Introduction to IPSL modeling tools and environment (modipsl and libIGCM)

Institut
Pierre-Simon
Laplace

January 29th 2021, GatherTown
IPSL « Plateforme » group

Outline

1. **Introduction**
2. IPSL models
3. High Performance Computing context
4. Which supercomputer(s) for us ?
5. Tools, configurations and performances
6. To go further
7. Now for today

What this training is for?
(and isn't)

Goals of this course:

- To have an overview of the tools used to launch Earth climate models, and to know how to use them.
- To know and to understand the environments at your disposal (supercomputers).
- To get an idea of the context at IPSL in terms of work teams and models.

Not seen:

- We will not explain how each model works (parameters, specific features), how to launch a zoom or a specific resolution.
- You will not see details about parallelisation.

=> look for dedicated trainings

Institut Pierre-Simon Laplace

Institut Simon Laplace (IPSL)

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

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

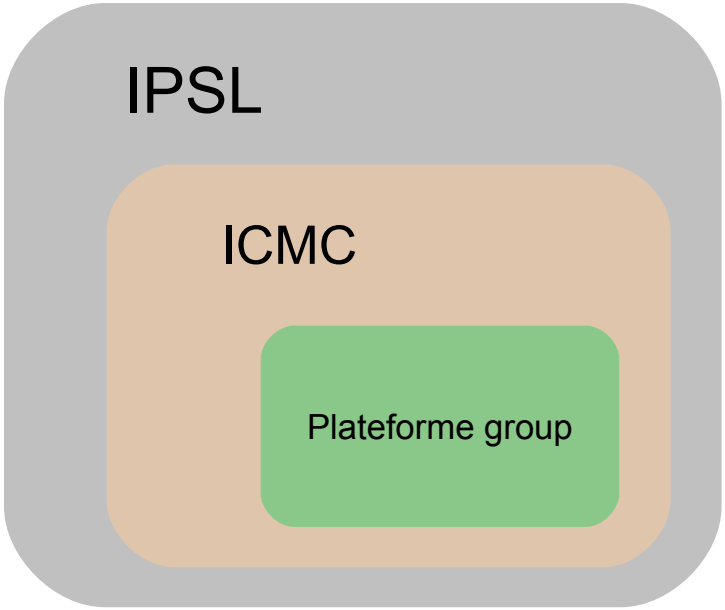
IPSL Climate Modeling Centre (ICMC http://icmc.ipsl.fr)

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



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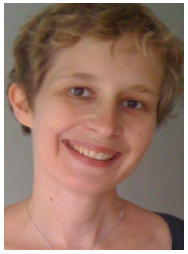
Plateforme-group members

Arnaud Caubel



Anne Cozic

Romain Pennel

Christian Ethé

Jérôme Servonnat

Simona Flavoni

Laurent Fairhead

Eliott Dupont

Josefine Ghattas

Nicolas Lebas

Yann Meurdesoif

Lola Falletti

Olivier Marti

Olivier Boucher

Thibaut Lurton

Sébastien Nguyen

Guillaume Levavasseur

Institut Pierre-Simon Laplace

Plateforme-group members

Arnaud Caubel	Coupled model / CMIP6 wokflow	**Josefine Ghattas**	Orchidee model
Anne Cozic	INCA model	**Nicolas Lebas**	Ensembles, StratAER (LMDZ)
Romain Pennel	Regional model	**Yann Meurdesoif**	Dynamico model / XIOS
Christian Ethé	NEMO & PISCES model	**Lola Falletti**	Reprobus model
Jérôme Servonnat	CliMAF / C-ESM-EP	**Olivier Marti**	weight on coupling
Simona Flavoni	Decadal and Ensembles	**Olivier Boucher**	ICMC director
Laurent Fairhead	LMDZ model	**Thibaut Lurton**	CIMP6 coupled simulations
Eliott Dupont	Data Management Project	**Sébastien Nguyen**	paleoclimate model
Guillaume Levavasseur	Thredds / Esgf		

\+ For all : libIGCM, modipsl, supercomputers, and lot of things

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IPSL Earth System Model

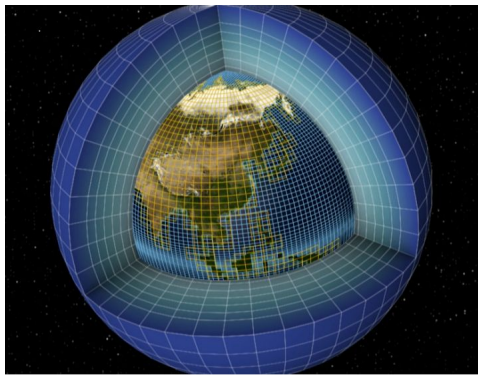
Control environment:
libIGCM/modipsl

In/Out server:
XIOS

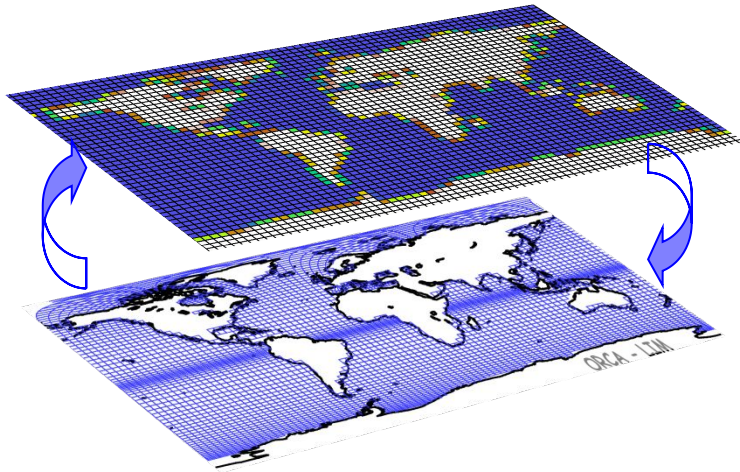
INCA/REPROBUS
(atmospheric chemistry, aerosols)

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*

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_v6.1.11	*ATM 144x144x79*
ICOLMDZOR_v7	
IPSLCM6.1.11-LR	*ATM 144x144x79 / OCE ORCA1*
IPSLCM6.2-MR1	*ATM 256x256x79 / OCE ORCA1*

https://orchidee.ipsl.fr

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:

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

LMDZOR_v6.1.11	*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_v6.1.11 *ATM 96x96x39 (AP) or 144x144x79 (NP)*
LMDZORINCA_v6.2 *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*

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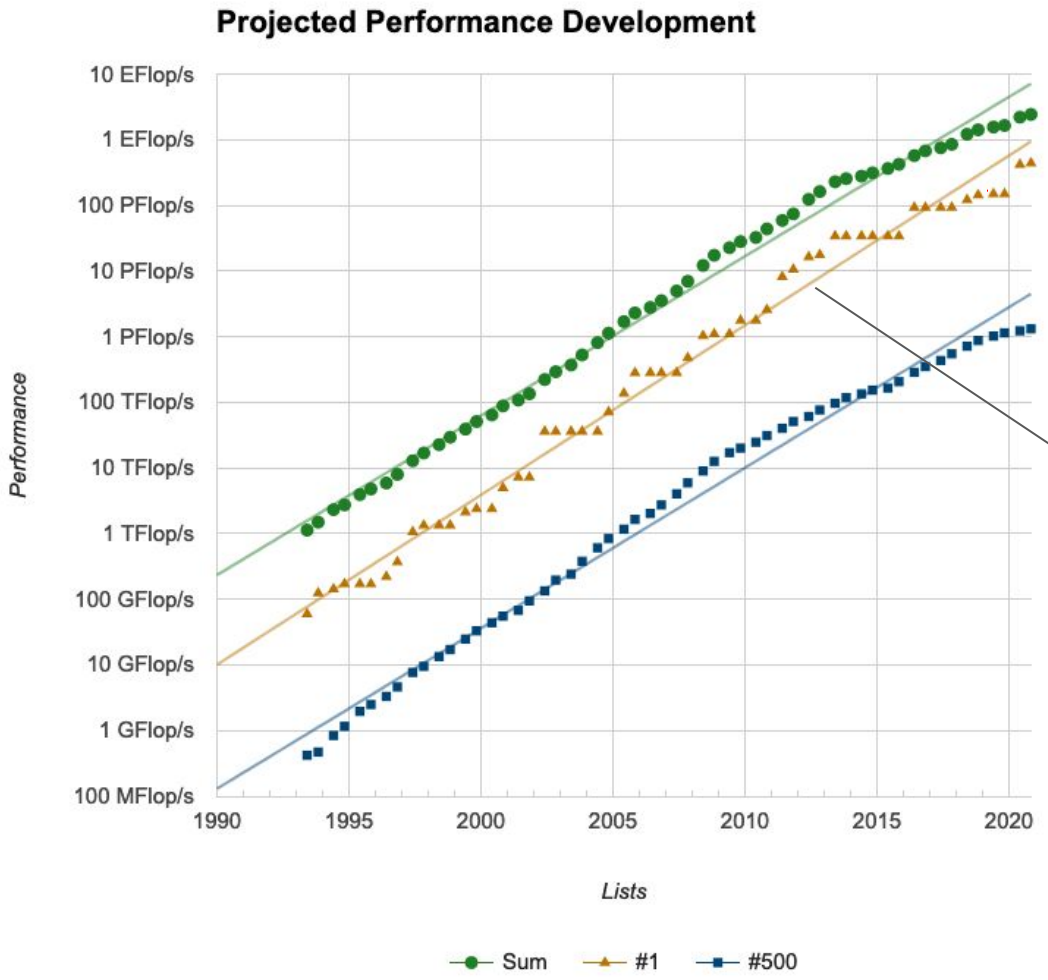
Supercomputer - *top500* timeline



Jean Zay & Joliot-Curie ROME/SKL

nov. 2020 TOP500.org

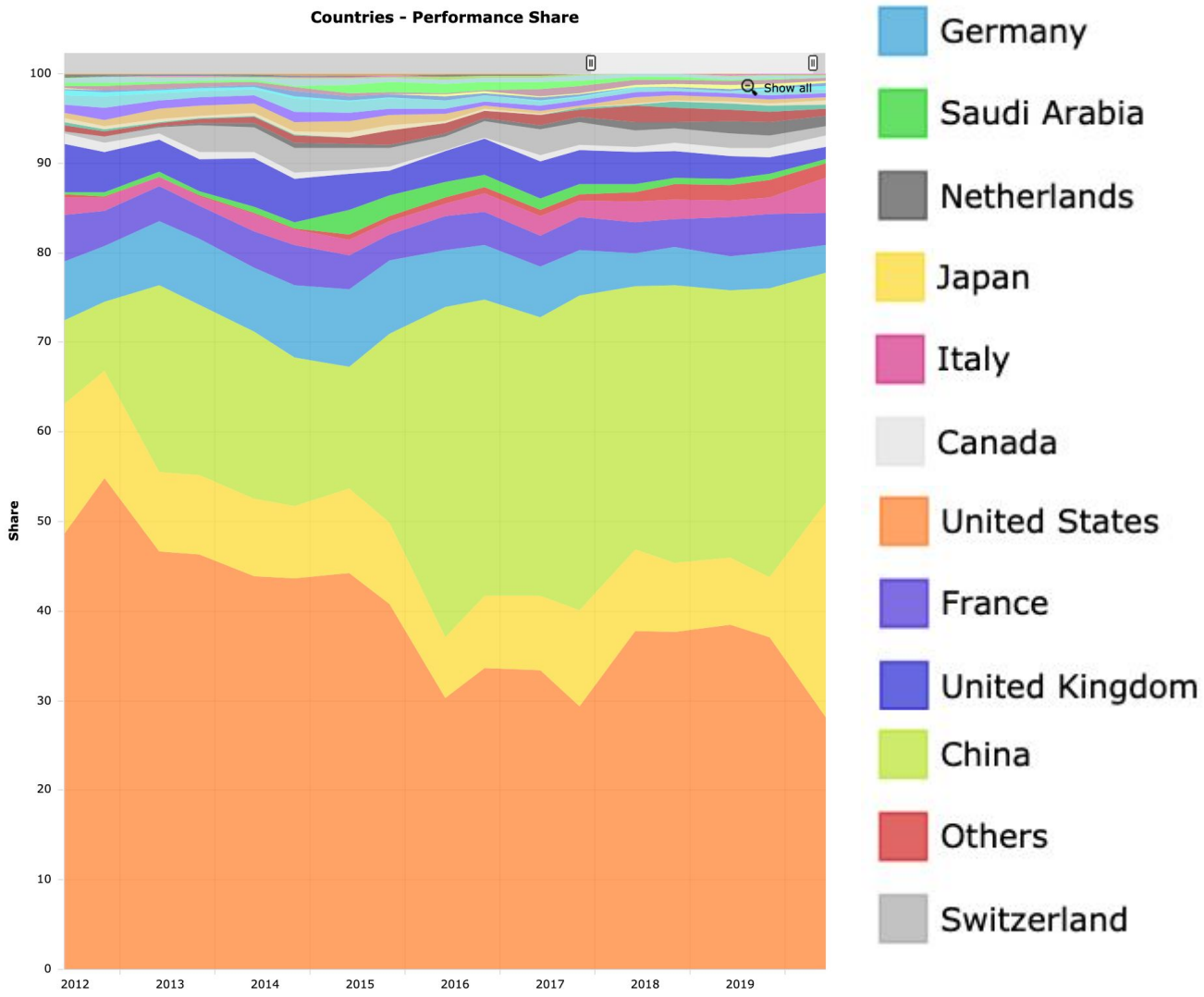
Supercomputer - *top500* ranking

Rank	Site	System	Cores	Rmax (TFlop/s)
1	**RIKEN Center for Computational Science Japan**	**Fugaku Supercomputer** Fujitsu	**7 630 848**	**442 010**
2	DOE/SC/Oak Ridge National Laboratory United States	**Summit** IBM / NVIDIA	2 414 592	148 600
3	DOE/NNSA/LLNL United States	**Sierra** IBM / NVIDIA	1 572 480	94 640
4	National Supercomputing Center in Wuxi China	**Sunway TaihuLight** Sunway MPP	10 649 600	93 014
5	NVIDIA Corporation United States	**Selene** AMD / NVIDIA	555 520	63 460

Supercomputer - *top500* ranking

Rank	Site	System	Cores	Rmax (TFlop/s)	Power (kW)
1	**Japan**	Fujitsu	7 630 848	442 010	29 899
2	**United States**	IBM	2 397 824	143 500	10 096
3	**United States**	IBM/NVIDIA	1 572 480	94 640	7 438
4	**China**	NRCPC	10 649 600	93 014	15 371
5	**United States**	NVIDIA	555 520	63 460	2 646
6	**China**	NUDT	4 981 760	61 444	18 482
7	**Germany**	Atos	449 280	44 120	1 764
8	**Italy**	Dell EMC	669 760	35 450	2 252
9	**United States**	Dell EMC	448 448	23 516	-
10	**Saudi Arabia**	Cray	672 520	22 400	-

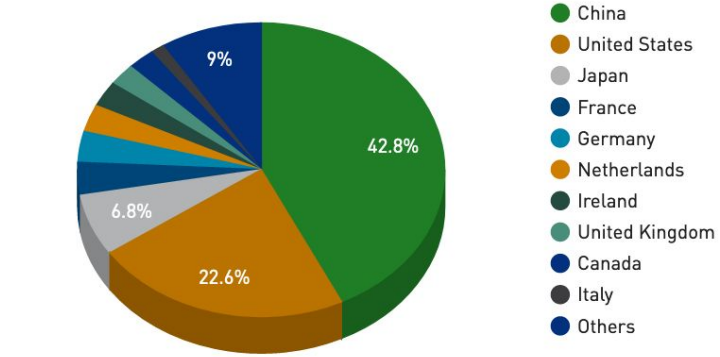
HPC performances / country



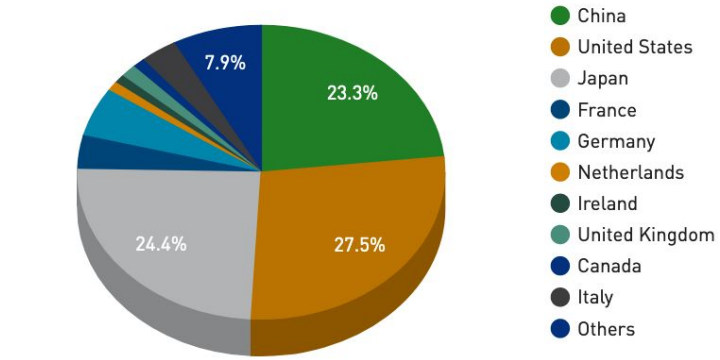
Cumulated performances by country over time

HPC systems & perfs / country

Countries System Share



Countries Performance Share



Supercomputer - Power efficiency

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x3 x3

Supercomputer - Power efficiency

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9	**United States**	Dell EMC	448 448	23 516	-
10	**Saudi Arabia**	Cray	672 520	22 400	-

x3 x3 == x2

Supercomputer - *green500* ranking

Rank	#Top 500	System	Rmax (TFlop/s)	Power (kW)	Power Efficiency (GFlops/watts)
1	**170**	**SuperPOD** NVIDIA - USA	**2 356**	**90**	**26.195**
2	330	**MN-3** Pref Networks - Japan	1 652	65	26.039
3	7	**JUWELS** Atos - Germany	44 120	1 764	25.008
4	146	**Spartan2** Atos - France	2 566	106	24.262
5	5	**Selene** NVIDIA - USA	63 460	2 646	23.983
...	...	...	...	...	...
10	**1**	**Fugaku** Fujitsu - Japan	442 010	29 899	15.418

Supercomputers in France

Rank	Site	System	Cores	Rmax (TFlop/s)	Power (kW)
1	RIKEN Center for Computational Science	**Fugaku** Fujitsu	7 630 848	442 010	29 899
…	…	…	…	…	
18	Total Exploration Production	**Pangea III** IBM	291 024	17 860	1 367
24	CEA	**Tera-1000-2** Atos	561 408	11 965	3 178
30	Meteo France	**Taranis** Atos	294 912	8 191	1 672
34	Meteo France	**Belenos** Atos	294 912	7 683	1 655
38	**CEA/TGCC-GENCI**	**Joliot Curie ROME** Atos	**197 120**	**6 988**	**1 436**
64	**CNRS/IDRIS-GENCI**	**Jean Zay** HPE	**93 960**	**4 478**	**-**
72	**CEA/TGCC-GENCI**	**Joliot Curie SKL** Atos	**79 488**	**4 065**	**917**

Why do we need supercomputer ?

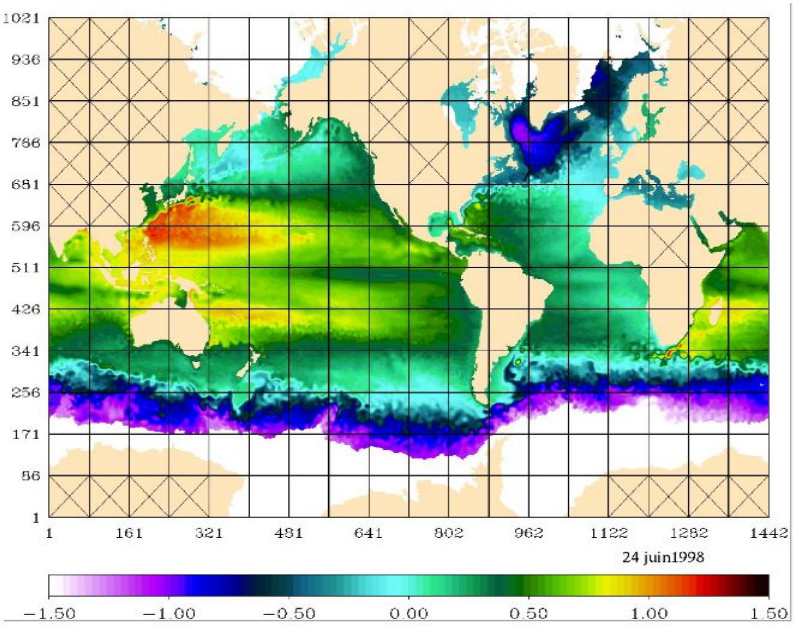
⇒ *parallelization*!

All models are parallelised with MPI or MPI+OpenMP.

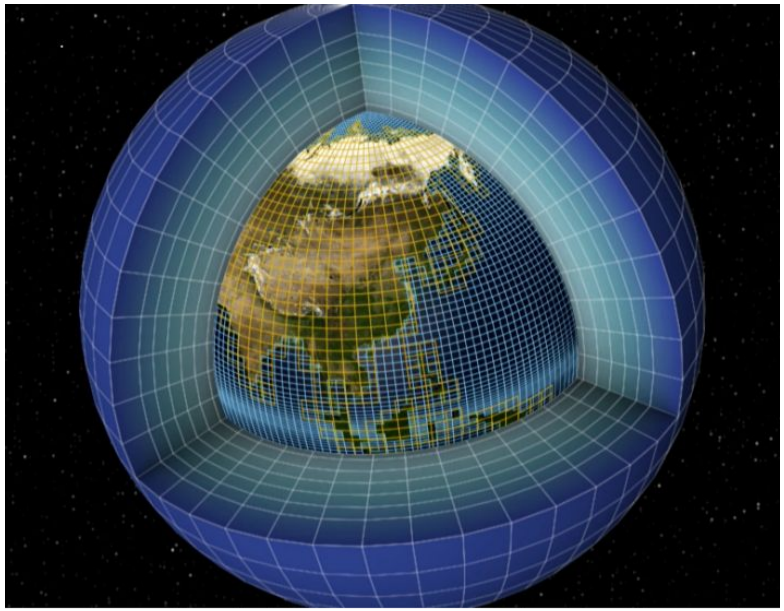
Parallelisation allows to run the same executable on several sub-domains to reduce the real time of the execution.

MPI (**M**essage **P**assing **I**nterface) is used to divide **lon/lat grid** splitting latitudes and **OpenMP** (**Open M**ulti-**P**rocessing) to parallelise the **vertical axis** through shared memory threads.

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



NEMO model parallelism (MPI only)



LMDZ model uses hybrid MPI/Open MP parallelisation

What does HPC usage imply for you? (1/2)

Environment:

- A supercomputer is not a personal computer! Each supercomputer is unique and has to have a dedicated staff to maintain its hardware and software.
- Its usage requires good skills to understand how to work well with.
- This is a very complex system that could implies an increase of instabilities on filesystem, computation nodes, high speed network...
- All resources are **SHARED** between all users (CPU hours, storage, bandwidth). *You need to adopt good practices to avoid to perturb other people. For example, you can be forced to clean your space very quickly if you didn't realize you used too much storage.*
- Computation centers have a **high level security policy**, so you can't connect to them from everywhere and you need to respect rules.

CPU hours on Tier-1 (national) and Tier-0 (European) centers:

- Computing hours are attributed through bi-annual GENCI or PRACE calls (technical and scientific goals, roadmap, code efficiency and evaluation)

What does HPC usage imply for you? (2/2)

General rules and advises:

- Quota: be careful with it! => Computing hours, storage, inodes (=number of file-system object such as file or directory)
- Jobs: priority algorithm between jobs (depending on the resources you request), max number of jobs running at the same time
- Use your computing hours regularly (to avoid peak usage of the machine)
- Security: never share your password!

If rules are not respected, computation centers could:

- remove amount of hours of the project
- block project jobs
- suspend account
- block filesystems (inodes or storage quota)

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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 ROME (197 120 cores, ~7 Pflops)**

2292 AMD Rome (Epyc) bi-processors nodes - 2,6 GHz, 64 cores/proc. 256 GB of DDR4 memory / node

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
  - http://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc/ComputingCenters/TGCC/Irene
  - http://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc/ComputingCenters/TGCC/IreneAmd
  - 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` (SKL)

  or `ssh -X login@irene-amd-fr.ccc.cea.fr` (ROME)
  - 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/Doc/ComputingCenters/IDRIS
  - 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/Doc/ComputingCenters/LSCE)
  - *Ciclad* and *ClimServ* – IPSL clusters (http://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc/ComputingCenters/IPSL)
- Following functionalities are adapted
  - Compilation
  - Computing job
  - Rebuild
  - TS-SE
- Not adapted : *pack, monitoring and full coupled-model*

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IPSL Compile and run environment

Software infrastructure based on **modipsl**, **libIGCM** and **XIOS** 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

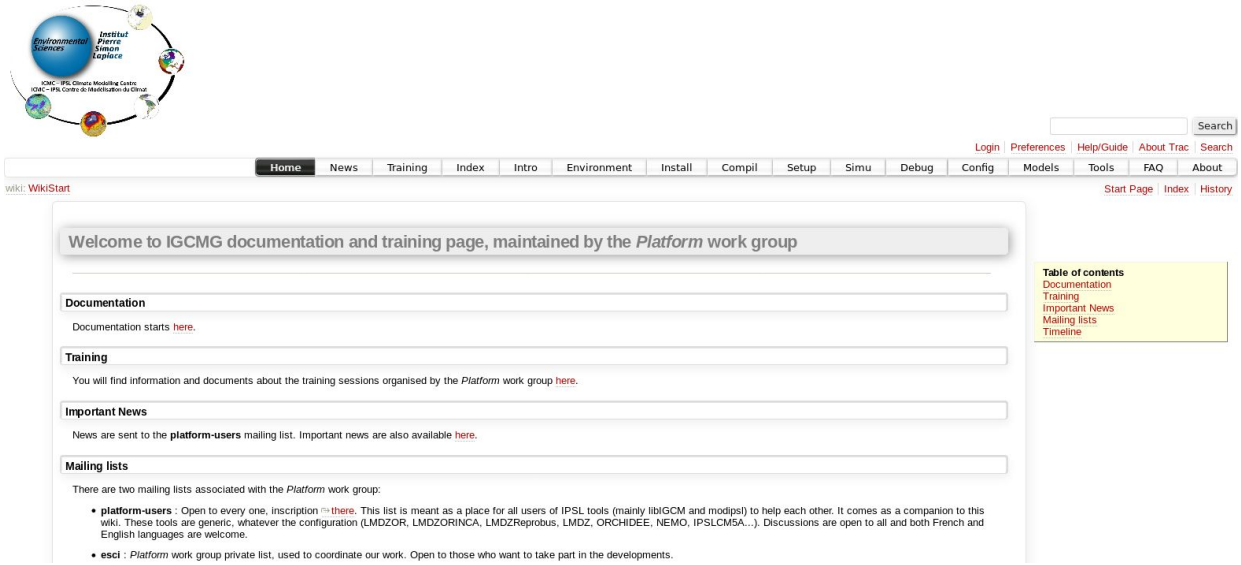
XIOS

- **read** input files
- **write** and **interpolate** results from models in parallel

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

Web documentations & mailing list

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



- **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 colleagues questions.

→ ***All users need to subscribe***

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 setups, input 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

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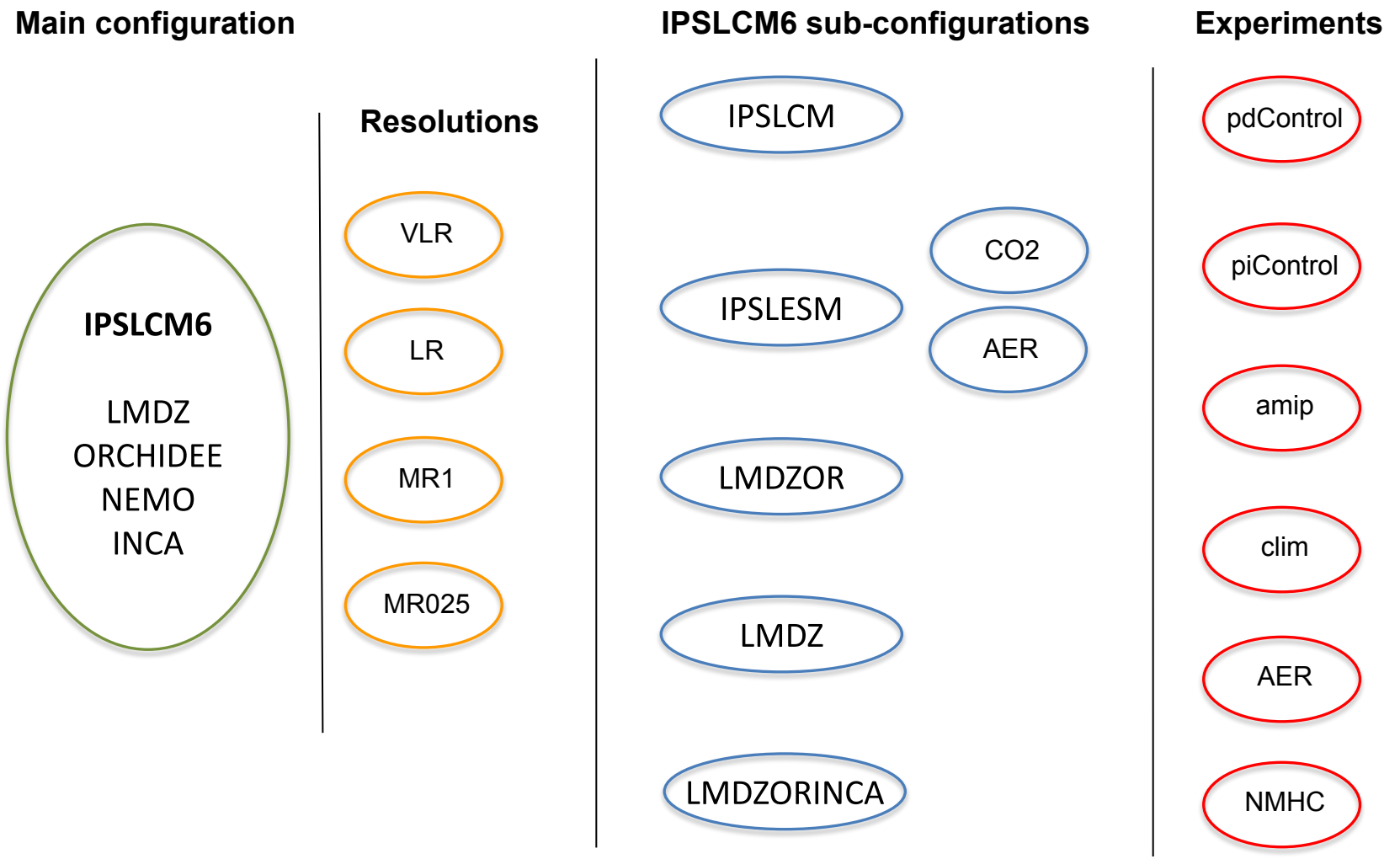
What is a configuration ? (2/2)



1 main configuration = 1 executable per resolution = several experiments (from sub-configurations)

Distributed configurations (1/3)

Actual configs : Recommended version of standard configurations. Parameters set up is the same for a component in all configurations of the "v6 family".

There are 3 type of v6 configurations:

1. v6.1 / v6.1.11 ⇒ versions used for CMIP6
2. v6.2 / v6.2_work ⇒ versions under development to improve CMIP6 version
3. v6.3 - 4 - 5 .. ⇒ versions to prepare next generation of configurations

Mains configurations proposed in this family are declined in v6.1 and several other types.

Distributed configurations (2/3)

IPSLCM6	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
LMDZREPR_v6	LMDZ_v6 coupled with REPROBUS Person in charge: L. Falletti

Distributed configurations (3/3)

IPSLCM5A2	Previous version of the coupled model (*IPSLCM5*) used on a very low resolution (VLR) grid. Person in charge : A. Caubel
IPSLCM5A2-CHM	coupled model in low resolution with an interactive atmospheric chemistry . Person in charge : A. Cozic
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 perfs: IRENE SKL

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 2021

IPSL-CM perfs: IRENE AMD

Configuration	Number of Core	Simulated Year Per Day
IPSL-CM6.2-MR1 *ATM: 256x256x79 / OCE: eORCA1*	**1196**	**8**
IPSL-CM6.1.11-LR *ATM: 144x144x79 / OCE: eORCA1*	**1952**	**24**
IPSL-CM5A2-VLR *ATM: 96x96x39 / OCE: ORCA2*	**604**	**97**
NEMO *eORCA1-LIM3-PISCES*	**640**	**23.5**
LMDZOR_v6.1.10-LR *LMDZ144x144x79*	**1136**	**25**

Benchmark in January 2021

IPSL-CM perfs: Jean Zay

Configuration	Number of Core	Simulated Year Per Day
IPSL-CM6.2-MR1 *ATM: 256x256x79 / OCE: eORCA1*	-	-
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 2021

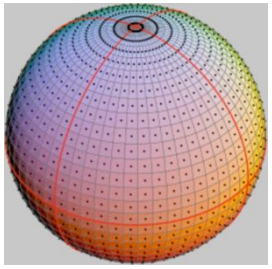
Outline

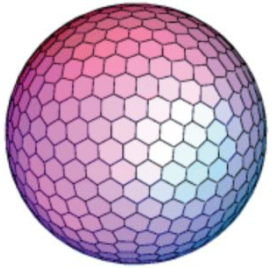
1. Introduction
2. IPSL models
3. High Performance Computing context
4. Which supercomputer(s) for us ?
5. Tools, configurations and performances
6. **To go further**
7. Now for today

IPSL ESM : ongoing developments

- **CMIP6 workflow**: integrate the CMIP6 specific workflow for “usual runs”
- **NEMO** v4 and **SI3** (new sea-ice model)
- **Next developments**
  - **XIOS 3.0** (XIOS multithreaded (OpenMP) to target « many cores » architectures, Coupling functionalities)
  - Ensemble runs (specific I/O design)
  - Zoomed configuration
  - **Atmospheric component : new dynamical core DYNAMICO**
    - better performances/scalability
    - new architectures (GPUs, MPPs, MICs…)

Lon-lat grid





Icosahedral grid

Training courses

Training courses at IPSL:

- *IPSL modeling tools and environment* (contact lola.falletti@latmos.ipsl.fr), current session
- *LMDZ training course* (contact Marie-Pierre.Lefebvre@lmd.jussieu.fr), next session in December 2021
- *ORCHIDEE Introduction* 2-days course (contact orchidee-help@ipsl.jussieu.fr), past session was in January 2021
- *CLIMAF/C-ESM-EP training course* (contact jerome.servonnat@lsce.ipsl.fr), next session in **April 2021**
- XIOS training course (contact yushan.wang@lsce.ipsl.fr), next sessions **March** (15-19) **and April** (12-16) **2021**

Other suggested training courses:

- *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 (not available actually)
- UNIX course
- http://formation-calcul.fr → give an inventory of training course (numeric – calcul – hpc) in France

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Now it's your turn to practice!

Advices and informations for this training:

- In **gather town**, each group have access to a document with informations for the training. Otherwise, you can also find some informations here: https://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc/Training
- **Not all exercises are meant to be done**: select topics based of your knowledge of modipsl/libIGCM (beginner or advanced user) and your needs.
- **Take your time to read everything in the doc!** All is explained.
- **Use your account on Jean Zay or Irene** (if you have one) in preference to Ciclad.

Don't hesitate to ask questions! ☺