What to do with Scientific Data?

by

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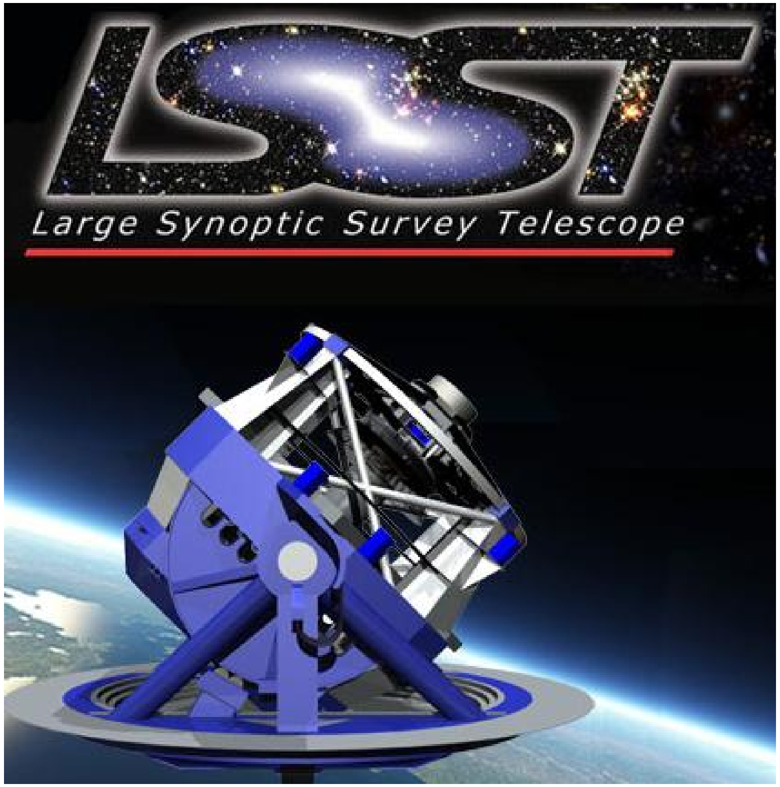
Outline

- Science data – what it looks like
- Hardware options for deployment
- Software options
  - RDBMS
  - Wrappers on RDBMS
  - SciDB



O(100) petabytes

Courtesy of LSST. Used with permission.

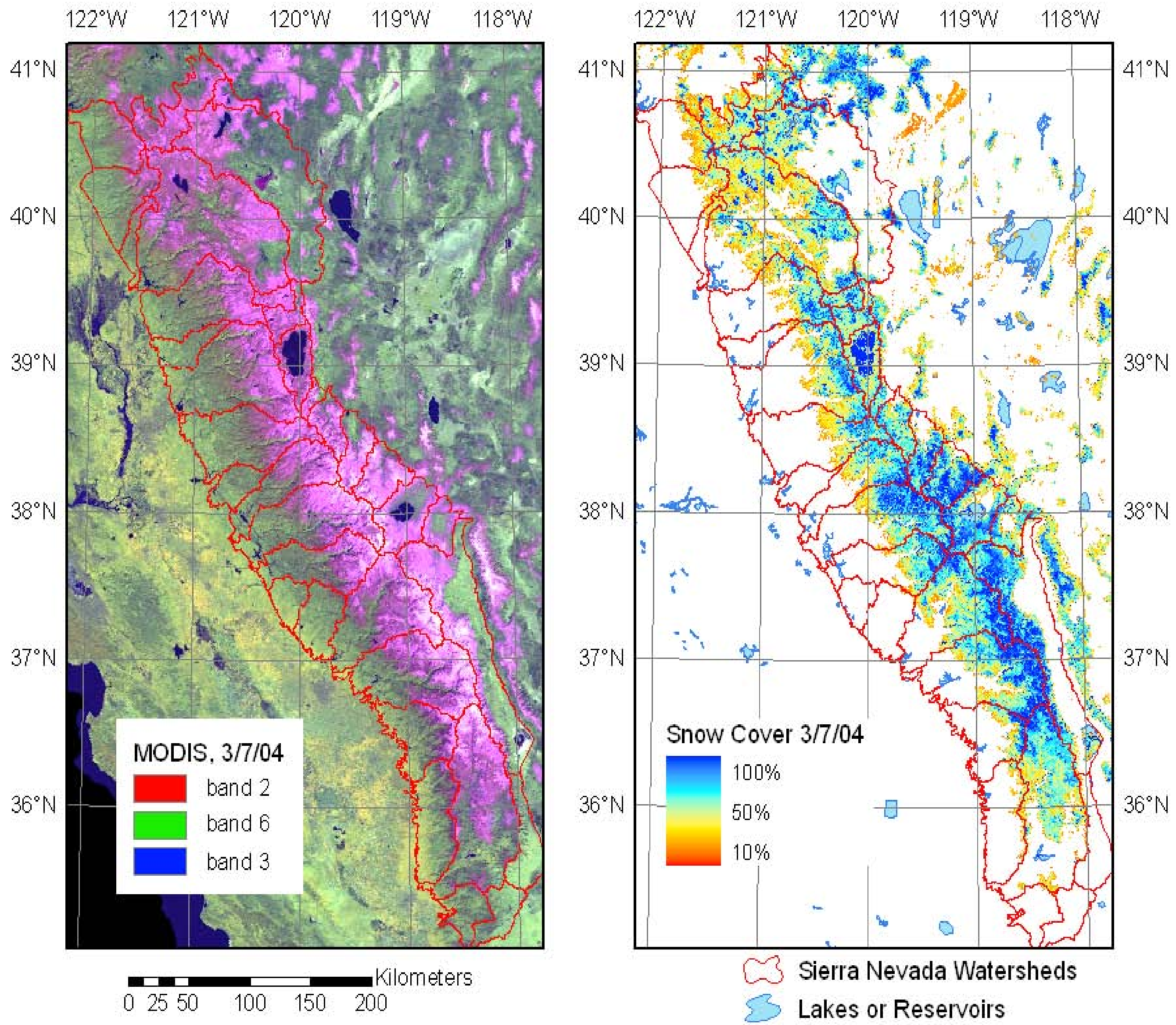
LSST Data

- Raw imagery
  - 2-D arrays of telescope readings
- "Cooked" into observations
  - Image intensity algorithm (data clustering)
  - Spatial data
- Further cooked into "trajectories"
  - Similarity query
  - Constrained by maximum distance

Example LSST Queries

- Recook raw imagery with my algorithm
- Find all observations in a spatial region
- Find all trajectories that intersect a cylinder in time

Snow Cover in the Sierras



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Satellite Imagery

- Raw data
  - Array of pixels precessing around the earth
  - Spherical co-ordinates
- Cooked into images
  - Typically “best” pixel over a time window
  - i.e. image is a composite of several passes
- Further cooked into various other things
  - E.g. polygons of constant snow cover

Example Queries

- Recook raw data
  - Using a different composition algorithm
- Retrieve cooked imagery in a time cylinder
- Retrieve imagery which is changing at a large rate

Chemical Plant Data

- Plant is a directed graph of plumbing
- Sensors at various places (1/sec observations)
- Directed graph of time series
- To optimize output plant runs “near the edge”
- And fails every once in a while – down for a week

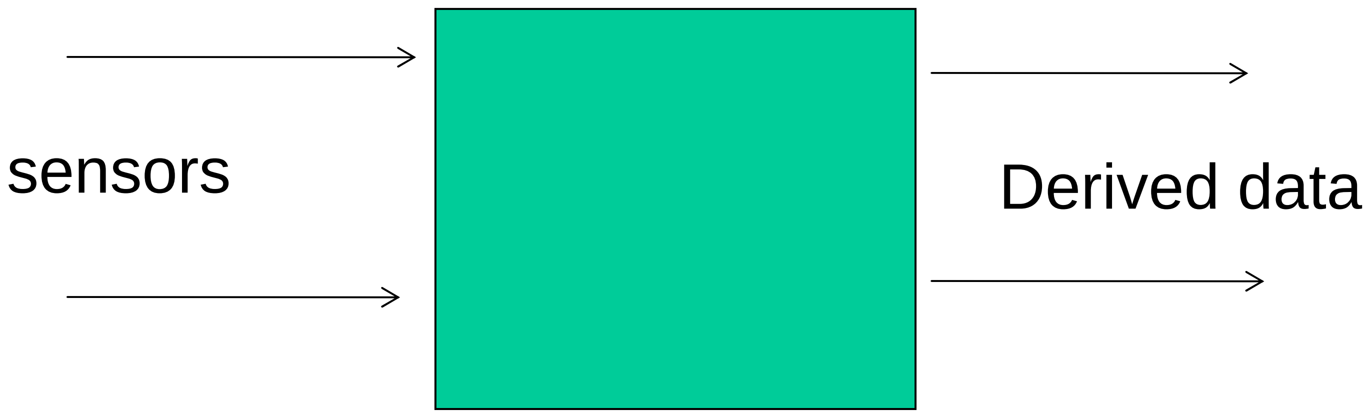
Chemical Plant Data

- Record all data

{(time, sensor-1, … sensor-5000)}

- Look for “interesting events – i.e. sensor values out of whack”
- Cluster events near each other in 5000 dimension space
- Idea is to identify “near-failure modes”

General Model



Cooking
Algorithm(s)
(pipeline)

Traditional Wisdom

- Cooking pipeline outside DBMS
- Derived data loaded into DBMS for subsequent querying

Problems with This Approach

- Easy to lose track of the raw data
- Cannot query the raw data
- Recooking is painful in application logic – might be easier in a DBMS (stay tuned)
- Provenance (meta data about the data) is often not captured
  - E.g. cooking parameters
  - E.g. sensor calibration

My preference

- Load the raw data into a DBMS
- Cooking pipeline is a collection of user-defined functions (DBMS extensions)
- Activated by triggers or a workflow management system
- ALL data captured in a common system!!!

Deployment Options

- Supercomputer/mainframe
- Individual project "silos"
- Internal grid (cloud behind the firewall)
- External cloud (e.g. Amazon EC20

Deployment Options

- Supercomputer/main frame
  - ($$$$)
- Individual project “silos”
  - Probably what you do now….
  - Every silo has a system administrator and a DBA (expensive)
  - Generally results in poor sharing of data

Deployment Options

- Internal grid (cloud behind the firewall)
  - Mimic what Google/Amazon/Yahoo/et.al do
  - Other report huge savings in DBA/SE costs
  - Does not require you buy VMware
  - Requires a software stack that can enforce service guarantees

Deployment Options

- External cloud (e.g. EC2)
  - Amazon can “stand up” a node wildly cheaper than Exxon – economies of scale from 10K nodes to 500K nodes
  - Security/company policy issues will be an issue
  - Amazon pricing will be an issue
  - Likely to be the cheapest in the long run

What DBMS to Use?

- RDBMS (e.g. Oracle)
  - Pretty hopeless on raw data
    - Simulating arrays on top of tables likely to cost a factor of 10-100
  - Not pretty on time series data
    - Find me a sensor reading whose average value over the last 3 days is within 1% of the average value over the adjoining 5 sensors

What DBMS to Use?

- RDBMS (e.g. Oracle)
  - Spatial data may (or may not) be ok
    - Cylinder queries will probably not work well
    - 2-D rectangular regions will probably be ok
  - Look carefully at spatial indexing support (usually R-trees)

RDBMS Summary

- Wrong data model
  - Arrays not tables
- Wrong operations
  - Regrid not join
- Missing features
  - Versions, no-overwrite, provenance, support for uncertain data, …

But your mileage may vary……

- SQLServer working well for Sloan Skyserver data base
- See paper in CIDR 2009 by Jose Blakeley

How to Do Analytics (e.g.clustering)

- Suck out the data
- Convert to array format
- Pass to MatLab, R, SAS, …
- Compute
- Return answer to DBMS

Bad News

- Painful
- Slow
- Many analysis platforms are main memory only

RDBMS Summary

- Issues not likely to get fixed any time soon
  - Science is small compared to business data processing

Wrapper on Top of RDBMS -- MonetDB

- Arrays simulated on top of tables
- Layer above RDBMS will replace SQL with something friendlier to science
- But will not fix performance problems!!

Bandaid solution……

RasDaMan Solution

- An array is a blob
  - or array is cut into chunks and stored as a collection of blobs
- Array DBMS is in user-code outside DBMS
  - Uses RDBMS as a reliable (but slow) file system
  - Grid support looks especially slow

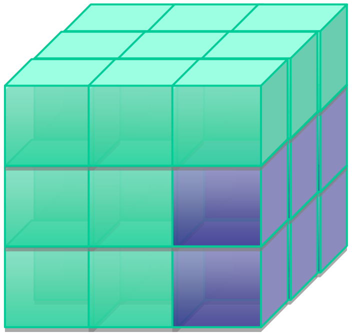
My Proposal -- SciDB

- **Build a commercial-quality array DBMS from the ground up.**

SciDB Data Model

- Nested multidimensional arrays
  - Augmented with co-ordinate systems (floating point dimensions)
  - Ragged arrays
- Array values are a tuple of values and arrays

Data Storage



- Optimized for both dense and sparse array data
  - Different data storage, compression, and access
- Arrays are "chunked" (in multiple dimensions)
- Chunks are partitioned across a collection of nodes
- Chunks have 'overlap' to support neighborhood operations
- Replication provides efficiency and back-up
- Fast access to data sliced along any dimension
  - Without materialized views

SciDB DDL

```
CREATE ARRAY Test_Array
    < A: integer NULLS,
      B: double,
      C: USER_DEFINED_TYPE >
     [I=0:99999,1000, 10, J=0:99999,1000, 10 ]
     PARTITION OVER ( Node1, Node2, Node3 )
     USING block_cyclic();
```

attribute names	index names	chunk size	overlap
A, B, C	I, J	1000	10

Array Query Language (AQL)

- Array data management (e.g. filter, aggregate, join, etc.)
- Stat operations (multiply, QR factor, etc.)
  - Parallel, disk-oriented
- User-defined operators (Postgres-style)
- Interface to external stat packages (e.g. R)

Array Query Language (AQL)

```
SELECT Geo-Mean ( T.B )
FROM Test_Array T
WHERE
  T.I BETWEEN :C1 AND :C2
AND T.J BETWEEN :C3 AND :C4
AND T.A = 10
GROUP BY T.I;
```

User-defined aggregate on an attribute B in array T

Subsample

Filter

Group-by

So far as SELECT / FROM / WHERE / GROUP BY queries are concerned, there is little logical difference between AQL and SQL

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Matrix Multiply

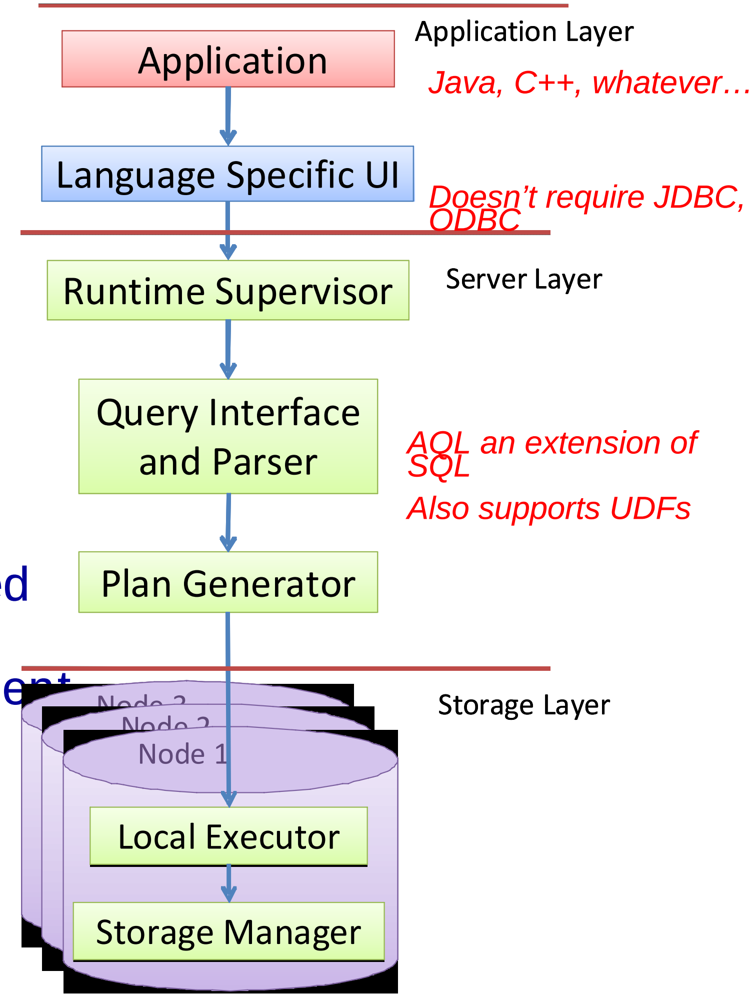
```
CREATE ARRAY TS_Data < A1:int32, B1:double >
                        [ I=0:99999,1000,0, J=0:3999,100,0 ]

Select  multiply (TS_data.A1, test_array.B)
```

- Smaller of the two arrays is replicated at all nodes
  - Scatter-gather
- Each node does its “core” of the bigger array with the replicated smaller one
- Produces a distributed answer

Architecture

- Shared nothing cluster
  - 10’s–1000’s of nodes
  - Commodity hardware
  - TCP/IP between nodes
  - Linear scale-up
- Each node has a processor and storage
- Queries refer to arrays as if not distributed
- Query planner optimizes queries for efficient data access & processing
- Query plan runs on a node’s local executor&storage manager
- Runtime supervisor coordinates execution



Other Features Which Science Guys Want (These could be in RDBMS, but Aren't)

- **Uncertainty**
  - **Data has error bars**
  - **Which must be carried along in the computation (interval arithmetic)**

Other Features

- **Time travel**
  - **Don’t fix errors by overwrite**
  - **I.e. keep all of the data**
- **Named versions**
  - **Recalibration usually handled this way**

Other Features

- Provenance (lineage)
  - What calibration generated the data
  - What was the “cooking” algorithm
  - In general – repeatability of data derivation