CDCS CENTER FOR DATA AND COMPUTING IN NATURAL SCIENCES



## **Databases Beyond Tables**

There's A System For Every Use-Case

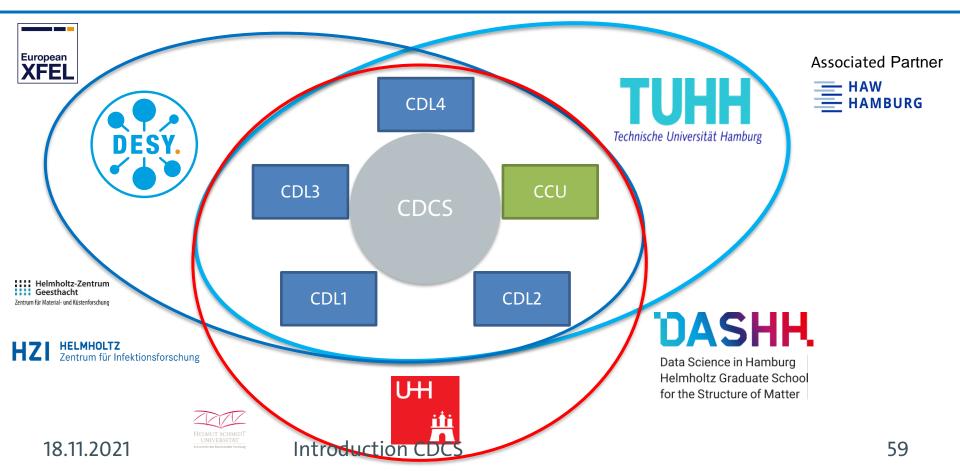
Annett Ungethüm, 06.01.2022



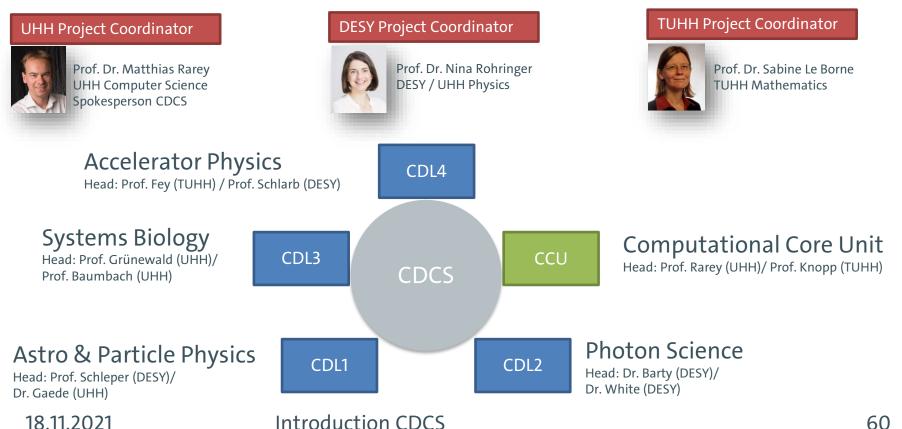




### **CDCS Hamburg-X Project (BWFGB)**

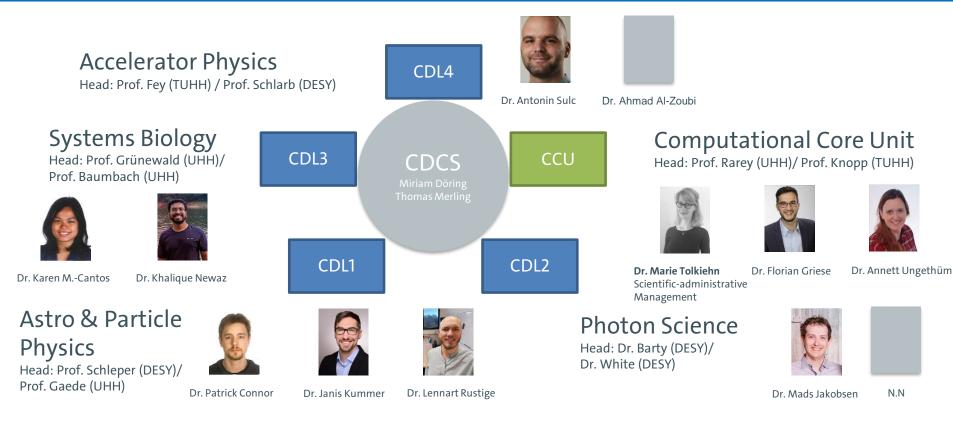


### **CDCS** Structure



### **CDCS and CDLs in Detail**

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18.11.2021

#### Introduction CDCS

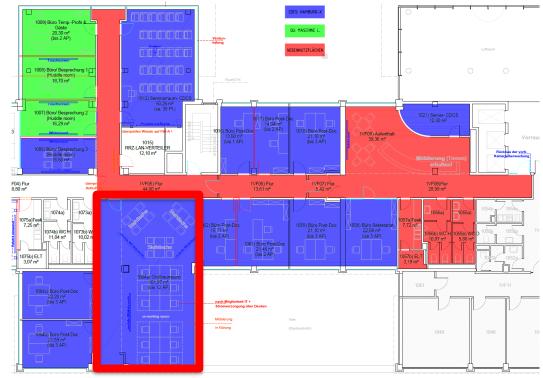
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### **The CDCS Office Space**

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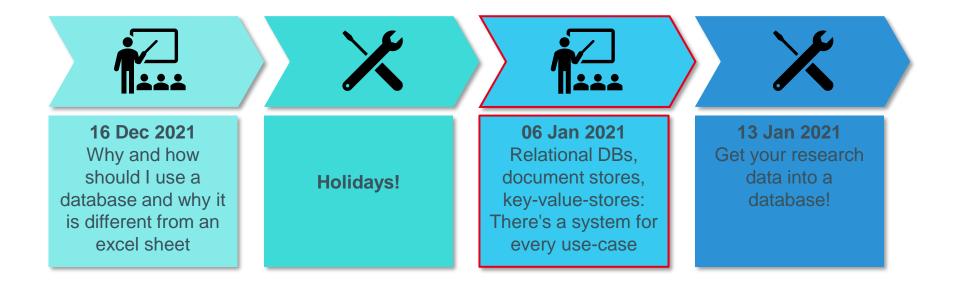
As a DASHH student you can get a transponder to the CDCS hot desk office space (room 1064) Ask our secretary Miriam Döring: miriam.doering@uni-hamburg.de

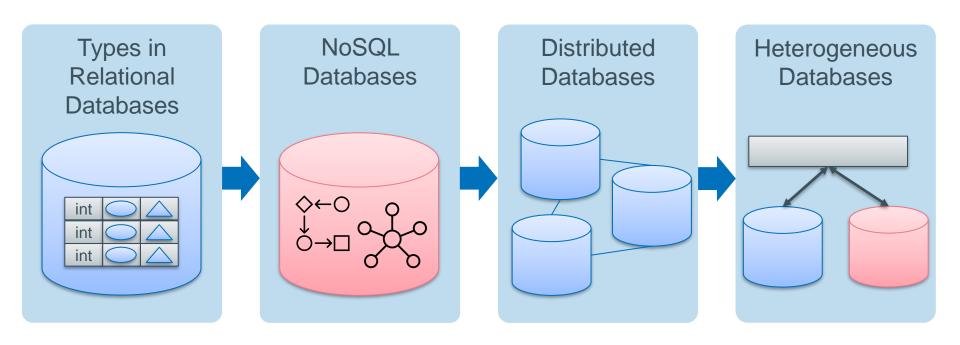


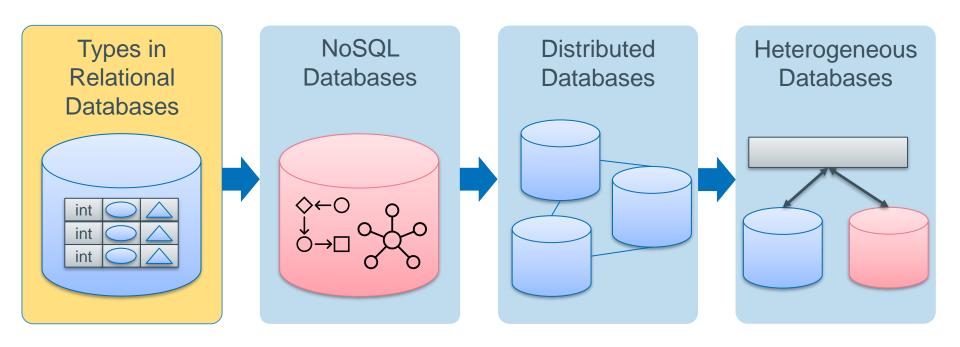
#### Introduction CDCS

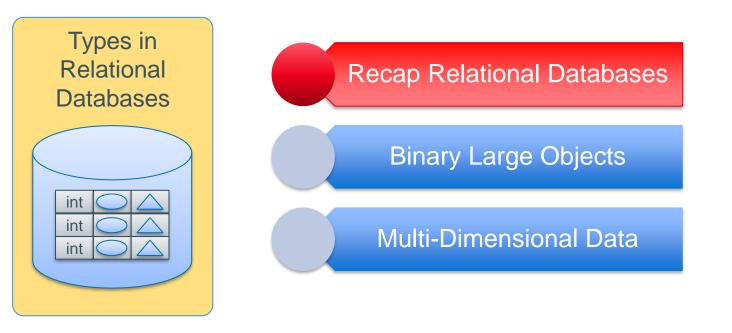
Topic of the month: Databases

You might want to send us your questions in advance to get more sophisticated answers









### **Recap Relational Databases**

This is a <b>relation</b> , defined as <i>MensaMeals(Meal,Price)</i>				-		MensaMeals	elational DBs, e.g. s WHERE PRICE <5; Price	
	are called relational Databases					Pasta Pie	4,90	
	Meal	Price			Meal and Price are the attributes of the			
	Pizza	zza 6,50			relation <i>MensaMeals</i>			
	Pasta		4,90	• Types here: <i>varchar</i> and <i>real</i>				
	Pie		1,20			• Types here: varchar and real		
	Potato Salad		5,80			h belongs to the		
	Pannfisch		7,90	relation MensaMeals				

Data is not always structured in tables containing plain numbers or text

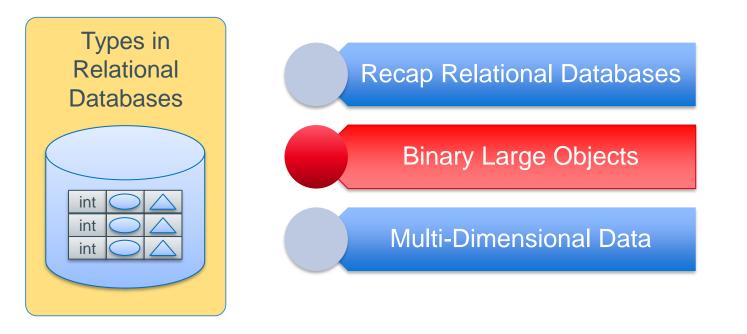
#### Standard types you may know:

CHAR, VARCHAR (aka TEXT or STRING), REAL, INTEGER, SMALLINT, BIGINT, FLOAT, DATE, TIME, INTERVAL,...

#### Standard types you may not know:

BINARY, BLOB (binary large object) MULTISET (collection of unordered values), ARRAY (array of another standard type), MDarray (multidimensional array, since 2019), JSON, ...

- Some systems support more types or alternative notations, e.g. TINYINT, MAP, LIST, ...
- Nesting of lists, structs and other composite types is supported by many systems



- Arbitrary binary data (e.g. images)
- "large" is a nebulous word → it's a bad idea to store a file with several GB of arbitrary binary data in a relational database
- Database does not know what your binary data represents
- Only the first x bytes are indexed
- Inserting data via command line might not be feasible → use the API
- Supported features vary heavily between systems → Client-Server systems usually come with a larger set of features

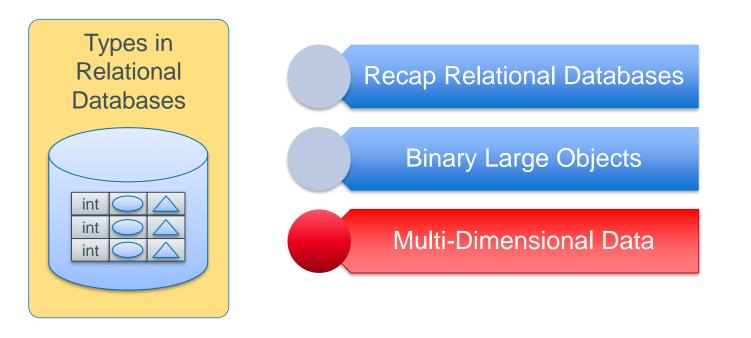
animal	picture
Duck	x0000FFFF00FF
Fish	x0000FFFF0000

Tasks:

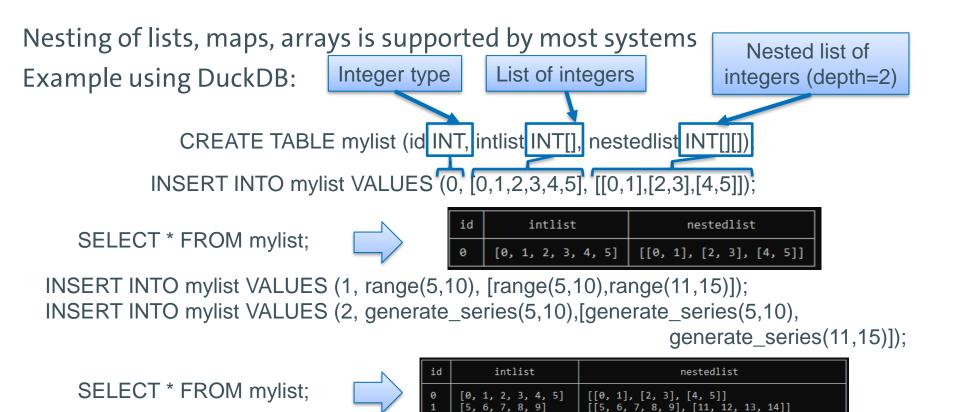
- 1. Insert data from file
- 2. Return something, e.g. blob size
- 3. Match a pattern, e.g.

#### **Blob Features**

Task	DuckDB (embedded, free)	MySQL (Client-Server, free)	Oracle (Client Server, \$\$\$)
1 insert	Use undocumented functions of backend or read and construct query yourself quick and dirty c++	<ul> <li>Same as DuckDB but with convenience function to escape special characters in strings (mysql_real_escape_string) OR</li> <li>Use LOAD_FILE('filename') → SQL extension</li> </ul>	Oracle SQL extension can be used (PL/SQL) InFile BFILE := BFILENAME('directory', 'fish_small.bmp');  DBMS_LOB.LOADFROMFILE( DEST_LOB => InBlob, SRC_LOB => InFile, AMOUNT => DBMS_LOB.GETLENGTH(InFile));
2 return	Limited choice of functions → check for equality and count of bytes (=size) SELECT animal, octet_length(picture) FROM pictures animal octet_length(picture) ARCHAR BIGINT [Rows: 1] Juck 2826	Blobs mostly treated like byte strings → use string operations	Extensive selection of functions in <i>dbms_lob</i> package, e.g. <i>getlength, get_storage_limit, compare,</i>
3 match	No support → Return blob and do it on your own	LOCATE (substring, string)	<ul> <li>Multiple ways to do this, e.g.:</li> <li>utl_raw.cast_to_raw() → get raw data format</li> <li>dbms_lob.instr() → compare content (alternative for LIKE)</li> </ul>



[[5, 6, 7, 8, 9, 10], [11, 12, 13, 14, 15]]

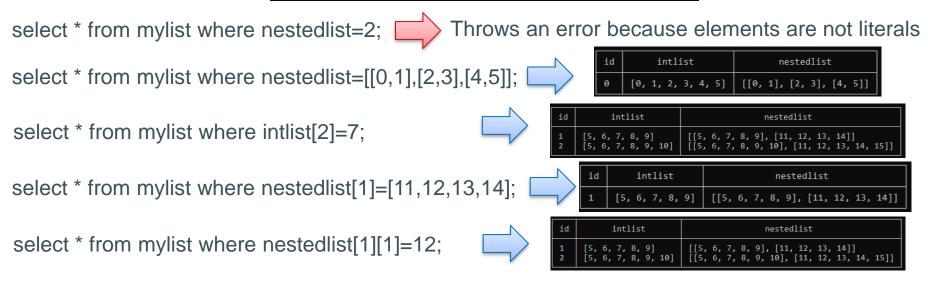


7, 8, 9, 10]

#### WHERE-clause and functions treat the whole element as one unit, e.g. the

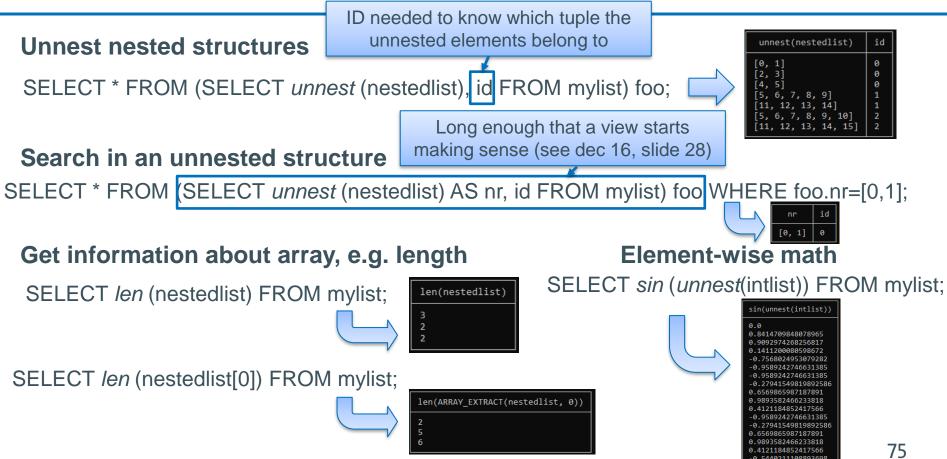
#### whole nested list

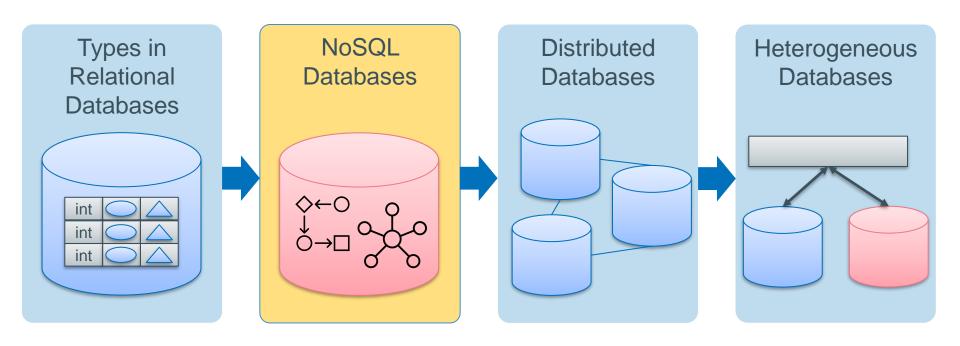
id	intlist	nestedlist
1	[5, 6, 7, 8, 9]	[[0, 1], [2, 3], [4, 5]] [[5, 6, 7, 8, 9], [11, 12, 13, 14]] [[5, 6, 7, 8, 9, 10], [11, 12, 13, 14, 15]]

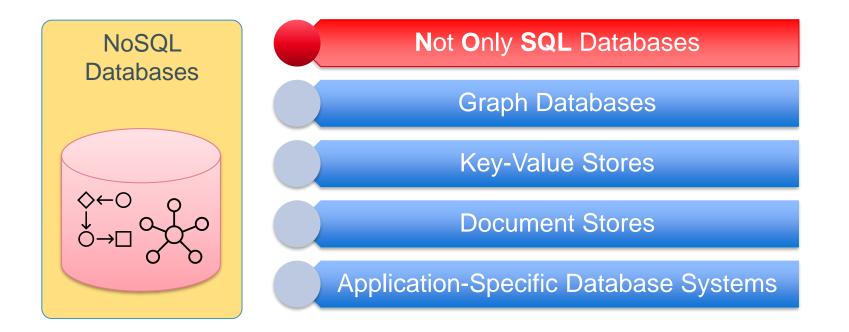


#### 23.12.2021

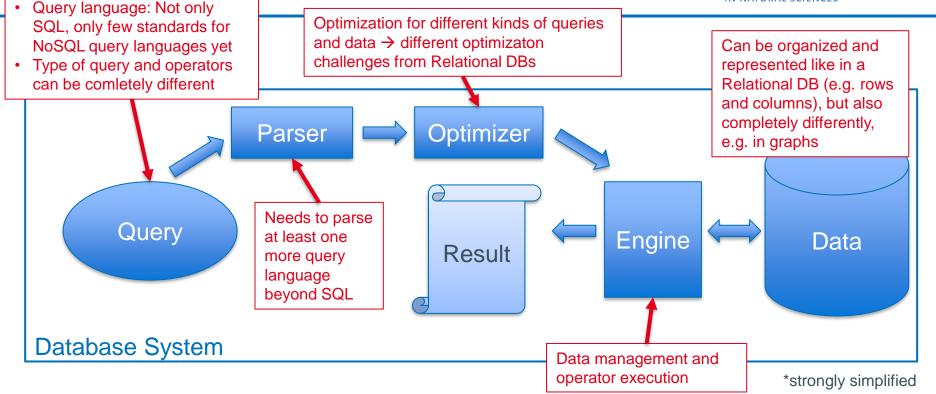
## **More Fun With Nested Lists**

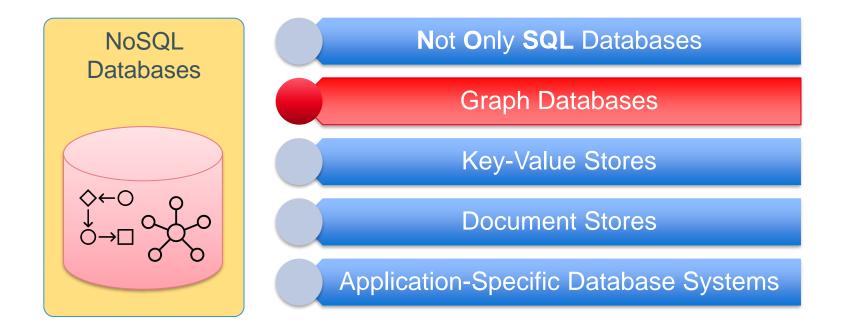




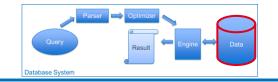


## Not only SQL Databases (NoSQL)

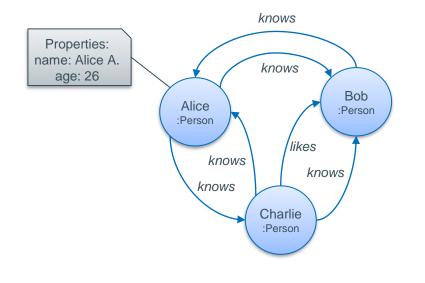




### **Graph Databases**



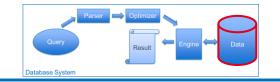
#### Most common logical representation: Property Graph Model



#### Parts of the Property Graph Model

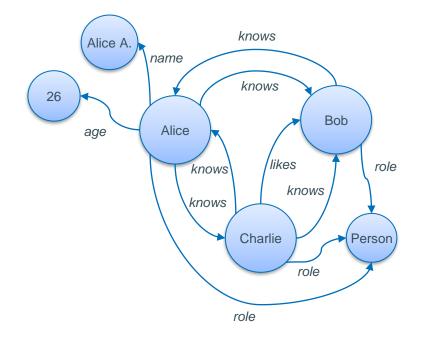
- Nodes (here: Alice, Bob, Charlie)
- Node properties/attributes (here: Name, Age)
- Node Label: describe the role of a node (here: Person)
- Directed and named edges between nodes (here: knows, likes)
- Edge properties/attributes (here: none)

### **Graph Databases**



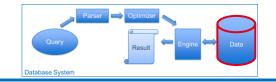
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Alternative representation: RDF (Resource Description Framework) → Triples



#### Parts of the RDF Model

- Source Predicate Object
   e.g. Charlie knows Alice
- No Properties → properties have to be expressed via triples, e.g. Alice – age – 26
- Each node and edge is just a unique label

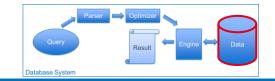


Node and Edge creation depends on System and preferred query language

• SPARQL uses INSERT DATA statement

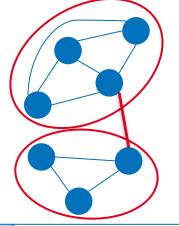
• Cypher uses CREATE statement

CREATE (eve:Person { name: "Eve V.", age: 45}) Physical representation in memory can be very different, e.g. as XML, in turtle syntax, a table in main memory, as a relational database (in all its variants),... →Neo4j uses different databases for nodes, properties, edges, and indexes



Partitioning of graphs when they become too big for one system

→ Sharding is an NP-hard problem → You won't always find the perfect solution, but you can find good solutions



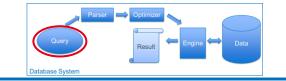
#### **Questions to answer**

- Where to cut the graph? (equal size, balance load, minimize inter-node edges, keep subgraphs at same node,...)
- How to cut the graph? (Through edges or through vertices)
- How to store the data, i.e. in which format

Sounds familiar?  $\rightarrow$  Blockchains are basically graphs. The blockchains of some crypto currencies have become really large, but a node still has to hold and synchronize the whole graph.  $\rightarrow$  Sharding with the added necessary security layer is the next big challenge for cryptos

#### 04.01.2022

## **Graph Databases**



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name

Alice

knows

knows

Alice A

age

26

knows

knows

Charlie

likes

knows

Bob

role

Persor

Query languages:

- Cypher (Neo4j)
- SPARQL (standardized by W3C)
- DSLs (e.g. Green-Marl), ...
- Example: Find all people Alice knows

Cypher: MATCH (:Person {name: ,Alice A.'}) -[:KNOWS]->(p:Person)

**Properties:** 

name: Alice A.

age: 26

Return p

SPARQL: PREFIX foaf: http://xmlns.com/foaf/0.1/

SELECT ?name WHERE {

- ?p foaf:name "Alice A.";
  foaf:knows ?o.
- ?o foaf:name ?name . }

foaf:

knows

knows

Charlie

:Persor

Alice

:Person,

knows

knows

Bob

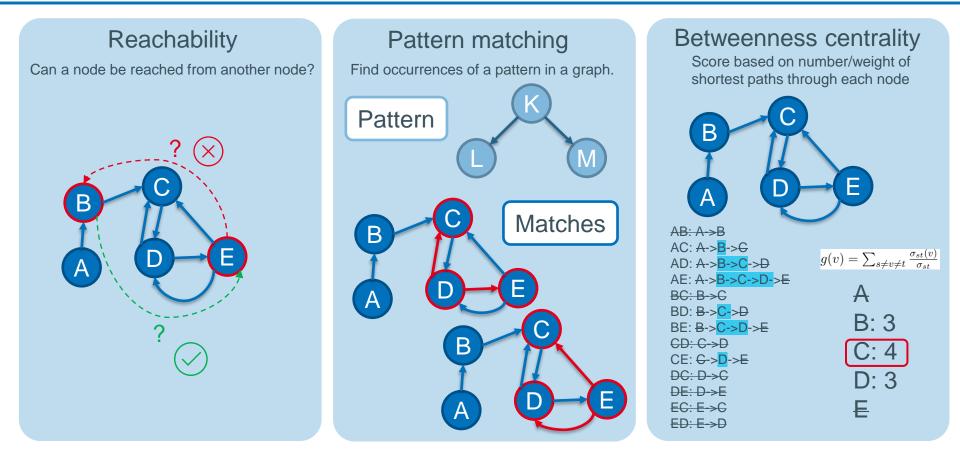
:Person

knows

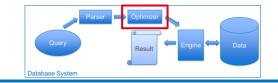
likes

- An ontology definition
- Short for friend of a friend
- Intentionally ignored in triple creation for comprehensibility

## **Different Queries in Graph DBs (Selection)**



## **Graph Databases**



Common optimization goal with Relational Databases: reduce runtime Common approach: Reduce work to do as early as possible Different challenge: in relational DBs, number of results is reduced as early as possible → in Graph DBs communication between vertexes/edges, nodes or clusters is reduced as early as possible



Query: Who likes Bob? Query Plan: Go through all triples or edges and find one with "likes" as poperty/label and "Bob" as objective Performance Bottleneck:

Broadcast the query to all triples

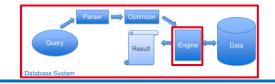
#### **Possible optimizations:**

- 1. Create inverted edges
- 2. Create and use an index on Bob's incoming edges
- Store entities with many connections close to each other (e.g. on the same node)

# Other common optimizations:

- Breadth First Search (BFS) or Depth First Search (DFS)
- Selection of starting node(s)
- Degree of parallelism

### **Graph Databases**



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Stand alone engines implementing a DSL, e.g. GreenMarl → no or very limited query optimization, requires additonal compiler to compile query

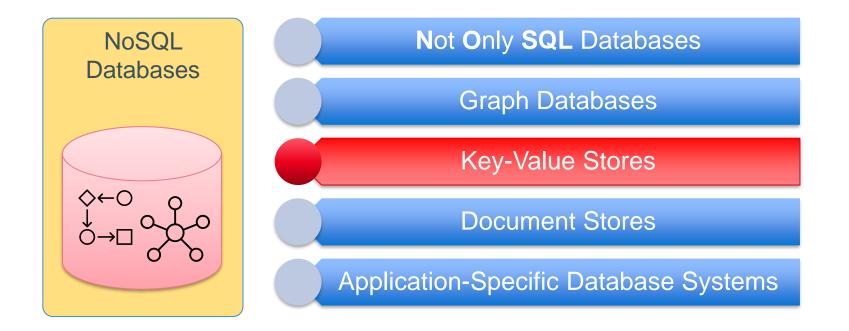
- Can (relatively) easily be integrated into own project, i.e. no system installation
- Rollout of own Software: No dependency on a fully fledged (potentially expensive) database system

Full Graph Database System, e.g. Neo4j, Pregel,...



- All-in-one solution including optimization
- May require root to install
- Can become expensive
- Licensing often more restrictive

#### 23.12.2021



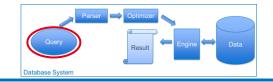
## **Key-Value Stores**



- Simple system for storing and retrieving (key,value)-pairs
- Extensions: sorting keys, two-dimensional (key,value)-pairs (aka widecolumn-stores),...
- Additional structures needed to find data fast, e.g. index on keys (e.g. as a tree structure), filters (e.g. bloom filters), ...
- Often used as embedded database
- Data can be organized write-optimized (as they are received) **or** readoptimized (in an organized structure, e.g. a tree or a sorted linked list)

→Data is often written into a write-optimized store and later migrated into a read optimized-store, e.g. when the system load is low

## **Key-Value Stores**



- 3 types of queries: put (add new pair), get (retrieve a pair), delete
- Query language depends on system, usually there is a system-specific API **Example: Memcached via telnet** → It has come a long way since ist time as a simple caching tool

Add a new KV-pair set AgeAlice 0 120 1 [Press Enter] 26 [Press Enter] Retrieve a KV-pair get AgeAlice Delete a KV-pair delete AgeAlice Syntax of set: set KEY META\_DATA EXPIRATION\_TIME\_IN\_S LENGTH\_IN\_BYTES [Press Enter] VALUE [Press Enter]



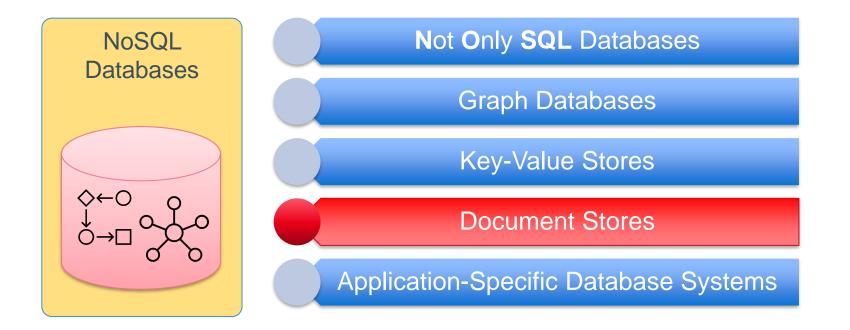


Query execution = Lookup of a key **or** add a key **or** remove a key

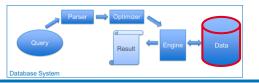
- → Stand-alone engine without optimization layer is not useful
- → Performance of operations depends on used storage layout and index structure

### Example systems:

- Memcached (<u>https://www.memcached.org/</u>, simple, open source, many supported languages, e.g. C/C++, Java, Python, Perl, Lisp,...)
- Redis (<u>https://redis.io/</u>, open source, many supported languages, e.g. C/C++, C#, Python, R, VB, Haskell, Prolog, Scala...)

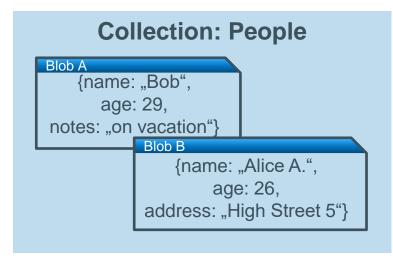


### **Document Stores**



Document stores are fancy key-value-stores:

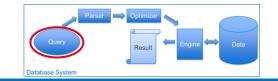
- → Values are blobs of data
- $\rightarrow$  Keys are usually assigned automatically



Collection of semi-structured data (e.g. JSON, XML)

- → Data is structured within each document
- → Structure can differ between documents

Insert data with MongoDB Create an empty collection with the name ,people': *use people* Insert data into collection people: *db.people.insert({name: "Bob", age: 29, notes: "on vacation"})* 



Query language depends on system, e.g. SPARQL, MongoDB Query Language (MQL), XQuery (for xml documents), DSLs, ...

## **Example: MQL**

Show active collection:

#### db

Show all documents in 'people' collection:

db.people.find({})

How many documents are in the 'people' collection?

db.people.find({}).count()

Show all documents in the 'people' collection where the name is 'Bob': <u>db.people.find({"name": "Bob"}</u>)

Sort all people called 'Bob' by their age in descending order: <u>db.people.find</u>({"name": "Bob"}).sort({age: -1})

23.12.2021

## **Document Stores**



- There are the usual optimizations (index usage, choice of operator implementation, ...)
- And there is a speciality of systems supporting full text search: the Inverted Index

Example: "This is a guy called Charlie. He knows this other guy called Bob."

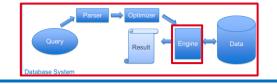
position	word	
1	This	
2	is	
3	а	
4	guy	
5	called	
6	Charlie	
7	He	
8	knows	
9	this	
10	other	
11	guy	
12	called	
13	Bob	

Normal index Mapping to the content of a document *Here:* position → word

Inverted index Mapping from the content of a document (from words, sentences, terms, whole documents,...) *Here:* word → position

word	position
This	1, 9
is	2
а	3
guy	4, 11
called	5, 12
Charlie	6
He	7
knows	8
other	10
Bob	13

- Not a new idea → oldest papers I found are from the 80s
- Progress during the last decades: compressed versions, support for different data types, inverted multi-indexes,...
- Data science is still slow when it comes to adaptation, e.g. "Realtime structural motif searching in proteins using an inverted index strategy", Bittrich et al., 2020

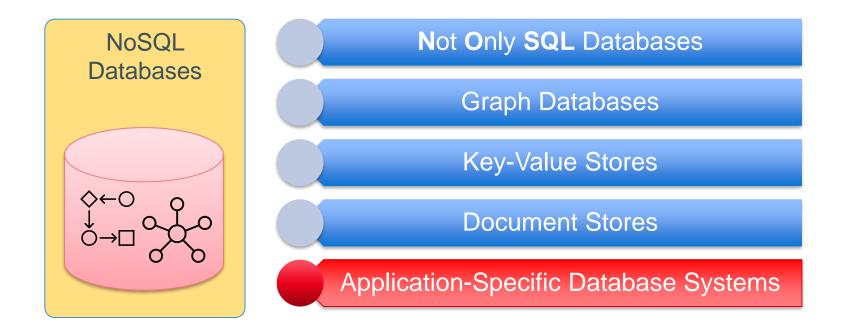


Usually rolled out as a full system or an extension for a relational database

Most popular stand-alone document store: MongoDB

Some other systems:

- Microsoft Azure Cosmos DB and Amazon DynamoDB (\$\$\$, supports JSON documents, cloud-only, supports other models, e.g. key-value, weird combination of table and document concept)
- Couchbase (open source, claims to scale better than MongoDB for large systems and many users)
- Oracle NoSQL (\$\$\$\$, supports other models, does not require a cloud)



## Example 1: SciDB

- Focuses on life sciences and healthcare
- Manages data as multidimensional arrays stored in columns
- Comes with ist own query language, e.g. scan instead of select \*
- Used to be open source, now you have to contact the company for them to install it on your vm (might not be free)
- Initial system paper: <a href="https://ieeexplore.ieee.org/document/6461866">https://ieeexplore.ieee.org/document/6461866</a>

## **Example 2: Oracles Spatial Database**

- Focuses on geospatial data and according tools, e.g. mapping services
- Part of Oracle's converged DB
  - → Like we learned last time, Oracle can deal with different types of data, but it comes at a high cost

Chances are there is already a system doing exactly what you need  $\rightarrow$  Try to get funding to pay for it **OR** 

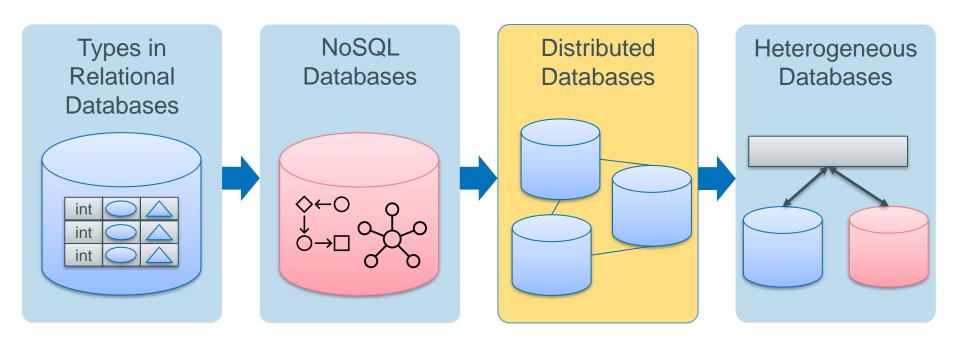
→ Read the system paper so you do not have to invent everything by yourself

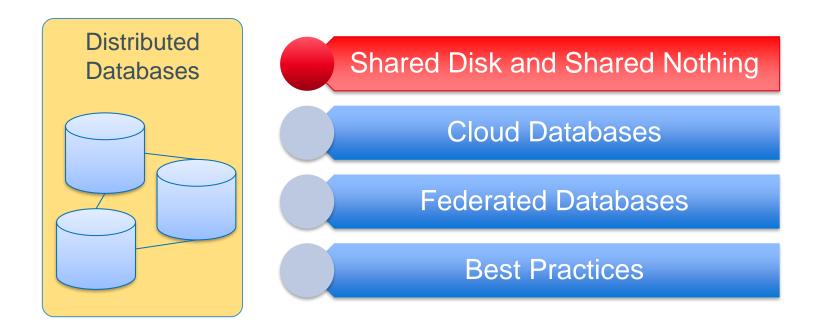
Many systems are forked from or inspired by open source and/or free systems. Try them before starting from scratch.

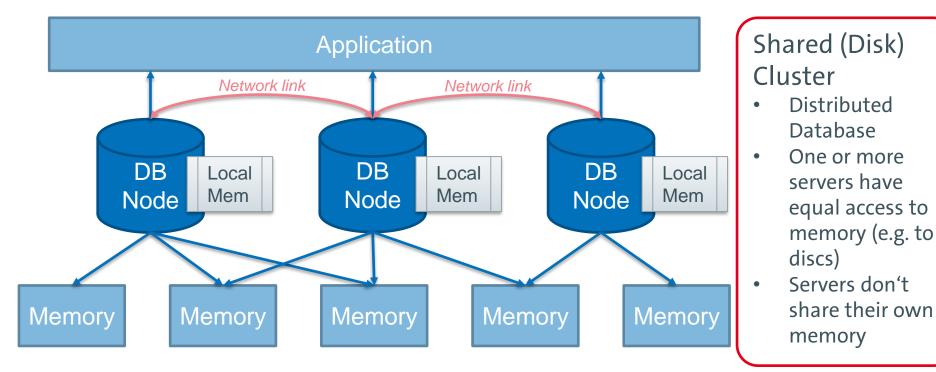
Initial system paper: https://ieeevplore.ieee.org/document/6/61866

#### More specialized DBs

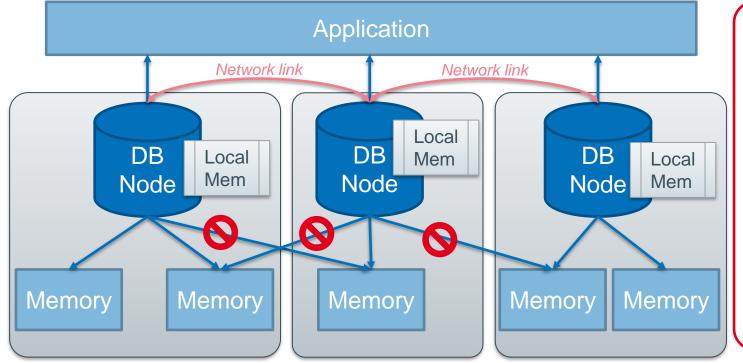
- Time series: InfluxDB (<u>https://github.com/influxdata/influxdb</u>, <u>https://www.influxdata.com/</u>)
- Search engine: Elasticsearch (<u>https://github.com/elastic/elasticsearch</u>, <u>www.elastic.co</u>)
- Spatial data:
  - Postgis (<u>https://postgis.net/</u>) → Extension for PostgreSQL
  - SpatiaLite (<u>https://www.gaia-gis.it/</u>) → Extension for SQLite (Postgis shows better benchmark results)





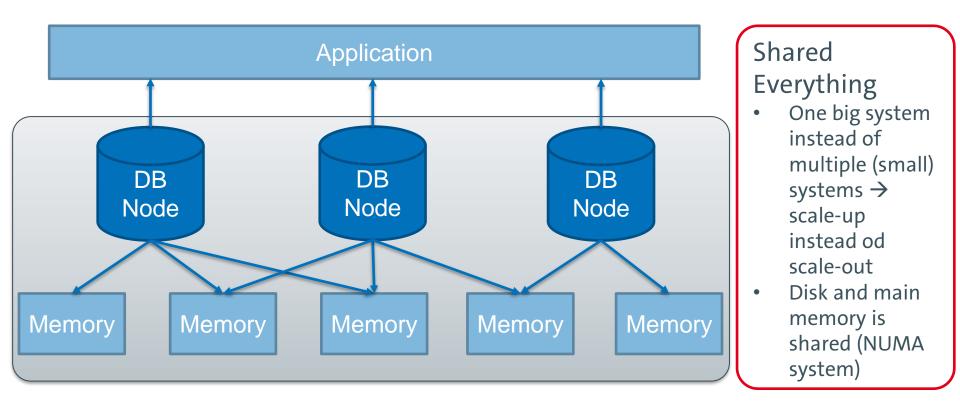


#### 102



## Shared Nothing

- Distributed
   Database
- Each node has exclusive access to its memory
- Servers don't share their own memory



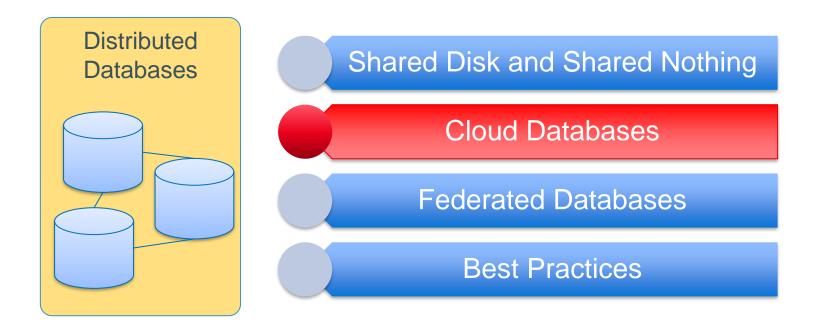
# To Share Or Not To Share

#### CDCS

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	Scale-out		Scale-up	
	Shared Disk	Shared Nothing	Share Everything	
Advantages	<ul> <li>Robust in case of node failure (discs can be accessed by another node)</li> <li>Usually easy to set up (if there is already a shared file system)</li> </ul>	<ul> <li>Robust in case of disk failure (frequently used data can be replicated across nodes)</li> <li>No distributed locking necessary</li> <li>High performance if query is executed on node where most of the data is</li> </ul>	<ul> <li>Comes for free with many systems → no additional setup</li> <li>Faster than accessing remote memory</li> </ul>	
Disadvantages	<ul> <li>Simultaneous disk access is a potential bottleneck</li> <li>Overhead to maintain cache consistency</li> <li>Requires complex locking mechanisms for updates</li> </ul>	- Partitioning (sharding) of data needs additional care to get optimal performance (store data where it is processed)	<ul> <li>Limited scaling possibilities</li> <li>Hardware for large systems becomes expensive</li> </ul>	
Example System(s)	<ul> <li>Add-on/Feature of data management systems, e.g. Microsoft Azure shared disk, Oracle RAC</li> <li>Hybrid Systems (SD &amp; SN), e.g. Snowflake</li> </ul>	Couchbase*, MariaDB SkySQL,	Each system working with NUMA architectures, e.g. MonetDB, PostgreSQL, SQL Server,	
Comments	Requires shared file system	Can be used for backup servers if full replication is enabled	Usually not noticed by the user	
*Couchbase white paper: http://info.couchbase.com/rs/porthscale/images/Couchbase_Architectural_Document_Whitepaper_2015.pdf				

\*Couchbase white paper: http://info.couchbase.com/rs/northscale/images/Couchbase\_Architectural\_Document\_Whitepaper\_2015.pdf

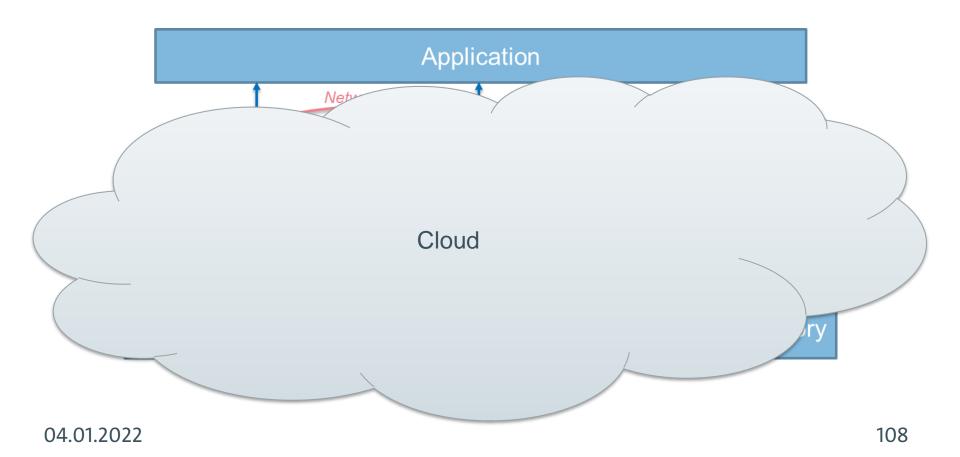


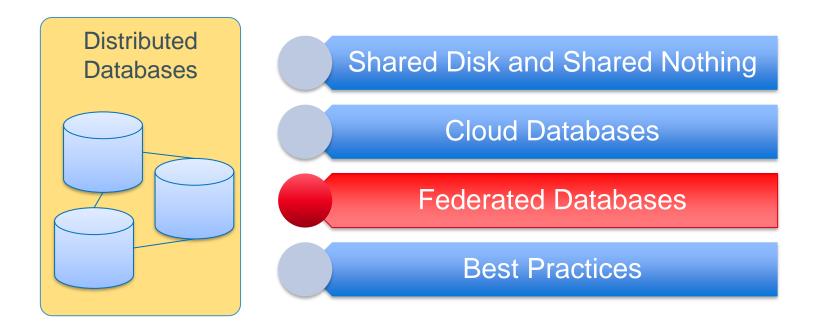
Cloud storages can be regarded as a special kind of shared disc storages with user management and some additional features:

- The cloud provider is an additional layer between the database and the application
  - Advantages: Cloud provider has to fix bugs, usually high availability due to large system with redundancies
  - Disadvantage: usually no physical access, provider must be trusted with security issues
- Cloud storage is usually remote whereas shared discs can be local
- A lot of marketing

Edge cloud  $\rightarrow$  process data close to its location (at the device of the end user) and make it available in the cloud and/or outsource work to the cloud

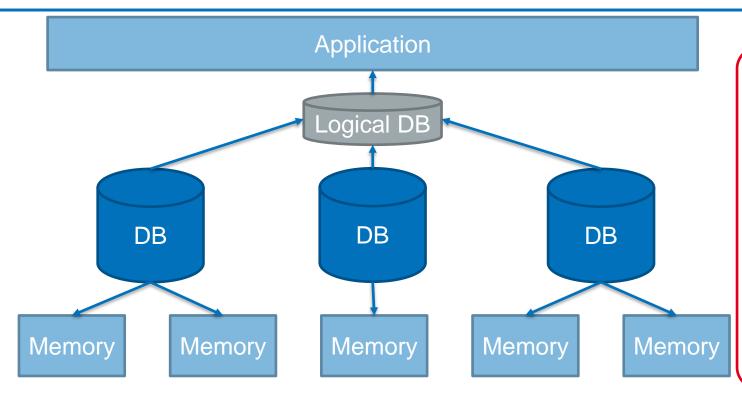
## **Cloud DBs**





## **Federated Databases**

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Federated Database

- Multiple
   Databases
- Databases are connected to one logical view
- Databases do not directly share data

## **Federated Databases**

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#### **Federated Database**

Multiple independet databases

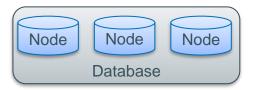


Explicit distinction between local and remote data

- $\rightarrow$  Not truely distributed, just coupled
- → Remote databases must be explicitly connected
- → No inconsistent states if individual databases are disconnected

#### **Shared Nothing**

One large distributed database



Data can become inconsistent if a node fails → Different nodes may have

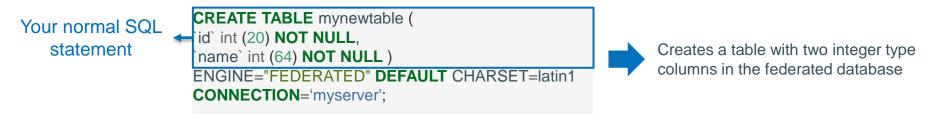
replicated different parts of the data and cannot synchronize with the base data when the node if offline

#### Step 1: Define the connection details of your (remote) database server

create Server 'myserver' foreign data Wrapper 'mysql' options (HOST '127.0.0.1', DATABASE 'mydb', USER 'root', PASSWORD '', PORT 3306, SOCKET '', OWNER 'root');

- Expects a local MySQL database called mydbat port 3306
- Connection will be available as ,myserver'

Step 2: Send your queries using the defined connection

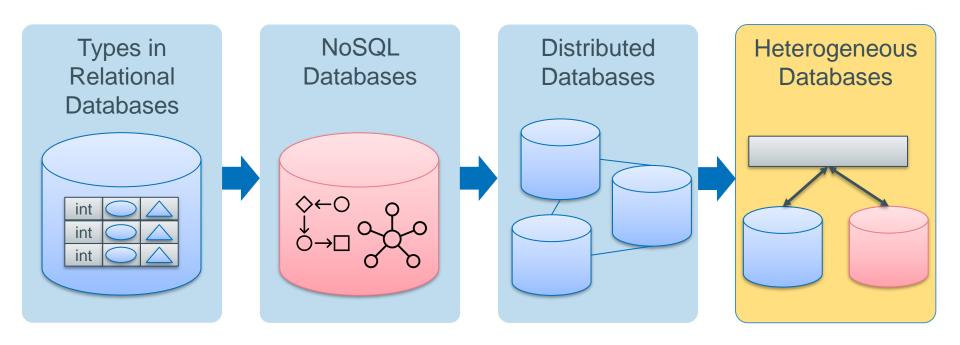


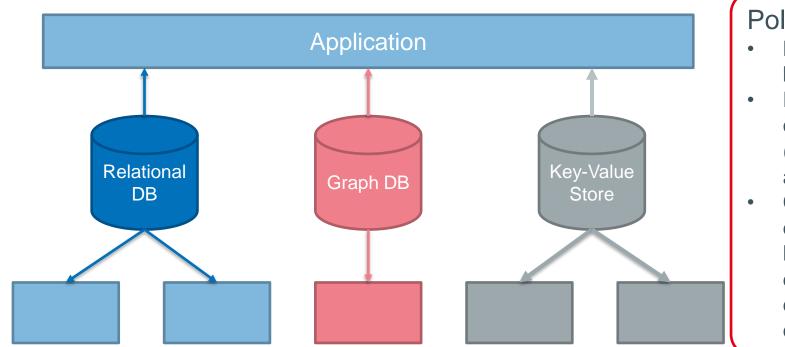
Step 3: Repeat with as many connections and/or queries as you like



Send one big query instead of several small queries

- Your optimizer will find a fast way to execute it, most probably better than you could do this
- You save time for transfering results between client and server
- If possible, save a copy of your data where you want to process it
  - Eliminates transfer between servers, especially useful during peak times
  - Hard to control when using a cloud





#### Polystore

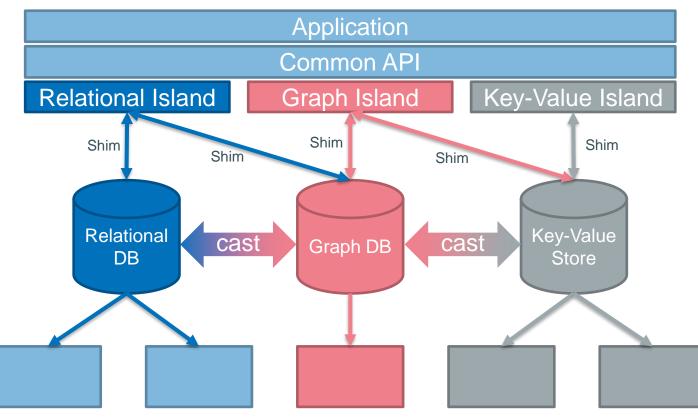
- May or may not be distributed
  - Different kinds of databases (e.g. relational and graph DBs)
- Challenges: different query languages, data models, query optimization,...

Interesting blog entry of Michael Stonebraker about Polystores: <u>http://wp.sigmod.org/?p=1629</u>

#### 23.12.2021

## Polystore

#### CDCS CENTER FOR DATA AND COMPUTING IN NATURAL SCIENCES



**Island:** An asbtraction of database systems which feature the same data model and query language

**Shim:** Query written in a query language but might be intended for a separate island

**Cast:** data transformation between different data models

- Currently supports PostgreSQL, SciDB, and Accumulo
- Other systems can be added with a bit of work as long as they fit into one of the existing islands (else, there is more work included)
- To get started, there is a tutorial which uses docker images
- $\rightarrow$  https://bigdawg-documentation.readthedocs.io/en/latest/getting-started.html MensaMeals

types (varchar and real)

Relational island, e.g. PostgreSQL (bdrel): Meal Pizza bdrel(SELECT meal FROM MensaMeals WHERE price<5) Pasta Array island, e.g. SciDB (bdarray): Pie bdarray(filter(MensaMeals, price<5) Selection on data on array island, projection on relational island: bdrel(SELECT meal FROM bdcast(bdarray(filter(MensaMeals, price<5), mytable, 'meal varchar, price REAL', relational) Cast to relational island and provide new table name (mytable), attributes(meal and price), and attribute

23.12.2021

# Price

Potato Salad	5,80
Pannfisch	7,90

6.50

4.90

1.20

