What Geoscientists Want: Short and Sweet Commands with Eco-friendly Data

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Abstract

The twin pressures to achieve mind-share and to harness available computing power drive the evolution of geoscientific data analysis tools. Such tools have enabled a remarkable progression in the atomic or fundamental unit of data they can easily analyze. In the mid-1980s we analyzed one or a few naked arrays at at time, and now researchers routinely intercompare climatological ensembles each comprising thousands of files of heterogeneous variables richly dressed in metadata. Two complementary semantic trends have empowered this analytical revolution: more intuitive and concise analysis commands that can exploit more standardized and brokered self-describing data stores. This talk highlights how tool developers can leverage these trends to successfully imagine and build the analysis tools of tomorrow by understanding the needs of domain researchers and the power of domain specific languages today. This talk will also highlight recent improvements in compression speed and interoperability that geoscientists can exploit to reduce our carbon footprint. Observations and simulations to advance Earth system sciences generate exabytes of archived data per year. Storage accounts for about 40% of datacenter power consumption, with its attendant consequences for greenhouse gas emissions and environmental sustainability. Precision-preserving lossy compression can further reduce the size of losslessly compressed data by 10-25% without compromising its scientific content. Modern lossless codecs (e.g., Zstandard or Zlib-ng) accelerate compression and decompression, relative to the traditional Zlib, by factors of 2-5x with no penalty in compression ratio. These proven modern compression technologies can help geoscientific datacenters become significantly greener.

ESSI 2021 Leptoukh Lecture
What Geoscientists Want: Short and Sweet Commands with Eco-friendly Data

Dr. Greg Leptoukh

Data management and analysis, large-scale computation and modeling, and hardware and software infrastructure profoundly affect the research capabilities of all AGU disciplines. The Earth and Space Science Informatics Focus Group established the **Leptoukh Lecture** in 2012 to recognize advances in these fields and their contributions to Earth and space science. Named in honor of the late Dr. Greg Leptoukh, a pioneer in satellite data quality and provenance, the Leptoukh Lecture aims to identify and support achievements in the computational and data sciences.

Charlie Zender

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Three Acts with the Theme of Interoperability

I. Role of Self-Describing Data Formats
II. Promise of Domain Specific Languages
III. Viability of Greener Computing and Compression

Act I:

Self-Describing Data Formats

Once Upon a Time in Boulder...

Climate data was stored in idiosyncratic model/dataset-specific formats understood by few mortals, accessible through monolithic tools...

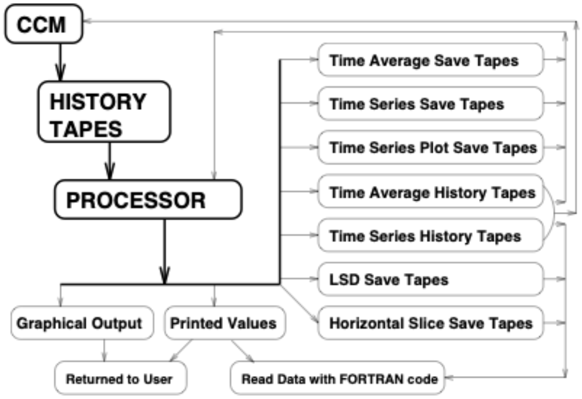
```
#!/bin/csh
#QSUB   -q econ  -lt 30  -lT 33  -lm 2Mw  -lM 2Mw   -eo
cd $TMPDIR

cat >! parms << 'END'
C
C plot.sh    read temperature from a history tape and plot
C
 TITLEA   = 'Plot.sh:  850,500,200mb T from the CCM2 Control Run'
 TAPESA   = '/CSM/ccm2/414/hist/h0002'
 DAYSA    =  11.,12.,13.,14.,15.
 FIELDA1 = 'T'
 PRESSLE =  850.,500.,200.
 HPROJ    = 'RECT'
 HPCINT   = 'T',850.,5., 'T',500.,10., 'T',200.,0.
 DPLTMF   = 'MP'
ENDOFDATA -----------------------------------------------------
'END'

/ccm/proc/Processor
exit
```

NCAR TECHNICAL NOTE

December 1992

Introduction to the UNICOS CCM Processor

LAWRENCE E. BUJA



CLIMATE AND GLOBAL DYNAMICS DIVISION

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BOULDER, COLORADO

...Analysis tools were powerful, but...

Climate data were stored in a proprietary model/dataset-specific history tape format understood by few mortals, accessible through the Fortran-based CCM Processor...

```
#!/bin/csh
#QSUB   -q econ  -lt 30  -lT 33  -lm 2Mw  -lM 2Mw   -eo
cd $TMPDIR

cat >! parms << 'END'
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 FIELDA1  = 'T'
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 HPROJ    = 'RECT'
 HPCINT   = 'T',850.,5., 'T',500.,10., 'T',200.,0.
 DPLTMF   = 'MP'
ENDOFDATA -----------------------------------------------------
'END'

/ccm/proc/Processor
exit
```

Extensible file lists, coordinate subsetting

Random access to variables

NCAR/TN-383+IA
NCAR TECHNICAL NOTE

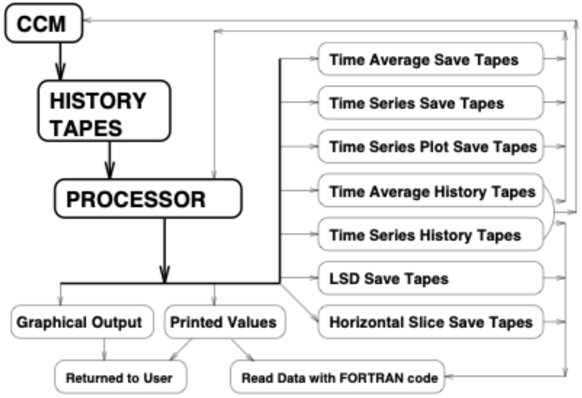
December 1992

OS-specific

Introduction to the UNICOS CCM Processor

Dataset-specific

LAWRENCE E. BUJA



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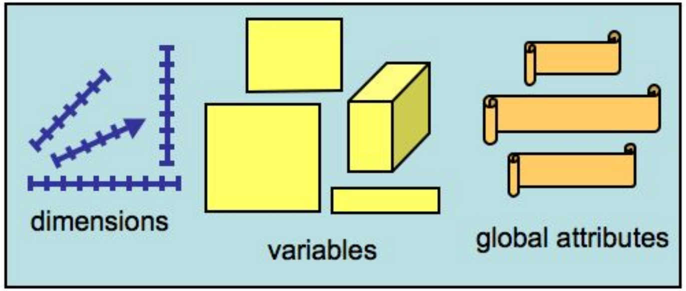
...When a legendary (well, to ESSI) team...

Unidata designed netCDF API/format to store datasets that fit the Common Data Model:



netCDF API enables clients to interrogate these "self-describing" files.

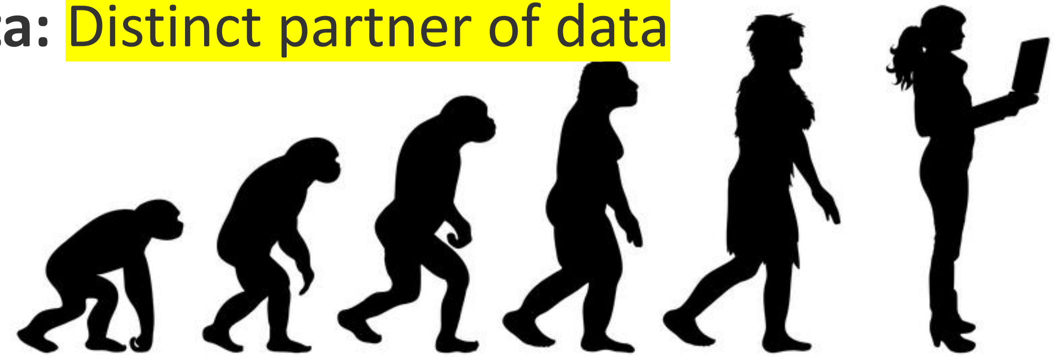
Harnett and Raphael, The School of netCDF, 1509-2021

…Other teams had similar aims...

NCSA developed the Hierarchical Data Format (HDF) and API, and a netCDF API for HDF. HDF is also self-describing. NASA chose HDF over netCDF for EOSDIS. In ~2007 the netCDF API married the HDF5 format, became netCDF4.

netCDF/HDF Make Data SPASSAM

- ***Self-Describing:** Queries reveal file contents*
- **Portable:** Allow different integer, character, FP formats
- **Archivable:** Guaranteed backwards compatibility
- **Scalable:** Efficiently access subsets/hyperslabs of datasets
- **Sharable:** SWMR access to the same file
- **Appendable:** No longer copy/redefine entire dataset
- **Metadata:** Distinct partner of data



Dataset Intercomparison Became Easier!

Ease of use, power of netCDF/HDF APIs led to rapid adoption:

- Tools: GrADS, IDL, NCL, NCO, …
- Producers: GISS, MPI, NASA, NCAR, UKMO
- Middleware: DODS-DAP
- Standards: COARDS, CF

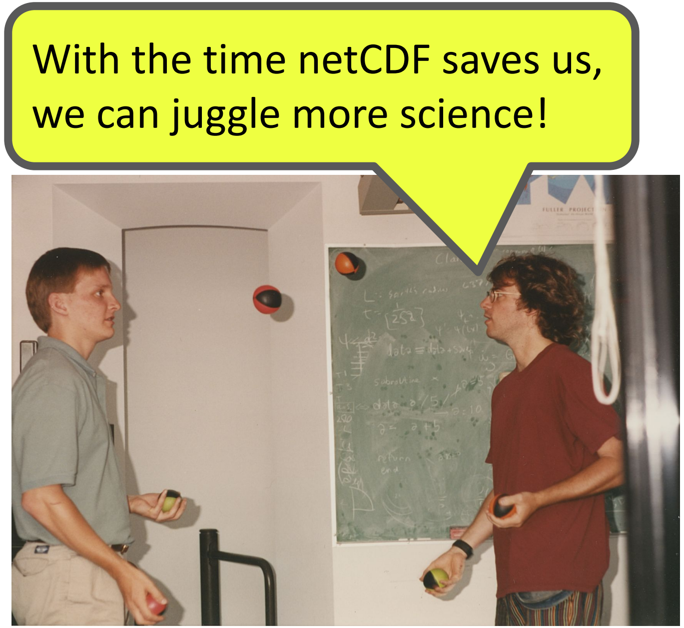
WCRP World Climate Research Programme CMIP6

xarray Iris

HYRAX DATA SERVER

What are the netCDF Operators (NCO)?

A) A modular set of tools for scriptable data analysis
B) A means to reduce future graduate suffering
C) A standard comparator for your newer, faster, better method
D) A way to treat files like atomic data
E) All of the above

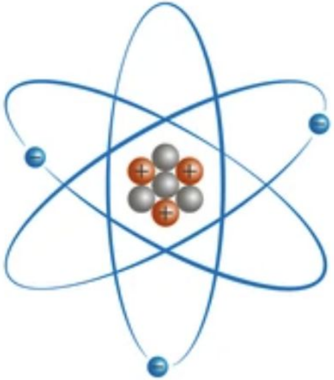


What are the netCDF Operators (NCO)?

- `ncap2` Arithmetic Processor
- `ncatted` ATTribute EDitor
- `ncbo` Binary Operator (differener)
- `ncclimo` CLIMatOlogy Generator
- `nces` Ensemble Statistics
- `ncecat` Ensemble conCATenator
- `ncflint` FiLe INTerpolator
- `ncks` Kitchen Sink
- `ncpdq` Permute Dimensions Quickly
- `ncra` Record Averager
- `ncrcat` Record conCATenator
- `ncremap` REMAPer
- `ncrename` RENAMEer
- `ncwa` Weighted Averager

Treat Datasets as Fundamental Units of Data

Every NCO operator can treat a dataset as a unit of data, independent of the numbers, types, and dimensionality of its variables

`data.nc =` 

$C = A - B$: `ncbo a.nc b.nc c.nc`

Act II: Domain-Specific Languages

What are the netCDF Operators (NCO)?

- ncap2 Arithmetic Processor
- ncatted ATTribute EDitor
- ncbo Binary Operator (differener)
- ncclimo CLIMatOlogy Generator
- nces Ensemble Statistics
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- ncks Kitchen Sink
- ncpdq Permute Dimensions Quickly
- ncra Record Averager
- ncrcat Record conCATenator
- ncremap REMAPer
- ncrename RENAMEer
- ncwa Weighted Averager

Domain Specific Language (DSL)

ncap2 is/as a Domain Specific Language

NCO's `ncap2` is ANTLR-based lexer/parser, uses netCDF API for I/O:

- C-like array-oriented language: `d=a+b(i,j)+c(:,:,3)`
- Loops, conditionals: `if(idx==sz) print("Finish")`
- Broadcast arrays to conform: `d3D=a1D+b2D+c3D`
- Common methods: `foo=bar.avg($time,$lon)`
- Special functions: `gsl_sf_legendre_Pl()`
- Autoload input, save output: `wind=U^2+V^2`
- Avoid disk, use RAM: `for(*idx=0;idx<sz;idx++)`
- Propagate metadata

NCL
NCAR Command Language

xarray

Short, Sweet Commands

Construct pressure field `p` in hybrid vertical coordinate system from `P0`, `PS(time,lat,lon)`, `hyam(lev)`, and `hybm(lev)`:

```
ncap2 -s 'p[time,lat,lon,lev]=P0*hyam+PS*hybm'
```

Broadcast RHS to shape of LHS, propagate attributes of first RHS variable. Output `p` has same attributes as `P0`!

High-level Workflows can be Short and Sweet

Create climatologies, or split and regrid CMIP6 timeseries:

```
ncclimo --case=foo --start=2001 --end=2020
--in_drc=raw --out_drc=clm --map=map.nc # Climo

ls *cam*h1*.nc | ncclimo -v T,Q,FSNT,FLNT
--start=1850 --end=2014 --map=map.nc # Splitter

ls *.nc | ncremap --map=map.nc # Regrid en-masse

ls *.nc | ncremap --dst=180x360 # Regrid swaths
```

NCO Ecosystem

NCO Workflow Scripts (ncremap, ncclimo)

ESMF_RegridWeightGen, TempestRemap

MPI

PyNCO

NCO Binary Executables (ncks, ncra, ncatted, nces, …)

ncap2 Binary (DSL)

CCR Libraries (BitGroom, Bzip2, Zstd, …)

NCO C Library

(OpenMP)

NCO C++ Library & ANTLR

netCDF C Library

Rx

UDUnits

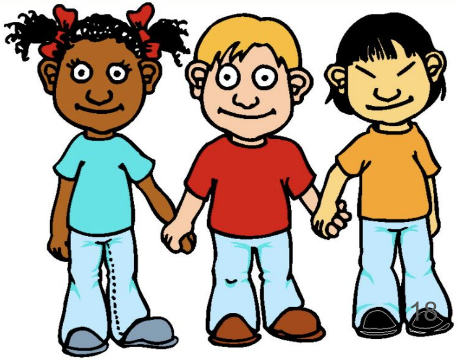
GSL

HDF5

HDF4

OPeNDAP

BLAS



Greg Leptoukh

On designing Giovanni v4 c.2008: “…*if we used NetCDF as our internal format, the entire library of NCO (NetCDF command operators) would be available to us, as well as the usual GrADS and IDL…*”

C. Lynnes, J. Acker pers. comm. 2021

Issues Solved by Conventions + DSLs

- Units conversion UDUnits
- Attach geophysical meaning CF `standard_name`
- Stitch datasets together CFA, `mfdataset()`, DAP/Hyrax
- Associate variables with formulae CF `formula_terms`
- Grid/projection ESMF, UGRID, CF `grid_mapping`, WKT-CRS

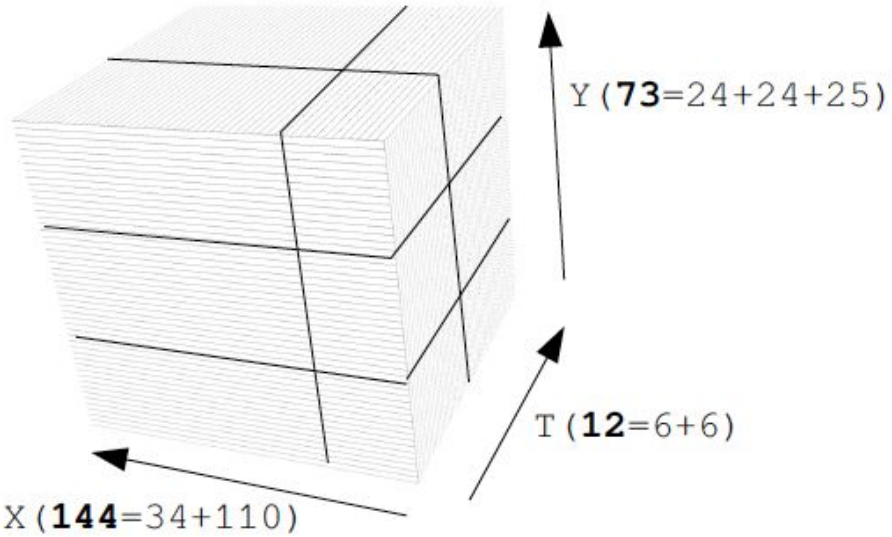
Powered By unidata UDUnits

ESMF

Open Geospatial Consortium

Climate and Forecast Aggregation (CFA) Conventions

```
aggregation_location = 6, 6, _,
                       24, 24, 25,
                       34, 110, _ ;
```




```
dimensions:
  time = 12 ;
  latitude = 73 ;
  longitude = 144 ;
  // Fragment dimensions
  f_time = 2 ;
  f_latitude = 1 ;
  f_longitude = 1 ;
  i = 3 ;
  j = 2 ;
variables:
  double temp ;
    temp:standard_name = "surface_temperature" ;
    temp:units = "K" ;
    temp:cell_methods = "time: mean" ;
    temp:aggregated_dimensions = "time latitude longitude" ;
    temp:aggregated_data = "location: aggregation_location
                            file: aggregation_file
                            format: aggregation_format
                            address: aggregation_address" ;
  double time(time) ;
    time:units = "days since 2001-01-01" ;
  double latitude(latitude) ;
    latitude:units = "degrees_north" ;
  double longitude(longitude) ;
    longitude:units = "degrees_east" ;
  // Aggregation definition variables
  int aggregation_location(i, j) ;
  string aggregation_file(f_time, f_latitude, f_longitude) ;
  string aggregation_format ;
  string aggregation_address(f_time, f_latitude, f_longitude) ;


// global attributes:
  :Conventions = "CF-1.9 CFA-0.6" ;
data:
  time = 0, 31, 59, 90, 120, 151, 181, 212, 243, 273, 304, 334 ;
  temp = _ ;
  aggregation_location = 6, 6,
                         73, _,
                         144, _ ;
  aggregation_file = "January-June.nc", "July-December.nc" ;
  aggregation_format = "nc" ;
  aggregation_address = "temp1", "tas" ;
```

Hassell, Gregory, Massey, Lawrence, Bartholomew 2021

Issues Solvable by Conventions + DSLs + AI/NL

"We should be able to treat climate datasets as atomic objects as well — namely, divorce the climate data from the number of time steps per file and which files contain which variables." — Paul Ullrich

Interpret intent: `phis(500hPa,JJA), MOC(2000-2010,NAtl),` `"plot monthly sensitivity of surface albedo to surface air temperature in all gridcells with snow and ice"`

Act III:

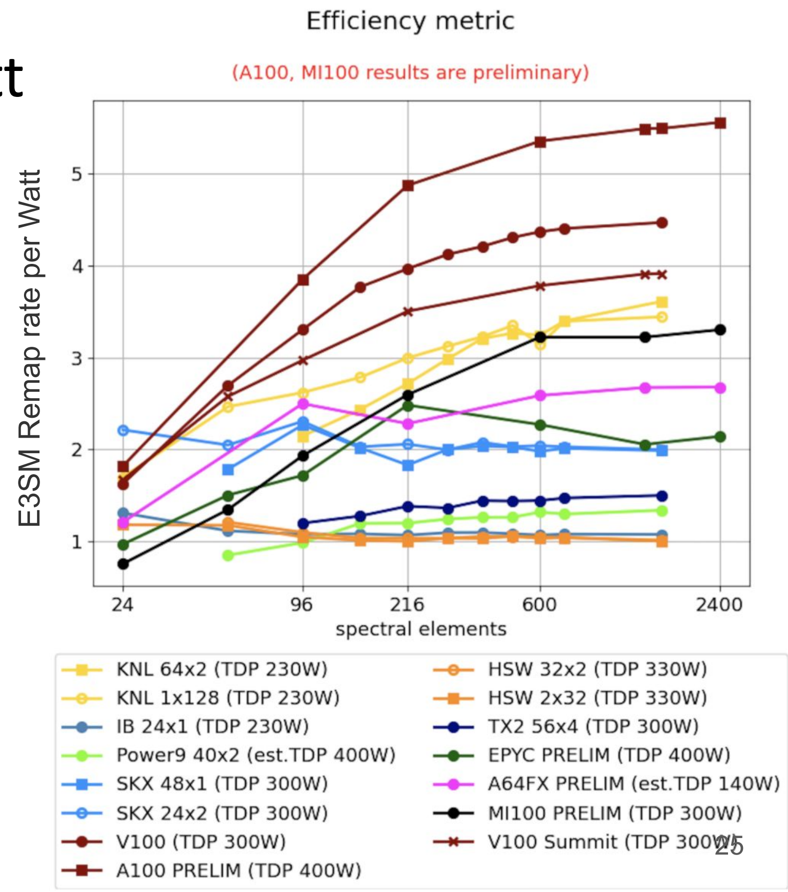
Green Computing and Storage

Why Reduce Computing Demands, Dataset Size?

1. Datacenters consume ~1-3% of global electrical power (~1% of global CO_2 emissions)
2. Storage accounts for ~40% of datacenter power, emissions
3. *Geoscience* computing is power-hungry, archives mostly false precision

ESM Energy Efficiency Tradeoffs: CPU vs. GPU

- Target Simulated Years per Day per Watt
- Optimize with hardware-agnostic APIs



Energy Efficiency of Programming Languages

- Dominated by execution time
- Total memory (DRAM) accounts for ~10%
- Compiled languages most efficient, C wins!

SLE'17, October 23–24, 2017, Vancouver, Canada R. Pereira et. al.

Table 5. Pareto optimal sets for different combination of objectives.

Time & Memory	Energy & Time	Energy & Memory	Energy & Time & Memory
C • Pascal • Go	C	C • Pascal	C • Pascal • Go
Rust • C++ • Fortran	Rust	Rust • C++ • Fortran • Go	Rust • C++ • Fortran
Ada	C++	Ada	Ada
Java • Chapel • Lisp • Ocaml	Ada	Java • Chapel • Lisp	Java • Chapel • Lisp • Ocaml
Haskell • C#	Java	OCaml • Swift • Haskell	Swift • Haskell • C#
Swift • PHP	Pascal • Chapel	C# • PHP	Dart • F# • Racket • Hack • PHP
F# • Racket • Hack • Python	Lisp • Ocaml • Go	Dart • F# • Racket • Hack • Python	JavaScript • Ruby • Python
JavaScript • Ruby	Fortran • Haskell • C#	JavaScript • Ruby	TypeScript • Erlang
Dart • TypeScript • Erlang	Swift	TypeScript	Lua • JRuby • Perl

Energy Efficiency of Programming Languages

Table 4: Normalized global results for Energy, Time, and Memory

Total					
	Energy (J)		Time (ms)		Mb
(c) C	1.00	(c) C	1.00	(c) Pascal	1.00
(c) Rust	1.03	(c) Rust	1.04	(c) Go	1.05
(c) C++	1.34	(c) C++	1.56	(c) C	1.17
(c) Ada	1.70	(c) Ada	1.85	(c) Fortran	1.24
(v) Java	1.98	(v) Java	1.89	(c) C++	1.34
(c) Pascal	2.14	(c) Chapel	2.14	(c) Ada	1.47
(c) Chapel	2.18	(c) Go	2.83	(c) Rust	1.54
(v) Lisp	2.27	(c) Pascal	3.02	(v) Lisp	1.92
(c) Ocaml	2.40	(c) Ocaml	3.09	(c) Haskell	2.45
(c) Fortran	2.52	(v) C#	3.14	(i) PHP	2.57
(c) Swift	2.79	(v) Lisp	3.40	(c) Swift	2.71
(c) Haskell	3.10	(c) Haskell	3.55	(i) Python	2.80
(v) C#	3.14	(c) Swift	4.20	(c) Ocaml	2.82
(c) Go	3.23	(c) Fortran	4.20	(v) C#	2.85
(i) Dart	3.83	(v) F#	6.30	(i) Hack	3.34
(v) F#	4.13	(i) JavaScript	6.52	(v) Racket	3.52
(i) JavaScript	4.45	(i) Dart	6.67	(i) Ruby	3.97
(v) Racket	7.91	(v) Racket	11.27	(c) Chapel	4.00
(i) TypeScript	21.50	(i) Hack	26.99	(v) F#	4.25
(i) Hack	24.02	(i) PHP	27.64	(i) JavaScript	4.59
(i) PHP	29.30	(v) Erlang	36.71	(i) TypeScript	4.69
(v) Erlang	42.23	(i) Jruby	43.44	(v) Java	6.01
(i) Lua	45.98	(i) TypeScript	46.20	(i) Perl	6.62
(i) Jruby	46.54	(i) Ruby	59.34	(i) Lua	6.72
(i) Ruby	69.91	(i) Perl	65.79	(v) Erlang	7.20
(i) Python	75.88	(i) Python	71.90	(i) Dart	8.64
(i) Perl	79.58	(i) Lua	82.91	(i) Jruby	19.84

Pereira et al., SCP, 2021

How much data do *geoscientists* store?

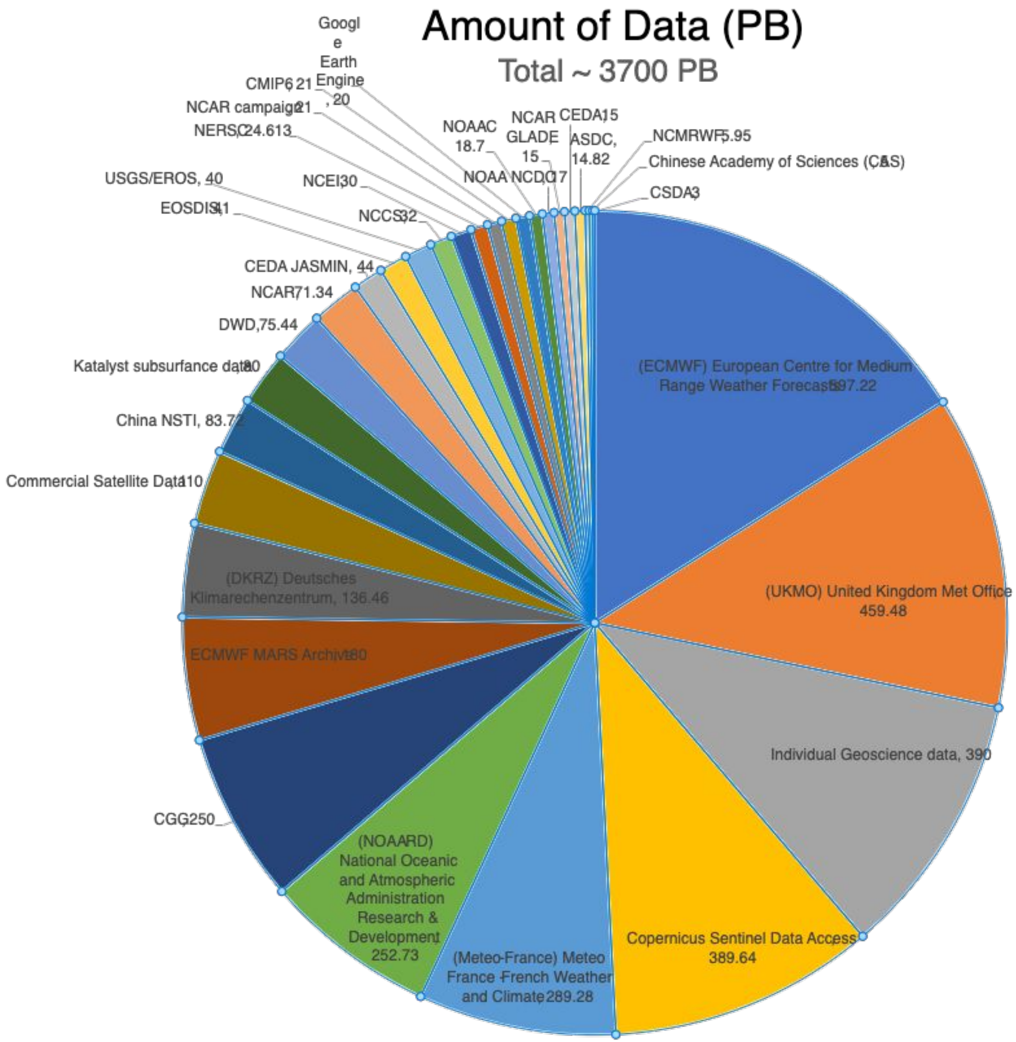
> 3700 PB

Assumes:

Data Centers ~3300 PB

130k AGU members @

3 TB on PCs ~400 PB



Trampush and Zender (2021), unpublished

CO2 Emissions from Geoscience Data Storage

> 10000 tCO_2e/yr

Assumes:

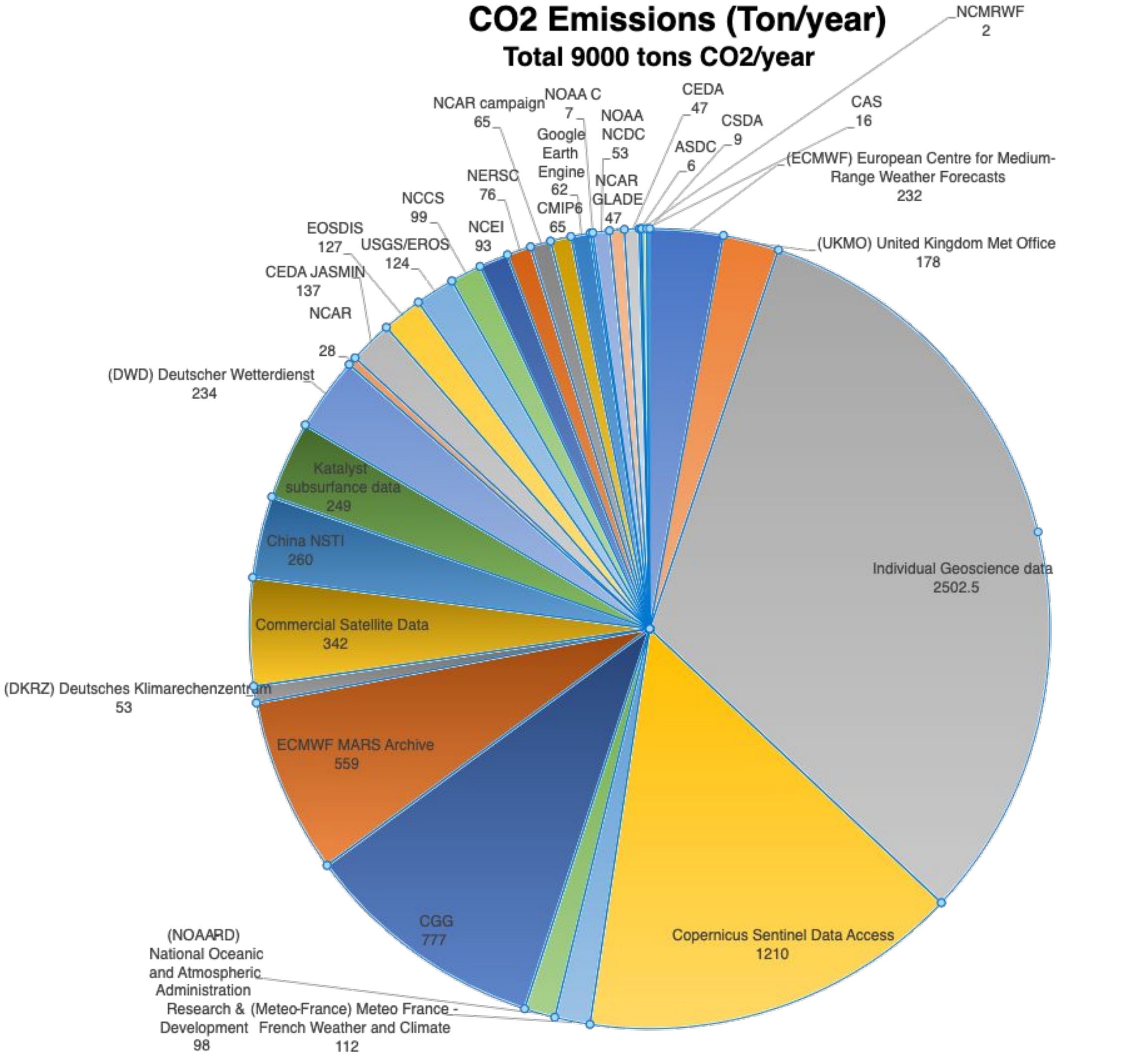
PC ~ 200 kWhr/TB/yr,

HDD ~ 7 kWhr/TB/yr,

Tape ~ 1 kWhr/TB/yr,

0.45 tCO_2eq/MWhr

Trampush and Zender (2021), unpublished



Barriers to Green Computing & Storage

- Accessing modern compressors (codecs) difficult
- Compression requires extra post-processing steps
- Traditional compression too slow
- Lossy compression discernibly distorts data
- How to identify false precision in model data?
- IEEE 64-bit, 32-bit formats are inflexible
- Culture of science encourages keeping false precision

Compression Capabilities of HDF5/netCDF4/Python

- HDF5 data chunks pass through "filters" (codecs)
- HDF5/netCDF4 APIs natively support checksum, shuffle, DEFLATE (aka zlib) filters, and szip (if built-in to HDF5)
- Python numcodecs: Zlib, BZ2, LZMA, ZFPY, Blosc
- *Interoperable, modern codec support has lagged in netCDF…*
  Until Recently! netCDF 4.8.2-develop supports new compression features: BitGroom, GranularBG PR, Zarr/numcodecs, CCR

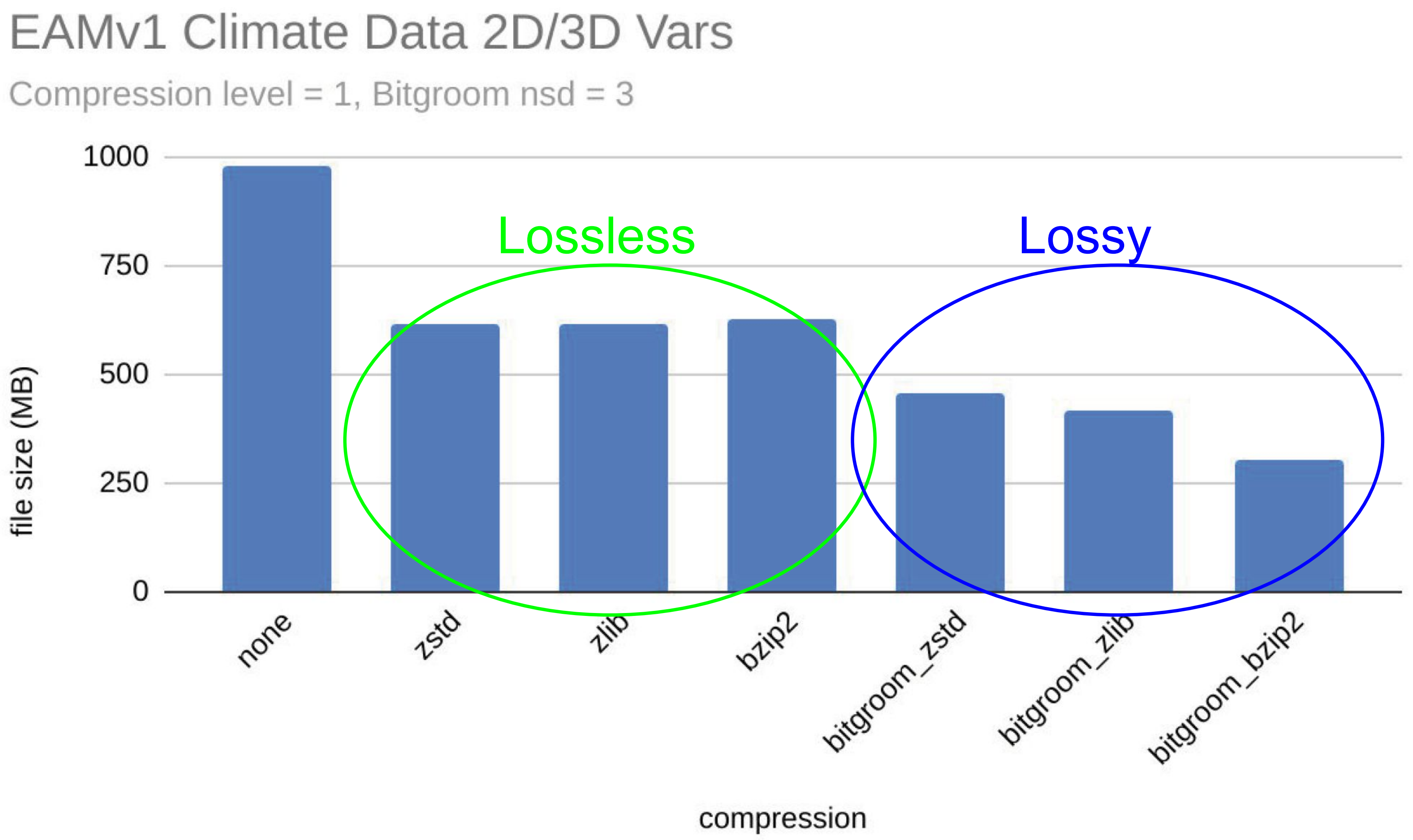
Zstandard

zfp

Community Codec Repository: Interoperable, End-to-End Compression for netCDF

- CCR builds filters, ccr library, netCDFish API
- Includes BitGroom, GranularBG, BZ2, Zstd
- Lossless+lossy I/O for C/Fortran:
  `nc_def_var_bitgroom(ncid,varid,level)`
  `nc_def_var_zstandard(ncid,varid,level)`
- Codec I/O is transparent to users
- *Efficient compression in production phase!*

Zender and Hartnett, CCR, 2020



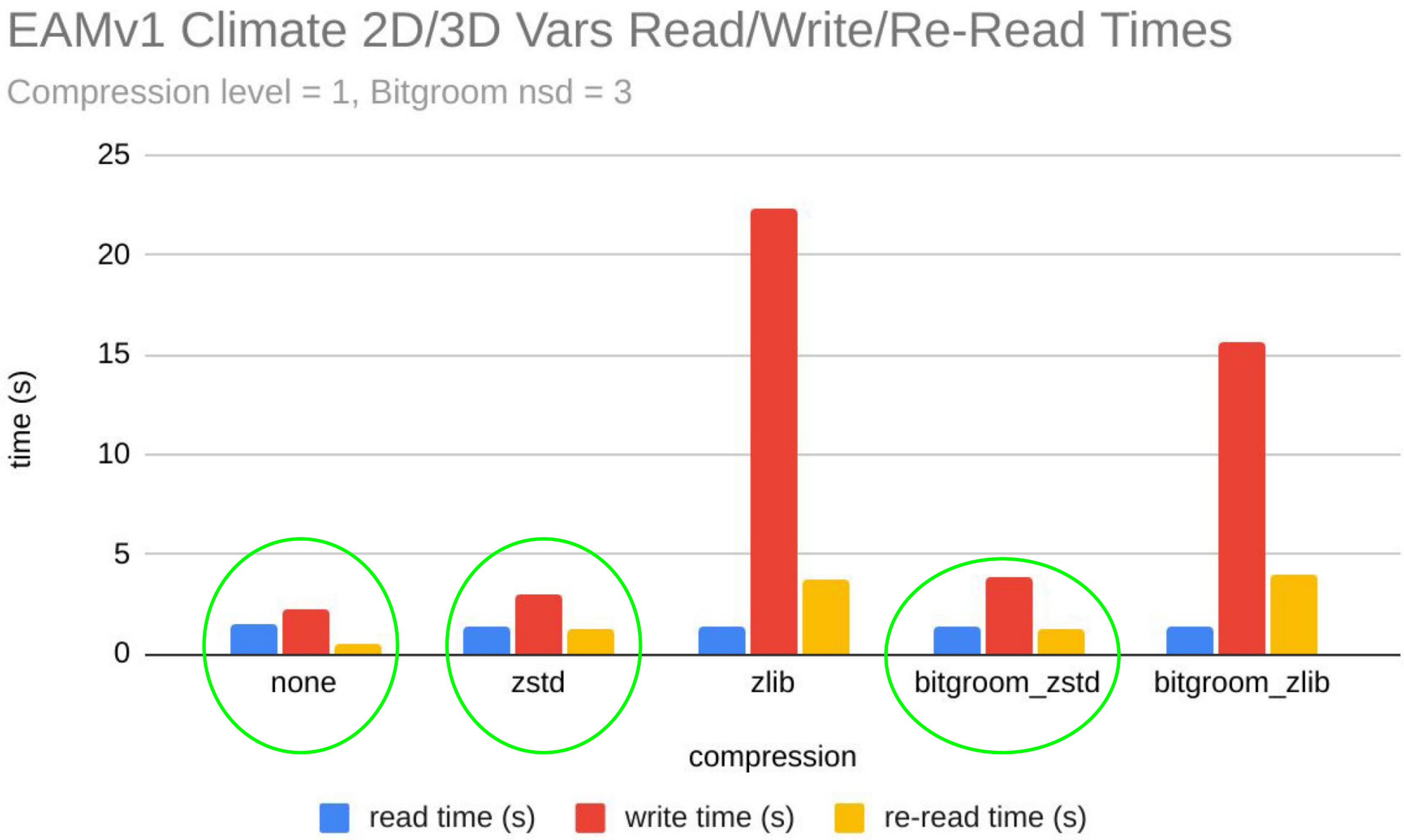
Harnett and Zender, AMS, 2021

Lossy Compression (e.g., BitGroom) as Pre-Filter

Sign	Exponent	Fraction (significand)	Decimal	Notes
0	10000000	10010010000111111011011	3.14159265	Exact
0	10000000	10010010000111111011011	3.14159265	* NSD = 8
0	10000000	10010010000111111011010	3.14159262	NSD = 7
0	10000000	10010010000111111011000	3.14159203	NSD = 6
0	10000000	10010010000111111000000	3.14158630	NSD = 5
0	10000000	10010010000111100000000	3.14154053	NSD = 4
0	10000000	10010010000000000000000	3.14062500	NSD = 3
0	10000000	10010010000000000000000	3.14062500	NSD = 2
0	10000000	10010000000000000000000	3.12500000	NSD = 1

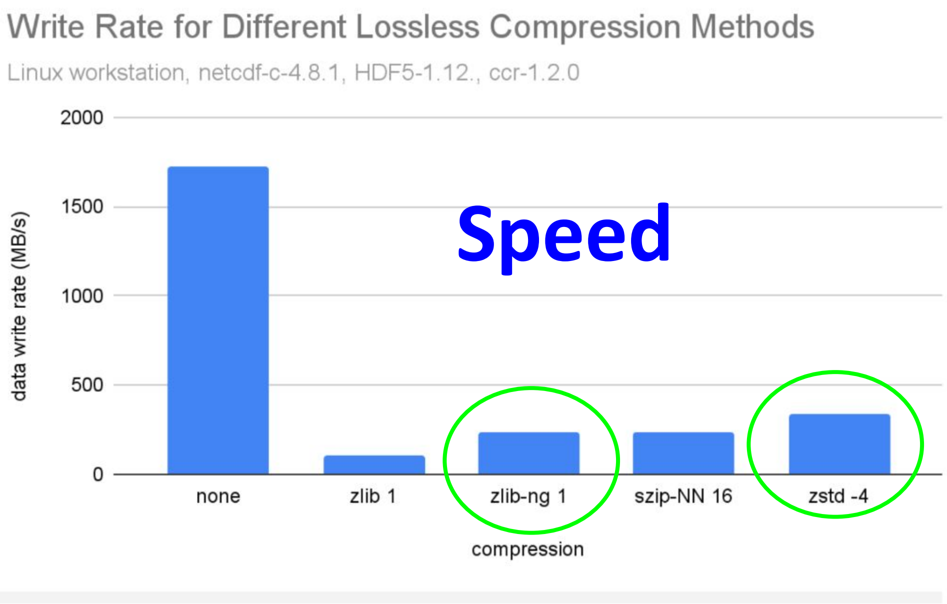
Zender, GMD, 2016

* *NSD* = Number of Significant Digits



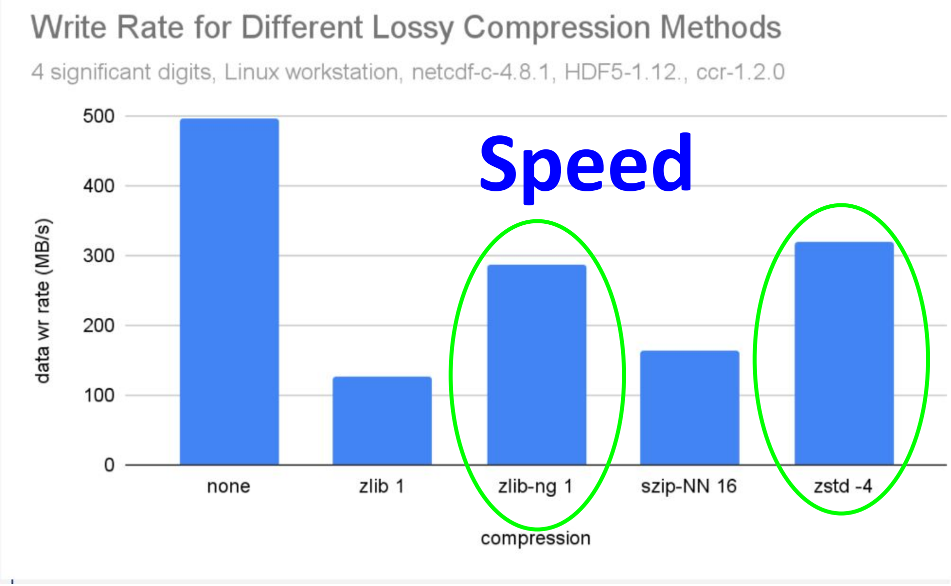
Harnett and Zender, AMS, 2021

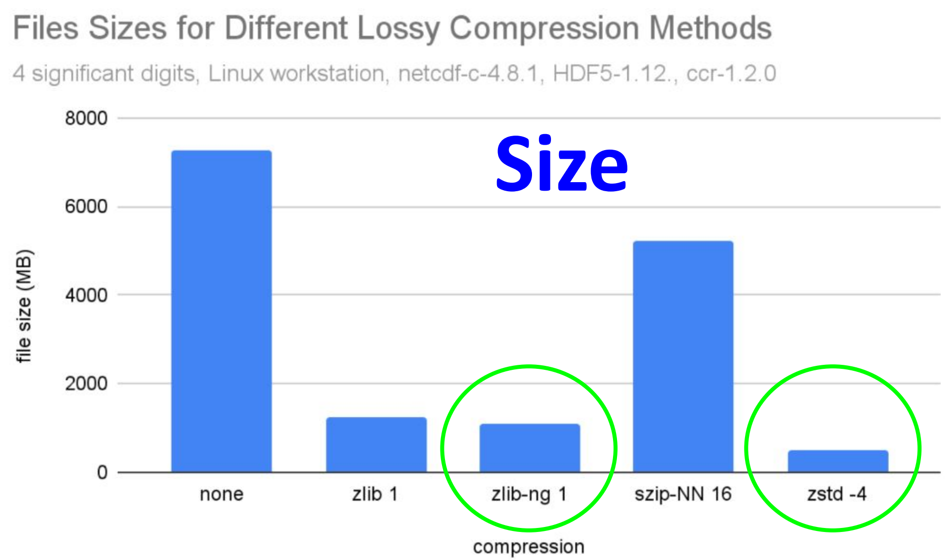
Lossless Compression



Harnett et al., AGU IN15A-05*, 2021*

Lossy Compression





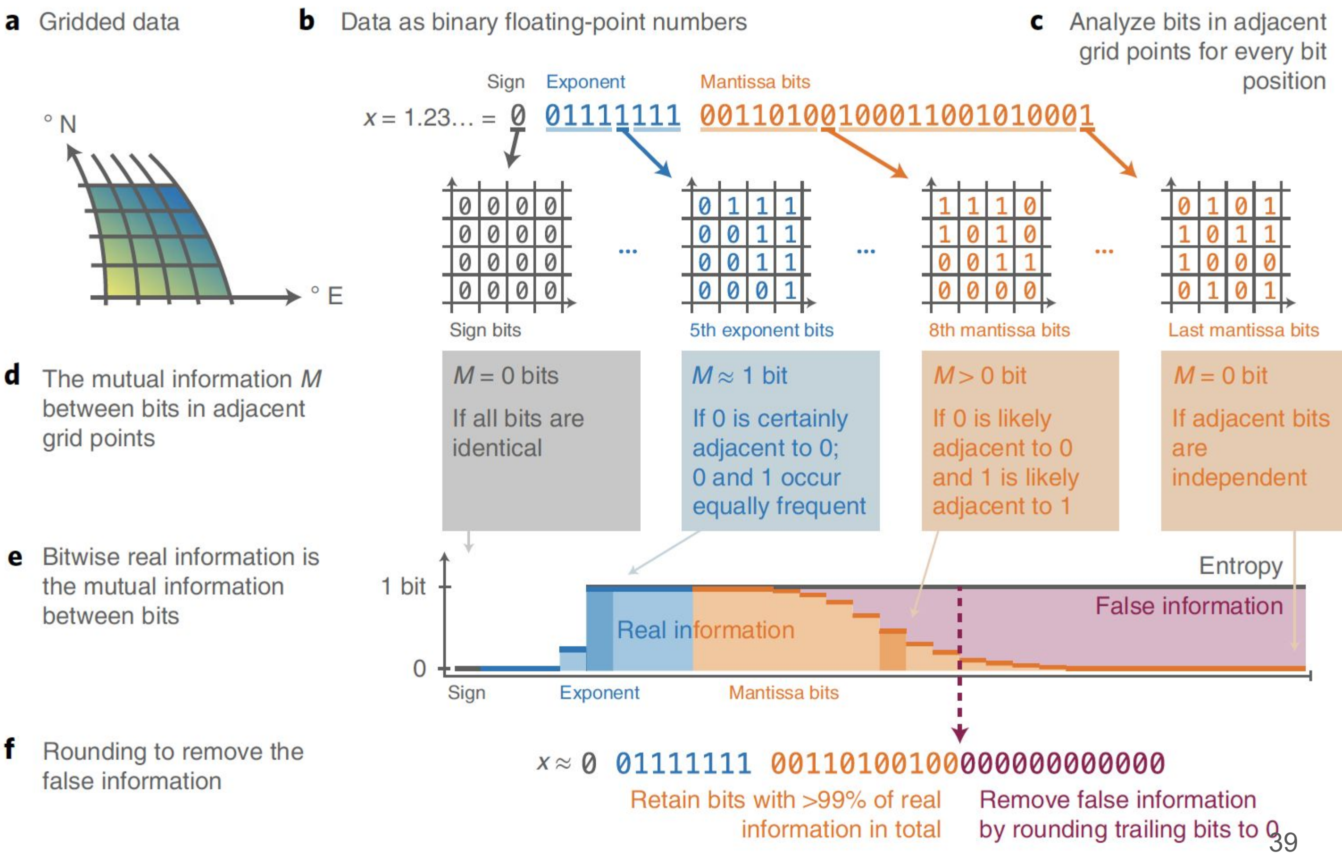
Harnett et al., AGU [IN15A-05](), 2021

Modern Codecs More Competitive

- Zlib-NG, Zstandard I/O speed 2-5x faster than Zlib
- Zlib-NG plug-compatible with Zlib thus netCDF/HDF!
- Zstandard+Bitgroom pre-filter CR ≳ 3x (*NSD* <= 4)
- Zstandard+GranularBG pre-filter CR ≳ 4x (*NSD* <= 4)
- Inflection point for adoption of lossy compression…

Compressing atmospheric data into its real information content

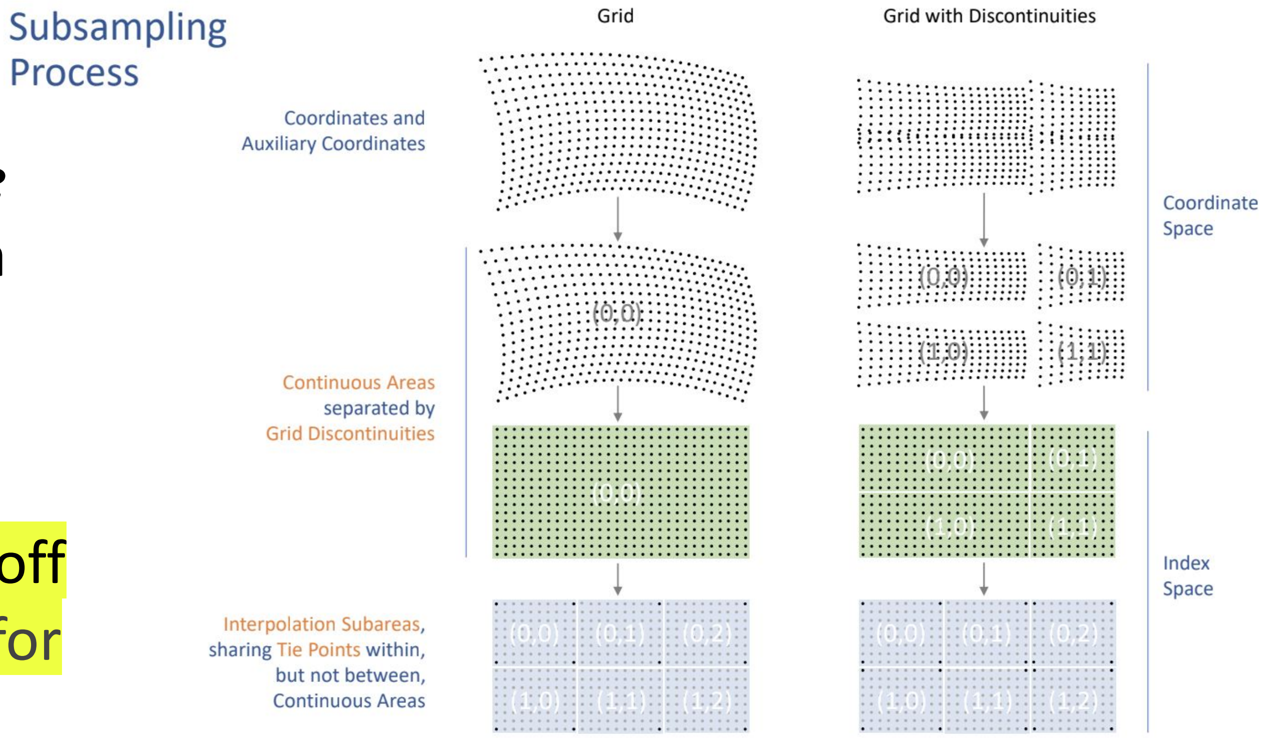
1. Determine # bits to preserve e.g. 99% *Information content* (IC) in adjacent cells
2. Round the rest (false precision)
3. CR ≳ 8x for 99% IC



Klöwer et al., NCS, 2021

Lossy Compression by Coordinate Subsampling

1. Store grid info. at *tie points*, reconstitute via interpolation
2. Preserves desired accuracy level.
3. Elegant for for one-off grids like RS. CR ~ 40x for VIIRS



Soerensen et al. (2021), CF, IN15A-06

Frontiers in Green Computing & Storage

- ~~Accessing modern codecs difficult~~ numcodecs, CCR, netCDF
- ~~Compression requires extra post-processing steps~~ CCR, netCDF
- ~~Traditional compression too slow~~ Modern codecs
- ~~Lossy compression discernibly distorts data~~ Pick *NSD*
- How to identify false precision in model data? Info. Content
- IEEE 64-bit, 32-bit formats are inflexible 16bit Posits?
- Culture of science encourages keeping false precision …

Ethical and Responsible Research (ER2)

PROGRAM SOLICITATION
NSF 22-526

Join our (hybrid vPICO) Session at EGU22

ESSI2.7: *Lossy and Lossless Compression for Greener Geoscientific Computing and Data Storage*

Conveners: Charlie Zender, Ed Hartnett, Bryan Lawrence, V. Balaji

Confirmed Invited Speaker: Milan Klöwer

Abstract Deadline: Jan. 12, 2022

Conclusions

- Self-describing formats (netCDF/HDF) enable tools and DSLs to treat complex datasets as atomic data. Untapped potential!
- End-to-End, model-to-archive compression now possible
- Modern compression nearly speed-competitive (within 2-5x)
- Lossy+Lossless can reduce (by $\gtrapprox$ 3x) scientific data storage (cost, power, GHGs) and retain all scientifically significant content

***Green Computing** has multiple benefits, few regrets!*

Appreciation

- Family: Shari, Olivia, Jinx, Ashley, Joel
- Advisors+Role Models
- ESS Department at UCI, Group Members
- Collaborators, Colleagues
- OpenSource Community
- Funding and Support

Resources

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That's all Folks!