I0U19A - Management of large-scale omics data

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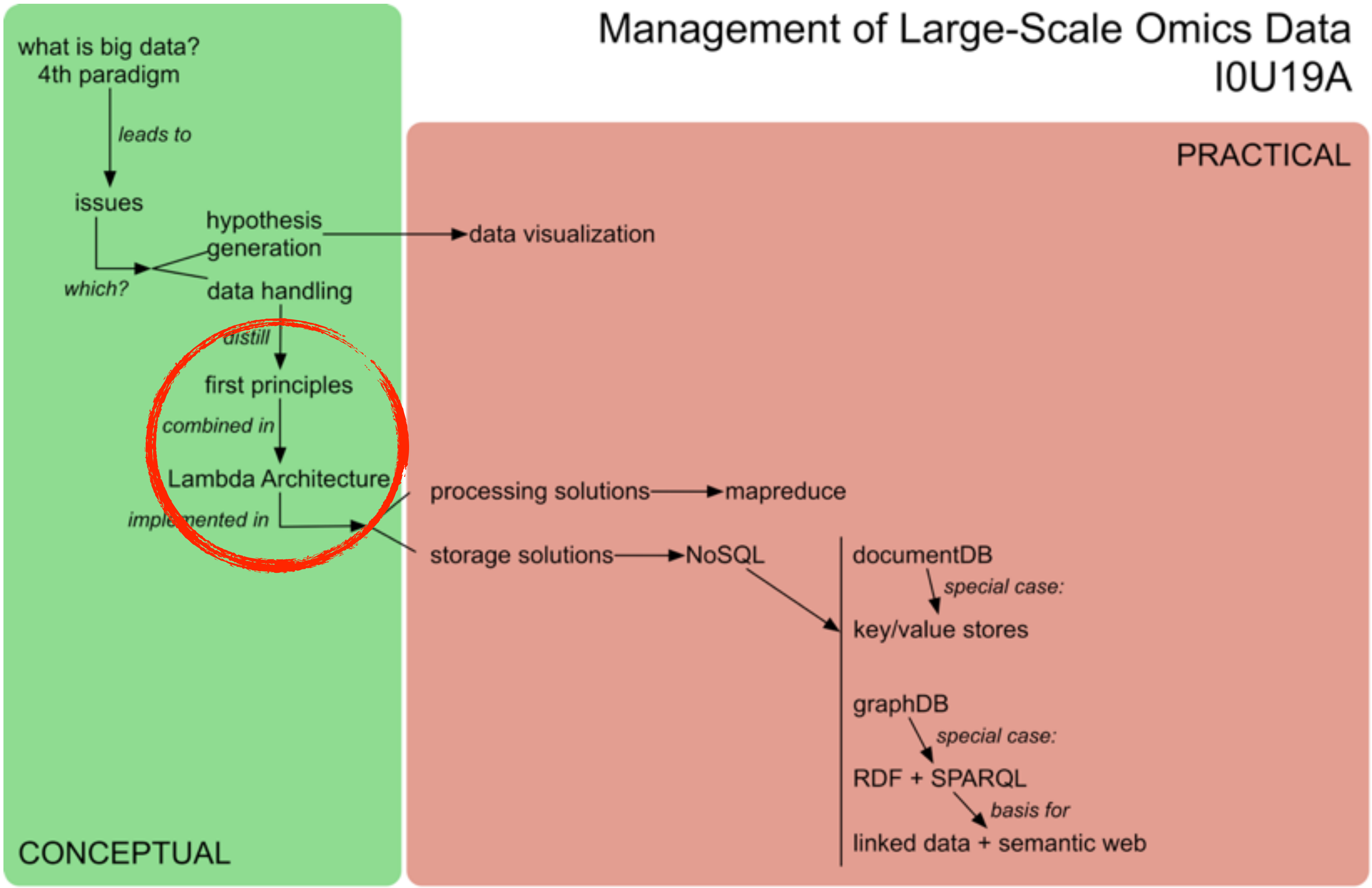
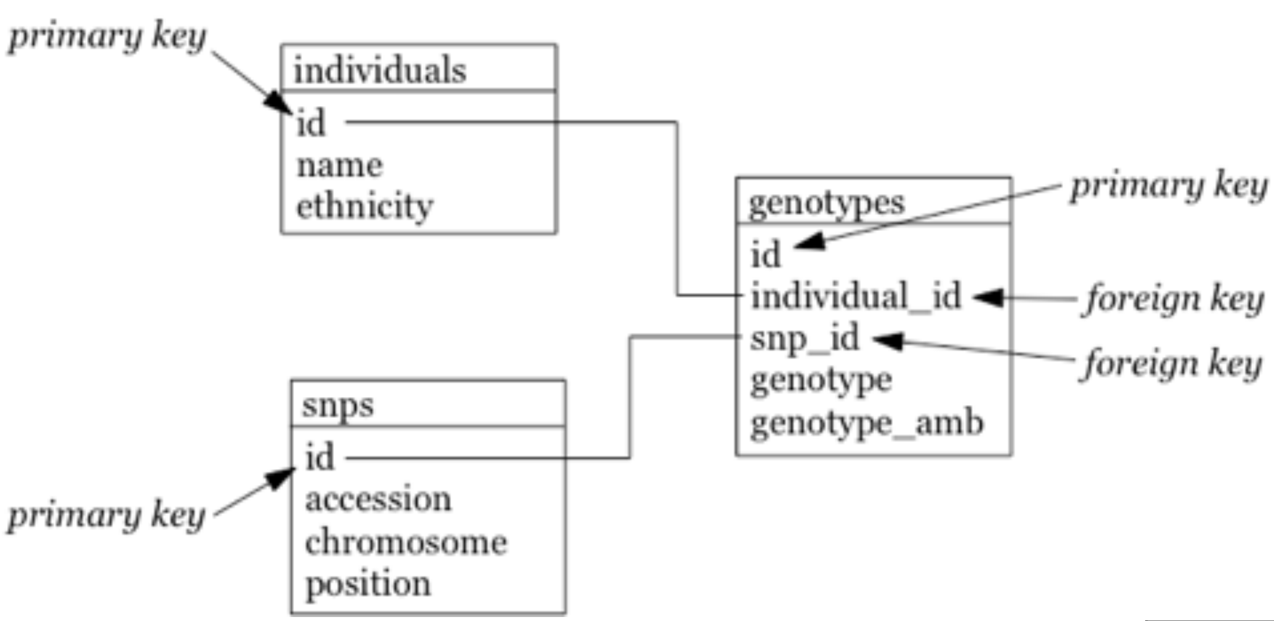
Today - Lambda architecture



Batch vs real-time

- Example Ensembl vs UCSC database showed that
  - Ensembl database allows for wider diversity in queries, but is therefore slower
  - UCSC database is optimized for speed (in a genome browser) but is less ideal for custom queries
- Issue gets more prominent once we get to really large datasets => we need a system that can compute any query (**query = function(all data)**) but at the same time be fast enough to allow interactivity (low latency)

individual	ethnicity	rs12345	rs12345_amb	chr_12345	pos_12345	rs98765	rs98765_amb	chr_98765	pos_98765	rs13579	rs13579_amb	chr_13579	pos_13579
individual_A	caucasian	A/A	A	1	12345	A/G	R	1	98765	G/T	K	5	13579
individual_B	caucasian	A/C	M	1	12345	G/G	G	1	98765	G/G	G	5	13579



individuals

id	name	ethnicity
1	individual_A	caucasian
2	individual_B	caucasian

genotypes

id	individual_id	snp_id	genotype	genotype_amb
1	1	1	A/A	A
2	1	2	A/G	R
3	1	3	G/T	K
4	2	1	A/C	M
5	2	2	G/G	G
6	2	3	G/G	G

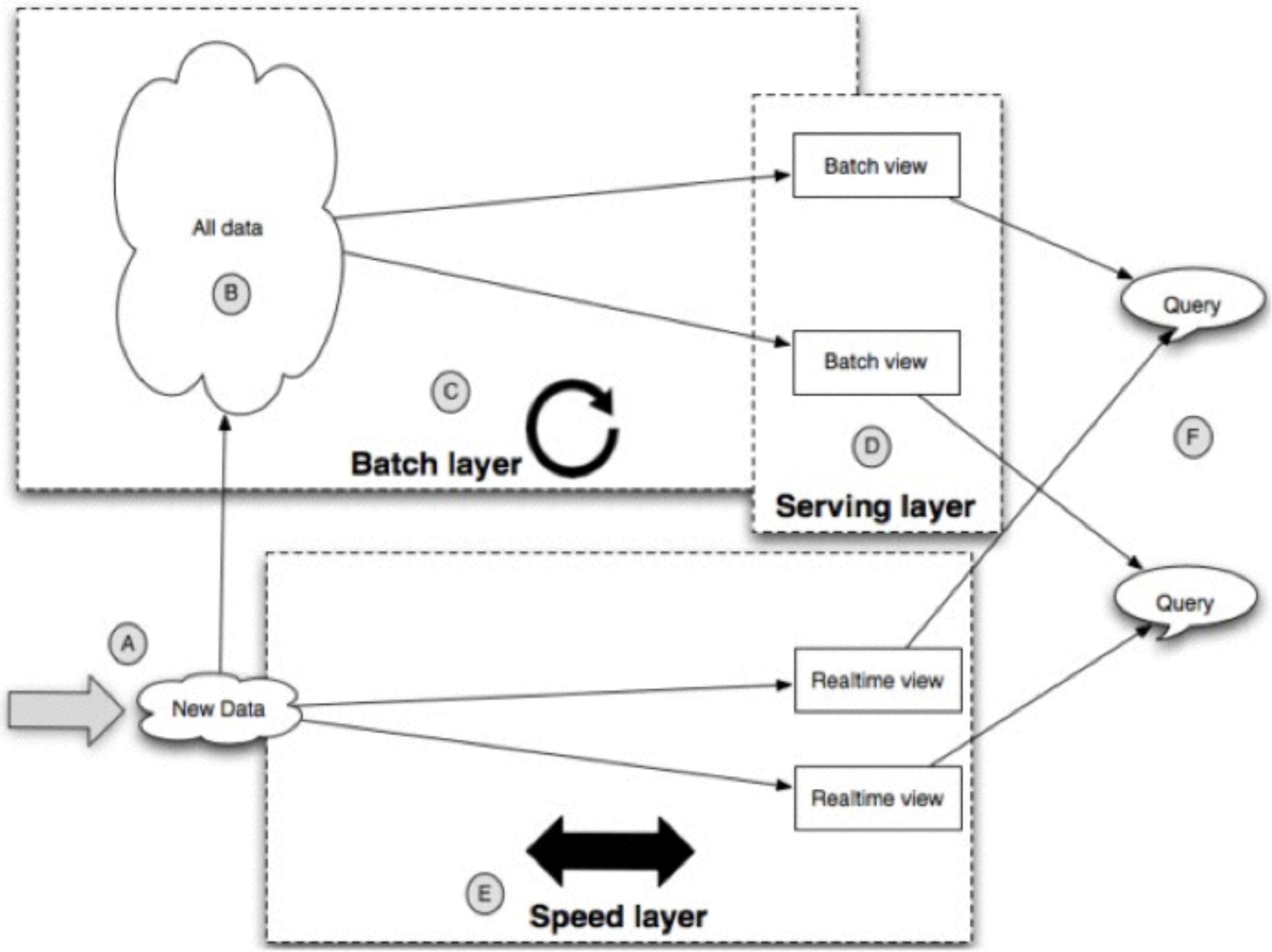
snps

id	accession	chromosome	position
1	rs12345	1	12345
2	rs98765	1	98765
3	rs13579	5	13579

3 layers in Lambda Architecture

- No single tool can provide a complete solution => use a variety of tools and techniques to build a complete Big Data system

- Lambda Architecture: decomposes the problem of computing arbitrary functions on arbitrary data in real-time by decomposing it into 3 layers:
    - **batch layer**
    - **serving layer**
    - **speed layer**



Lambda Architecture diagram (from Big Data, Marz & Warren)

1. Batch layer

- needs to be able to (1) **store** an **immutable**, constantly growing **master dataset**, and (2) compute **arbitrary functions** on that dataset
- “batch processing systems”, *e.g.* Hadoop
- continuously **recomputes** “views” that are exposed to the serving layer => **“batch views”**
- very **simple**: computations are single-threaded programs, but automatically parallelize across a cluster => scales to datasets of any size

2. Serving layer

- load views from batch layer and make them queryable through indexing
- together with batch layer: satisfy almost all properties we need
- only requires batch updates and random reads (does not need to support random writes)

batch layer

raw data

can be files on file system, …

id	who	timestamp	action	who
1	Tom	20100402	add	Frank
2	Tony	20100404	add	Frank
3	Tom	20100407	remove	Frank
4	Tim	20100409	add	Frank
5	Tom	20100602	add	Freddy
6	Tony	20100818	add	Francis
7	Tom	20100819	add	Frank
8	Tony	20101021	add	Flint
9	Tony	20110101	add	Fletcher

no updates!

serving layer

friend counts

name	friends
Tom	2
Tim	1
Tony	4

How many friends does Tom have?

friend lists

name	friends
Tom	[Frank, Freddy]
Tim	[Frank]
Tony	[Frank, Fletcher, Flint, Francis]

Is Fletcher a friend of Tim?

Batch & serving layers satisfy almost all properties

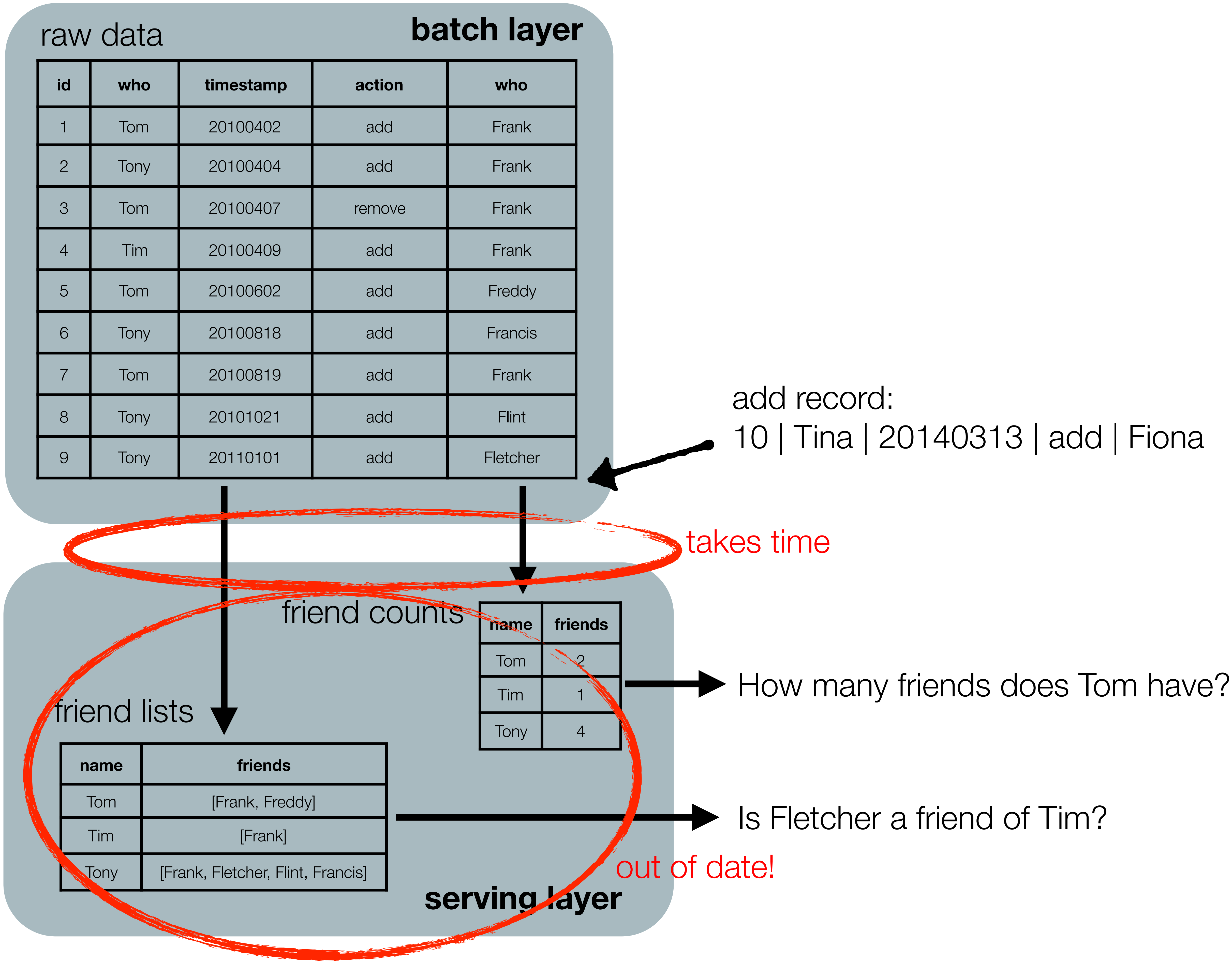
- **robust & fault tolerant**: simple system; views can be recomputed; easily distributable
- **scalable**: can be implemented as fully distributed systems
- **general**: can compute and update arbitrary views of arbitrary data
- **extensible**: adding new view = adding new function on data
- **allows ad hoc queries**: batch view allows any function
- **minimal maintenance**: very few pieces
- **debuggable**: you always have the inputs and outputs of computations run on the batch layer (<-> traditional DBs: you *update* the data)

3. Speed layer

- Serving layer updates whenever batch layer finishes precomputing views => the only data not represented in the batch views is the data that came in while the precomputation was running

  => only have to compensate for these last few minutes/hours of data

- speed layer is similar to batch layer: produces views based on data it receives



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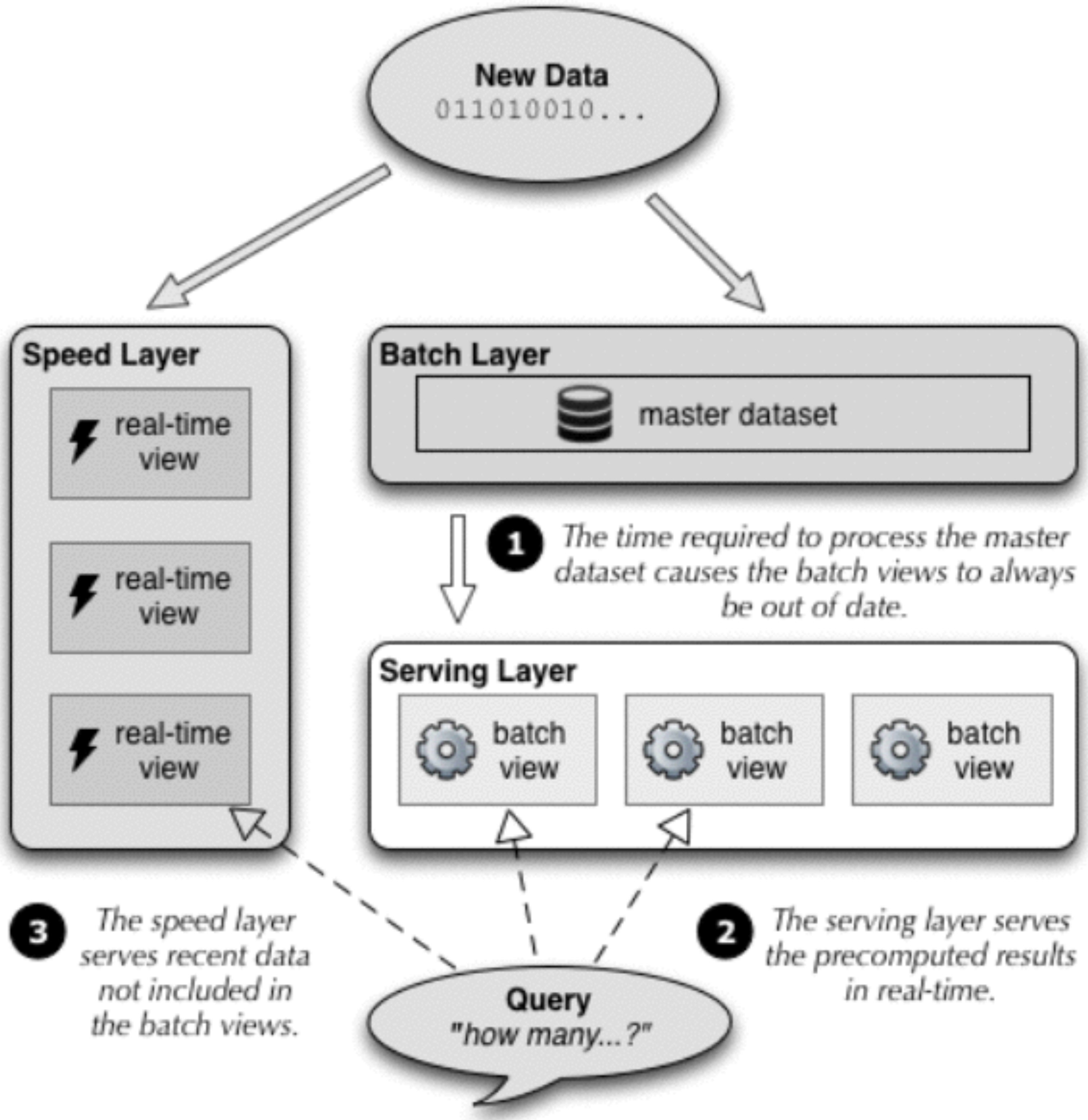


Serving layer provides low-latency access to results of calculations performed on master dataset. Serving layer views are slightly out-of-date due to time required for batch computation.

- Fundamental different approach than batch and serving layers: **incremental updates** (<-> batch/serving: **recomputation updates**)

- Consequence: significantly more complex!

    - reason: needs random reads and random writes

- Fortunately: narrow requirements => important **advantages**:

    - speed layer is only responsible for data that is not yet included in serving layer => vastly **smaller dataset**

    - speed layer views are transient => any **errors are short-lived**

- **complexity isolation**: complexity is pushed into a layer whose results are only temporary

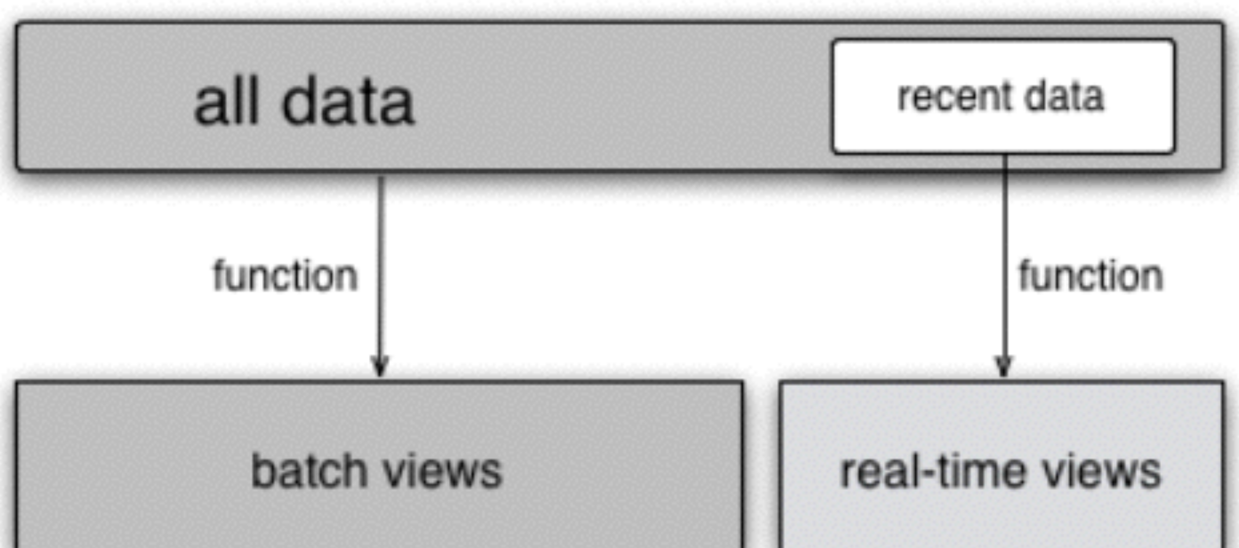
- last piece of Lambda Architecture: merging results from serving and speed layers

how to compute real-time views

- simple approach: same *recomputation* function as batch layer, but only on recent data => real-time view = function(recent data)

- problem: will still have some latency => sub-second speed is difficult

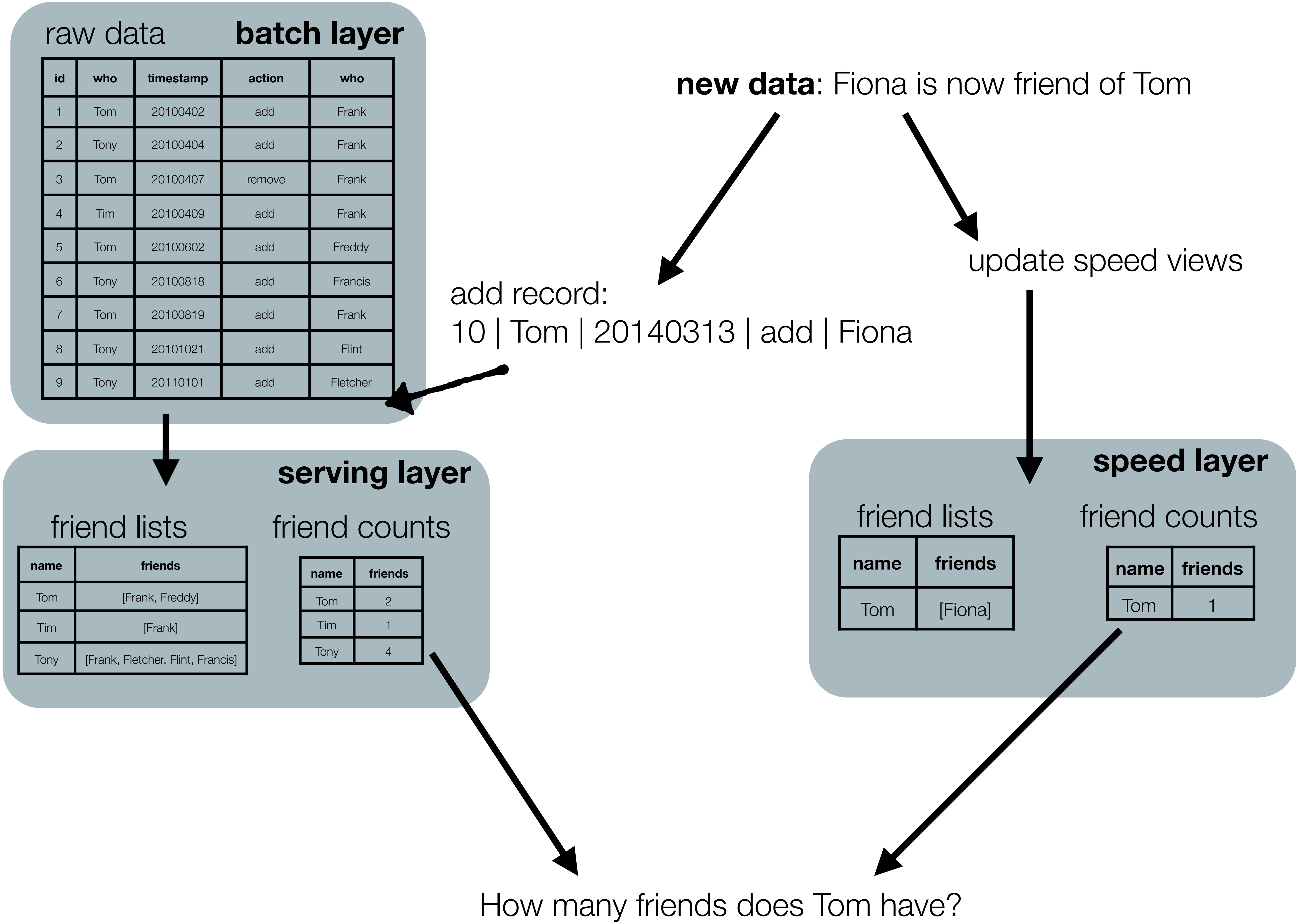
=> we need *incremental algorithm*: does not need to constantly recompute when new data arrives



a simple strategy mirrors the batch/serving layer and computes the real-time views using all recent data as input

how to store real-time views

- storage layer must meet these requirements:
    - *random reads* - data must be indexed
    - *random writes* - must be possible to modify a real-time view with low latency
    - *scalability* - real-time views can be distributed across many machines
    - *fault tolerance* - data must be replicated across machines in case one machine fails


raw data
batch layer
id | who | timestamp | action | who
1 | Tom | 20100402 | add | Frank
2 | Tony | 20100404 | add | Frank
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4 | Tim | 20100409 | add | Frank
5 | Tom | 20100602 | add | Freddy
6 | Tony | 20100818 | add | Francis
7 | Tom | 20100819 | add | Frank
8 | Tony | 20101021 | add | Flint
9 | Tony | 20110101 | add | Fletcher
new data: Fiona is now friend of Tom
update speed views
add record:
10 | Tom | 20140313 | add | Fiona
serving layer
friend lists
name | friends
Tom | [Frank, Freddy]
Tim | [Frank]
Tony | [Frank, Fletcher, Flint, Francis]
friend counts
name | friends
Tom | 2
Tim | 1
Tony | 4
speed layer
friend lists
name | friends
Tom | [Fiona]
friend counts
name | friends
Tom | 1
How many friends does Tom have?

eventual accuracy

- often very difficult to incrementally compute functions which are easily computed in batch (*e.g.*: word count)

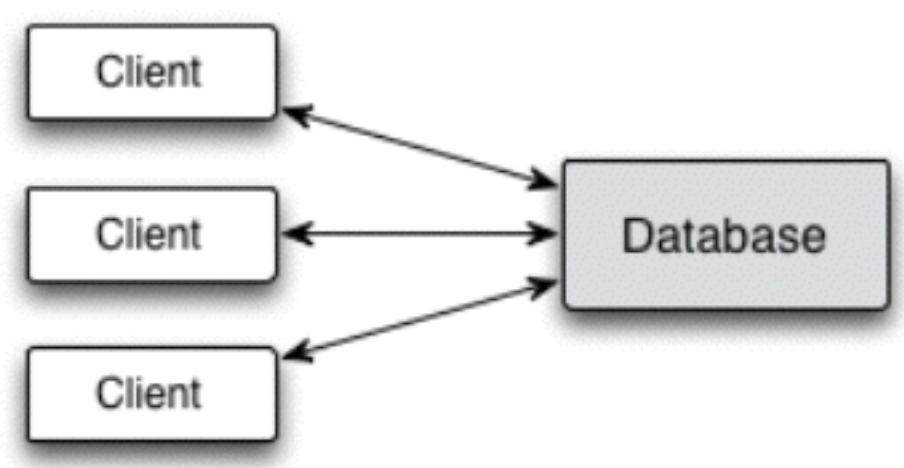
- possible approach: *approximate* the correct answer

  - will be continuously corrected through batch/serving

  - common with sophisticated queries such as those requiring real-time machine learning

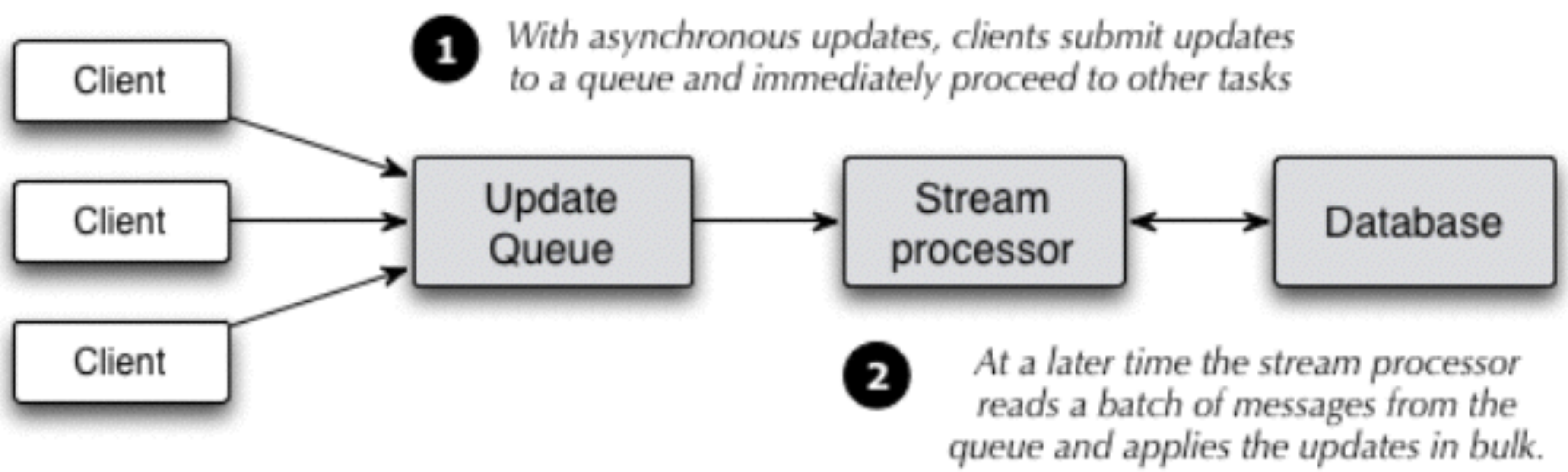
asynchronous vs synchronous updates

- synchronous update: application issues request directly to the database and *blocks* until the update is processed
  - update can be coordinated with other aspects of the application (such as displaying a spinning cursor while waiting for the update to complete)



With synchronous updates, clients communicate directly with the database and block until the update is completed

- <u>asynchronous</u> requests: put in *queue*
    - impossible to coordinate with other actions since you cannot control when they are executed
    - but advantages: greatly increases throughput + can handle varying load more easily



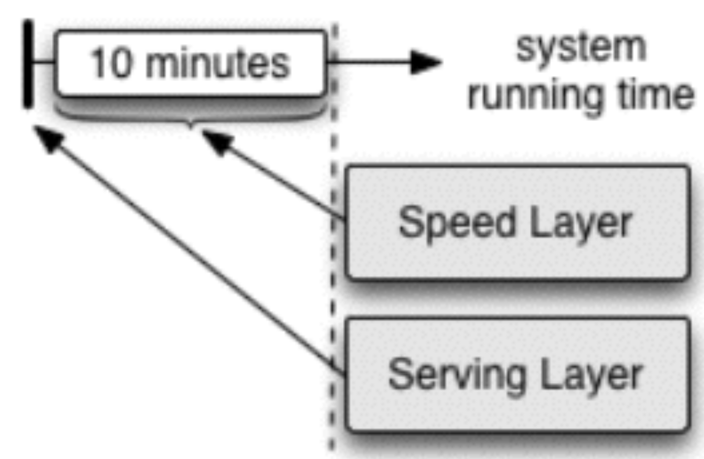
which do you use when?

- synchronous update: typical for transactional systems that interact with users and require coordination with user interface
- asynchronous update: typical for analytics-oriented workloads or workloads not requiring coordination
- asynchronous is architecturally simpler => use asynchronous unless you have a good reason not to do so

how to expire real-time views

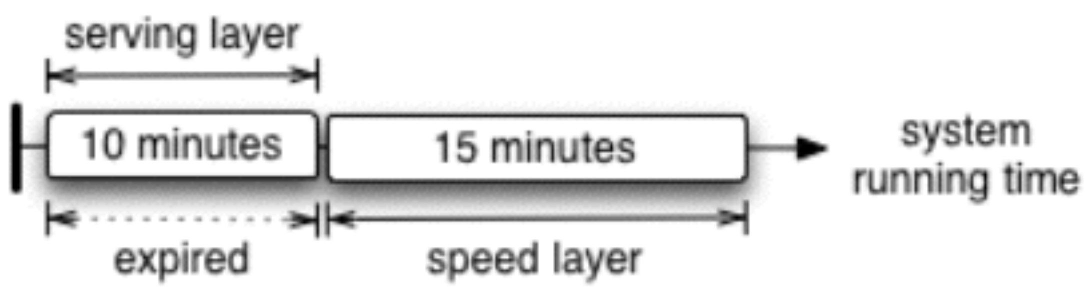
- once batch computation run finishes: you can discard a portion of the speed layer views, but you need to keep everything else => what exactly needs to be expired?

- suppose: just turned on application => no data
  => when batch layer runs **first**: operates on no data
  => if batch takes 10 minutes: when finished: batch views empty + 10min worth of data in speed



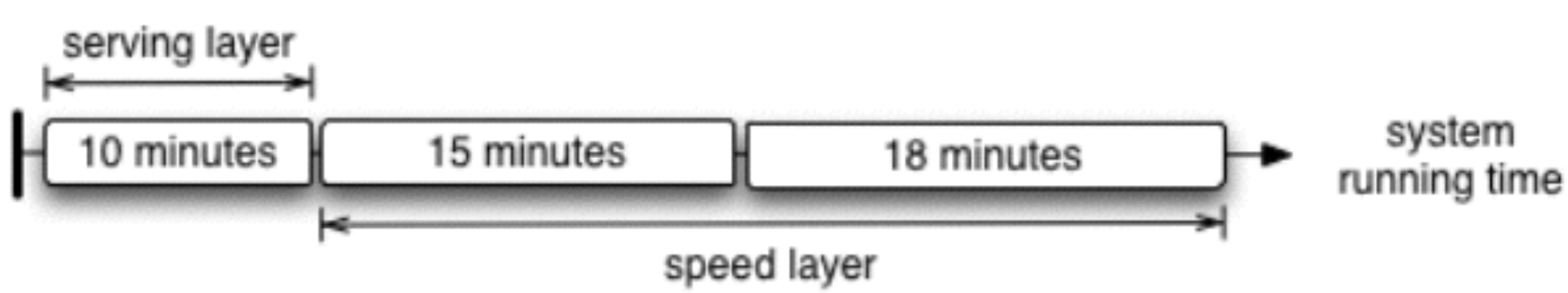
After the first batch computation run, the serving layer remains empty but the speed layer has processed recent data.

=> **2nd batch run** starts immediately after 1st
=> say 2nd run takes 15 minutes => when finished: batch view covers 1st 10 minutes + speed layer views represent 25 minutes of data
=> first 10 minutes can be expired



When the second batch computation run finishes, the first segment of data has been absorbed into the serving layer and can be expired from the speed layer views.

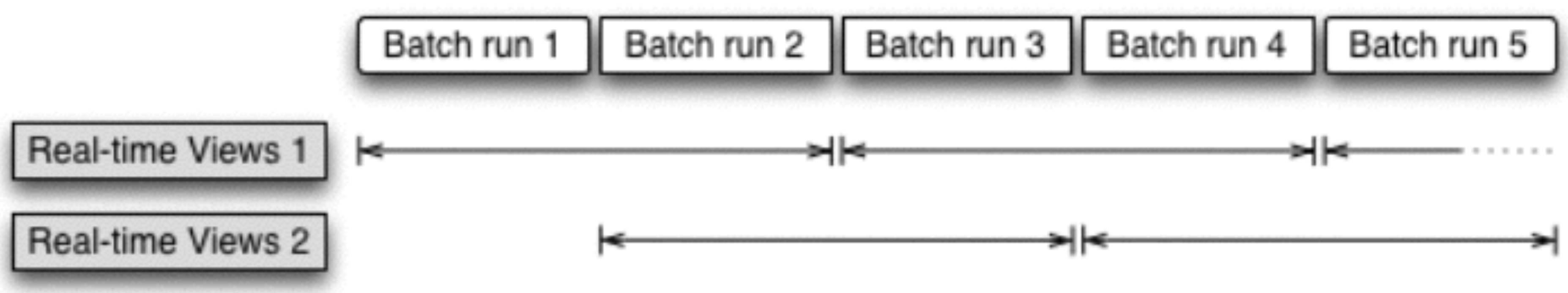
=> **3rd batch run** starts immediately after 2nd
=> say 3rd run takes 18 minutes
=> just after 3rd run started: speed layer responsible for single run (i.e. 2nd)
=> just *before* completion: speed layer responsible for data that accumulated in previous 2 runs
=> when 3rd run completes: data from 3 runs ago can be discarded

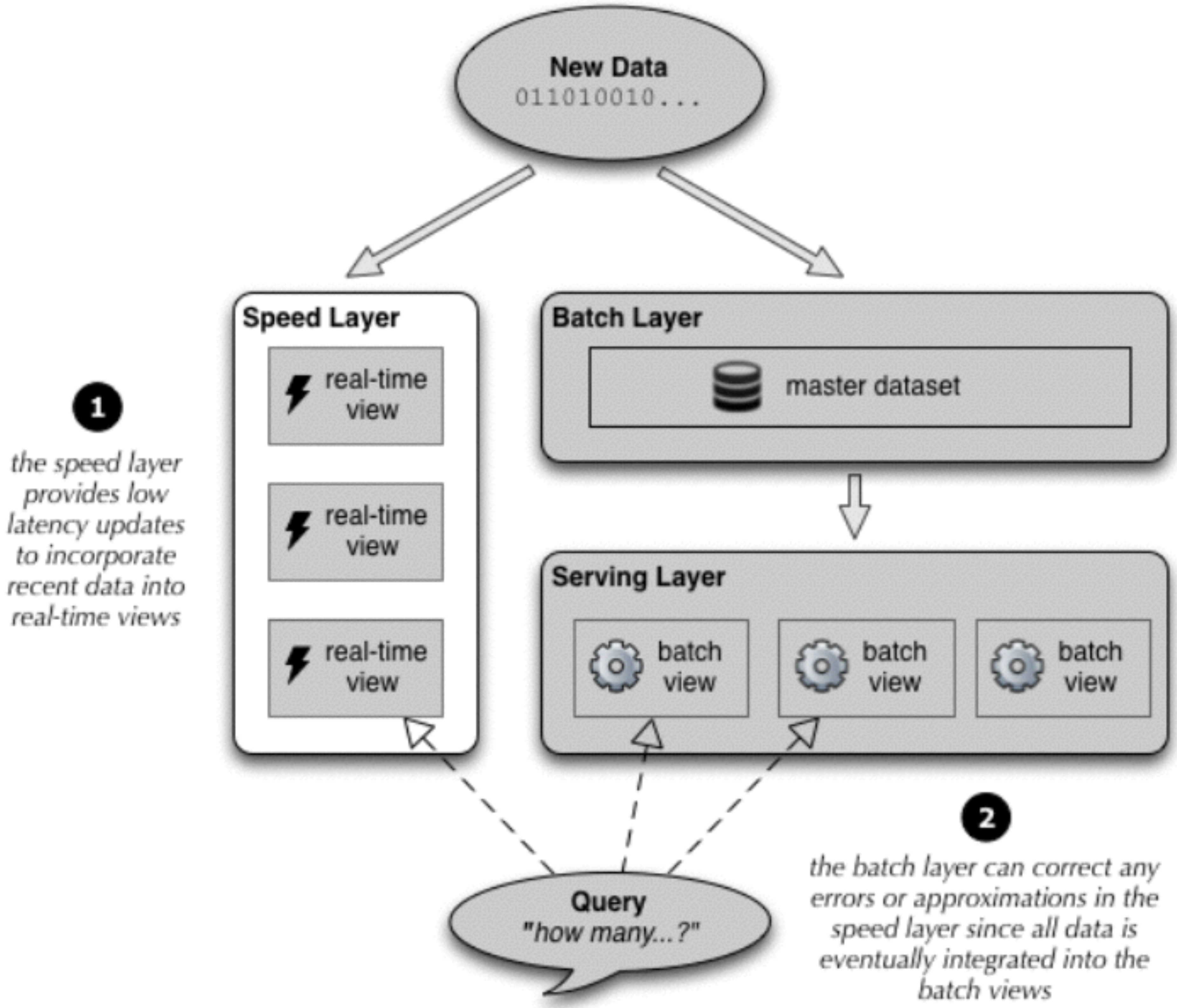


Just prior to the completion of the batch layer computation, the speed layer is responsible for data that accumulated for the prior two runs.

simplest way to do this: maintain *two* sets of real-time views and alternate clearing them after each batch run

=> after each batch layer run: application should switch to reading from the real-time view with more data





Speed layer allows Lambda Architecture to serve low-latency queries over up-to-date data

Brewer's CAP theorem: understanding trade-offs in **distributed systems**

- Using a formal process to understand the trade-offs in your selection process will help drive your focus towards things most important.

- "When a distributed data system is partitioned, it can *consistent* or *available*, but *not both*.

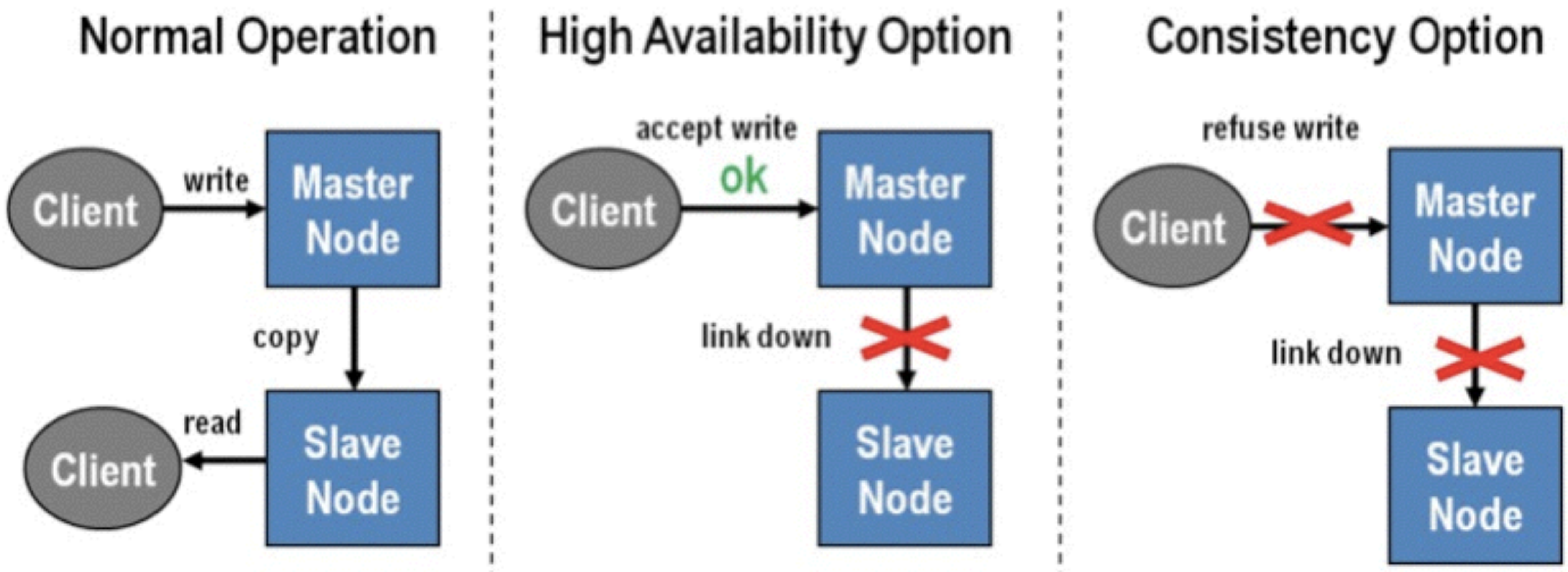
- **Consistency** (!= the consistency in ACID) - multiple clients reading the same items from **replicated partitions** get consistent results

- **high Availability** - knowing that the distributed database will always allow database clients to update items without delay (=> internal communication failures between replicated data should not prevent updates)

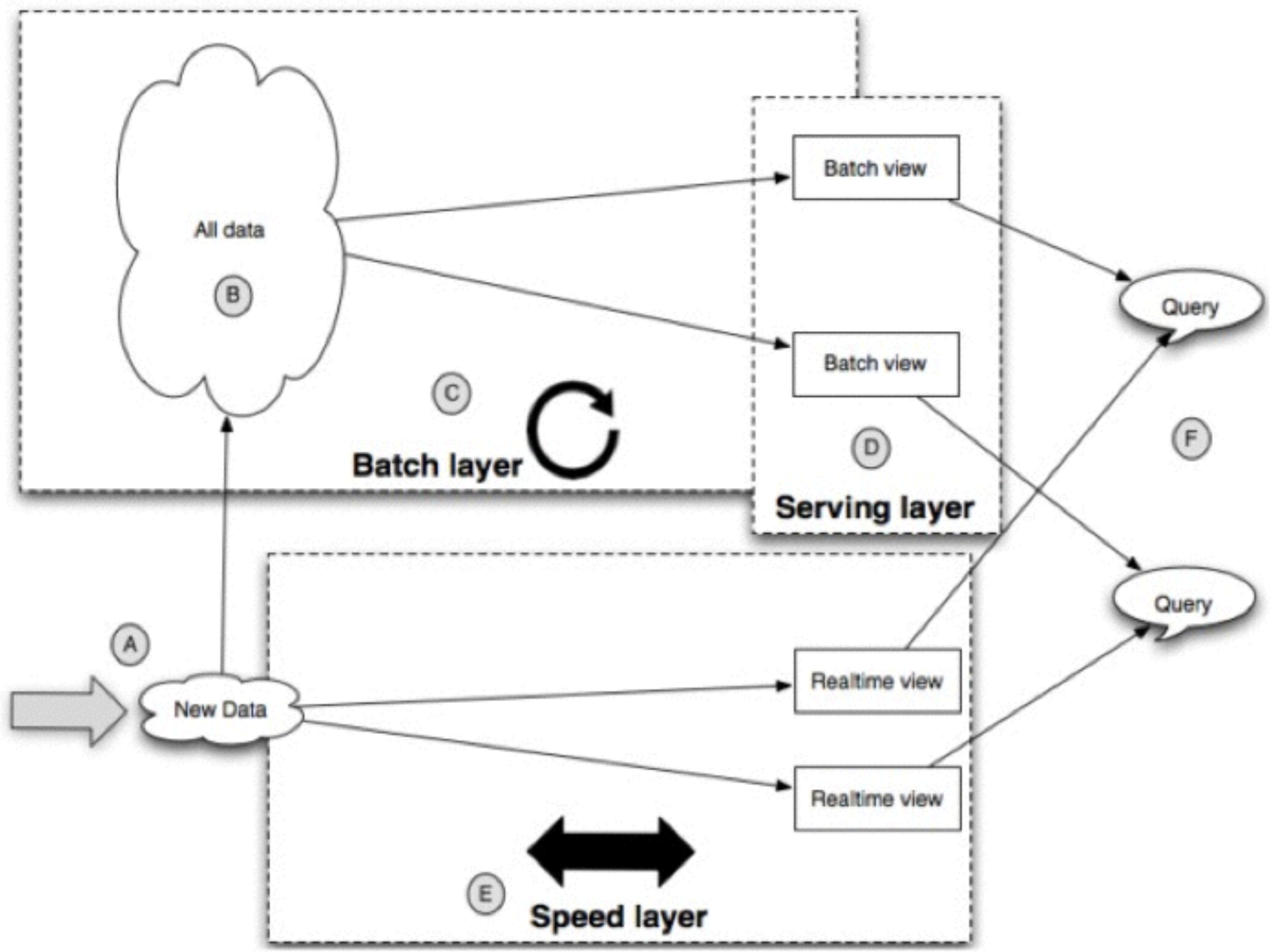
- **Partition tolerance** - ability for the system to keep responding to client requests even if there is a communication failure between database partitions

- CAP theorem only applies when something goes wrong in communication => the more reliable your network the less chance you need to think about CAP

- => CAP theorem helps you understand that once you partition your data you must consider the availability <-> consistency spectrum in case of network failure



• to recapitulate:



Data Processing in Lambda Architecture

- batch systems: mapreduce
  - very simple conceptually: map phase + reduce phase
- real-time systems: spark, storm, …
  - technologically much more complex

see next 2 sessions

Data Storage in Lambda Architecture

NoSQL - Not Only SQL

See following lectures

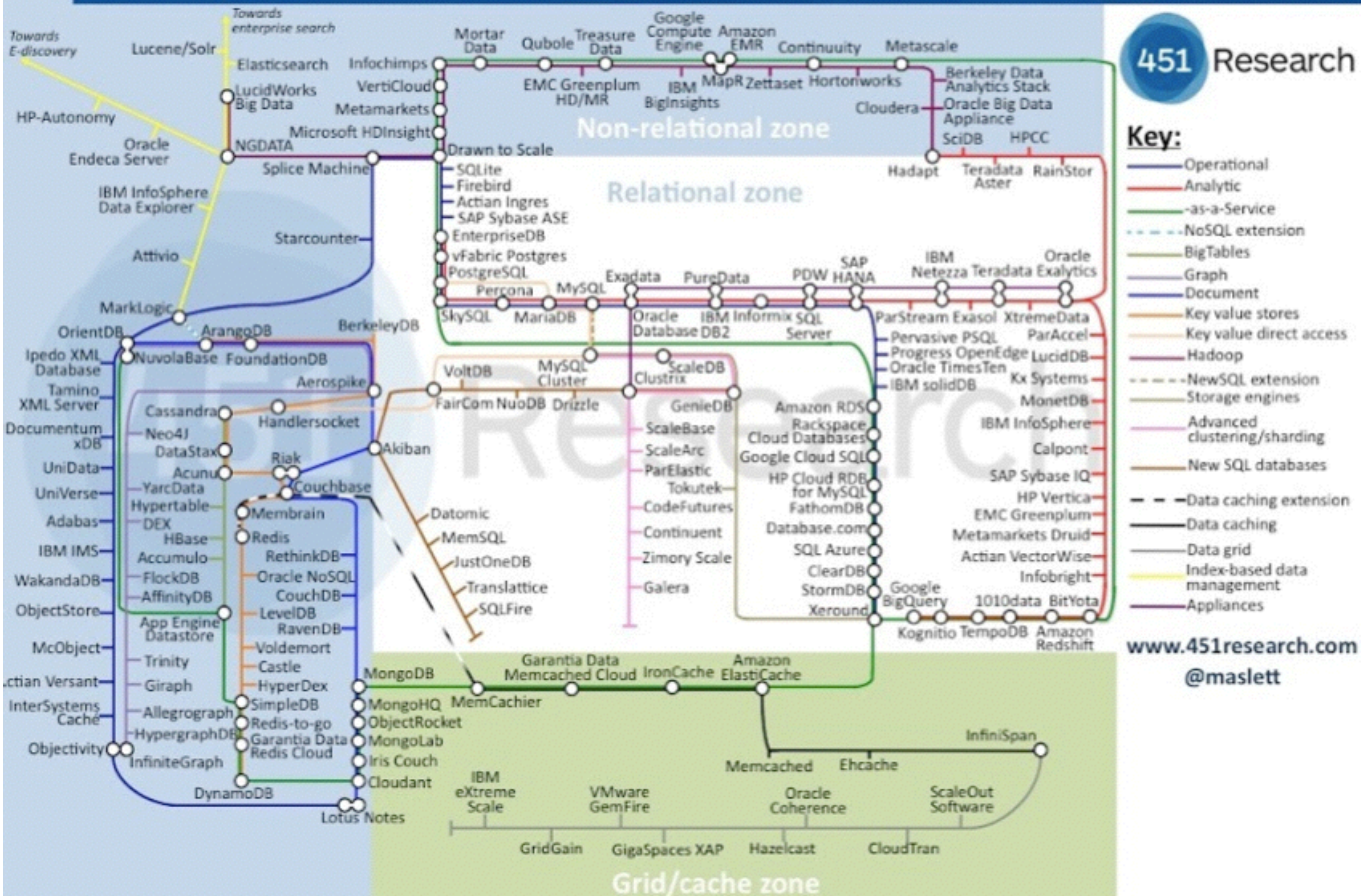
= set of concepts that allow the rapid and efficient processing of datasets with a focus on performance, reliability and agility. Core themes:

- free of joins
- schema-free
- works on many processors
- uses shared-nothing commodity computers
- supports linear scalability

Types of NoSQL data stores

- **document stores**: for storing hierarchical data structures (*e.g.* document search)
- **key/value stores**: simple data storage systems that use a key to access a value (*e.g.* image stores, Amazon S3)
- **column stores**: sparse matrix systems that use a row and column as key
- **graph stores**: for relationship intensive problems (*e.g.* social network, gene network)

Database Landscape Map – February 2013



document stores

- focus on storage of *documents* rather than rows and columns
- some: provide SQL-like interface
- some: provide mapreduce processing

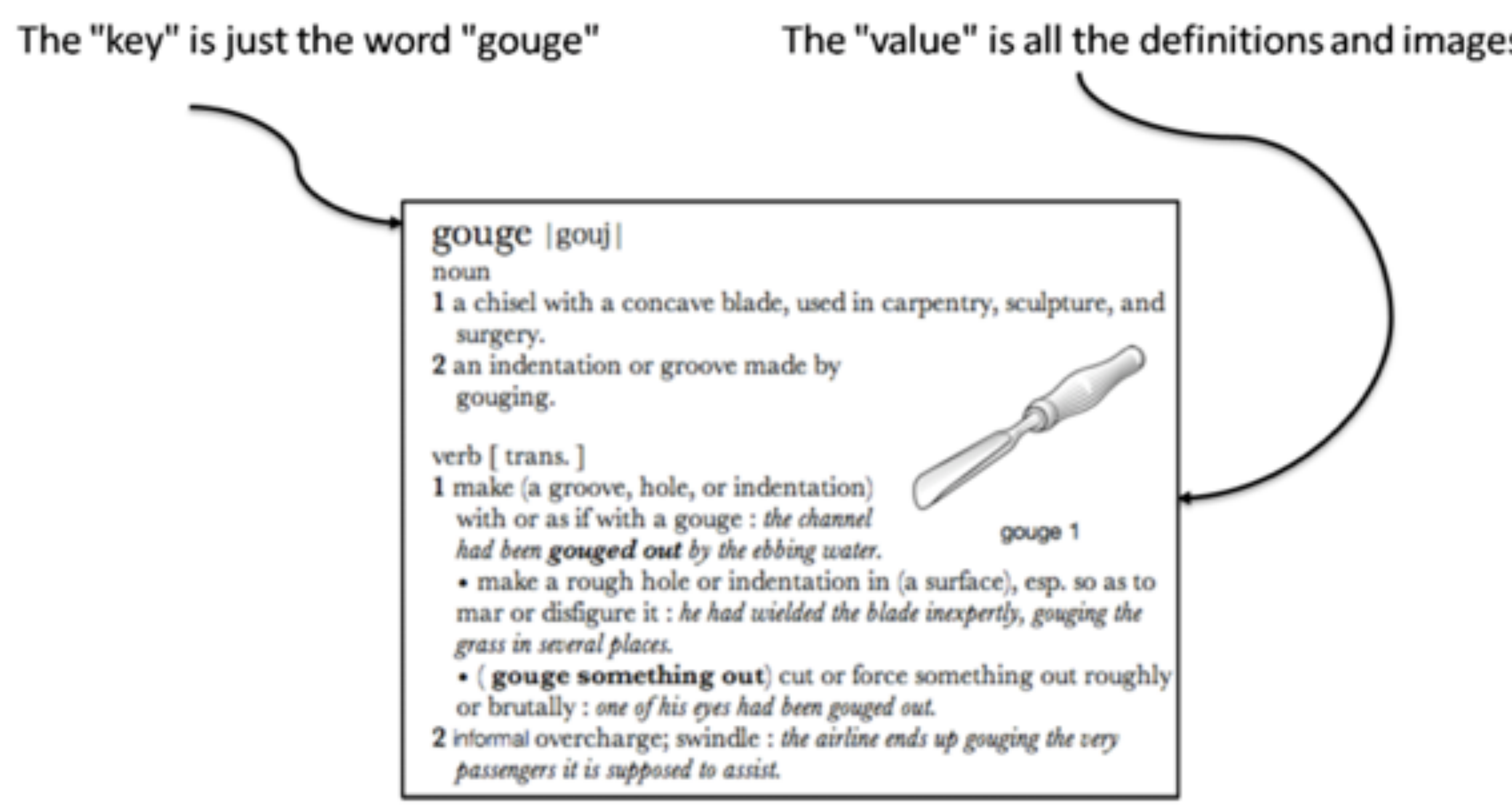
key/value stores

- very specific use
  - provide only a single way to access values (only commands: `put`, `get`, `delete`)
  - not possible to query value
- very simple
- very fast

- simple database that when presented with a simple string (the key) returns an arbitrary large blog of data (the value)

- has no query language; can only put stuff in and get stuff out

- like a dictionary



- very scalable: fast retrieval of values regardless of the number of items in your store

- don’t have to specify data type for the value => you can store whatever you want

  - system stores the information as a blob (*e.g.* Amazon S3)

  - up to the application to determine what type of data it is and what to do with it

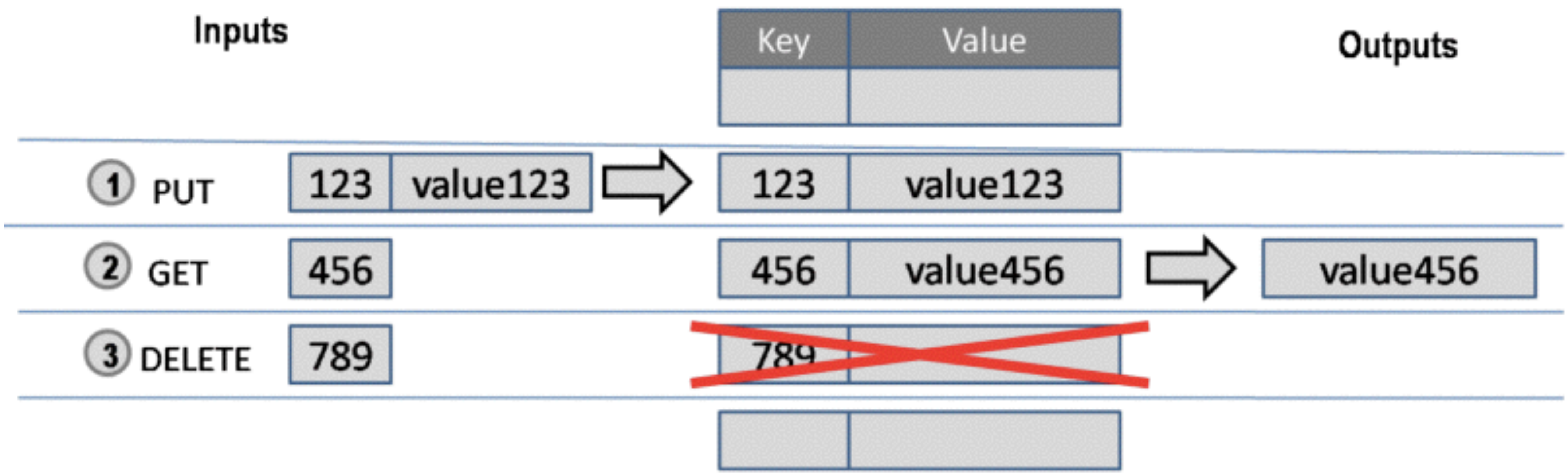
  - keys can be many things: path names to files, artificially generated strings, SQL queries (as string), ...

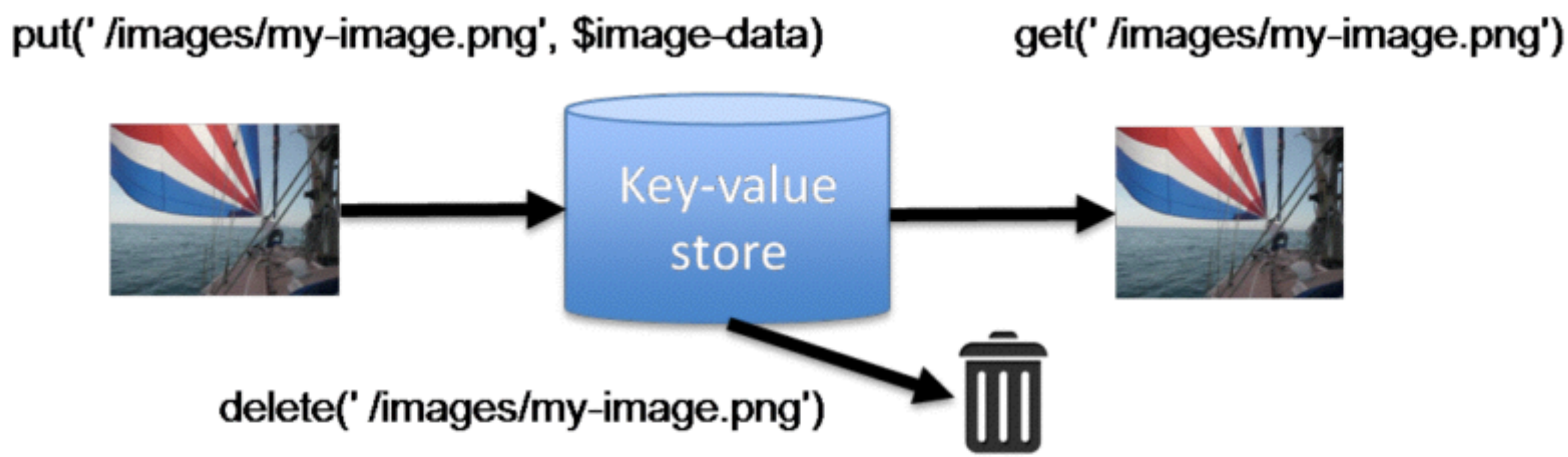
Benefits of key/value stores

- scalable and reliable
  - reason: very simple database interface
- portable and low operational costs
  - simple to plug in different store (or application) because only `put` and `get`

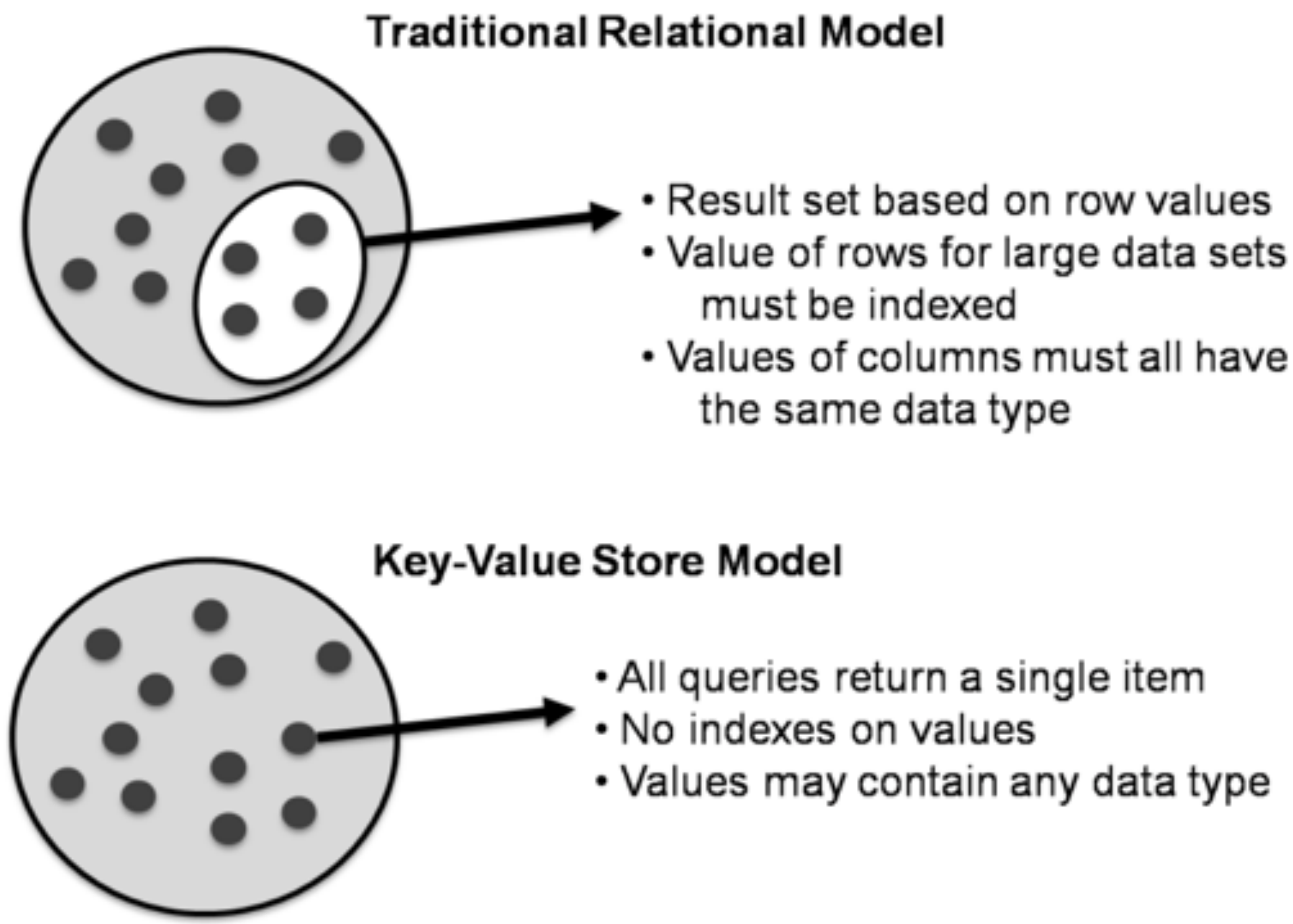
Using a key/value store

- only 3 operations in API: `put`, `get` and `delete`




put(' /images/my-image.png', $image-data)
get(' /images/my-image.png')
Key-value store
delete(' /images/my-image.png')

- only 2 rules:
  - distinct keys: you can never have two items with the same key
  - no queries on values: you cannot select a key/value pair using the value <-> RDBMS: you can constrain a result set using the `WHERE` clause



Use cases

- storing web pages
    - key = URL; value = HTML code of webpage
- Amazon Simple Storage Service (S3)
    - uses a simple REST API (see later in course)
    - = key/value store, plus metadata and access control

Redis

- http://redis.io

redis Commands Clients Documentation Community Download Support License

Redis is an open source (BSD licensed), in-memory **data structure store**, used as database, cache and message broker. It supports data structures such as strings, hashes, lists, sets, sorted sets with range queries, bitmaps, hyperloglogs and geospatial indexes with radius queries. Redis has built-in replication, Lua scripting, LRU eviction, transactions and different levels of on-disk persistence, and provides high availability via Redis Sentinel and automatic partitioning with Redis Cluster.

- http://try.redis.io

```
> set server:name "fido"
OK
> get server:name
"fido"
> SET tom '{name: "Tom Willems", age: 47}'
OK
> get tom
"{name: \"Tom Willems\", age: 47}"
```

- Python API

```
$ sudo pip install redis
```

```
>>> import redis
>>> r = redis.StrictRedis(host='localhost', port=6379, db=0)
>>> r.set('foo', 'bar')
True
>>> r.get('foo')
'bar'
```

column store / “BigTable” database

- proprietary Google BigTable implementation
- database = multiple tables, each containing addressable rows, each row with a set of values in columns
- important differences with RDBMS:
  - each row can have a different set of columns (but common set of “column groups”)
  - tables are intended to have many (>1,000-1,000,000) columns

graph stores

- use *nodes*, *edges* and *properties* as primary elements
- different underlying infrastructures

NoSQL concepts

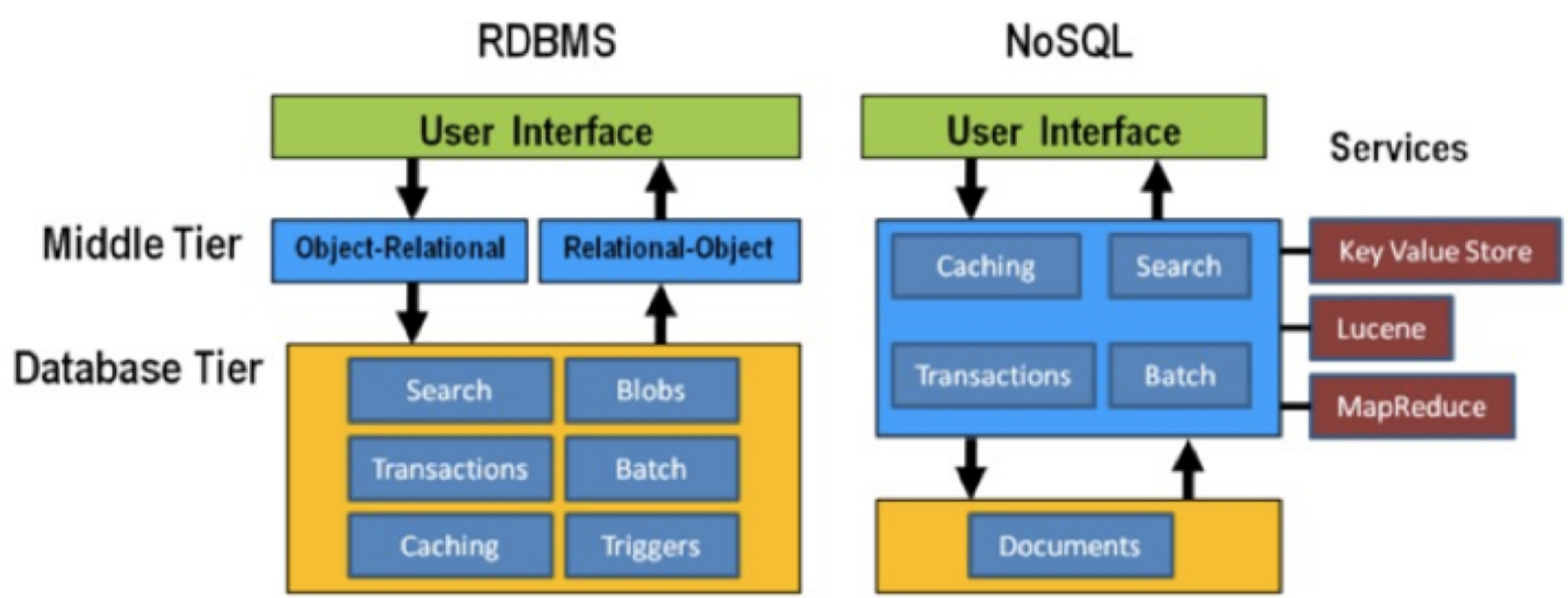
1. keeping components simple to promote reuse: linux pipe philosophy

- NoSQL systems are often created by integrating a large number of modular functions that work together <=> traditional RDBMS: mammoth system
  `cat data.csv | grep “chr1” | cut -f 2 | sort | uniq -c`
- *e.g.* one function allows sharing of objects in RAM, another function to run batch jobs, yet another function for storing documents
- NoSQL system interfaces are broader than regular STDIN and STDOUT (*i.e.* using line delimiters): can be documents, REST, JSON, XML, … services

2. using **application tiers** to simplify design

- by segregating an application into tiers you have the option of modifying or adding a specific layer instead of reworking an entire application => **separation of concerns**
  - Lambda Architecture
  - user interface <-> middle tier <-> database layer (e.g LocusTree)

- where do you put functionality? trade-offs
  - RDBMS: have been along for long time and are mature => much functionality added to database tier
  - NoSQL: most of application functionality is in middle tier



3. speeding performance by **strategic use of RAM, SSD, and disk** (e.g. Spark)

- you: in Leuven
    - getting something from RAM = your backyard
    - getting something from SSD (solid state drive) = somewhere in your neighbourhood
    - getting something from disk = traveling to Saudi Arabia
    - getting something from the network = traveling to Jupiter

4. using **consistent hashing** you keep your cache current

- hash string or checksum = process that calculates sequence of letters by looking at each byte of a document (*e.g.* MD5, SHA-1)

- consistent hashing: quickly tells you if a new query or document is the same as one already in your cache. Consistent hashing occurs when two different processes running on different nodes in your network create the same hash for the same object

- changing a single bit in the object/file changes the MD5 sum

```
md5sum my_file.txt => 5a13448726555d031061aef7432b45c3
```

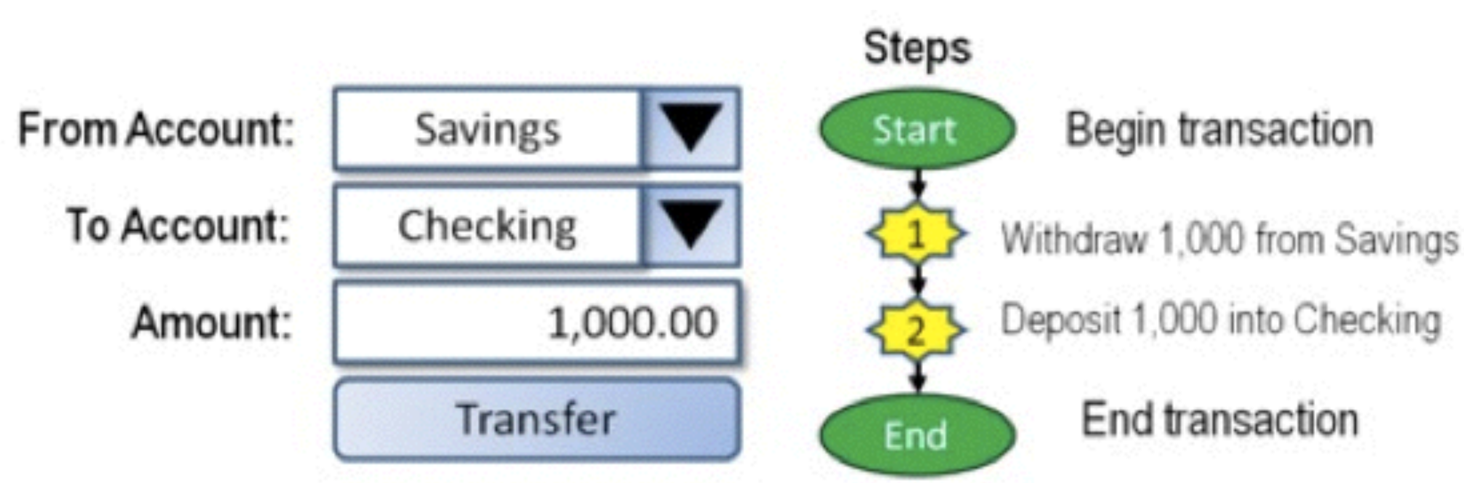
- in principle: possible that 2 different documents create the same hash value = **hash collision**

    - MD5 algorithm: 128 bit string => occurs once every 10^38 documents => if you generate a billion documents a second it would take 10 trillion times the age of the universe for a single accidental collision to occur

- consistent hashing: can also be used to assign documents to specific database nodes

5. **ACID vs BASE** - two methods of reliable database transactions

- ACID & BASE = “transaction control models”
- RDBMS:ACID
  NoSQL: BASE
- example: bank transaction: making sure that the two processes in figure happen either together or not at all



- **ACID**

- **Atomicity** - exchange of funds in example must happen as an all-or-nothing transaction

- **Consistency** - your database should never generate a report that shows a withdrawal from saving without the corresponding addition to the checking account => block all reporting during atomic operations (=> impact on speed!)

- **Isolation** - each part of the transaction occurs without knowledge of any other transaction

- **Durability** - once all aspects of transaction are complete, it’s permanent

- software to handle these rules = very complex (50-60% of the codebase => new databases often do not support database-level transaction management in their first release)

- all transaction control strategies: depend on resource locking

- ACID systems: focus on consistency and integrity of data above all other considerations (temporarily blocking reporting mechanisms is a reasonable compromise to ensure systems return reliable and accurate information) => *pessimistic*

- **BASE**
  - **Basic Availability** - information and service capability are “basically available” (you can *always* generate a report)
  - **Soft-state** - some inaccuracy is temporarily allowed and data may change while being used to reduce the amount of consumed resources
  - **Eventual consistency** - eventually, when all service logic is executed, the systems is left in a consistent state

e.g. shopping carts: no problem if back-end reports are inconsistent for a few minutes; it’s more important that the customer can actually purchase things

- ACID: focuses on consistency <-> BASE: focuses on availability

- BASE = *optimistic*: eventually all systems will catch up and be consistent

- BASE systems tend to be much simpler and faster <= don’t have to write code that deals with locking and unlocking resources

- ACID vs BASE != black vs white; continuum

6. **Horizontal scalability** through **database sharding**

- In RDMBS: automatic sharding
- As number of servers grows: higher chance that one will go down => duplicate data to backup or mirrored system = data **replication**

An example - small scale

Employee database

- Database containing all information about employees: name, address, contract(s), …
  - One individual can have several subsequent contracts
- Can be kept in relational database (e.g. mysql), but we can still use Lambda Architecture principles
  - key: immutability

Using *views*

ID	name	phone	address
1	Tim Janssen	+32 272618273	St-Jobsweg 143, Berchem
2	Filip Beckaert	+32 918274917	Karmstraat 2, Vissenaken
3	Bart Willard	+32 726291726	Kipdorpstraat 101, St Niklaas
...	...	...	...

individuals

contracts

ID	individual_id	start_date	stop_date
1	1	20141001	20150930
2	1	20151001	20160930
3	2	20140401	20150331
...	...	...	...

```sql
CREATE VIEW v_current_individuals AS
SELECT i.id, i.name, i.phone, i.address
FROM individuals i
WHERE EXISTS (
  SELECT * FROM contracts c
  WHERE c.individual_id = i.id
  AND c.start_date <= CURDATE()
  AND CURDATE() <= c.stop_date
)
```

v_current_individuals

ID	name	phone	address
1	Tim Janssen	+32 272618273	St-Jobsweg 143, Berchem
3	Bart Willard	+32 726291726	Kipdorpstraat 101, St Niklaas
...	...	...	...

Filip Beckaert (ind 2) doesn't work here anymore

=> every individuals who ever worked at the company stays in the "individuals" table

An example - larger scale

What do we have? What do we need?

- The data: twitter at Belgian scale (= not optimised/tweaked)
  - profile data (username, real name, gender, language, …)
  - user clicks “follow” on profile of other user
  - actual (re)tweets (timestamp, sender, text)
- The uses
  - key influencers (= those with most retweets)
  - suggest new people to follow
  - what are the trending hashtags?
  - twitter analytics

Batch layer - the ground truth

- immutable; add, don’t update
  - necessary for profile data?
  - can e.g. be regular csv files

name, twitter handle, gender, language

profile

```
Tim Janssen;tjanssen;male;Dutch
Filip Beckaert;beck;male;Dutch
Bart Willard;bartw;male;English
...
```

timestamp, twitter handle, object, action

followers

```
20150105T0345;tjanssen;bartw;follow
20150105T0532;tjanssen;beck;follow
20150512T1917;tjanssen;realdonaldtrump;follow
20150512T1921;tjanssen;realdonaldtrump;unfollow
20150512T2331;bartw;tjanssen;follow
...
```

timestamp, twitter handle, text

tweets

```
20150105T0348;tjanssen;"Just followed @bartw"
20150105T0529;bartw;"Moules-frites… The best…"
20150512T1924;tjanssen;”Is anyone going to #tedxbrussels?"
20150513T0815;bartw;"#crispr now identified in viruses as well"
...
```

Serving layer

- convert data in batch layer into form that can answer the uses

- **Twitter analytics**

One per month: run over data in batch layer and count => store in key-value store

```
tjanssen_201602
  => {tweets: 14,
      impressions:10391,
      visits: 591,
      mentions: 12,
      new_followers: 16}
bartw_201602
  => ...
```

- **trending hashtags**

Trends · Change
#TwoWordTrump
#power2women
#BANvPAK
#GPSamyn
#COP21
Adam Johnson
Nina Simone
FAN FASTEST 100K LIKES
Greece
Finding Dory

```
20150105T0348;tjanssen;"Just followed @bartw"
20150105T0529;bartw;"Moules-frites… The best…"
20150512T1924;tjanssen;”Is anyone going to #tedxbrussels?"
20150513T0815;bartw;"#crispr now identified in viruses as well"
...
```

```
Greece;2837
Nina Simone;5922
#crispr;1998
#GPSamin;9283
#TwoWordTrump;27102
#tedxbrussels;2692
...
```

Continuously: run over data in batch layer, count and sort;

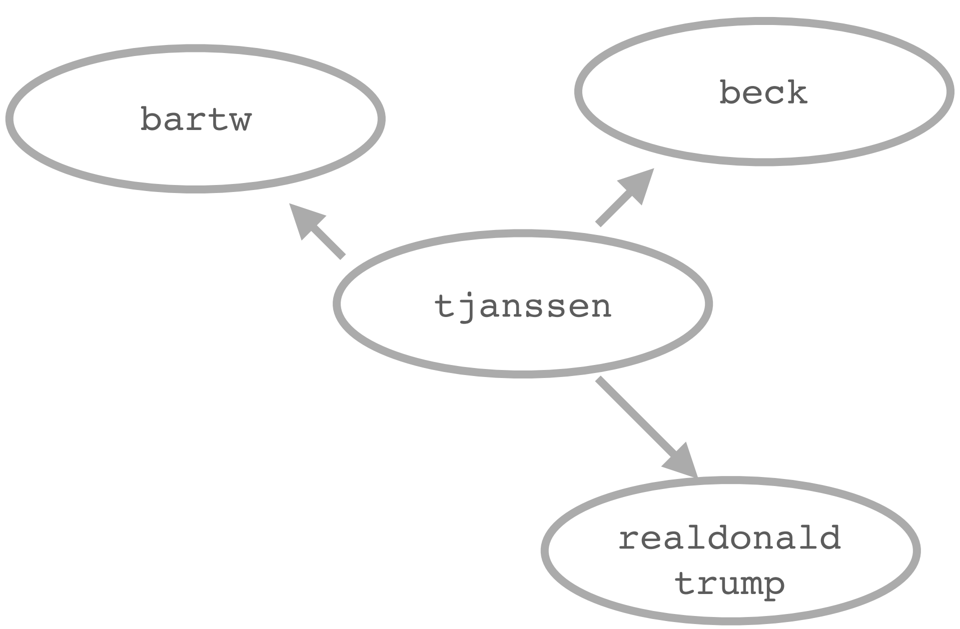
if takes too long: include speed layer (either same computation as serving but only on new data, or completely different incremental algorithm)

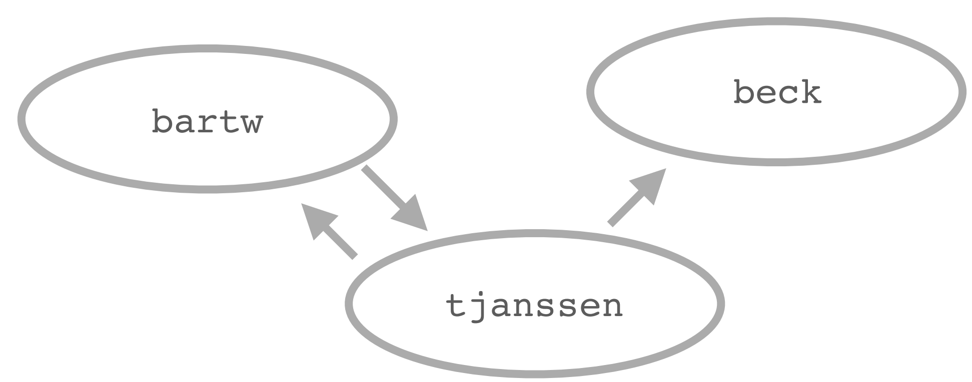
- **suggest new people to follow**
  who are key influencers?
  who are more popular?

Continuously: run over data in batch layer, create nodes and links in graph

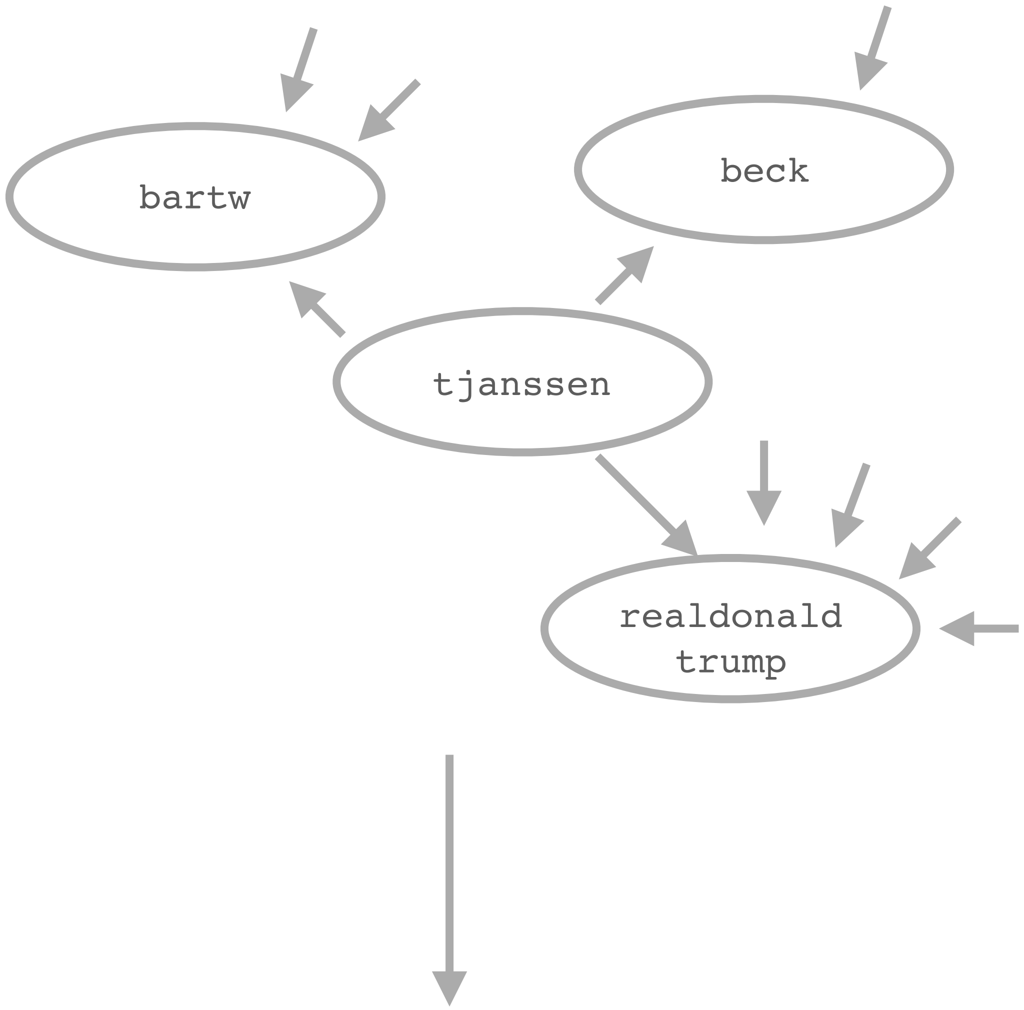
```
20150105T0345;tjanssen;bartw;follow
20150105T0532;tjanssen;beck;follow
20150512T1917;tjanssen;realdonaldtrump;follow
20150512T1921;tjanssen;realdonaldtrump;unfollow
20150512T2331;bartw;tjanssen;follow
...
```

depending on when process is run





in graph database (e.g. Neo4j)



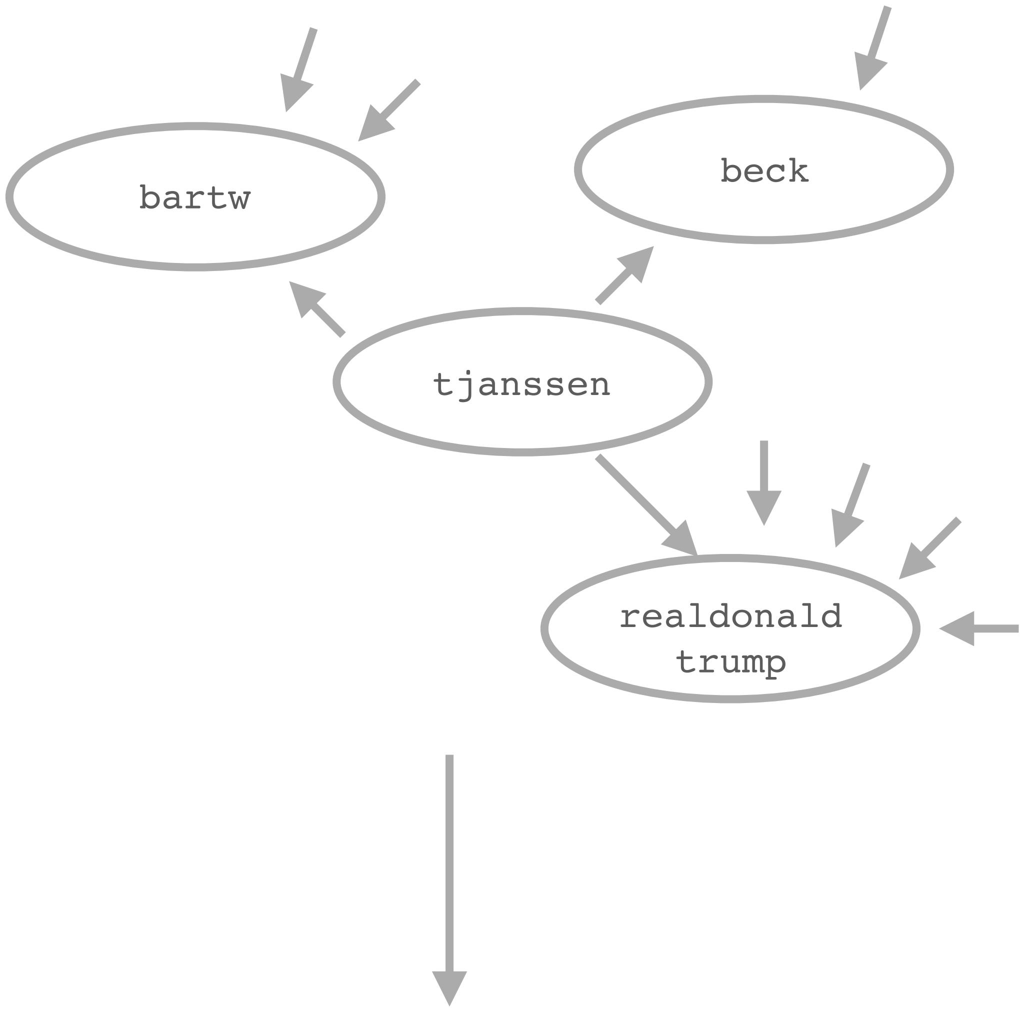
- **who are more popular?**

```
tjanssen => 1,928
realdonaldtrump => 6,570,000
bartw => 3,102
beck => 2,281
…
```

in key/value store?
cannot sort by value

```
tjanssen;1928
realdonaldtrump;6570000
bartw;3102
beck;2281
…
```

in file?



- **who are key influencers?**

e.g. defined as how many followers in three steps?

(easy when using graph database; see later)

in file?

```
tjanssen;24918
realdonaldtrump;87102817
bartw;28172
beck;49812
…
```

in SQL database?

handle	influences
tjanssen	24918
realdonaldtrump	87102817
bartw	28172
beck	49812
…	…