Training session
Introduction to IPSL tools

January 14th & 15th 2020, IDRIS

IPSL « Plateforme » group – Lola Falletti & Nicolas Lebas

Outline

1. **Introduction**
2. HPC context
3. Which supercomputer(s) for us ?
4. Tools, configurations and performances
5. Perspectives

Institut Simon Laplace (IPSL)

IPSL gathers 9 laboratories whose research topics concern the global environment.

CEREA / GEOPS / LERMA / LATMOS / LISA / LMD / LOCEAN / LSCE / METIS

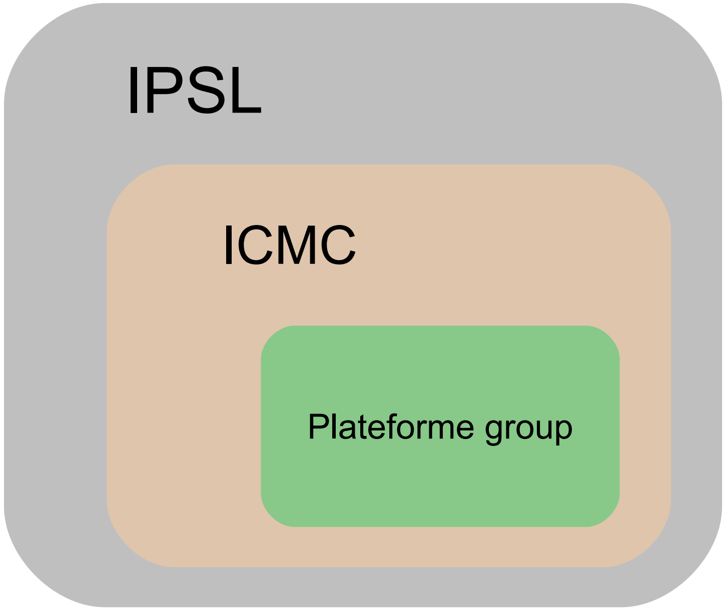
IPSL Climate Modeling Centre (ICMC http://icmc.ipsl.fr)

Activities articulated around

- The development of an integrated model of the Earth system
- To run and analyse climate simulations
- Working groups to share skills
- A scientific expertise

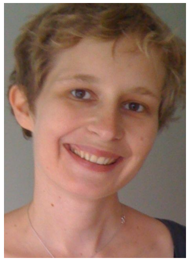
To be involved in ICMC activities, subscribe to the mailing list ***ipsl_cmc@listes.ipsl.fr***

IPSL Plateforme group : in charge of the development of modipsl, libIGCM, XIOS usage, metrics tools deployment



Plateforme-group members


Arnaud Caubel


Anne Cozic


Romain Pennel


Christian Ethé


Jérôme Servonnat


Laurent Fairhead


Eliott Dupont


Josefine Ghattas


Nicolas Lebas


Yann Meurdesoif


Simona Flavoni


Olivier Marti


Olivier Boucher


Thibaut Lurton

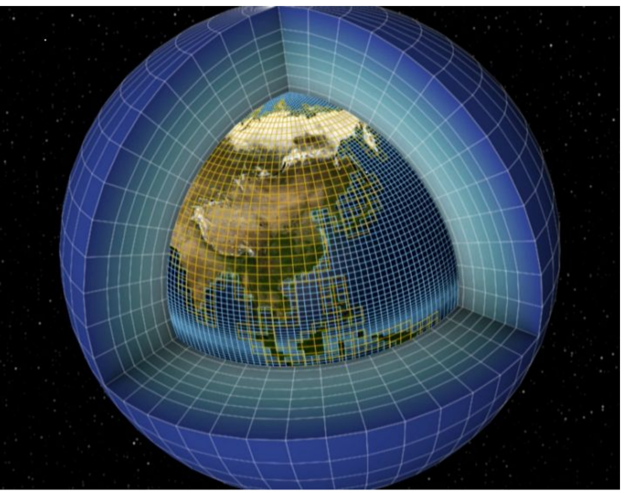

Lola Falletti

IPSL Earth System Model

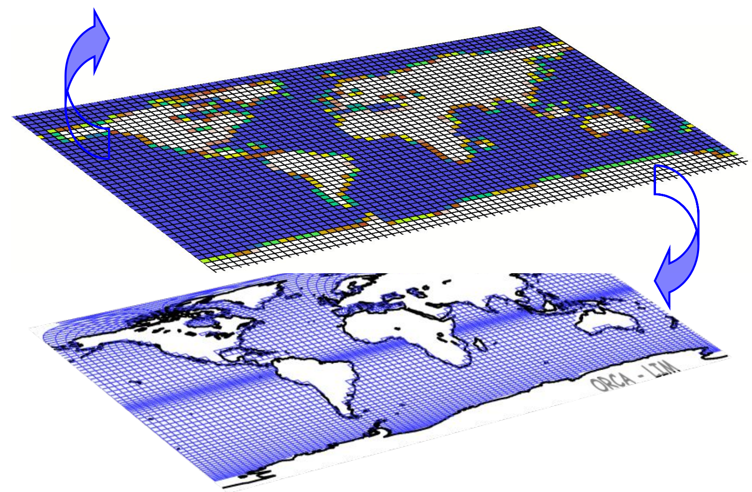
INCA/REPROBUS
(atmospheric chemistry, aerosols)

LMDZ
(atmosphere)

ORCHIDEE
(land surfaces, vegetation)



OASIS3-MCT
(coupler)



OPA
(ocean)

PISCES
(marine biogeochemistry)

LIM
(sea ice)

NEMO

https://www.nemo-ocean.eu

NEMO (**N**ucleus for **E**uropean **M**odelling of the **O**cean) is a state-of-the-art modelling framework for research activities and forecasting services in ocean and climate sciences, developed in a sustainable way by a European consortium.

3 main components:

- **OPA**: models the ocean {thermo}dynamics and solves the primitive equations
- **LIM**: models sea-ice {thermo}dynamics, brine inclusions and subgrid-scale thickness variations
- **PISCES**: models the {on,off}line oceanic tracers transport and biogeochemical processes

NEMO_v5	*OCE ORCA2*
NEMO_v6	*OCE ORCA1*

LMDZ

http://lmdz.lmd.jussieu.fr

LMDZ (**L**aboratoire de **M**étéorologie **D**ynamique **Z**oom model) is a general circulation model (or global climate model) developed since the 70s at the LMD, which includes various variants for the Earth and other planets (Mars, Titan, Venus, Exoplanets). It is first and foremost a research tool.

2 dynamic cores:

- **Actual**: based on regular LatxLon grid. Easy to use but limited in terms of parallelization on actual machines.
- **DYNAMICO**: icosaedric grid that allows very high scalability on HPC machines (still in development).

LMDZOR_v6.1.10	*ATM 144x144x79*
ICOLMDZOR_v7	
IPSLCM6.1.10-LR	*ATM 144x144x79 / OCE ORCA1*
IPSLCM6.2-MR1	*ATM 256x256x79 / OCE ORCA1*

ORCHIDEE

https://orchidee.ipsl.fr

ORCHIDEE
LAND SURFACE MODEL

ORCHIDEE (**O**rganising **C**arbon and **H**ydrology **I**n **D**ynamic **E**cosystems) represents the state of the art in global land surface modelling. It solves the water-energy-carbon budget, represents the ecosystem in terms of a range of Plant Functional Types and vegetation with a big leaf approach. It uses precipitation, air temperature, wind, solar radiation, humidity and atmospheric CO_2 as forcing data and computes its own phenology.

2 major components:

- **Seschiba**: water and energy budgets
- **Stomate**: biogeochemical and anthropogenic processes

LMDZOR_v6.1.10	*ATM 144x144x79 / ORCHIDEE_2_0*
LMDZOR_v6.2	*ATM 144x144x79 / ORCHIDEE_2_2*
LMDZOR_v6.3	*ATM 144x144x79 / ORCHIDEE trunk*
ORCHIDEE_2_2	
ORCHIDEE_trunk	

INCA / REPROBUS

http://inca.lsce.ipsl.fr

INCA (**IN**teraction with **C**hemistry and **A**erosols) is a chemistry and aerosol model coupled to General Circulation Model, LMDz. LMDzINCA accounts for emissions, transport (resolved and sub-grid scale), photochemical transformations, and scavenging (dry deposition and washout) of chemical species and aerosols interactively in the GCM. INCA is often coupled to the ORCHIDEE biosphere model in order to determine interactively the exchange of chemical species (emissions, deposition) between the atmosphere and the surface.

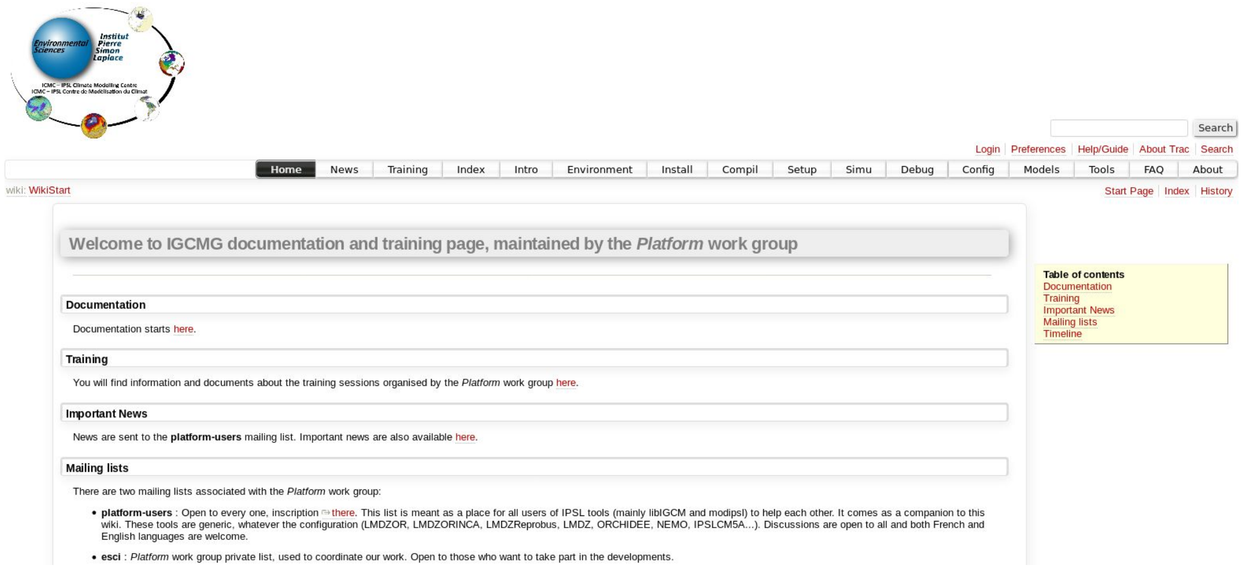
LMDZORINCA_v6.1.10 *ATM 96x96x39 (AP) or 144x144x79 (NP)*

REPROBUS model (**RE**active **P**rocesses **R**uling the **O**zone **BU**dget in the **S**tratosphere) coupled with the general circulation atmosphere model LMDz is a 3-D model designs to solve the dynamic and chemistry in the stratosphere in order to study ozone layer and its interactions with climate.

LMDZREPR_v6 (in prep.) *ATM 144x144x79*

Web documentations & mailing list

- **Modipsl / libIGCM**: http://forge.ipsl.jussieu.fr/igcmg_doc



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Welcome to IGCMG documentation and training page, maintained by the *Platform* work group

Table of contents
Documentation
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Mailing lists
Timeline

Documentation

Documentation starts here.

Training

You will find information and documents about the training sessions organised by the *Platform* work group here.

Important News

News are sent to the **platform-users** mailing list. Important news are also available here.

Mailing lists

There are two mailing lists associated with the *Platform* work group:

- **platform-users** : Open to every one, inscription there. This list is meant as a place for all users of IPSL tools (mainly libIGCM and modipsl) to help each other. It comes as a companion to this wiki. These tools are generic, whatever the configuration (LMDZOR, LMDZORINCA, LMDZReprobus, LMDZ, ORCHIDEE, NEMO, IPSLCM5A...). Discussions are open to all and both French and English languages are welcome.
- **esci** : *Platform* work group private list, used to coordinate our work. Open to those who want to take part in the developments.

- **Platform-users**: https://listes.ipsl.fr/sympa/info/platform-users

Community list for communication between all IPSL tools users. All of them can ask questions and answer his/her collegues questions.

→ ***All users need to subscribe***

Training

Training courses at IPSL :

- *Training course : IPSL tools and environments*
- *LMDZ training course* (contact Marie-Pierre.Lefebvre@lmd.jussieu.fr) next session in december
- *ORCHIDEE Introduction* 2-days course (contact orchidee-help@ipsl.jussieu.fr) next session after tomorrow
- *CLIMAF hands-on sessions*, every thursday in Jussieu/Saclay/Toulouse (contact jerome.servonnat@lsce.ipsl.fr)

Other suggested training :

- *Programming in Fortran* (niv1, niv2), *MPI, OpenMP and Hybrid MPI/OpenMP* at IDRIS twice a year www.idris.fr
- Training course for using the computer centres
- UNIX course
- http://formation-calcul.fr → give an inventory of training course (numeric – calcul – hpc) in France

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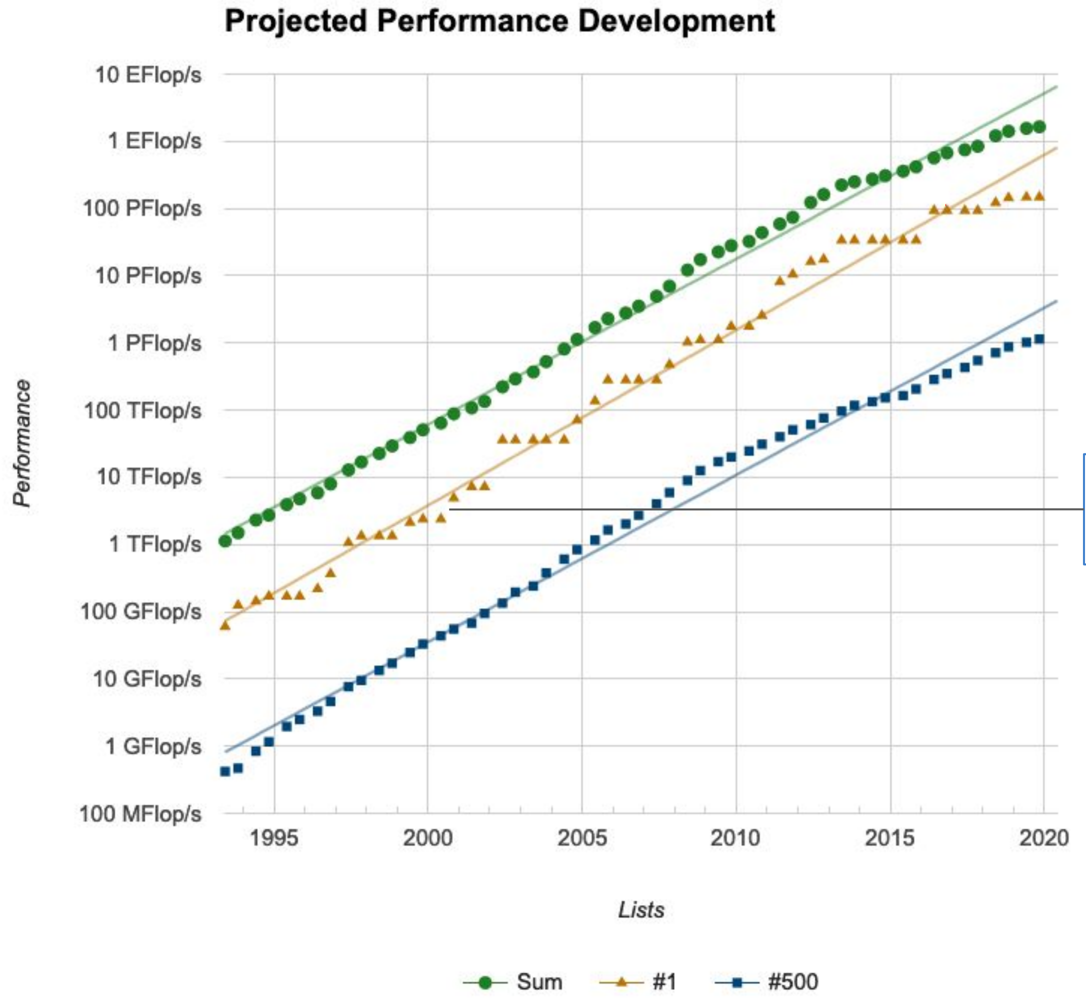
Supercomputers timeline: top 500

Factor 6/4 years



JeanZay & Joliot-Curie SKL

nov. 2019 TOP500.org

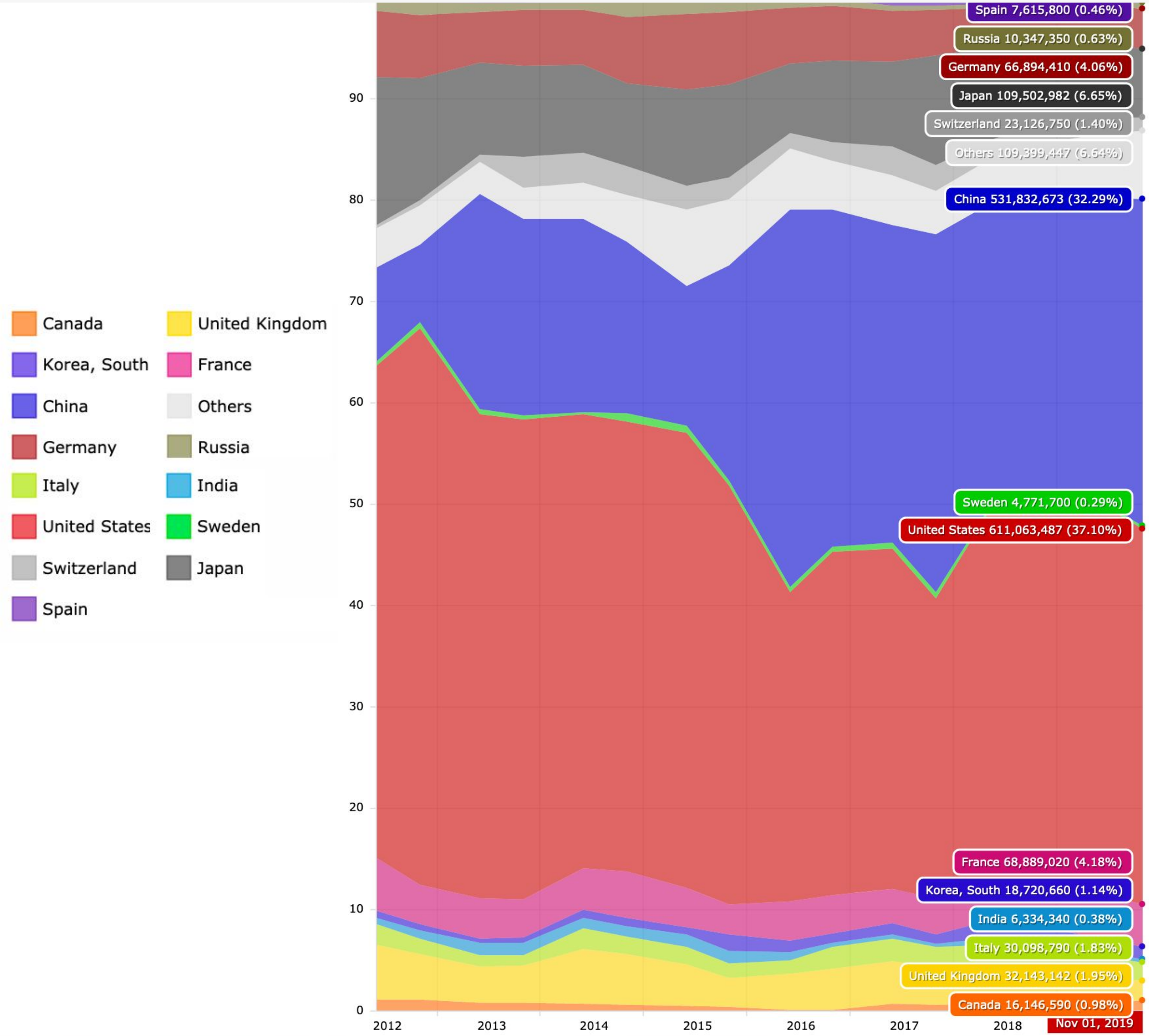
Supercomputers (ranking)

Rank	Site	System	Cores	Rmax (TFlop/s)
1	**DOE/SC/Oak Ridge National Laboratory United States**	**Summit** IBM / NVIDIA	**2,414,592**	**148,600**
2	DOE/NNSA/LLNL United States	**Sierra** IBM / NVIDIA	1,572,480	94,640
3	National Supercomputing Center in Wuxi China	**Sunway TaihuLight** Sunway MPP	10,649,600	93,014
4	National Super Computer Center in Guangzhou China	**Tianhe-2A** TH-IVB-FEP (Intel)	4,981,760	61,444
5	Texas Advanced Computing Center/Univ. of Texas United States	**Frontera** Dell C6420	448,448	23,516

Supercomputers (countries)

Rank	Site	System	Cores	Rmax (TFlop/s)	Power (kW)
1	**United States**	IBM	2,397,824	143,500	10,096
2	**United States**	IBM/NVIDIA	1,572,480	94,640.0	7,438
3	**China**	NRCPC	10,649,600	93,014.6	15,371
4	**China**	NUDT	4,981,760	61,444.5	18,482
5	**United States**	Dell EMC	448,448	23,516.4	-
6	**Switzerland**	Cray/HPE	387,872	21,230.0	2,384
7	**United States**	Cray/HPE	979,072	20,158.7	7,578
8	**Japan**	Fujitsu	391,680	19,880.0	1,649
9	**Germany**	Lenovo	305,856	19,476.6	-
10	**United States**	Cray	560,640	17,590.0	8,209

Performances by country



Cumulated performances by country over time

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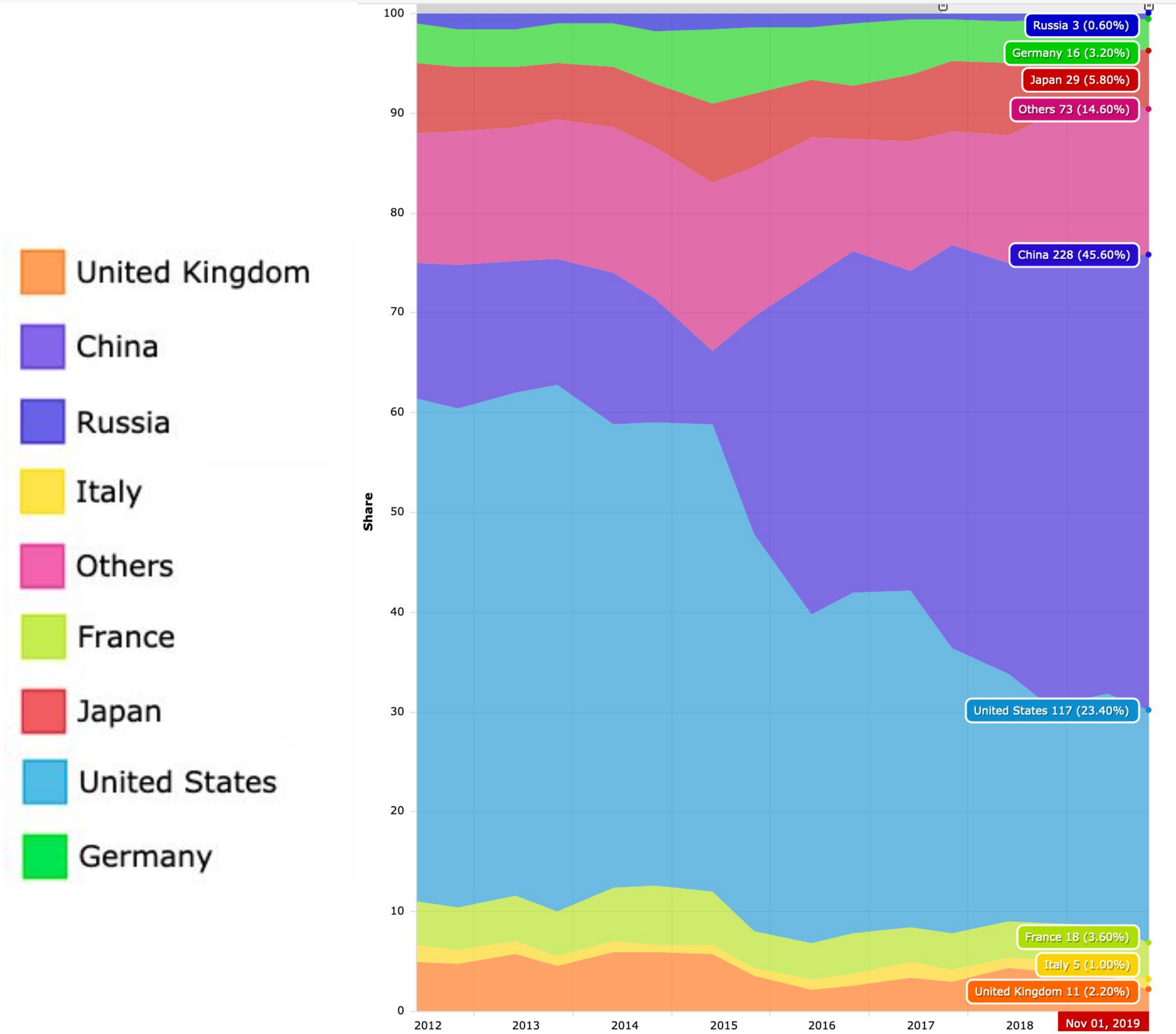
Number of HPC systems by country



Number of HPC systems by country over time

nov. 2019 TOP500.org

Supercomputers in France

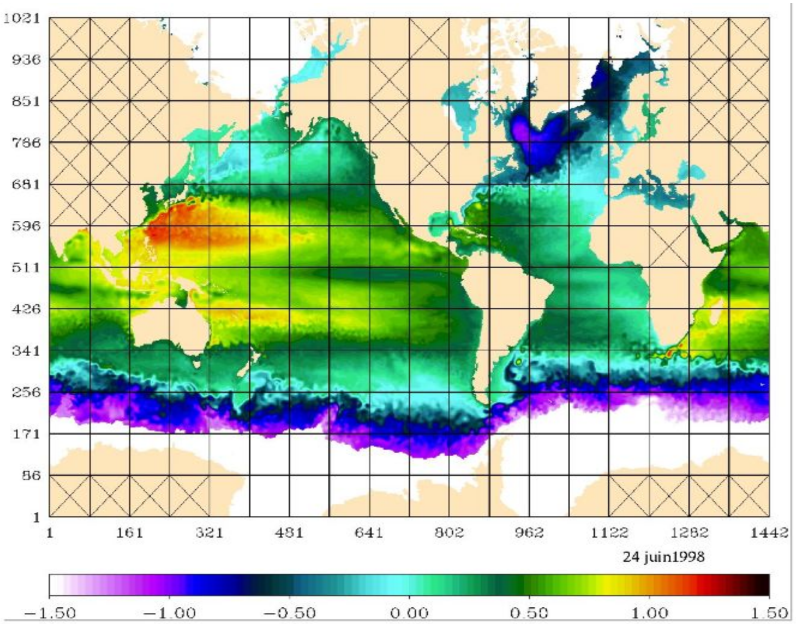
Rank	Site	System	Cores	Rmax (TFlop/s)	Power (kW)
1	DOE/SC/Oak United States	**Summit** IBM / NVIDIA	2,414,592	148,600	10,096
…	…	…	…	…	
11	Total Exploration Production	**Pangea III** IBM	291,024	17,860	1,367
17	CEA	**Tera-1000-2** Atos	561,408	11,965	3,178
41	Total Exploration Production	**Pangea** HPE	220,800	5,283	4,150
46	**CNRS/IDRIS-GENCI**	**Jean Zay** Intel/NVIDIA	**93,960**	**4,478**	**-**
52	**CEA/TGCC-GENCI**	**Joliot Curie SKL** Atos	**79,488**	**4,065**	**917**
59	**CEA/TGCC-GENCI**	**Joliot Curie ROME** Atos	**160,000**	**3,686**	**795**
79	**CNRS/IDRIS-GENCI**	**Jean Zay** Intel	**61,120**	**3,054**	**-**

Why do we need supercomputer ? ⇒ parallelization!

All models are parallelised.

MPI parallelisation implemented in our models allows to run the same executable on several core MPI to reduce the real time of the execution.

→ The global domain is divided into sub-domains, each core treats one sub-domain

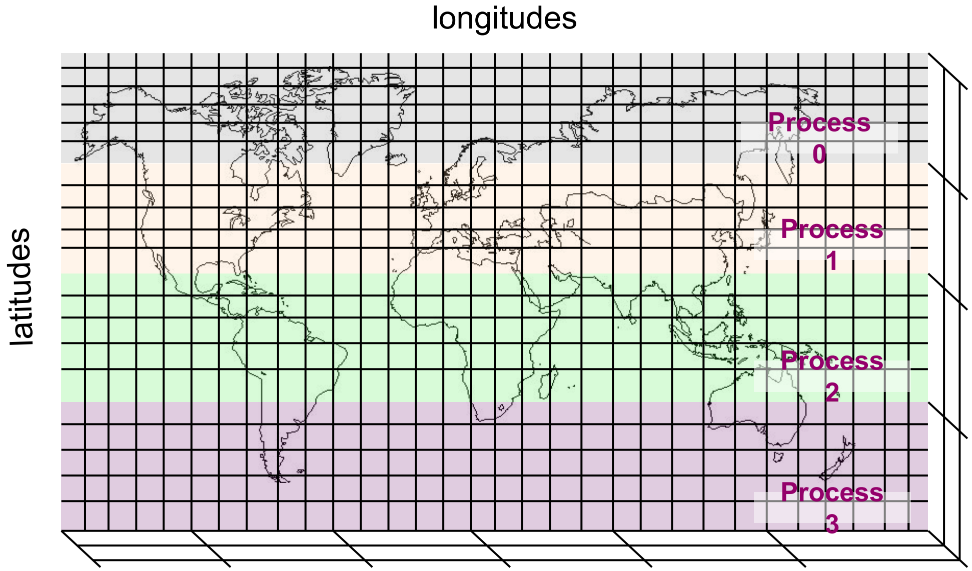


NEMO parallelism

Why do we need supercomputer ? ⇒ parallelization!

LMDZ model use hybrid MPI/Open MP parallelisation

MPI used to divide lon/lat grid splitting latitudes and Open MP to parallelise the vertical axis through shared memory threads.



LMDZ parallelisation grid

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National computing centers

Computing **Jean Zay Intel/NVIDIA (93 960 cores, 4,48 Pflops)** :

1528 nodes, 2 proc. Intel Cascade Lake 6248 2,5 Ghz (20 cores/node), 192Go/node (4,8Go/core)
261 converged nodes XA780i, 2 proc. Intel Cascade Lake 6248 & 4 GPUs Nvidia V100 SXM2 32 Go

Post : 4 fat nodes (4 proc. Intel Skylake 6132 12 cores 3,2 GHz, 1 GPU Nvidia V100 (62 Go/core)
Dods files : coming soon…
Assistance : assist@idris.fr or 01-69-35-85-55
Infos : www.idris.fr

Computing **Irene Joliot-Curie SKL (79 488 cores, 4,1 Pflops)**

1 656 Intel Skylake 8168 bi-processors nodes - 2,7 GHz, 24 cores/proc. 192 GB of DDR4 memory / node

Post : Irene xlarge
Dods files : http://vesg.ipsl.upmc.fr/… (only WORK space)
Assistance : hotline.tgcc@cea.fr or 01-77-57-42-42
Infos : irene.info or http://www-hpc.cea.fr/fr/complexe/tgcc.htm

TGCC (1/2)

- Filesystems:
  - *HOME : small space, back up*
  - *WORKDIR : working space and archiving of small files – quota 1Tb, no back up, no purge*
  - *STOREDIR : only for archive of big files – min 1Gb – quota 100 000 inodes, on tape*
  - *SCRATCHDIR : big working space, can be purged after 40 days*

- We advise you to copy the **IPSL plateforme environment** in the `HOME` of your account and install models into your project `WORK`. All information is in the IPSL Documentation:

https://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc/ComputingCenters/TGCC

TGCC (2/2)

- Documentation :
  - https://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc/ComputingCenters/TGCC and http://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc/ComputingCenters/TGCC/Irene
  - Command on irene : irene.*info*
  - *https://www-tgcc.ccc.cea.fr* (private access for user only)

- Assistance : 01 77 57 42 42, hotline.tgcc@cea.fr

- Connexion :
  - ssh -X login@irene-fr.ccc.cea.fr
  - for group quota, use *ccc_quota -g genXXXX*
  - for personal quota, only use *ccc_quota* to check

Quota are attributed for each project for all the group and not individually, so be careful of your own practices to avoid blocking all the group

IDRIS (1/2)

- Filesystems:
  - *HOME : small space, back up*
  - *WORK : working space, no back up, no purge*
  - *STORE : for archive, no back up*
  - *SCRATCH : big working space, is purged after 30 days, not save*
  - *JOBSCRATCH : temporary execution directory (for batch jobs),destroyed at the end of the job*

We advise you to copy the IPSL platform environment in the HOME of your account :

https://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc/ComputingCenters/IDRIS

IDRIS (2/2)

- Documentation :
  - https://forge.ipsl.jussieu.fr/igcmg_doc/wiki/DocBenvAidris
  - http://www.idris.fr
- Assistance : 01 69 35 85 55, assist@idris.fr
- Connexion :
  - `ssh -X login@jean-zay.idris.fr` *(JeanZay)*
  - `ssh -X login@jean-zay-pp.idris.fr` *(JeanZayPP)*

- The password is the same on *jeanzay* and *jeanzaypp*. Use *passwd* on one of the machines to change it.

- Quota for the whole group. Use *idrquota -s* and *idrquota -w* to check for $STORE and for $WORK.

Quota are attributed for each project for all the group and not individually, so be careful of your own practices to avoid blocking all the group

MesoScale clusters

- Modipsl and libIGCM are also adapted to be used at
  - *Obelix* – LSCE cluster
    (http://forge.ipsl.jussieu.fr/igcmg_doc/wiki/DocBenvClsce)
  - *Ciclad* and *ClimServ* – IPSL clusters
    (http://forge.ipsl.jussieu.fr/igcmg_doc/wiki/DocBenvDipsl)
- Following functionalities are adapted
  - Compilation
  - Computing job
  - Rebuild
  - TS-SE
- Not adapted : pack, monitoring and full coupled-model

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Sciences de l'environnement

IPSL Compile and run environment

Software infrastructure based on **modipsl** and **libIGCM** tools which allow to :

modipsl

- **predefine** and **extract** standard configurations
- **compile** sources from different components, coupling interfaces

libIGCM

- **adapt** and **launch** predefined experiments
- **monitor** simulations
- **produce** and **store** results from models
- **produce**, **store** and **distribute** some analysis

Tools available for usage at TGCC, IDRIS, LSCE and IPSL cluster.

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What is a configuration ? (1/2)

A configuration is a combination of one or several models (components) coupled together

- For example the configuration LMDZOR contains the two models LMDZ and ORCHIDEE.

A configuration can be used for different experiments, using different set up, choice of parameters, etc.

- For example with the configuration LMDZOR you can run experiments with different parameterizations for the physics in the atmosphere.

- For example with the configuration LMDZOR you can run an experiment with only LMDZ

What is a configuration ? (2/2)

IPSLCM6.2

- LMDZ (Atmosphere)
- ORCHIDEE (Surface)
- NEMO – LIM – PISCES (Ocean)
- INCA (chemistry – aerosol Tropo)

→

IPSL.ESM.6
LMDZ + ORCHIDEE + NEMO – LIM – PISCES + INCA

IPSLCM6
LMDZ + ORCHIDEE + NEMO – LIM – PISCES

LMDZORINCA
LMDZ + ORCHIDEE + INCA

LMDZOR
LMDZ + ORCHIDEE

LMDZ
LMDZ

1 configuration – 1 executable

Distributed configurations (1/2)

Actual configs : Recommended version of standard configurations. Parameters set up is the same for a component in all configurations of the “v6 family”. v6 configurations are actually use for CMIP6.

IPSLCM6.1.X-LR	Version uses for CMIP6 of the coupled model *(currently IPSLCM6.1.11-LR)* Person in charge: A. Caubel
NEMO_v6	Forced ocean model OPA-LIM3-PISCES. Person in charge: C. Ethé.
LMDZOR_v6	LMDZ coupled with ORCHIDEE. Person in charge: J. Ghattas
LMDZORINCA_v6	LMDZOR_v6 coupled with INCA. Person in charge: A. Cozic

Distributed configurations (2/2)

LMDZREPR_v6	LMDZ coupled with REPROBUS Person in charge: L. Falletti
IPSLCM5A2	Previous version of the coupled model (*IPSLCM5*) used on a very low resolution (VLR) grid. Person in charge : A. Caubel
ORCHIDEE_trunk/ ORCHIDEE_2_0	Forced continental surfaces model ORCHIDEE, with latest version on the trunk of ORCHIDEE or tag 2_0. Person in charge: J. Ghattas.
RegIPSL	Regional coupled climate model of IPSL. Person in charge: R. Pennel.

General recommendation :

- *inform person in charge* before launching new studies based on one of these configurations, especially for coupled models.
- Read model and configuration documentation before using it !!!

IPSL-CM performances: IRENE

Configuration	Number of Core	Simulated Year Per Day
IPSL-CM6.2-MR1 *ATM: 256x256x79 / OCE: eORCA1*	1200	8.8
IPSL-CM6.1.11-LR *ATM: 144x144x79 / OCE: eORCA1*	976	16
IPSL-CM5A2-VLR *ATM: 96x96x39 / OCE: ORCA2*	437	95
NEMO *eORCA1-LIM3-PISCES*	433	20
LMDZOR_v6.1.10-LR *LMDZ144x144x79*	576	20

Benchmark in January 2019

IPSL-CM performances: JeanZay

Configuration	Number of Core	Simulated Year Per Day
IPSL-CM6-MR1 *ATM: 256x256x79 / OCE: eORCA1*	**1248**	
IPSL-CM6.1.11-LR *ATM: 144x144x79 / OCE: eORCA1*	**1071**	**24**
IPSL-CM5A2-VLR *ATM: 96x96x39 / OCE: ORCA2*	**399**	**93**
NEMO *eORCA1-LIM3-PISCES*	**428**	**40**
LMDZOR_v6.1.11-LR *ATM: 144x144x79*	**711**	**23**

Benchmark in January 2020

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HPC performances

System factors

- Architecture : CPU (SMP, MPP), accelerators (GPU, MIC)
- Memory hierarchy (register - cache - main memory - disk)
- I/O configuration- Parallel file system (supporting parallel I/O)
- Compiler
- Connecting network between processors

Application factors

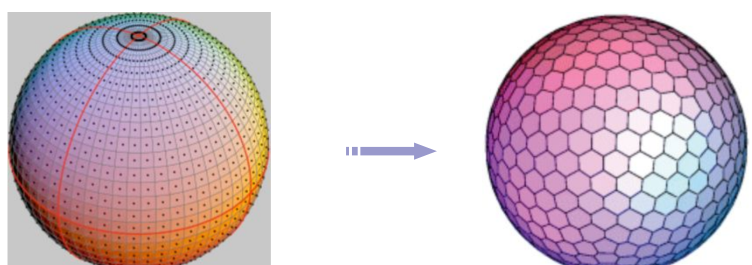
- Programming language (C/C++, Fortran, CUDA, ...)
- Algorithms and implementation
- Memory management
- Libraries (e.g. math libraries)
- **Compiler optimization flags**
- **Use of I/O**
- **MPI / OpenMP**

IPSL ESM : HPC perspectives

- **CMIP6 workflow** : integrate the CMIP6 specific workflow for “usal runs”
- **Next developments**
  - **XIOS 3.0**
    - XIOS multithreaded (OpenMP) to target « many cores » architectures
    - Coupling functionalities
  - **Atmospheric component : new dynamical core DYNAMICO** (early 2020 in IPSLCM6)
    - better performances/scalability
    - MPPs, MICs, GPUs architectures.

→ *A working configuration currently exist: ICOLMDZOR_v7_work*

Lon-lat grid



Icosahedral grid