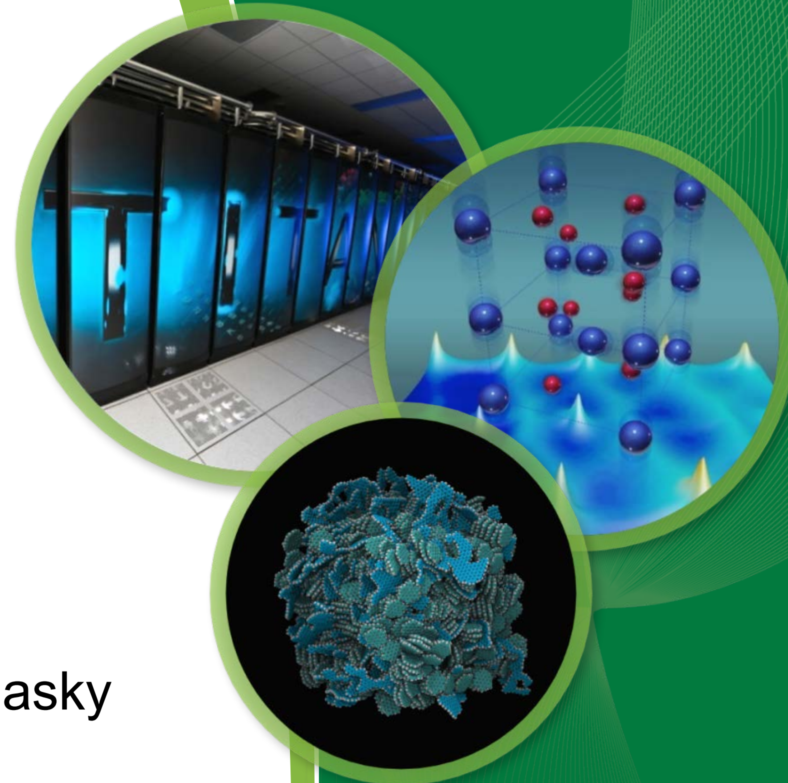
Data Reduction with Applied Statistics and Machine Learning for Computational Climate Science



George Ostrouchov,

Jong Y. Choi, Eric Suchyta, and Scott Klasky

Scientific Data Group

Computer Science and Mathematics Division

Oak Ridge National Laboratory

ORNL is managed by UT-Battelle
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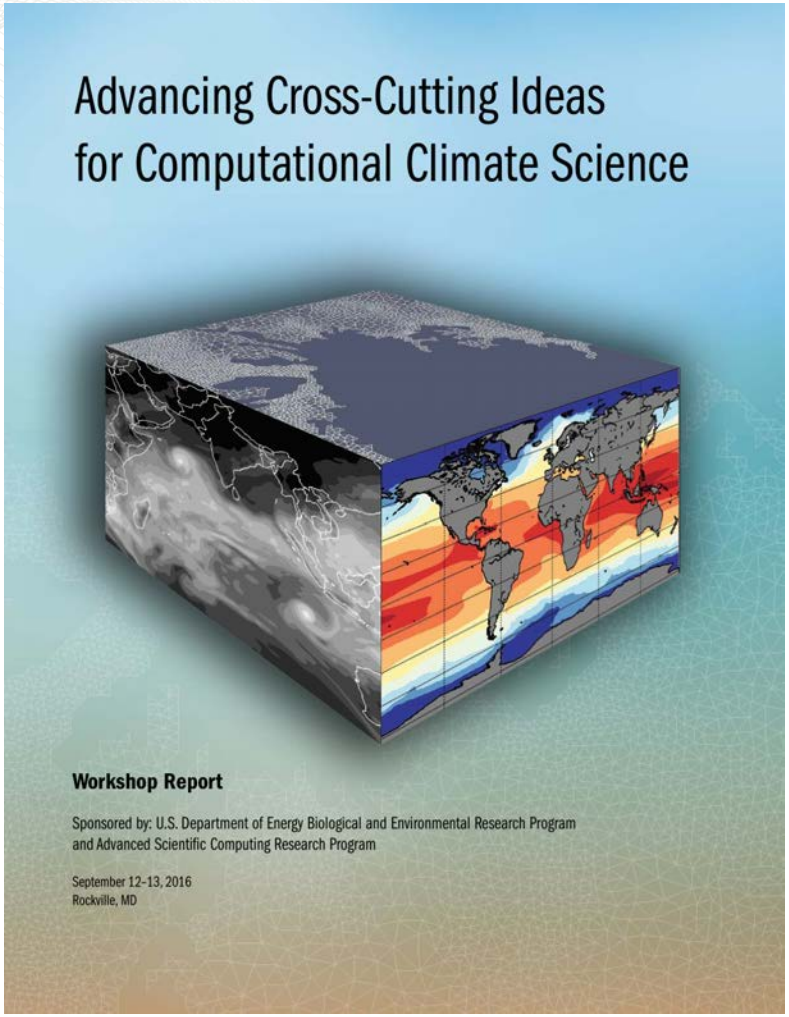
A Three Component Talk

- AXICCS workshop
  - Climate simulation data analysis communities
  - Data reduction in climate science
- The CODAR ECP project
  - I/O reality at exascale
  - Reduction methods
- Applied statistics and machine learning for reduction
  - Data analysis for data reduction
  - Tradeoffs between interpretability and reduction performance
  - A functional data analysis future

AXICCS Workshop



Workshop Chairs

Esmond G. Ng (Lawrence Berkeley National Laboratory)

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George Ostrouchov (Oak Ridge National Laboratory)

Raymond Tuminaro (Sandia National Laboratories)

Paul Ullrich (University of California, Davis)

Stefan M. Wild (Argonne National Laboratory)

Samuel Williams (Lawrence Berkeley National Laboratory)

DOE/ASCR Point of Contact

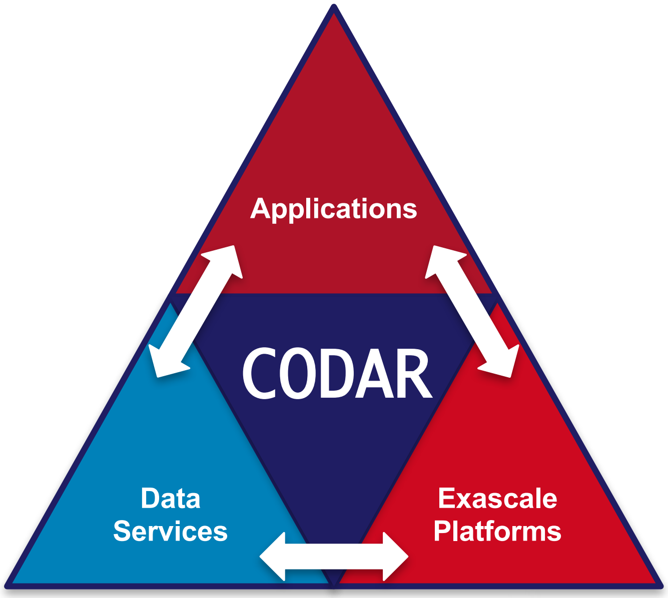
Randall Laviolette

DOE/BER Point of Contact

Dorothy Koch

CODAR:
Center for Online Data Analysis and Reduction, an ECP Codesign Center

Ian Foster, PI
Scott Klasky, Kerstin Kleese Van Dam, Todd Munson, Co-Is



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Stony Brook University

AXICCS: Climate Simulation Data

Unique among simulations:

- Scale of data production, retention, and throughput
- Serves diverse international communities
- Tasked to answer a broad array of questions
- Can not anticipate all uses or users

Common data reduction:

- Decimation: output fewer time steps
  - Short simulation with frequent output
  - Long simulation with less frequent output
- Averaging
  - Monthly averages for long simulations
  - Hourly averages for short simulations

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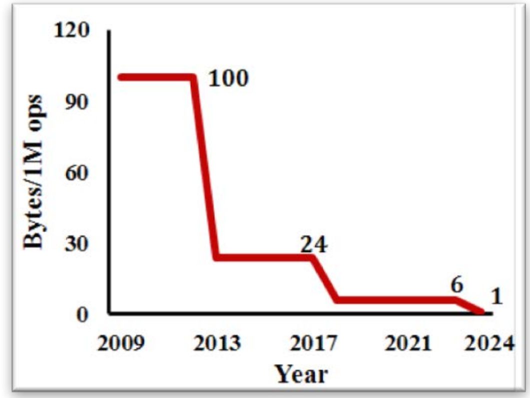
Why Reduce?

- CPU advances faster than bandwidth advances
- Bits per FLOP decreasing
- Reduce I/O with compression CPU cycles

“Compute-Data Gap”



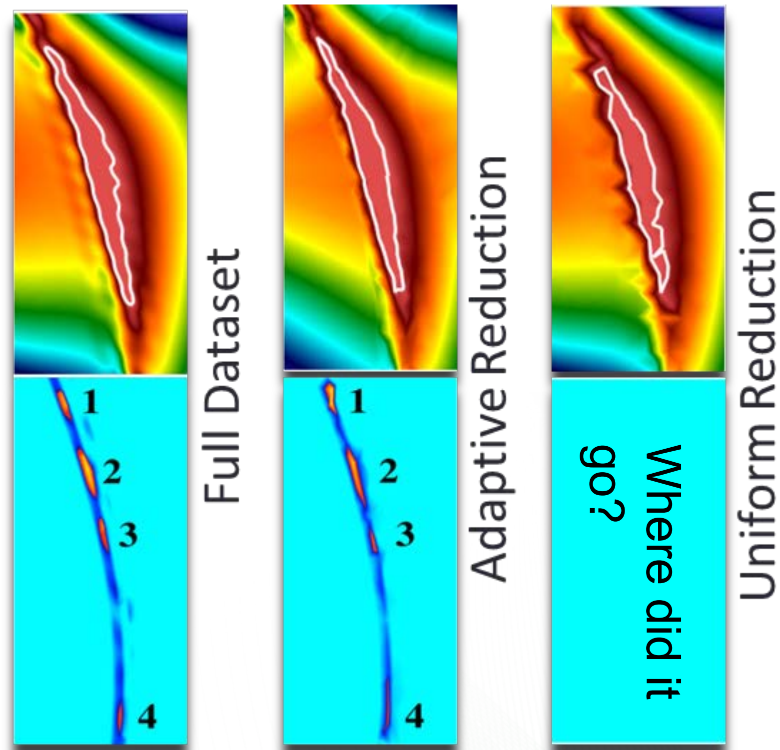
System attributes	NERSC Now	OLCF Now	ALCF Now	NERSC Upgrade	OLCF Upgrade	ALCF Upgrades	
Name Planned Installation	Edison	TITAN	MIRA	Cori 2016	Summit 2017-2018	Theta 2016	Aurora 2018-2019
System peak (PF)	2.6	27	10	> 30	150	>8.5	180
Peak Power (MW)	2	9	4.8	< 3.7	10	1.7	13
Total system memory	357 TB	710TB	768TB	~1 PB DDR4 + High Bandwidth Memory (HBM)+1.5PB persistent memory	> 1.74 PB DDR4 + HBM + 2.8 PB persistent memory	>480 TB DDR4 + High Bandwidth Memory (HBM)	> 7 PB High Bandwidth On-Package Memory Local Memory and Persistent Memory
Node performance (TF)	0.460	1.452	0.204	> 3	> 40	> 3	> 17 times Mira
Node processors	Intel Ivy Bridge	AMD Opteron Nvidia Kepler	64-bit PowerPC A2	Intel Knights Landing many core CPUs Intel Haswell CPU in data partition	Multiple IBM Power9 CPUs & multiple Nvidia Voltas GPUS	Intel Knights Landing Xeon Phi many core CPUs	Knights Hill Xeon Phi many core CPUs
System size (nodes)	5,600 nodes	18,688 nodes	49,152	9,300 nodes 1,900 nodes in data partition	~3,500 nodes	>2,500 nodes	>50,000 nodes
System Interconnect	Aries	Gemini	5D Torus	Aries	Dual Rail EDR-IB	Aries	2nd Generation Intel Omni-Path Architecture
File System	7.6 PB 168 GB/s, Lustre®	32 PB 1 TB/s, Lustre®	26 PB 300 GB/s GPFS™	28 PB 744 GB/s Lustre®	120 PB 1 TB/s GPFS™	10PB, 210 GB/s Lustre initial	150 PB 1 TB/s Lustre®

Reduction comes with challenges

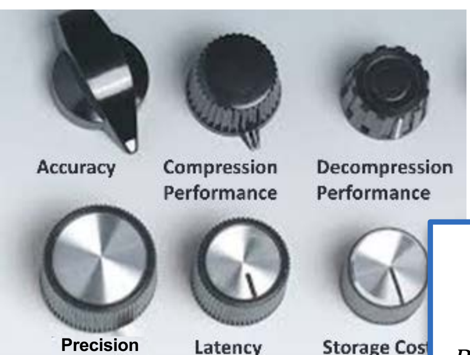
- Handling high entropy
- Performance – no benefit otherwise
- Not only errors in variable itself
  - $\|f(x,t) - \hat{f}(x,t)\|$
- must also consider impact on derived quantities:
  - $\|g(f) - g(\hat{f})\|$

$$f = \bar{B}$$

$$g(f) = \frac{\nabla\phi \times B}{\|B\|}$$



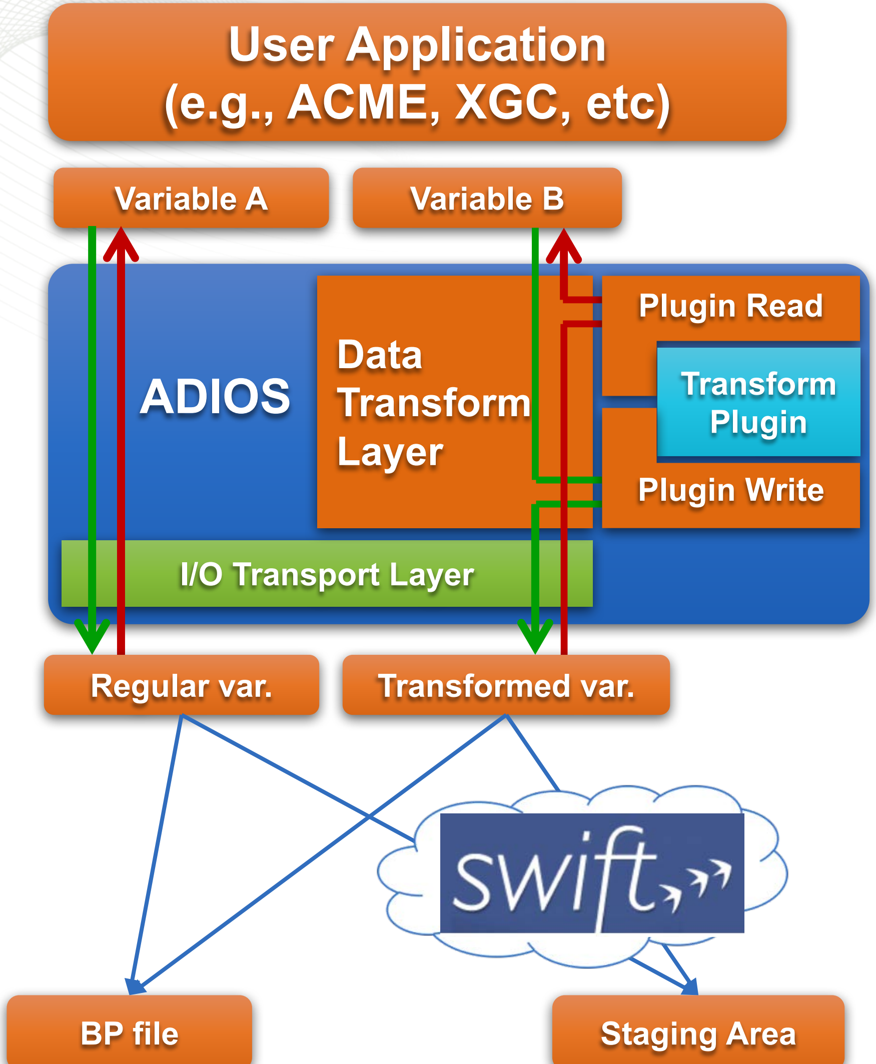
400 X reduction techniques



$$Accuracy \text{ “=“ } \frac{1}{Bias}$$

$$Precision \text{ “=“ } \frac{1}{Variability}$$

Adios Data Reduction Layer



- Designed for data conversions, compression, and transformation
- Transparent for users
  - User code read/write the original untransformed data
- Applications
  - Compressed output
  - Data Reduction
- Analysis on staging area
  - CODAR project
  - Dynamic management
  - Can be managed by Swift-T

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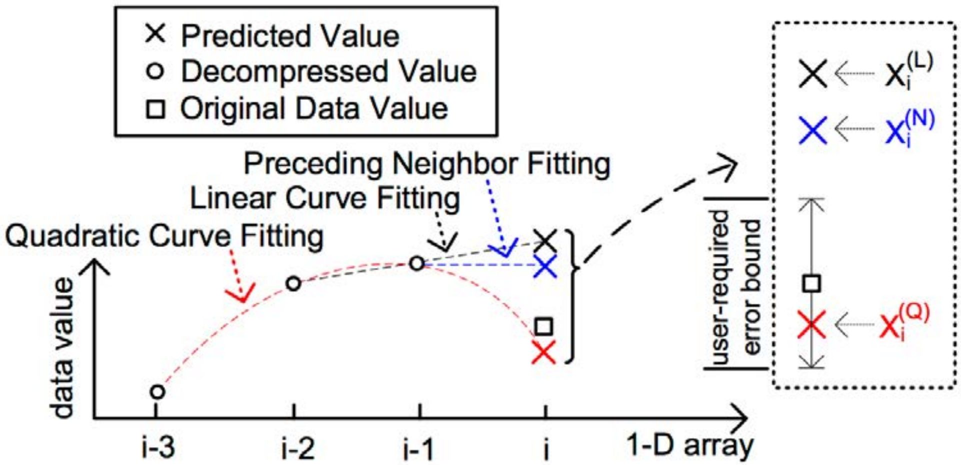
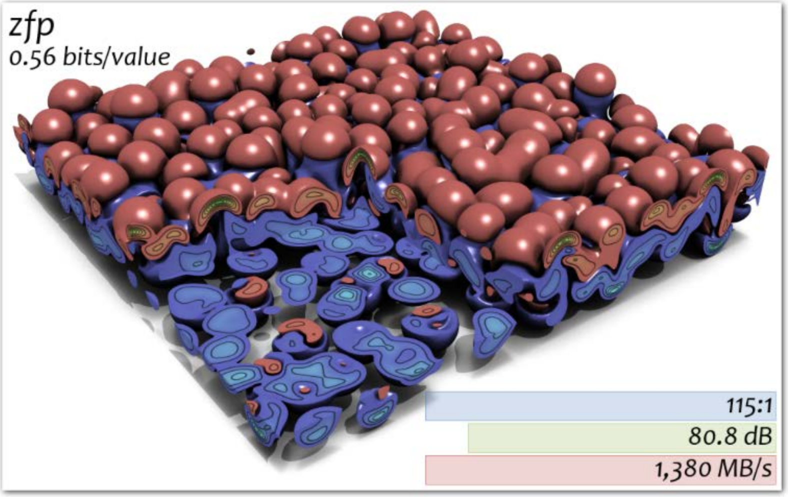
Adios With Data Reduction Methods

- Adios integrates with reduction methods
  - SZ: Best-fit curve-fitting compression
  - ZFP: Fixed-rate floating point Compression
  - Lossless: bzip2, szip, szip, …



SZ Curve-fitting illustration
(Sheng Di, PDPS 2016)



ZFP for fixed-rate compression
(http://computation.llnl.gov/projects/floating-point-compression)

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PCA of Time Varying Spatial Data

Same Concept → Different Context → Many Names

- Spectral Decomposition:1700-1800
- Singular Value Decomposition (SVD): 1900
- Principal Component Analysis (PCA):1902, 1935, Statistics/Psychology
- Karhunen-Loeve Decomposition (KL): 1946, 1955 Probability/Mathematics
- Empirical Orthogonal Functions (EOF): 1956, Climate
- Proper O
- Probabili

$n \times p$ matrix with entries $F(x,t)$ at grid locations $\{x_1, x_2, \ldots, x_p\}$ and times $\{t_1, t_2, \ldots, t_n\}$.

$F_c = V S U^T$ (center data: $F_c = (I - n^{-1} 1 1^T) F$)

$VS = F_c U$ p time series

$US = F_c^T V$ n images

VS and US have same units as F

Reduction:

- k components extract k-dimensional linear subspace
- $k(p + n + 1) < pn$ for $k \ll p$ or n
- Linearizing transformations, centering, and scaling reduces k needed for fixed error budget

Distributed PCA
Tradeoffs for Data Reduction

Global PCA across data partitions

- Approximate methods acceptable
- Requires communication across nodes
- Enables interpretation over full spatial domain

Local PCA within data partitions

- Approximate methods acceptable
- Faster and more scalable
- Avoids cross-node communication
- Interpretation limited to local spatial domain
- Postprocessing global PCA from local PCA possible but costly

A Scalable Platform for Novel Algorithmic Development on Big Data Analytics!

HPCwire

July 6, 2016

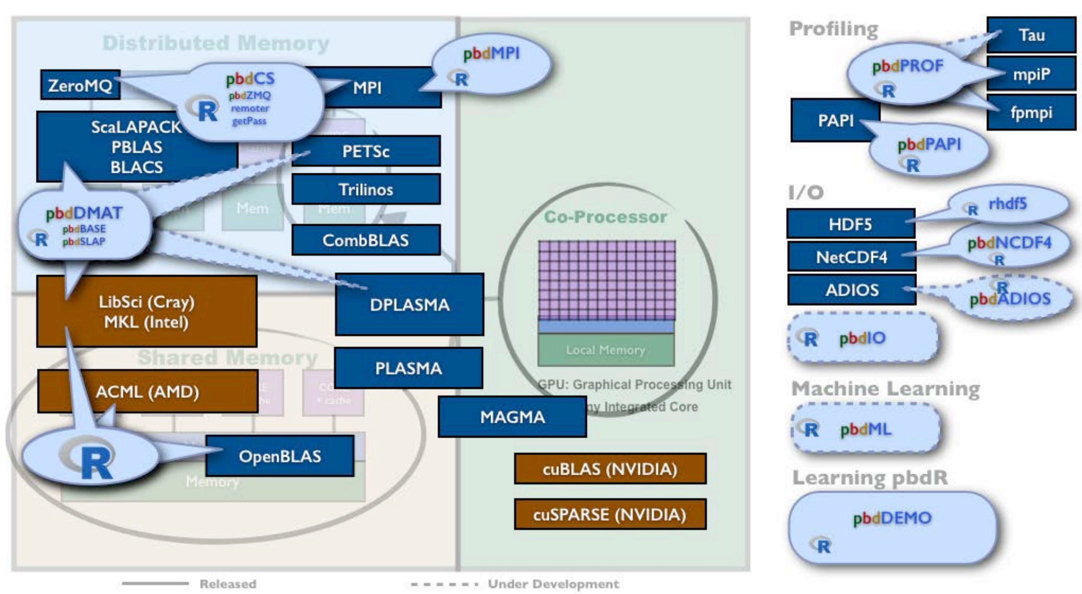
"OLCF Researchers Scale R to Tackle Big Science Data Sets"
"***for situations where one needs interactive near-real-time analysis, the pbdR approach is much better*** *[than Apache Spark–like frameworks].*"
PCA of a 134 GB matrix: "*several hours on . . . Apache Spark, . . . less than a minute using R.*"

Modern statistical algorithm + pbdR infrastructure + HPC Libraries + HPC Hardware

pbdR
Programming with Big Data in R

http://pbdr.org

- Engage parallel math libraries at scale
- R language unchanged
- New distributed concepts
- New profiling capabilities
- New interactive SPMD parallel
- In-situ distributed capability
- In-situ staging capability via ADIOS
- 2016 ORNL Significant Event Award



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Functional Data Analysis (FDA): From Euclidean Space of Points to Hilbert Space of Functions

- Euclidean space
  - N items
  - Each with *p* grid points (in time, over spectrum, in space)
  - Finer discretization increases *p*
  - Each item a point in Euclidean *p*-space
- Hilbert space
  - N items
  - Each a function over domain (time, spectrum, space)
  - Implicitly $p = \infty$
  - Each item a point (function) in Hilbert space
- Nature (physics) does not change with sampling rate!
- Replacing memory/data with mathematical complexity

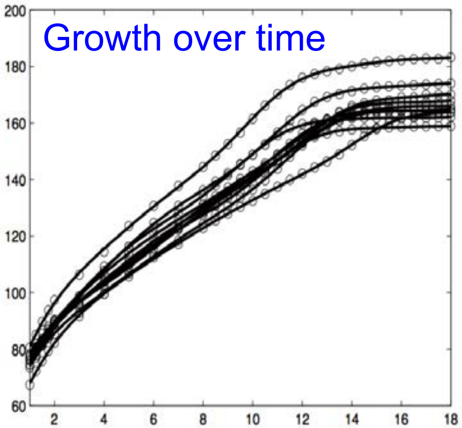
FDA: Simple Point Data to Rich Functional Data

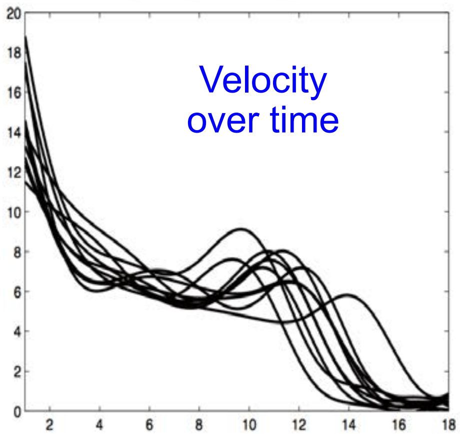
- Physical constraints
  - E.g. monotone growth, positive velocity
- Smoothing, roughness penalties crossvalidation
  - Splines, Fourier, wavelets, Gaussian process, etc.
- Quantified u

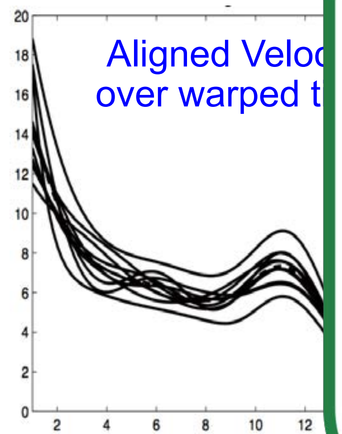
What is new?

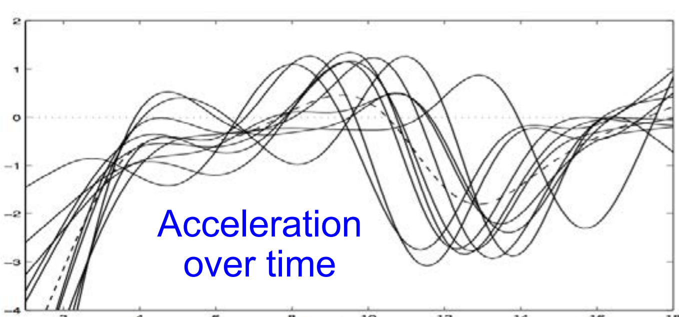
- Access to new information
- Represent with more parsimony
- Phase space alignment

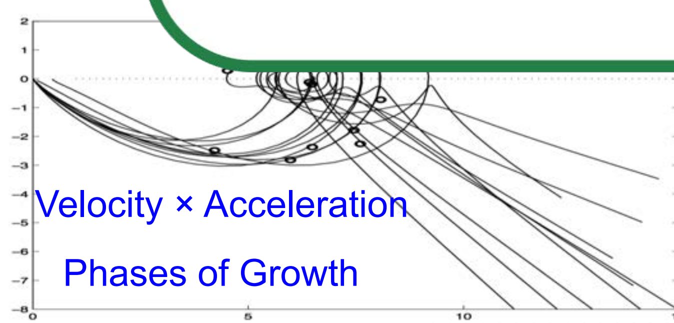
- Computationally demanding but potentially highly parallel











Landmark
Registration

Figures adapted from Ramsay & Hermanussen, 2014.

Reducing Functional Data Representations

- Stage I: Spline knot placement optimization and knot reduction
  - Related to sparse estimation
  - Optimality is difficult but near optimality good enough
  - Fine use of additional compute cycles
  - Potentially highly parallel
- Stage II: Phase alignment
- Stage III: Functional PCA for finite basis construction
  - Better reduction properties than Euclidean PCA
- Fast reconstruction for visualization
  - Potential for higher resolution with less data
  - Not unlike transition from bitmap fonts to scalable Bezier curve fonts

Functional Data Analysis Brings

- Reduced data movement and reduced storage
- Analysis performed in functional space
  - Smaller memory footprint than traditional methods
  - Added mathematical complexity
  - Tools exist for common analytics such as variability attribution, principal components, canonical correlation, clustering, and many other multivariate methods
  - New techniques unique to functional data
- Principled model component coupling at any resolution
- Rigorous interpolation schemes for visualization
- Fallback to traditional methods, data reconstructed at any resolution
- Potential connections to finite element methods

Thank You!

This research was supported by the Exascale Computing Project (ECP), Project Number: 17-SC-20-SC, a collaborative effort of two DOE organizations -- the Office of Science and the National Nuclear Security Administration -- responsible for the planning and preparation of a capable exascale ecosystem -- including software, applications, hardware, advanced system engineering, and early testbed platforms -- to support the nation's exascale computing imperative.