zfp 000000000 Topological compression

Summary o

Lossy data compression

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Summary o

Zoom controls

- Please mute your microphone and camera unless you have a question
- To ask questions at any time, type in Chat, or Unmute to ask via audio
 - please address chat questions to "Everyone" (not direct chat!)
- Raise your hand in Participants



- Email training@westdri.ca
- Our winter/spring training schedule https://bit.ly/wg2024a
 - webinars, courses, summer school at SFU on June 3-7

Numerical simulations produce too much data! (challenge to write and store long-term)

- Store every 100th timestep
- Store only selected variables
- In-situ visualization
- Data compression

Intro o●o Topological compression

Summary o

Compression techniques: lossless compression of 3D data

- Tools like gzip, bzip2, xz and many others
- Use general-purpose algorithms; replace recurrent bit patterns in the data by references to a single copy of the pattern
- Often included into the file format (NetCDF, HDF5, VTK)
- For typical datasets (such as CFD) $\sim 40 50\%$ reduction in size
- Very high compression rates when a high redundancy is present in the data
 - e.g. the Mandelbulb on the right: 800³ in single precision ⇒ 1.9G, actual NetCDF file 12M
 - effectively, a litmus test for the efficiency of your data storage (if stored uncompressed)



Compression techniques: lossy compression of 3D data

- Lower resolution and/or precision
- Orthogonal transformation-based algorithms, e.g. zfp (based on local block transforms, similar to discrete cosine transforms)
- Topological compression
- Compression via ML

- 1D / 2D / 3D scalar fields
- Can this be applied to other data, e.g. MD trajectories?

zfp: compressed floating-point and integer arrays

https://computing.llnl.gov/projects/zfp

- Developed at LLNL, supported by the U.S. DOE's Exascale Computing Project
- Open source https://github.com/LLNL/zfp
- Lossless and lossy
- Very good documentation https://zfp.readthedocs.io
- Written in C/C++
- Bindings in C, C++, Python, Fortran; Python interface is called zfPy
- Built into ~63 projects

https://computing.llnl.gov/projects/floating-point-compression/related-projects

- For faster (de)compression supports several backends: OpenMP, CUDA, HIP (C++ runtime for AMD and NVIDIA GPUs), FPGAs
- Reported throughputs up to 2 GB/s per CPU core, 800 GB/s aggregate throughput on GPUs

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Algorithm

- Details at https://zfp.readthedocs.io/en/release1.0.1/algorithm.html#lossy-compression
- Relies on orthogonal transforms, keeping only significant transform coefficients
- The transform coefficients are encoded into a losslessly-compressed bit stream that can be truncated in one of three ways, giving a user three "non-expert" compression modes:
 - fixed-rate mode controlled by a double-precision parameter (*rate*) giving a fixed number of bits per floating number
 - **fixed-precision mode** controlled by an integer parameter (*precision*) specifying the number of bit planes for the transform coefficients
 - **fixed-accuracy mode** controlled by a double-precision parameter (*tolerance*) specifying the max point-wise variable error

zfp

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Summary o

Using zfp via Python: tiny 1D array

import numpy as np, zfpy

```
# next, lossy compression
rate = 4 # number of bits per each floating number
initial = np.arange(1, 11, dtype=np.float32)
compressed = zfpy.compress_numpy(initial, rate=rate)
decompressed = zfpy.decompress_numpy(compressed)
print("rate_=", rate, "-->", str(len(compressed))+"B", "decompressed_=", decompressed)
```

```
file = open("compressed.zfp", "wb")
file.write(compressed)
file.close()
```



Note: the compressed file also includes some overhead beyond individual elements, the relative size of which will decrease for bigger data (next slide)

Topological compressio

zfp 000●000000

Using zfp via Python: large 3D array

→ 3D sine envelope wave function defined inside a unit cube ($x_i \in [0, 1]$)

$$f(x_1, x_2, x_3) = \sum_{i=1}^{2} \left[\frac{\sin^2 \left(\sqrt{\xi_{i+1}^2 + \xi_i^2} \right) - 0.5}{\left[0.001(\xi_{i+1}^2 + \xi_i^2) + 1 \right]^2} + 0.5 \right], \text{ where } \xi_i \equiv 15(x_i - 0.5)$$

- Discretized at 300^3 Cartesian grid in double precision double300.nc \Rightarrow 206M
- Lossless compression: double300.nc.gz 125M, double300.nc.bz2 119M
- NetCDF's compression='zlib' 159M
- NetCDF's compression='zlib', significant_digits=3 (very aggressive compression) 33M

```
import netCDF4 as nc, zfpy
import netCDF4 as nc, zfpy
                                                       file = open("compressed.zfp", "rb")
f = nc.Dataset('double300.nc')
rho = f.variables['density'][:]
                                                       decompressed = zfpy.decompress_numpy(compressed)
compressed = zfpy.compress numpy(rho, rate=2.0)
print(len(compressed)) # in bytes => 6.4M
                                                       f = nc.Dataset('compressed.nc', 'w', format='NETCDF4')
                                                       nx, ny, nz = decompressed.shape
file = open("compressed.zfp", "wb")
                                                       f.createDimension('x', nx)
                                                       f.createDimension('z', nz)
                                                       rho = f.createVariable('density', 'f4', ('x', 'y', 'z'))
     Demo rate=2.0, rate=1.0, rate=0.5
                                                       rho[:,:,:] = decompressed
```

Summa

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Summary o

Other notable storage formats supporting zfp

https://computing.llnl.gov/projects/floating-point-compression/related-projects

- https://h5z-zfp.readthedocs.io
- VTK-m supports zfp for (de)compressing arrays
- ZfpCompression.jl provides Julia bindings for zfp
- TTK without topological compression (will demo next)

Topological compression

Summary o

Using zfp in Julia

- ZfpCompression.jl is a wrapper around the C zfp library
- Use one of tol::Real, precision::Int, and rate::Real
- Optionally pass nthreads=... argument for multithreading, if ZfpCompression compiled with OpenMP (not enabled on MacOS by default)

```
using ZfpCompression
# (1) lossless compression
print(sizeof(initial), "....", sizeof(compressed)) # 40000 and 34040 bytes
decompressed = zfp_decompress(compressed);
initial == decompressed # true
# (2) lossy compression
compressed = zfp compress(initial, tol=1e-3);
decompressed = zfp_decompress(compressed);
maximum(abs.(initial - decompressed)) # 0.0003338
                                                       initial = Array{Float32,2}(undef, 100, 100);
                                                       read!("111.bin", initial);
print(sizeof(initial), ",, sizeof(compressed))
                         # 40000 and 17512 bytes
                     # Vector{UInt8}
                                                       decompressed = zfp decompress(compressed);
write("111.bin", initial)
                               # 40000 bytes
                                                       maximum(abs.(initial - decompressed)) # 0.0003338
write("111.zfp", compressed)
                               # 17512 bytes
```

Topological compression

Using zfp via TTK's TCWriter without topological compression In ParaView GUI

TopologicalCompressionWriter

- 1. Enable TTK plugin (more on it later in the talk)
- 2. File | Save Data, for file type select TTK Compressed Image Data (*.ttk)
- 3. Check ZFP compressor only, set ZFP Relative Error Tolerance

Using zfp via TTK's TCWriter without topological compression In pvpython

To enable parallel mode, rebuild TTK with "-DTTK_ENABLE_OPENMP=ON"

ZFPRelativeErrorToleranceextra	50% (default)	20%	10%	5%	3%
File size	1.6M	2.0M	2.5M	3.1M	4.4M
Compression ratio	129	103	82	66	47
Quality	noisy	quite noisy	small noise	very small noise, acceptable	excellent

Topological compression

Summary o

Deep water impact dataset

IEEE Vis 2018 contest https://sciviscontest2018.org

- One timestep, all variables, single-precision compressed VTK: 1.3G
- As far as I can tell, TTK's TopologicalCompressionWriter requires double precision input ⇒ stored sound speed as a double-precision VTK file (snd.vti)

uncompressed (500 ³)	gzip-compressed	LZMA-compressed	ZLib-compressed
954M	245M	178M	258M

```
from paraview.simple import *
data = XMLImageDataReader(FileName='snd.vti')
SaveData('zfp50.ttk', proxy=data, ScalarField=['POINTS', 'sound'],
```

```
ZFPRelativeErrorToleranceextra=50,
```

UseZFPcompressoronlynotopologicalcompression=1)

ZFPRelativeErrorToleranceextra	90%	50% (default)	30%	20%	10%	5%
File size	1.2M	2.0M	3.3M	5.3M	8.1M	12M
Compression ratio	795	477	289	180	117	80

Telltale sign of zealous zfp compression: negative sound speeds (check zfp50.ttk and zfp10.ttk)

Topological compression ••••••••

Topology-based analysis

This slide is based on Attila Gyulassy's introductory topology tutorial (U. of Utah)

- Phenomenon of interest in a scalar field in the data ⇒ derive its measurable topological equivalent or abstraction
- Measurable topological attributes:
 - measurement of connectedness: pick any two points + find an inside path to connect them
 - count non-contractable cycles: pick a closed loop inside that you can't squeeze down to a point
 - and many others
- Applications in:
 - molecular analysis: e.g. pick up atomic bonds, atoms from the 3D electronic probability density
 - materials analysis: porosity measurement, battery design, defect identification, cavity deformation
 - neural pathways (connectomics)
 - CFD: turbulence and vorticity, buble formation rate, ocean eddies
 - combustion analysis: ignition kernels
 - geological features
 - image segmentation

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Summary o



Figure copied from David Cohen-Steiner's slides on Topological Persistence

- Evolution of the topology of connected components during a filtration from $-\infty$ to $+\infty$
- Pair thresholds (critial points) that create components with those that destroy them
- Component persistence = difference in function value between component's birth and death

zfp 000000000 Topological compression

Summary o



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Persistence diagram



Figure copied from David Cohen-Steiner's slides on Topological Persistence

- Persistence diagram: x = function value at feature's birth, y = function value at feature's death
- Small features are mapped closer to the diagonal
- Critical points in 1D: minima and maxima
- Domain segmentation (monotone regions) between critical points, based on the gradient sign
- Mountains = monotone pieces around maxima, basins = monotone pieces around minima

Top

Topological compression

• Sweep in function value from $-\infty$ to $+\infty$

- Coloured regions shows the subdomain with function value lower than the sweep value
- This time single component with multiple holes that
 - split at the saddles
 - disappear at the maxima
- Critical points in 2D: minima, maxima, and saddle points
- Domain segmentation (monotone regions) between integral lines (orthogonal to the contours), based on the gradient sign
- Same definition for mountains and basins, but there are also ridge lines and valley lines



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- The topology becomes more complex
- 4 types of critical points: minima, maxima, and two kinds of saddles
 - 1-saddles are located between 2 minima, 2-saddles are located between 2 maxima
- Domain segmentation (monotone regions) between integral surfaces, based on the gradient sign
- Monotone regions combined into mountains and basins, with ridge lines and valley lines and saddle connector lines, ridge surfaces (separating the mountains) and valley surfaces (separating the basins)



Figure copied from Guoning Chen's slides on Morse-Smale Complex

Topological compression

Summary o

TTK = the Topology ToolKit

- Topological analysis of multi-dimensional scalar functions
- https://topology-tool-kit.github.io
 - great documentation, many tutorials and step-by-step videos
- Open source, development since 2014, first public release in 2017
- Lead author Julien Tierny + active development community
- Some workflows in this presentation were taken from the excellent half-day TTK tutorial at IEEE VIS 2020
- Interfaces:
 - pure C++
 - VTK/C++ (~3X shorter code)
 - ParaView Python (~5X shorter code) and ParaView plugin, and ParaView GUI

Topological compression algorithm

- 1. Topological simplification
 - remove all topological features below a user persistence tolerance ϵ
- 2. Domain quantization
 - break the domain into regions by the number of components
 - initially, in each region the data are represented by a constant plane (that could span multiple components)
- 3. Approximate data in each domain with an adaptive step function
 - each plane's vertical value is set to the data average over that region
 - each plane's horizontal extent is set to the data extent over that region
 - keep the original critical points in non-simplified regions
 - in each region compute the max pointwise error on the grid (data minus the planes / critical points); if larger than the specified error ⇒ subdivide that region in two (double the number of its planes approximating the non-simplified data) and repeat the procedure
- 4. Lossless compression of all elements
- 5. Optionally combine with zfp compression

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Summary o

Topological simplification in 1D



SFU webinar - slides at https://bit.ly/lossycom

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Summary 0

Topological simplification in 2D



On presenter's laptop:

cd ~/tmp/lossy
open s??.png

SFU webinar - slides at https://bit.ly/lossycom

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Topological compression

Summary o

Topological compression in 1D



zfp 00000000c Topological compression

Topological compression in 1D and 2D



Figure copied from Soler et al., IEEE PacificVis, 2018

SFU webinar - slides at https://bit.ly/lossycom

Topological compression

Using TTK's topological compression via ParaView GUI

- 1. Enable TTK plugin
- 2. Load double300.nc
- 3. File | Save Data, for file type select TTK Compressed Image Data (*.ttk)
- 4. Select topological persistence tolerance and max pointwise error
- 5. Optionally select ZFP Relative Error Tolerance

Topological compression

Using TTK's topological compression via pvpython

Topological compression

Using TTK's topological compression via C++/VTK

Step 1: install TTK (could not use x86-compiled MacOS binary \Rightarrow compile)

```
wget https://github.com/topology-tool-kit/ttk/archive/1.2.0.tar.gz
tar xvfz 1.2.0.tar.gz && cd ttk-1.2.0
brew install vtk libomp llvm cmake
mkdir ttk_install build && cd build
FLAGS=(
    -DTTK_BUILD_PARAVIEW_PLUGINS=OFF
    -DCMAKE_INSTALL_PREFIX=$HOME/tmp/ttk
)
export OpenMP_ROOT=$(brew --prefix)/opt/libomp
cmake .. "${FLAGS[@]}"
make -j4
make install
```

ztp 000000000

Topological compression

Using TTK's topological compression via C++/VTK (cont.)

Step 2: write the code and compile it against TTK

#include <CommandLineParser.h>
#include <vtkSmartPointer.h>
#include <vtkNew.h>
#include <vtkNmageData.h>
#include <vtkWnGenericDataObjectReader.h>
#include <ttkTopologicalCompressionWriter.h>
#include <string>

int main(int argc, char **argv) {
 ttk::CommandLineParser parser;
 std::string inputFile, outputFile, tolerance, error;
 parser.setArgument("i", śinputFile, "Path to input VTI file");
 parser.setArgument("c", śotlerance,
 "Topological persistence tolerance percentage", true);
 }
}

```
parser.setArgument("e", &error, "Maximum error", true);
parser.parse(argc, argv);
```

```
// read the data
auto reader = vtkSmattPointer<vtkXMLGenericDataObjectReader>::New();
reader->SetFileName(inputFile.data());
reader->Update();
```

```
auto inputDataObject = reader->GetOutput();
```

```
if(!inputDataObject)
```

```
cout << "Unable to read input file " + inputFile << endl;</pre>
```

```
return
```

```
auto inputAsVtKDataSet = vtkDataSet::SafeDownCast(inputDataObject),
auto pointData = inputAsVtkDataSet->GetPointData();
cout < "kead '" << pointData->GetArrayName(0) << "' array" << end;</pre>
```

vtkNew<ttkTopologicalCompressionWriter> topoWriter{}; topoWriter->SetInputArrayToProcess(0, 0, 0,

vtkDataObject::FIELD_ASSOCIATION_POINTS, pointData->GetArrayName(0)); topoWriter->SetInputData(inputAsVtkDataSet);

```
// set parameters
```

```
if (tolerance.length() > 0) // persistence %; default 10
  topoWriter->SetTolerance(std::stod(tolerance));
```

```
if (error.length() > 0) // relative error; default 10
topoWriter->SetMaximumError(std::stod(error));
topoWriter->Set2EPTolerance(-1); // no zfp compression
topoWriter->SetSubdivide(true);
topoWriter->SetUseTopologicalSimplification(true);
```

```
// write compressed TTK file
topoWriter->SetFileName(outputFile.c_str());
topoWriter->Write();
```

```
return 0
```

zfp 00000000c Topological compression

Summary o

Using TTK's topological compression via C++/VTK (cont.)

Step 3: run the code

(cd ~/tmp/lossy && make)
./main -i double300.vti -t 10 -e 10 -o double300.ttk

Two parameters: topological persistence tolerance and max error

- Both as percentages (defaults: 10% and 10%)
- Original dataset: 206M, rendering similar to the lower right panel



Deep water impact dataset

IEEE Vis 2018 contest https://sciviscontest2018.org

Recall: double-precision, single-variable VTK file (snd.vti)

uncompressed (500 ³)	gzip-compressed	LZMA-compressed	ZLib-compressed
954M	245M	178M	258M

Demoing with C++/VTK:

```
cd ~/tmp/deepWaterImpact
```

../lossy/main -i snd.vti -t 10 -e 10 -o t10e10.ttk

Arguments	-t 10 -e 10 (default)	-t 5 -e 10	-t 10 -е 5	-t 20 -е 10	-t 30 -е 10
File name	t10e10.ttk	t5e10.ttk	t10e5.ttk	t20e10.ttk	t30e10.ttk
File size	9.6M	16M	9.8M	4.2M	1.7M
Compression ratio	99	60	97	227	561
Quality	looks great, colour a little quantized	looks identical, so t10 is already good	looks identical, so e10 is already good	somewhat compressed	quantized colours, defi- nitely compressed

- \sim 1 min to compress and \sim 1 min to uncompress (or load into ParaView)
- Compare two 3D distributions (snd.vti vs. t10e10.ttk): paraview --script=compare.py
- Variable bounds kept constant

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Summary o

Deep water impact dataset (cont.)



- Both methods (zfp and TC) are quite comparable in output file quality and sizes
- Both can *reliably* achieve ~20-30X compression, without any visible data degradation and sometimes as high as ~80-200X
- Compression artifacts show in very different ways
- Can combine the two for improved quality and compression (they operate on different bits), see some comparison at https://topology-tool-kit.github.io/examples/persistenceDrivenCompression
- TC is much slower, both during compression and decompression
 - however, it provides more control (two parameters vs. one)
 - it preserves variable bounds
 - in certain cases it can achieve much higher compression, esp. if interested only in certain components
- Both algorithms act on scalar arrays, not files
- zfp: C/C++, Fortran, Python, built into many third-party packages, can compress integer, single- and double-precision datasets
- TC: only one widely accessible implementation (TTK), available via C++, ParaView (GUI and scripting), double precision only?
- In principle, TC should be able to compress AMR (multi-resolution) data in one go, as it does not rely on spatial wavelengths, although this would require some effort

