# An Introduction to Databases

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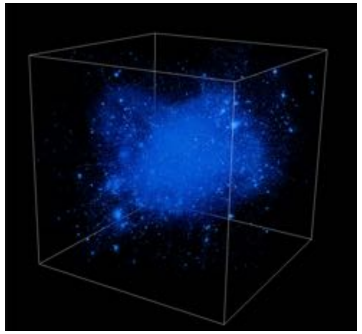
# A Brief History of Science

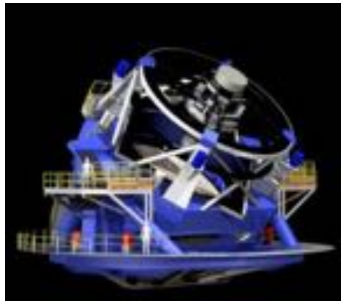
**THOUSAND YEARS AGO**
science was empirical
describing natural phenomena

$$\left(\frac{\dot{a}}{a}\right)^2 = \frac{4\pi G\rho}{3} - \mathrm{K}\frac{c^2}{a^2}$$

**LAST FEW HUNDRED YEARS**
theoretical branch using models, generalizations

**LAST FEW DECADES**
computational branch simulating complex phenonmena





**TODAY**
data intensive science synthesizing experiment and computation with statistics ▶ *new way of thinking required!*

(*Courtesy*: A. Szalay)

# The Scope of the Problem

In 2000, before the Sloan Digital Sky Survey started collecting data, astronomers had photometric data for

**~ 200,000 galaxies**

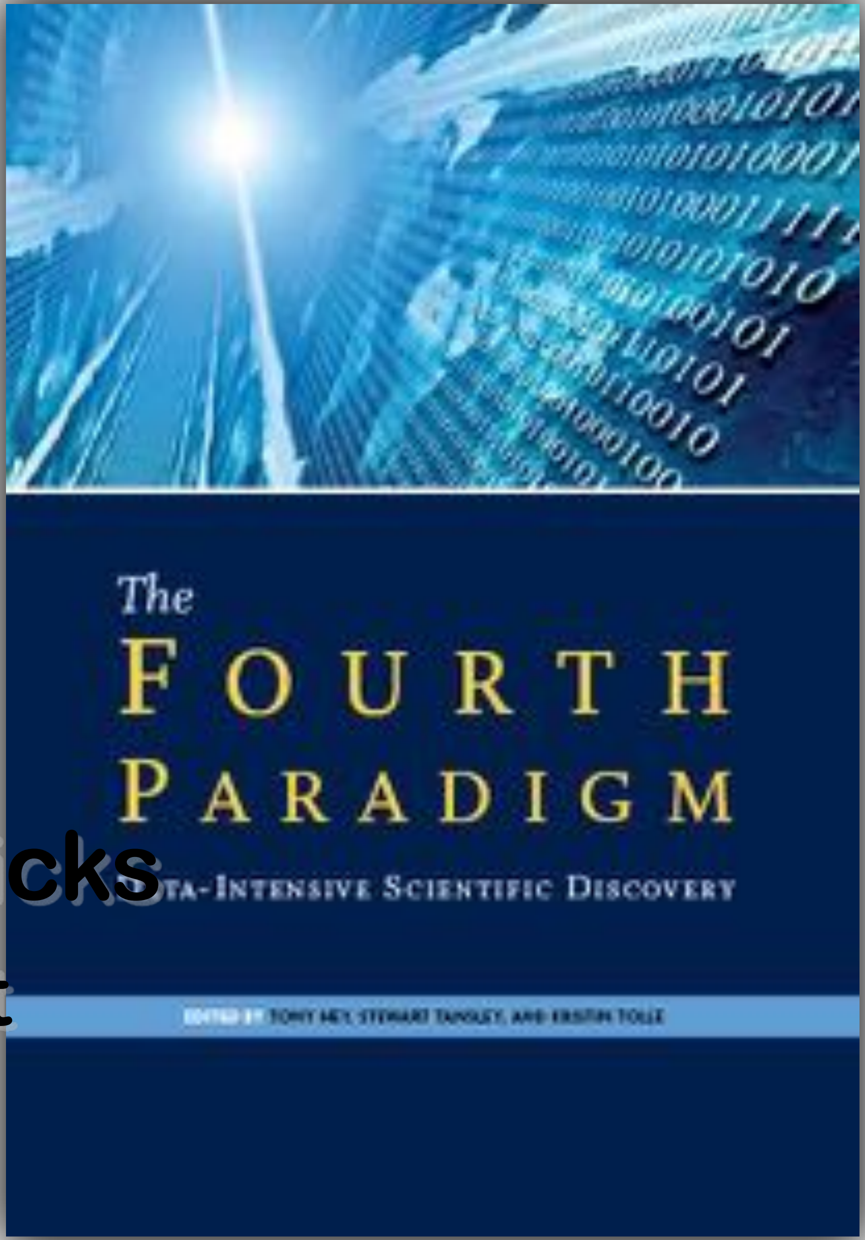
By 2005, SDSS-I had collected photometric data for

**> 200,000,000 galaxies**

**A thousand-fold increase over 5 years!**

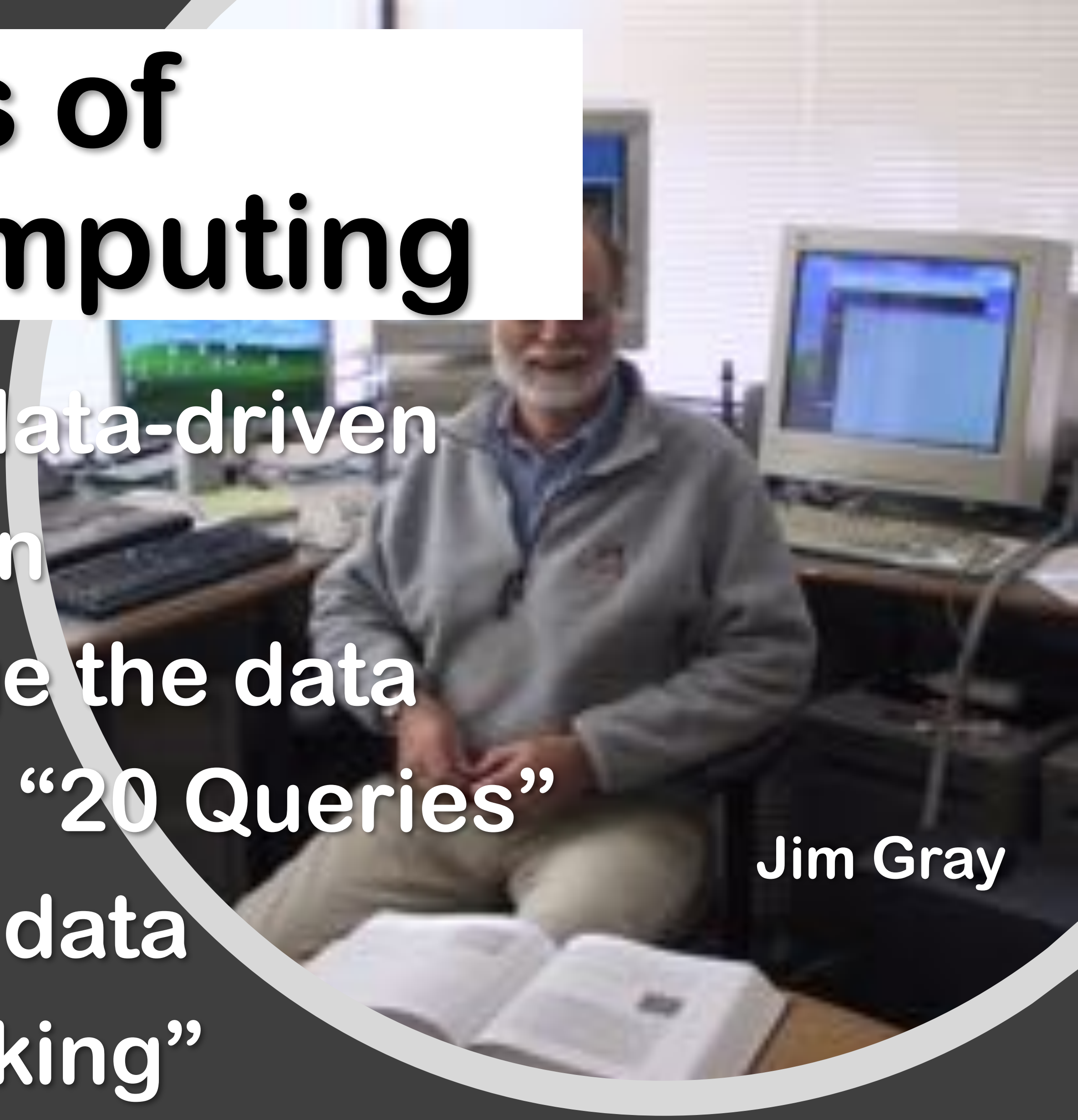
# eScience

- X-Info in addition to Comp-X
  - BioInformatics, Comp. Biology
  - AstroInformatics, Comp. Astro.
- Data retrieval hits the wall
- Scientists need to learn new tricks
  - Can’t download data to the client
  - Can’t reduce data on your own



# Gray's Laws of Data-centric Computing

- Science is increasingly data-driven
- "Scale out" is the solution
- Use databases to manage the data
- Start the design with the "20 Queries"
- Bring the analysis to the data
- Go from "working to working"



Jim Gray

# Original 20 Queries for SDSS

1. Find all galaxies without unsaturated pixels within 1 arcsecond of a given point in the sky (right ascension and declination).
2. Find all galaxies with blue surface brightness between and 30 and 40, and -10<super galactic latitude (sgb) <10, and declination less than zero.
3. Find all galaxies brighter than magnitude 22, where the local extinction is >0.75.
4. Find galaxies with a surface brightness greater than 24 with a major axis 30"<d<1', in the red-band, and with an ellipticity>0.5.
5. Find all galaxies with a deVaucouleours profile (r^< falloff of intensity on disk) and the photometric colors consis-tent with an elliptical galaxy.
6. Find galaxies that are blended with a star, output the deblended magnitudes.
7. Provide a list of star-like objects that are 1% rare for the 5-color attributes.
8. Find all objects with spectra unclassified.
9. Find quasars with a line width >2000 km/s and 2.5<redshift<2.7.
10. Find galaxies with spectra that have an equivalent width in Ha >40A (Ha is the main hydrogen spectral line.)
11. Find all elliptical galaxies with spectra that have an anomalous emission line.
12. Create a gridded count of galaxies with u-g>1 and r<21.5 over 60<declination<70, and 200<right ascen-sion<210, on a grid of 2', and create a map of masks over the same grid.
13. Create a count of galaxies for each of the HTM trian-gles (hierarchal triangular mesh) which satisfy a certain color cut, like 0.7u-0.5g-0.2and i-magr<1.25 and r-mag<21.75.
14. Provide a list of stars with multiple epoch measure-ments, which have light variations >0.1 magnitude.
15. Provide a list of moving objects consistent with an asteroid.
16. Find all star-like objects within DetaMagnitde of 0.2 of the colors of a quasar at 5.5<redshift<6.5.
17. Find binary stars where at least one of them has the colors of a white dwarf.
18. Find all objects within 1' of one another other that have very similar colors: that is with the color ratios u-g, g-r, r-I are less than 0.05m. (Magnitudes are logarithms so these are ratios.)
19. Find quasars with a broad absorption line in their spectra and at least one galaxy within 10". Return both the quasars and the galaxies.
20. For a galaxy in the BCG data set (brightest color gal-axy), in 160<right ascension<170, 25<declination<35, give a count of galaxies within 30" which have a photoz within 0.05 of the BCG.

# 20 Queries for WFIRST Archive

## (Galaxy Formation & Evolution as provided by EXPO SIT)

1. What are the abundances of bright galaxies and quasars at $z>6$?
2. How does the intergalactic medium affect the Lyman-alpha lines of galaxies during the reionization?
3. How does the spatial distribution of bright galaxies correspond to the structure of ionized regions (as measured by, e.g., the spin-flip transition of neutral hydrogen) during reionization?
4. How does the NII/Hα line ratio in galaxies evolve with z?
5. How does the NII/Hα line ratio correlate with stellar mass?
6. How does the NII/Hα a line ratio depend on env. density?
7. How does the Hα line strength-inferred star formation rate depend on environmental density?
8. How does the Balmer decrement (Hα vs. Hβ line strengths, relative to the theoretical expectation) depend on galaxy mass or environment at $z\sim2$ (where both lines fall on the WFIRST grism)?
9. How does the width of the star-forming galaxy main sequence depend on redshift?
10. How do the morphological properties of galaxies at fixed stellar mass depend on environmental density?
11. How do the near-IR colors of galaxies at fixed stellar mass depend on environmental density?
12. How does the weak-lensing estimate dark matter halo mass for galaxies compare with the halo mass inferred from spatial clustering at fixed stellar mass?
13. How does the inferred SNIa rate in host galaxies depend on stellar mass?
14. How does the inferred SNIa rate in host galaxies depend on stellar age?
15. What are the typical host galaxies of Pair Instability or Pulsation Pair Instability supernovae, if they are discovered by WFIRST?
16. What is the evolution in the faint-end slope of the galaxy luminosity function at redshifts $z>7$?
17. What is the evolution in the faint-end of the quasar luminosity function at redshifts $z>6$?
18. What is the typical dark matter halo mass that hosts luminous quasars, and how does this evolve with redshift?
19. What is the abundance and mass-spectrum of dark matter substructure in lens halos discovered through galaxy-galaxy gravitational lensing?
20. How do star-forming galaxies at $z\sim1.8$, where Hα, Hβ , NII, and OII can all be measured by the WFIRST grism, populate the line excitation (“BPT”) diagram?

*(Courtesy*: A. Szalay)

# Why Databases?

## Searchability and Performance

- Ask a data question and get an answer in a reasonable amount of time (mins vs hrs)
- Performance irrespective of size and complexity
- Nothing filters and returns the *minimum* amount of data quite like a database

## Data Integrity and Security

- Self-consistency of data relationships
- Handle concurrency (transaction model)
- Avoid data loss and corruption
- Insulated from Web and application layers

# What is a database?

- Colloquially, “database” means
  – Any sizable store of valuable information
- Formally, “database” is short-hand for
  – A DataBase Management System (DBMS)
- DBMS components include
  – The actual bits: the storage engine
  – The Query Engine (incl. optimizer)
  – The performance and admin tools
  – The UI

# Database Features

- Data and metadata
    - Co-located, self-consistent and queryable
- Built-in indexing for performance
- Data curation and management
    - Backup and recovery tools
        - Full and differential backups
    - Performance tuning tools

| OODBMS (Object Oriented DBMS) | RDBMS (Relational DBMS) |
| --- | --- |
| • Container based distributed architecture<br>• Objects map to real world<br>• Object Query Language (OQL)<br>• Much less market share | • Table-based architecture<br>• Relationships between table entities<br>• Transaction model for concurrent updates<br>• By far the most commonly used DBMS |

# Database Technologies

# RDBMS technology

- Millions of man-hours of development
- Based on mathematical theory (set theory)
- Technology tested in real life critical applications for decades now
  - May be a blunt instrument at times
  - But utterly reliable and mature
- Built on transaction model
  - Originally formulated by Jim Gray et al.
  - Entire banking industry relies on it

# Relational Databases

## Everything is a table

## Entity-Relationship Diagrams

## Relationships between table columns

- One-many, many-one, many-many
- Unique and non-unique
- Primary keys (PKs) and foreign keys (FKs)

## Indexing for performance

- Clustered indices
- Non-clustered indices

# Database Systems

- RDBMS
  - MySQL, PostgreSQL (open source)
  - SQL Server, DB2, Oracle (commercial)
- OODBMS
  - Objectivity, Versant
- MonetDB (column store)
- SciDB (MIT, under development)
- Many others …

# Discussion

- What are the most popular DBMS platforms today?
  – Which ones have you used of or are familiar with?
- What functionality is available for free?
  – What do you have to pay for?

# Notable among the “others”

- Google BigTable
  - Well suited to the online search data that Google manages
    - Unstructured for the most part
    - One of the application spaces that traditional databases do not map so well to
  - Uses SQL-like BigQuery
    - Latest version of BigQuery supports standard SQL
  - If you’re Google, you can
    - Write your own DBMS
    - Scale out ad infinitum (MapReduce)

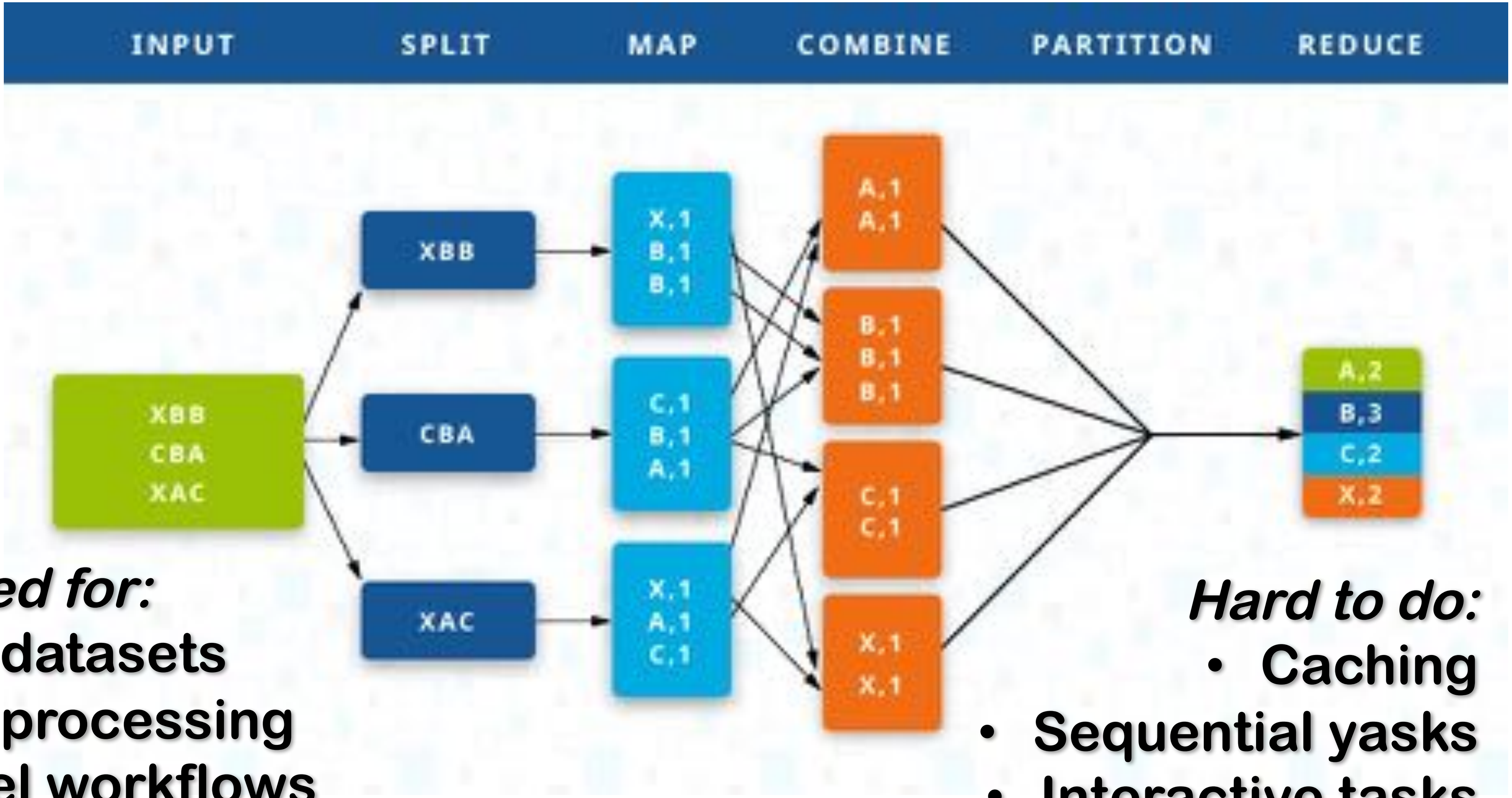
# Free RDBMS Versions

- Microsoft: SQLite, SQL Server Express
- IBM: DB2 Express-C
- Oracle: XE-Express Edition

# Alternatives to Databases

- MapReduce is probably the biggest one out there
  - A programming paradigm for scale-out, originally Google
  - But now most popular implementation is Apache HADOOP
    - MapReduce is at the heart of HADOOP, open-source
    - Hive for SQL-like querying and analysis
    - Hbase storage/database engine, HDFS file system
  - Other implementations, including Amazon/AWS
- NoSQL (Not only SQL, No SQL?)
  - Seeking simplicity & flexibility
  - Different data structures, not restricted to tables
- Each has its own application space

The devil, as usual, is in the details




*Optimized for:*
- Large datasets
- Batch processing
- Parallel workflows

*Hard to do:*
- Caching
- Sequential yasks
- Interactive tasks

# MapReduce

# NoSQL Platforms

- MongoDB – probably the most prominent one
- Apache
  - Cassandra
  - HBase
- Oracle NoSQL
- Amazon DynamoDB
- Couchbase
- Some technologies pre-dating RDBMS also qualify

# DIscussion

- **Which Big Data technologies are most suitable for LSST-scale astronomy?**
  - **Is this even a well-formulated question?**

# Transactions

- Integral to database consistency and concurrency
- "The" book on OLTP: Jim Gray and Andreas Reuter
- ACID properties
  - Atomicity
  - Consistency
  - Isolation
  - Durability

## Atomicity

All or nothing

All parts of transaction must succeed

Else roll back to previous state

Once you COMMIT a transaction, you cannot roll back

## Isolation

No inference across transactions

Even if they are concurrent

Each transaction proceeds without any interference, as if other concurrent transactions have not been started yet

## Consistency

Data always meets the constraints defined on it

According to validation rules

It will never be in an inconsistent state

See PK and FK constraints (below)

## Durability

Committed transactions guaranteed to survive

Even after power failures and other exceptions

Errors, HD failures etc.

# ACID Properties

# Transaction Logs

- **Every transaction is logged**
  - For rollback, backup and recovery
  - Different logging models
    - E.g., Simple, Bulk, Full
    - Depends on how much protection you want against failures
    - Trade-off is speed and size of logs
    - The more scrupulously you log, the slower the transactions
  - You can control logging ad hoc with the lock level you select (see next slide)

# Locking and Concurrency

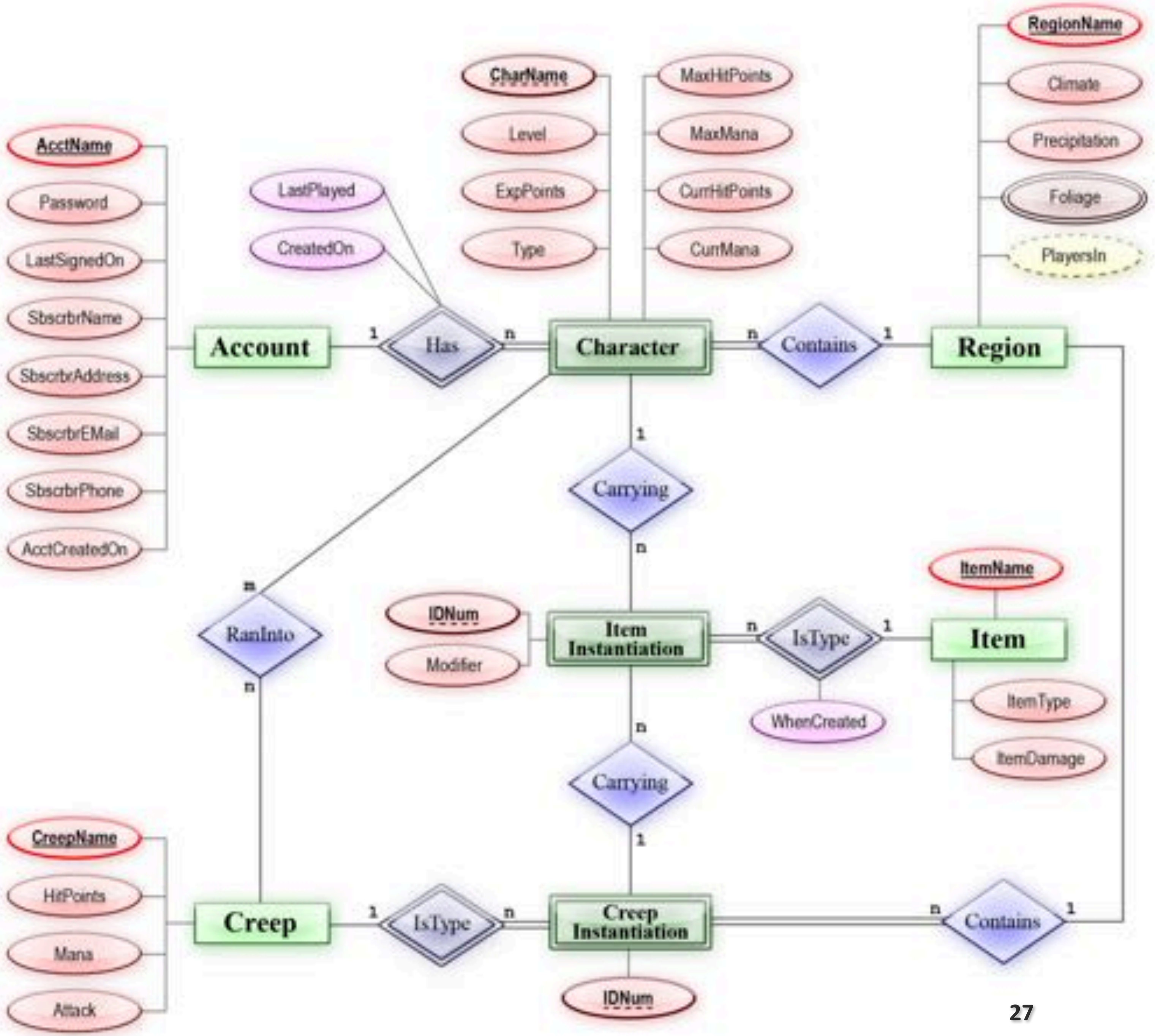
- Every transaction runs in locked mode
  - The data being accessed is locked for duration of transaction
  - Lock can be table, page or row level
  - Higher the granularity, more the logging
    - E.g. TABLE LOCK is least logging (hence fastest) option
- Deadlock
  - When 2 transactions are depending on each other to complete

# Transactions in action

- When you are at the ATM
- Every action you perform is a transaction
- Transaction steps
  - BEGIN transaction
  - COMMIT transaction
  - ROLLBACK transaction
- Ensures integrity of your data (your money!) while millions of concurrent transactions are being performed

# ER Diagrams

- ER diagrams are NOT DB schema diagrams
- They are more general
- They describe the nature of the relationships between entities
- Entities in RDBMSs are represented by tables
- Relationships are represented by keys



# Primary and Foreign Keys

- Every table must have a primary key
  - Even if DBMS does not require it
  - Makes searching faster
  - Unique identifier of a table row
    - Ideally an existing tabel column
- Foreign key defines a relationship
  - Between 2 tables
  - FK must reference PK or unique column in parent table

# PK and FK constraints

- PK constraint is essentially uniqueness
- FK constraint defines one-one or one-many relationship
  - E.g. multiple spectra associated with a single image
- Data integrity and correctness checks
  - Invaluable for checking data validity

# Database Indices

- Clustered (PK) index
  - Index leaf nodes ARE the actual data pages on disk
    - Hence there can only be ONE clustered index per table
    - Data stored on disk in order of PK
    - Hence redoing PK index is a lot of work (reorder data on disk)
- Non-clustered indices
  - Index leaf nodes POINT TO data pages on disk (bookmarks)
  - FK index
    - Fast lookup for linked table, but not created by default
  - Covering index (unique or non-unique)
    - Index defined on a few selected columns for specific query patterns
    - Usually a frequently requested set of columns (e.g. coords, mags)
    - Always includes the PK

# Discussion Items

- Do you think databases are the best option for large astronomical data sets going forward (LSST)?
- What are the one or two things that make them good?
- What are the alternatives?
- What do you think the situation will be 10 years from now?