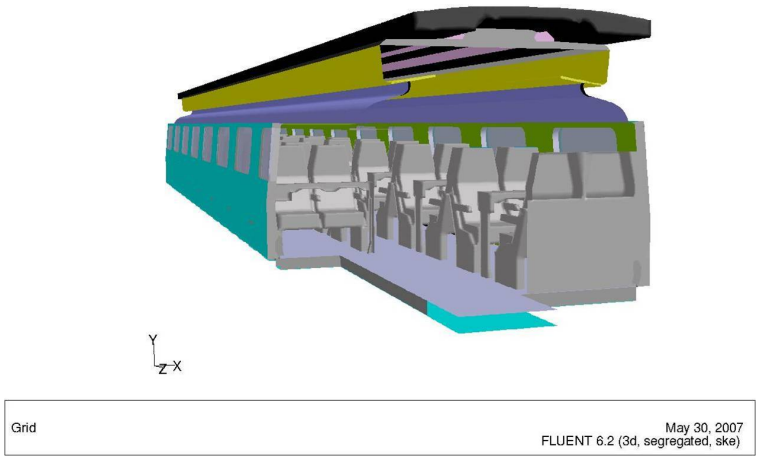
Porting Cetma-ENEA Grid

The aim of the activity is to connect the ENEA grid infrastructure to the single design work stations and to the CVRC (CETMA VIRTUAL REALITY CENTRER) located at CETMA site.
Post processing and full understanding of the results is allowed through the capabilities of the virtual reality environment provided by the CVRC while reduction of running time is obtained through the parallel computing environment provided by the Grid.

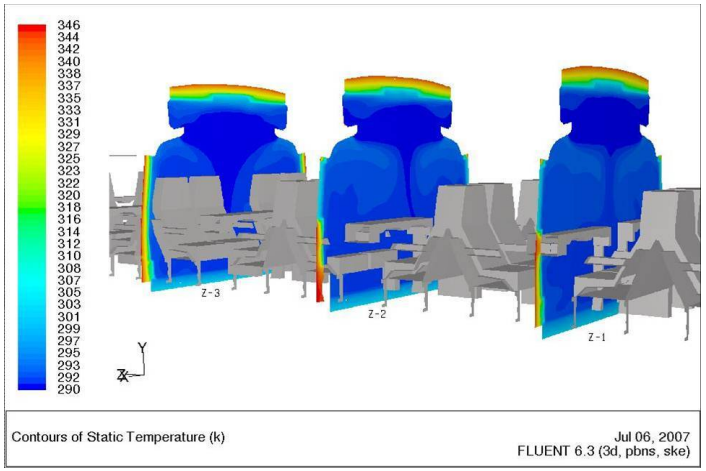


Layout of the various phases of the porting CVRC-Grid ENEA

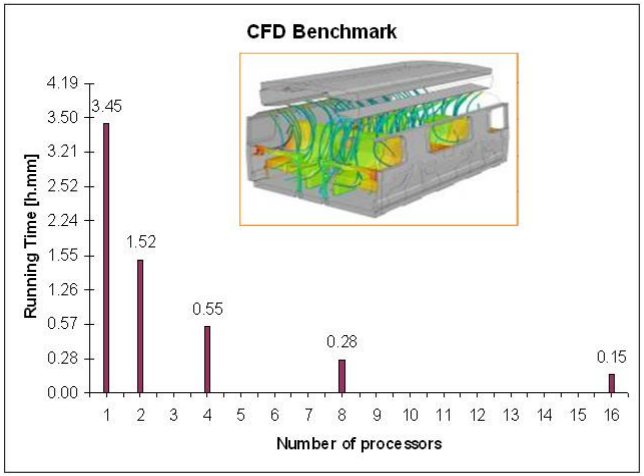
CFD case study 1: Thermal Fluid Dynamic ANALYSIS OF A PASSANGER COACH



3D CFD Model

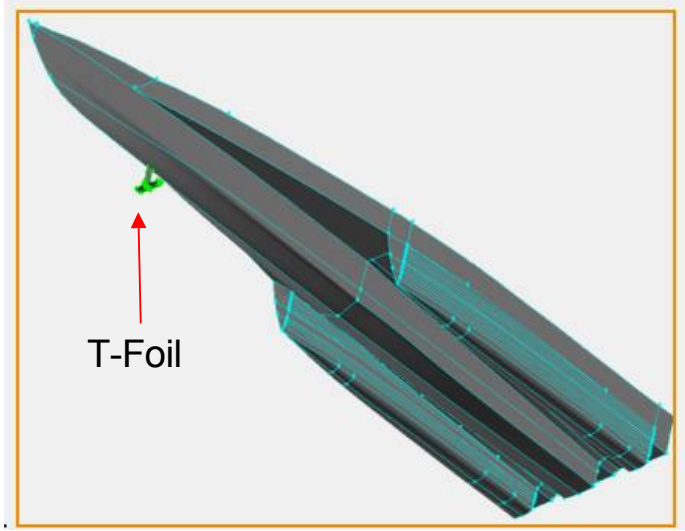


Air Temperature Contours

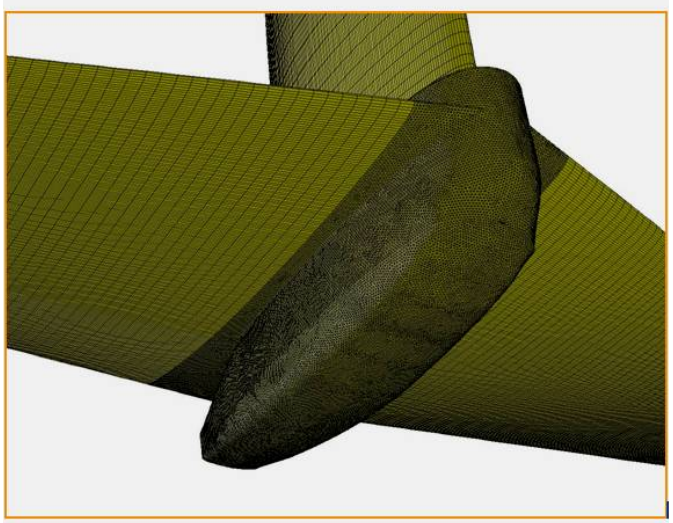


HPC: reduction of running time for a 3D CFD model when the number of processors increase (from 1 to 16)

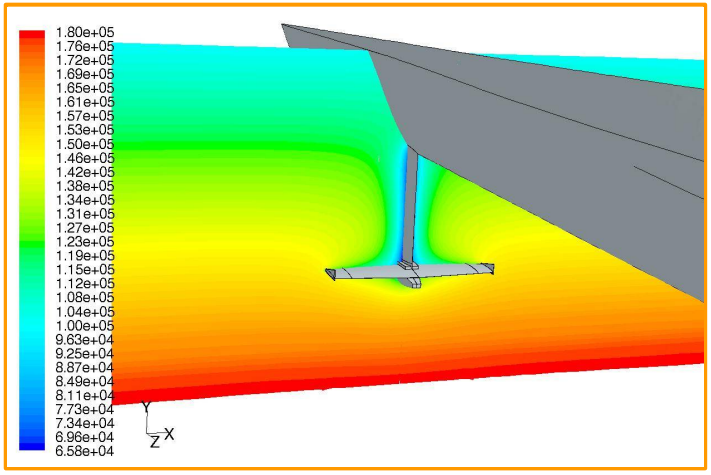
CFD case study 2: hydro-dynamics analyses of Fast Ship T-Foil system



3D Model: trimaran + T-foil



Detail of T-foil mesh



Results: pressure contour (Pa): flap 0° , cruising speed 31.5 knots

Mesh: 15 Millions of cells with dimensions ranging from 1 mm to 550 mm

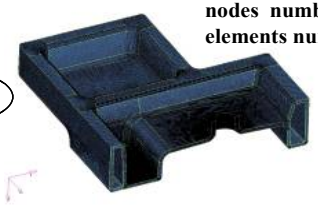
Need of HPC: ENEA GRID

The analyses were carried out using 16 CPUs on ENEA GRID with a total running time of 70 h.

Structural analysis case study: Development of numerical models for the simulation of ceramic components during sintering

FE solver was used to simulate and visualize the system deformations during sintering. Some tools were developed to achieve better results: user subroutines to correctly represent the constitutive material law and macro to allow post-processing for mould design.

Pre Processor



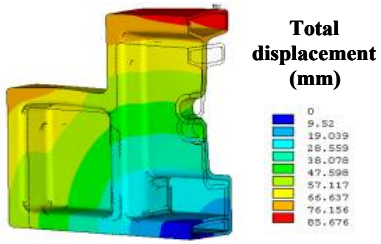
nodes number: 1272783
elements number: 792674

Solver

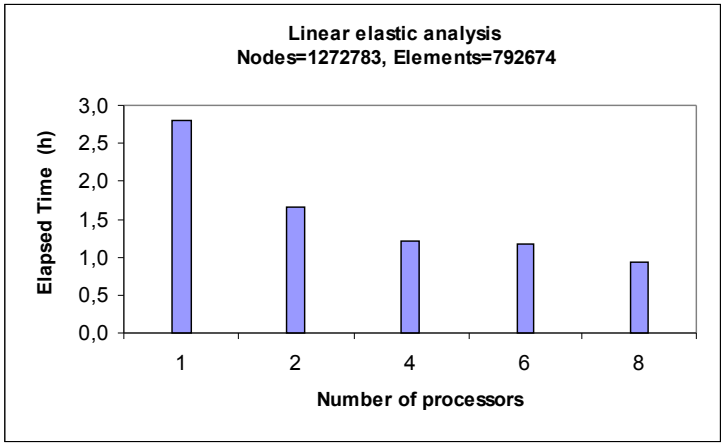
Olevsky costitutive law for ceramics materials

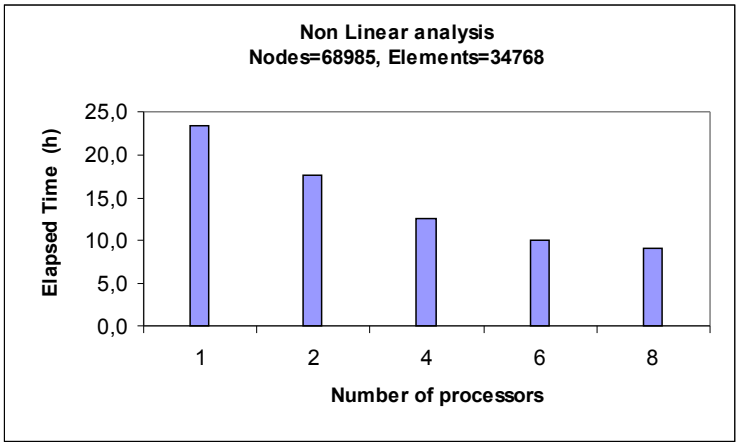
$$\sigma_{ij} = \frac{\sigma(W)}{W}\left[\varphi\dot{\varepsilon}_{ij} + \left(\psi - \frac{1}{3}\varphi\right)e\delta_{ij}\right] + P_L\delta_{ij}$$

Post Processor



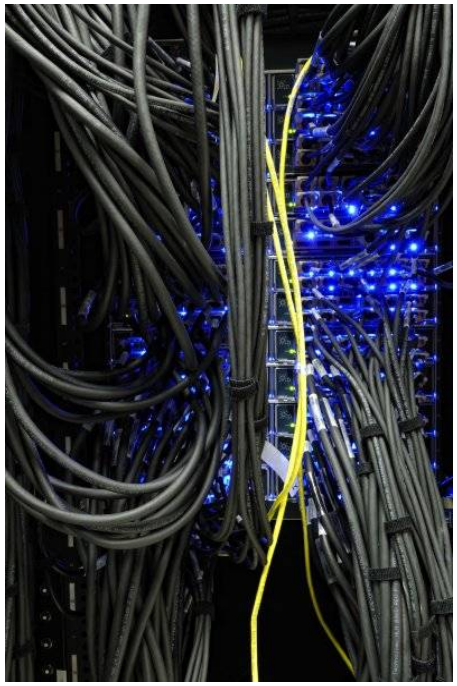
Design of new ceramic shapes (washbasin) through numerical simulation





HPC: reduction of running time for linear and non linear mechanical analyses when the number of processors increase (from 1 to 8)

Il sistema HPC CRESCO



I processori di CRESCO

2720 cores in totale: ad oggi: HPL 17.1 Tflops

Sezione 1: 672 cores

42 fat nodes IBM x3850/x3950-M2, 4 Xeon Quad-Core Tigerton E7330 processors (2.4GHz/1066MHz/6MB L2), 32 GB RAM (4 extra-fat nodes with 64 GB RAM, 2 coupled node(x3) 48 cores/192 GB, 1 coupled node (x2) 32 cores /128 GB.

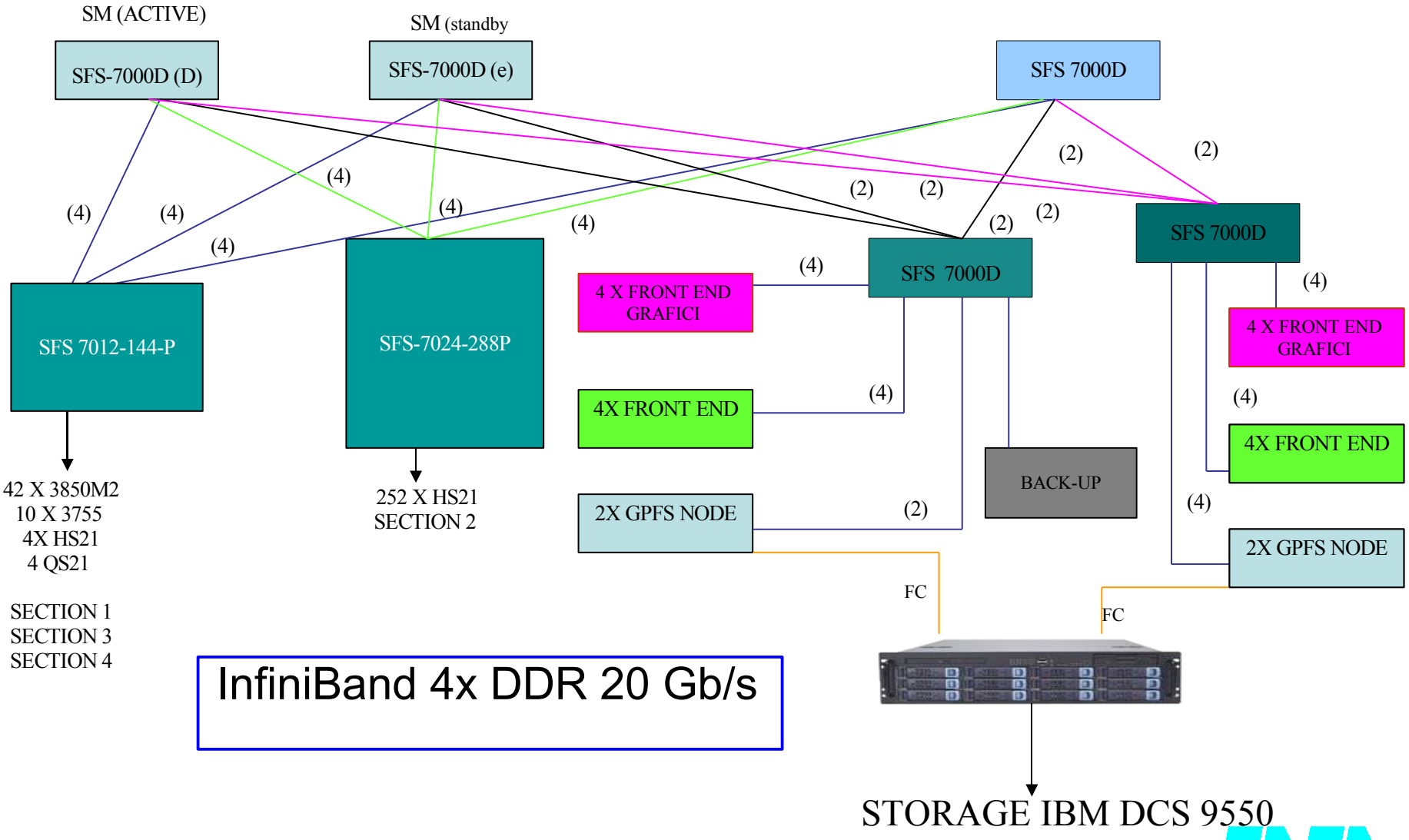
Sezione 2: 2048 cores

256 blades IBM HS21, Xeon Quad-Core Clovertown E5345 processors (2.33GHz/1333MHz/8MB L2), 16 GB RAM

Sezione sperimentale

- 4 blades IBM QS21, 2 Cell BE Processors 3.2 Ghz
- 6 nodes IBM x3755, 4 sockets AMD Dualcore 8222, FPGA VIRTEX5 LX330
- 4 node IBM x 3755, 4 sockets AMD Dualcore 8222, NVIDIA Quadro FX 4500 X2 video card

Rete INFINBAND CRESCO



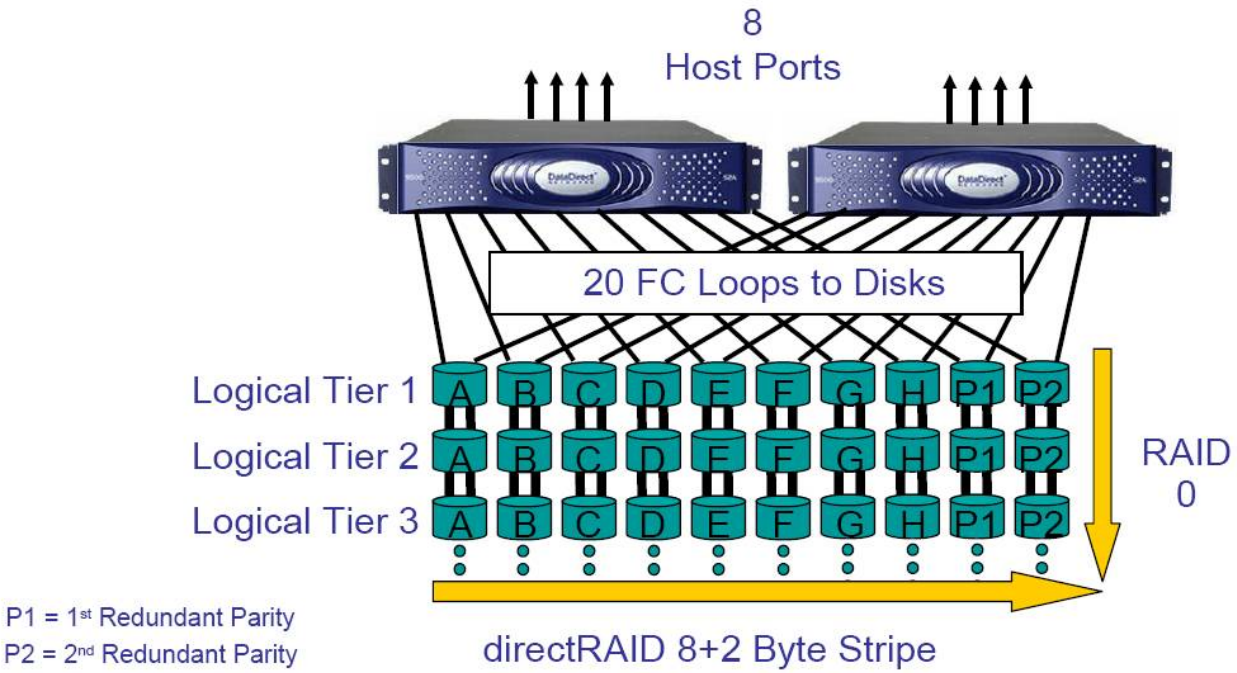
Storage IBM/DDN: 160 TB raw

Storage di CRESCO

File sistem parallelo GPFS: 120 TB 2 GB/s aggregato, 0.6 GB/s da singolo client

OpenAFS per software e le HOME degli utenti: su fileserver locali fino a 40 MB/s

directRAID6 S2A9550



ENEA-GRID: il salto di qualità di CRESCO

- Il sistema CRESCO fornisce risorse con un aumento di un ordine di grandezza nelle prestazioni disponibili
  - 17.1 Tflops Rmax nel test HPL
  - 120 TB storage su file system parallelo GPFS
  - La connettività su WAN è stata incrementata significativamente

- L'inserimento di CRESCO in ENEA-GRID
  - Le modalità di lavoro per l'utente rimangono sostanzialmente inalterate
  - Consolidamento della infrastruttura e nuovi strumenti di amministrazione
  - Gli assegnisti di CRESCO: uno nucleo di competenza
  - Visibilità nazionale come elemento di attrazione

Ringraziamenti

in ENEA

S. Taglienti, R. Guadagni, A. Perozziello, A. De Gaetano, S. Pecoraro, T. Bastianelli, G. Mencuccini, M. Caiazzo, A. Palumbo, G.Tommasino, G. Elmo, M. Impara, V.Lusani, G. Furini, C. Zini, C. Mercuri, U. Ferrara, A. Santoro,..

Supporto e collaborazioni:

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Installazione e configurazione CRESCO:

ComputerVar e IBM