How to connect to today's training account?

Informations for today's training:

Today's on **JeanZay specific training accounts**:

- Connect on "**`ipcours22.`**....." session.
- Your login: use the **`cforXXX`** login/password provided to you *(complete the form with your name and signature)*

If you need to **switch between qwerty** and **azerty** you can use the command **`alt+shift`**.

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

Institut
Pierre-Simon
Laplace

January/February 2024, IDRIS
IPSL « Platforme » group

Training timetable

Schedule for these 2 days:

- 9am-9:30am welcome ; 9:30am-5:30pm training.
- Lunch around 11:45
- After this presentation, all training will be practical work. Take breaks at your convenience.

Don’t hesitate to ask questions during the training!

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 is not)

Objectives of this course:

- Have an overview of the tools used to launch Earth climate models, and to know how to use them.
- Know and understand the environments at your disposal (supercomputers).
- 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 non-standard resolution.
- You will not see details about parallelisation.

=> look for dedicated trainings!

Institut Pierre-Simon Laplace

Institut Simon Laplace (IPSL)

IPSL gathers 8 laboratories for which research topics concern the global environment.

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

IPSL Climate Modeling Centre (ICMC https://cmc.ipsl.fr/)

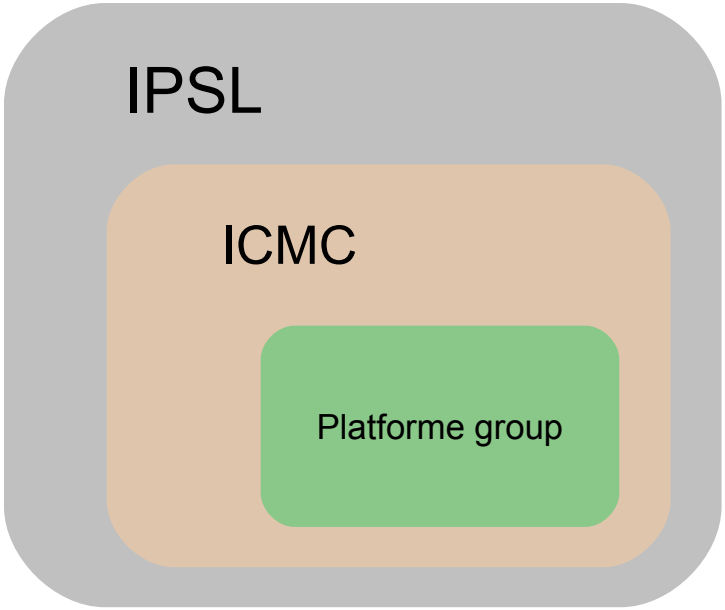
Activities articulated around :

- The development of an integrated model of the Earth system
- Running and analysing 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 Platforme group : in charge of the development of modipsl, libIGCM, XIOS usage, metric tools deployment

To contact the list: ***platform-users@listes.ipsl.fr***



Institut Pierre-Simon Laplace

Platform-group members


Arnaud Caubel


Anne Cozic


Romain Pennel


Christian Ethé


Jérôme Servonnat


Laurent Fairhead


Olivier Marti


Josefine Ghattas


Nicolas Lebas


Lola Falletti


Thibaut Lurton


Sébastien Nguyen


Guillaume Levavasseur


Patricia Cadule


Renaud Person

Platform-group members

Patricia Cadule	Orchidee model	**Arnaud Caubel**	Coupled model / CMIP6 wokflow
Anne Cozic	INCA model	**Christian Ethé**	NEMO & PISCES model
Laurent Fairhead	LMDZ model	**Lola Falletti**	REPROBUS model
Josefine Ghattas	ORCHIDEE model	**Nicolas Lebas**	Ensembles, StratAER (LMDZ)
Guillaume Levavasseur	Thredds / Esgf	**Thibaut Lurton**	CMIP6 coupled simulations
Olivier Marti	Weight on coupling	**Sébastien Nguyen**	Paleoclimate model
Romain Pennel	Regional model	**Renaud Person**	NEMO & PISCES model
Jérôme Servonnat	CliMAF / C-ESM-EP		

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

ICMC head : Masa Kageyama, Julie Dehayes, Laurent Bopp, Christian Ethé

Outline

1. Introduction
2. **IPSL models**
3. High Performance Computing context
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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 / SI3** : 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_v6.2	*NEMO 3.6*
NEMO_v7	*NEMO 4*

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 several variants for the Earth and other planets (Mars, Titan, Venus, Exoplanets). It is first and foremost a research tool.

2 dynamic cores:

- **Regular**: based on regular Lat x Lon 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_v6.2.2	*ATM 144x144x79*
IPSLCM7	*ATM 144x144x79 (reg) or ATM nbp40 (ico)*
IPSLCM6.2.2	*ATM 144x144x79 / OCE ORCA1*
	ATM 256x256x79 / OCE ORCA1
LMDZORINCA_v6.2.2	*ATM 144x144x79*
LMDZREPR_v6.2.2	*ATM 144x144x79*

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

IPSLCM7	*ORCHIDEE_2_2 (default) or ORCHIDEE_4 trunk*
LMDZOR_v6.2.2	*ATM 144x144x79 / ORCHIDEE_2_2*
LMDZOR_v6.4_work	*ATM 144x144x79 / ORCHIDEE trunk*
ORCHIDEE_4_1	*ORCHIDEE offline latest tag*
ORCHIDEE_trunk	*ORCHIDEE offline with the 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_v6.2.2	*ATM 96x96x39 (AP) or 144x144x79 (NP)*
IPSLCM7	*ATM 144x144x79 regular and ico*

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_v6.2	*ATM 144x144x79*

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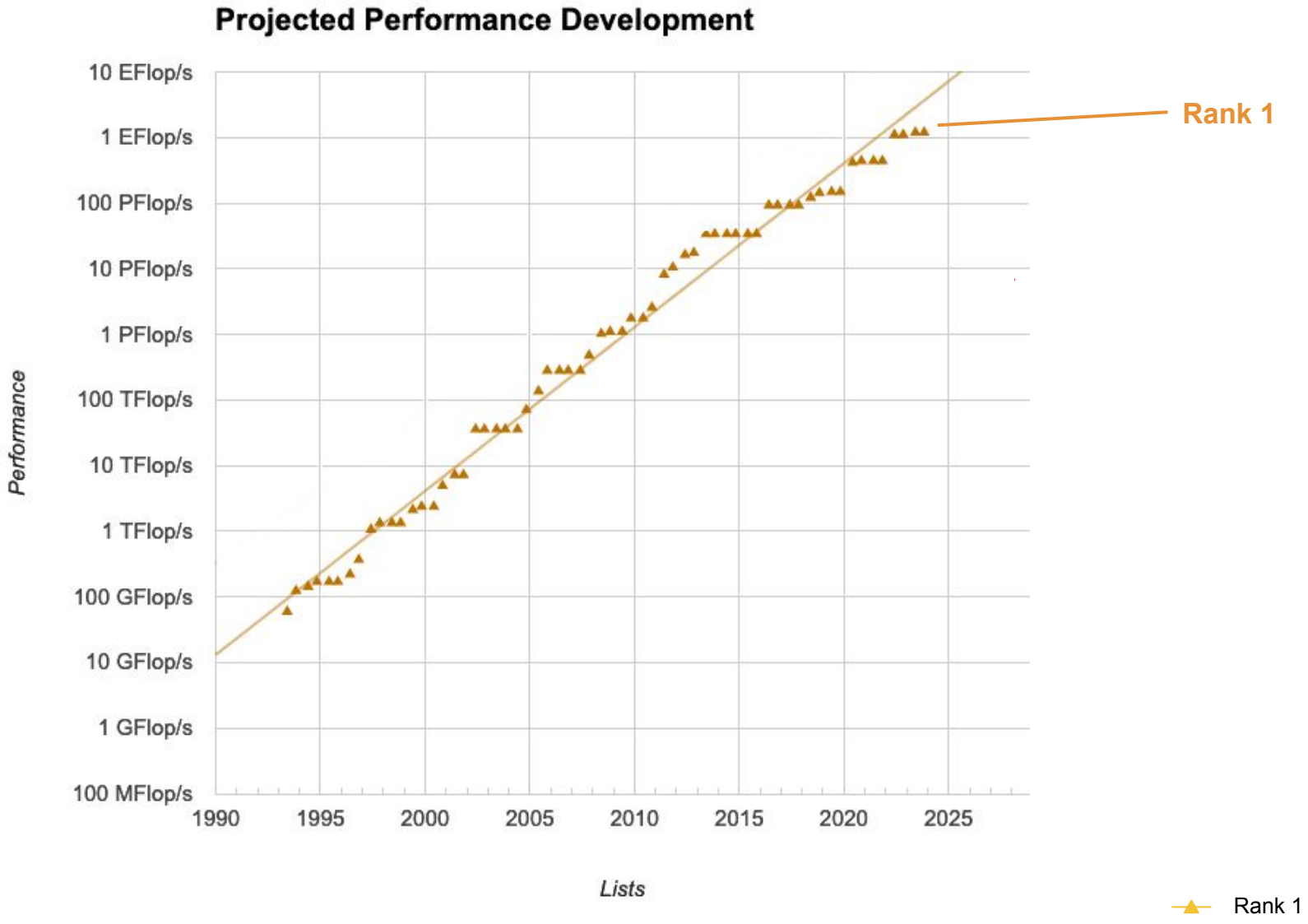
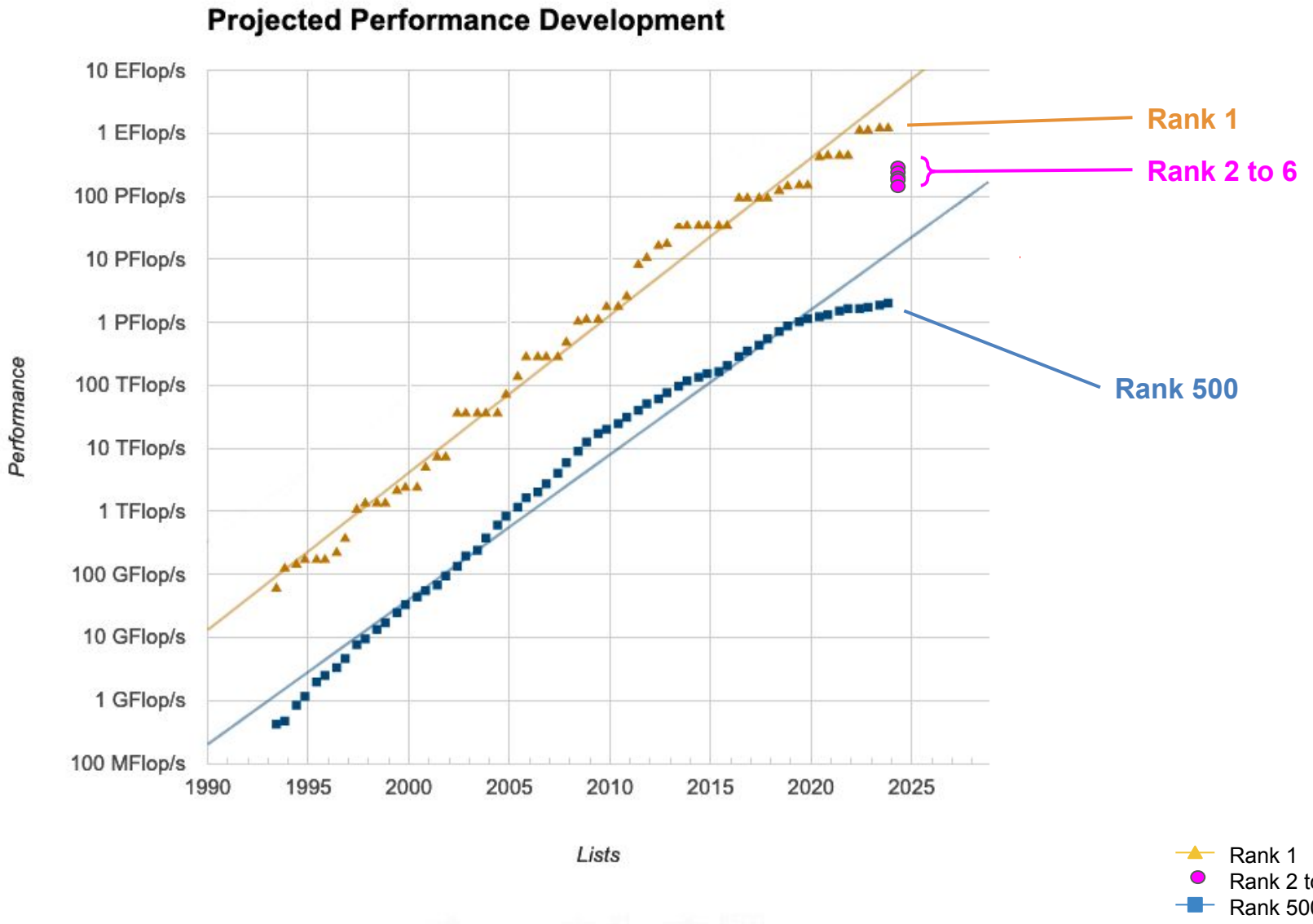
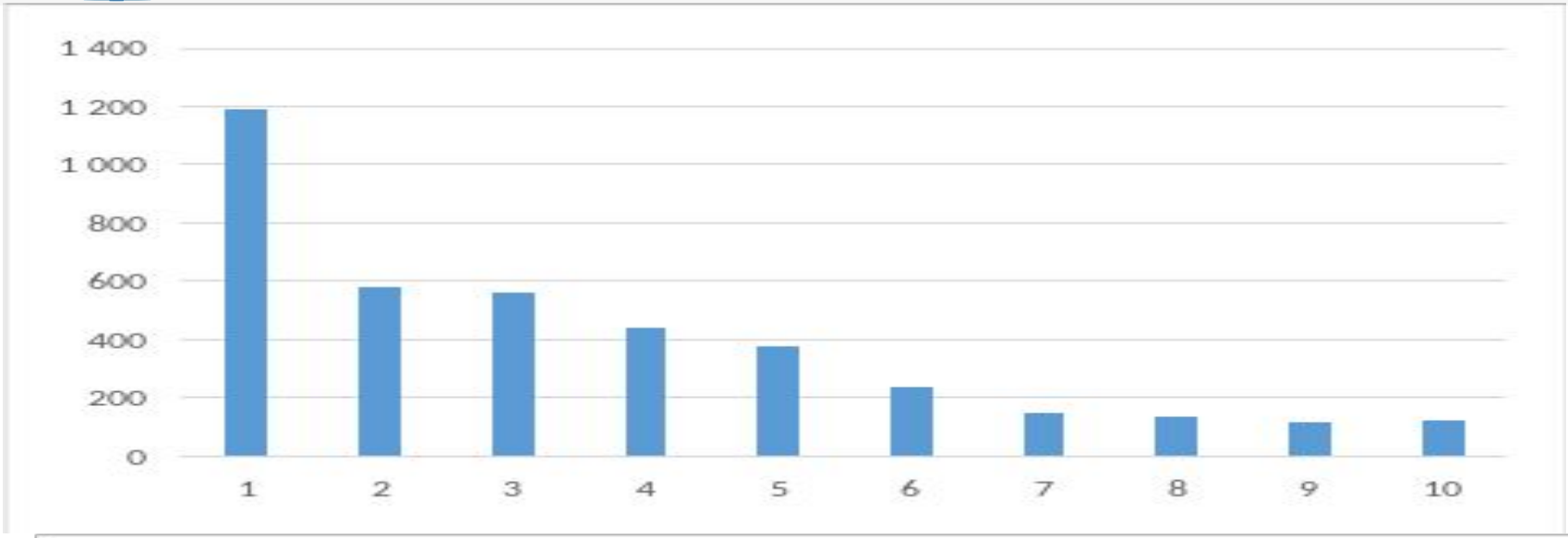
Supercomputer - *top500* timeline

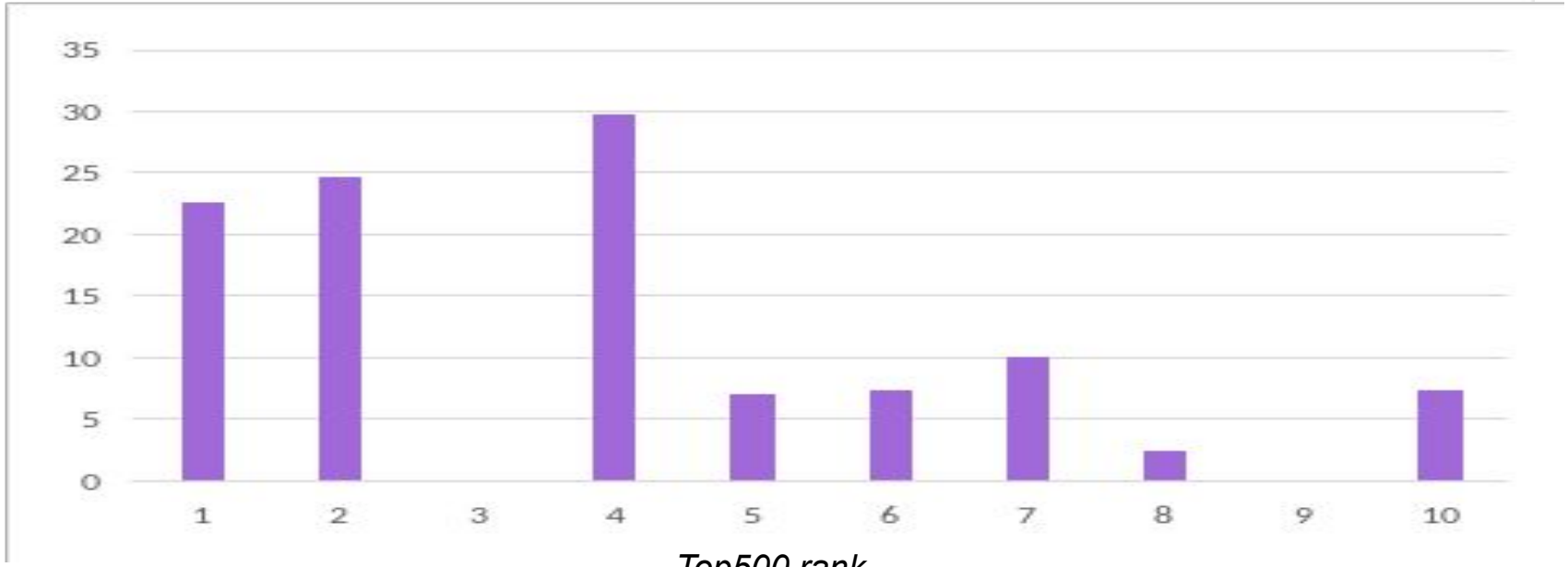


Supercomputer - *top500* timeline

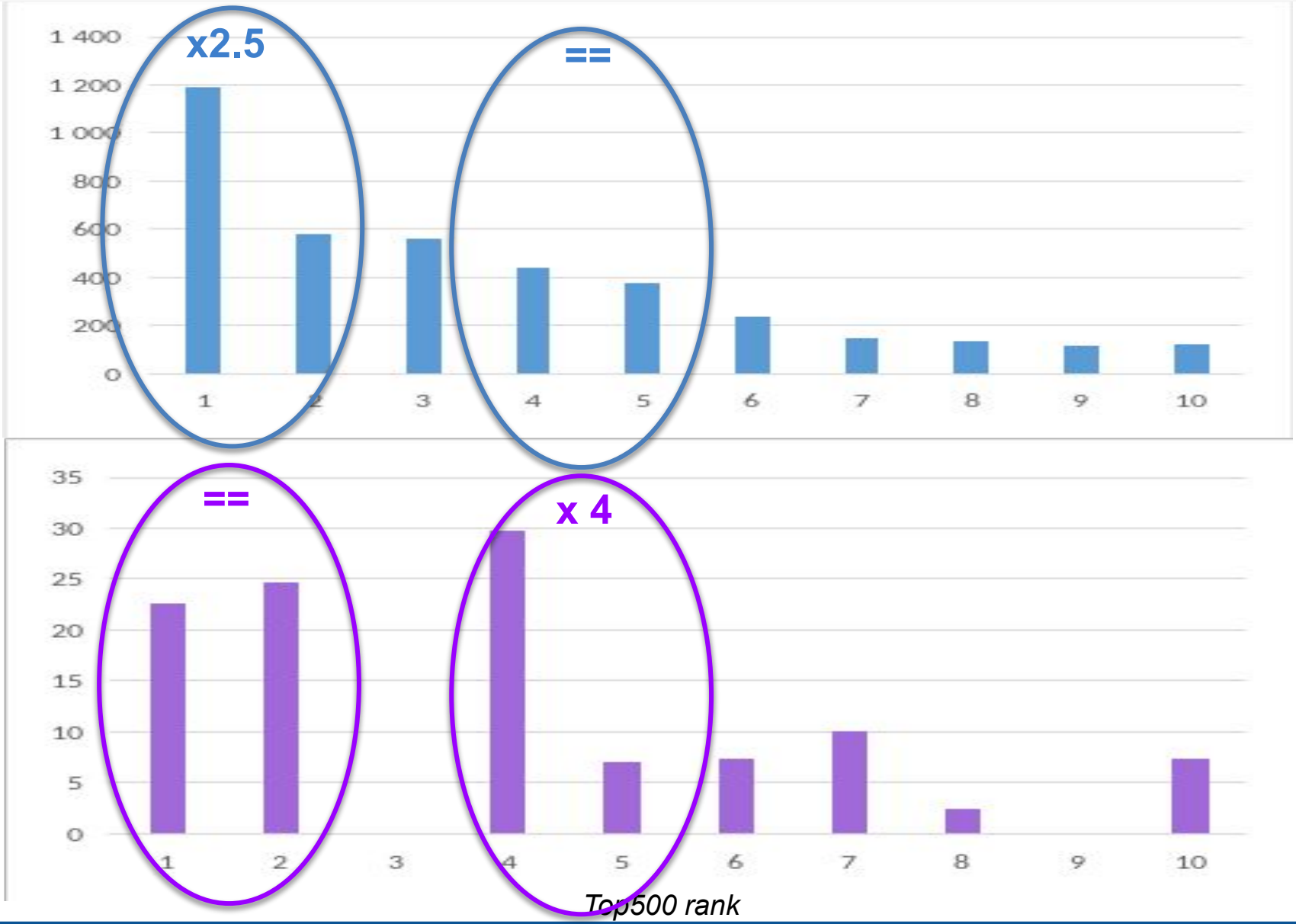


Supercomputer - Power efficiency

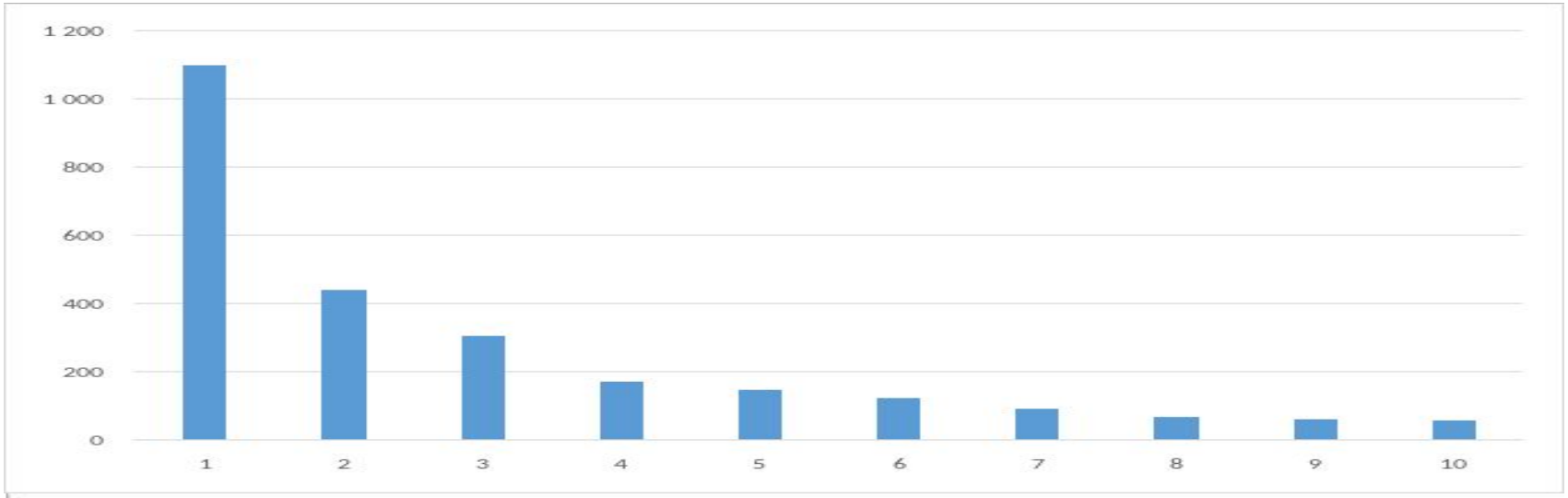


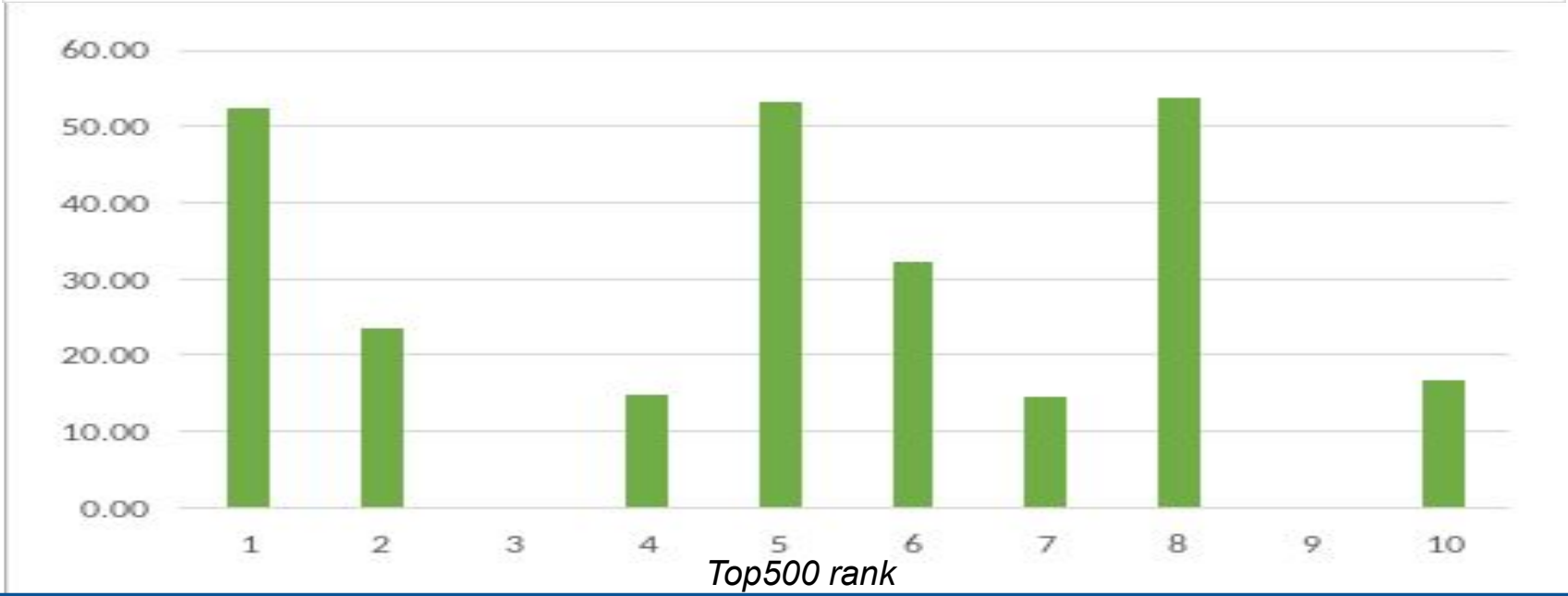


Supercomputer - Power efficiency



Supercomputer - Power efficiency

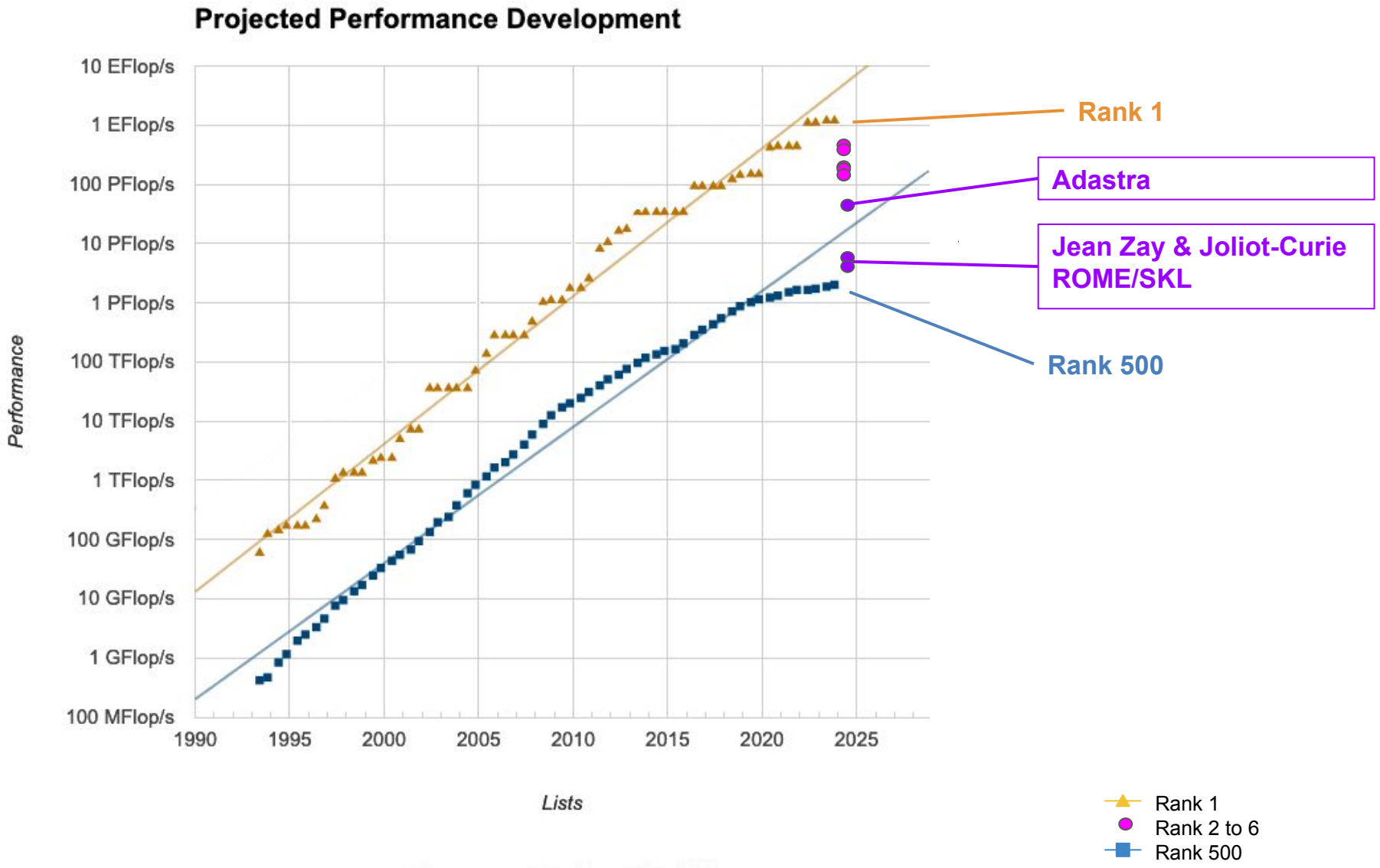




Supercomputer - *green500* ranking

Rank	#Top 500	System	Cores	Rmax (PFlop/s)	Power (MW)	Efficiency (GFlops/W)
1	**293**	**Henri** Lenovo - USA	**8 288**	**2.88**	**0.044**	**65.4**
2	44	**Frontier TDS** Cray - USA	120 832	19.2	0.31	62.68
3	17	**Adastra** Cray - France	319 072	46.1	0.92	58.02
4	25	**Setonix GPU** Cray - Australia	181 248	27.16	0.48	56.98
5	92	**Dardel GPU** Cray - Sweden	52 864	8.26	0.15	56.5
6	8	**MareNostrum** Bull - Spain	680 960	138	2.56	53.98
7	5	**LUMI** Cray - Finland	2 752 704	379.7	7.11	53.43
8	1	**Frontier** Cray - USA	8 699 904	1 194	22.7	52.59

Supercomputer - *top500* timeline



Why do we need supercomputer ?

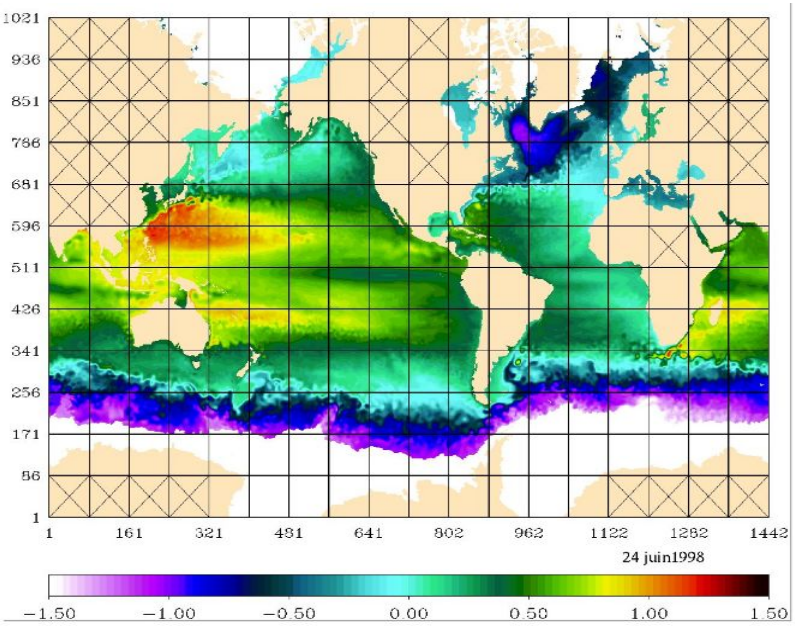
⇒ *parallelization*!

All models are parallelized with MPI or MPI+OpenMP.

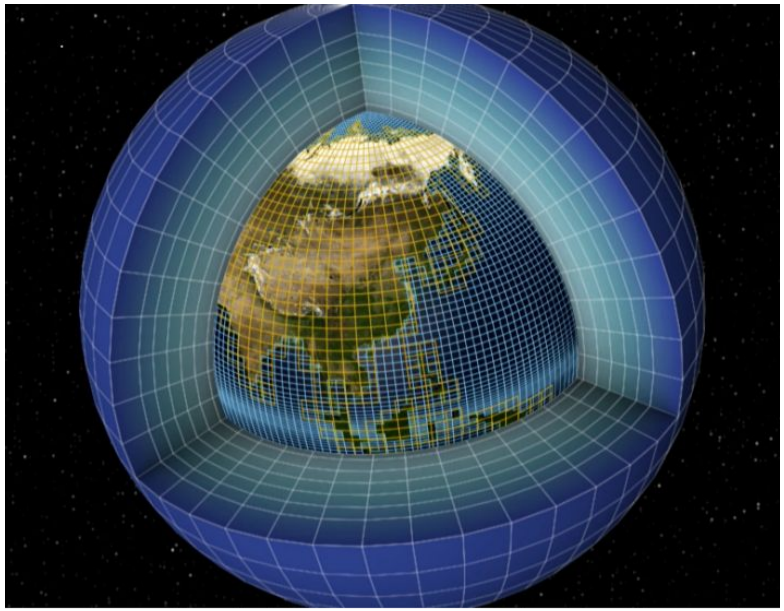
Parallelization allows to run the same executable on several sub-domains to reduce the real time of the execution.

MPI (**M**essage **P**assing **I**nterface) is used to divide **lon/lat grid** splitting latitudes and **OpenMP** (**Open M**ulti-**P**rocessing) to parallelize 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 parallelization

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

Environment:

- A supercomputer is not a personal computer! Each supercomputer is unique and requires a dedicated staff to maintain its hardware and software.
- Its usage requires good skills to understand how to work with it properly.
- 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 cannot 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)
- Dynamical access (all year long) for project with <500 kh CPU or 50 kh GPU

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, computing centers could:

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

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Where can you use IPSL tools?

National centers

Jean Zay

Irene Joliot-Curie (ROME and SKL)

Meso-center

Spirit(x)

Local cluster

Obelix

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 saved*

We advise you to copy the **IPSL platform environment** in the `HOME` of your account and **install** models into your project `WORK`.

- Partitions:
  - Jean Zay CPU: scalar computing nodes for launching simulations
  - Jean Zay pre-post-processing: large memory nodes for pre and post processing tasks (such as compilation)

IDRIS (2/2)

- Documentation:
  - https://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc/ComputingCenters/IDRIS
  - https://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc/ComputingCenters/IDRIS/JeanZay
  - http://www.idris.fr (useful cheat sheet : http://www.idris.fr/jean-zay/cheat-sheet.html)
- 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

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 10Gb – quota 100 000 inodes, on tape*
  - *SCRATCHDIR : big working space, may be purged after 40 days*

We advise you to copy the **IPSL platform environment** in the `HOME` of your account and **install** models into your project `WORKDIR`.

- Partitions:
  - Irene Joliot-Curie SKL: AMD Rome (Epyc) bi-processors nodes
  - Irene Joliot-Curie Rome: Intel Skylake 8168 bi-processors nodes
  - xlarge nodes: large memory nodes for pre and post processing tasks

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) or http://www-hpc.cea.fr/docs/userdoc-tgcc-public.pdf (public access)
- 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

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
  - *spirit* and *spiritx* : IPSL clusters (ESPRI mesocenter)
    http://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc/ComputingCenters/ESPRImesocenter
- 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 mainly on **modipsl**, **libIGCM** and **XIOS** tools which allow to :

modipsl

- **predefine** and **extract** standard configurations and **compilation** scripts

libIGCM

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

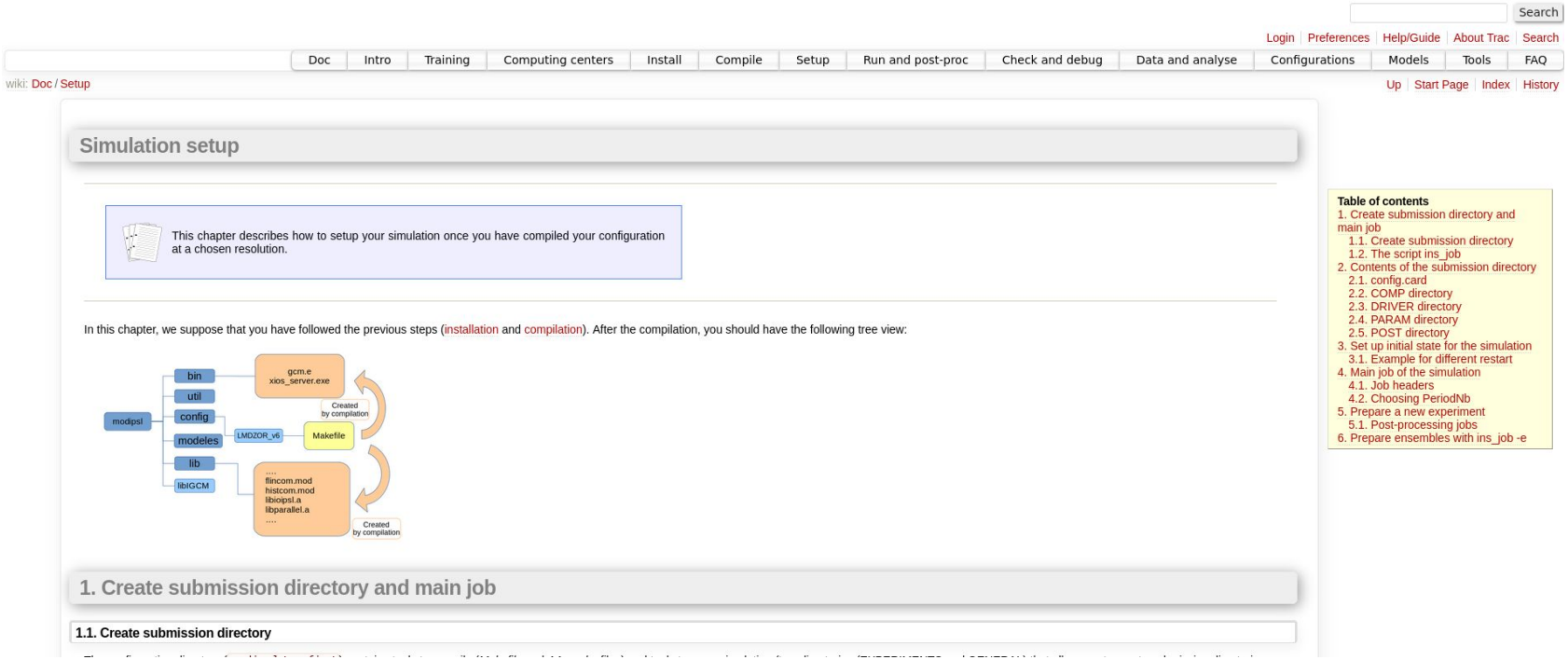
XIOS

- **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. Anyone 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 LMDZOR configuration contains the two models LMDZ and ORCHIDEE.

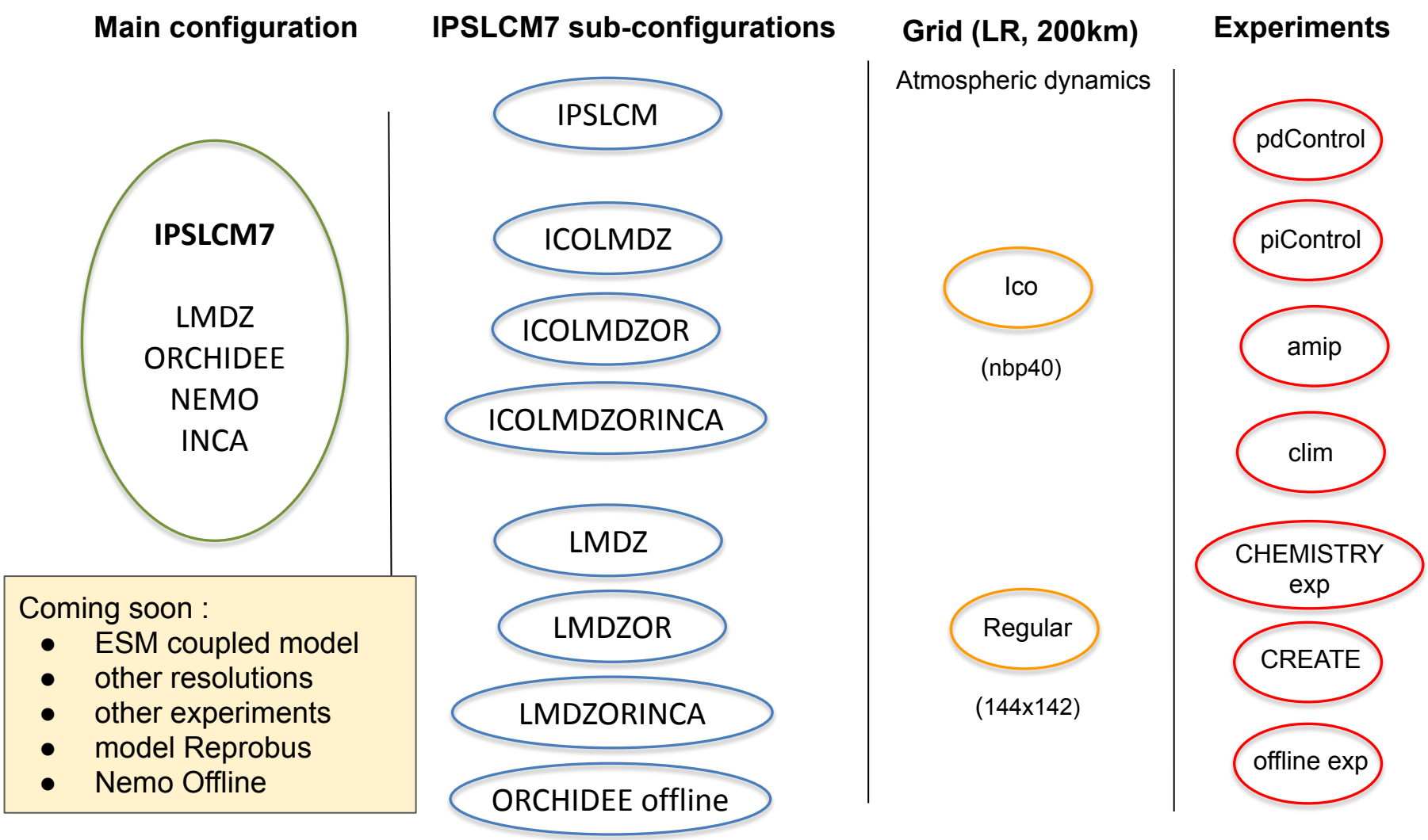
A configuration can be used for different experiments, using different setups, input parameters, etc.

For example with the LMDZOR configuration you can:

- *run experiments with different parameterizations for the physics in the atmosphere.*
- *and/or run an experiment with only LMDZ*

Institut Pierre-Simon Laplace

What is a configuration? (2/2)



1 main or 1 sub configuration = 1 executable per grid ico or reg = several experiments (from sub-configurations)

Distributed configurations (1/3)

Actual configs => recommended version of standard configurations.

There are 4 types of used 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 - to be used only for dev
4. v7 ⇒ newest configurations (DYNAMICO and NEMO4 and all v6.2 experiments)

General recommendations:

- *Inform person in charge* before launching new studies based on a specific configuration, especially for coupled models.
- Read model and configuration documentation before using it!!!

Distributed configurations (2/3)

IPSLCM7	New working configuration of the coupled model, including DYNAMICO core. *Persons in charge: A. Caubel, J. Ghattas, A. Cozic, C. Ethé*
IPSLCM6	Version of the coupled model used for CMIP6 (currently IPSLCM6.2.2) *Person in charge: A. Caubel*
NEMO_v6	Forced ocean model OPA-SI3-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	LMDZ6 coupled with REPROBUS *Person in charge: L. Falletti*

Distributed configurations (3/3)

IPSLCM5A2	Previous version of the coupled model (*IPSLCM5*) VLR grid. *Person in charge : S. Nguyen*
IPSLCM5A2-CHT	coupled model in low resolution with an interactive atmospheric chemistry. *Person in charge : A. Cozic*
ORCHIDEE_trunk/ ORCHIDEE_4_1	Forced continental surfaces model ORCHIDEE, with latest version on the trunk of ORCHIDEE or tag 4_1. *Person in charge: J. Ghattas*
RegIPSL	Regional coupled climate model of IPSL. *Person in charge: R. Pennel*
ICOLMDZOR_LAM	Limited Area Model (DYNAMICO-LMDZ-ORCHIDEE). *Person in charge: A. Caubel*

IPSL-CM perfs: IRENE SKL

Configuration	Number of Cores	Simulated Year Per Day
IPSL-CM7 LR (DYNAMICO - NEMO4) *ATM: 200km - 79 / OCE: eORCA1*	**1000**	**20**
IPSL-CM6 LR *ATM: 144x144x79 / OCE: eORCA1*	**1000**	**20**
IPSL-CM5A2-VLR *ATM: 96x96x39 / OCE: ORCA2*	**437**	**95**
NEMO *eORCA1-LIM3-PISCES*	**433**	**20**
LMDZOR_v6.1.10-LR *LMDZ144x144x79*	**576**	**20**
ICOLMDZOR *NBP 40 (~200 km)*	***680***	***40***

Benchmark in January 2021

IPSL-CM perfs: IRENE AMD

Configuration	Number of Cores	Simulated Year Per Day
IPSL-CM7 LR (DYNAMICO - NEMO4) *ATM: 200km - 79 / OCE: eORCA1*	-	-
IPSL-CM6 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 Cores	Simulated Year Per Day
IPSL-CM7 LR (DYNAMICO - NEMO4) *ATM: 200km - 79 / OCE: eORCA1*	-	-
IPSL-CM6-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

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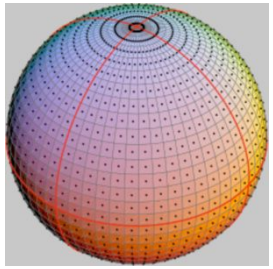
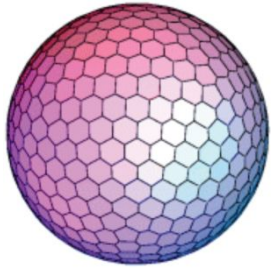
New developments

- **Atmospheric dynamical core DYNAMICO**
  - better computing performances/scalability
  - new architectures (GPUs, MPPs, MICs)

Lon-lat grid   ***Icosahedral grid***

- **NEMO v4** and **SI3** (new sea-ice model)
- **Limited Area Model** (available with ICOLMDZOR configurations)
- **CMIP6 workflow**: to integrate the CMIP6 specific workflow (outputs) for "usual runs", available and already used for specific cases
- **Ensemble runs** (specific I/O design)
- **C-ESM-EP** in libIGCM

Ongoing developments

- **XIOS 3.0** (XIOS multithreaded (OpenMP) to target « many cores » architectures, coupling functionalities)
- **StratAer:** config with stratospherical microphysics
- Improve **zoomed** configuration
- Study of the use of **Cylc** tool to manage simulations

Training courses

Training courses at IPSL:

- IPSL climate modeling: training in simulation tools (contact platform-training-team@listes.ipsl.fr), current session
- LMDZ training course (contact Laurent.Fairhead@lmd.jussieu.fr), last session in January 2024
- ORCHIDEE Introduction 2-days course (contact orchidee-help@ipsl.jussieu.fr), next session in February 2024
- XIOS training course (contact xios-team@forge.ipsl.jussieu.fr), past sessions in 2021
- PISCES training course (contact formation_pisces@locean.ipsl.fr), past session in October 2023

Other suggested training courses:

- *MPI, OpenMP and Hybrid MPI/OpenMP* at IDRIS twice a year www.idris.fr
- Training course for using the computer centres (not available actually, usually at TGCC)
- UNIX course
- https://calcul.math.cnrs.fr/category/formation.html→ give an inventory of training course (numeric – calcul – hpc) in France

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**

Now it's your turn to practice!

Informations for today's training (1/2):

Today's on **JeanZay specific training accounts**:

- Connect on "`ipcours22.....`" session.
- Your login: use the `cforXXX` login/password provided to you *(**please complete the form with your name and signature!**)*
- Note that everything in these accounts will be erased after the training.

If you need to **switch between qwerty and azerty** you can use the command **`alt+shift`**.

Download training_exercises_2024.pdf, training_exercises_answers_2024.pdf and main_commands_summary_2024.pdf at:

http://forge.ipsl.jussieu.fr/igcmg_doc/wiki/Doc/Training

Now it's your turn to practice!

Advices and informations for this training(2/2):

- **Not all exercises are meant to be done**: select topics based on your knowledge of modipsl/libIGCM and your needs.

BEGINNER	INTERMEDIATE	SPECIALIZED
0. Introduction 1. Check your quota 2. Installing and compiling 3. Basic simulations	4. Debug 5. Post-processing (TS&C-ESM-EP) 6. Monitoring and Inter-monitoring 7. How to REDO part of a simulation 8. Modify output using XIOS 9. Output files manipulations	10. Install and run NEMO-PISCES 11. Ensembles 12. Coupled model 13. ICOLMDZOR configuration

Beginner: to be done by everyone, in this order.
Intermediate and **specialized**: depending of your level and your needs, not meant to be done in this order.

- **Take your time to read everything in the doc!** All is explained.

Do not hesitate to ask questions! ☺