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Data Formats and Databases

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How will you store your data?

- Binary data is compact but not portable
  - Machine readable only
  - Byte-order issues: big endian (IBM) vs. little endian (Intel)
- Formatted text is portable but not compact
  - Need to know all the details of formatting to read the data
  - 1 byte of ASCII text stores only a single decimal digit (~3 bits)
  - Compression can help, but is slow and often impractical for large files
- Need to consider how data will be used
  - Is portability an issue?
  - Will your favorite analysis tools be able to read the data?
  - Are there storage constraints?

Data Preservation and Discovery

- NSF requires a data management plan with all grant proposals
    - Metadata
    - Formats used
    - Data location
    - Discovery and access plans
    - https://confluence.cornell.edu/display/rdmsgweb/Home

- Large Research Projects
    - Personnel
    - Long time horizons
    - Distant collaborators

- Scientific data formats address some of these issues…

Hierarchical Scientific Data Formats

Data Format	Academic Discipline	Parallel I/O	Software Interfaces	Comments
HDF5	2D and higher dimensional data	yes	C, C++, Fortran, Java, Python, Perl, IDL, Matlab, Mathematica	developed at NCSA
NetCDF	Earth Sciences	yes	C, C++, Fortran, Java, Python, Perl, Ruby, IDL, R, Matlab, ArcGIS	developed at UCAR
FITS	Astrophysics	no	C, C++, Fortran, Java, Python, Perl, IDL, R, Matlab, Mathematica	developed at NASA
Silo	General Visualization	yes	VisIt	developed at LLNL

Scientific Data Formats: HDF5

- Versatile data model that can represent complex data objects and metadata
- Portable file format with no limit on the number or size of data objects
- Open software library that runs on platforms from laptops to massively parallel systems
- Integrated performance features that optimize access time and storage space
- Tools and applications for managing, manipulating, viewing, and analyzing the data in the collection

Source: www.hdfgroup.org/hdf5

HDF5 Features

- *Headers* include extensive metadata (datatypes, dimensionality, storage layout); files are self-documenting
- *Virtual file layer* provides flexible storage and transfer capabilities: Standard (Posix), Parallel, and Network I/O file drivers
- *Compression & chunking* increase access and storage efficiency
- *Datatype transformations* can be performed during I/O operations
- *Subsetting* reduces transferred data volume & improves access speed during I/O operations

Source: www.hdfgroup.org/hdf5

Scientific Data Formats: netCDF

- Similar to HDF5; newest version uses the HDF5 format
- Used extensively in the Earth Sciences community for time varying geospatial data; most data from NOAA is in netCDF format
- NetCDF has good tools for geo-gridded data
  - *Panoply* (http://www.giss.nasa.gov/tools/panoply/) focuses on the presentation of geo-gridded data.
  - *Ferret* (http://ferret.wrc.noaa.gov/Ferret/) offers a Mathematica-like approach to analysis. Variables and expressions may be defined interactively; calculations may be applied over arbitrarily shaped regions; geophysical formatting is built in.
  - *Parallel-NetCDF* (http://trac.mcs.anl.gov/projects/parallel-netcdf/) is built upon MPI-IO to distribute file reads and writes efficiently among multiple processors.

netCDF Features

- *Self-Describing*—files include information about the data they contain
- *Portable*—endian problems handled automatically
- *Direct-access*—subsets of a larger dataset can be accessed without reading through all the preceding data
- *Appendable*—data may be appended to a properly structured netCDF file without copying the dataset or redefining its structure
- *Shareable*—one writer and multiple readers may simultaneously access the same netCDF file
- *Archivable*—netCDF will always be backwards compatible

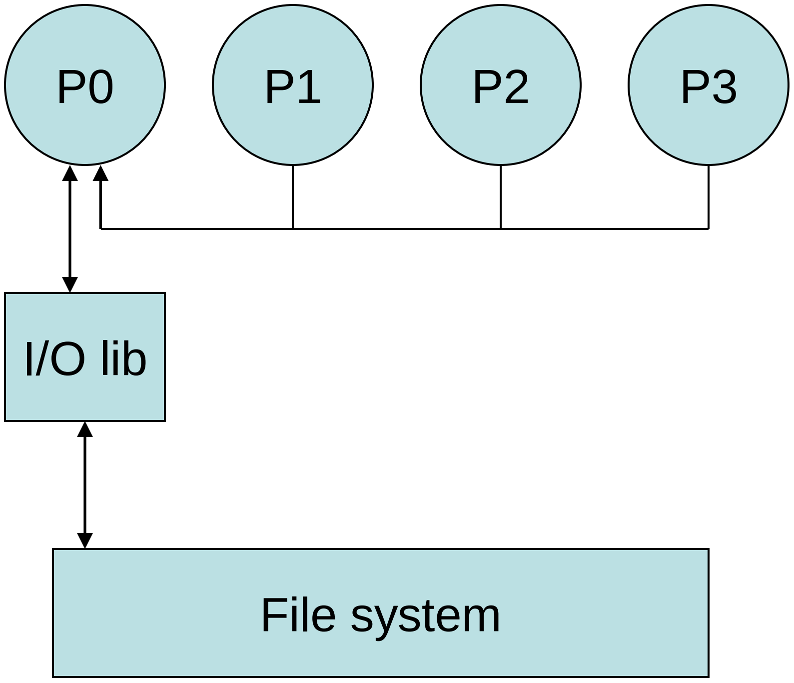
Source: http://www.unidata.ucar.edu/software/netcdf

Scientific Data Formats: Silo

- Silo is a library for reading and writing scientific data to binary disk files
- Silo supports point meshes, structured and unstructured meshes in 2D and 3D
- Two layers
  - API with Fortran, C, and Python interfaces
  - I/O driver (HDF5 is one of these drivers)
- Primary file format for VisIt

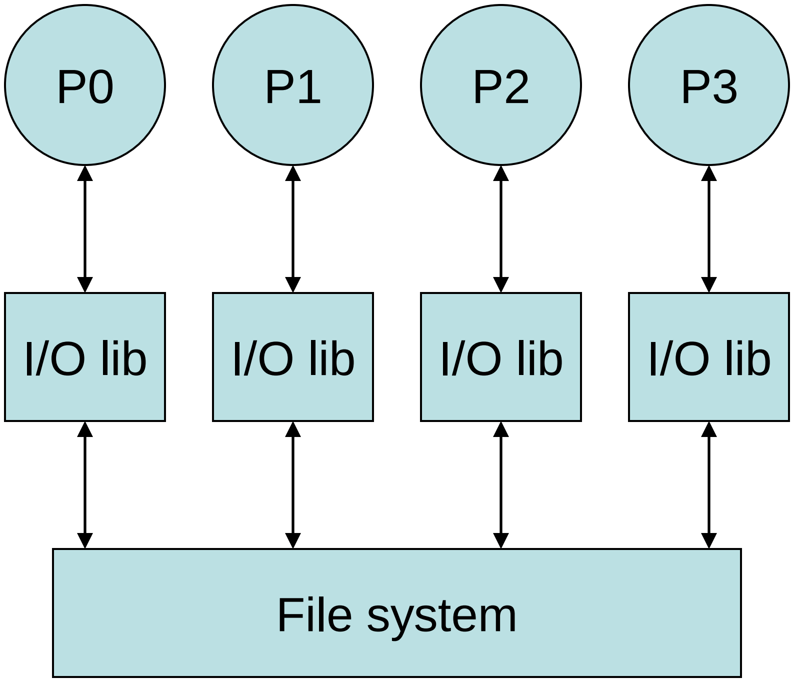
https://wci.llnl.gov/codes/silo/index.html

Why Parallel I/O is important



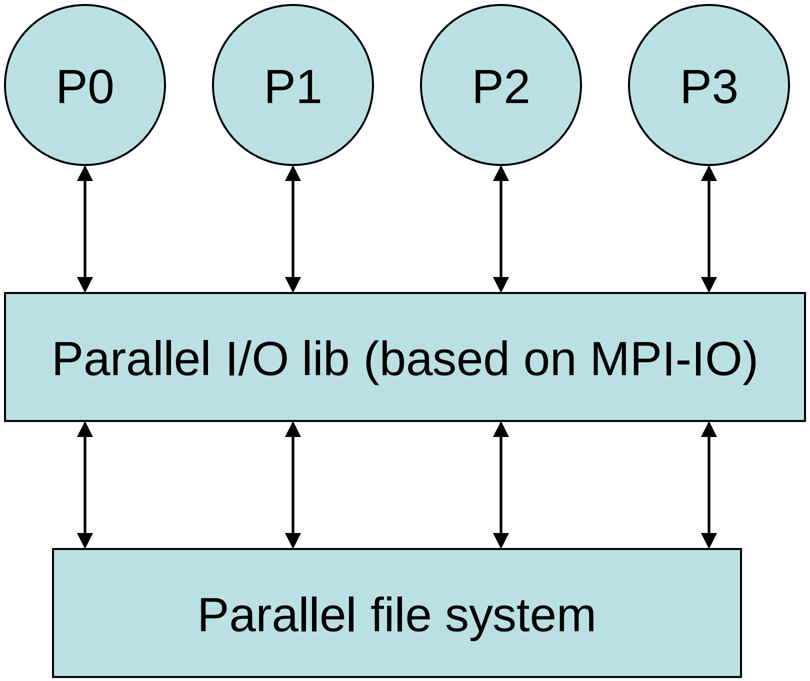
- P0 may become bottleneck
- System memory may be exceeded on P0

Why Parallel I/O is important – part 2



- Possible to achieve good performance
- May require post-processing
- More work for applications, programmers

Why Parallel I/O is important – part 3



- HDF5, netCDF and Silo can take the place of a parallel I/O library - they've linked the parallel I/O library for you
- Variant: only P1 and P2 act as parallel writers; they gather data from P0 and P3 respectively (chunking)

Scientific Data Formats: Scientific Databases

- What is a database?
  - from Wikipedia—an organized collection of data
- When to use a database
  - Data hierarchy more complicated than space/time dimensions
- Database added value
  - Built-in data integrity checks
    - Management of row duplication
    - Enforcement of data ranges and types
  - Enforces planning about the data to be stored
    - Data types (integer, decimal, datetime), scale, precision
    - Missing data (null values)
  - Scalability

Scientific Databases vs. Hierarchical Data Formats

- Academic Disciplines

  All with any kind of hierarchical data

- Parallel I/O

  Available from many commercial vendors and open sources

- Software interfaces to SQL databases

  C, C++, C#, Fortran, Java, Python, Perl, Ruby, IDL, R, Matlab, ArcGIS, Excel

- Advanced query capabilities

  Fine grained ability to extract subsets of the data efficiently

Relational Database Software

- Enterprise-class relational database systems
  - Oracle
  - Microsoft SQL Server
  - MySQL
  - PostgreSQL

- Small, light-weight relational database systems
  - SQLite (C based)
  - SmallSQL (Java based)
  - Apache Derby (Java based)
  - Gadfly (Python based)

Real life example

- A Facebook application that allows people to show their arXiv.org papers on their Facebook profile page
- The application needs to store information about papers so that it can extract these papers based on queries about authors
- Conceptually we have a couple of objects we want to connect:
  - Authors (Facebook ID, arXiv info, etc.)
  - Papers (title, abstract, journal reference, etc.)
- Two approaches to this problem

Approach one – Delimited flat file

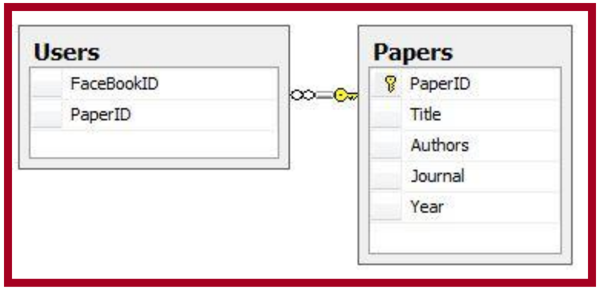
- Add a row to the table for every unique paper an author has written
- Search the table for all rows that have the appropriate ID

Facebook ID	Paper ID	Paper Title	Paper Authors
2341234	http://arxiv.org/abs/5234	Particle Pleasantry	CH Foo
2341234	http://arxiv.org/abs/3234	Reading is neat	CH Foo, RG Fields
1234123	http://arxiv.org/abs/4321	Science in Teaching	DS Henry, RG Fields
1234123	http://arxiv.org/abs/3234	Reading is neat	CH Foo, RG Fields
12341345	http://arxiv.org/abs/4321	Science in Teaching	DS Henry, RG Fields

- Benefits:
  - Easy to add new entries (depending on sorting); harder with more entries
  - Simple to code the read/write functions
- Problems:
  - A row is duplicated for every author of a paper (e.g., *Reading is neat*)
  - To match a given Facebook ID, a linear scan of the entire file is required

Approach two – Relational database

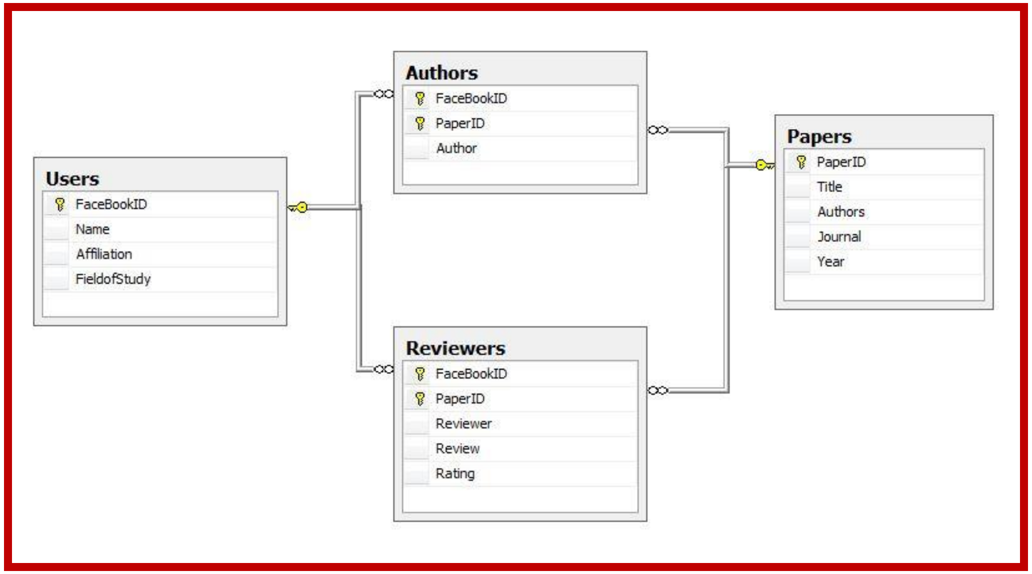
- Define *two* tables
  - Users/Authors table and Papers table
- Link them together by the paperID
  - ***PaperID*** in Papers is a ***Primary Key***; it uniquely identifies a row
  - ***PaperID*** in Users is a ***Foreign Key***; it points to a row in another table



- Benefits
  - Fast retrevial of papers for an author
  - Easy to add fields to the Users and Papers tables
- Problems
  - Database management

More relationships

- We can create relationships that are much more fined-grained
  - Make the Users table more general
  - Create a separate Authors table and a Reviewers table for reviews

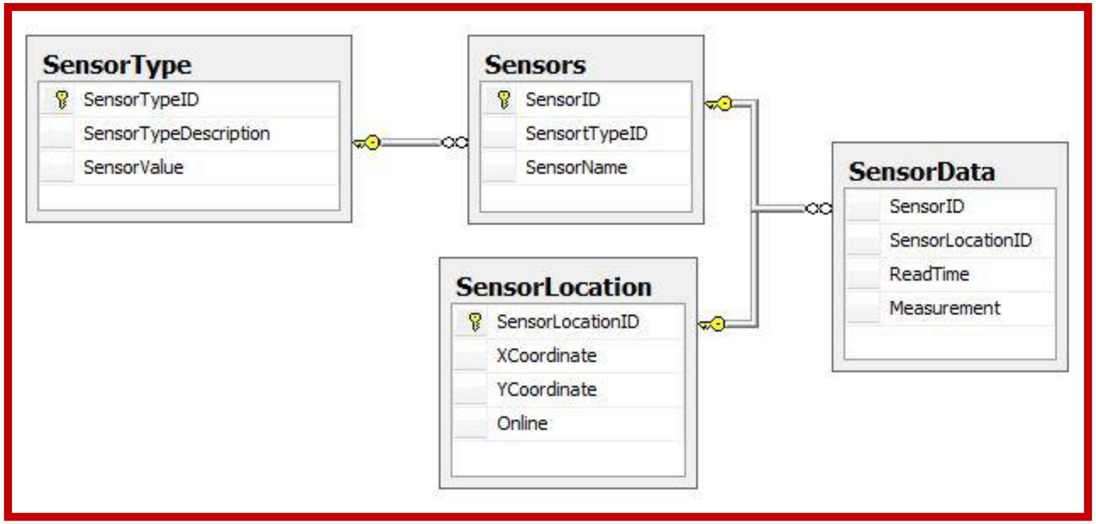


Relational databases

- Relational databases are based on the *relational model*--data is expressed by a set of binary relationships

Flat files would replicate columns of metadata for each row

The replication gets worse when the metadata is hierarchical



Flat file or database?

- Flat files are useful for
  - Small datasets
  - Static dumping of data
- Databases are useful for
  - Evolving data
  - Data where searching/querying is important/complex
  - Expressing relationships that are not captured in a row-based table
- Other factors to consider:
  - Database overhead
  - Expectations about sharing data

Interacting with a database – SQL

- **SQL – Structured Query Language**

  A programming language designed for the creation, management, modification and retrieval of data from a database

  All databases speak SQL, though many also provide non-standard extensions

  Using a database requires a basic knowledge of SQL

  Designing a database requires extensive knowledge of SQL

- **PL/SQL** and **SQL/PSM**

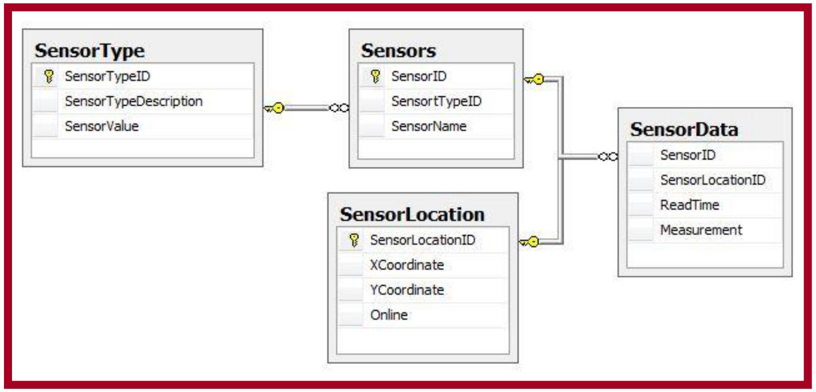
  Database extensions for creating stored procedures

SQL language – Select, Where

Select & Where control what subset of data to obtain from the database

Retrieve sensor locations

```
SELECT XCoordinate, YCoordinate
FROM SensorLocation
```



Retrieve sensor data for a one sensor

```
SELECT * FROM SensorData
WHERE SensorID = 200
```

Retrieve sensor data for a one time period

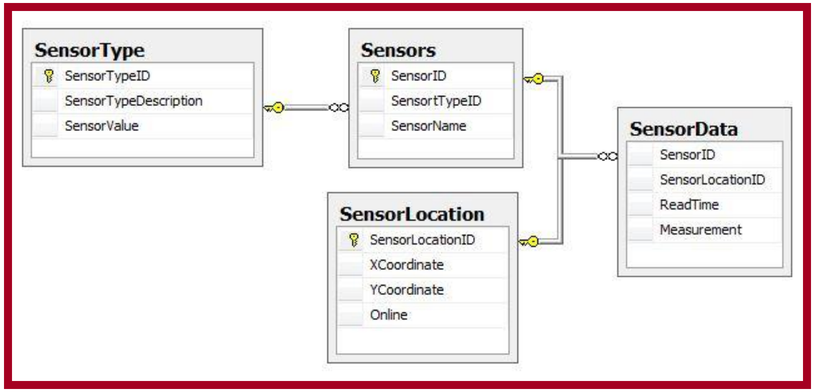
```
SELECT * FROM SensorData
WHERE ReadTime = ‘1/1/2012’
```

SQL language – Join

Use Join to retrieve data from more than one table

Retrieve sensor data with locations

```
SELECT SensorID, ReadTime,
Measurement, Xcoordinate,
YCoordinate
FROM SensorData SD
INNER JOIN SensorLocation SL
ON SD.SensorLocationID =
SL.SensorLocationID
```



Retrieve sensor data with sensor types

```
SELECT SD.SensorID, ReadTime, Measurement, SensorValue
FROM SensorData SD
INNER JOIN Sensors S
ON SD.SensorID = S.SensorsID
INNER JOIN SensorType ST
ON S.SensorTypeID = ST.SensorTypeID
```

SQL language – insert, update, commit

New rows can be inserted and existing rows can be updated

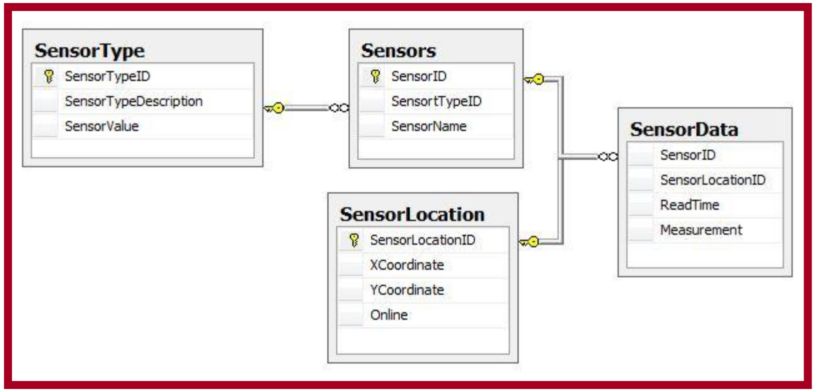
Insert a new sensor

```
INSERT INTO SensorType (SensorTypeID,
SensorTypeDescription, SensorValue)
Values(1001,'Heat Sensor',20)
```

```
INSERT INTO Sensors
Values(89019, 1001, 'Cayuga')
```

Update the sensor data

```
UPDATE Sensors
SET SensorName = 'Cayuga Lake"
WHERE SensorID=89019
```



Commit the transactions

```
COMMIT
```

SQL language – delete, order, etc.

Dropping rows from a table mirrors SELECTing

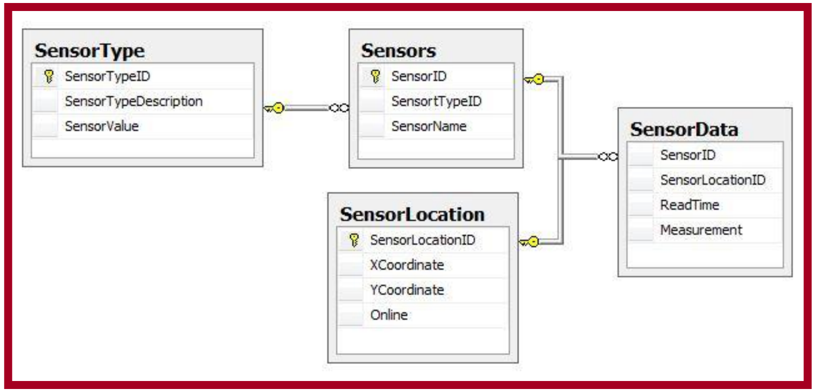
- Delete data for a particular day

```
DELETE FROM SensorData
WHERE ReadTime = ‘1/1/2011’
```

No assumptions can be made about the order that rows are retrieved

- Sort rows by location and within location by time

```
SELECT * FROM SensorData
ORDER BY SensorLocationID, ReadTime
```



Using SQL in application code

- Most programming languages have SQL interfaces which are software modules that provide a connection to the database and a cursor

```
import MySQLdb
conn = MySQLdb.connect(host=“h”, user=“u”, passwd=“p321”, db=“test”)
cursor = conn.cursor()
cursor.execute(“SELECT * FROM SensorData WHERE SensorID = 1234”)
row = cursor.fetchone()
cursor.execute (“SELECT * FROM SensorLocations”)
row = cursor.fetchall()
cursor.close()
conn.close()
```

- Note: Many interfaces have a special executeQuery function which returns an iterable to retrieve rows (res->next())

SQL language assessment

- Benefits:
  - SQL is a relatively simple language
  - Interfaces exist from many programming languages to every type of database; all reasonable databases support SQL; therefore SQL is a ubiquitous choice
  - Lines of code can be drastically reduced by taking advantage of powerful SQL commands for searching and retrieving objects from a database
- Problems:
  - SQL queries can be amazingly inefficient ; there are tools for optimization
  - Another language to learn

Object-relational mapping

- Object-relational mapping (also ORM and O/R mapping) converts data between a database and an object-oriented programming language

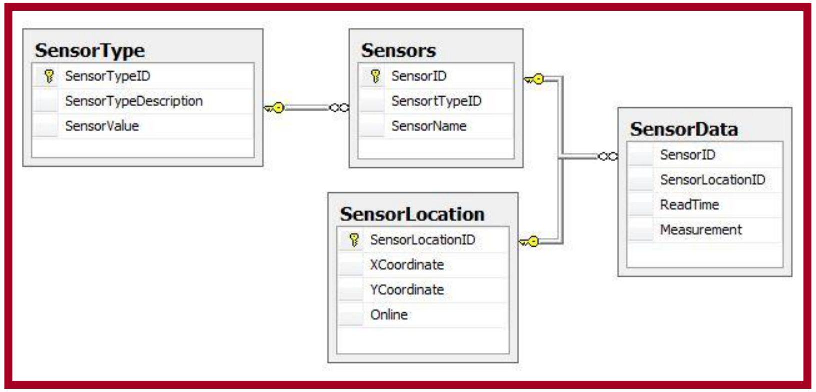
- An ORM tool lets you create and use a database within a standard OO programming paradigm
  - Database tables are created from class definitions
  - SQL queries are basically written for you by the tool

- The ORM tools also allow you direct SQL access where optimized queries are needed

OR mapping

Script to create database tables

```
Begin;
CREATE TABLE 'SensorType' (
    'SensorTypeID'  integer  NOT NULL  PRIMARY KEY,
    'SensorTypeDescription'  varchar(100)  NOT NULL,
    'SensorValue'  integer  NOT NULL);

CREATE TABLE 'Sensors' (
    'SensorID'  integer  NOT NULL  PRIMARY KEY,
    'SensorTypeID'  integer  NOT NULL,
    'SensorName'  varchar(100)  NOT NULL);

CREATE TABLE 'SensorLocation' (
    'SensorLocationID'  integer  NOT NULL  PRIMARY KEY,
    'XCoordinate'  integer  NOT NULL,
    'YCoordinate'  integer  NOT NULL,
    'Online' integer NOT NULL;)

CREATE TABLE 'SensorData' (
    'SensorID'  integer  NOT NULL,
    'SensorLocationID'  integer  NOT NULL,
    'RealTime'  datetime  NOT NULL,
    'Measurement'  integer  NOT NULL;)

ALTER TABLE 'SensorData' ADD CONSTRAINT SensorID_refs_id
    FOREIGN KEY ('SensorID' REFERENCES 'Sensors' ('SensorID');

COMMIT
```



OR mapping – data structure

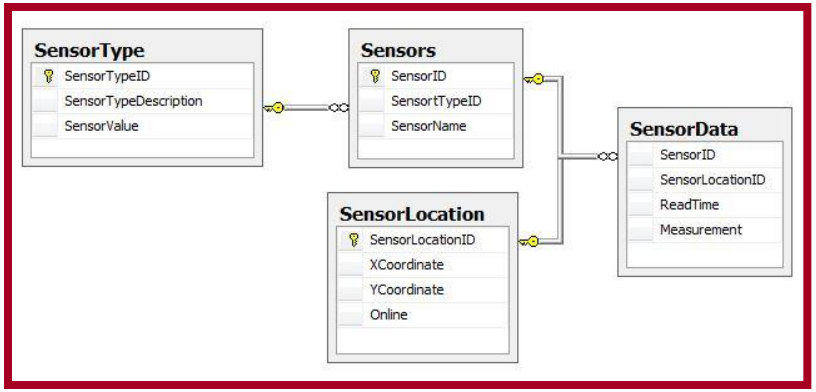
The structure of the data is specified using classes and member variables

Null-ability, default values, primary and foreign keys are easily specified

Specify the primary key (otherwise one is generated)

This means varchar(100)

```
class  SensorType (Model):
SensorTypeID = models.IntegerField (primary_key =True)
SensorTypeDescription = models.CharField(max_length=100, null =False)
SensorValue = models.IntegerField (null=False)
```



OR mapping – programming

The notation for dealing with an OR-mapped version is relatively simple but has several important features

- Transactions/sessions are managed by the mapper
- Type checking is enforced by the language rather than at runtime by SQL
- Changing data tables means changing the class structure

Summary – databases

- Databases can be an effective way to improve your ability to share and manage your data.

- Databases and database technologies are increasingly embedded in a variety of systems and technology stacks to support easy use of these systems are increasingly omnipresent.

- Database languages and tools can help reduce the amount of code you manage in your projects.