BSC-Microsoft Research Centre Overview

Osman Unsal

Moscow 11.June.2009

Outline

- Barcelona Supercomputing Center
- BSC – Microsoft Research Centre

Barcelona Supercomputing Center

- Mission
  - *Investigate, develop and manage technology to facilitate the advancement of science.*

- Objectives
  - Operate national supercomputing facility
  - R&D in Supercomputing and Computer Architecture.
  - Collaborate in R&D e-Science

- Consortium
  - the Spanish Government (MEC)
  - the Catalonian Government (DURSI)
  - the Technical University of Catalonia (UPC)

MINISTERIO DE EDUCACION Y CIENCIA

Generalitat de Catalunya
Departament d'Universitats, Recerca i Societat de la Informació

UNIVERSITAT POLITÈCNICA DE CATALUNYA

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Location

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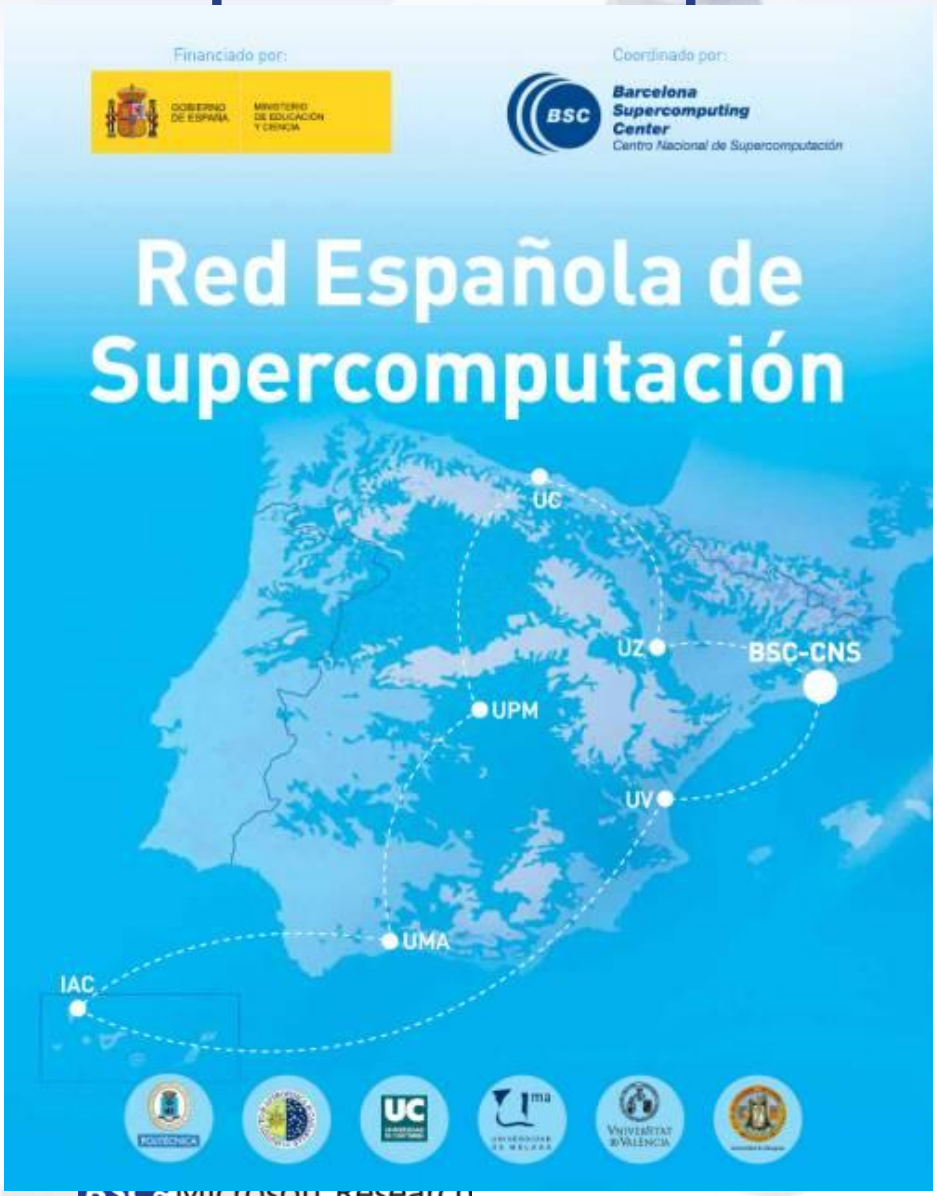
MareNostrum

- MareNostrum 2006
  - 10240 PowerPC 970 cores
    - 2560 JS21 2.3 GHz
    - 20 TB of Memory
    - 8 GB per node
  - 380 TB Storage Capacity
  - 3 networks
    - Myrinet
    - Gigabit
    - 10/100 Ethernet
  - Operating System
    - Linux 2.6 (SuSE)

Spanish Supercomputing Network



Magerit

Altamira

CaesarAugusta

LaPalma

Picasso

Tirant

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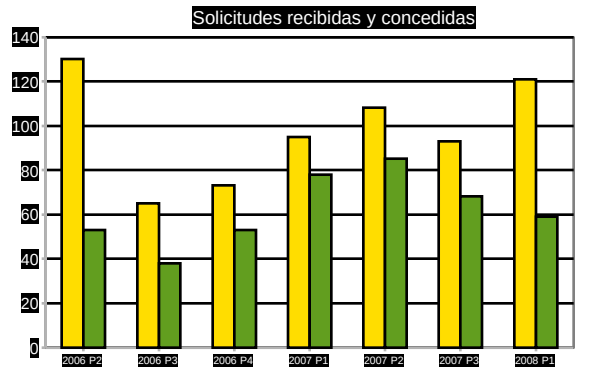
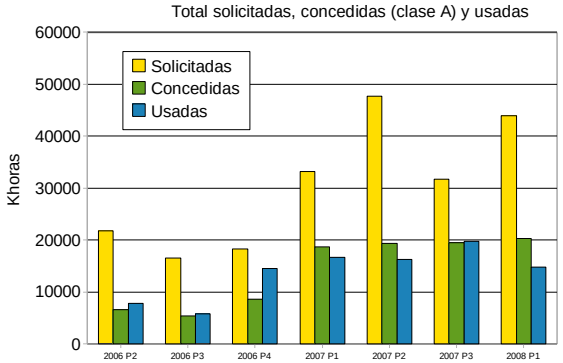
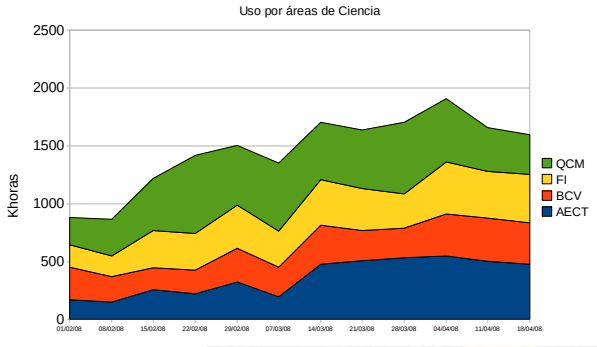
Access Committee Resource utilization

- Resource distribution
  - 20% internal use
  - 80% assigned via Access Committee
- Unique Access Committee
  - 44 Spanish researchers
    - Core Team
    - 4 panels
      - Astrophysics, Space, and Earth Sciences
      - Biomedicine and Life Sciences
      - Physics and Engineering
      - Chemistry and New Materials
  - New applications every four months
  - Committee renewed every 2 years
  - Designated by the Spanish Ministry
  - Technical assistance by BSC staff







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Industry using MareNostrum

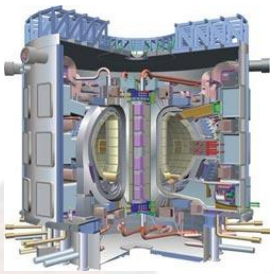
AIRBUS

- Average utilization of 1000 processors
- Using dedicated network

- Oil prospection using 2000 processors, each execution lasts for 5 weeks

repsolypf.com

ITER



- Provide HPC computing resourceswith the following specifications:
  - 1 Million CPU-hours
  - Disk space: 2 Terabytes capacity
  - Disaster Back-up for 20 Terabytes capacity

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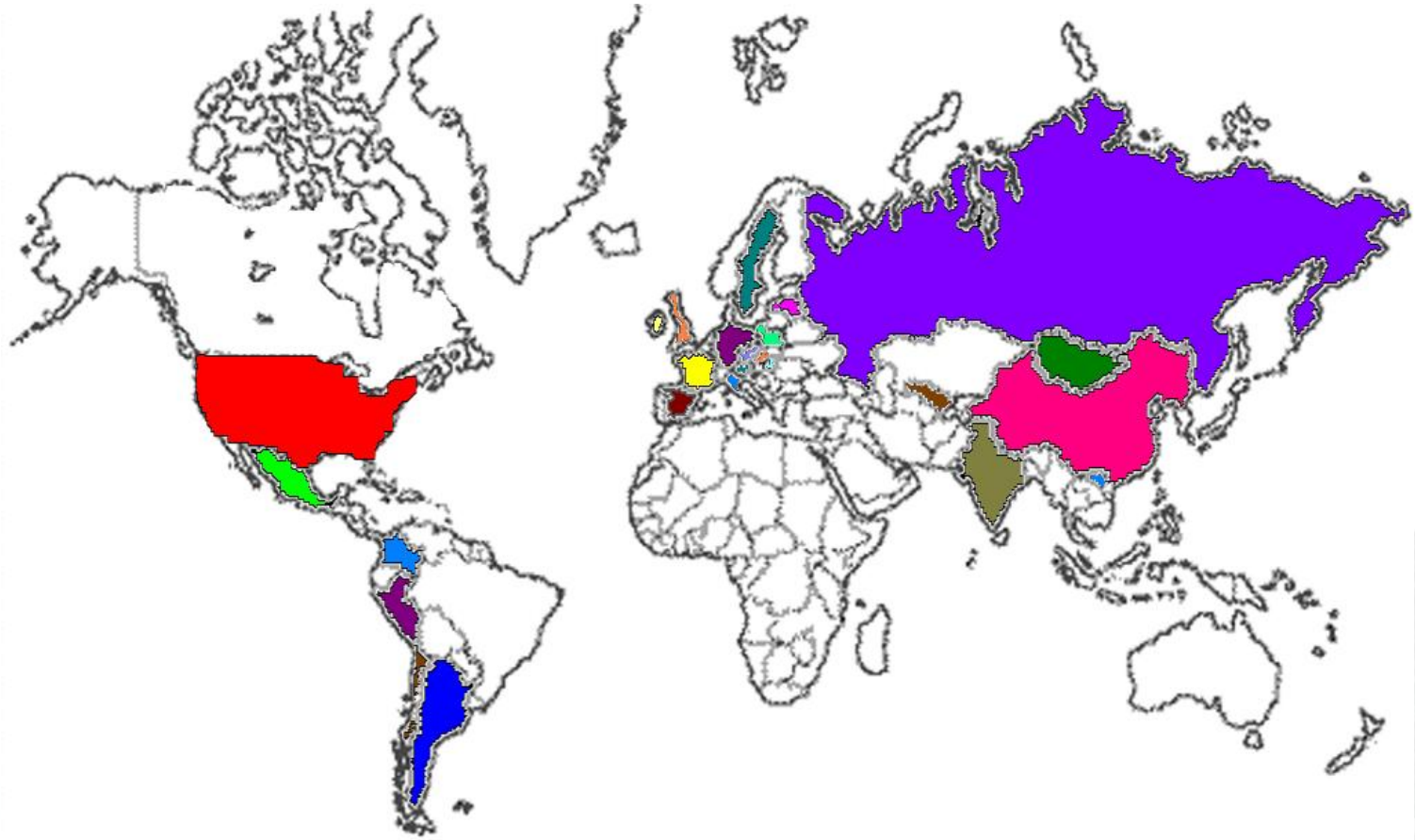
Staff Evolution

BSC-CNS has 195 members at October of 2007 and hailed from 21 different countries (Argentina, Belgium, Brazil, Bulgaria, Colombia, China, Cuba, France, Germany, India, Ireland, Italy, Lebanon, Mexico, Poland, Russia, Serbia, Turkey, the United Kingdom, the United States and Spain).



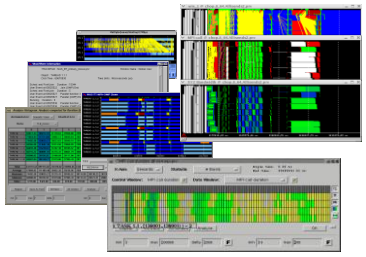
BSC Departments

- Computer Science
  - Computer Architecture
- Life Sciences
- Earth Sciences
- Computer Applications

Towards Petaflop computing systems

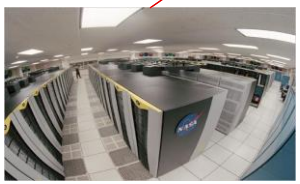
Analysis and prediction of:

- Applications
- Parallel execution environments
- OS activity



eNANOS

The Grid



Distributed-memory programming model

- Scalable MPI

Future Petaflop systems

Shared-memory programming models

- Mercurium OpenMP compiler

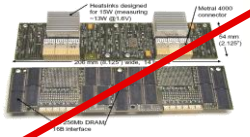
- NthLib

- NanosDSM

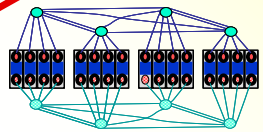
- Transactional memory

Small DMM

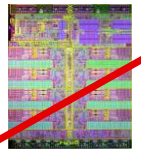
Large cluster systems



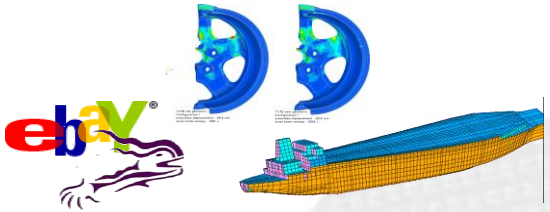
On-board SMP



cc-NUMA



10s, 100s, 1000s, … cores, multithreaded chip



Hardware and software technologies for:

- Grand Challenge applications
- Killer applications (Google, Amazon, eBay, …)

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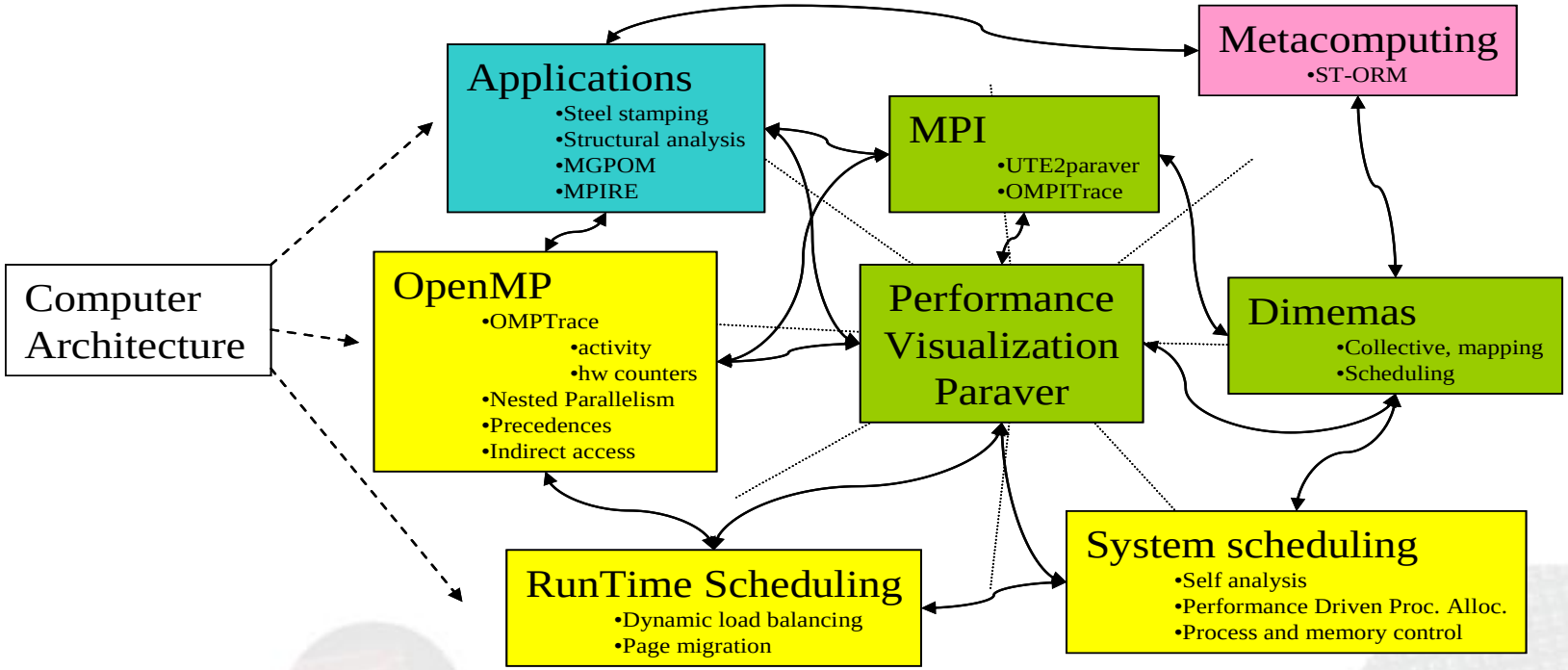
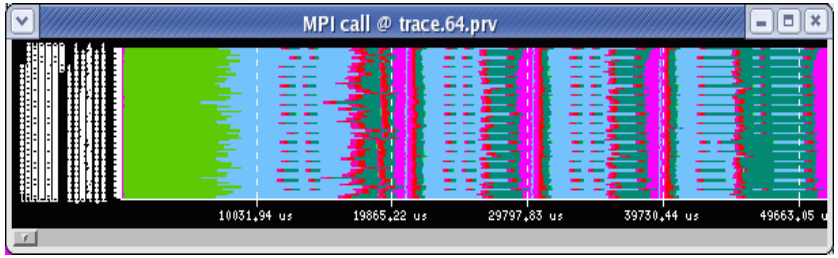
CIRI R&D Philosophy

- Technology Web

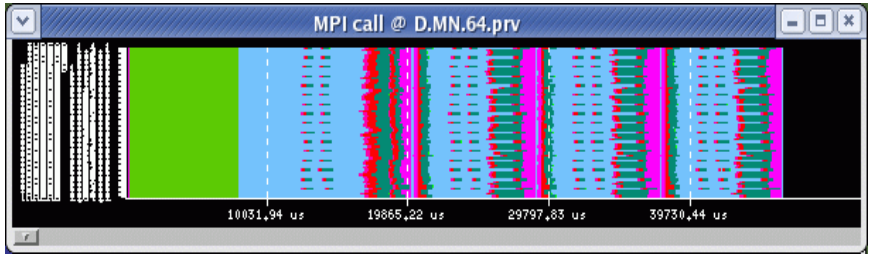


Amber

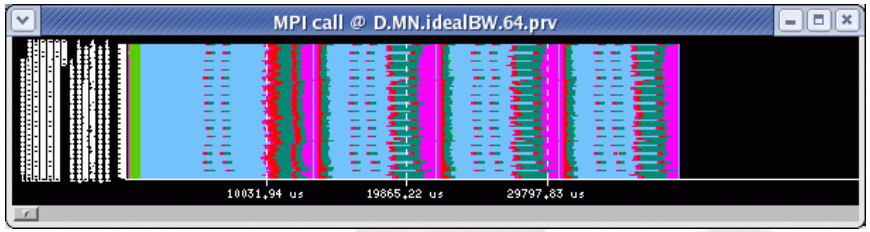
Marenostrum



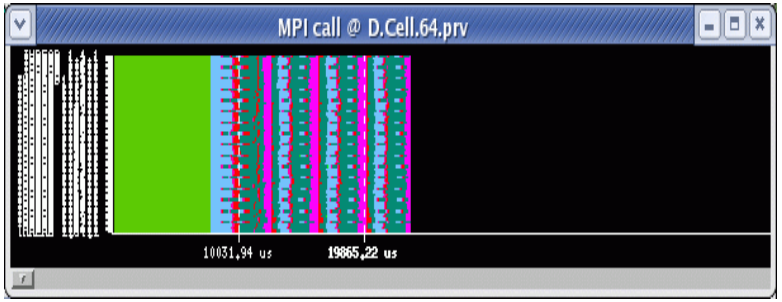
MN prediction



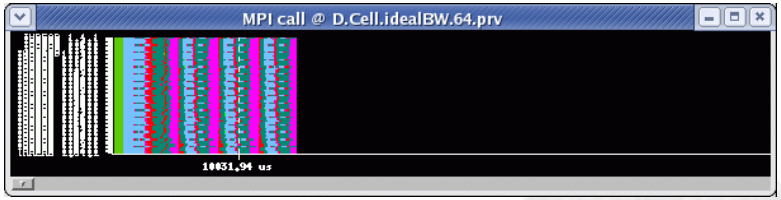
MN prediction Ideal BW



5x CPU?



5x CPU Ideal BW?



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BSC Departments

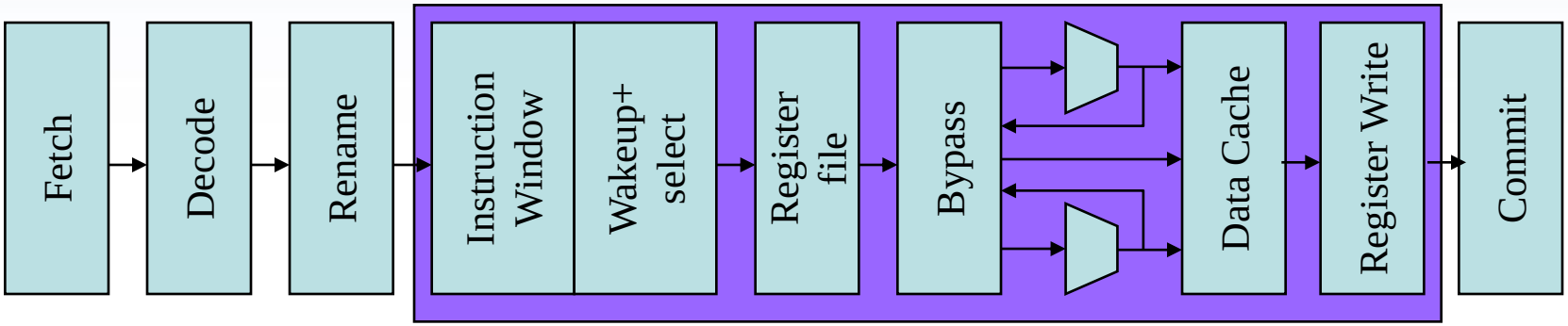
- Computer Science
  - Computer Architecture
- Life Sciences
- Earth Sciences
- Computer Applications

Computer Architecture is .....

- About the interface between what technology can provide and what the people/market demand
- At that interface we have our design point:
  - Reliability
  - Availability
  - Cost
  - Power
  - Performance

Yale Patt, University of Austin at Texas

Superscalar Processor

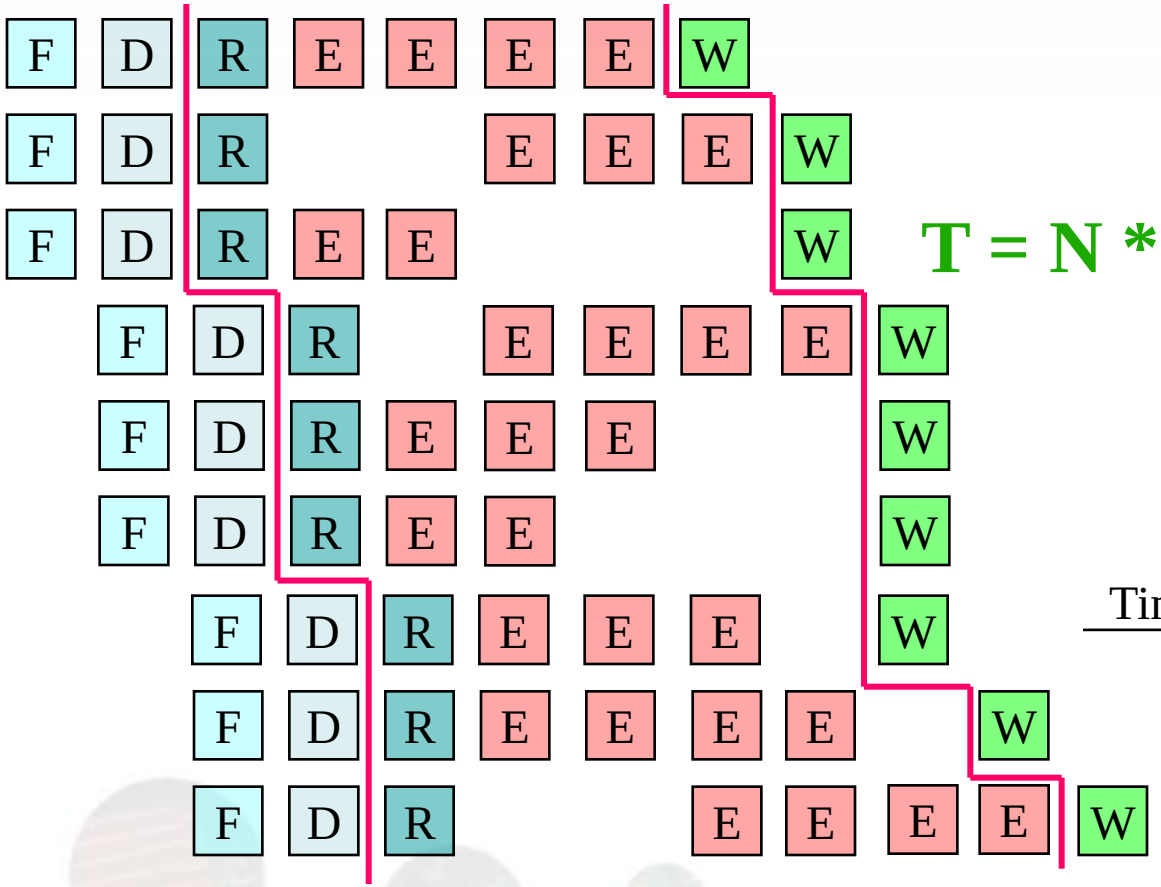


Fetch of multiple instructions every cycle.
Rename of registers to eliminate added dependencies.
Instructions wait for source operands and for functional units.
Out- of -order execution, but in order graduation.
Predict branches and speculative execution

J.E. Smith and S.Vajapeyam.¨Trace Processors…¨ IEEE Computer.Sept. 1997. pp68-74.

Superscalar Processors

- Out of order (IPC <= 3)



$$T = N * \frac{1}{IPC} * t_c$$

Future High-Performance Processors

- Future Applications: Integer, FP, Commercial and Multimedia
- Future Technology: Moore´s Law
- No New Paradigm for Computing
- Pipeline Design and Optimization:
  - Memory Hierarchy: Cache, Prefetching
  - Branch Predictors
  - Wire Delays
  - Power
  - Design
  - Verification
- ILP improvements

Future Architectures

- Superscalar
- VLIW (EPIC)
- Multithreaded
- Multiprocessors on a chip

Which is the Architecture that will dominate the future??

Advanced ILP Techniques for Superscalar Processors

- Value Prediction
- Reuse
- Helper Threads
- Trace Processor
- Control/Data Speculation
- Kilo-instruction Processors

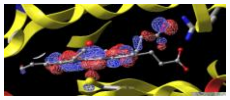
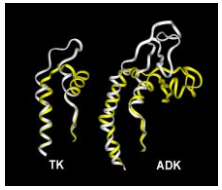
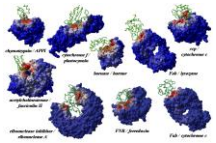
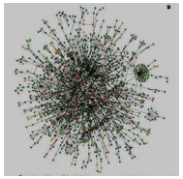
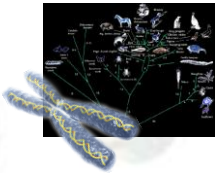
BSC Departments

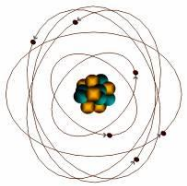
- Computer Science
  - Computer Architecture
- Life Sciences
- Earth Sciences
- Computer Applications

Life Sciences Department

Our goal is to understand Biology from a biomedical, molecular and evolutionary point of view

Covering from the atom to the earth

Group		Research Line
Victor Guallar	 	Atomic (and electronic) modeling of protein biochemistry and biophysics
Modesto Orozco	 	Molecular dynamics: understanding the motion of proteins
Juan Fernández	 	Identification of the structural bases of protein-protein interaction
Patrick Aloy	 	Protein-protein interaction networks
Josep Ll. Gelpí	 	Web services
David Torrents	 	Analysis of genomes and networks to model diseases, systems and evolution of organisms



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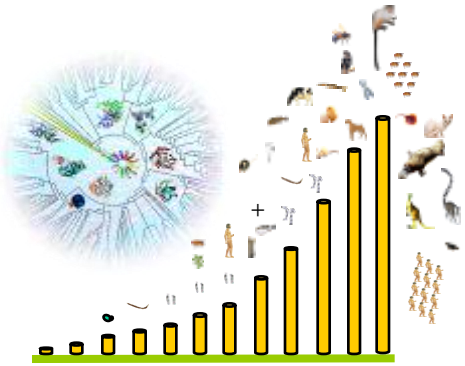
Analysis of protein and function diversity on earth

Computational genomics group (collaboration with EMBL, Heidelberg)

Identification and classification of new and known proteins from known genomes and metagenomic data



IMPACT FIELDS

Molecular Biology

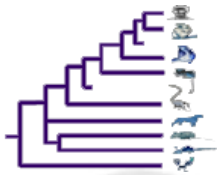
Providing new functional associations and hypothesis for basic research

BioMedicine

FP7 European project

Identification of new microorganisms, pathways, proteins and molecules. New therapeutic molecules (antibiotics, protein targets)

Evolution



Understanding the mechanisms of evolution of proteins and organisms

Ecology

Identification of new pathways and organisms for new possibilities in biodegradation.

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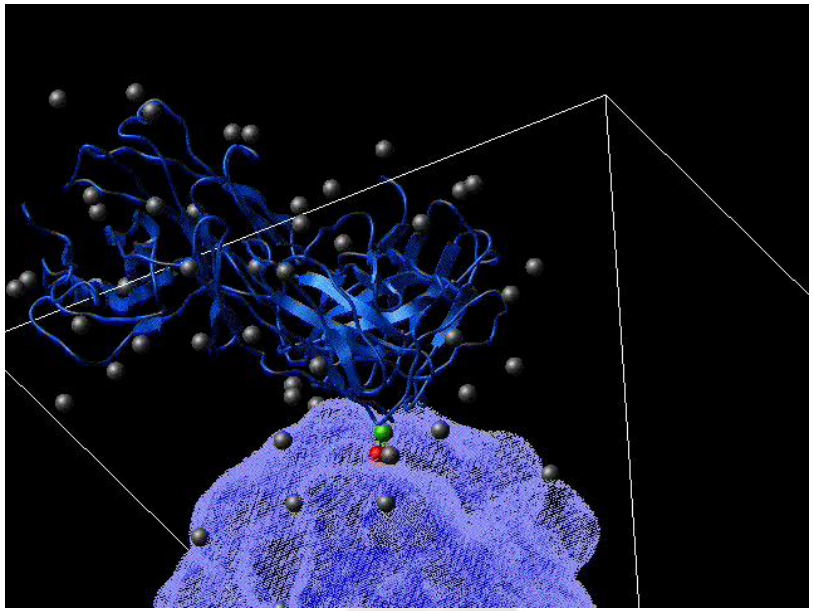
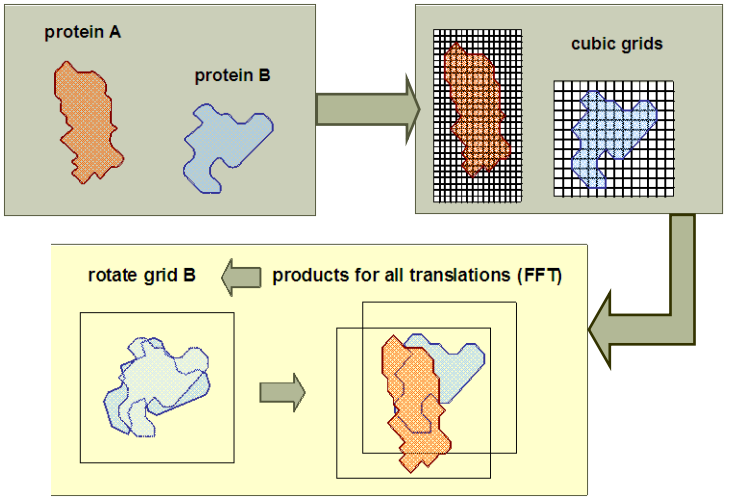
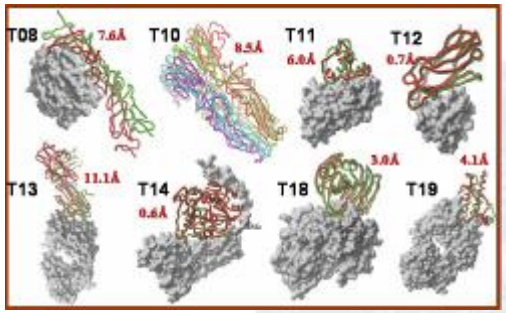
Understanding the structural basis of the interaction between proteins and with therapeutic drugs

Biomedical and molecular goals:

- Drug design
- Identification of therapeutic protein targets
- Finding functional associations between proteins
- Function prediction for new proteins
- Structure prediction of proteins







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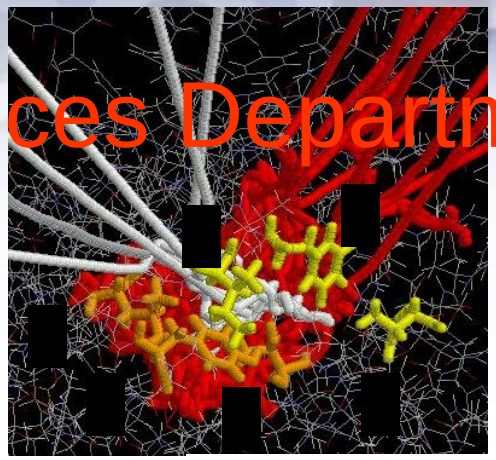
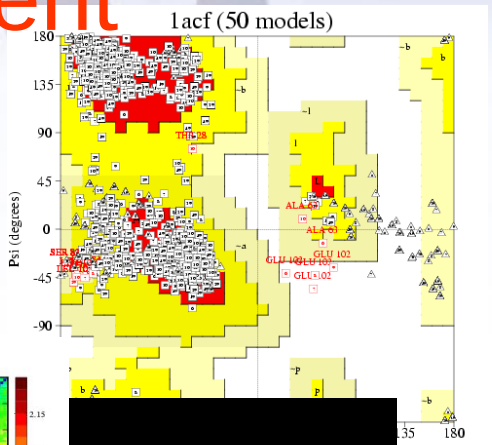
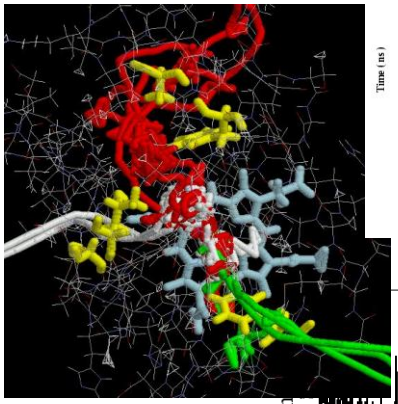
Life Sciences Department

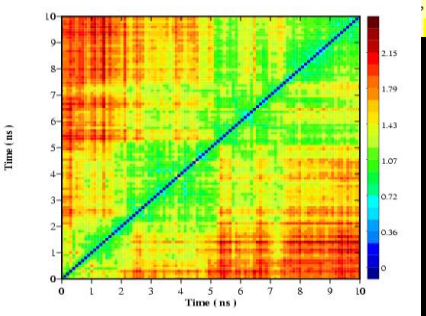
MoDEL

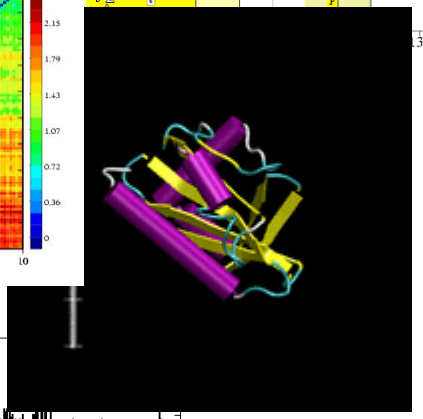
- Library of protein MD simulations
- 1400 at the moment
- >900 CPU years.
- 10 Tb of data



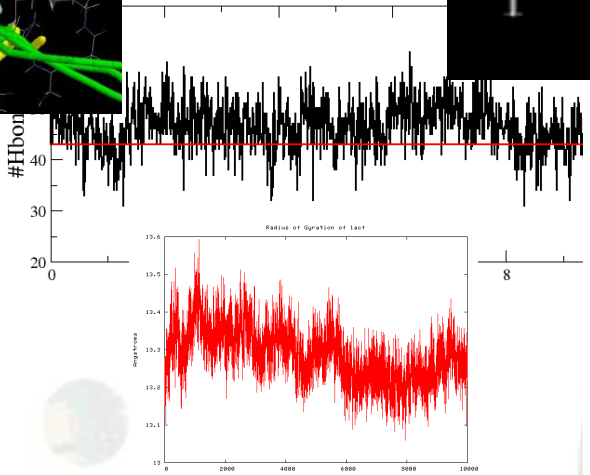


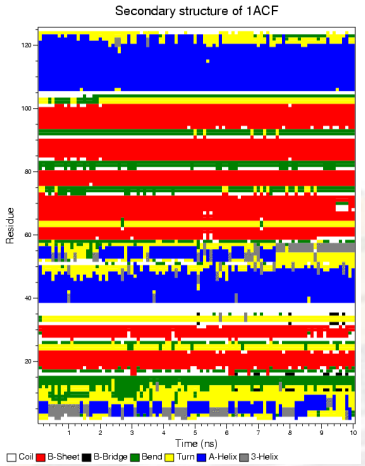


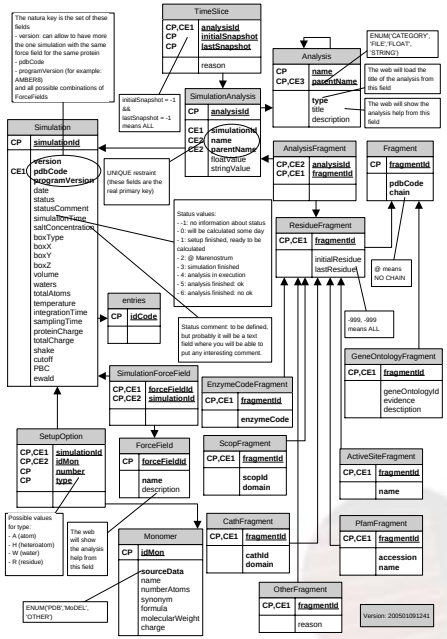




Hbonds of 1acf







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Rueda et al., PNAS 2007

BSC: Life Sciences R&D

THE ENCODE PROJECT

THE EARTH PROTEOME

- Genome all organisms + all metagenomes
- $1.4x10^6$ sequences
- 32 Tb of RAM used
- 4000 processors
- 38 CPU years
- 9 Tb of output data
- G-Superscalar
- 3.5 days job!

EMBL-EBI

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BSC Departments

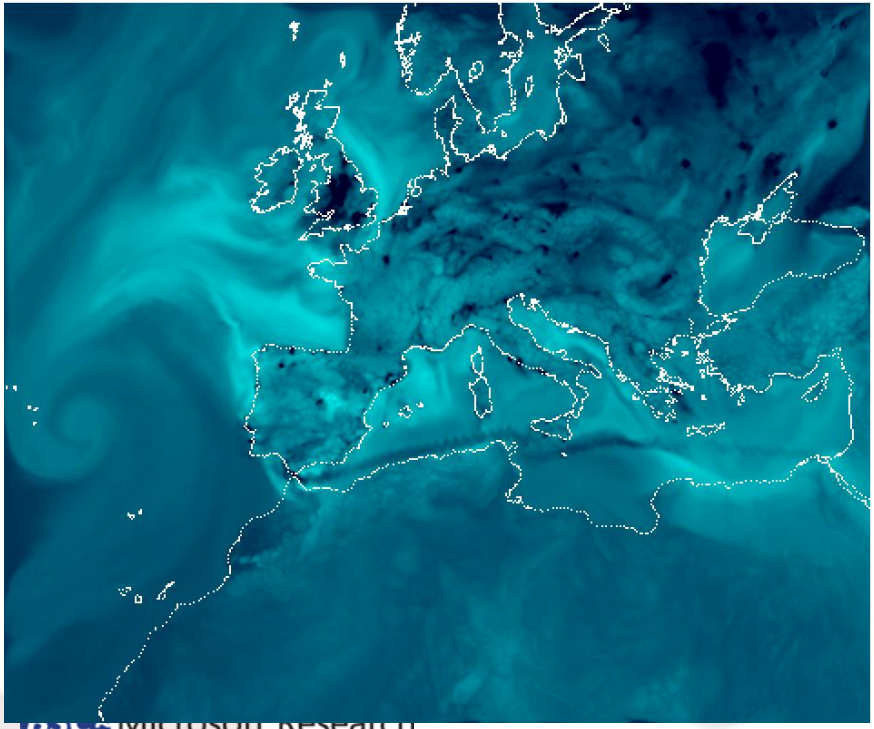
- Computer Science
  - Computer Architecture
- Life Sciences
- Earth Sciences
- Computer Applications

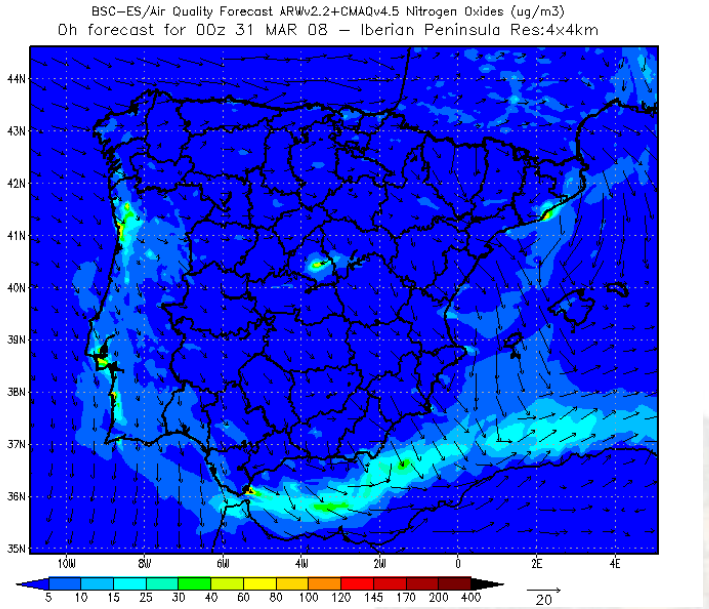
BSC Earth Sciences Department

Air Quality and Meteorological Modelling:

✓ The group offers a pan-European (12 km) and Spain (4 km) Air Quality forecasting and assessment service to end-users that takes advantage of the high spatial and temporal resolution of the air quality modelling system.
(http://www.bsc.es/caliope).

✓Development of the HERMES high-resolution emission model for Spain (1 km and 1 hr).





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Centre

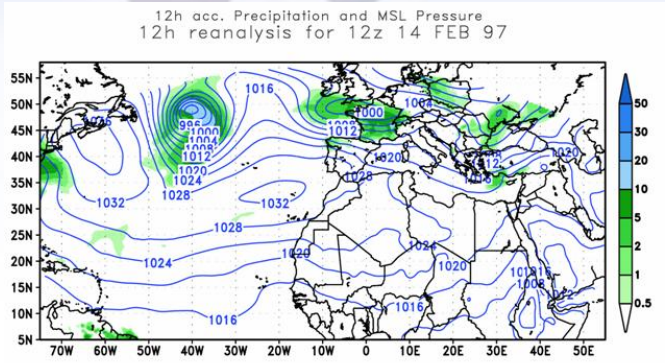
BSC Earth Sciences Department

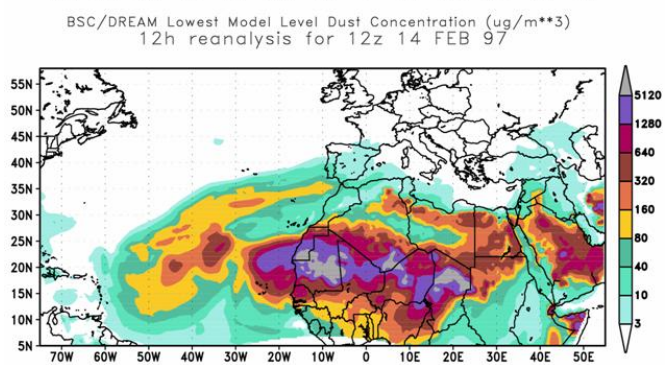
Mineral Dust:

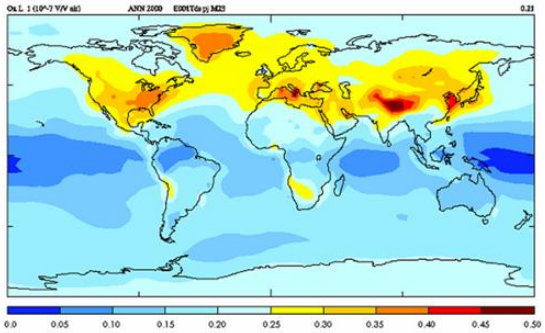
✓ Daily operational forecasts of mineral dust for the Euro-Mediterranean and the East Asia region based DREAM Model (http://www.bsc.es/projects/earthscience/DREAM).

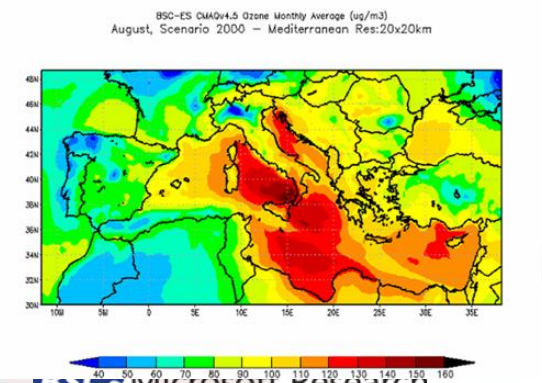
✓ Leading initiative: World Meteorological Organization initiative to create a Regional Centre for Sand and Dust Storm Warning System.

✓ Initial steps for the development of a global-to-regional / hydrostatic-non hydrostatic dust model based on the UMO.









Climate Modelling:

✓ Global Climate Modelling with NASA GISS ModelE and NCAR WACCM in MareNostrum supercomputer with a resolution of 2ºx2.5º.

✓ Implementation of a regional climate model (RCM) based on the WRF/CMAQ/DREAM system for the Mediterranean Sea and Europe (20 km resolution) in order to simulations to ascertain the regional impact of climate change in the trends of extreme events.

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Asia dust forecasting at BSC

SDS WS Operational products

http://www.bsc.es/projects/earthscience/DREAM/

Model predictions (72-h):

Horizontal distribution

- ➢ PM2.5, PM10, TSP at surface and height
- ➢ Total column mass (dust load)
- ➢ Dust aerosol optical depth
- ➢ Wet, dry, total deposition
- ➢ Visibility (soon available)
- ➢ Meteorological variables

✓ **Vertical distribution**

- ➢ Cross sections
- ➢ Fixed point/time profiles

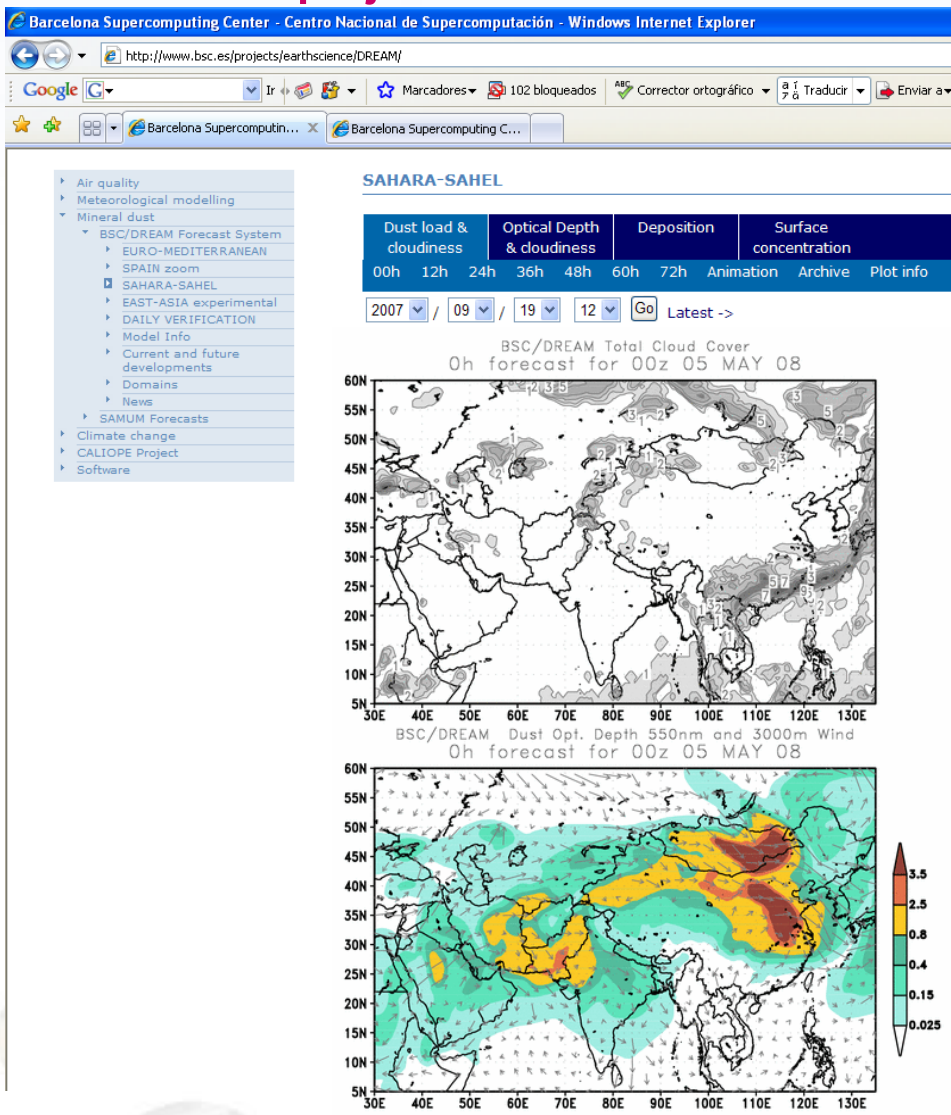
✓ **Fixed point (selected sites/cities)**

- ➢ Dustgrams
- ➢ Meteograms

Request-only basis:

✓ **Numerical data**

✓ **Climatology**



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World Meteorological Organization (WMO): Sand and Dust Storm Warning and Assessment System (SDS-WAS)

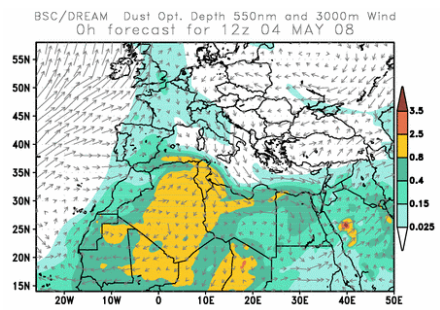
- To enhance the ability of participating countries to establish and improve systems for forecasting and warning to suppress the impact of Sand and Dust Storm

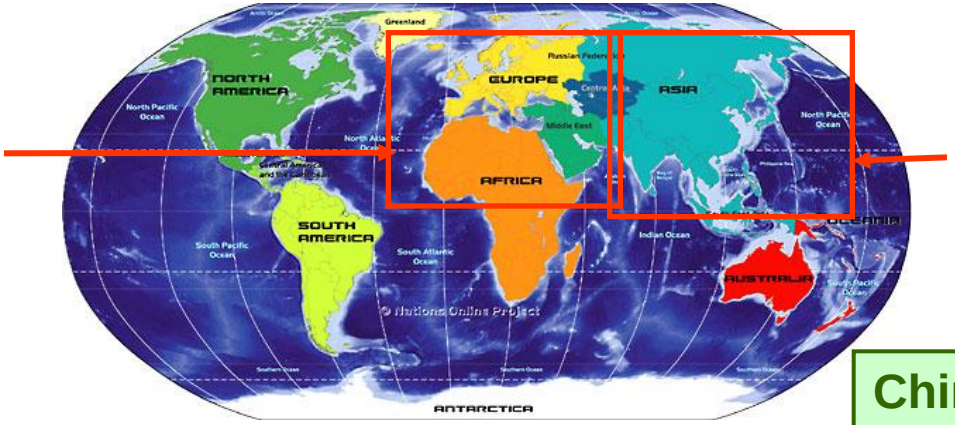
by

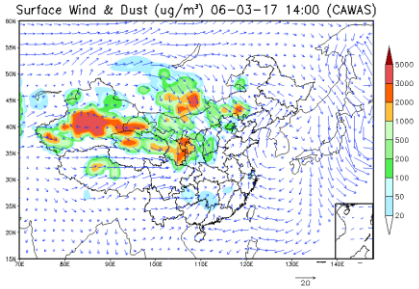
- Establishing a coordinated global network of Sand and Dust Storm forecasting centers delivering products useful to a wide range of users in understanding and reducing the impacts of SDS

North Africa, Middle East and Europe

Asia







BSC
AEMET
CSIC, Spain

China Meteorological Administration (CMA)
Xiao Ye Zhang
xiaoye@cams.cma.gov.cn

WMO REGIONAL CENTRES

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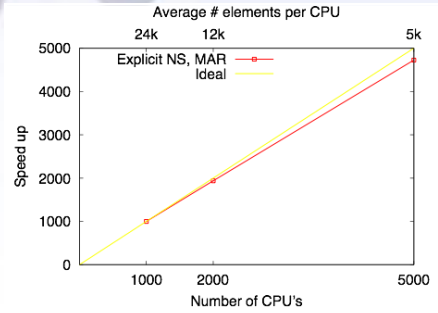
BSC Departments

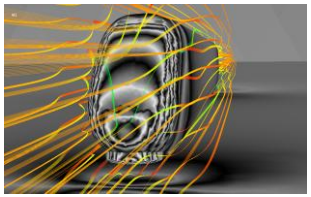
- Computer Science
  - Computer Architecture
- Life Sciences
- Earth Sciences
- Computer Applications

CASE R&D lines

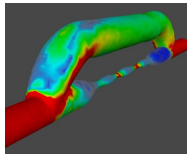
- Objective: Grand Challenge problems with quasi linear scalability
  - 10,000 processors with 95% parallel efficiency



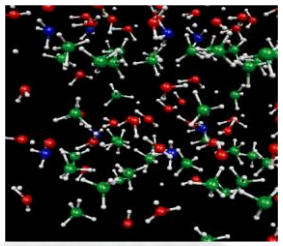
- Flow coupled problems (Aero Acoustics, Reactive flows, building energetic efficiency, …)



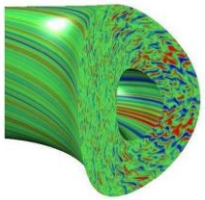
- Biomechanics (Haemodynamics, Cardiac model, Nasal airflow, …)



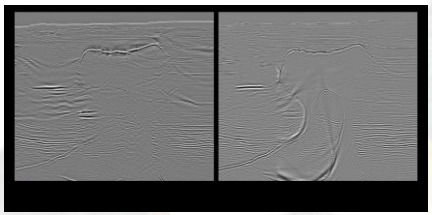
- Ab-initio Molecular dynamics and spectroscopy



- Plasma physics (Gryro-kinetic PIC codes,…)



- Seismic imaging (RTM, tomography,…)



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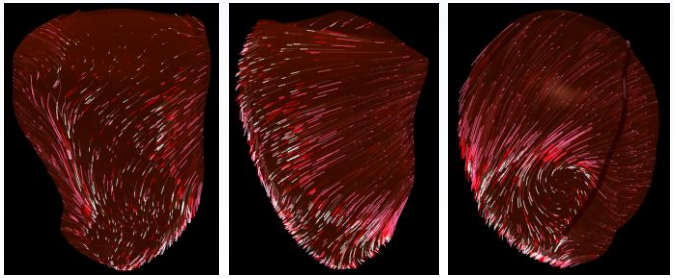
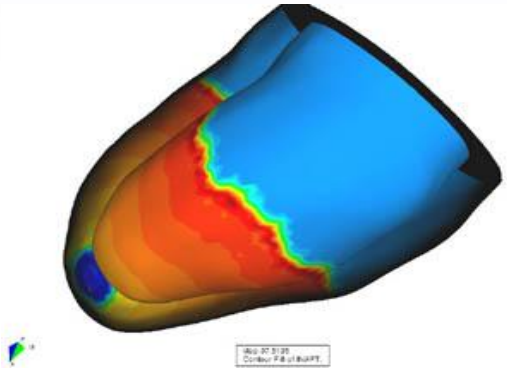
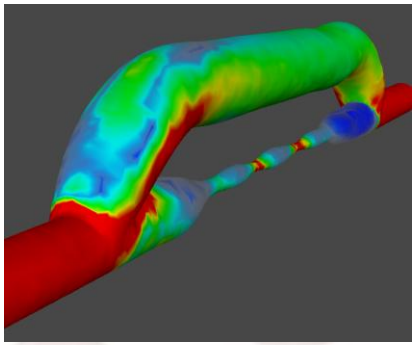
Biomechanics

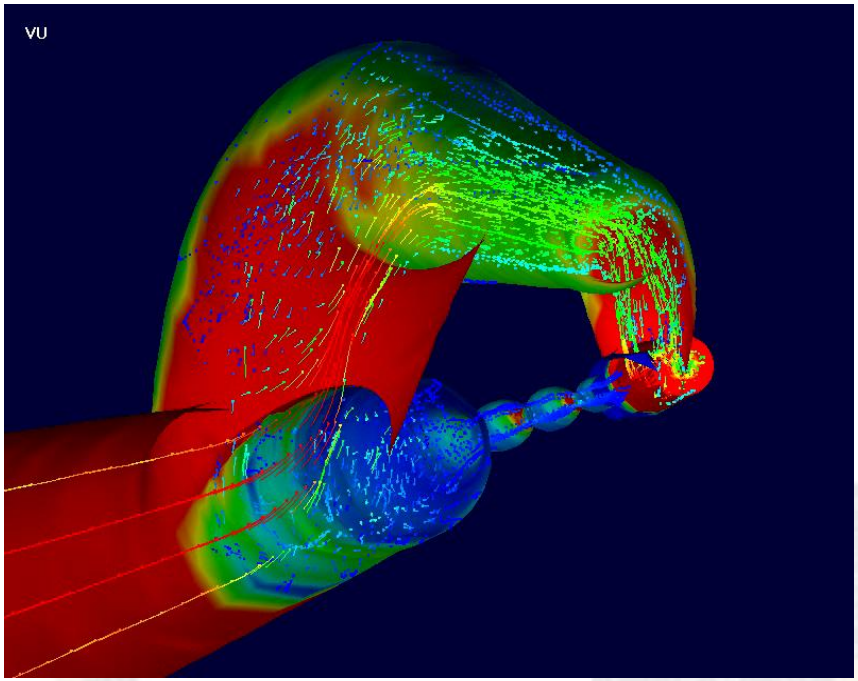
- Cardiac Simulator





- By-pass Blood flow





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CASE R&D connection with China

Invited speakers in:

AEROCHINA-2 Short Course, co-funded by Min. of Science

and Technology of China and European Commission

Topics: Complex multi-physics HPC simulations in Aerospace

Engineering

BSC talk: “HPC in Aerospace Industry for Large Scale

Supercomputers: Aerodynamics and Aeroacoustics”

Marseille, June 16-18, 2008

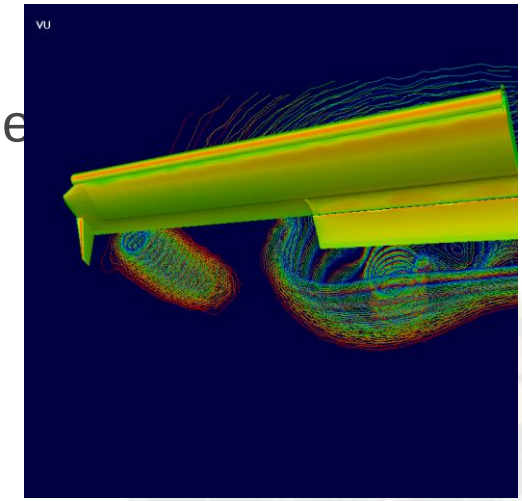
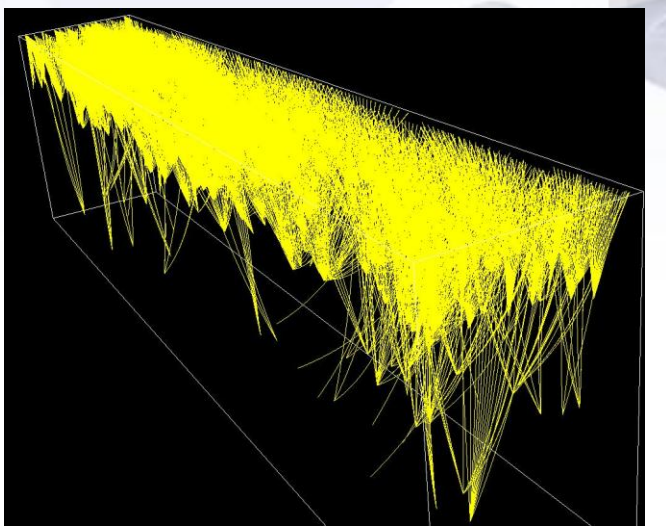
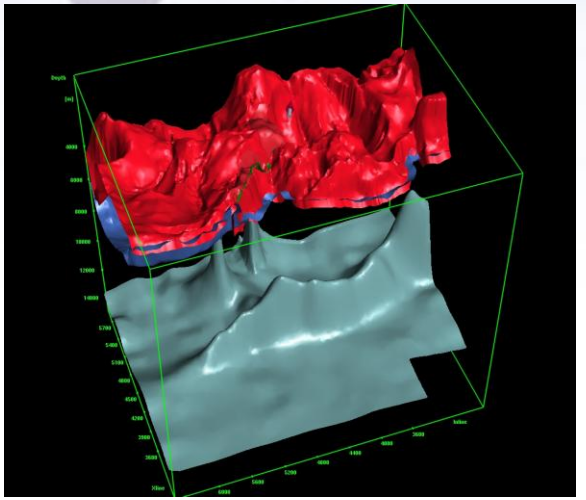


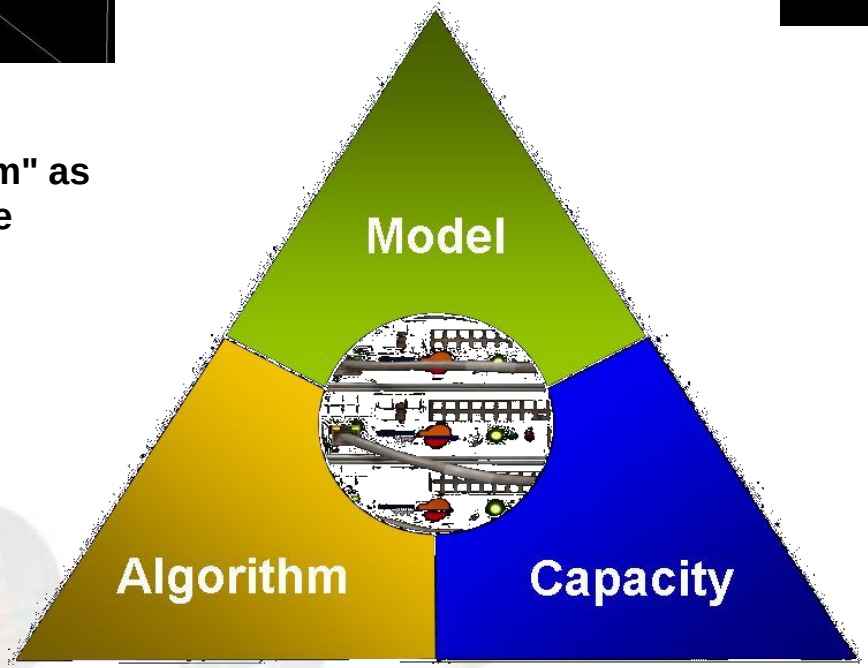
Imagen Sísmica: Proyecto Calidoscopio





REPSOL YPF

Selected by "IEEE Spectrum" as one of the 5 most-innovative technologies in 2007



3DGEO DEVELOPMENT INC.

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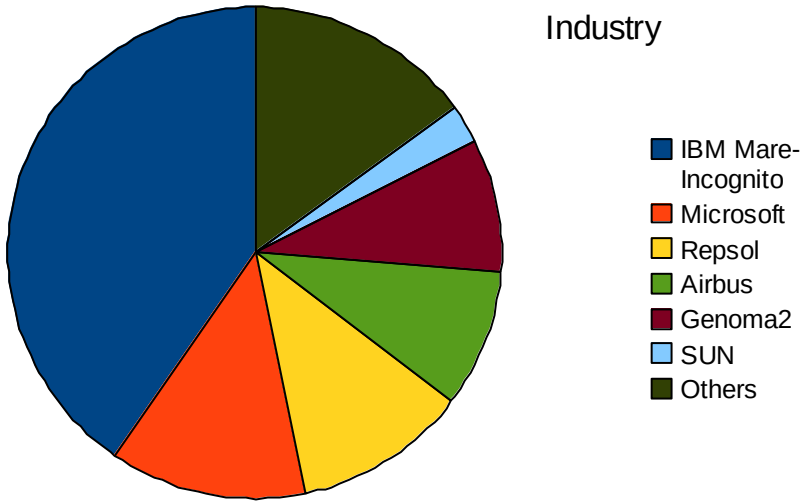
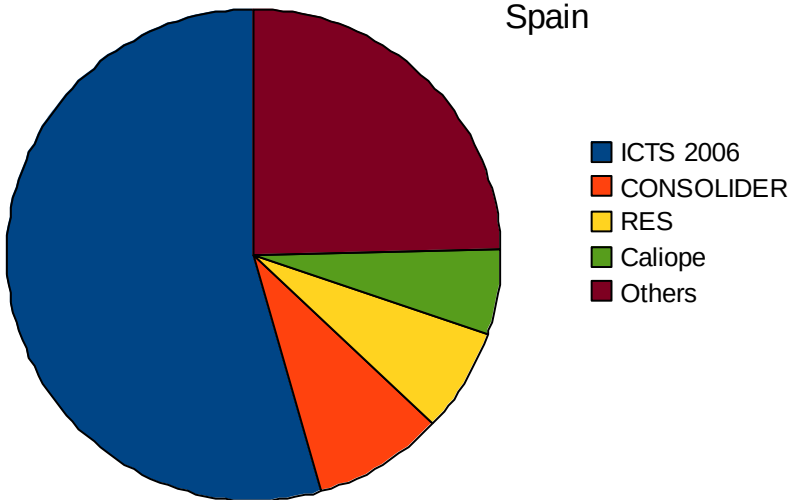
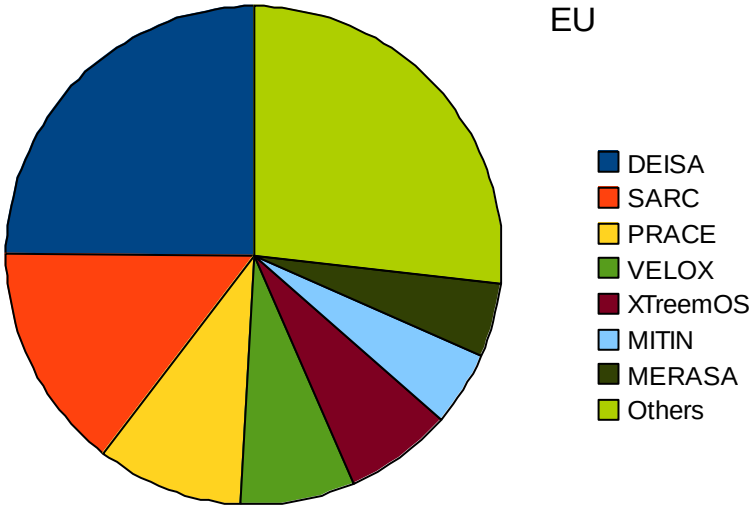
BSC General Information

BSC Projects income





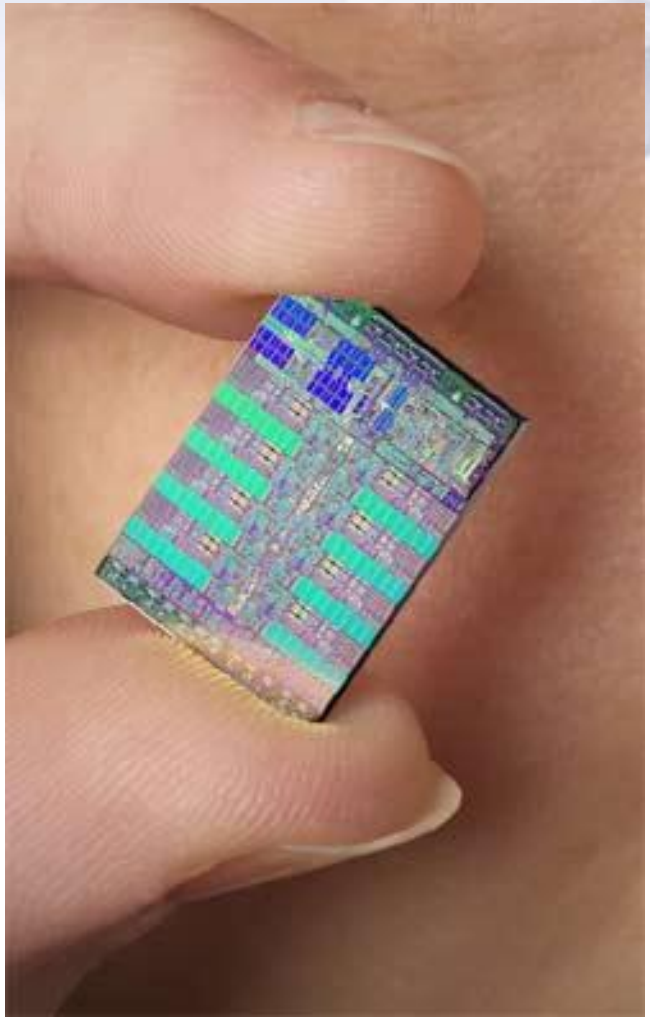


	Total income
Industry	11.368.925 €
EU	8.445.744 €
Spain	3.735.332 €

Objective

- **Design a 10+ Petaflops Supercomputer for 2010-11**
- **BSC – IBM Cooperation**
- **Spanish position with PRACE**

CELL processor



235 Mtransistors
235 mm^2

Roadrunner supercomputer
at
Los Alamos National Laboratory

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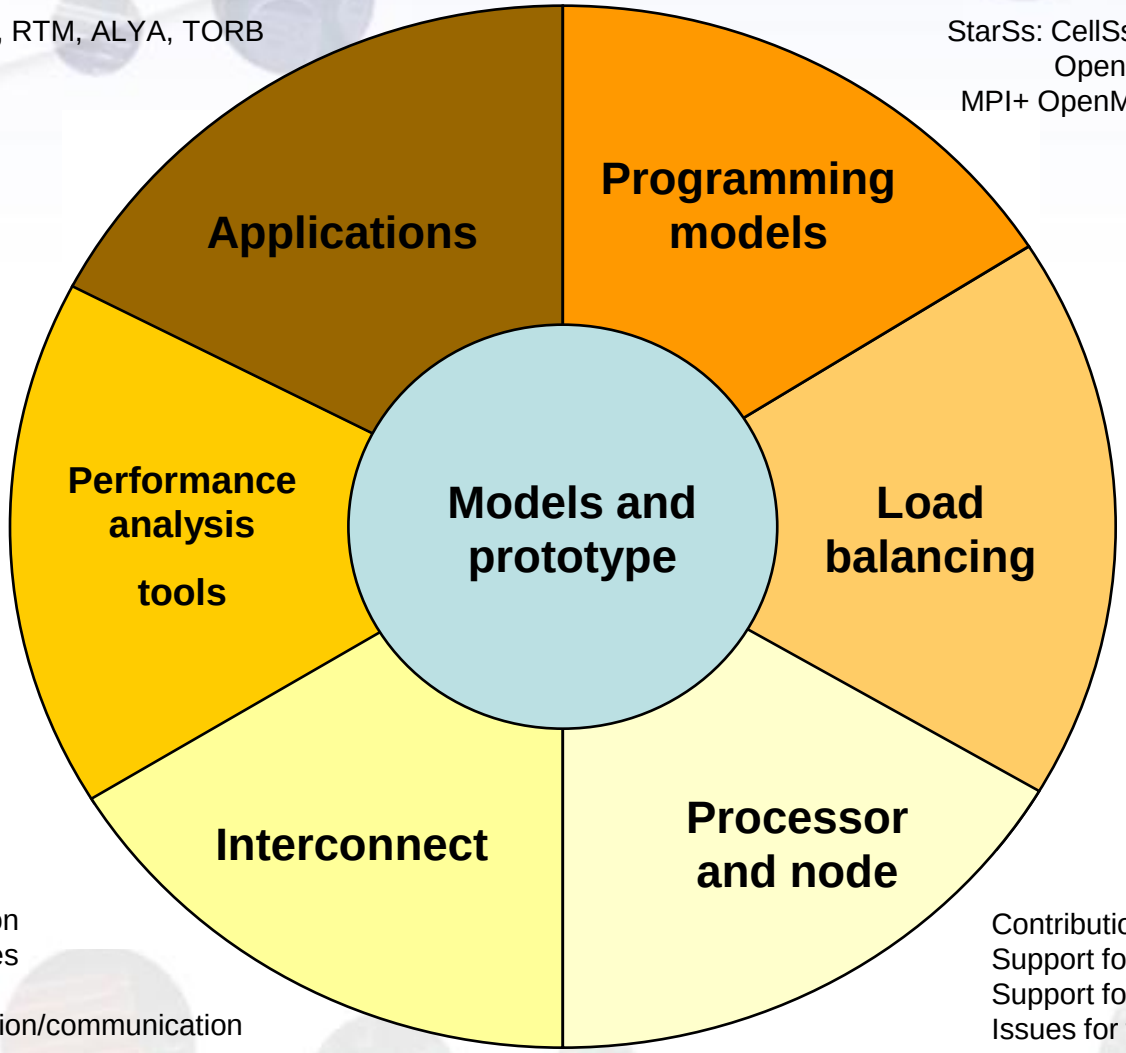
Project structure

4 relevant apps: SIESTA, RTM, ALYA, TORB
General kernels

StarSs: CellSs, SMPSs
OpenMP@Cell
MPI+ OpenMP/StarSs



Automatic analysis
Coarse/fine grain prediction
Sampling
Clustering
Integration with Peekperf

Coordinated scheduling:
Run time,
Process,
Job
Power efficiency

Contention
Collectives
Overlap
computation/communication

Contribution to new Cell design
Support for programming model
Support for load balancing
Issues for future processors

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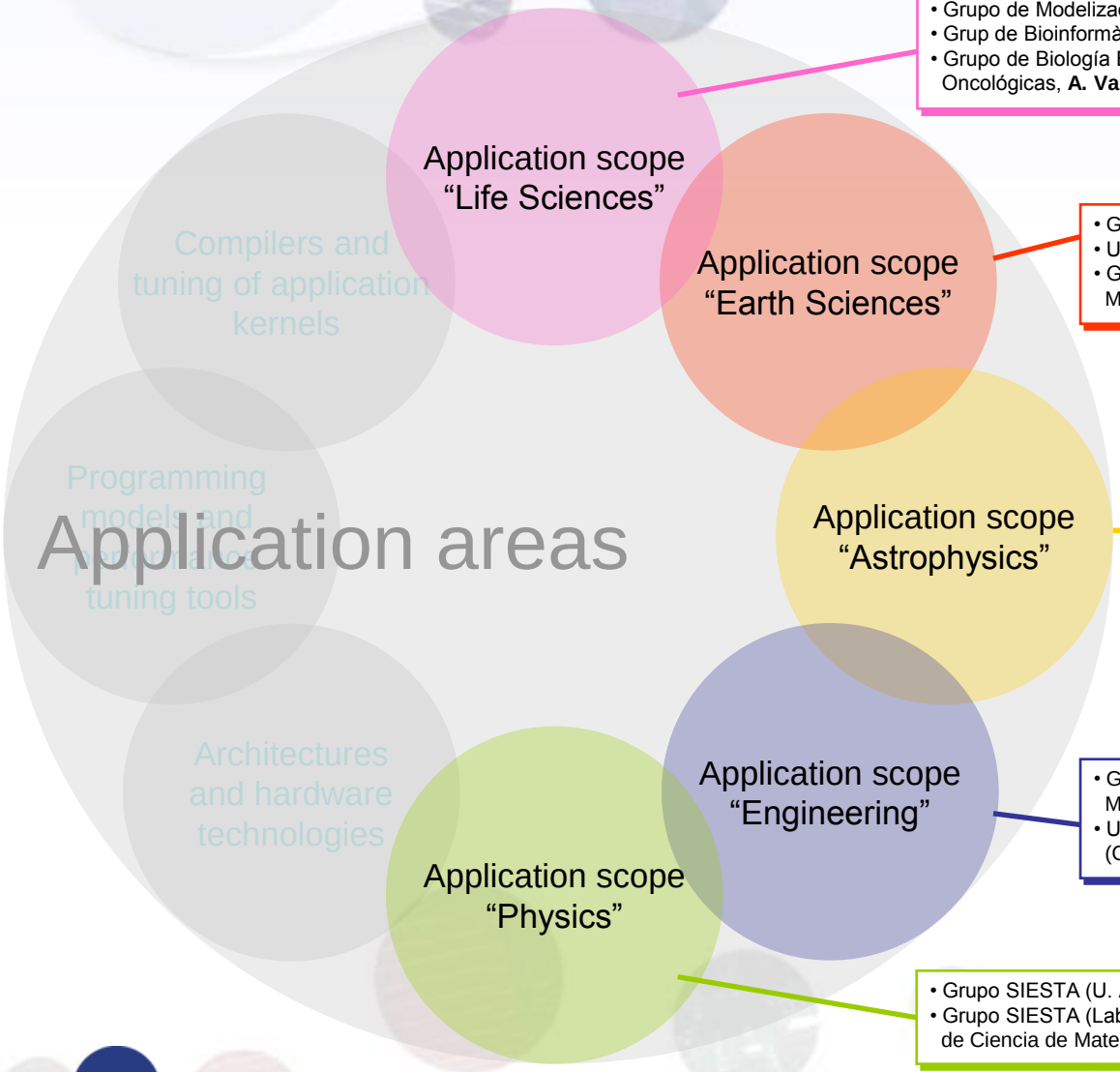
Supercomputing and e-Science: research areas and groups (1)



- Grupo de Modelización Molecular y Bioinformática (U. de Barcelona, **M. Orozco**)
- Grup de Bioinformàtica del Genoma (Centre de Regulació Genòmica, **R. Guigó**)
- Grupo de Biología Estructural Computacional (Centro Nacional de Investigaciones Oncológicas, **A. Valencia**)

- Grupo de Ciencias de la Tierra (BSC-CNS, **J. M. Baldasano**)
- Unidad de Contaminación Atmosférica (CIEMAT, **F. Martín**)
- Grupo de Diagnóstico y Modelización del Clima (U. Complutense de Madrid, **R. García-Herrera**)

- Grupo de Astrofísica Relativista y Cosmología (U. de Valencia, **J. M. Ibáñez**)
- Grupo de Simulación Numérica de Procesos Astrofísicos (Instituto de Astrofísica de Canarias, **F. Moreno**)
- Grupo GAIA de Astronomía Galáctica (U. de Barcelona, **J. Torra**)
- Grupo de Cosmología Computacional (U. Autónoma de Madrid, **G. Yepes**)

- Grupo de Mecánica de Fluidos Computacional (U. Politécnica de Madrid, **J. Jiménez Sendín**)
- Unidad de Simulación Numérica y Modelización de Procesos (CIEMAT, **M. Uhlmann**)

- Grupo SIESTA (U. Autónoma de Madrid, **J. M. Soler**)
- Grupo SIESTA (Laboratorio de Estructura Electrónica de los Materiales del Instituto de Ciencia de Materiales de Barcelona ICMAB-CSIC, **P. J. Ordejón**)

Supercomputing and e-Science: research areas and groups (2)

- Departamento de Tecnologías de la Información (BSC-CNS, **M. Valero**)
- Grupo Computación de Altas Prestaciones (U. Politècnica de Catalunya, **J. M. Llabería**)
- Grupo de Arquitectura y Tecnología de Sistemas Informáticos (U. Complutense de Madrid, **F. Tirado**)
- Grupo de Arquitectura de Computadores (U. de Malaga, **E. López Zapata**)

Compilers and tuning of application kernels

- Departamento de Tecnologías de la Información (BSC-CNS, **M. Valero**)
- Grupo Computación de Altas Prestaciones (U. Politècnica de Catalunya, **J. M. Llabería**)
- Parallel Processing and Distributed Systems group (U. Autónoma de Barcelona, **A. Ripoll**)

Programming models and performance tuning tools

- Departamento de Tecnologías de la Información (BSC-CNS, **M. Valero**)
- Grupo Computación de Altas Prestaciones (U. Politècnica de Catalunya, **J. M. Llabería**)
- Grupo de Arquitectura de Computadores (U de Zaragoza, **V. Viñals**)
- Grupo de Arquitectura y Tecnología de Sistemas Informáticos (U. Complutense de Madrid, **F. Tirado**)
- Grupo de Arquitectura y Tecnología de Computadores (U. de Cantabria, J. R. **Beivide**)
- Grupo de Arquitectura de Computadores (U. de Malaga, **E. López Zapata**)
- Grupo de Arquitectura de Computadores (U. de Las Palmas de Gran Canaria, Instituto Universitario de Ciencias y Tecnologías Cibernéticas, **E. Fernández**)

Architectures and hardware technologies

Application scope "Life Sciences"

Application scope "Earth Sciences"

Application scope "Astrophysics"

Application scope "Engineering"

Application scope "Physics"

Basic research in supercomputing

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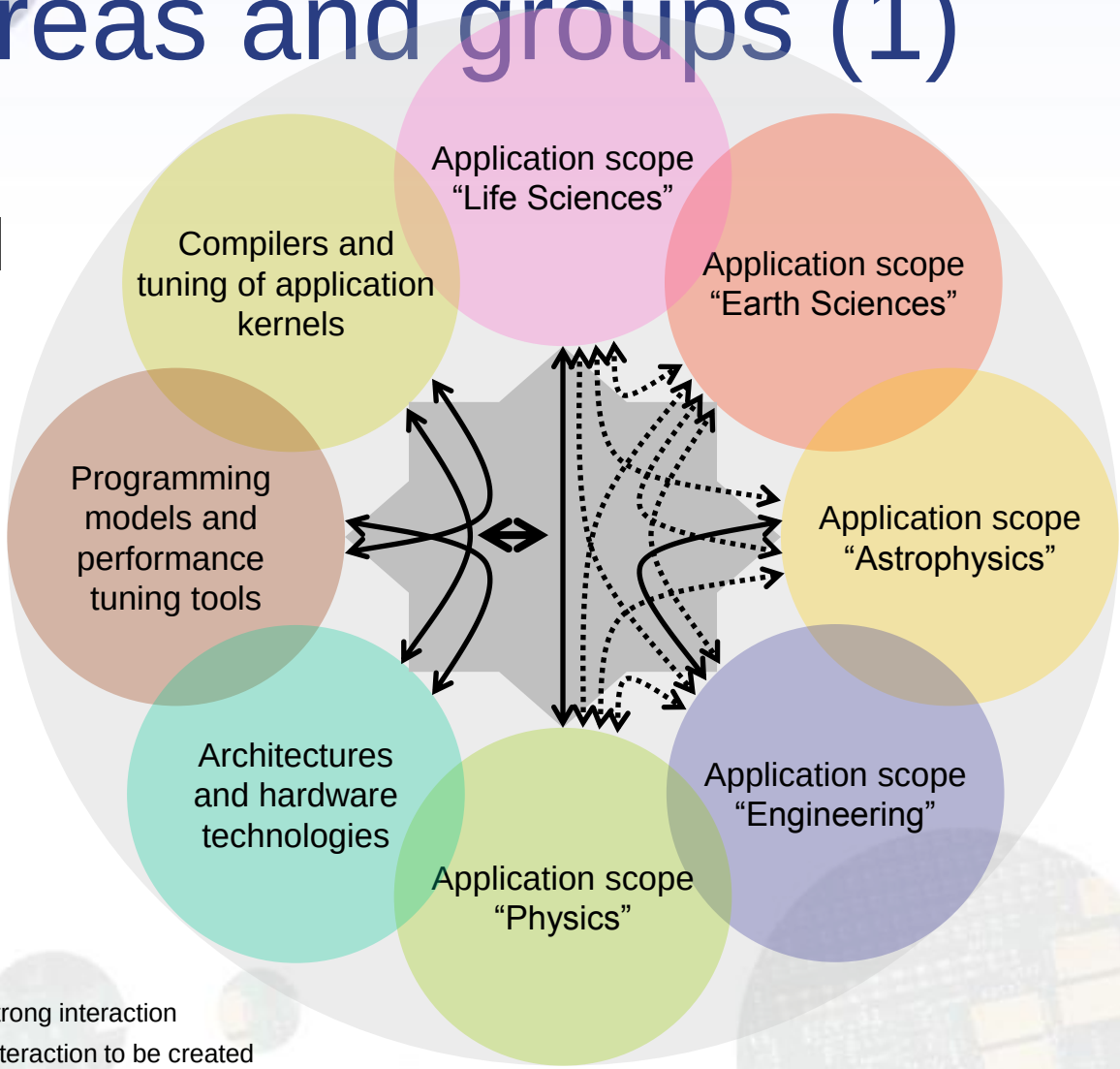
Supercomputing and e-Science: research areas and groups (1)

- Consolider program proposal
- 22 groups
- 119 senior researchers
- Work structured around:
  - 10 workpackages
  - 29 tasks
  - 3 grand challenges



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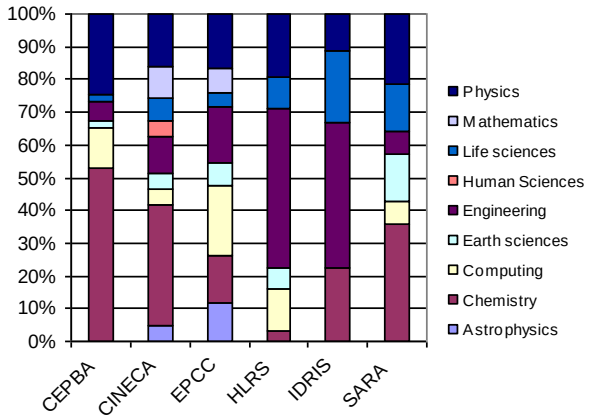
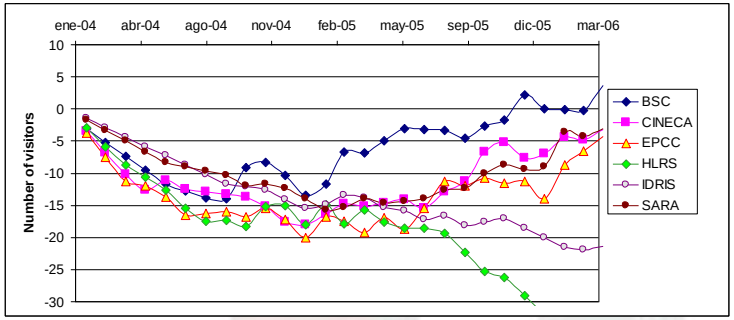
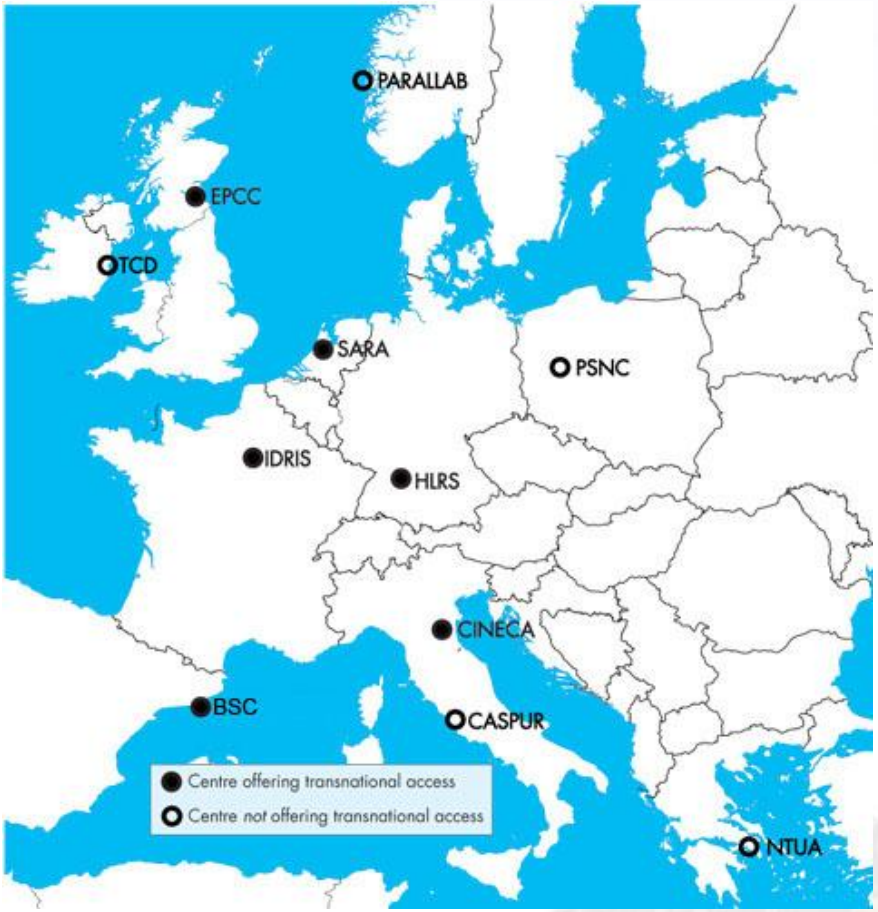
BSC in Europe - DEISA

Mobility – HPC - Europa

HPC-Europa
Pan-European Research Infrastructure on High Performance Computing







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Outline

- Barcelona Supercomputing Center
- BSC – Microsoft Research Centre

The motivation

- Top-down architecture, include:
  - Application
  - Debugging
  - Programming models
  - Programming languages
  - Compilers
  - Operating Systems
  - Runtime environment
- As design drivers

Microsoft- BSC Project: A quick snapshot

- Project started in April 2006
- Two-year initial duration
- Initial topic:Transactional Memory
- BSC – Microsoft Research Centre inaugurated January 2008

BSC Microsoft Research Centre

BSC Contributors

Mateo Valero	Professor	Spain	Part-time
Eduard Ayguade	Professor	Spain	Part-time
Adrian Cristal	Doctor	Argentina	Full-time
Osman Unsal	Doctor	Turkey	Full-time
Alex Pajuelo	Doctpr	Spain	Part-time
Xavier Verdu	Doctor	Spain	Part-time
Enrique Vallejo	PhD Student	Spain	Part-time
Srdjan Stipic	PhD Student	Serbia	Full-time
Ferad Zyulkyarov	PhD Student	Bulgaria	Full-time
Sasa Tomic	PhD Student	Serbia	Full-time
Nehir Sonmez	PhD Student	Turkey	Full-time
Cristian Perfumo	PhD Student	Argentina	Full-time
Sutirtha Sanyal	PhD Student	India	Full-time

Vladimir Gajinov	PhD Student	Serbia	Full-time
Gokcen Kestor	PhD Student	Turkey	Full-Time
Chinmay Kulkarni	Undergraduate	India	Intern
Azam Seyedi	PhD Student	Iran	Full-Time
Nikola Markovic	PhD Student	Serbia	Full-Time
Gulay Yalcin	PhD Student	Turkey	Full-Time
Vesna Smiljovic	PhD Student	Serbia	Full-Time
Nebosja Miletic	PhD Student	Serbia	Full-Time
Oriol Arcas	M.S. Student	Spain	Intern
Adria Armejach	M.S. Student	Spain	Intern
Otto Pflucker	M.S. Student	Spain	Intern
Vasilis Karakostas	M.S. Student	Greece	Intern
Jasmina Tomic	Webmaster	Serbia	Part-time

Microsoft Contributors

Technical

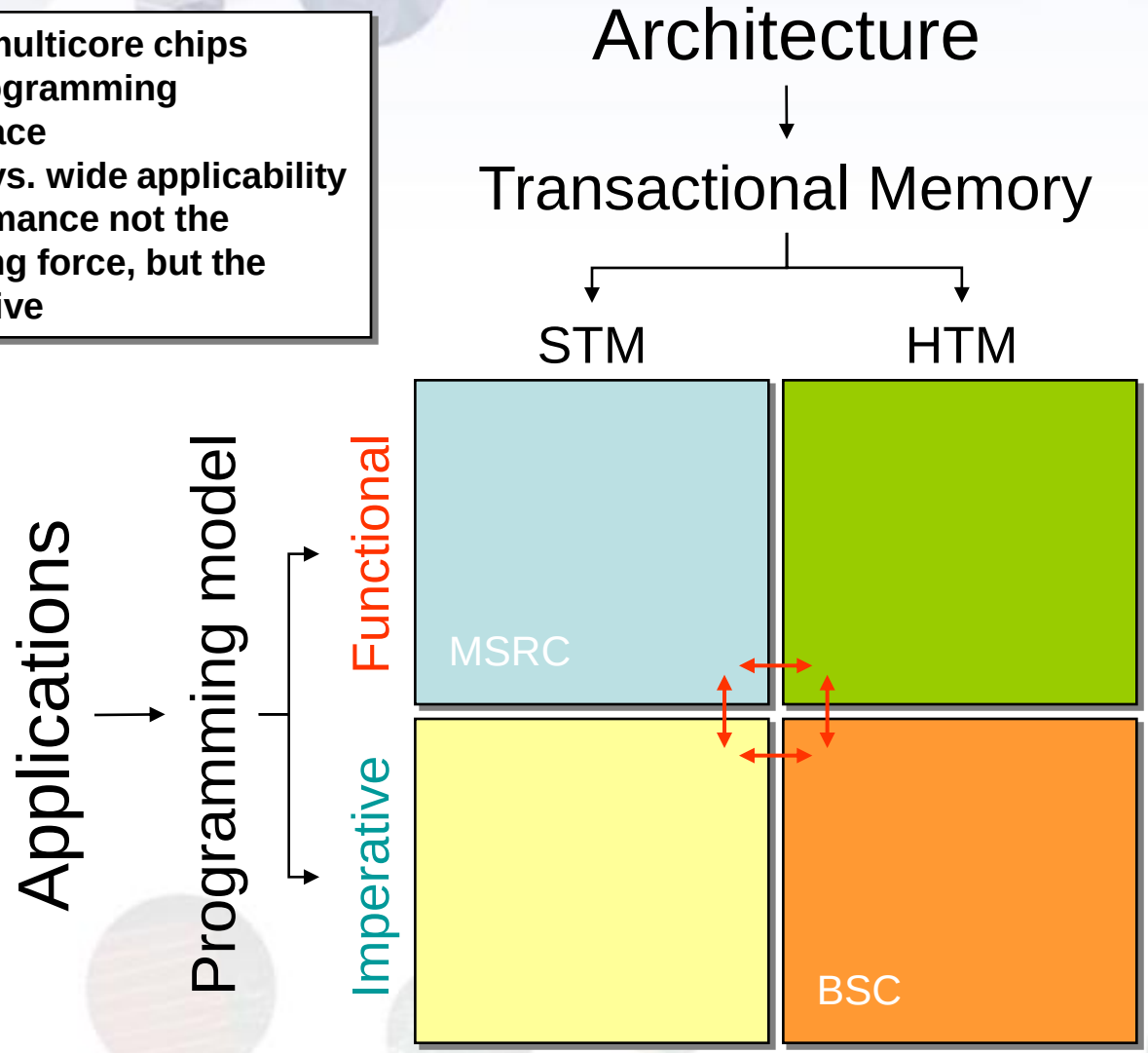
Tim Harris
Satnam Singh
Doug Burger

Management (Executive and Advisory Board)

Fabrizio Gagliardi
Andrew Herbert
Tony Hey
Avi Mendelson
Daniel Reed

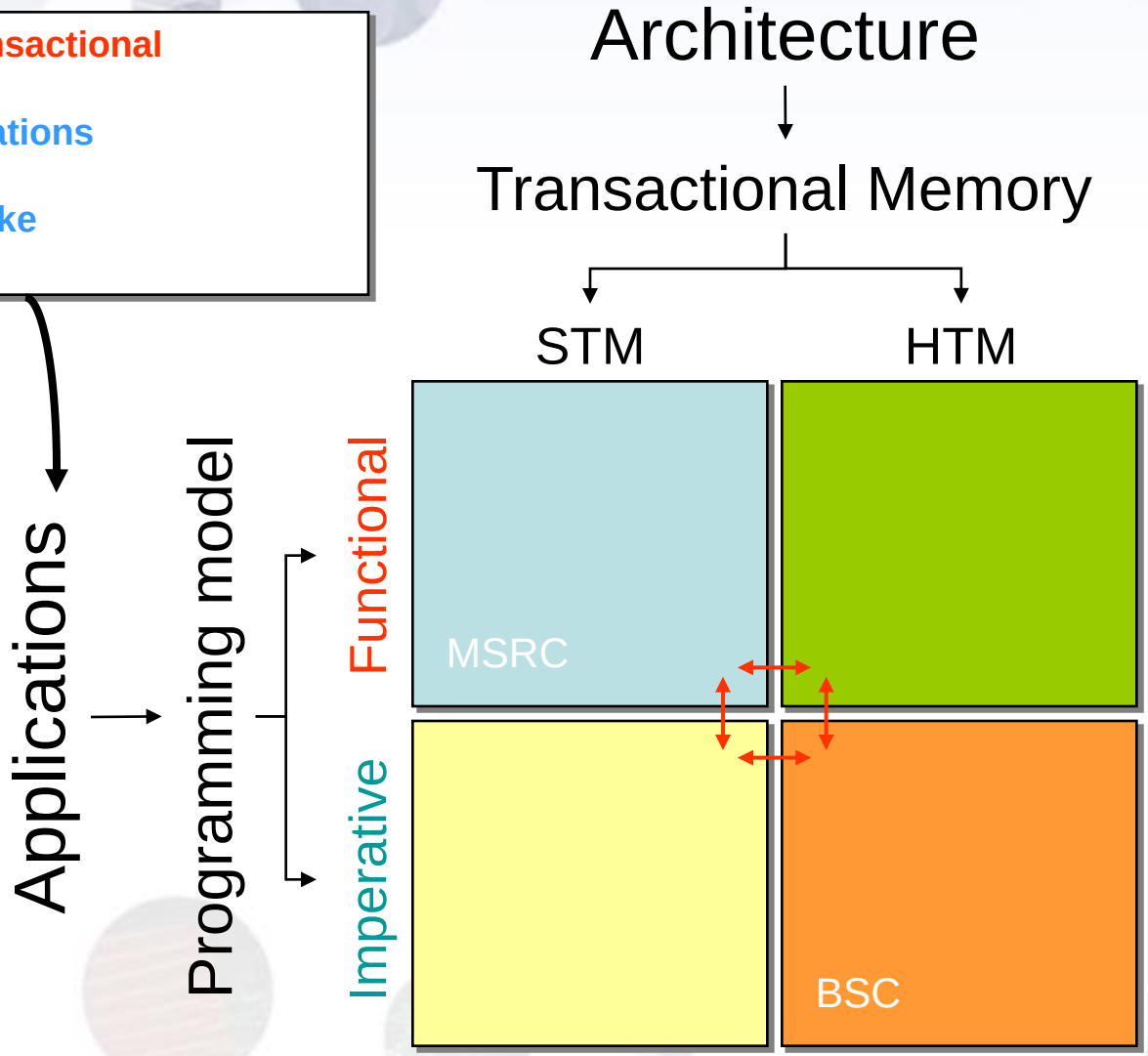
Transactional Memory

- **Advent of multicore chips**
- **Parallel programming commonplace**
- **Simplicity vs. wide applicability**
- **Full performance not the initial driving force, but the final objective**



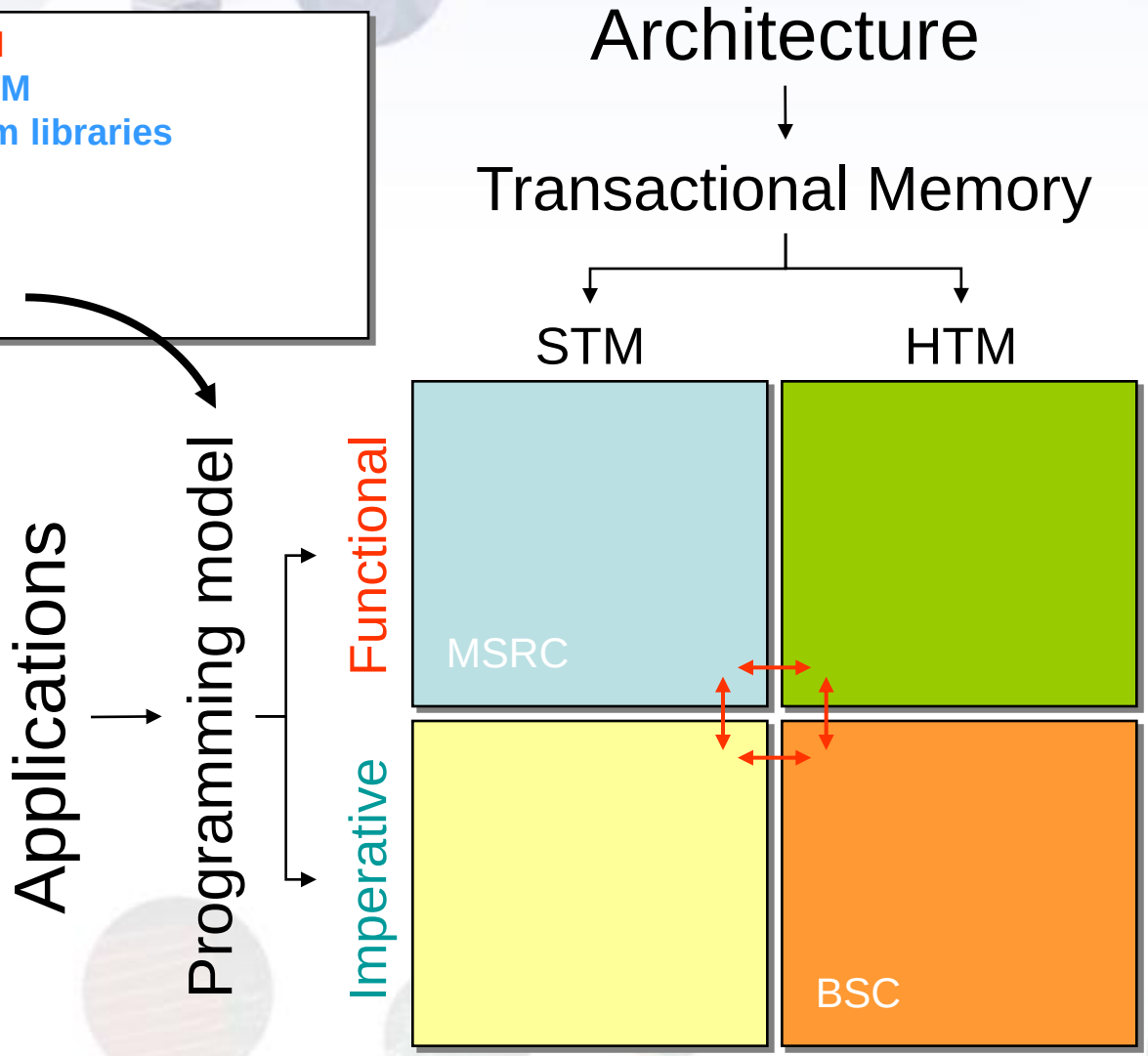
Research onTM

- **Haskell Transactional Benchmark**
- **RMS applications**
- **Quake-TM**
- **Atomic-Quake**
- **Wormbench**



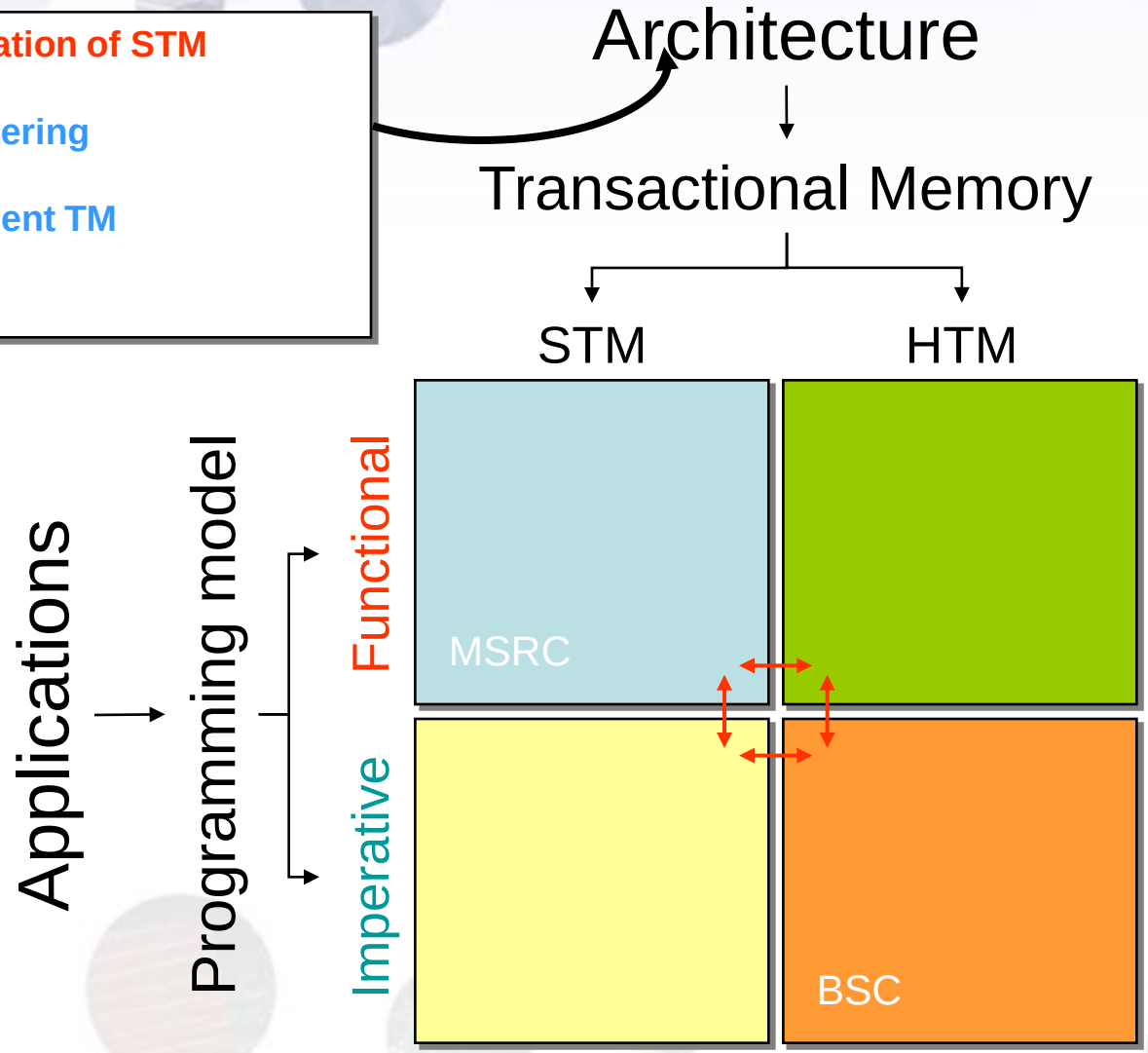
Research on TM

- **Haskell STM**
- **OpenMP + TM**
- **TM in system libraries**



Research on TM

- **HW acceleration of STM**
- **Simulators**
- **Dynamic filtering**
- **Eazy HTM**
- **Power-efficient TM**



Major focus on TM applications

- Haskell STM benchmark, RMS-TM, Wormbench, QuakeTM, Atomic Quake
- Requested ahead of time by Intel, SUN, …
- Released publicly through www.bscmsrc.eu

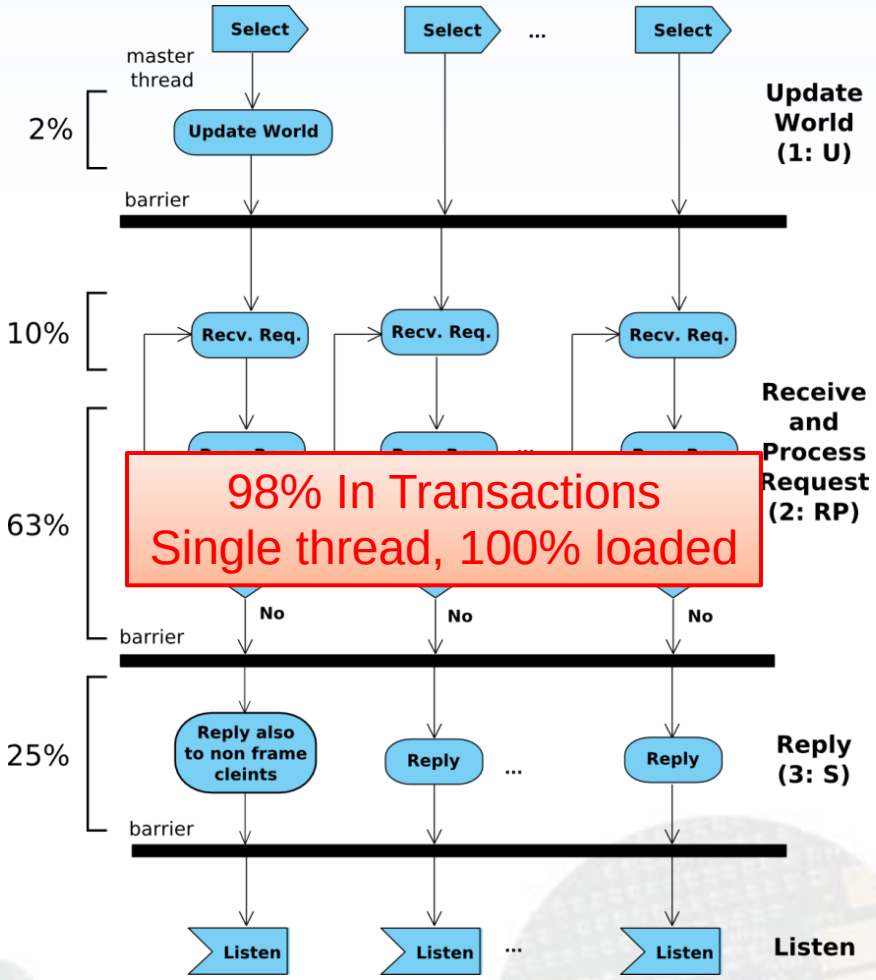
Quake

- Interactive first-person shooter game
- Very popular among gamers
- Challenge for multi-core processors

- Two versions:
  - Atomic Quake
  - Quake TM

Atomic Quake – General Overview

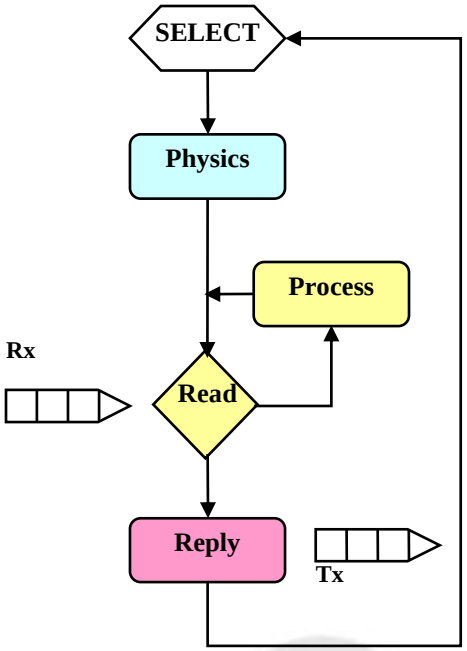
- 10 man months
- 27,400 Lines of C code
- 56 files
- 63 atomic blocks
- Irregular parallelism
  - Requests are dispatched to their handler functions.



Quake-TM: The Server

- The main server task - computing a new frame

Frame execution diagram



We concentrate on the request processing stage

Execution breakdown

Stage	Time [%]
Request Processing	87.8
Reply	3.1
Physics Update	2.1
Measuring and Info	5.3
Other	1.7

Sequential server execution with 8 connected clients.

Quake-TM Parallelization

- Each of three main frame phases can be parallelized separately.
  - No intersection between parallel regions
  - We parallelize only request processing stage
- OpenMP to start parallel execution.
- Transactions for synchronization.
- Macros to start transactions.
  - Support for various kinds of transactional systems.

Results: TM and OpenMP

- BSC-Microsoft led the first proposal to integrate TM with OpenMP; the industrial standard for writing shared-memory parallel programs
- Prototype uses in-house tools: Mercurium (S2S OpenMP)

#pragma omp task transaction [exclude(list)|only(list)] structured-block

- Suitable for the upcoming updates to the OpenMP standard which includes tasking
- Simplifies writing code with tasks and critical sections

- Cooperating with other players in the field
- On-track to define a unified OpenMP-TM standard
- Participating on the appropriate forums (GCC, OpenMP) to push for industry adoption

Haskell STM

- TM a first-class language for Haskell for a long time
  - Many STM applications developed

- UnreadTVar: delisting a variable from the readset
- Limits of STM
- AB-based application profiling
- Dynamic switching between pessimistic and optimistic concurrency

Selected Publications on TM

V. Gajinov, F. Zyulkyarov, A. Cristal, O. Unsal, T. Harris, M. Valero, “QuakeTM: Parallelizing a Complex Serial Application Using Transactional Memory”, 23rd International Conference on Supercomputing (ICS 2009), June 2009.

N. Sonmez, A. Cristal, T. Harris, O. Unsal, M. Valero, “Taking the heat off transactions: dynamic selection of pessimistic concurrency control”, 23th International Parallel and Distributed Systems Symposium, (IPDPS 2009), May 2009,

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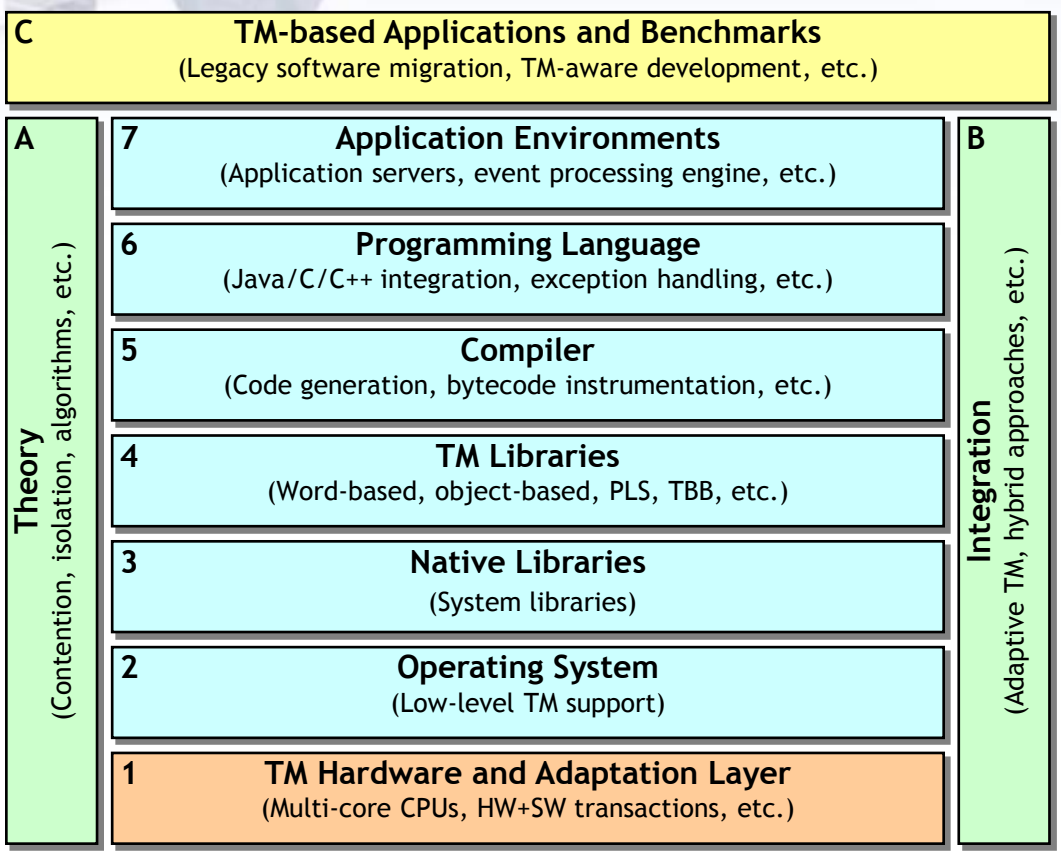
FP7 TM-Project VELOX

- Goal: Unified TM system stack, Duration: 2008-2011, Budget: 5M Euros
- BSC involvement initiated through BSC-MSR Centre
- Project participants:
  - BSC
  - EPFL
  - University of Neuchatel
  - Technical University of Dresden
  - Tel Aviv University
  - Chalmers Institute of Technology
  - AMD
  - Red-Hat
  - VirtualLogix
- Project observers:
  - Microsoft
  - Intel
  - SUN

Empowering TM across the system stack



http://www.velox-project.eu/

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Barcelona Multi-core Workshop BMW June 2008

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Thanks!

http://www.bscmsrc.eu