## Can we Aggressively Reduce Scientific Data Without Losing Science?

- Why lossy data reduction?
- SZ lossy compressor
- Z-checker: reduction error analysis
- Compression vs. Decimation

Franck Cappello

Argonne National Laboratory

University of Illinois at Urbana Champaign

With major contribution from: Sheng Di<sup>#</sup>, Dinwen Tao<sup>+</sup>

#ANL, +U. California Riverside.





# Why do we need to reduce scientific datasets?

Image from the Argonne Photon Source

# Scientific Simulations and Experiments: the flood of data!

- Today's scientific research is using simulation or instruments and produces extremely large of datasets to process/analyze
- Feasibility problems:
  - Cosmology Simulation:
    - A total of >20PB of data when simulating trillion of particles
    - Petascale systems FS ~20PB (you will never have 20PB of scratch for one application)
    - On Blue Waters (1TB/s file system), it would take 20 X 10^15 / 10^12 seconds (5h30) to store the data
  - Data reduction of a bout a factor of 10 is needed
    - $\rightarrow$  currently drop 9 snapshots over 10 (also called decimation in time)









# Data reduction is needed for many scientific simulations



- High-resolution CESM simulation (1/10° ocean-ice, 1/4° atmosphere)
   → 1 TB of data generated per compute day
- IPCC Coupled Model Comparison Projects (CMIPs)
  - Phase 5 (2013)  $\rightarrow$  2.5 PB of output
  - Phase 6 (2018)  $\rightarrow$  >10 PB expected!
- The relative cost of storage is increasing...
  - Previous NCAR platform (2013): ~20% of hardware budget
  - Current NCAR platform (2017): ~50% of hardware budget
    - $\rightarrow$  Work of Allison H. Baker, NCAR, on compression of climate datasets (HPDC2014)
    - $\rightarrow$  Data reduction of about a factor of 10 is needed



# Data reduction is also needed for experimental sciences

- APS-U (next-generation APS project at Argonne):
  - Brain Initiatives: in the order of **100PB** of storage: hundreds of specimens, each requiring 150TB of storage.
  - Data analysis is performed on ANL Mira (several miles)
  - Connection between APS and Mira: 100Gb/s
    - Would take ~10^17/10^10 = 10^7 seconds to transfer the data: 115 days to move the data
    - There is no 100PB buffer at the APS.
- APS-U users need to use filters to reduce the data size

→ Data reduction of about a factor of 100 is needed











## When data is too big

It cannot be communicated, stored or processed plain  $\rightarrow$  Data needs to live in reduced version

#### **CISCO** statistics:

- Annual global IP traffic: 2.3 ZB (10^21) in 2020
- IP video traffic will be 82 percent of all IP traffic
- $\rightarrow$  >>80% of the IP traffic will be compressed!
- → >>80% of the files exchanged in the Internet will exist (probably only) in compressed version







### Data reduction techniques

#### • Generic Decimation:

- Just remove m datum over n. Typical example: remove 9 data over 10. 90% loss
- In space (e.g. coarser mesh size) and/or in time (remove snapshots)

#### • Specific filtering:

- E.G. ATLAS raw data per event: 1MB at 100Mhz (Run 2).
- Run 3 (2021) will produce events at 60TB/s!!

 $\rightarrow$ Goal is to reduce data rate to storage to 20 GB/s (/1000).

 O2 framework design: 463 FPGAs detector for readout and fast cluster finding, 100,000 cores to compress 1.1 TB/s streams.

#### Generic / customizable compression







Generic/Customizable Compression of Scientific Data

Image from Nek5000 Fuild Dynamic Simulation

#### Data compression

- A form of data reduction
- ~40 years old (LZ77, 1977), ~70 years (Shannon's information theory, 1948)
- Systematically (almost) used for files (e.g. GZIP), digital photos (e.g. JPEG), movies (e.g. MP4), music (e.g. MP3)
- Very effective on images
- A priori compression algorithms are generic and applicable to many applications
  - In practice they are combined and optimized for specific usages





### Compression

- Lossless:
  - The data is compressed and decompressed in such a way that the decompressed data is **identical** to the initial data (there is no alteration, deviation, distortion)
  - Best example: Gzip (will have a slide on it)
- Lossy:
  - The data is altered during compression: some piece of information is removed (lost): the original data cannot be retrieved.
  - If user can control the accuracy of the compressed data, then lossy compression is a trade-off between compression factor and loss of accuracy
  - Best example: JPEG (will have a slide on it)





# General Compression Process for scientific data

• Two or three main stages (each stage may use multiple sub-stages)







### What scientific data looks like?

EXASCALE COMPLITING PRO 160



 Floating point datasets looks very random at first sight (except for the sign and the exponent)



## **Entropy of Datasets**

Entropy of the string of symbols:

$$H = -\sum p(x)\log p(x)$$

p(x) being the probability of occurrence of x in the string log p(x): information quantity carried by observing x

Maximum compression factor of ~2 according to Shannon Entropy (datasets are 64 bits)

Note:  $25.17 = Log_2(dataset size)$  384 x 384 x 256  $\rightarrow$  Every value is unique

From: Lindstrom, Peter, and Martin Isenburg. "Fast and efficient compression of floating-point data." *Visualization and Computer Graphics, IEEE Transactions on* 12.5 (2006): 1245-1250.



data set							
name	unique (%)	entropy (bits)	range (bits)	min	max	size (MB)	
m2d density	3.89	3.49	21.83	8.7E-01	1.2E + 00	19.6	
m2d vorticity	99.20	22.25	31.05	-1.4E + 02	2.5E + 01	19.6	
m3d density	7.67	5.16	23.60	1.0E + 00	3.0E + 00	364.8	
m3d pressure	27.29	23.91	31.06	-3.7E+00	2.3E + 03	364.8	
m3d diffusivity	36.87	23.19	30.02	0.0E + 00	6.8E + 00	364.8	
m3d viscocity	50.07	24.86	28.59	8.6E-15	2.9E + 00	364.8	
h3d temp	65.70	23.54	31.56	-7.7E + 01	1.0E + 35	95.4	
h3d pressure	81.82	24.13	31.58	-3.4E+03	1.0E + 35	95.4	
h3d $x$ velocity	84.18	24.18	31.55	-5.3E+01	1.0E + 35	95.4	
h3d $y$ velocity	84.32	24.18	31.55	-4.6E+01	1.0E + 35	95.4	
h3d $z$ velocity	86.82	24.24	31.54	-3.2E+00	1.0E + 35	95.4	
M3d density	40.14	18.84	52.59	1.0E + 00	3.0E + 00	288.0	
M3d pressure	100.00	25.17	63.00	-2.2E+00	2.2E + 00	288.0	
M3d $x$ velocity	100.00	25.17	63.00	-2.2E+00	2.3E + 00	288.0	
M3d y velocity	100.00	25.17	63.00	-2.1E+00	2.3E + 00	288.0	
M3d $z$ velocity	100.00	25.17	63.00	-5.2E+00	9.0E + 00	288.0	
a3d $x$ position	61.10	23.82	31.01	-4.8E-02	4.6E + 02	107.'	
a3d $y$ position	45.90	23.32	26.99	3.7E-02	2.1E + 03	107.'	
a3d $z$ position	61.68	23.84	27.48	9.1E-05	4.6E + 02	107.'	
a3d $y$ velocity	64.65	23.87	30.96	-1.5E-01	1.4E-01	107.'	
a3d temp	64.91	23.94	27.41	3.0E-03	7.1E + 03	107.'	
a3d energy	3.45	18.57	21.79	-3.6E+00	-2.7E+00	107.'	
lucy	61.39	24.38	31.09	-6.1E + 02	1.2E + 03	160.8	
$david_{1mm}$	25.23	17.08	31.11	-4.4E+03	1.8E + 03	322.	
torso	84.72	18.48	31.08	-2.7E+02	5.8E + 02	1.9	
rbl	71.90	20.14	25.99	1.48E + 00	3.6E + 02	8.4	

### What advanced lossless compressors?

3 years ago

Scheme	Transformation Applied	Algorithm	Compression Ratio
FPC [8]	not used	it first predicts values sequentially using two predic- tors (FCM and DFCM), and subsequently selects the closer predicted value to the actual. Lastly, it XORs the selected predicted value with the actual value, and leading-zero compresses the result.	1.02x~1.96x
ISOBAR [30]	divide byte-columns into compressible and incompressibles	apply zlib, bzlib2, (fpzip, FPC) on all compressible (af- ter discarding noisy byte-columns). zlib is the main com- pression algorithm; others are for comparison purposes	1.12x~1.48x
PRIMACY [31]	frequency based permutation of ID values	apply zlib on transformed data	1.13x~2.16x
ALACRITY [19]	split floating-point values into sign, exponent, and significands	unique-value encoding of the most significant bytes (as- suming high-order bytes (sign and exponents) are easy to compress); low-order bytes are compressed using ISO- BAR	1.19x~1.58x
CC [6]	XOR on $\Delta$ of neighboring data point in the same iteration	apply zero-filled run length encoding	up to 2.13x
IOFSL [36]	not used	integration of LZO, bzip2, zlib within the I/O forward- ing layer	~1.9x
Binary Masking [5]	bit masking (XOR)	apply zlib on bit masked data in order to partially de- creases the entropy level	1.11x~1.33x
MCRENGINE [18]	variable merging in the same group	apply parallel gzip on the merged variables across pro- cesses	up to 1.18x

Son, S. W., Chen, Z., Hendrix, W., Agrawal, A., Liao, W. K., & Choudhary, A. (2014). Data Compression for the Exascale Computing Era-Survey. *Supercomputing frontiers and innovations*, 1(2), 76-88.





# Anatomy of one of the best available lossy compressors

Image from Combustion Simulation

## ANL SZ Lossy compressor

#### Design considerations:

- Effective: compete with the best existing lossy compression algorithms
- Efficient, fast: only use linear complexity steps (no sorting)
- Strict respect of error bounds set by users
- Allow different types of error bounds: absolute, relative, relative to value range (request from users), PSNR
- Target all types of scientific data: 1D to nD, Structured, Unstructured, Particles, Instruments (images)



Produce acceptable distortions (error autocorrelation, spectral, derivatives)



#### How do we compress (leverage redundancy)

Similarities, autocorrelation, smoothness

Value

Data

Smoothness → Prediction



Not smooth → Deal with prediction error



## SZ Design Principles

- Prediction based lossy compressor
- Multi-stages



## Controlling the compression error

- SZ provides point wise error controls (input parameters)
- Three types of error (E: error, V: intial dataset, V': decompressed dataset)
  - Absolute error: (small value range),
  - Relative error: (large value range),
  - Relative to value range:

$$\mathsf{E}_{\mathsf{a}} = |\mathsf{V} - \mathsf{V'}|$$

$$E_r = \frac{|V - V'|}{V}$$

$$E_{vr} = |V - V'|$$

Vmax-Vmin







EXASCALE COMPLITING PROJECT

D. Tao, S. Di, Z. Chen, F. Cappello, Significantly Improving Lossy Compression for Scientific Datasets Based on Multidimensional Prediction and Error-Controlled Quantization, **IEEE IPDPS 2017** 





**Relative Error Bound** 

## SZ Coding Stage

#### 3) Variable length coding (Huffman)

We built the Huffman tree using a symbol size corresponding to the number of bits needed to code the bin numbers



Reduce the number of bits needed to represent values

#### 4) Unpredictable data analysis





Reduce the number of bits needed to represent unpredictable data (<1%)

5) Optional GZIP (L77 + Huffman coding): improve the compression by about 10%, but also slowdown Both on result of the Huffman coding and the array of unpredictable data







### **Lossy Compression Performance**

#### Argonne SZ 1.4 lossy compressor



All these apps need at least a factor of 10 compression

E
EXASCALE COMPUTING PROJECT

S. D., F. Cappello, Optimization of Error-Bounded Lossy Compression for Hard-to-Compress HPC Data, **IEEE TPDS**, to appear.



## **Surprisingly Good Compression Performance**

#### **Quantum Chemistry**

All properties of the quantum mechanical system are determined by the wave functions which are obtained by solving the Schrödinger Equation.

Computing two-electron repulsion integrals is the most time-consuming step in solving Schrödinger Equation.

Typically, integrals cannot fit into memory and iterative solutions requires recalculating integrals every iteration.

Much better strategy: compute election repulsion integrals once, compress and store them in memory, and read ERIs from memory every time we need them.

→ But a factor of 10 compression is needed (at least)
 → Designed a new predictor using pattern matching





A. Murat Gok, D. Tao, S. Di, V. Mironov, Y. Alexeev, F. Cappello, PaSTRI: A Novel Data Compression Algorithm for Two-Electron Integrals in Quantum Chemistry, **IEEE/ACM SC17** 

#### Some datasets are very hard to compress e.g. Particle datasets -FPZIP

AMDF Molecular Dynamics code (Accelerated Molecular **Dynamics Family**) A compression factor of 10 is needed

Compression ratio/rate (AMDF), REB: 10<sup>-4</sup> Compression Ratio

Compression Rate





 $\rightarrow$  We need to find a new way to compress these particles datasets



D. Tao, S. Di, Z. Chen, and F. Cappello, In-Depth Exploration of Single-Snapshot Lossy Compression Techniques for N-Body Simulations, Submitted



#### Some datasets are much easier to compress

In some situation, SZ 1.4 compression factor can be >100. And the difference is barely noticeable. SZ = 14.8

#### E.G. Miranda dataset\*

Miranda is a radiation hydrodynamics code designed for large-eddy simulation of multicomponent flows with turbulent mixing.

Example of Rayleigh-Taylor instability simulation involving two fluids of different density.

→ Compression factor of 110 with acceptable distortions

\*Figure from Peter Lindstrom, LLNL





Can we Aggressively Reduce Scientific Data Without Losing Science?

Image from HACC Cosmology Simulation

#### How Lossy Compression Distorts Scientific Data?

- Lossy compressors using different algorithms are likely to distort the dataset differently
- Very few studies (mostly on climate datasets) analyze compression quality
- We need to compare the different compressors scientifically (fairly)
- We need to share common metrics quantifying the lossy compression error

→ We need a methodology (metrics and tools) to assess the nature of the error introduced by lossy compressors.





### ANL Z-checker (ECP CODAR)

Analysis Kernels:

- 1. Initial Data Property Analyzer
- 2. Compression Error Analyzer

#### Incremental design:

• Metrics and interface defined with users Integrates analysis functions in C and R



#### 2 modes:

- With SZ and ZFP integrated (1 input file), compression is run several times for RD
- 2 input files (does not provide rate-distortion analysis)

Currently accepts only data sources in binary format (big/little endian), 32 or 64 bits.



Z-Checker is supported by the DOE/NNSA ECP CODAR Project.

I. Foster, M. Ainsworth, B. Allen, J. Bessac, F. Cappello et al. Computing Just What You Need: Online Data Analysis and Reduction at Extreme Scales, **Europar 2017** 



#### Z-checker Example: Climate and Severe Weather

- Experimental data (single-floating point)
  - Climate: ATM: 2D datasets from climate/atmosphere simulations (pseudo 3D)
  - Weather: hurricane: 3D datasets from Hurricane Isabel simulation

	Data Source	Dimension Size	Data Size	File Number
ATM	Climate simulation	$1800 \times 3600$	2.6 TB	11400
Hurricane	Hurricane simulation	$100 \times 500 \times 500$	1.2 GB	624

Notes: Tested many different datasets:

- Particle datasets (Cosmology, Molecular Dynamics)
- Quantum Chemistry
- Datasets from Instrument (Argonne APS, Berkeley Linac Coherent Light Source)







## Z-checker: Compression ratios (factors)



- Value-range-based (VRB) relative error bound: (ratio of absolute error bound to data value range)
- E.g., VRB relative error bound = 1E-3

EXASCALE COMPUTING PROJEC

- > ATM: SZ-1.4: CF=14  $\rightarrow$  2x of ZFP
- > Hurricane: SZ-1.4: CF=33  $\rightarrow$  2.5x of ZFP



### Z-checker: Rate Distortion

$$R_X = x_{max} - x_{min}$$

$$psnr = 20 \cdot log_{10}(\frac{R_X}{rmse}) \quad rmse = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (e_{abs_i})^2}$$



- SZ-1.4: 14 dB higher than ZFP on ATM
- > SZ-1.4: 11 dB higher than ZFP on Hurricane
- PSNR is logarithmic scale
- PSNR  $\rightarrow$  RMSE: 14 dB ~ 5x, 11 dB ~ 3.5x





## Z-checker: Distribution of Compression Error



EXASCALE COMPLITING PRO 1601

Distribution plot informs about the nature of the noise that the lossy compressor adds to the dataset. It also shows how the errors are distributed around 0. SZ and ZFP provide symmetric errors: Good. We need to know what type of distribution is better for users: Uniform or Gaussian Argonne

### **Z-checker: Spectral Alteration**

We want to know how the compression affects the different components of the signal (frequency domain)

8%

7%

6%

5%

4%

Compute the Fourier Spectrums for

- the initial dataset
- the decompressed dataset

Plot the amplitude difference for each frequency (normalized from the initial dataset)

In general, we want to preserve as much as possible the spectral properties of the signal



Value-rang-based relative error bound = 1E-2

Value-rang-based relative error bound = 1E-3



## Z-checker: Pearson Correlation of Initial and Decompressed Datasets

Considering a dataset  $\{x_1,...,x_n\}$  containing *n* values and another dataset  $\{y_1,...,y_n\}$  containing *n* values



Pearson correlation coefficient measures the linear correlation between two variables *X* and *Y*.

- $r = +1 \le Value \le -1$ ,
- 1: total positive linear correlation,
- 0: no linear correlation,
- -1: total negative linear correlation



#### We want a maximum correlation (~1) between the initial and decompressed datasets

Maximum	ATM			Maximum	Hurricane		
$e_{rel}$	SZ-1.4	ZFP	SZ-1.1	$e_{rel}$	SZ-1.4	ZFP	SZ-1.1
$3.3 \times 10^{-3}$	0.99998	0.9996	0.99998	$2.4 \times 10^{-3}$	0.998	0.99995	0.998
$4.3 \times 10^{-4}$	$\geq 1 - 10^{-6}$	$\geq 1 - 10^{-7}$	$\geq 1 - 10^{-6}$	$1.8 \times 10^{-4}$	$\geq 1 - 10^{-5}$	$\geq 1 - 10^{-6}$	$\geq 1 - 10^{-5}$
$2.6 \times 10^{-5}$	$\geq 1 - 10^{-8}$	$\geq 1 - 10^{-9}$	$\geq 1 - 10^{-9}$	$2.5 \times 10^{-5}$	$\geq 1 - 10^{-6}$	$\geq 1 - 10^{-8}$	$\geq 1 - 10^{-5}$
$3.4 \times 10^{-6}$	$\geq 1 - 10^{-10}$	$\geq 1 - 10^{-11}$	$\geq 1 - 10^{-11}$	$2.6 \times 10^{-6}$	$\geq 1 - 10^{-8}$	$\geq 1 - 10^{-9}$	$\geq 1 - 10^{-7}$
$4.1 \times 10^{-7}$	$\geq 1 - 10^{-12}$	$\geq 1 - 10^{-13}$	$\geq 1 - 10^{-13}$	$2.9 \times 10^{-7}$	$\geq 1 - 10^{-10}$	$\geq 1 - 10^{-11}$	$\geq 1 - 10^{-11}$

#### Z-checker: Autocorrelation of the Compression Error

Compression introduces autocorrelation that was not there before

EXASCALE COMPUTING PROJECT



SZ introduce a much lower and shorter autocorrelation compared to ZFP



## Z-checker: Preservation of Derivatives



Compute the derivatives on each point of the original and Decompressed dataset.

Plot the result.

Note that we could have plotted the difference instead of the two figures

 $\rightarrow$  SZ does not visually alter the first and second derivatives





## Lossy Compression vs. Decimation

Image from Halo finder in Cosmology Simulation

### Decimation vs. Compression (Z-checker analysis)

Lossless Spatial Decimation + Linear Interpolation  $\rightarrow$  The most common reduction technique Lossy compression with SZ 1.4 Rate distortion

ATM dataset: ATM CLDLOW Decimation/compression factor: 6

→ Much better rate-distortion for SZ
 → Much lower autocorrelation for SZ
 → Much lower spectral alteration for SZ
 → Compression outperforms decimation









SZ: <u>https://github.com/disheng222/SZ</u>

**Z-checker:** <u>https://github.com/CODARcode/Z-checker</u>

SC17 Tutorial on lossy compression for scientific data: http://sc17.supercomputing.org/presentation/?id=tut106&sess=sess205

Soon: a repository with reference datasets, compressors, configurations, results





#### Conclusion

- Aggressive data reduction is needed and will be critical to advance science
- All IT domains use lossy compression when data becomes too large
- Lossy compressors are available for scientific data (simulation and instruments)
- They produce excellent results: performance, speed, distortions
- The current popular technique of **decimation is far inferior to** lossy compression
- As we progress in the use of lossy compression in scientific application, we should continue developing the evaluation methodology (metrics, tools, benchmarks, etc.)

By the way, compression is also an art



