Earth Science Research at the Barcelona Supercomputing Center

Dr. José M. Baldasano
jose.baldasano@bsc.es

Barcelona Supercomputing Center-Centro Nacional de Supercomputación (BSC-CNS)
Earth Sciences Department, Barcelona, Spain

29th HPC User Forum – September 8 to 10, 2008 – In Tucson, Arizona
A unique place .............
MareNostrum

- 10240 IBM Power PC 970MP processors at 2.3 GHz (2560 JS21 blades).
- 20 TB Main Memory.
- 94,219 Tflops (peak performance).
- 280 + 90 TB disk.
- Interconnection networks:
  - Myrinet
  - Gigabit
- Linux cluster (SuSe).
- Diskless network support.
MareNostrum’s evolution:

<table>
<thead>
<tr>
<th>List</th>
<th>World Position</th>
<th>Europe Position</th>
</tr>
</thead>
<tbody>
<tr>
<td>November 2004</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>June 2005</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>November 2005</td>
<td>8</td>
<td>1</td>
</tr>
<tr>
<td>June 2006</td>
<td>11</td>
<td>3</td>
</tr>
<tr>
<td>November 2006</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>June 2007</td>
<td>9</td>
<td>1</td>
</tr>
<tr>
<td>November 2007</td>
<td>13</td>
<td>3</td>
</tr>
</tbody>
</table>
Spanish Supercomputing Network (RES)

**MareNostrum**
- Processors: 10240 PowerPC 970 2.3 GHz
- Memory: 20 Tbytes
- Disc: 280 + 90 Tbytes
- Networks: Myrinet, Gigabit, 10/100
- Operating System: Linux

**CeSViMa**
- Processors: 2408 PowerPC 970 2.2 GHz
- Memory: 4.7 Tbytes
- Disc: 63 + 47 Tbytes
- Networks: Myrinet, Gigabit, 10/100
- Operating System: Linux

**IAC, UMA, UNICAN, UNIZAR, UV**
- Processors: 512 PowerPC 970 2.2 GHz
- Memory: 1 Tbyte
- Disc: 14 + 10 Tbytes
- Networks: Myrinet, Gigabit, 10/100
- Operating System: Linux
The BSC-IBM MareIncognito project

- 10 Petaflop research project (2010)
- Port/develop applications to reduce time-to-production once installed
- Programming models
- Tools for application development and to support previous evaluations
- Evaluate node architecture
- Evaluate interconnect options
Which countries joined PRACE

HPC NEWS

PRACE selects Petaflop's HPC sites
1 September 2008

PRACE (Partnership for Advanced Computing in Europe) has selected a broad coverage of promising architectures for Petaflop-class systems to be deployed in 2009 and 2010. Prototypes will be installed at six partner sites starting in 2008.

PRACE analysed key scientific applications and mapped them to suitable architectures. As a result six prototypes were selected including more advanced hybrid systems.

‘Our objective is to build the best set of prototypes for preparing a timely and seamless deployment of production systems in 2009 and 2010 – not to attempt to select the best individual prototypes’, said François Robin, from CEA/GENCI. The prototypes will be installed at the following PRACE partner sites:

- BSC (Barcelona Supercomputing Center, Spain), installs a hybrid prototype combining IBM Cell and Power6 processors. The Cell processors are used for computation and the Power6 processors for service.

- CEA (French Atomic Energy Commission, France) and FZJ (Forschungszentrum Jülich, Germany) jointly use Intel Nehalem/ Xeon processors in their systems. Two shared-memory multiprocessors (thin node clusters) will be distributed over the two sites; a prototype produced by Bull at CEA and a larger system of the same architecture at FZJ.

- CSC (The Finnish IT Center for Science, Finland) and CSCS (Swiss National Supercomputing Centre, Switzerland) jointly evaluate the Cray XT3 architecture. This Massively Parallel Processing (MPP) prototype will be installed at CSC’s facilities.

- FZJ provides its already installed IBM BlueGene/P system, as a Massively Parallel Processing prototype.

- HLRS (High Performance Computing Center Stuttgart, Germany) offers a NEC SX-9 and an x86-based cluster as a hybrid prototype.

- NCF (Netherlands Computing Facilities Foundation, The Netherlands) evaluates the IBM Power6 architecture, a shared-memory multiprocessor (fat node cluster). This prototype will be installed in SARA Computing and Networking Services facilities in Amsterdam.

These prototypes will be used to evaluate the architectures in near-production situation with regard to application performance and scalability, as well as total cost of ownership and energy consumption. They will make also possible the evaluation of software for managing the distributed infrastructure, the preparation of benchmarks for future Peta-scale systems allowing better understanding of user requirements, the scaling and optimization of libraries and codes and the definition of technical requirements and procurement procedures for the PRACE Petaflop’s production systems for 2009/2010.

Related internet links

PRACE
Workflow of a 48 h high-resolution simulation of Europe at 12 km and Spain at 4 km

<table>
<thead>
<tr>
<th>Computational requirements</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Meteorology</strong></td>
</tr>
<tr>
<td>wrf-Control</td>
</tr>
<tr>
<td>real.exe</td>
</tr>
<tr>
<td>Europe-12 km</td>
</tr>
<tr>
<td>real.exe + ndown.exe</td>
</tr>
<tr>
<td>Spain-4 km output</td>
</tr>
<tr>
<td>WRFtoHERMES</td>
</tr>
<tr>
<td>HERMES</td>
</tr>
<tr>
<td>MCIP Europe-12 km</td>
</tr>
<tr>
<td>Emissions Europe 12 km</td>
</tr>
<tr>
<td>CCTM Europe 12 km</td>
</tr>
<tr>
<td>Images Europe 12 km</td>
</tr>
<tr>
<td><strong>Emissions</strong></td>
</tr>
<tr>
<td>MCIP Spain 4 km</td>
</tr>
<tr>
<td>Emissions Spain 4 km</td>
</tr>
<tr>
<td>BCON Spain 4km</td>
</tr>
<tr>
<td>CCTM Spain 4 km</td>
</tr>
<tr>
<td>Images Spain 4 km</td>
</tr>
<tr>
<td><strong>Chemistry</strong></td>
</tr>
<tr>
<td>Total</td>
</tr>
</tbody>
</table>

1 hour - 5 min division

1 CPU
8 CPUs
128 CPUs
192 CPUs
258 CPUs

4 h 55 min
Enhancing spatial resolution - towards a new generation air quality modeling system

Resolution improved to 12 km for all Europe, 4 km for the Iberian peninsula, and 1 km for hot spot regions within MareNostrum Supercomputer

http://salam.upc.es/caliopesalam.upc.es/caliope
**Definition of the study cases:**
- Europe at 12 km horizontal resolution: WRF-ARW, WRF-NMM
- Iberian peninsula at 4 km horizontal resolution: WRF-ARW, WRF-NMM
- North America at 12 km horizontal resolution: WRF-ARW
- Analysis of European and Iberian peninsula domains

**WRF computational needs depend on:**
- 1) Domain size
- 2) Topography
- 3) Meteorological conditions

<table>
<thead>
<tr>
<th>Domain</th>
<th>Europe</th>
<th>Iberian peninsula</th>
<th>Europe</th>
<th>Iberian peninsula</th>
<th>USA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model</td>
<td>WRF-ARW</td>
<td>WRF-ARW</td>
<td>WRF-NMM</td>
<td>WRF-NMM</td>
<td>WRF-ARW</td>
</tr>
<tr>
<td>NX</td>
<td>400</td>
<td>400</td>
<td>400*</td>
<td>400*</td>
<td>425</td>
</tr>
<tr>
<td>NY</td>
<td>400</td>
<td>400</td>
<td>400*</td>
<td>400*</td>
<td>300</td>
</tr>
<tr>
<td>NZ</td>
<td>38</td>
<td>38</td>
<td>38</td>
<td>38</td>
<td>35</td>
</tr>
<tr>
<td>Resolution (km)</td>
<td>12</td>
<td>4</td>
<td>12</td>
<td>4</td>
<td>12</td>
</tr>
<tr>
<td>Hours of simulation</td>
<td>9-12h</td>
<td>15-18h</td>
<td>9-12h</td>
<td>15-18h</td>
<td>0-3h</td>
</tr>
<tr>
<td>Microphysics</td>
<td>WSM 3class</td>
<td>WSM 6class</td>
<td>Ferrier</td>
<td>Ferrier</td>
<td>Ferrier</td>
</tr>
<tr>
<td>LSM</td>
<td>Noah</td>
<td>Noah</td>
<td>Noah</td>
<td>Noah</td>
<td>5-layers</td>
</tr>
<tr>
<td>PBL</td>
<td>YSU</td>
<td>YSU</td>
<td>MYJ</td>
<td>MYJ</td>
<td>YSU</td>
</tr>
<tr>
<td>Cu</td>
<td>KF</td>
<td>Explicit</td>
<td>BMJ</td>
<td>Explicit</td>
<td>KF</td>
</tr>
</tbody>
</table>
Performance in MareNostrum Supercomputer:

- Reduced scalability of atmospheric WRF codes (30-40%) in current HPC environments
  - Over 128 cpus, reduced speedup

- Similar codes have large difference in performance computing.
  Differences between NMM and ARW dynamical cores:
  - ARW: load balancing and communications problems. Low Instructions per cycle. Sensitive to contention.
  - NMM: code replication major point.

- Limitation of coding paradigm finite difference schemes
  - Replication of code for communication exchange
  - Strong scalability limitation in current HPC environment
Database information management

**Biogenic emissions**
- Land use map
- Emission factors and biomass
- Meteorological information (air temperature, solar radiation)

**On road, ships and aircrafts traffic**
- Roads (urban streets, roads, etc.), LTO cycles and ships routes
- Hourly, weekly and monthly profiles
- Distribution of the vehicles
- Velocity by road type
- Meteorological information (air temperature)
- Type of combustibles

**Industry and electric generation**
- Location (point/area)
- Production / electric generation
- Emission factors – energetic intensity
- Chimney height / diameter

**Residential and commercial**
- Density population map
- Combustibles consume
- Emission factors
- Solvent use
- Waste generation

Emission computation and speciation

- BVOCs
- NOx, VOCs, CO, SO2, particulate matter, CO2, CH4 and N2O
- NOx, VOCs, CO, SO2, particulate matter, CO2, CH4 and N2O
- NOx, VOCs, CO, SO2, particulate matter, CO2, CH4 and N2O

Speciation

Management of the emission information

- Visualization and analysis of the results
- Management information tool

Management of emission data for air quality modelling

- Hourly aggregation of archives (4x4 km, 1x1 km grid size)
- Height desaggregation (vertical layers)
- Database resolution (1 - 4 km grid size)
- Generation of netCDF emission files
HERMES: Emissions for Europe, 12 km, disaggregated from EMEP (50 km), 01-02 October 2007, pollutant: NO
1. Operational meteorological validation: MSG
2. Operational meteorological validation: RADAR
3. Operational air quality validation: OMI NO$_2$ tropospheric column
The Canary Islands are located in the middle-east of the Atlantic Ocean in front of the southern coast of Morocco. They are the most distant archipelago of Spain constituted of seven islands of volcanic origin with very complex topography. La Palma, which is a very steep island, and Tenerife, the largest island (1929 km²) with the highest peak (3718 m a.s.l.) of Spain (Teide volcano), were the most affected for the synoptic situation of Delta storm.
Methods

- Weather Research and Forecasting (WRF) Model
  - ARW dynamics solver
  - Microphysics: single-moment 3-class scheme
  - Cumulus: Kain-Fritsch
  - PBL: Yonsei University PBL scheme
  - LSM: Rapid Updated Cycle LSM
  - Radiation: RRTM for LW, Dudhia scheme for SW
  - IC & BC: ECMWF IFS-0.25° forecast, BC every 3h.

- Conducted numerical simulations:
  - Base case run: three nested high-resolution domains 9, 3, 1 km
  - Experimental run without Canary Islands topography
  - 00 UTC 28 November 2005 – 00 UTC 30 November 2005

- Domains:
  - D1: 300 x 230 grid points at 9 km
  - D2: 340 x 226 grid points at 3 km
  - D3: 337 x 292 grid points at 1 km
  - 40 sigma vertical levels;
  - model top at 50 hPa
Operational forecast products

SDS WS Operational products

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

http://www.bsc.es/projects/earthscience/DREAM/
Dust forecast and validation system

Model has shown very good agreement with observations in a number of studies of single events (e.g., Ansmann et al., 2003, Papayannis et al., 2005; Pérez et al., 2006a;b; Jiménez et al, 2006 …)

Current users of the system:
- Scientific (aerosols, ocean, health, …)
- Experimental campaigns (TROMPETA, SAMUM, …)
- Observational Networks: Earlinet (European Lidar Network), AERONET and in-situ observations
- Satellite community
- Spanish administration: alert system

Implementation of aerosol and chemistry module into the most recent parallelized and non-hydrostatic version of the NMW NCEP model, with application either as a limited area or global model

→ Increasing resolution
→ Global model domain
→ High resolution dust forecast

<table>
<thead>
<tr>
<th>Eta model</th>
<th>ESMF/NMM-b model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Regional model</td>
<td>Global/Regional model</td>
</tr>
<tr>
<td>Hydrostatic</td>
<td>Non-hydrostatic</td>
</tr>
<tr>
<td>Eta coordinate</td>
<td>Sigma coordinate</td>
</tr>
<tr>
<td>Arakawa E-grid</td>
<td>Arakawa B-grid</td>
</tr>
<tr>
<td>Convection</td>
<td>Microphysical</td>
</tr>
<tr>
<td>parameterization</td>
<td>convection</td>
</tr>
</tbody>
</table>

Temperature field from UMO

- New generation of Earth system modelling framework (ESMF) in MARENOSTRUM parallelized environment
- Implementation of mineral dust module
- Implementation of full chemistry component online
- Code improvement after benchmark and performance studies
PRELIMINARY RESULTS WITH DUST COMPONENT

Simulation set-up:
Global
Cycle 20080124 12 UTC
60 hours forecast
160 CPU’s
8 dust bins
769x541 64 sigma layers

Cycle 20080124_12
54h forecast
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

China Meteorological Administration (CMA)
Xiao Ye Zhang
xiaoye@cams.cma.gov.cn
Global Circulation Model: EC-Earth (ECMWF), GISS ModelE (NASA)

Climate modeling system at BSC-CNS:
- Global Circulation Model
- Regional Climate Model

Meteorology: WRF-ARW / WRF-NMM

Regional modelling system

Mineral Dust: DREAM

Chemistry Transport: CMAQ / CHIMERE

Emissions: HERMES, EMEP
GISS ModelE at BSC-CNS Precipitation Anomaly mm/day (1951–1980)
Year 2010, BAU scenario – Global Res: 2° x 2.5°
Combination of Collaborative Project and Coordination and Support Action for Integrating Activities

FP7 INFRASTRUCTURES 2008-1
INFRA-2008-1.1.2. Targeted approach: Integrating Activities

INFRA-2008-1.1.2.21: “Establishing an European e-Infrastructure for earth system’s understanding and modelling”

InfraStructure for the European Network for Earth System Modelling

IS-ENES

Coordinator: Dr Sylvie Joussaume

<table>
<thead>
<tr>
<th>Participant no.</th>
<th>Participant organisation name</th>
<th>Part. Short Name</th>
<th>Country</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (Coordinator)</td>
<td>Centre National de la Recherche Scientifique - IPSL</td>
<td>CNRS - IPSL</td>
<td>France</td>
</tr>
<tr>
<td>2</td>
<td>Max-Planck-Gesellschaft zur Förderung der Wissenschaften e.V.</td>
<td>MPG</td>
<td>Germany</td>
</tr>
<tr>
<td>3</td>
<td>Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique</td>
<td>CERFACS</td>
<td>France</td>
</tr>
<tr>
<td>4</td>
<td>Deutsches Klimarechenzentrum GmbH</td>
<td>DKRZ</td>
<td>Germany</td>
</tr>
<tr>
<td>5</td>
<td>Finnish Meteorological Institute</td>
<td>FMI</td>
<td>Finland</td>
</tr>
<tr>
<td>6</td>
<td>University of Manchester</td>
<td>UNIMAN</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>7</td>
<td>Academy of Athens – Centre for Atmospheric, Physics and Climatology</td>
<td>AA - CAPC</td>
<td>Greece</td>
</tr>
<tr>
<td>8</td>
<td>Science and Technology Facilities Council</td>
<td>STFC</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>9</td>
<td>Centro Euro Mediterraneo per i Cambiamenti Climatici</td>
<td>CMCC</td>
<td>Italy</td>
</tr>
<tr>
<td>10</td>
<td>METOFOICE</td>
<td>METOFOICE</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>11</td>
<td>Koninklijk Nederlands Meteorologisch Instituut</td>
<td>KNMI</td>
<td>Netherlands</td>
</tr>
<tr>
<td>12</td>
<td>Météo France – Centre National de Recherches Meteorologiques</td>
<td>MF - CNRM</td>
<td>France</td>
</tr>
<tr>
<td>13</td>
<td>Sveriges Meteorologiska och Hydrologiska Institut</td>
<td>SMHI</td>
<td>Sweden</td>
</tr>
<tr>
<td>14</td>
<td>NEC Laboratories Europe - IT Research Division</td>
<td>NLE-IT</td>
<td>Germany</td>
</tr>
<tr>
<td>15</td>
<td>Linköpings Universitet</td>
<td>LIU</td>
<td>Sweden</td>
</tr>
<tr>
<td>16</td>
<td>Barcelona Supercomputing Centre</td>
<td>BSC</td>
<td>Spain</td>
</tr>
<tr>
<td>17</td>
<td>Wageningen Universiteit</td>
<td>WU</td>
<td>Netherlands</td>
</tr>
<tr>
<td>18</td>
<td>Instituto Nacional de Hidrologia y Geodinamica en Espacio</td>
<td>INHGA</td>
<td>Romania</td>
</tr>
<tr>
<td>19</td>
<td>Deutsches Zentrum Für Luft- und Raumfahrt in der Helmholtz Gemeinschaft</td>
<td>DLR</td>
<td>Germany</td>
</tr>
<tr>
<td>20</td>
<td>Program for Climate Model Diagnosis and Intercomparison</td>
<td>PCMDI</td>
<td>United States of America</td>
</tr>
</tbody>
</table>
Thanks you for the attention

CONTACT
jose.baldasano@bsc.es