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2007

V. Galiano

Introduction

PyACTS

PyPnetCDF

Applications

Conclusions

Parallel Access to netCDF files in High Performance Applications from High-Level Frameworks

V. Galiano

joint work with H. Migallón, V. Migallón and J. Penadés

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Elche (Alicante), Spain

Harrachov, Czech Republic
August 24, 2007

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3 PyPnetCDF

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- EOFs Analysis

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Scientific and engineering applications usually ...

- Require knowledges about an specific programming language.
- Use libraries developed by others.
- Are platform dependent.
- Computational requirements grow with size of the problem.

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Scientific and engineering applications usually ...

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Scientific and engineering applications usually ...

- Require knowledges about an specific programming language.
- Use libraries developed by others.
- Are platform dependent.
- Computational requirements grow with size of the problem.

High Performance Computing Systems *HPC*

- More complexity in libraries
- Need the execution in a multiprocessor system with ...
 - Shared memory
 - Distributed memory
- Require Data distribution
- Syncronize Parallel execution

Example of computational requirements and motivation I

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PyClimate

- Sequential application programmed in Python.
- Designed to accomplish some usual tasks during the analysis of climate variability.
- Open source and free distribution.

PyClimate 1.2

PyClimate

- Sequential application programmed in Python.
- Designed to accomplish some usual tasks during the analysis of climate variability.
- Open source and free distribution.

Utilities:

- Empirical Orthogonal Functions (EOFs) Analisys.
- Canonical Correlation Analysis (CCA).
- SVD of coupled datasets.
- Simple multivariate statistical tools
- Digital filters.
- Input/Output functions.

Example of computational requirements and motivation II

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EOFs Analysis

- Delete redundant information with minimum lost of variability.
- Efficient method for data compression.
- Useful in high dimensionality spaces.
- We can get EOFs analysis based on the Singular Value Decomposition *SVD*.

Example of computational requirements and motivation II

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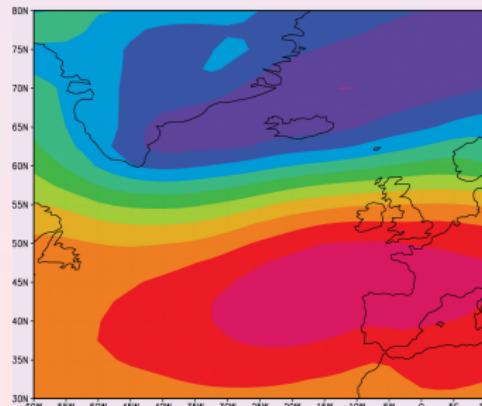
Applications

Conclusions

EOFs Analysis

- Delete redundant information with minimum lost of variability.
- Efficient method for data compression.
- Useful in high dimensionality spaces.
- We can get EOFs analysis based on the Singular Value Decomposition SVD.

Analisis of a netCDF file containing sea level pressure in NAO region



1st EOF accounting for
55,81% of the variance

Example of computational requirements and motivation II

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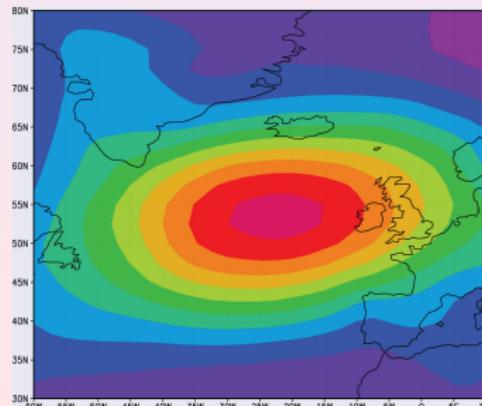
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EOFs Analysis

- Delete redundant information with minimum lost of variability.
- Efficient method for data compression.
- Useful in high dimensionality spaces.
- We can get EOFs analysis based on the Singular Value Decomposition SVD.

Analisis of a netCDF file containing sea level pressure in NAO region



2nd EOF accounting for
20,38% of the variance

Example of computational requirements and motivation II

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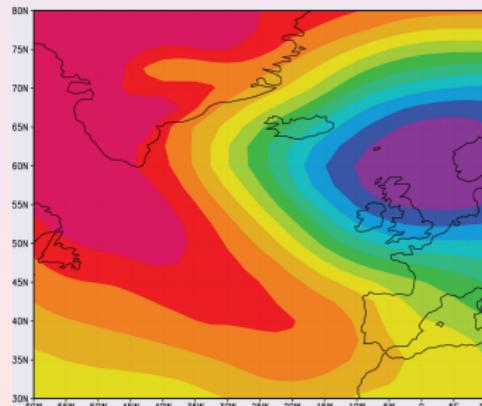
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- Delete redundant information with minimum lost of variability.
- Efficient method for data compression.
- Useful in high dimensionality spaces.
- We can get EOFs analysis based on the Singular Value Decomposition SVD.

Analisis of a netCDF file containing sea level pressure in NAO region



3rd EOF accounting for
el 11,62% of the variance

Example of computational requirements and motivation II

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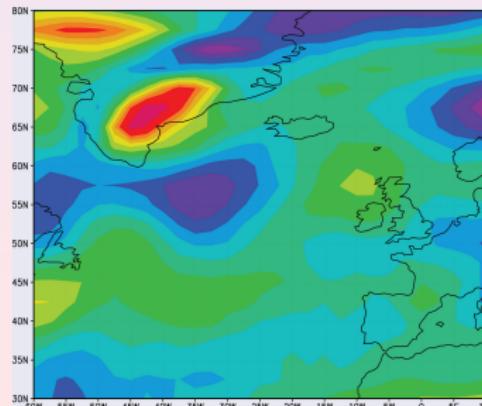
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EOFs Analysis

- Delete redundant information with minimum lost of variability.
- Efficient method for data compression.
- Useful in high dimensionality spaces.
- We can get EOFs analysis based on the Singular Value Decomposition SVD.

Analisis of a netCDF file containing sea level pressure in NAO region



20th accounting for
el 0,03% of the variance

¿Scalability?

- NetCDF files obtained from Climate Diagnostics Center (www.cdc.noaa.gov).
- Extending data grid 144×73 .
- Including Data grids at different elevations $17 \times 144 \times 73$.
- Increasing time axis.
 - `air.mon.ltm.nc`:
 - `air.day.ltm.nc`:
 - `air.mon.mean.nc`:
 - `air.1988to2005.nc`

EOFs Analisys with PyClimate

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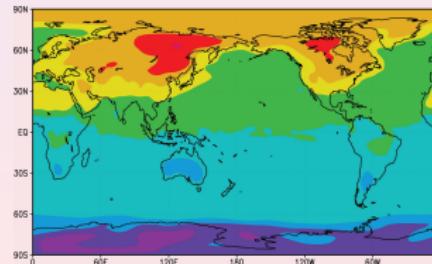
PyPnetCDF

Aplications

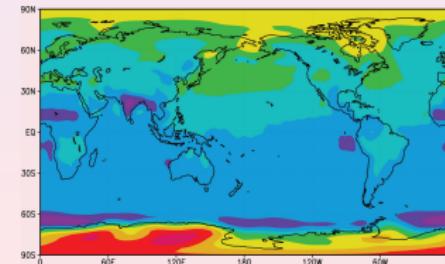
Conclusions

¿Scalability?

- NetCDF files obtained from Climate Diagnostics Center (www.cdc.noaa.gov).
- Extending data grid 144×73 .
- Including Data grids at different elevations $17 \times 144 \times 73$.
- Increasing time axis.
 - air.mon.ltm.nc: $\rightarrow 17 \times 12 \times 144 \times 73$ 8,5MB
 - air.day.ltm.nc:
 - air.mon.mean.nc:
 - air.1988to2005.nc



1^a EOF (90,64%)



2^a EOF (7,19%)

EOFs Analisys with PyClimate

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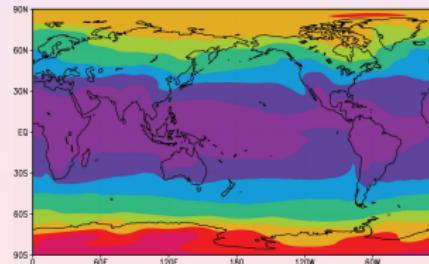
PyPnetCDF

Aplications

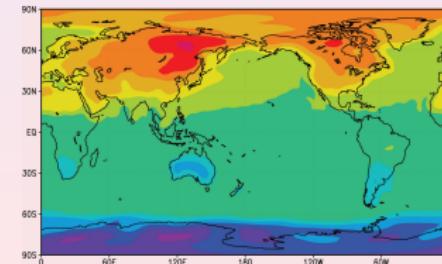
Conclusions

¿Scalability?

- NetCDF files obtained from Climate Diagnostics Center (www.cdc.noaa.gov).
- Extending data grid 144×73 .
- Including Data grids at different elevations $17 \times 144 \times 73$.
- Increasing time axis.
 - air.mon.ltm.nc:
 - air.day.ltm.nc: $\rightarrow 17 \times 365 \times 144 \times 73$ 1,3GB
 - air.mon.mean.nc:
 - air.1988to2005.nc



1^a EOF (99,72%)



2^a EOF (0,253%)

EOFs Analisys with PyClimate

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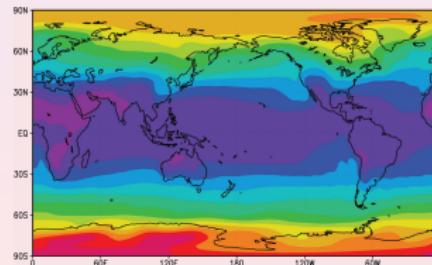
PyPnetCDF

Aplications

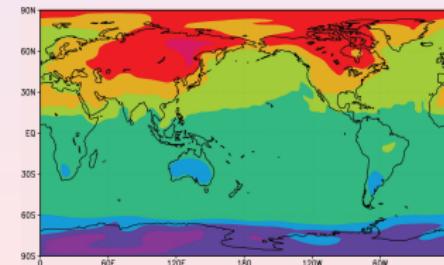
Conclusions

¿Scalability?

- NetCDF files obtained from Climate Diagnostics Center (www.cdc.noaa.gov).
- Extending data grid 144×73 .
- Including Data grids at different elevations $17 \times 144 \times 73$.
- Increasing time axis.
 - air.mon.ltm.nc:
 - air.day.ltm.nc:
 - air.mon.mean.nc: $\rightarrow 17 \times 703 \times 144 \times 73$ 2,5GB
 - air.1988to2005.nc



1^a EOF (99,60%)



2^a EOF (0,34%)

EOFs Analisys with PyClimate

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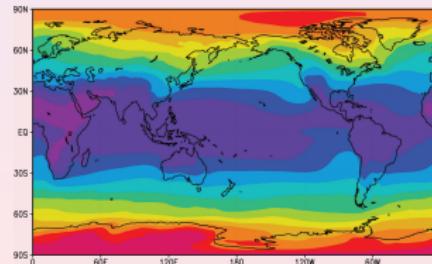
PyPnetCDF

Aplications

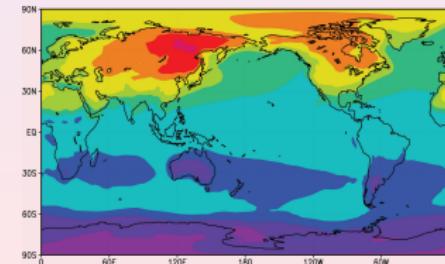
Conclusions

¿Scalability?

- NetCDF files obtained from Climate Diagnostics Center (www.cdc.noaa.gov).
- Extending data grid 144×73 .
- Including Data grids at different elevations $17 \times 144 \times 73$.
- Increasing time axis.
 - air.mon.ltm.nc:
 - air.day.ltm.nc:
 - air.mon.mean.nc:
 - air.1988to2005.nc → $17 \times 2922 \times 144 \times 73$ 4,17GB



1^a EOF (99,87%)



2^a EOF (0,08%)

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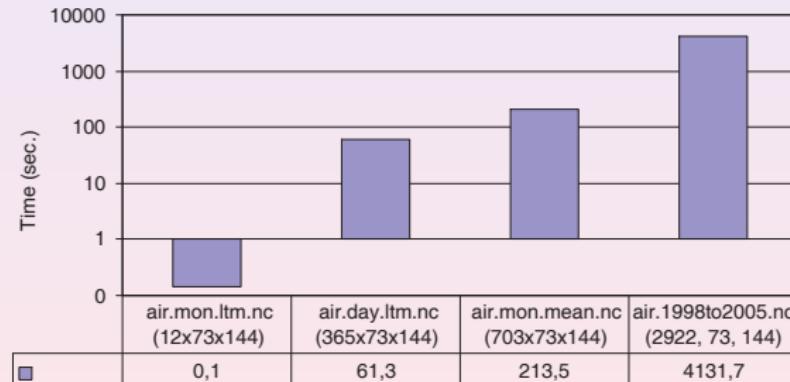
PyPnetCDF

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¿Scalability?

- Increasing execution times.
- Limited memory resources.



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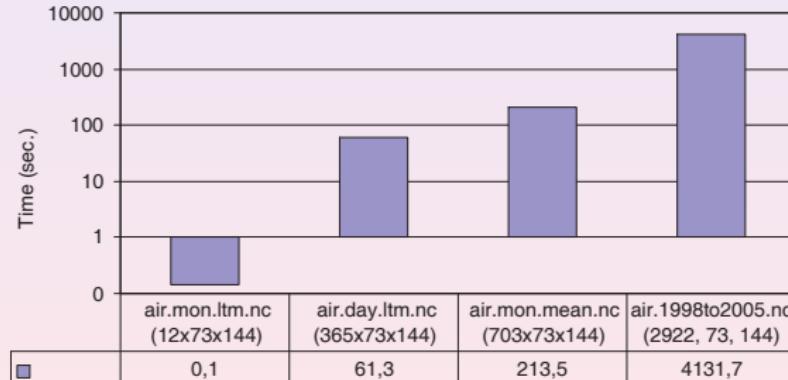
PyPnetCDF

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¿Scalability?

- Increasing execution times.
- Limited memory resources.



We need an scalable solution to obtain EOFs Analisys

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Python Introduction

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Python is

- Free Distribution.
- Scripting language: No compile or link steps.
- No type declarations.
- High-level data-types and operations.
- Extending and embedding in C as system bond.
- Run in either batch mode or interactive mode.

Execution Modes

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- Batch Mode.
- Interactive mode

Execution Modes

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- Batch Mode.

```
vgaliano@node0:~$ python hello.py
Hello World
```

- Interactive mode

Execution Modes

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- Batch Mode.

```
vgaliano@node0:~$ python hello.py
Hello World
```

- Interactive mode

```
vgaliano@node0:~$ python
Python 2.4.3 (#4, May 12 2006, 19:00:23)
[GCC 3.3.5 (Debian 1:3.3.5-13)] on linux2
Type "help", "copyright", "credits" or "license" for
more information.
>>> print "Hello World"
Hello World
```

Main used packages: Numeric Python

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Numeric Python

- Adds a fast multidimensional array facility to Python.
- array object : homogeneous collections of potentially large numbers of numbers.
- Similar arrays management like Matlab, Fortran, Basis and others.
- Operations performed *elementwise* on the arguments of the operation
- Same data types between C/Fortran y Python.
- Contiguous arrays performs better times
(`PyArray_ContiguousFromObject()`).

Main used packages: Numeric Python

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(`PyArray_ContiguousFromObject()`).

```
>>> from Numeric import *
>>> vector1 = array([1,2,3,4,5])
>>> print vector1
[1 2 3 4 5]
```

Main used packages: Numeric Python

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Numeric Python

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- Operations performed *elementwise* on the arguments of the operation
- Same data types between C/Fortran y Python.
- Contiguous arrays performs better times
(`PyArray_ContiguousFromObject()`).

```
>>> a = arrayrange(9)
>>> a.shape = (3,3)
>>> print a
[[0 1 2]
 [3 4 5]
 [6 7 8]]
>>> print a[0]
[0 1 2]
>>> print a[1,0]
3
```

Main used packages: Numeric Python

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- Operations performed *elementwise* on the arguments of the operation
- Same data types between C/Fortran y Python.
- Contiguous arrays performs better times (`PyArray_ContiguousFromObject()`).

```
>>> print a
[1 2 3]
>>> print a * 3
[3 6 9]
>>> print a + 3
[4 5 6]
>>> print sin(a)
[ 0.84147098  0.90929743  0.14112001]
```

Main used packages: Numeric Python

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(`PyArray_ContiguousFromObject()`).

```
>>> print a
[1 2 3]
>>> print a * 3
[3 6 9]
>>> print a + 3
[4 5 6]
>>> print sin(a)
[ 0.84147098  0.90929743  0.14112001]
```

Main used packages: Numeric Python

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- Similar arrays management like Matlab, Fortran, Basis and others.
- Operations performed *elementwise* on the arguments of the operation
- Same data types between C/Fortran y Python.
- **Contiguous arrays performs better times**
`(PyArray_ContiguousFromObject ())`.

```
>>> a=reshape(range(9), [3,3])
>>> a
array([[0, 1, 2],
       [3, 4, 5],
       [6, 7, 8]])
>>> b=a[:,0]
>>> b
array([0, 3, 6])
>>> print a.iscontiguous(), b.iscontiguous()
1 0
```

Main used packages: Scientific Python y pyMPI

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Scientific Python

- Collection of Python modules that are useful for scientific computing.
- `ScientificPython.MPI`.
- `ScientificPython.IO.NetCDF`.

Main used packages: Scientific Python y pyMPI

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Scientific Python

- Collection of Python modules that are useful for scientific computing.
- `ScientificPython.MPI`.
- `ScientificPython.IO.NetCDF`.

pyMPI

- Integrating the Message Passing Interface (MPI) into the Python interpreter.
- Asynchronous interactive execution.

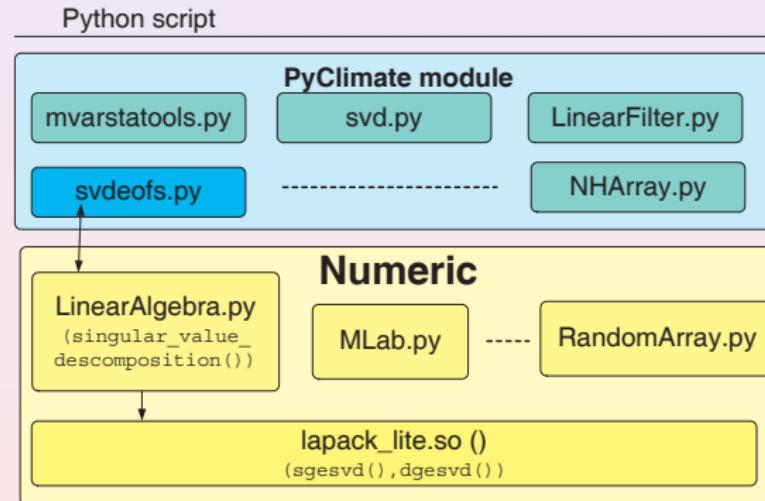
PyClimate structure

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Software libraries used in EOFs Analysis

- NetCDF access: ScientificPython.
- Numeric Modules: Numeric Python (actually Numarray).
- C libraries: `lapack_lite.so`.



PyClimate structure

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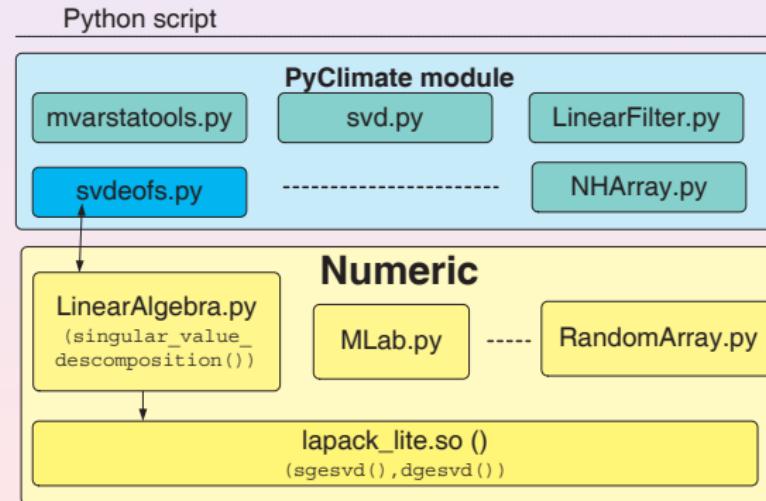
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Parallelization of EOFs Analysis



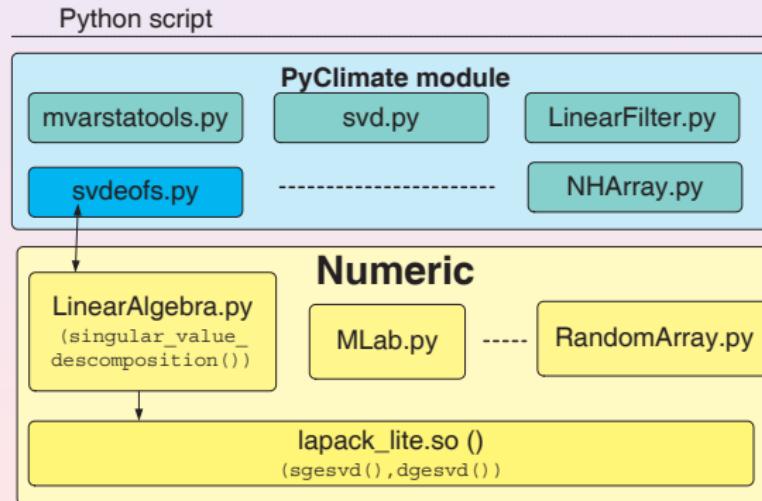
PyClimate structure

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Parallelization of EOFs Analysis

- Messages Passing Interface (PVM, MPI, ...)
- $X_{gesvd} \in \text{LAPACK} \implies pX_{gesvd} \in \text{ScalAPACK}$



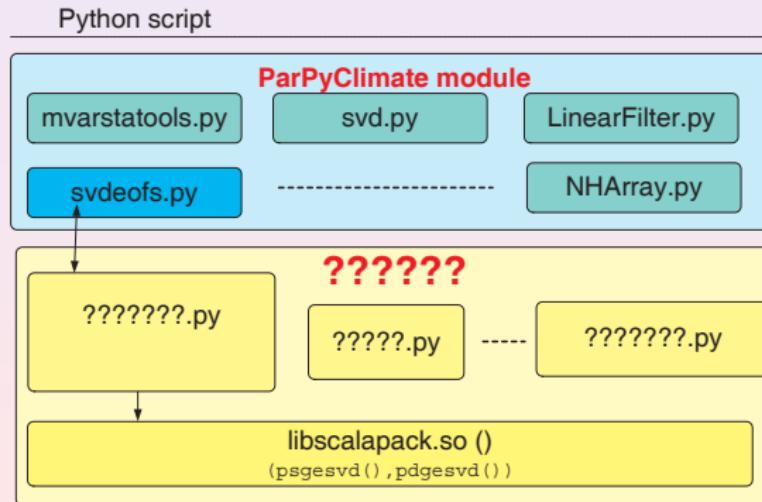
PyClimate structure

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Parallelization of EOFs Analysis

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- $X_{gesvd} \in \text{LAPACK} \implies pX_{gesvd} \in \text{ScalAPACK}$



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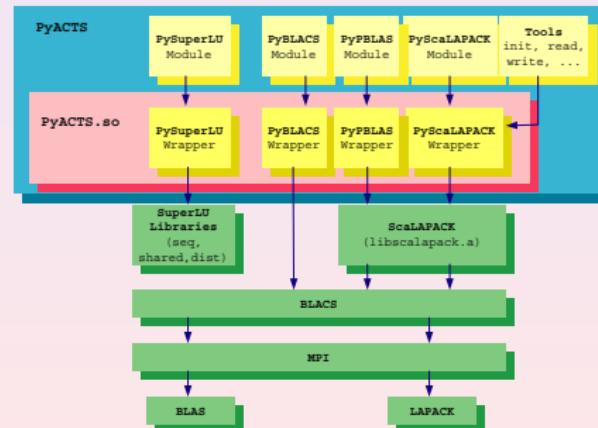
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High Level Interfaces and Auxiliary routines to the ACTS Collection:

- PyBLACS.
- PyPBLAS.
- PyScalAPACK.



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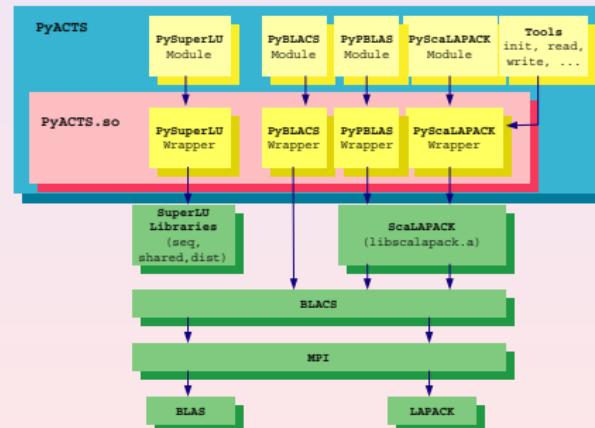
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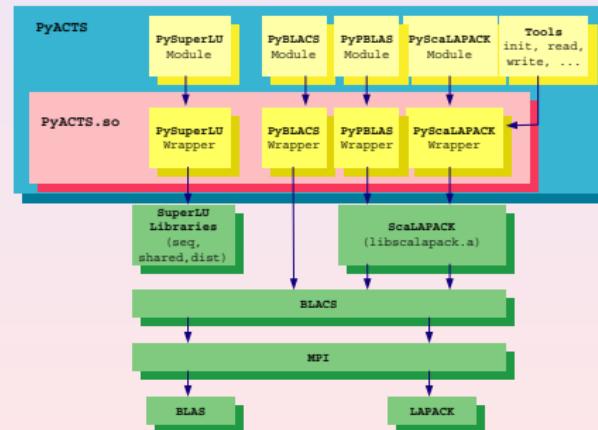
PyPnetCDF

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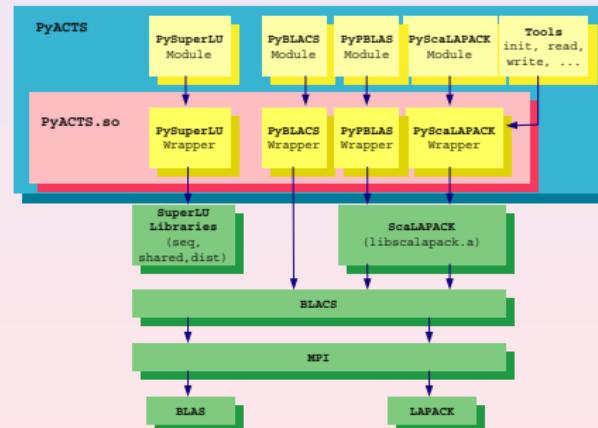
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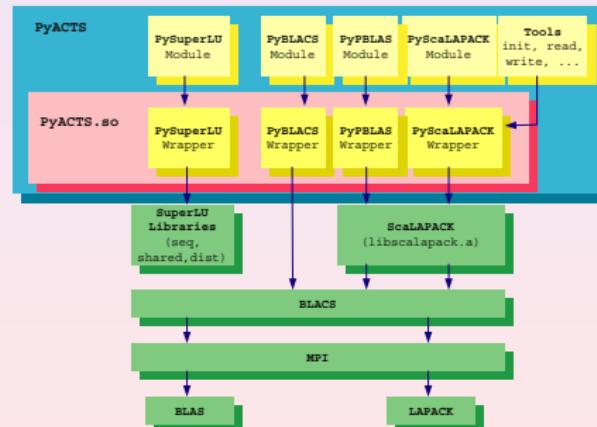
PyPnetCDF

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High Level Interfaces and Auxiliary routines to the ACTS Collection:

- PyBLACS.
- PyPBLAS.
- PyScalAPACK.
- **Support functionality:**
 - Basic Services
 - I/O Services
 - Errors and Exceptions



Plattforms used in tests

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Cluster-umh

Seaborg

6 Intel Pentium 4, 2 GHz with 1 Gbyte RAM connected with a Switch Gigabit Ethernet and with operative system Linux (Debian distribution). Node0 shares its hard disk with NFS.

Plattforms used in tests

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Cluster-umh

Seaborg

IBM SP RS/6000 with 6080 processors. Each processor has a peak performance of 1.5 GFlops and the processors are distributed among 380 compute nodes with 16 processors per node. Disk Access with **Global Parallel File System**

Communications about PyACTS

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- L. A. Drummond, V. Galiano, V. Migallón, and J. Penadés. *High Level User Interfaces for High Performance Libraries in Linear Algebra: PyBLACS and PyPBLAS*. In *12th International Linear Algebra Society Conference*, University of Regina, Regina, Saskatchewan, Canada, June 2005.
- L. A. Drummond, V. Galiano, V. Migallón, and J. Penadés. Improving ease of use in BLACS and PBLAS with Python. *Proceedings of the International Conference ParCo*. September 2005.
- L. A. Drummond, V. Galiano, V. Migallón, and J. Penadés. PyACTS: A High-Level Framework for Fast Development of High Performance Applications. In *Proceedings from Seventh International Meeting on High Performance Computing for Computational Science - VECPAR'06*, pages 373–378, Rio de Janeiro, Brazil, July 2006.
- L. A. Drummond, V. Galiano, J. Penadés, and V. Migallón. An introduction to PyACTS. In *SIAM Conference on Computational Science and Engineering*. SIAM Activity Group on Computational Science and Engineering, Orlando, Florida, February 2005.
- L. A. Drummond, V. Galiano, J. Penadés, and V. Migallón. High Level User Interfaces for Numerical Linear Algebra Libraries: PyScalAPACK. In *Proceedings of the Fifth International Conference on Engineering Computational Technology*, pages 1–10. Civil-Comp Ltd., September 2006.

Communications about PyACTS

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PyScaLAPACK

PyPnetCDF

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- L. A. Drummond, V. Galiano, J. Penadés, and V. Migallón. PyACTS: A High-Level Framework for Fast Development of High Performance Applications. In *Proceeding of the SIAM Conference on Parallel Processing for Scientific Computing*. SIAM Activity Group on Supercomputing, San Francisco, California, February 2006.
- L. A. Drummond, V. Galiano, J. Penadés, and V. Migallón. High-level User Interfaces for the DOE ACTS Collection. In *PARA06: Proceeding of the Workshop on state-of-the-art in scientific and parallel computing*. Umea University, Sweden, June 2006.

PyACTS Publications

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- L. A. Drummond, V. Galiano, V. Migallón, and J. Penadés. PyACTS: A High-Level Framework for Fast Development of High Performance Applications. In *Lectures Notes in Computer Science*, 4395: 417–425, 2007.
- L. A. Drummond, V. Galiano, J. Penadés, and V. Migallón. High-level User Interfaces for the DOE ACTS Collection. To appear in *Lecture Notes in Computer Science*.
- L. A. Drummond, V. Galiano, V. Migallón, and J. Penadés. Improving ease of use in BLACS and PBLAS with Python. In G.R. Joubert, W.E. Nagel, F.J. Peters, O. Plata, P. Tirado, and E. Zapata, editors, *Parallel Computing: Current & Future Issues of High-End Computing*, volume 33. NIC series, September 2006. ISBN 3-00-017352-8.
- L. A. Drummond, V. Galiano, J. Penadés, and V. Migallón. High Level User Interfaces for Numerical Linear Algebra Libraries: PyScalAPACK. Submitted to *International Journal of Computers and Structures (CAS)*.

PyScaLAPACK Module

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- Transparent and simplified access to ScalAPACK from Python.

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- Transparent and simplified access to ScaLAPACK from Python.
- Same names than in ScaLAPACK.

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- Transparent and simplified access to ScaLAPACK from Python.
- Same names than in ScaLAPACK.
- Interaction with PyBLACS and PyPBLAS.

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- Transparent and simplified access to ScaLAPACK from Python.
- Same names than in ScaLAPACK.
- Interaction with PyBLACS and PyPBLAS.
- **PyScaLAPACK is classified in two groups:**

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- Transparent and simplified access to ScaLAPACK from Python.
- Same names than in ScaLAPACK.
- Interaction with PyBLACS and PyPBLAS.
- PyScaLAPACK is classified in two groups:
 - Driver Routines
 - 1 Linear Equations
 - 2 Linear Least Squares Problems
 - 3 Standard Eigenvalue and Singular Value Problems
 - 4 Generalized Symmetric Definite Eigenproblems (GSEP)

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- Transparent and simplified access to ScaLAPACK from Python.
- Same names than in ScaLAPACK.
- Interaction with PyBLACS and PyPBLAS.
- PyScaLAPACK is classified in two groups:
 - Driver Routines
 - 1 Linear Equations
 - 2 Linear Least Squares Problems
 - 3 Standard Eigenvalue and Singular Value Problems
 - 4 Generalized Symmetric Definite Eigenproblems (GSEP)
 - Computational Routines
 - 1 Linear Equations
 - 2 Orthogonal Factorizations and Linear Least Squares Problems
 - 3 Generalized Orthogonal Factorizations
 - 4 Symmetric Eigenproblems
 - 5 Nonsymmetric Eigenproblems
 - 6 Singular Value Decomposition
 - 7 Generalized Symmetric Definite Eigenproblems

Driver Routines for Standard Eigenvalue and Singular Value Problems

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Standard Eigenvalue and Singular Value Problems

- Simmetric Matrix.

- Simple: `w,z,info= pvsyev(a[, jobz='N', uplo='U'])`
- Advanced: `m,nz,w,z,ifail,ioclustr,gap,info=pvsyevx(a [, jobz='N', range='A', uplo='U', orfac=0, rcond=0, vl=None, vu=None, il=None, iu=None, abstol=0])`

- General Matrix.

- Simple: `s,u,vt,info= pggesvd(a[, jobu='N', jobvt='N'])`

Singular value decomposition Example with pvgesvd

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$$A = U\Sigma V^T, A \in \mathbb{R}^{m \times n}$$

```
from PyACTS import *
import PyACTS.PyScalAPACK as PySLK
from Numeric import *
n=8
PyACTS.gridinit()
if PyACTS.iread==1:
    a=8*identity(n,Float)
    print "a=",a
else:
    a=None
ACTS_lib=1
a=Num2PyACTS(a,ACTS_lib)
s,u,vt,info=PySLK.pvgesvd(a,'V','V')
u_num=PyACTS2Num(u)
vt_num=PyACTS2Num(vt)
if PyACTS.iread==1:
    print "s'=",transpose(s)
    print "u=",u_num
    print "vt=",vt_num
PyACTS.gridexit()
```

```
$ mpirun -np 4 mpipython pvgesvd.py
a= [[ 8.  0.  0.  0.  0.  0.  0.  0.  0.]
 [ 0.  8.  0.  0.  0.  0.  0.  0.  0.]
 [ 0.  0.  8.  0.  0.  0.  0.  0.  0.]
 [ 0.  0.  0.  8.  0.  0.  0.  0.  0.]
 [ 0.  0.  0.  0.  8.  0.  0.  0.  0.]
 [ 0.  0.  0.  0.  0.  8.  0.  0.  0.]
 [ 0.  0.  0.  0.  0.  0.  8.  0.  0.]
 [ 0.  0.  0.  0.  0.  0.  0.  8.  0.]
 [ 0.  0.  0.  0.  0.  0.  0.  0.  8.]]
s'= [ 8.  8.  8.  8.  8.  8.  8.  8.  8.]
u= [[ 1.  0.  0.  0.  0.  0.  0.  0.  0.]
 [ 0.  1.  0.  0.  0.  0.  0.  0.  0.]
 [ 0.  0.  1.  0.  0.  0.  0.  0.  0.]
 [ 0.  0.  0.  1.  0.  0.  0.  0.  0.]
 [ 0.  0.  0.  0.  1.  0.  0.  0.  0.]
 [ 0.  0.  0.  0.  0.  1.  0.  0.  0.]
 [ 0.  0.  0.  0.  0.  0.  0.  1.  0.]
 [ 0.  0.  0.  0.  0.  0.  0.  0.  1.]
 [ 0.  0.  0.  0.  0.  0.  0.  0.  1.1]]
vt= [[ 1.  0.  0.  0.  0.  0.  0.  0.  0.]
 [ 0.  1.  0.  0.  0.  0.  0.  0.  0.]
 [ 0.  0.  1.  0.  0.  0.  0.  0.  0.]
 [ 0.  0.  0.  1.  0.  0.  0.  0.  0.]
 [ 0.  0.  0.  0.  1.  0.  0.  0.  0.]
 [ 0.  0.  0.  0.  0.  1.  0.  0.  0.]
 [ 0.  0.  0.  0.  0.  0.  0.  1.  0.]
 [ 0.  0.  0.  0.  0.  0.  0.  0.  1.]
 [ 0.  0.  0.  0.  0.  0.  0.  0.  1.1]]
Info: 0
```

SVD Execution times

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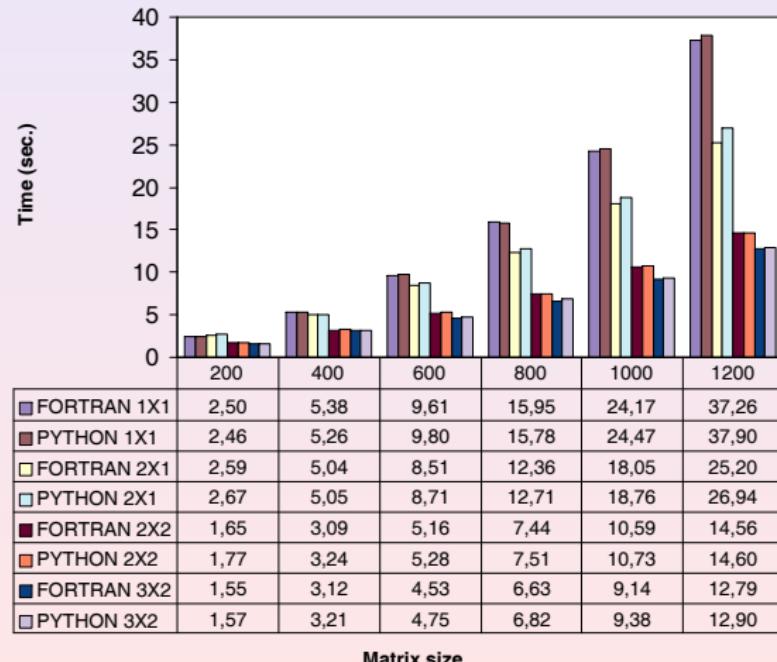
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Comparative Fortran vs Python: `pvgesvd` vs `PDGESVD`

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Seaborg



SVD Execution times

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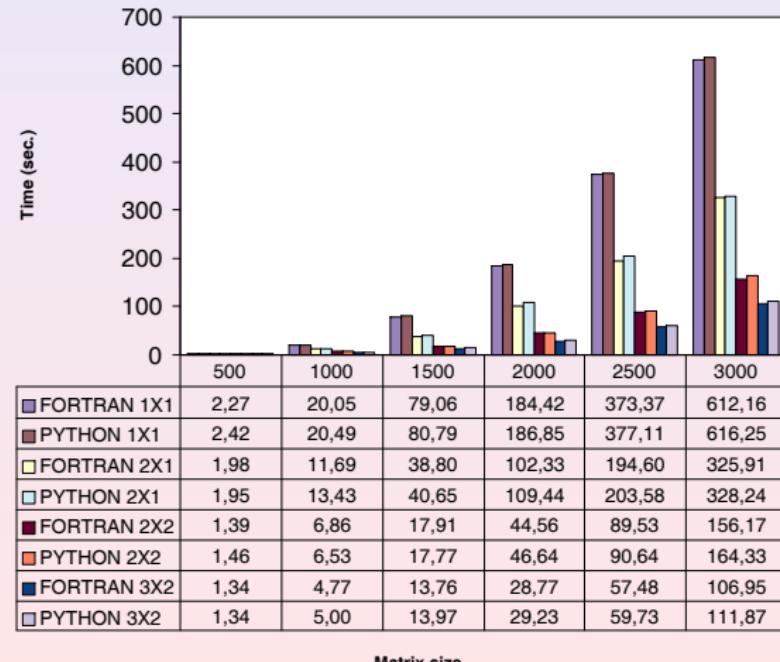
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Comparative Fortran vs Python: `pvgesvd` vs `PDGESVD`

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3 PyNetCDF

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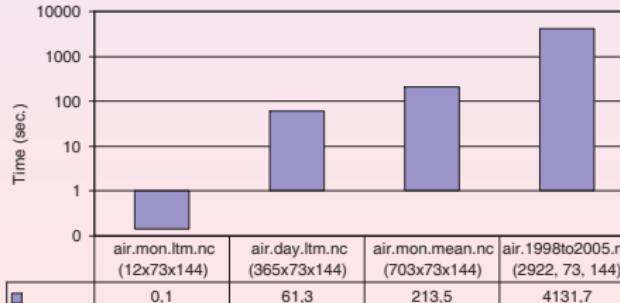
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¿Scalability?

- NetCDF files obtained from Climate Diagnostics Center (www.cdc.noaa.gov).
- Extending data grid 144×73 .
- Including Data grids at different elevations $17 \times 144 \times 73$.
- Increasing time axis.
 - `air.mon.ltm.nc` → $17 \times 12 \times 144 \times 73$ 8,5MB
 - `air.day.ltm.nc` → $17 \times 365 \times 144 \times 73$ 1,3GB
 - `air.mon.mean.nc` → $17 \times 703 \times 144 \times 73$ 2,5GB
 - `air.1988to2005.nc` → $17 \times 2922 \times 144 \times 73$ 4,17GB



Remembering scalability problems in EOFs Analysis

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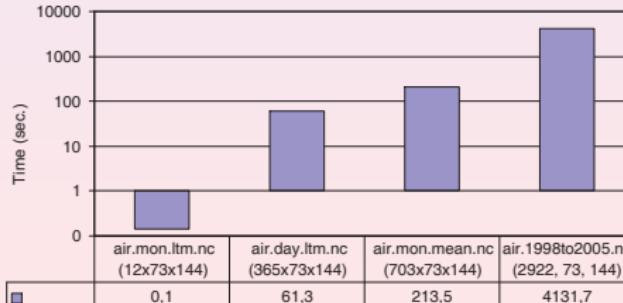
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¿Scalability?

- NetCDF files obtained from Climate Diagnostics Center (www.cdc.noaa.gov).
- Extending data grid 144×73 .
- Including Data grids at different elevations $17 \times 144 \times 73$.
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 - $\text{air.mon.ltm.nc} \rightarrow 17 \times 12 \times 144 \times 73$ 8,5MB
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 - $\text{air.1988to2005.nc} \rightarrow 17 \times 2922 \times 144 \times 73$ 4,17GB



An scalable solution also requires a parallel access to disk and data distribution

Introduction to netCDF

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netCDF: network Common Data Format

- Popular package for storing data files in scientific applications.
- NetCDF consists of both an API and a portable file format.
- NetCDF file format guarantees data portability and self defined.
- API libraries for C/C++/F77/F90.
- Support from Unidata.
- Many organizations rely on the netCDF data access standard for data storage.
 - Easy to learn.
 - Widely used in climate community .

Data structure and file format

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Data structure

- Dimensions.
- Variables.
- Attributes.

```
ejemplo_netCDF {
dimensions:
    lat = 5, lon = 10;
    level = 4, time = unlimited;
variables:
    float temp(time,level,lat,lon);
    temp:long_name = "Temperature";
    temp:units = "° Celsius";
    float rh(time,lat,lon);
    rh:long_name = "Relative Hum.";
    rh:valid_range = 0.0, 1.0;
// Global Attributes:
    :source = "Output Model";
data:
    temp = 3.2, ..., 15.1,
        ...
        1.6, ..., 2.4;
    rh = .5,.2,.4,.2,.3,.2,.4,.5,.6,.7,
        ...
        0,.1,.2,.4,.4,.4,.4,.7,.9,.9;
}
```

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Data structure

- Dimensions.
- Variables.
- Attributes.

```
ejemplo_netCDF {  
dimensions:  
    lat = 5, lon = 10;  
    level = 4, time = unlimited;  
variables:  
    float temp(time,level,lat,lon);  
    temp:long_name = "Temperature";  
    temp:units = "° Celsius";  
    float rh(time,lat,lon);  
    rh:long_name = "Relative Hum.";  
    rh:valid_range = 0.0, 1.0;  
// Global Attributes:  
    :source = "Output Model";  
data:  
temp = 3.2, ..., 15.1,  
      ...  
      1.6, ..., 2.4;  
rh = .5,.2,.4,.2,.3,.2,.4,.5,.6,.7,  
      ...  
      0,.1,.2,.4,.4,.4,.7,.9,.9;  
}
```

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Data structure

- Dimensions.
- Variables.
- Attributes.

```
ejemplo_netCDF {  
dimensions:  
    lat = 5, lon = 10;  
    level = 4, time = unlimited;  
variables:  
    float temp(time,level,lat,lon);  
    temp:long_name = "Temperature";  
    temp:units = "° Celsius";  
    float rh(time,lat,lon);  
    rh:long_name = "Relative Hum.";  
    rh:valid_range = 0.0, 1.0;  
// Global Attributes:  
    :source = "Output Model";  
data:  
temp = 3.2, ..., 15.1,  
      ...  
      1.6, ..., 2.4;  
rh = .5,.2,.4,.2,.3,.2,.4,.5,.6,.7,  
      ...  
      0,.1,.2,.4,.4,.4,.7,.9,.9;  
}
```

NetCDF access from Python

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ScientificPython Package

- `Scientific.IO.NetCDF`.
- NetCDF metadata is managed with:
 - `NetCDFFile`
 - `NetCDFVariable`

NetCDF access from Python

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ScientificPython Package

- `Scientific.IO.NetCDF`.
- NetCDF metadata is managed with:
 - `NetCDFFile`
 - `NetCDFVariable`

```
import sys, string
from Numeric import *
from Scientific.IO.NetCDF import NetCDFFile
file = NetCDFFile('test.nc', 'w')
file.title = "Example file"
file.version = 42
file.createDimension('xyz', 3)
file.createDimension('n', 20)
file.createDimension('t', None)
foo = file.createVariable('foo',
                         Float, ('n', 'xyz'))
foo.units = "arbitrary"
foo[:, :] = 1.
foo[0:3, :] = [42., 42., 42.]
foo[:, 1] = 4.
foo[0, 0] = 27.
file.close()
file2 = NetCDFFile('test.nc', 'r')
print file2.variables.keys()
print file2.dimensions.keys()
for varname in file2.variables.keys():
    var1 = file2.variables[varname]
    print varname, ":", var1.shape
    foo = file2.variables['foo']
    data1 = var1.getValue()
    print "Datos:", data1
file2.close()
```

NetCDF access from Python

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ScientificPython Package

- `Scientific.IO.NetCDF`.
- **NetCDF metadata is managed with:**
 - `NetCDFFile`
 - `NetCDFVariable`

```
$ python read_netcdf.py test.nc
['foo']
['xyz', 't', 'n']
foo : (20, 3)
Datos: [[ 27.   4.  42.]
 [ 42.   4.  42.]
 [ 42.   4.  42.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 [ 1.   4.  1.]
 ...
 [ 1.   4.  1.]]
```

```
import sys, string
from Numeric import *
from Scientific.IO.NetCDF import NetCDFFile
file = NetCDFFile('test.nc', 'w')
file.title = "Example file"
file.version = 42
file.createDimension('xyz', 3)
file.createDimension('n', 20)
file.createDimension('t', None)
foo = file.createVariable('foo',
                         Float, ('n', 'xyz'))
foo.units = "arbitrary"
foo[:, :] = 1.
foo[0:3, :] = [42., 42., 42.]
foo[:, 1] = 4.
foo[0, 0] = 27.
file.close()
file2 = NetCDFFile('test.nc', 'r')
print file2.variables.keys()
print file2.dimensions.keys()
for varname in file2.variables.keys():
    var1 = file2.variables[varname]
    print varname, ":", var1.shape
    foo = file2.variables['foo']
    data1 = var1.getValue()
    print "Datos:", data1
file2.close()
```

Parallel access to netCDF files

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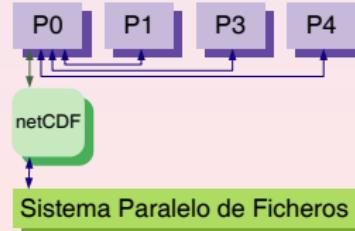
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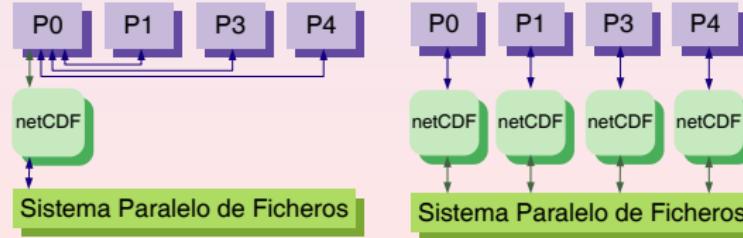
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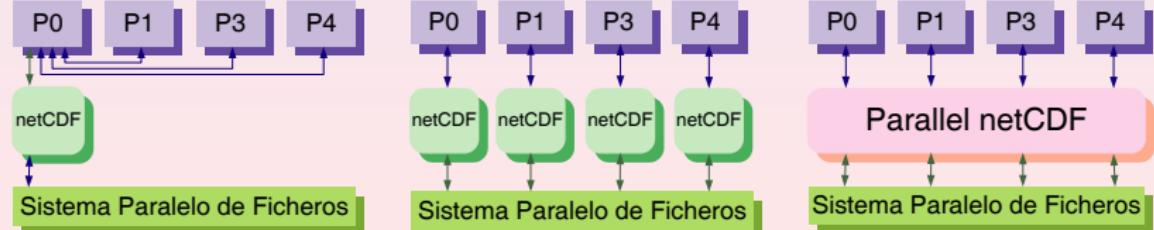
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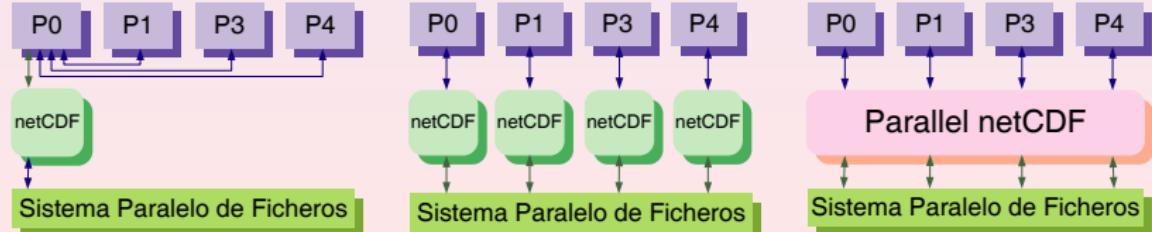
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PnetCDF library

- Parallel interface to netCDF files.
- Call MPI-IO routines.
- Similar syntax than netCDF.
- Very similar to the sequential version netCDF.
- Interfaces for Fortran (`nfmpi`) y C (`ncmpi`).

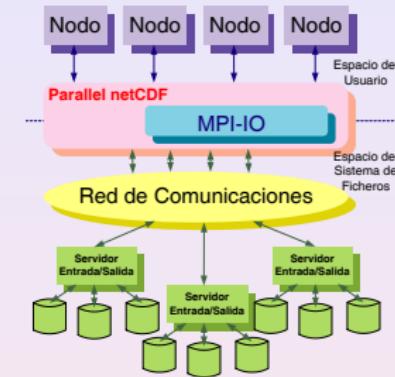
netCDF files management in parallel architectures



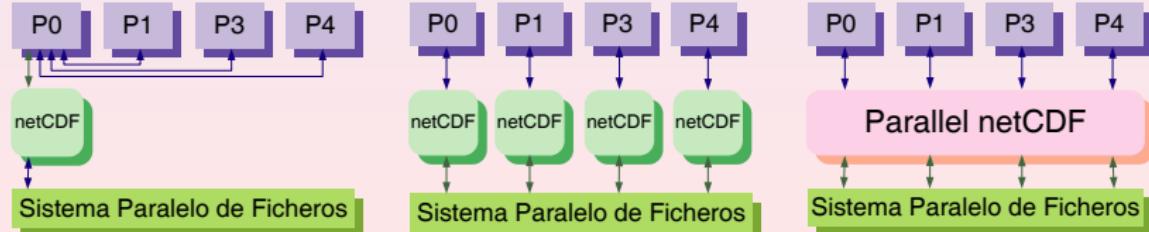
Parallel access to netCDF files

PnetCDF library

- Parallel interface to netCDF files.
- Call MPI-IO routines.
- Similar syntax than netCDF.
- Very similar to the sequential version netCDF.
- Interfaces for Fortran (`nfmpi`) y C (`ncmpi`).



netCDF files management in parallel architectures



Parallel access to netCDF files

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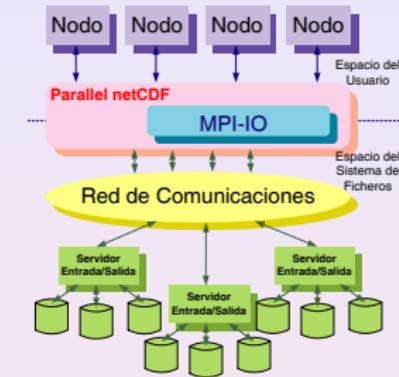
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PnetCDF library

- Parallel interface to netCDF files.
- Call MPI-IO routines.
- Similar syntax than netCDF.
- Very similar to the sequential version netCDF.
- Interfaces for Fortran (ncmpi) y C (ncmpi).



Write

```
ncmpi_create(MPI_Comm, filename, 0,  
            MPI_Info, &file_id)  
  
ncmpi_def_var(file_id, ...)  
  
ncmpi_enddef(file_id)  
  
ncmpi_put_vara_all(file_id, var_id, start[],  
                   count[], buffer, bufcount, MPI_Datatype)  
  
ncmpi_close(file_id)
```

Read

```
ncmpi_open(MPI_Comm, filename, 0,  
          MPI_Info, &file_id)  
  
ncmpi_inq(file_id, ... );  
  
ncmpi_enddef(file_id)  
  
ncmpi_get_vara_all(file_id, var_id,  
                   buffer, bufcount, start[], count[],  
                   stride[], MPI_Datatype)
```

Motivation

- NetCDF access from Python, only sequential .
- Limited in parallel applications with Python
- ... but PnetCDF library is ...
 - Free distribution and Open Source.
 - Interfaces for C/C++/F77/F90.
- Create an interface for access to `libpnetcdf.a` from Python.
- Python Module hide parallelism and simplify synchronizing tasks.
- Functionality and sintaxis similar to ScientificPython.
- Object oriented programming:
 - `PNetCDFFile`
 - `NetCDFVariable`
- Integration with PyACTS.

Motivation

- NetCDF access from Python, only sequential .
- Limited in parallel applications with Python
- ... but PnetCDF library is ...
 - Free distribution and Open Source.
 - Interfaces for C/C++/F77/F90.
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PyPnetCDF: parallel access to netCDF files from Python

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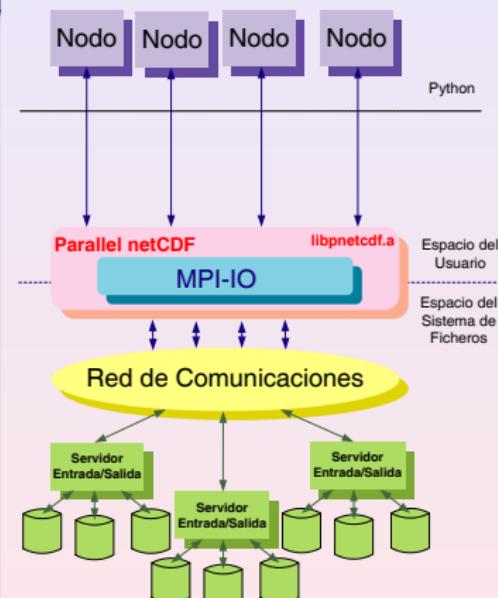
Tests

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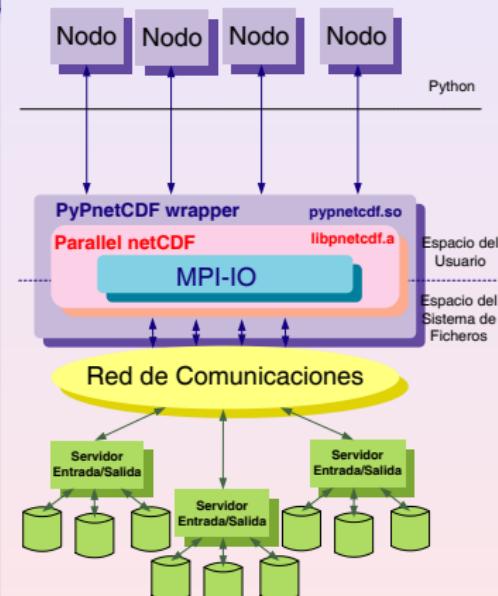
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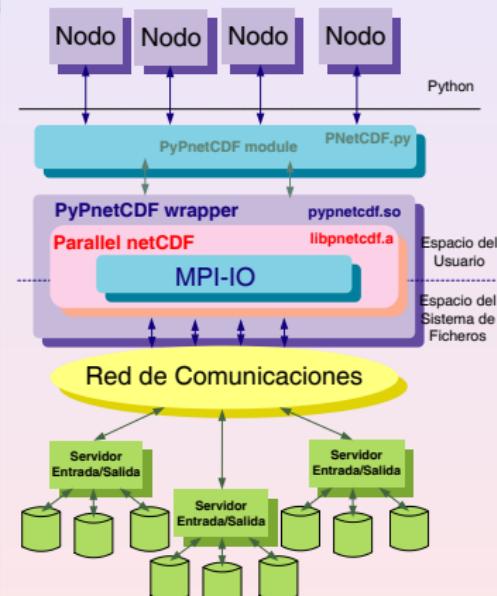
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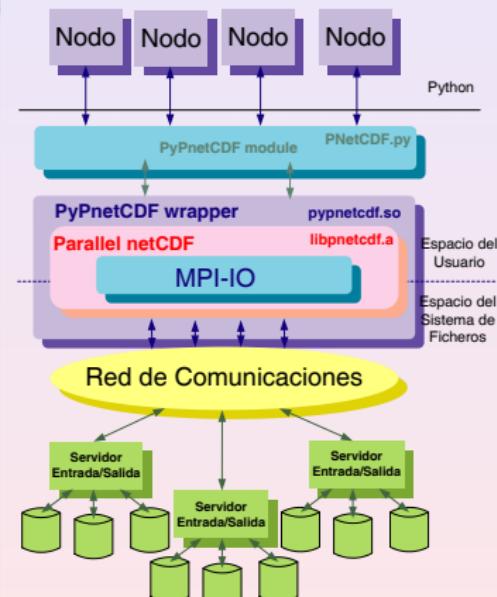
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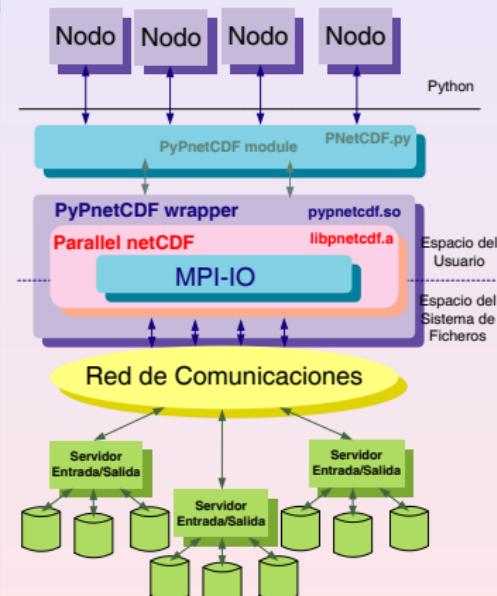
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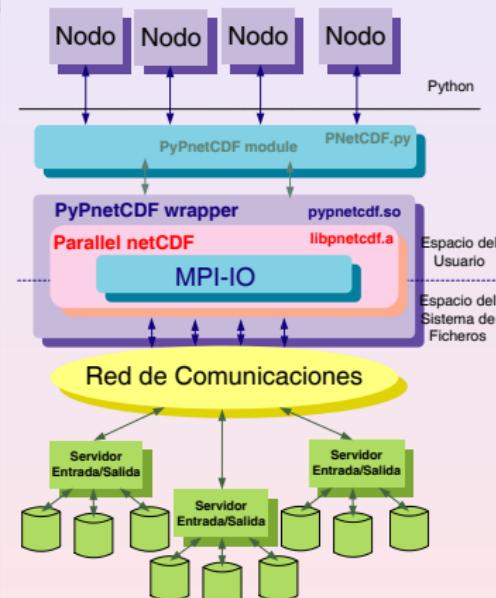
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Parallel access from Python using PyNetCDF

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```
from Numeric import *
from PyPNetCDF.PNetCDF import *
import PyACTS

file = PNetCDFFile('test.nc', 'w')
file.title = "Just some useless junk"
file.version = 42

file.createDimension('xyz', 3)
file.createDimension('n', 20)
# Dimension ilimitada
file.createDimension('t', None)
dfoo={'n','xyz'}
foo=file.createVariable('foo',Float,dfoo)
foo.units = "arbitrary"

foo[:,::] = 1.
foo[0:3,:] = [42., 42., 42.]
foo[:,1] = 4.
foo.data[0,0] = PyACTS.iam
file.enddef()
foo.setValue()
file.close()
```

```
file2 = PNetCDFFile('test.nc', 'r')
print "*"*10," Proceso ",PyACTS.iam,"/",PyACTS.nprocs,"*"*10
print ncfile1.variables.keys()
print ncfile1.dimensions.keys()
for varname in file2.variables.keys():
    var1 = file2.variables[varname]
    print varname,":",var1.shape,";",
          var1.units
    foo = file2.variables['foo']
    data1 = var1.getValue()
    print "Datos:",data1
file2.close()
```

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```
$mpirun -np 4 mpipython read_pnetcdf.py ./test.nc
```

```
***** Proceso 0 / 4 *****
['foo']
['xyz', 't', 'n']
foo : (20, 3) ; arbitrary
Datos: [[ 0.  4.  42.]
       [ 42.  4.  42.]
       [ 42.  4.  42.]
       [ 1.  4.  1.]
       [ 1.  4.  1.]]
*****
Proceso 3 / 4 *****
['foo']
['xyz', 't', 'n']
foo : (20, 3) ; arbitrary
Datos: [[ 3.  4.  1.]
       [ 1.  4.  1.]
       [ 1.  4.  1.]
       [ 1.  4.  1.]]
```

```
***** Proceso 2 / 4 *****
['foo']
['xyz', 't', 'n']
foo : (20, 3) ; arbitrary
Datos: [[ 2.  4.  1.]
       [ 1.  4.  1.]
       [ 1.  4.  1.]
       [ 1.  4.  1.]]
*****
Proceso 1 / 4 *****
['foo']
['xyz', 't', 'n']
foo : (20, 3) ; arbitrary
Datos: [[ 1.  4.  1.]
       [ 1.  4.  1.]
       [ 1.  4.  1.]
       [ 1.  4.  1.]]
```

PyPnetCDF Scalability

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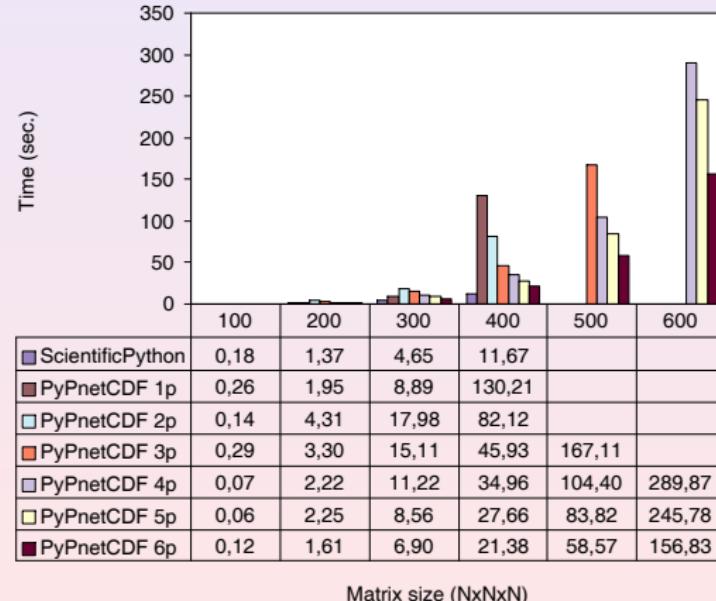
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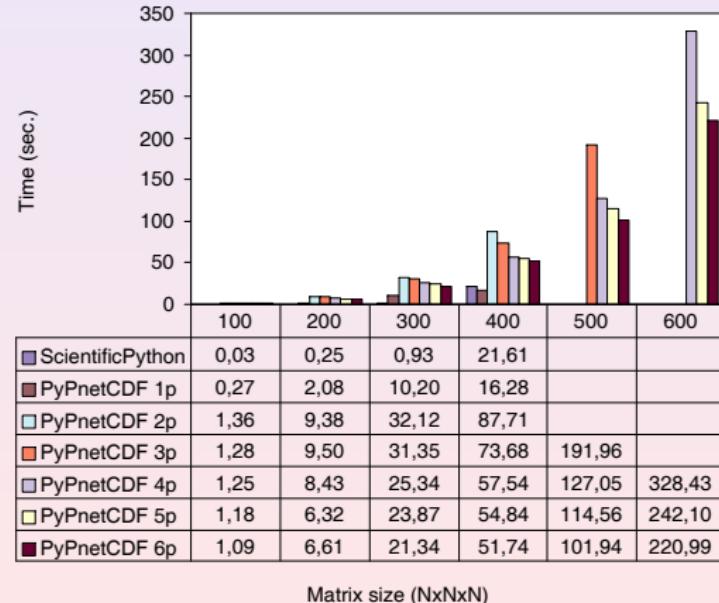
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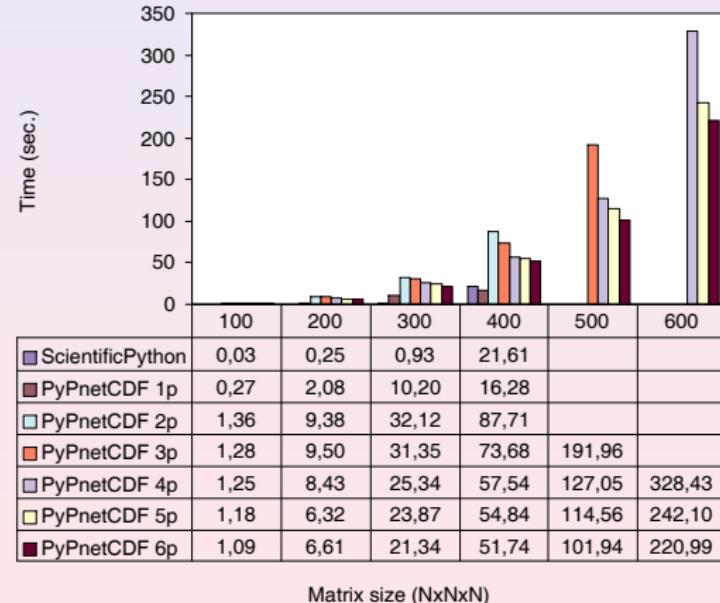
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PyPnetCDF scales with the number of processors

Writing Times in Cluster-umh



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Remembering EOFs Analysis

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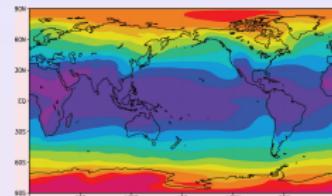
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EOFs Analysis with PyClimate

- Delete redundant information with minimum lost of variability.



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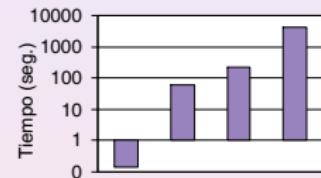
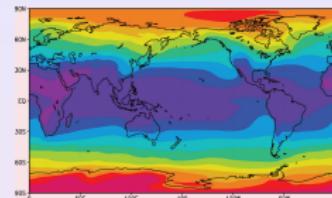
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EOFs Analysis with PyClimate

- Delete redundant information with minimum lost of variability.
- Scalability problem with huge data volume.



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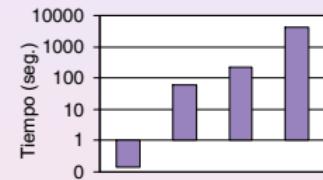
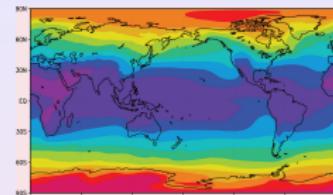
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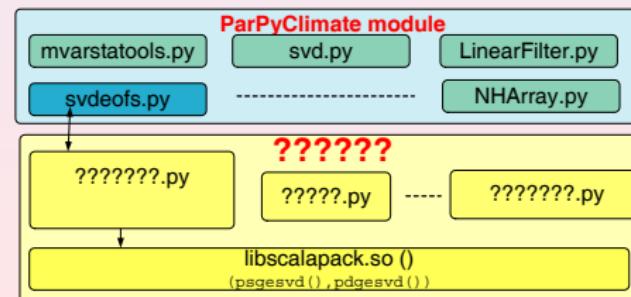
Conclusions

EOFs Analysis with PyClimate

- Delete redundant information with minimum lost of variability.
- Scalability problem with huge data volume.
- We didn't have appropriate Python tools.



Python script



Remembering EOFs Analysis

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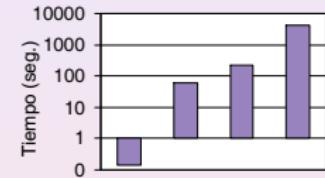
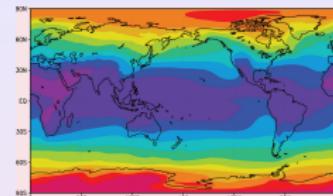
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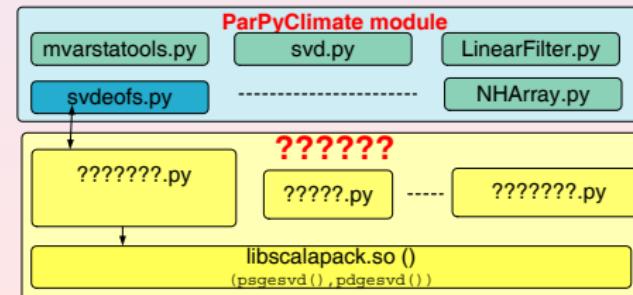
Conclusions

EOFs Analysis with PyClimate

- Delete redundant information with minimum lost of variability.
- Scalability problem with huge data volume.
- We didn't have appropriate Python tools.
- But with PyACTS and PyPnetCDF we can build and scalable EOFs analysis.



Python script



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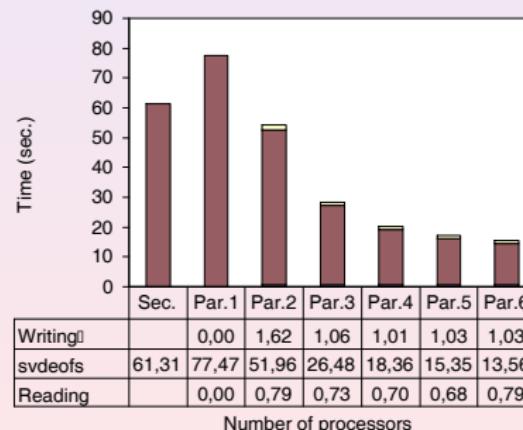
air.day.ltm.nc

air.mon.mean.nc

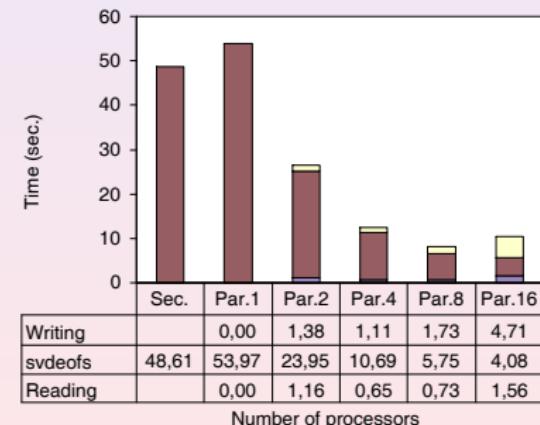
air.1988to2005.nc

$17 \times 365 \times 144 \times 73$, 1.3GB

Cluster



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Scalability with *ParPyClimate*

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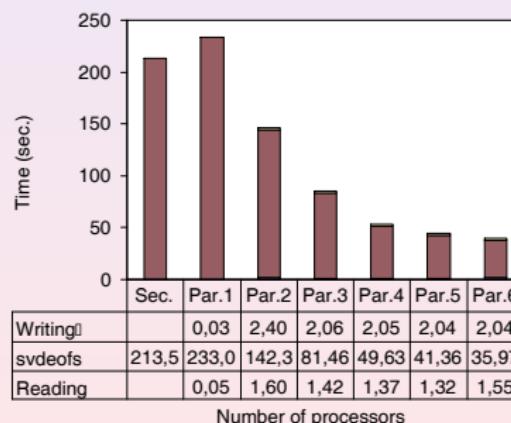
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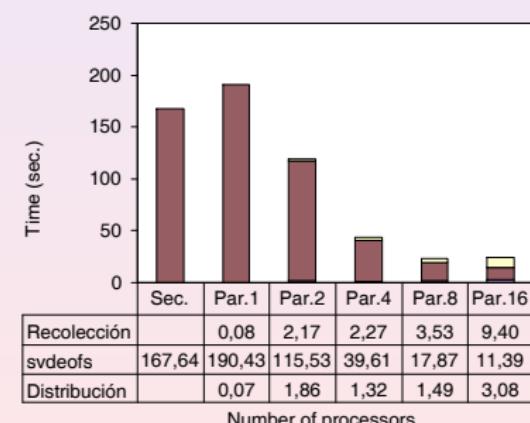
air.1988to2005.nc

$17 \times 703 \times 144 \times 73$, 2.5GB

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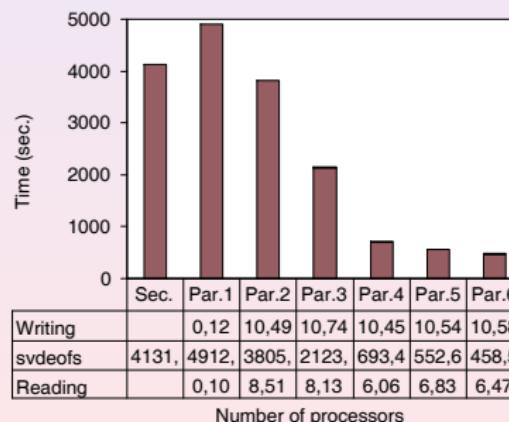
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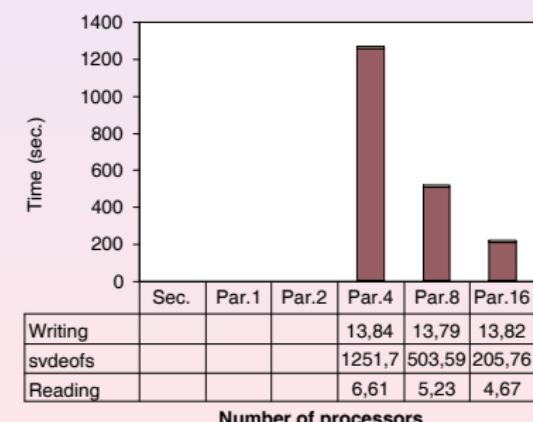
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Goals

- We can manage huge datasets in a parallel execution with a intuitive language.

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Goals

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- Hide parallelism and data distribution if the users that don't want to know about it.
- New applications, not only in climate area.

PyACTS and PyPnetCDF Distribution

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- Web site.
- Mail List and mail support.
- Backup in sourceforge.net
- Documentation and quickguide in PDF & HTML.
- Referenced from Python and Unidata.

<http://www.pyacts.org>
<http://www.pyacts.org/pypnetcdf>

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Testing PyBLACS and PyPBLAS
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<http://sourceforge.net/projects/pypnetcdf>

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Manual de Referencia de PyACTS: PyBLACS, PyPBLAS y PyScalAPACK

Release 1.0

Vicente Galiano
Violeta Migallón
Jose Penadés
Tony Drummond

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Release 1.0

Vicente Galiano
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Tony Drummond

And of course, ...

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DÊKUJI

DANKE

THANKS

GRACIAS