

# Parallel I/O for Earth System Modelling

Luis Kornblueh, Deike Kleberg and Uwe Schulzweida

Max Planck Institute for Meteorology

supported by

Mathias Pütz, CRAY

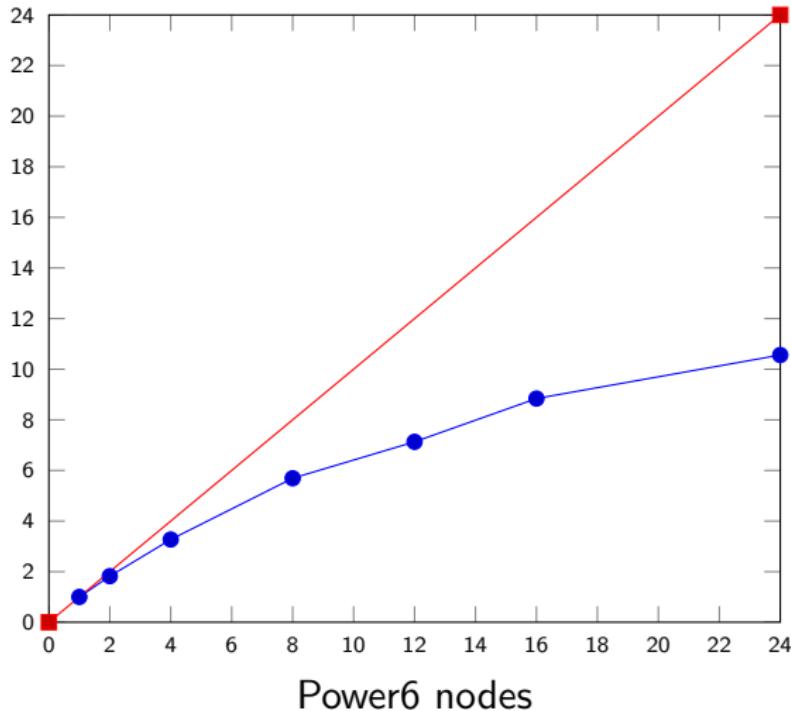
Christoph Pospiech, IBM

Thomas Jahns, Moritz Hanke, Jörg Behrens, and Mathis Rosenhauer, DKRZ

October 3, 2012

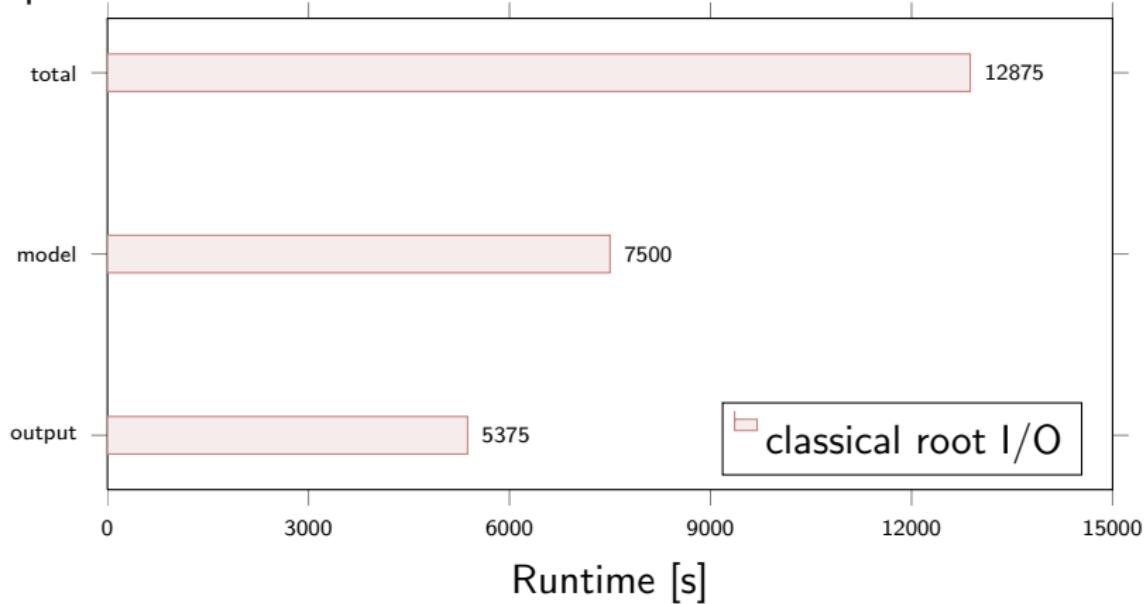
# Scaling optimization required

Scaling



# Classical root I/O explains scaling

Model part



# Atmospheric and Oceanographic Data

## Constraints

- Large amounts of data
- Comparable small spatial extent ( $O(2, \dots, 4)$ )
- Large Time extent ( $O(4, \dots, 7)$ )
- Large Number of variables ( $O(2, \dots, 3)$ )

... continued ...

## Requirements

- long term metadata and data storage
- standardization
- compression

## Solutions

- WMO GRIB standard
- lowest entropy data subsampling
- two stage compression: lossy entropy based and lossless compression of resulted *image* — metadata uncompressed!

# I/O improvements possible

## Improvement by additional packing of the BDS data

Resolution	GRIBZip2d	grib-szip	gzip (external)
Source	Frauenhofer	MPI-M	GNU
T42 L19	2.32	2.13	2.06
T63 L31	1.85	1.78	1.35
T106 L60	5.17	4.75	3.81
T213 L31	3.09	3.06	2.41
mean	3.03	2.93	2.15

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### Remark 1

netCDF stores 4 byte, grib in average 2 byte — compression ratio given with respect to the later.

### Remark 2

szip has a patent and copyright issue. We (most work by Mathis Rosenhauer) reimplemented the scheme from the CCSDS reference with the extensions from May 2012. The license is the BSD license now!

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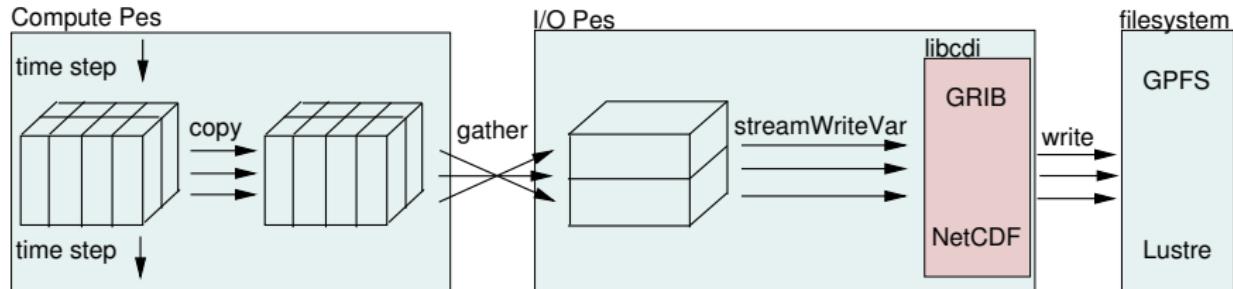
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- ⑥ write ... sort of

# File writing in ECHAM based on cdi-pio



- After calculating one I/O timestep the compute processes copy their data to a buffer and go on calculating till the next I/O timestep.
- I/O processes fetch the data using MPI one sided communication.
- Gather and transpose of the data is based on callback routines supplied by the model.

## Most important property

Compute processes are not disturbed by file writing.

## Known difficulties

- single offload step requires large memory on offload-node (requires eventually changes for Linux cluster and Cray XT architecture type machines, and maybe for IBM BlueGene)
- generates network jitter (RMA access to all compute nodes concurrent with computing nodes internal communication)
- filesystem jitter due to system bottlenecks (total bandwidth 30 GB/s, 2 GB/s per node, but 256 nodes)

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- ⑤ track down to *offending* level
- ⑥ check selected counters for *offending* code part

# I/O capabilities

## An example: DKRZ

- 256 compute nodes, 12 file server, 6 PB filesystem, 4 HPSS server, 60 PB tape archive
- total I/O bandwidth to disk 30 GB/s
- per node max. I/O bandwidth 2 GB/s
- 1600 users
- max. 96 post-processing jobs
- unknown number of production jobs

# Offending code parts

## Legacy in libraries

- portable double to float conversion (199x) taking into account CRAY, VAX , IBM, and IEEE FP formats
- C max/min search loop
- encoding kernel
  - ▶ mixed floating point/integer operation
  - ▶ very small number of operations

# Analysis for optimization strategy

## Caution: Assembler reading required

- understand roughly how your CPU works
- need to *read* Assembler (not that bad, feels like using a pocket calculator), you get an idea what the compiler is doing
- compare code of different optimization levels
- try to find the patterns, you would expect for fast code

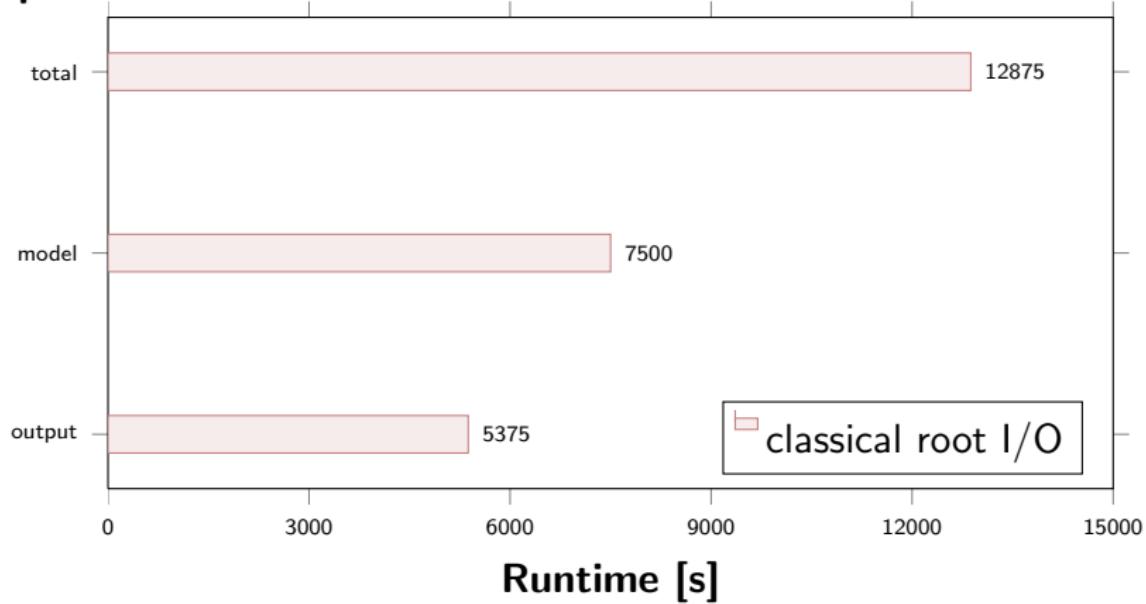
## An example

```
/* datatype information only */
long datasize
double data[datasize];
unsigned char *lGrib;
long i, z;
unsigned long ival;
double dval, reference, factor;

/* offending code */
for ( i = 0; i < datasize; i++ )
{
    dval = ((data[i] - reference) * factor + 0.5);
    ival = (unsigned long) dval;
    lGrib[z] = ival >> 8;
    lGrib[z+1] = ival;
    z += 2;
}
```

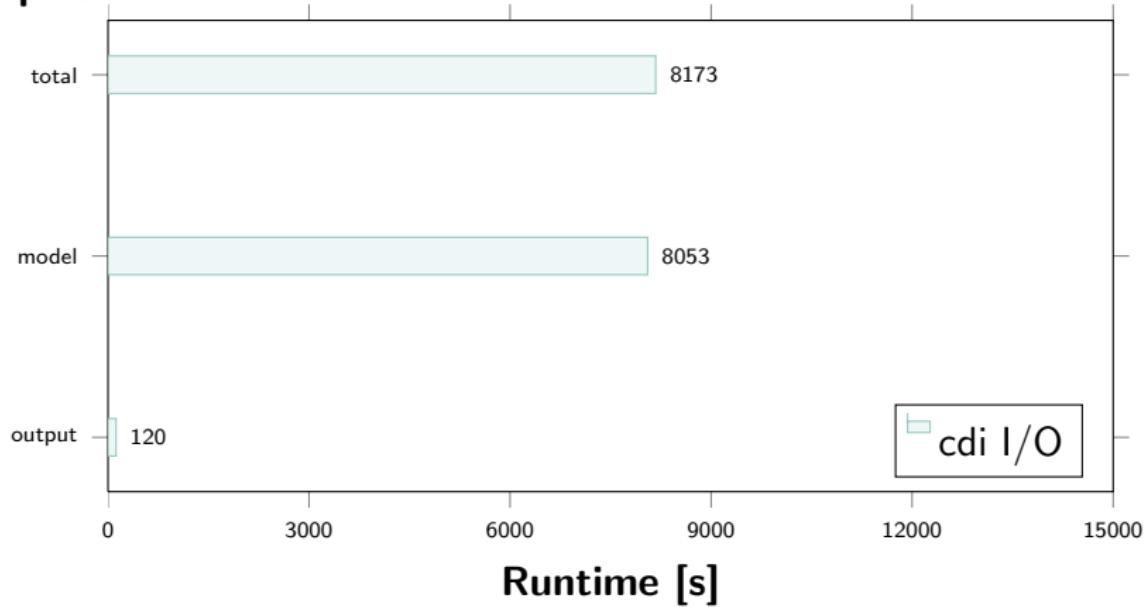
# Classical root I/O

## Model part



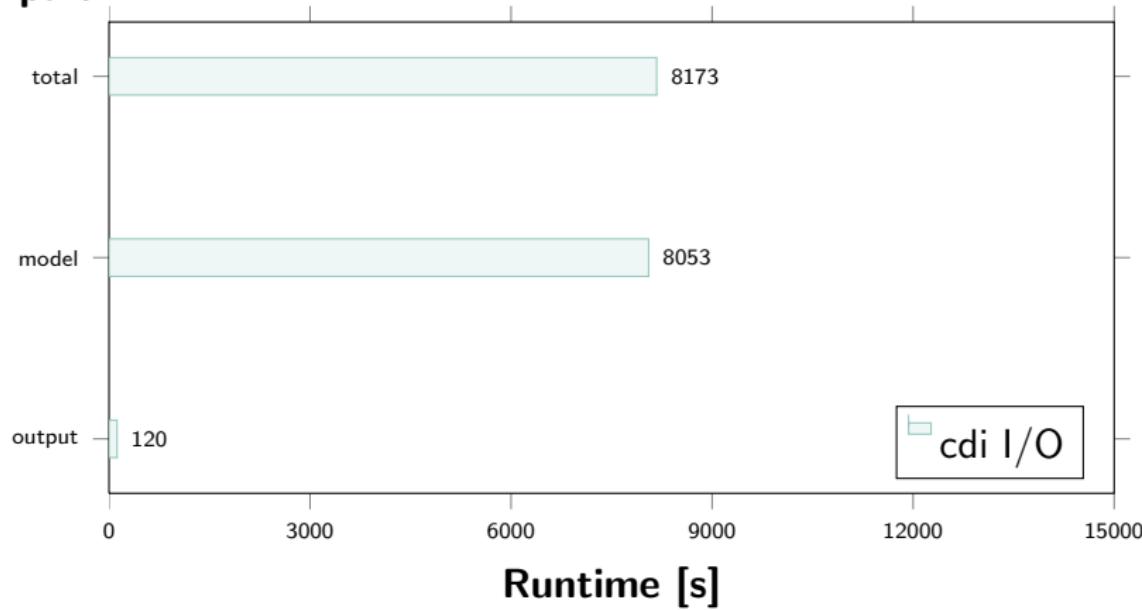
# cdi based asynchronous parallel I/O

## Model part



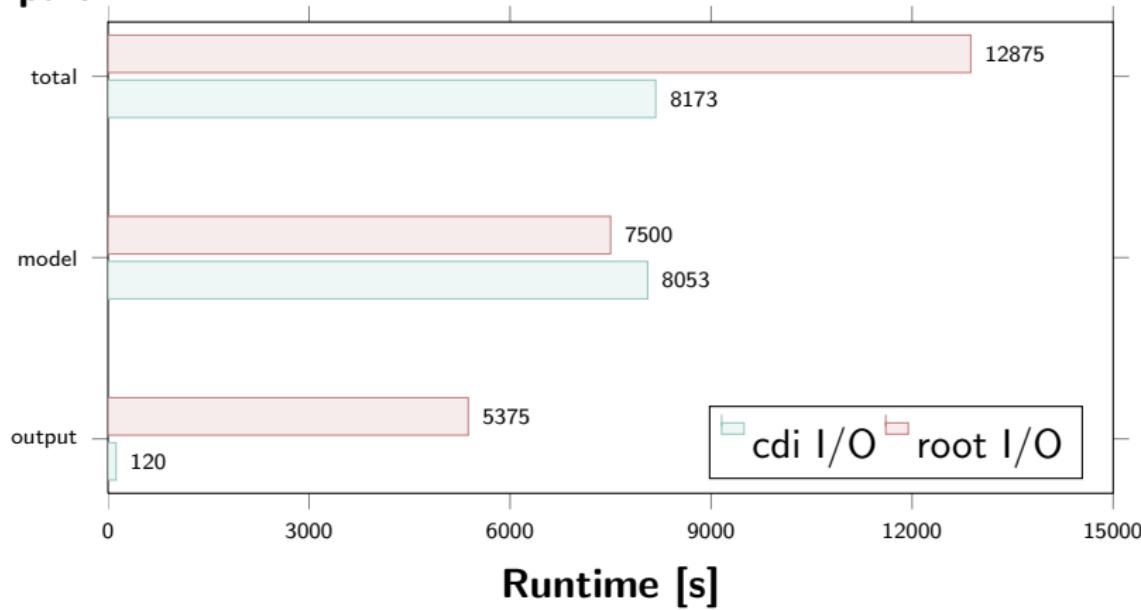
# Compare

## Model part



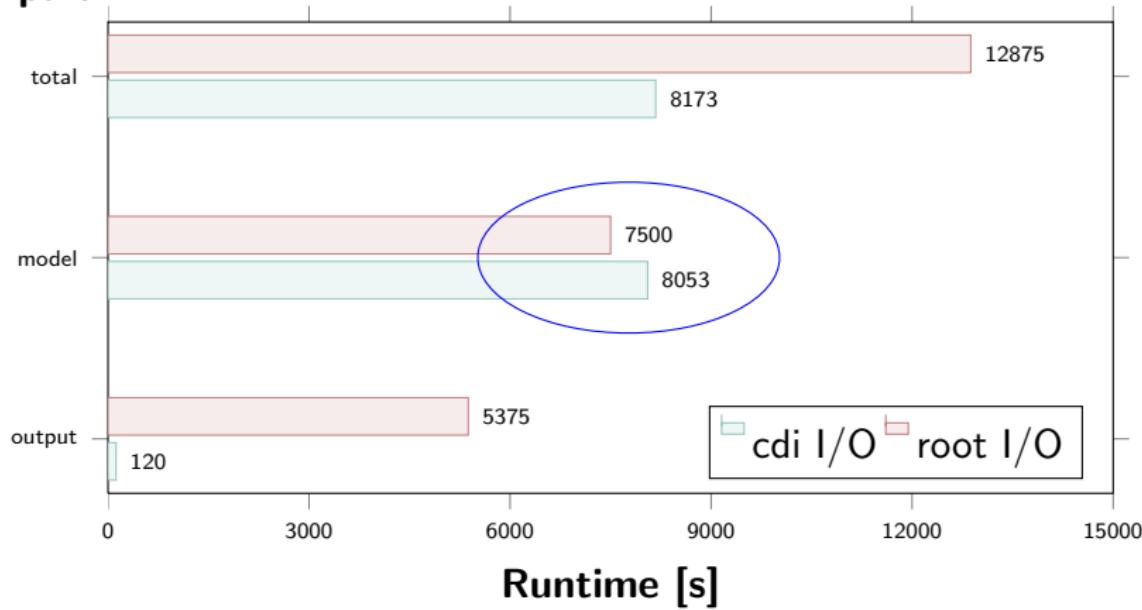
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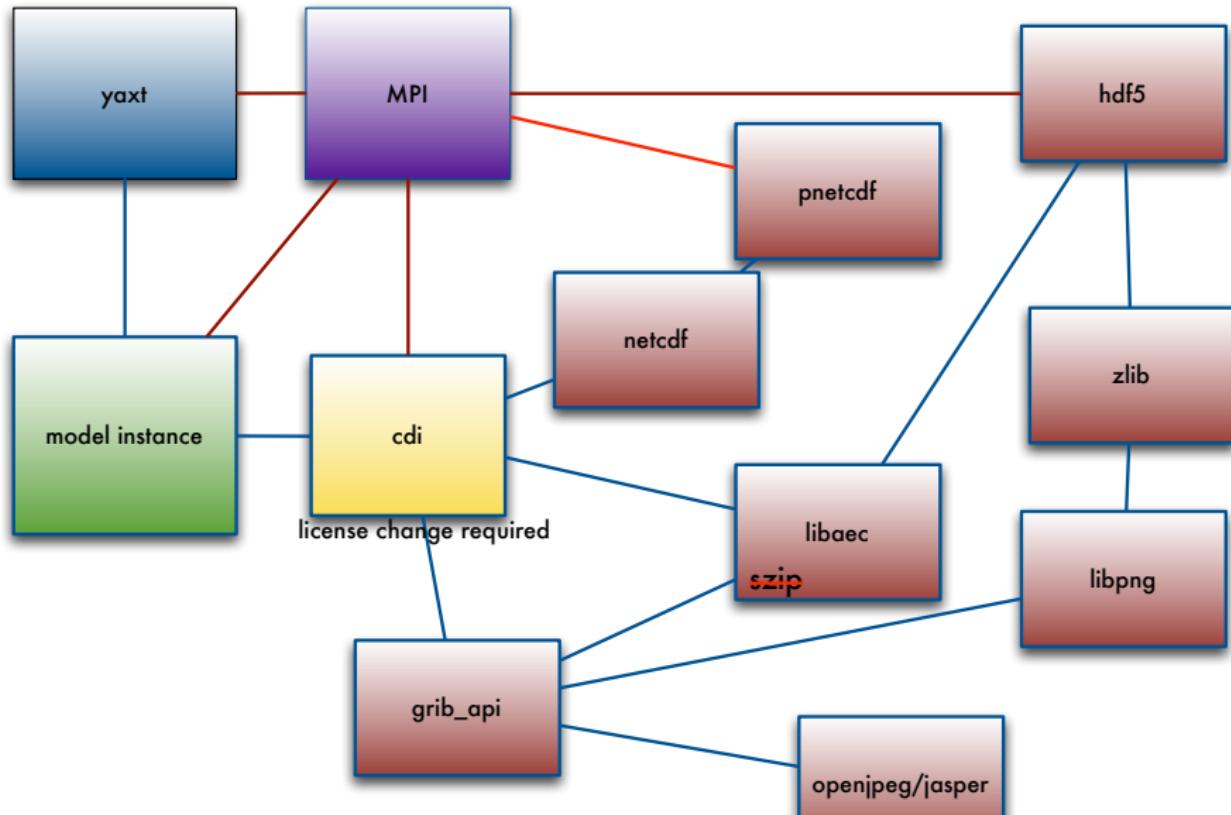
## Model part



## What next?

- Scaling experiments
- Further optimizations of details
- Implementation in all MPIM models
- Finish Implementation in EC-Earth
- Optimize GRIB decoding
- Optimize libaec
- Intensivy collaboration on solving issues in each single component
- Get library zoo manageable

# Library zoo



# What is CDO ?

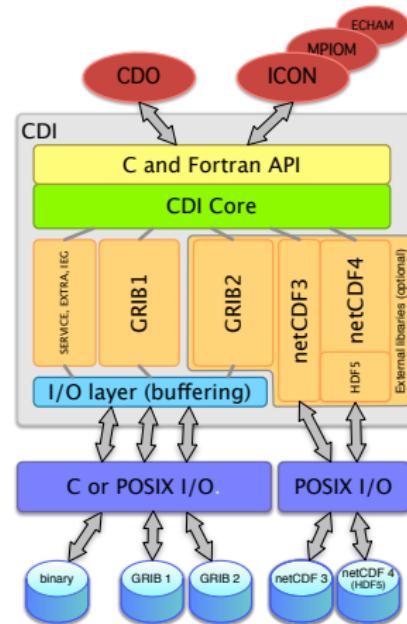
CDO is a collection of tools to process and analyze data from climate and NWP models.

- File format conversion: GRIB  $\Leftrightarrow$  netCDF
- Interpolation between different grid types and resolution
- Portability (ANSI C99 with some POSIX extention)
- Performance (fast processing of large datasets, multi-threaded)
- Modular design and easily extendable with new operators
- UNIX command line interface
- Tested on many UNIX/Linux systems, Cygwin, and MacOS-X

# Data I/O Interface

Part of CDO is the I/O interface CDI (Climate Data Interface) which it shares with all major MPI-M climate models.

- GRIB1 via CGRIBEX (MPI-M)
- GRIB2 via GRIB\_API (ECMWF)
- netCDF, CF-convention (UNIDATA)
- SERVICE, EXTRA, IEG (MPI-M binary formats)



GRIB support includes highly efficient, fast compression algorithms.

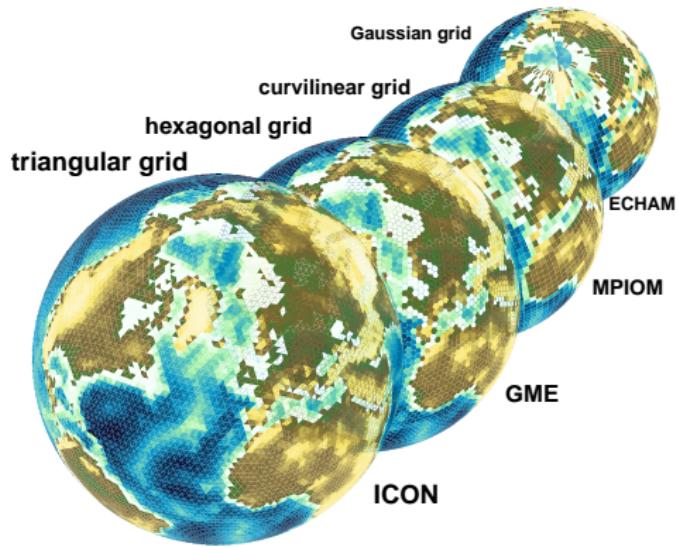
# Available Operators

CDO provides more than 400 operators which can be pipelined on thread level. CPU time intensive operators are OpenMP parallelized.

Main categories	Description
File information	Print information about datasets
File operations	Copy, split and merge datasets
Selection	Select parts of a dataset
Comparision	Compare datasets
Modification	Modify data and metadata
Arithmetinc	Arithmetically process datasets
Statistical values	Ensemble, field, vertical and time statistic
Interpolation	Horizontal, vertical and time interpolation
Import/Export	HDF5, binary, ASCII
Climate indices	ECA Indices

# Supported Grids

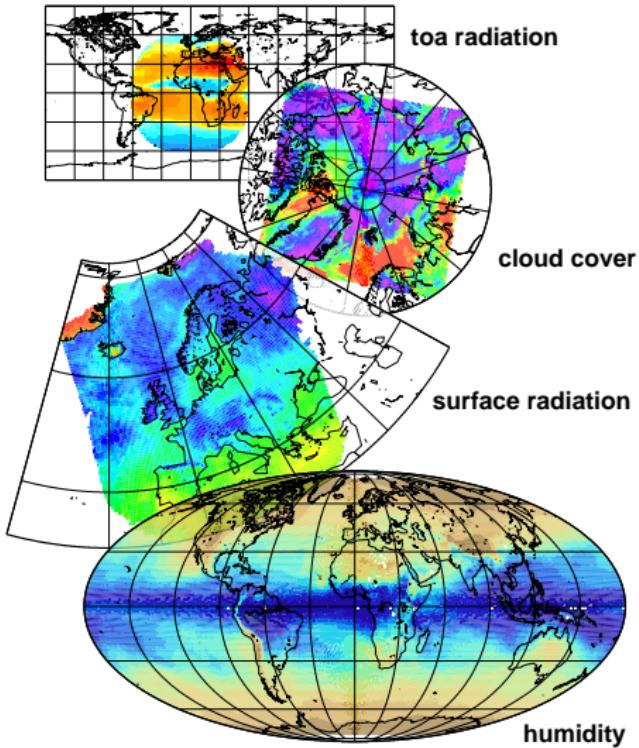
A large set of grids is supported including spectral- and Fourier-coefficients. Gaussian grids, regular and rotated lat-lon grids, conformal mapped quadrilateral grids, and finally general unstructured grids.



All major models world wide are supported (COSMOS, CLM, ECHAM, GME, HIRLAM, ICON, IFS, MPIOM, NEMO, and REMO — only to mention those used mostly in Germany).

# Satellite-data Support

EUMETSAT's Climate Monitoring Satellite Application Facility provides satellite-derived geophysical parameter for climate monitoring. Data sets contain several cloud parameters, surface albedo, radiation fluxes, temperature and humidity profiles. These products are stored in HDF5. DWD has funded an import CDO operator  
import\_cmsaf.



# Community Support

The rapidly increasing number of CDO installations and users create a very high demand of support. A fully featured development platform is available to support the community. The CDO community page was funded by the European Commission infrastructure project IS-ENES.

The screenshot shows the homepage of the CDO project. At the top, there's a navigation bar with links for Home, Projects, Help, and a user sign-in/register section. Below the navigation is a search bar. The main content area has several sections:

- Welcome to the Climate Data Operators**: A brief introduction to CDO, mentioning it's a large tool set for working on climate and NWP model data, supporting NetCDF 3/4, GRIB 1/2 (including SZIP and JPEG compression), EXTRAP, SERVICE and IEG are supported as IO-formats. It notes that CDO can be used to analyse any kind gridded data not related to climate science. It also mentions small memory requirements and can process files larger than the physical memory.
- CDO is open source and released under the terms of the GNU General Public License Version 2 (GPL).**
- Documentation**: A list of operators for the following topics:
  - File information and file operations
  - Selection and Comparison
  - Modification of meta data
  - Mathematical analysis
  - Statistical analysis
  - Regression and Interpolation
  - Vector and General Transformations
  - Format and I/O
  - Climate indices
- Known Problems**: A list of known issues with CDO, including:
  - Using netCDF variables after processing with CDO
  - Static build with netcdf 4.1.1 incl. dep. on MPI causes errors with mixed precision
  - CDO mailing lists
  - Using CDO at MPIM and DKRZ
- Wiki**: Links to Start page, Index by title, and Index by date.
- Forums**: A link to the forums.
- Files**: A link to the download area.

At the bottom left, there's a note about full documentation being available as [HTML](#) or [PDF](#). The bottom right contains a search bar with the placeholder "oko -> [operator]".

- User wiki
- Documentation
- Bug tracking system
- User forums
- Download area
- Repository access

<http://code.zmaw.de/projects/cdo>

## What comes next?

- Web Services (EUDAT, EU funded)
- Script-language interface (Python, Perl, Ruby, ...)
- Add simple standardized plotting capabilities (Magics++, ECMWF)
- Add more functionalities
- Performance improvements (ENES funded)
- Parallel asynchronous CDI, Deike Kleberg and Luis Kornblueh  
(ScaLES, BMBF funded)