On the Role of Indexing for Big Data in Scientific Domains

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BIGDATA and EXTREME-SCALE COMPUTING

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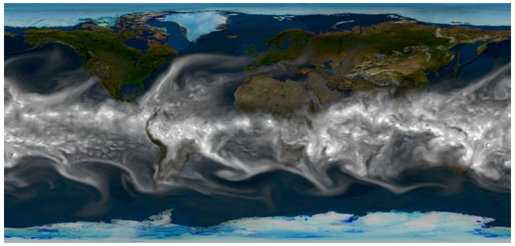
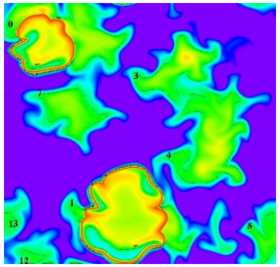
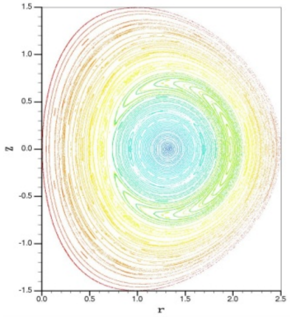
Outline

- ❑Examples of indexing needs in scientific domains
- ❑ Scientific Indexing requirements
- ❑Bitmaps indexing as a promising technology



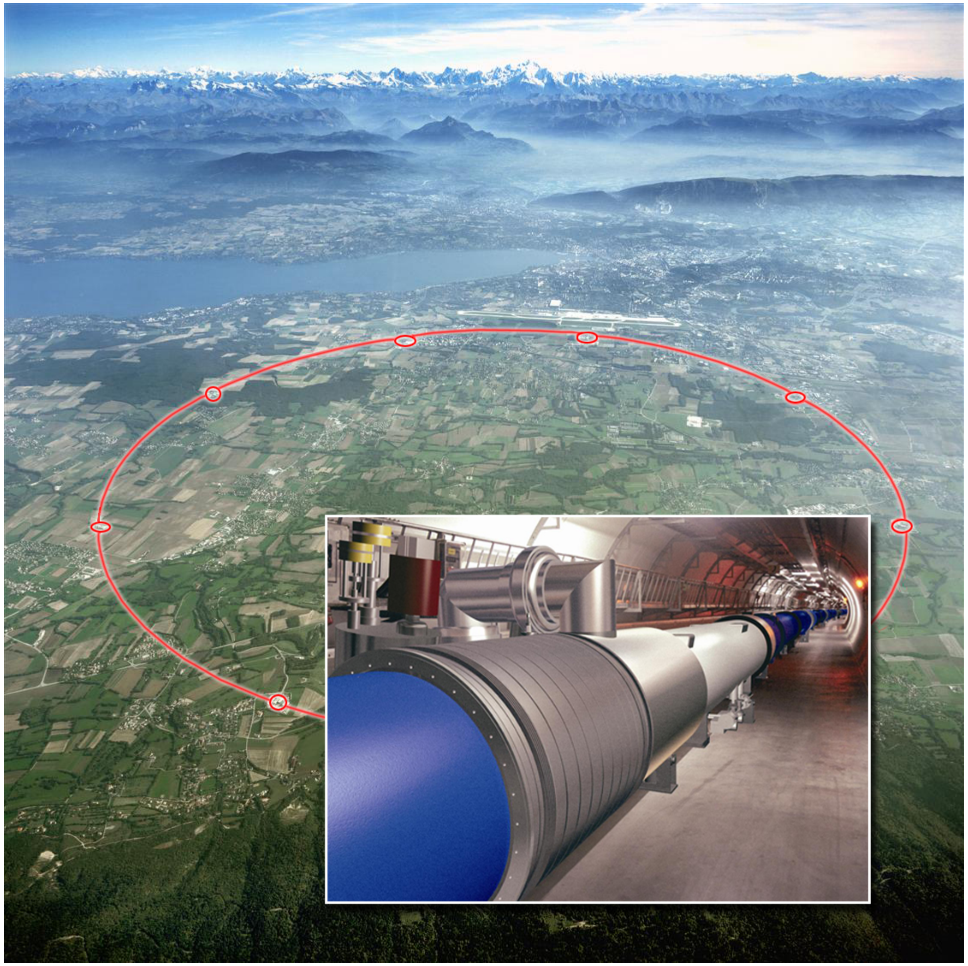




Example of Big Data in Science

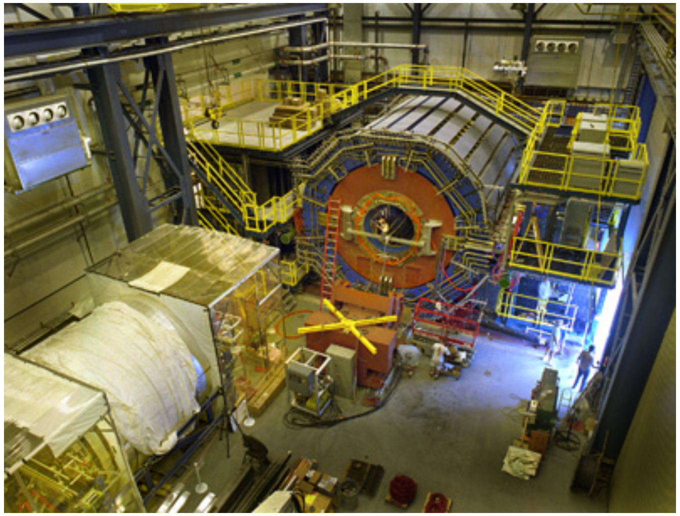
Large Hadron Collider: to find the God particle

- **15 PB** per year – sensors capable of 140PB/s
- 27 km tunnel
- ~10,000 superconducting magnets
- Operating temperature 1.9 Kelvin
- Construction cost:
  US$9Billion
- Power consumption: ~120 MW



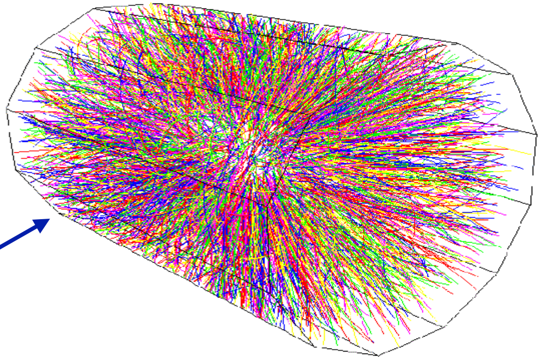
Typical Event Figures

Experiment	# members /institutions	Date of first data	# events/ year	volume/year- TB
STAR	350/35	2001	10^8-10^9	500
PHENIX	350/35	2001	10^9	600
BABAR	300/30	1999	10^9	80
CLAS	200/40	1997	10^{10}	300
ATLAS	1200/140	2008	10^{10}	5000



STAR: Solenoidal Tracker At RHIC
RHIC: Relativistic Heavy Ion Collider

LHC: Large Hadron Collider
Includes: ATLAS, CMS, …



A mockup of
An “event”

What are the indexing challenges?

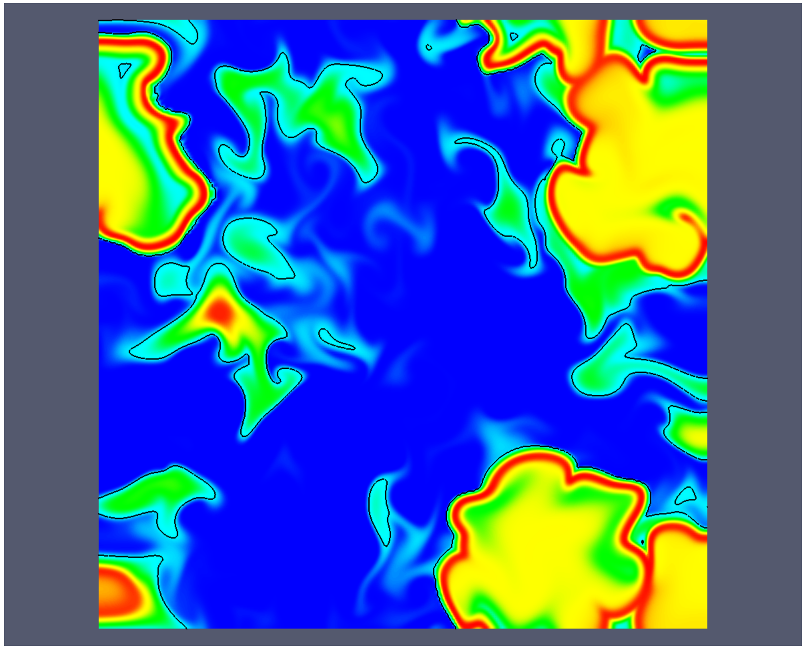
- Generate large amounts of raw data – referred to as “events”
  - Collected from simulations and experiments
- Post-processing of data
  - Identify elements in data (find particles produced, tracks)
  - generate summary variables per event
    - e.g. momentum, no. of pions, transverse energy
    - Number of variables is large (50-100)
- Analyze data
  - use summary variables to characterize events
  - extract subsets from the large dataset
    - Need to access events based on partial variable specification (range queries)
    - e.g. $((0.1 < AVpT < 0.2) \wedge (10 < Np < 20)) \vee (N > 6000)$
- Challenges
  - Search over billions of events
  - Multi-variable search, but only over a subset of the variable
  - Type of query: a needle-in-the-haystack
  - Another type of query: larger subsets for statistical properties
  - Search over numerical values (integers, floating point)

Combustion simulation example

- Combustion simulation: 1000x1000x1000 mesh with 100s of chemical species over 1000s of time steps – 10^{14} data values
- This is an image of a <u>single</u> variable (temperature)
- What's needed is search over multiple variables, such as:

  Temperature > 1000
  AND pressure > 106
  AND HO2 > 10^{-7} AND HO2 > 10^{-6}

- Challenges
  - Multi-variable queries from a subset of variables
  - Search over numerical values
  - Identify large number of regions



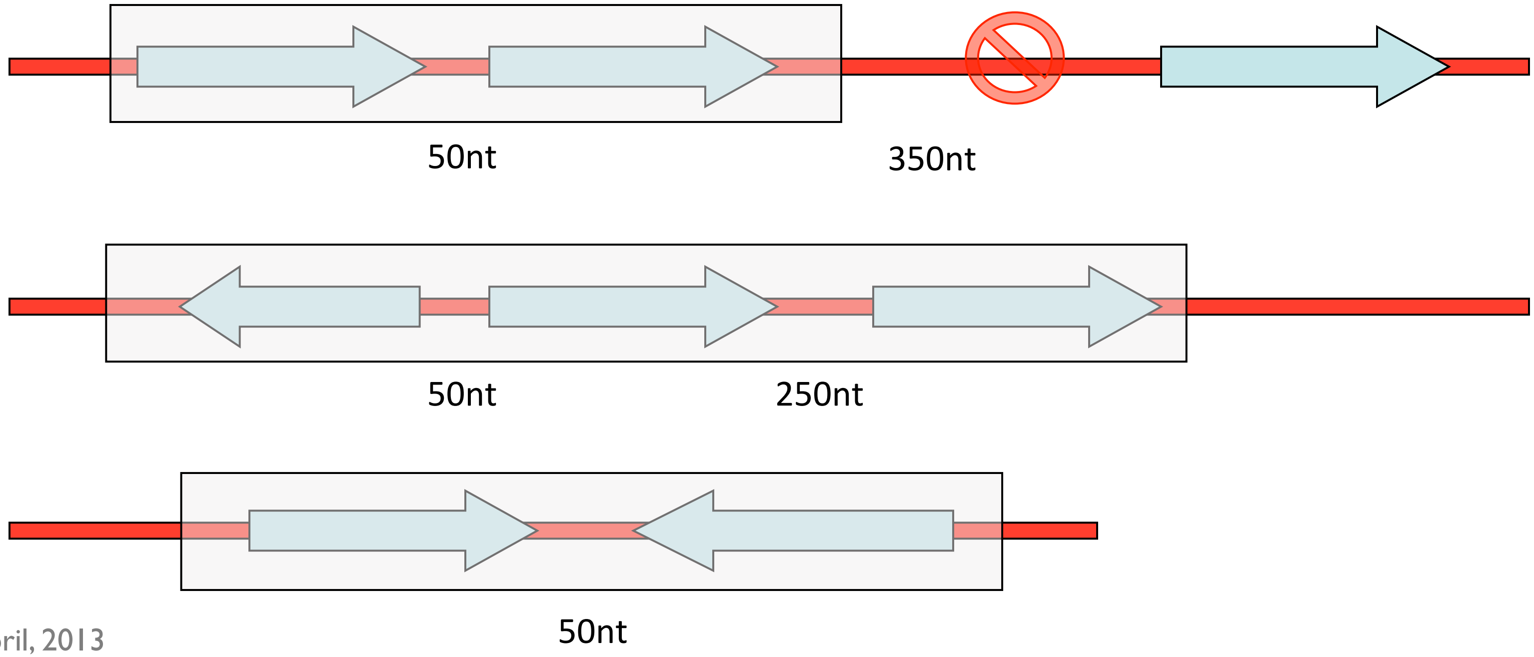
Gene functional annotation

Sequence similarity

Gene context provide information for the function of genes.

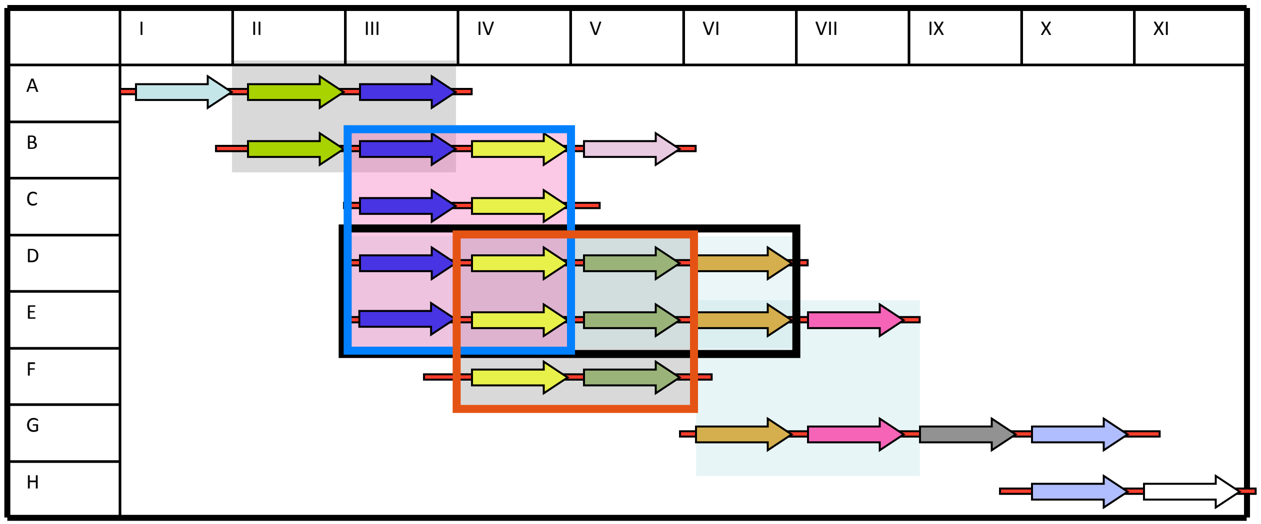
Functionally related genes are frequently found in the same chromosomal neighborhood.

- **Cassette Definition**
  - **Parallel or Divergent orientation**
  - **Distance < 300nt**



Conserved chromosomal cassettes

- Genes are replaced by protein families (COGs, pfams, IMG ortholog families). One gene → multiple families.
- We refer to these as "properties", such as "cog0087 cog0088 cog0089 pfam00181 pfam00189 pfam00203 pfam00237"



- Boxes that share two cassettes and two genes, if the genomes are distant phylogenetically (more than species)
- E.g. for black box: blue and red are 1st step relatives.

Why is this problem hard?

- Size
  - ✧ 100 million cassettes, with properties from about 25,000 possible values (currently).
  - ✧ Total number of elements: 2.5×10^{12}

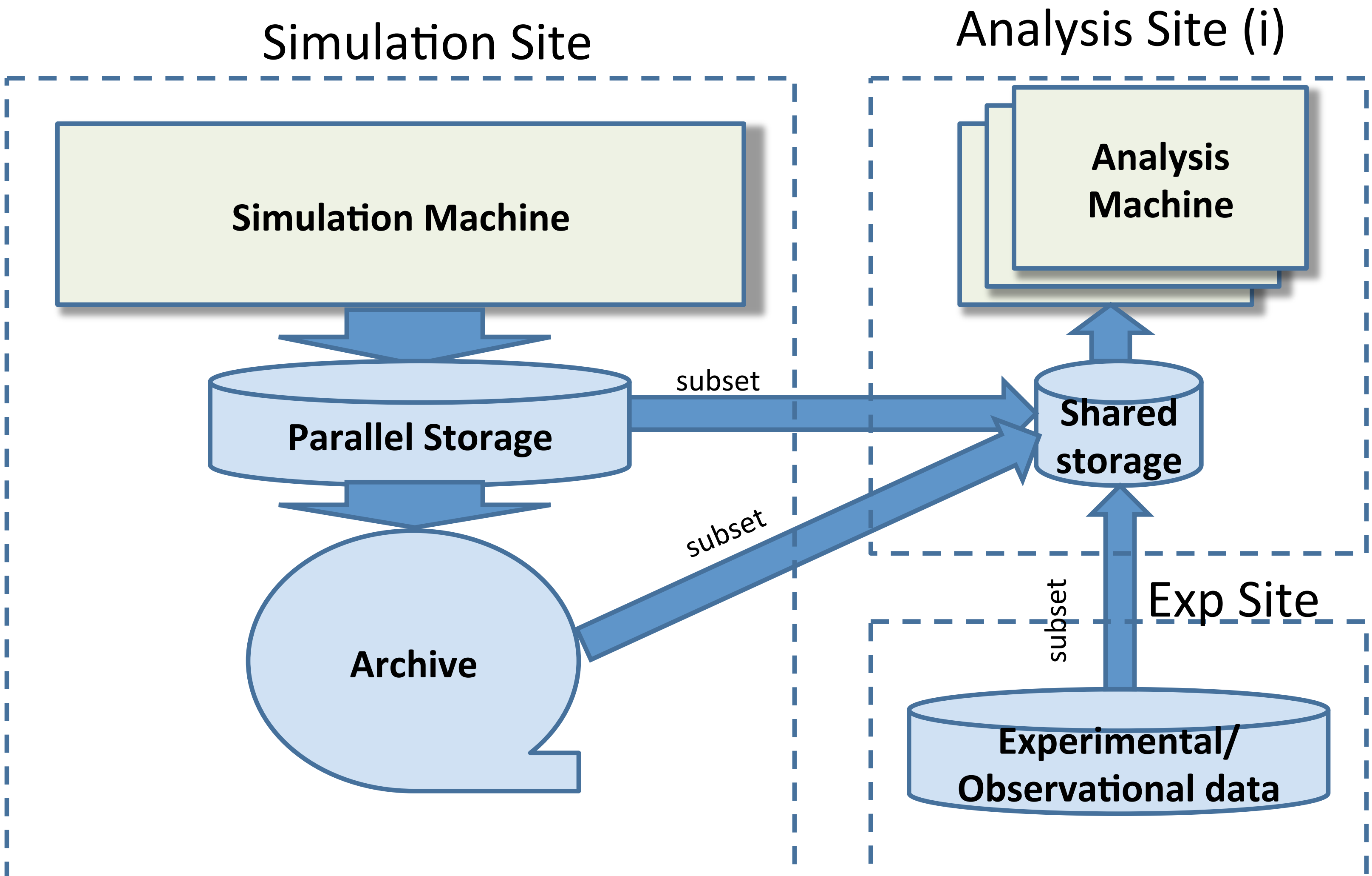
Challenge

- Query types
  - ✧ Given a cassette find all cassettes that have the same properties in common
    - That is a massive multi-value search
  - ✧ Given a cassette find all cassettes that have 2-or-more properties in common (in general k-or-more)
    - Explosive search of all possible combinations of 2-or-more

Big Data Indexing Requirements

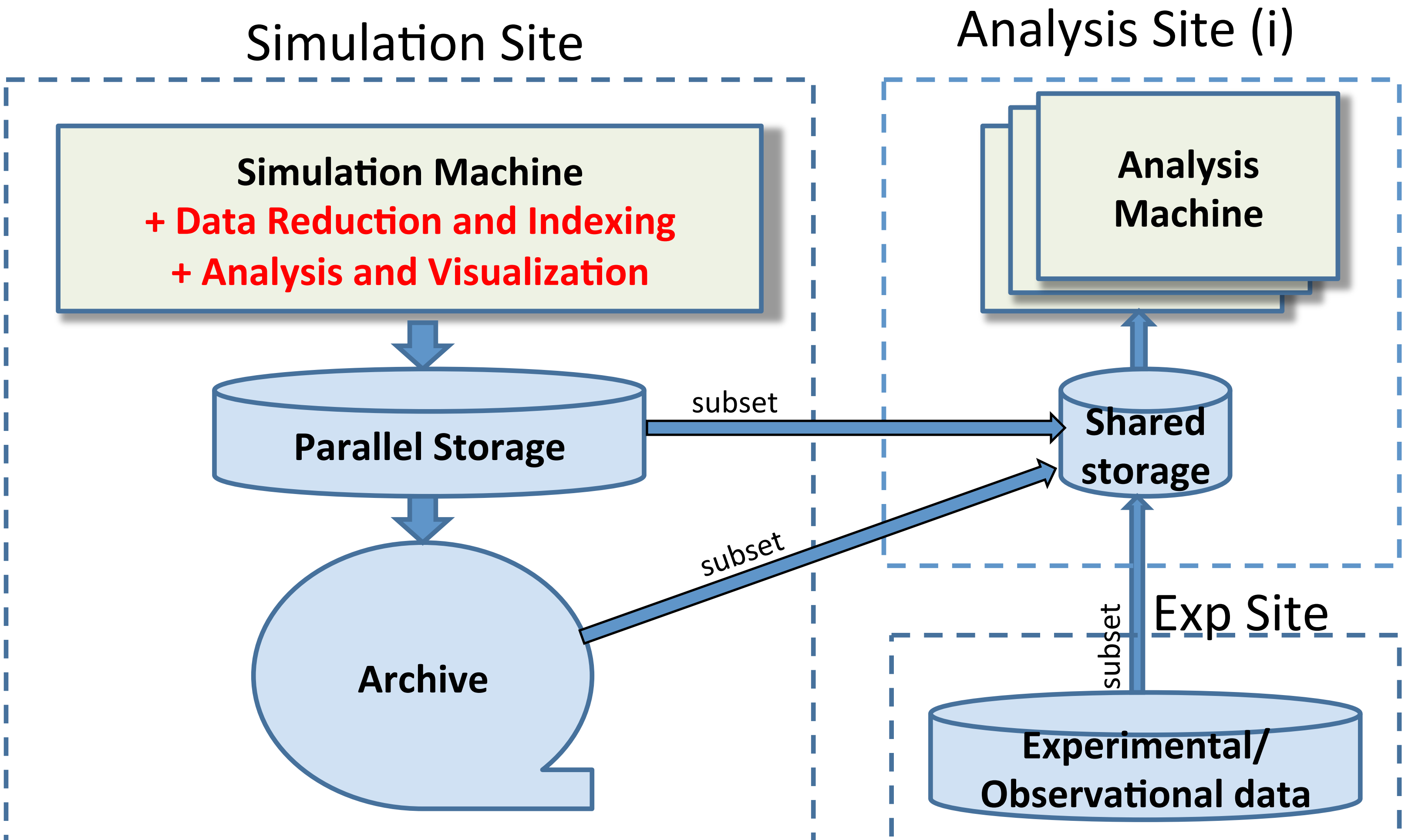
- ❑ Speed of search
  - ✧ Search over billions – trillions data values in seconds
- ❑ Multi-variable queries
  - ✧ Be efficient for combining results from individual variable search results
- ❑ Size of index
  - ✧ Index size should be a fraction of original data
- ❑ Granularity
  - ✧ Ability to produce smaller indexes when granularity can be reduced, such as 1 decimal points, for example
- ❑ Parallelism
  - ✧ Should be easily partitioned into sections for parallel processing
- ❑ Speed of index generation
  - ✧ For in situ processing, index should be built at the rate of data generation

Scaling simulations generates a data volume challenge (PBs)



What Can be Done?

- Perform some data analysis and visualization on simulation machine (in-situ)
- Reduce Data and prepare data for further analysis (in-situ)



Data Analysis

- ❑ Two fundamental aspects
  - ✧ Pattern matching: Perform analysis tasks for finding known or expected patterns
  - ✧ Pattern discovery: Iterative exploratory analysis processes of looking for unknown patterns or features in the data
- ❑ Ideas for the analysis of Big Data
  - ✧ Perform pattern matching tasks in the simulation machine
    - “In situ” analysis
  - ✧ Prepare data for pattern discovery on the simulation machine, and perform analysis on mid-size analysis machine
    - “In-transit” data preparation
    - “Off-line” data analysis

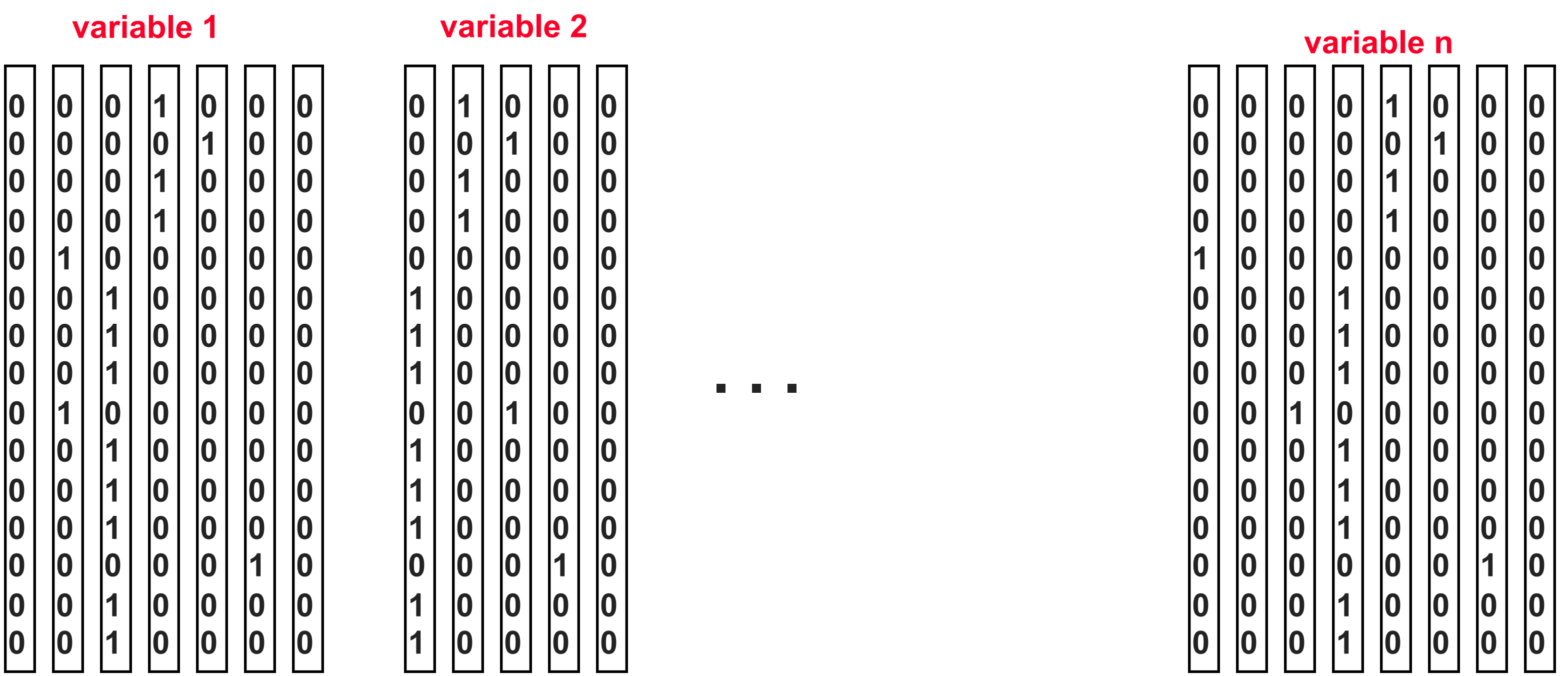
Index:

A Data Structure for Accelerating Data Accesses

- ❑ Tree-based indexes
  - ✧ E.g. family of B-Trees
  - ✧ Commonly used database management systems
  - ✧ Sacrifice search efficiency to permit dynamic update
- ❑ Multi-dimensional indexes
  - ✧ E.g. R-tree, Quad-trees, KD-trees, …
  - ✧ Don't scale for large number of dimensions
  - ✧ Are inefficient for partial searches (subset of attributes)
- ❑ Hashing
  - ✧ Predictable performance
  - ✧ Good for locating individual data records
- ❑ Bitmap indexes:
  - ✧ Good for read-mostly data
  - ✧ Handle partial range queries efficiently
  - ✧ May have trouble handling data with a large number of distinct values

Bitmap index for each variable

- Take advantage that index need to be is append only
- Generate a bitmap for each possible value of each variable
  - (e.g. for 0<Np<300, have 300 bitmaps)
- compress each bit vector (some version of run length encoding)
- Need to touch only bitmaps for the specified search



Basic Bitmap Index

Data values	b_0 =0	b_1 =1	b_2 =2	b_3 =3	b_4 =4	b_5 =5
0	1	0	0	0	0	0
1	0	1	0	0	0	0
5	0	0	0	0	0	1
3	0	0	0	1	0	0
1	0	1	0	0	0	0
2	0	0	1	0	0	0
0	1	0	0	0	0	0
4	0	0	0	0	1	0
1	0	1	0	0	0	0

A < 2   2 < A

- <u>Easy to build</u>: faster than building B-trees
- <u>Efficient for querying</u>: only bitwise logical operations
  - $A < 2 \rightarrow b_0$ OR b_1
  - $A > 2 \rightarrow b_3$ OR b_4 OR b_5
- Efficient for multi-dimensional queries
  - Use bitwise operations to combine the partial results
- Size: one bit per distinct value per object
  - Definition: Cardinality == number of distinct values
  - Need to control size for high cardinality attributes
- Main idea:
  - highly efficient compression method
  - Compute friendly – can perform operations directly on compressed data

FastBit properties – highly efficient and compact

Main idea:

- ✧ **Invented specialized compression methods (was patented) that:**
  - **Can perform logical operations directly on compressed bitmaps**
  - **Excels in support of multi-variable queries**
  - **Can partition and merge bitmaps without decompression – essential for parallelization of indexes**

FastBit takes advantage of append only data to achieve:

- ✧ **Search speed by 10x – 100x than best known bitmap indexing methods**
- ✧ **On average about 1/3 of data volume compared to 2-3 times in common indexes because of compression method**
- ✧ **Proven to be theoretically optimal – data search time is proportional to size of the result**

Usage

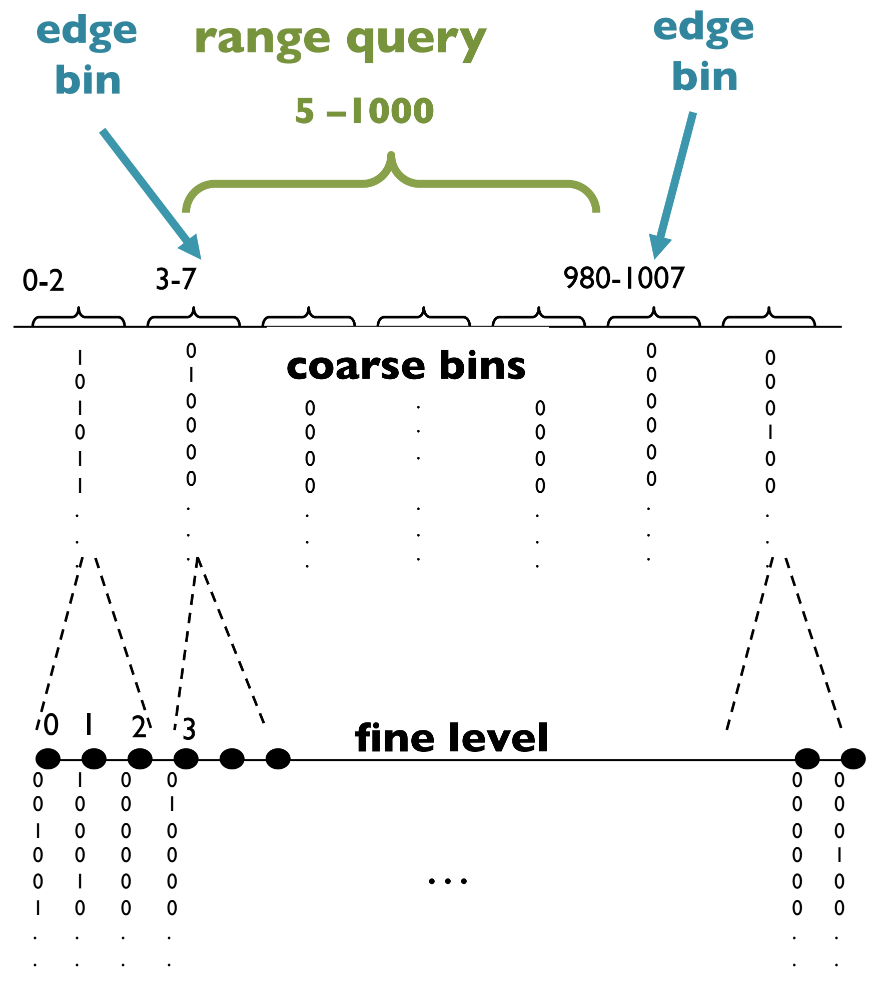
- ✧ **In multiple scientific application in DOE**
- ✧ **Embedded into in situ frameworks**
- ✧ **Thousands of downloads around the world (open source under source forge), including commercial companies**

Methods to Improve Bitmap Index

- **Compression**
  - FastBit compression method: Word-Aligned Hybrid (WAH) code
  - 10x speedup over Byte-aligned Bitmap Code
- **Encoding**
  - Multi-level encoding
  - Reduce bitmaps needed for a query
  - 5x speedup
- **Binning**
  - Some times we choose to use bins at the fine level to reduce index size
  - Problem: if query falls in the middle of edge bins
  - Solution: Order-preserving Bin-based Clustering (OrBiC)
  - 5x speedup for searching bins

Improving Bitmap Indexes: Multi-Level Encoding

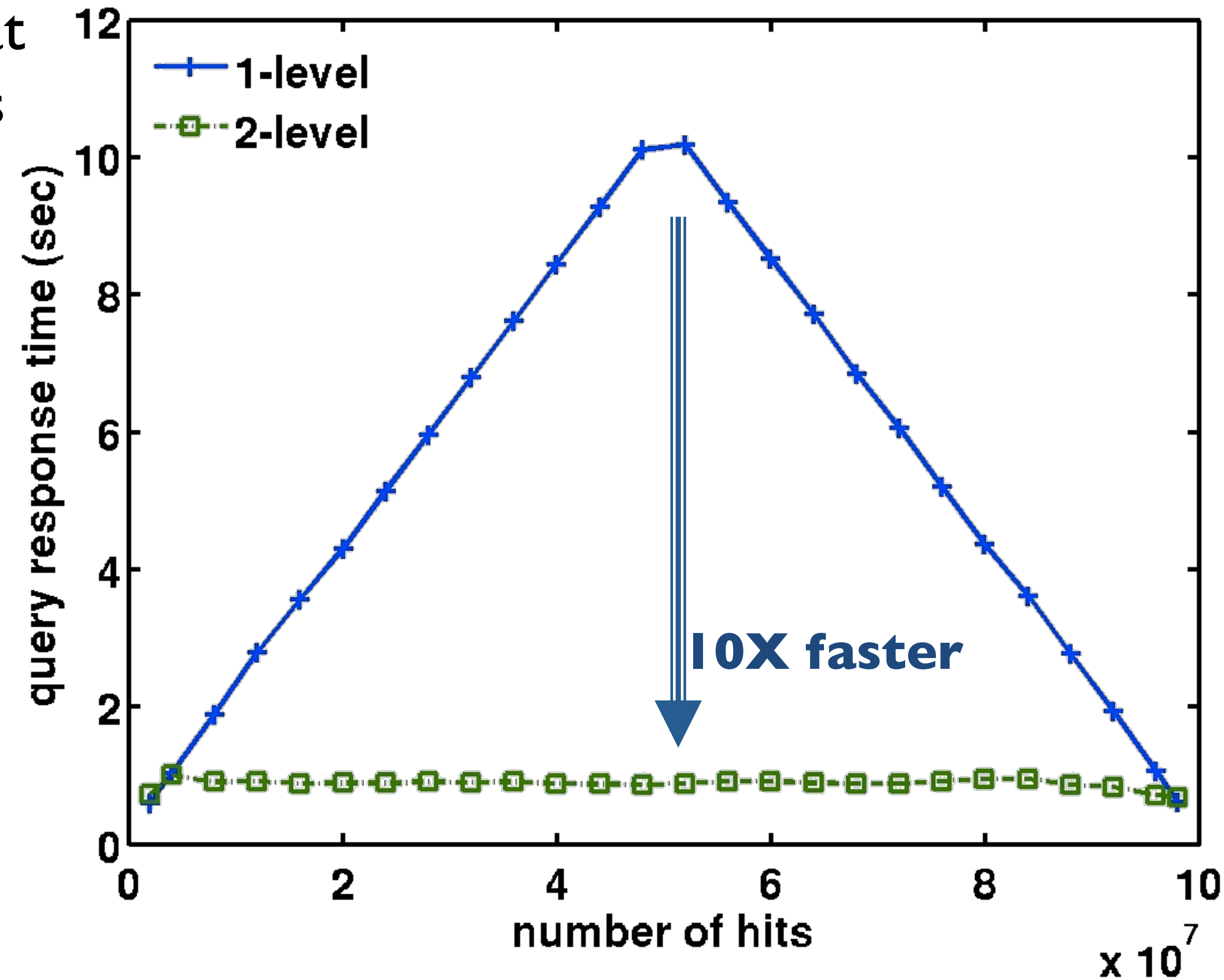
- The finest-level may be precise or binned
- Coarse levels are always binned
- Each coarse bin contains a number of fine bins/values
- Queries can be processed with a combination of coarse and fine bitmaps
- Only edge bins need to be resolved at the fine level
- Analysis revealed how to construct the coarse level in order to reduce the query processing time



[Wu, Shoshani and Stockinger 2010]

Two Levels Are Better Than One

- Prove theoretically that the second level needs to have only a small number of bins (15 ~ 50 depending on data)
- Only two levels are necessary
- Result: 5X speedup on average (over WAH compressed 1-level index)



[Wu, Shoshani and Stockinger 2010]

Domain-Specific Challenges – current and future

- Generate index at the rate of data generation in situ
  - Increase level of parallel processing
  - Perform partial index generation per node
  - Take advantage of local NVRAM
- Adapt indexing methods to a variety of data models
  - Irregular grids, geodesic meshes, toroidal meshes
    - How to linearize the space
  - Multi-level grid, such as adaptive-mesh-refinement (AMR)
- Use results of index in subsequent operations
  - Statistical summaries
  - Region growing, region overlaps, …
- Adapt indexing to specialized operations
  - Searches for k-or-more matches
  - Searches based on formulas (plug-in-codes)

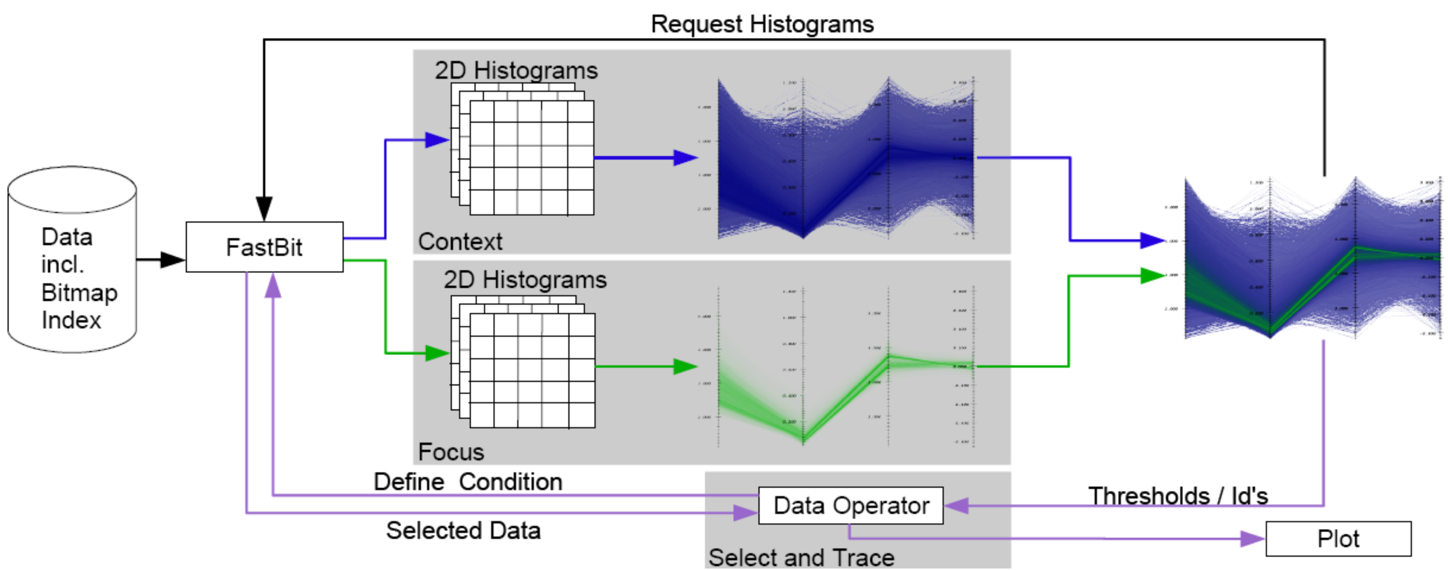
FastBit in support for Query-Driven Visualization

Collaboration between SDM and Vis groups

- Use FastBit indexes to efficiently select the most interesting data for visualization

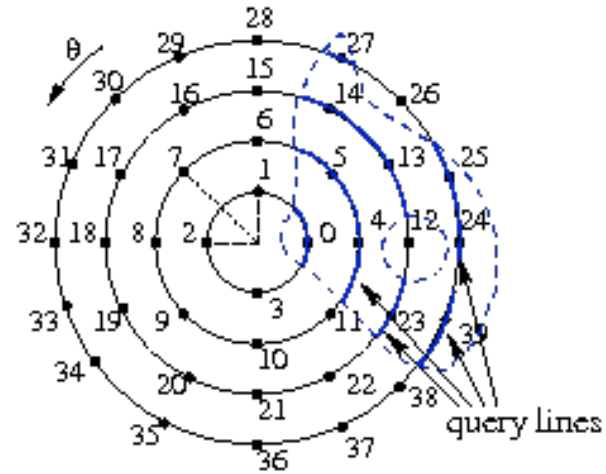
Example: laser wakefield accelerator simulation

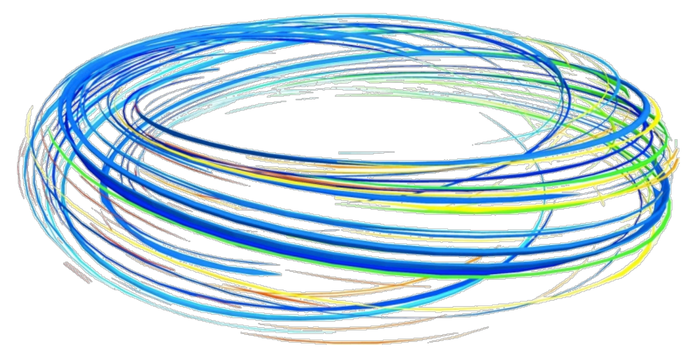
- VORPAL produces 2D and 3D simulations of particles in laser wakefield
- Finding and tracking particles with large momentum is key to design the accelerator
- Brute-force algorithm is quadratic (taking 5 minutes on 0.5 mil particles), FastBit time is linear in the number of results (takes 0.3 s, 1000 X speedup)



FastBit adaptation to toroidal meshes

- Extended FastBit indexing capability to search for regions of interest defined on toroidal meshes used for fusion simulations
- Developed algorithms to take full advantages of the regularity present in the magnetic coordinates but not in the Cartesian coordinates
- Much more compact than the general connectivity graph: ~ 200 numbers vs. 6 million numbers
- Labeling query lines using magnetic coordinates is 600-1000 x faster than using connectivity graph
- Developed new Connected Component Labeling algorithm
  - Recently used in Atmospheric Rivers project





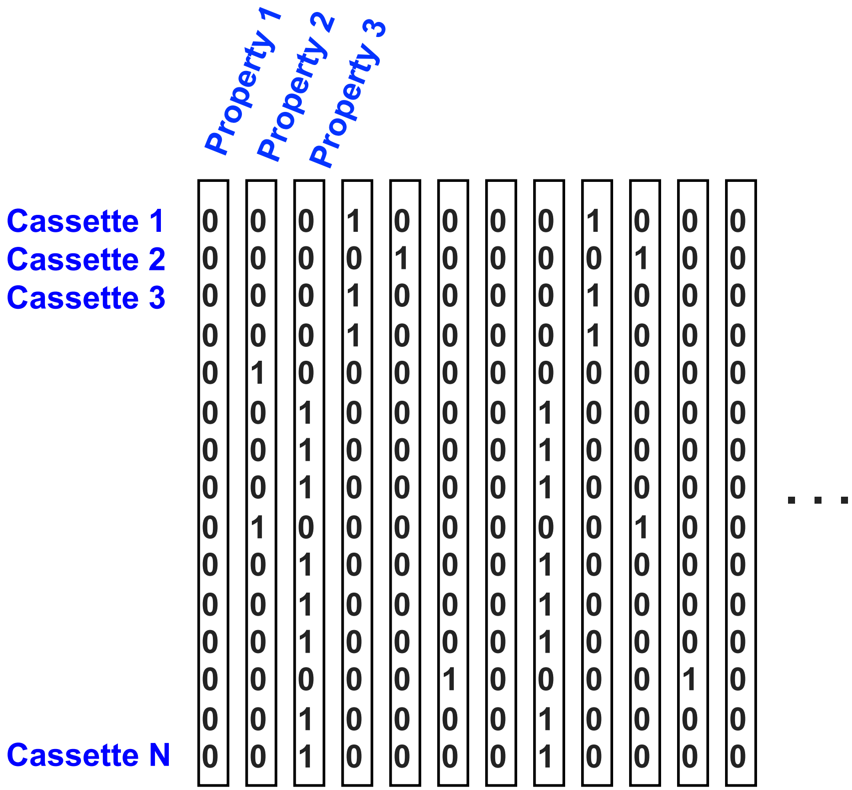
Adapting to cassette searches

Results: (1) given a cassette, search all cassettes with the same properties

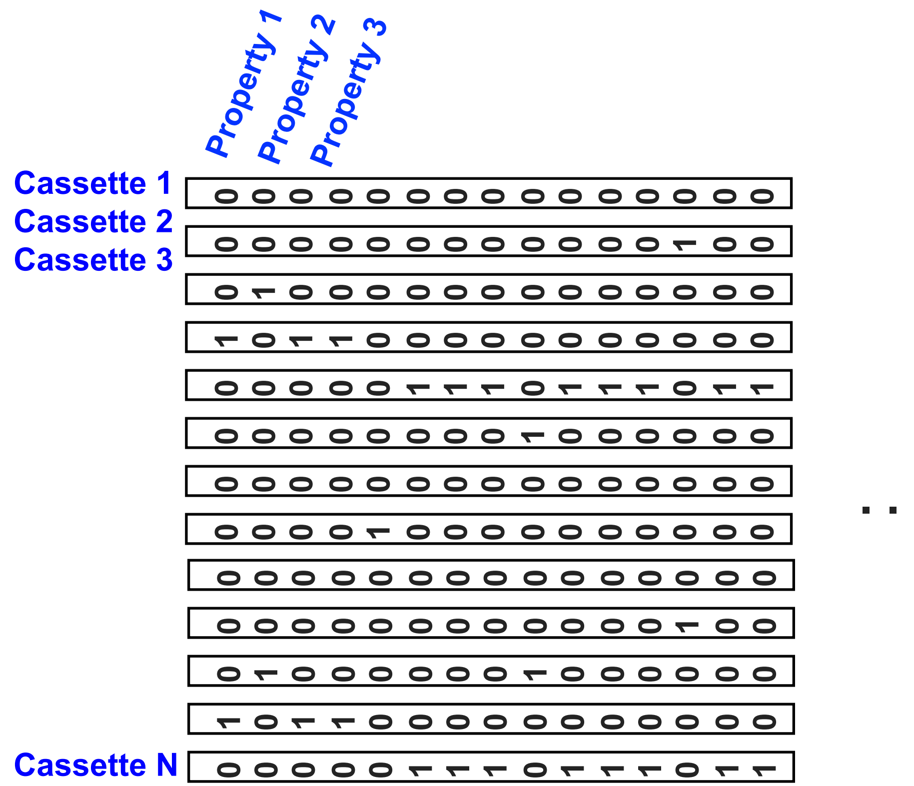
Done in about 0.07 second (using vertical bitmaps)

(2) Find similar cassettes with 2 or more properties

Done in about 10-15 seconds (using horizontal bitmaps)

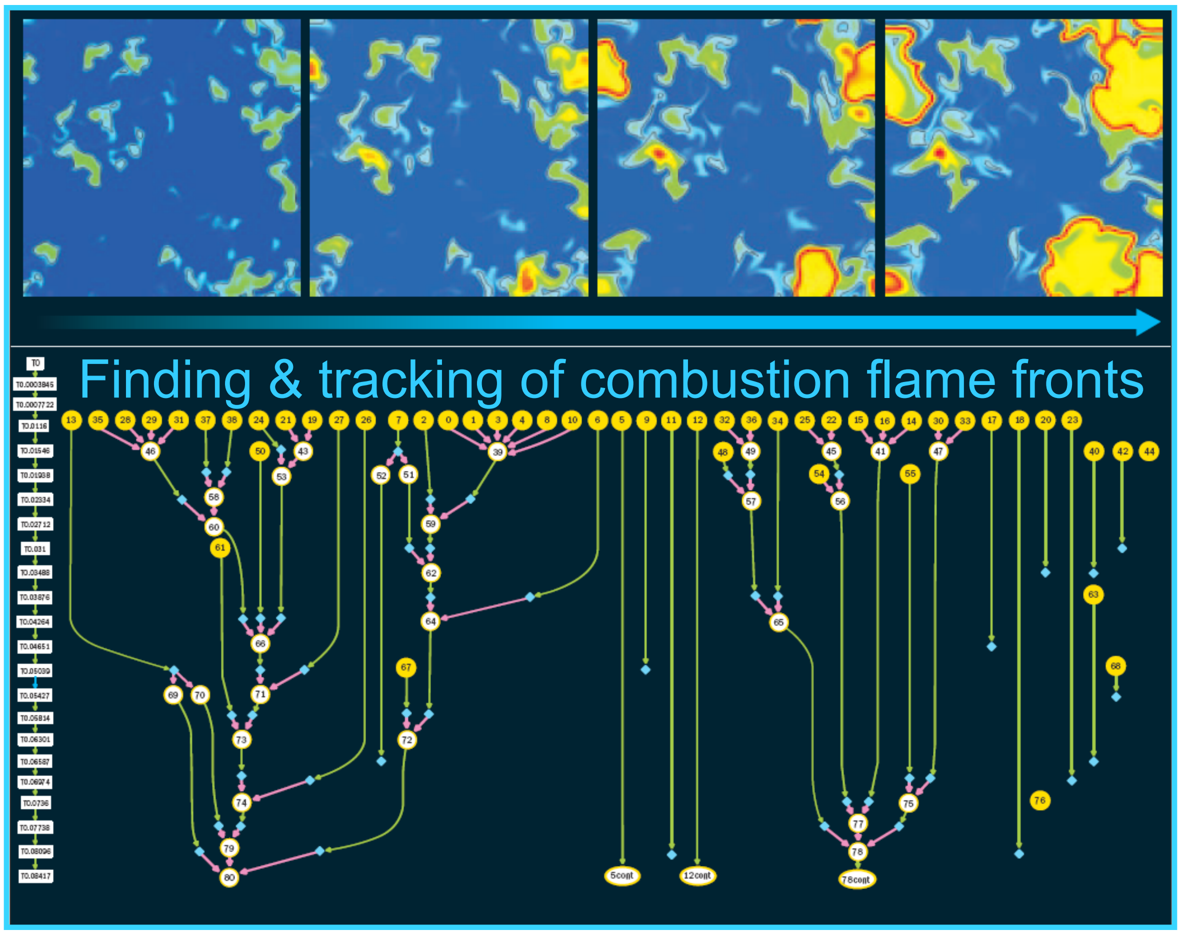


Vertical Organization



Horizontal Organization

Flame Front Tracking in Combustion



Challenges

✧**Cell identification**

✧Identify all cells that satisfy range conditions

✧**Region growing**

✧Connect neighboring cells into regions

✧**Region tracking**

✧Track the evolution of the features through time

Big Data Indexing Requirements: Bitmap indexing advantage

- Speed of search
  - Search over billions – trillions data values in seconds
    - Yes, with compute-friendly compression
- Multi-variable queries
  - Be efficient for combining results from individual variable search results
    - Yes, combining results for each variable as bitmaps is very efficient
- Size of index
  - Index size should be a fraction of original data
    - Yes, compression of bitmap index is essential
- Granularity
  - Ability to produce smaller indexes when granularity can be reduced, such as 2 decimal points, for example
    - Yes, binning over multiple values proved very effective
- Parallelism
  - Should be easily partitioned into sections for parallel processing
    - Yes, if compressed bitmaps can be easily combined (WAH has this property)
- Speed of index generation
  - For in situ processing, index should be built at the rate of data generation
    - OK for billions of values, but a trillion value index took 10 minutes (still a challenge)

Architectural Changes that Could Benefit in situ indexing

- NVRAM on each node
  - Can be used to build partial indexes over multiple time steps
  - Can be used to accelerate in-situ index generation
- Take advantage of GPUs
  - Assign index generation for each variable to separate GPUs
- NVRAM between machine and storage system
  - Can be used for generating indexing for post-processing while data is streaming out to be stored on disk

THANKS!

Co-authors:

E. W. Bethel, S. Byna, J. Chou, W. S. Daughton, M. Howison, H. Karimabadi, K.-J. Hsu, K.-W. Lin, V. Markowitz, K. Mavrommatis, Prabhat, A. Romosan, V. Roytershteynz, O. Rübel, A. Shoshani, A. Uselton

FastBit software http://sdm.lbl.gov/fastbit/

FastQuery software http://goo.gl/iBw6V

Scientific Data Management group http://sdm.lbl.gov/