Execution of WRF workflows on local and distributed resources with WRF4G

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Thanks to:
V. Fernández-Quiruelas
C. Blanco
A.S. Cofiño
L. Fita
M. García-Díez
• Motivation

• WRF4G
  • Accessing distributed resources
  • Workflow
  • Experiment types
  • Side-products
  • Projects supporting WRF4G

• The Grid
  • Grid computing for meteo/climate apps

• Conclusions
Reanalysis/Reforecasts/Hindcast

- High number (~10^4) of independent simulations
- High volume of output data (>TB)
- Requires scalability

Regional climate simulation

- Long, continuous simulations; weeks of walltime
- High volume of output data (>TB)
- Recovering system for simulation restart

Weather Forecasting

- QoS and optimal resources: **deadline for delivery**

Sensitivity/ensemble studies

- Physical schemes, initial conditions and boundary conditions: uncertainty sampling
- Resource demanding experiments composed of many **independent simulations**
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Reanalysis/Reforecasts/Hindcast

● SEAWIND project
  • 21 years of daily reforecasts (36h each)
  • 7,665 independent simulations

Regional climate simulation

● ESCENA project
  • 50 years (continuous run, 28-day restarts)
  • 650 dependent simulations

Sensitivity/ensemble studies

● CORWES project
  • Physics sensitivity study for CORDEX-Africa
  • 8-member ensemble of 5-year continuous simulations
  • 8 independent groups of 65 dependent simulations
Computer resource scenarios

**Desktop/Laptop (UI)**
- Low computational power and storage
- **User interface** to other computer resources

**Workstation**
- Multi-core, shared memory, moderate storage
- ssh access

**Local group/institutional cluster**
- Multi-node, distributed memory, large storage
- ssh access, **batch system** (PBS, SGE, ...) to submit jobs

**Mainframe/HPC site**
- Different architectures and memory arrangements
- ssh or higher security access

**Grid infrastructure**
- “Cluster of clusters”, geographically distributed
- Huge amount of **computational power** and storage (not trivial to take advantage of it for meteo/climate apps)
**WRF4G**, developed by the Santander Meteorology Group, provides:

- Flexible WRF experiment **design, execution** and **monitoring**, and ...

- … the ability of running these experiments on different computing resources at the same time in a **transparent** way.

It is, currently, a set of **command line tools** (Web interface planned)

**WRF** is **not installed in the host resources**. Binaries are transferred for each simulation.

The **output and log files are centralized** in a single repository

A broken experiment (due to a temporal failure of the resources) is **restarted by resubmitting the whole experiment**: only the unfinished simulations will be restarted from their last restart file
WRF4G, developed by the Santander Meteorology Group, provides:

- Flexible WRF experiment design, execution and monitoring, and ...

- … the ability of running these experiments on different computing resources at the same time in a transparent way.

The only dependencies to be met by the host are:

- python (usually present, no need to install)
- python-mysql bindings (to be removed in the future)
WRF4G, developed by the Santander Meteorology Group, provides:

- Flexible WRF experiment **design**, **execution** and **monitoring**, and ...

- ... the ability of running these experiments on different computing resources at the same time in a **transparent** way.
DRM4G (Distributed Resource Manager) allows the user to merge different computing resources at hand in a transparent way:

**Local** resources (UI)

- Directly in a shell session
- Interacting with LRMS
  - PBS
  - SGE
  - SLURM
  - ...

User application (WRF)

Resources
DRM4G (Distributed Resource Manager) allows the user to merge different computing resources at hand in a transparent way:

- **Local** resources (UI)
- **Remote** resources (via ssh)

- Directly in a shell session
- Interacting with LRMS
  - PBS
  - SGE
  - SLURM
  - ...

![Diagram showing DRAM4G integration with local and remote resources](image-url)
DRM4G (Distributed Resource Manager) allows the user to merge different computing resources at hand in a transparent way:

**Local** resources (UI)

**Remote** resources (via ssh)

**Grid** infrastructures (via Globus)

- Directly in a shell session
- Interacting with LRMS
  - PBS
  - SGE
  - SLURM
  - ...
wrf4gframework.conf

[Computing Resources]
mycomputer       local://localhost?
    LRMS_TYPE=none;
    NODECOUNT=1;

myworkstation    ssh://workstation.unican.es?
    LRMS_TYPE=none;
    NODECOUNT=16;

PBS_cluster      ssh://pbs.cluster.edu?
    LRMS_TYPE=pbs;
    QUEUE_NAME=long;
    NODECOUNT=256;

SGE_cluster      ssh://sge.cluster.edu?
    LRMS_TYPE=sge;
    PROJECT=1.project;
    NODECOUNT=256;
WRF4G, developed by the Santander Meteorology Group, provides:

- Flexible WRF experiment design, execution and monitoring, and ...

- ... the ability of running these experiments on different computing resources at the same time in a transparent way.
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Gridded Data: NAM, GFS, RUC, AGRMET, etc.

Static geographical data

WRF Preprocessing System

WRF ARW

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WRF4G

wrf4g_prepare

resources.wrf4g
experiment.wrf4g

Monitor DB (MySQL)

WRF4G_DOMAINS
geo_em.nc
namelist.wps

WRF4G_INPUT
Gridded Data: NAM, GFS, RUC, AGRMET, etc.

Static geographical data

Locally processed

WRF Preprocessing System

ungrib → metgrid
real → wrf

gribgrid
namelist.wps

WRF ARW

WRF4G_APPS
WRF4G-1.0.tgz
WRFbin-3.1.1r274.tgz
nco.tgz
cdo.tgz
grib_api.tgz

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WRF4G DOMAINS
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WRF4G_INPUT
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Static geographical
data
Locally processed

WRF4G
resources.wrf4g
experiment.wrf4g

wrf4g_prepare

wrf4g_submit
Target resource abstraction layer (DRM4G)
Monitor DB (MySQL)

WRF Preprocessing System
ungrib
metgrid

WRF ARW
real
wrf

WRF4G_APPS
WRF4G-1.0.tgz
WRFbin-3.1.1r274.tgz
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# WRF4G version to use (packed scripts must be in $WRF4G_APPS)
WRF4G_VERSION="1.0"

# Name of the packed WRF binaries (the file must be in $WRF4G_APPS)
WRF_VERSION="3.1.1_r832INTEL_OMPI"

# Common path to save all output and log files
WRF4G_BASEPATH="/oceano/gmeteo/WORK/ASNA/WRF/experiments"

# Path to the preconfigured WRF domains
WRF4G_DOMAINPATH="/oceano/gmeteo/WORK/ASNA/WRF/domains"

# Path to the global data for the boundary and initial conditions
WRF4G_INPUT="/oceano/gmeteo/DATA"

# Path to the packed binaries (WRF4G script, WRF, cdo (preprocessor), ..)
WRF4G_APPS="/oceano/gmeteo/WORK/wrf4g/repository/apps"

# Number of parallel processors (cores) per simulation
NP=8

# Computer resources to use
RESOURCES="myworkstation,PBS_cluster"

# Fine tuning
ENVIRONMENT='MAXWALLTIME = 36000, MAXMEMORY = 1000'
Configuration files

```bash
# WRF4G version to use (packed scripts must be in $WRF4G_APPS)
WRF4G_VERSION="1.0"

# Name of the packed WRF binaries (the file must be in $WRF4G_APPS)
WRF_VERSION="3.1.1_r832INTEL_OMPI"

# Common path to save all output and log files
WRF4G_BASEPATH="rsync://my.storage.edu/path/to/WRF/experiments"

# Path to the preconfigured WRF domains
WRF4G_DOMAINPATH="rsync://other.computer.edu/path/to/WRF/domains"

# Path to the global data for the boundary and initial conditions
WRF4G_INPUT="rsync://other2.computer.edu/path/to/input/DATA"

# Path to the packed binaries (WRF4G script, WRF, cdo (preprocessor), ..)
WRF4G_APPS="rsync://other3.computer.edu/path/to/apps"

# Number of parallel processors (cores) per simulation
NP=8

# Computer resources to use
RESOURCES="myworkstation,PBS_cluster"

# Fine tuning
ENVIRONMENT='MAXWALLTIME = 36000, MAXMEMORY = 1000'
```
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---

wrf4gframework.conf
resources.wrf4g
experiment.wrf4g

---

**experiment_name** = "MyExperiment"
**domain_name** = "Europe15km"
**max_dom** = 2

**extdata_vtable** = "ECMWF"  # Vtables must exist as Vtable.[input_extdata]
**extdata_path** = ":\WRF4G_INPUT\ECMWF\INTERIM"
**extdata_interval** = 21600  # Seconds between global analysis input times
**extdata_preprocessor** = "ECMWF"
**postprocessor** = "SEAWIND2"

**start_date** = "1989-01-01_06:00:00"
**end_date** = "2001-01-02_00:00:00"
**chunk_size_h** = 36

**multiple_dates** = 1
  **simulation_interval_h** = 24
  **simulation_length_h** = 1*chunk_size_h

**multiple_parameters** = 0
  **multiparams_variables** = "mp_physics,cu_physics,e_vert"
  **multiparams_nitems** = "${max_dom},${max_dom},${maxdom}"
  **multiparams_combinations** = "3,1,28 / 3,3,28 / 4,1,36 / 3,1,36"
  **multiparams_labels** = "WSM3_KF_L28/WSM3_GD_L28/WSM5_KF_L36/WSM3_KF_L36"

### Override namelist.input variables here ###

# Single valued:
**NI_restart_interval** = 2880  # minutes
**NI_spec_bdy_width** = 10
**NI_spec_zone** = 1
**NI_relax_zone** = 9
**NI_sst_update__physics** = 1

# One value per domain:
**NIM_history_interval** = 180,60  # minutes
**NIM_frames_per_outfile** = 4,12

# One value per domain; but all equal (provide a single value here):
**NIN_e_vert** = 42

---

Boundary data

Experiment dates

Multi-parameter experiment

namelist.input modifications
WRF4G framework

- WRF4G splits a regular WRF simulation **experiment** into:
  - **realizations**
    - A realization is any **independent WRF simulation**, which does not need as input the output (e.g. restart file) of another simulation.
  - **chunks**
    - For convenience, a WRF realization can be split into chunks. By definition, a chunk is a **dependent simulation** and requires the previous chunk to finish.

- Chunks are convenient to create WRF jobs finishing before the job is kicked out of a queue. Also, they allow fine tuning of the size of the input files.
Experiment definition

```
multiple_dates = 1
multiple_parameters = 0
```
Experiment definition

Days

start_date

end_date

simulation_length_h

multiple_dates = 1
multiple_parameters = 0
Experiment definition

- start_date
- end_date
- multiple_dates = 1
- multiple_parameters = 0
- simulation_interval_h
Experiment definition

Days

start_date

end_date

multiple_dates = 1
multiple_parameters = 0

simulation_interval_h

simulation_length_h
Experiment definition

- start_date
- end_date
- multiple_dates = 1
- multiple_parameters = 0
- simulation_interval_h
- simulation_length_h
Experiment definition

- `start_date` to `end_date`
- `simulation_interval_h`
- `simulation_length_h`
- `multipleDates = 1`
- `multipleParameters = 0`
Experiment definition

Months

- start_date
- end_date
- simulation_interval_h
- simulation_length_h
- multiple_dates = 1
- multiple_parameters = 0
- chunk_size_h
Experiment definition

Months

start_date

end_date

simulation_interval_h

multiple_dates = 1
multiple_parameters = 0

simulation_length_h

chunk_size_h

WRF4G_BASEPATH
wrfout_*
wrfrst_*
wrfinput_*
wrfbdy_*
Example:

```
multiple_parameters = 1
multiparams_variables = "mp_physics,cu_physics,eVert"
multiparams_nitems = "$\{max\_dom\},\{max\_dom\},\{max\_dom\}"
multiparams_combinations = "3,1,28 / 3,3,28 / 4,1,36 / 3,1,36"
multiparams_labels = "WSM3\_KF\_L28/WSM3\_GD\_L28/WSM5\_KF\_L36/WSM3\_KF\_L36"
```
Multi-parameter & multi-date

multiple_dates = 1
multiple_parameters = 1
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Multi-parameter & multi-date

Months

start_date

param1

param2

param3

param4

end_date

multiple_dates = 1
multiple_parameters = 1

simulation_interval_h
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Climate simulation (continuous)

Years

start_date

chunk_size_h

end_date

multiple_dates = 0
multiple_parameters = 0
Years


\[
\text{start_date} \quad \text{chunk_size_h} \quad \text{simulation_interval_h} \quad \text{simulation_length_h} \quad \text{end_date}
\]

\[
\text{multiple_dates} = 1 \\
\text{simulation_length_h} = 22 \times \text{chunk_size_h} \\
\text{simulation_interval_h} = 20 \times \text{chunk_size_h} \\
\text{multiple_parameters} = 0
\]
Monitoring

Shell$ wrf4g_status -e example

<table>
<thead>
<tr>
<th>Realization</th>
<th>GW</th>
<th>Stat</th>
<th>Chunks</th>
<th>Comp. Res</th>
<th>WN</th>
<th>Run. Sta</th>
<th>ext</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>example__ph1</td>
<td>-</td>
<td>P</td>
<td>0/4</td>
<td>-</td>
<td>-</td>
<td>Prepared</td>
<td>-0.00</td>
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</tr>
<tr>
<td>example__ph2</td>
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<td>Prepared</td>
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<tr>
<td>example__ph3</td>
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<td>Prepared</td>
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<td>example__ph4</td>
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<td>Prepared</td>
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</tr>
<tr>
<td>example__ph5</td>
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<td>-</td>
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<td>Prepared</td>
<td>-0.00</td>
<td></td>
</tr>
</tbody>
</table>
### Monitoring

Shell:

```
wrf4g_status -e example
```

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</tr>
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<tbody>
<tr>
<td>example__ph1</td>
<td>32</td>
<td>R</td>
<td>1/4</td>
<td>mycomputer</td>
<td>legolas</td>
<td>metgrid</td>
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<tr>
<td>example__ph2</td>
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<tr>
<td>example__ph4</td>
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### Monitoring

Shell:

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$ wrf4g_status -e example
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Shell$ `wrf4g_status -e example`

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Outline

- Motivation
- WRF4G
  - Accessing distributed resources
  - Workflow
  - Experiment types
  - Side-products
  - Projects supporting WRF4G
- The Grid
  - Grid computing for meteo/climate apps
- Conclusions
Useful tools developed

- **vcp**
  - **Virtual copy**
  - **Provides transparent copy between any of:**
    - local file
    - gridftp URL
    - ssh host (via rsync)
    - local link (as destination)
  - **E.g:**
    - `vcp /local/file /other/local/path/`
    - `vcp /local/file rsync://remote.comp.edu/remote/path/`
    - `vcp rsync://remote.comp.edu/remote/path ln:/local/path`  # (copies)
    - `vcp /local/file ln:/other/local/path`  # (links)
    - `vcp -r /local/dir gridftp://server:port/remote/path`
    - `vcp gridftp://srv1:port/rmt/file gridftp://srv2:port/other/file`
Useful tools developed

• fortmnl
  • Fortran namelist
  • Provides Fortran namelist manipulation from the command line along with some WRF namelist checks.
  • E.g:

```bash
fortmnl -f namelist.input
fortmnl --wrf -f namelist.input
fortmnl -f namelist.input -s variable value
fortmnl -f namelist.input -s variable value1 value2 value3 ...
fortmnl -f namelist.input -s variable@record value
```
European commission (7FP):

**EELA2**: E-science grid facility for Europe and Latin America

Partners: 52 institutions in Latin America and Europe

Spanish Ministry of Science and Innovation:

**WRF model port to Grid infrastructures and proof-of-concept for a high-resolution wind hindcast over Europe**

*Universidad de Cantabria*

**Coordinated regional climate downscaling experiment using WRF:**

A contribution to the CORDEX initiative by the Spanish WRF community

Partners: 3 Spanish universities and a supercomputing center
WRF modifications and tools

Coordination / dissemination

Grid computing

ROMS

Canary islands

WRF4G
CLWRF
Pre- & post-process tools

WRF
Grid computing is a computational paradigm taking advantage of geographically distributed computer resources.

A software layer (middleware) provides **transparent access** to the distributed resources.

The access to the resources is **secure**

Users are organized in **virtual organizations**
Example: EGI infrastructure

Status Jan 2011
- 340 sites
- 56 countries
- 288000 LCPUs (cores)
- 117 PB disk
- 91 PB tape
- 13800 users
- 28 million jobs/mon
- 217 VOs (30 active)

Another example: Earth System Grid (only storage)
- Infrastructure shared between several NL in the US
- Holding the PCMDI CMIP3, CMIP5 and many other databases
Not trivial for climate...

- Large input and output data transfer
- Long running times
- Very intensive: CPU and memory (requires parallel execution in order to finish in a reasonable time)
More than 1000 years simulated with a global model (CAM, T62) in less than 4 days

Benefits and requirements of grid computing for climate applications. An example with the community atmospheric model

V. Fernández-Quiruelas, J. Fernández, A.S. Cofiño, L. Fita, J.M. Gutiérrez
Conclusions

• The WRF user usually:
  • designs experiments where several (many?) simulations are required
  • has several computer resources available for her simulations

• WRF4G simplifies the design, execution and monitoring of WRF on several computer resources

• WRF4G is freely available for use...

www.meteo.unican.es/software/wrf4g
Thank you! Takk!

Contact: fernandej@unican.es

More info: www.meteo.unican.es/software/wrf4g
Three realizations split into two chunks each:
Three realizations split into two chunks each:

- exp__rea1
- exp__rea2
- exp__rea3

WPS+real
WRF

Model time step (no output)
Three realizations split into two chunks each:

exp__rea1

exp__rea2

exp__rea3
Three realizations split into two chunks each:

exp__rea1

exp__rea2

exp__rea3

Storage Element - METEO4G/WRF/experiments/exp

exp__rea1

exp__rea2

exp__rea3

output restart wpsout output restart wpsout output restart wpsout

wrfinput_t0 wrfbdy_t0
Three realizations split into two chunks each:

exp__rea1

exp__rea2

exp__rea3

Storage Element - METEO4G/WRF/experiments/exp

exp__rea1

output restart wpsout

exp__rea2

output restart wpsout

exp__rea3

output restart wpsout

wrfout_t0
wrfout_t1

wrfinput_t0
wrfbdy_t0
Three realizations split into two chunks each:

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exp__rea2

exp__rea3

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exp__rea3

Storage Element - METEO4G/WRF/experiments/exp

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output restart wpsout

exp__rea3

output restart wpsout

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wrfout_t2

wrfout_t3

wrfout_t4

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wrfrst_t4

wrfbdy_t0

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wrfbdy_t4
Three realizations split into two chunks each:

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Three realizations split into two chunks each:

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Three realizations split into two chunks each:

- exp__rea1
- exp__rea2
- exp__rea3

Storage Element - METEO4G/WRF/experiments/exp

- exp__rea1: output, restart, wpsout
- exp__rea2: output, restart, wpsout
- exp__rea3: output, restart, wpsout

Files:
- wrfout_t0, wrfout_t1, wrfout_t2, wrfout_t3, wrfout_t4, wrfout_t5, wrfout_t6, wrfout_t7, wrfout_t8
- wrfrst_t2, wrfrst_t4, wrfrst_t6, wrfrst_t8
- wrfinput_t0, wrfbdy_t0, wrfinput_t4, wrfbdy_t4
Three realizations split into two chunks each:

exp__rea1

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Storage Element - METEO4G/WRF/experiments/exp

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