[tile]DB

Using TileDB with R

An Introductory Tutorial

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Overview

Outline

Brief Introduction

Key Topics

- Dense Arrays
- Sparse Arrays
- Full TileDB API
- S3 Access
- Arrow Format
- Time Travel
- Encryption

Applications

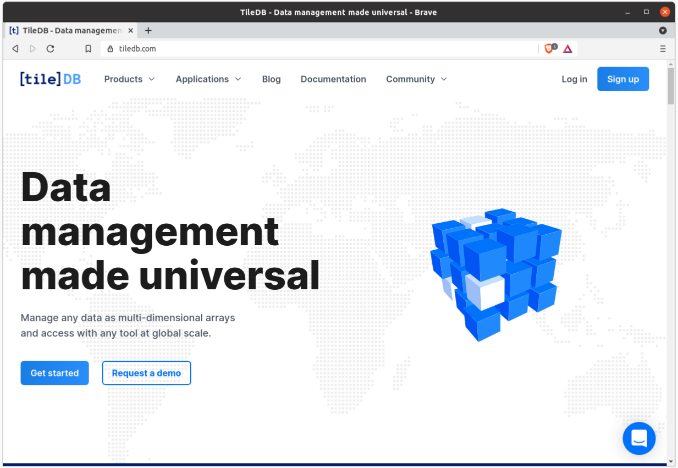
- SQL Access Example
- Data Science with Flights
- LiDAR / Geospatial
- Finance / Time Series
- Genomics: GWAS

Wrap-Up

Further References

Introduction

TileDB



Universal Data Management

Any Data in Multi-Dimensional Arrays

Serverless, and at scale

In this tutorial with an R focus

Tutorial Resources

To install the package with code examples and the slides, use

```
remotes::install_github('eddelbuettel/tiledb-user2021')
```

or

```
repos <- c("https://eddelbuettel.github.io/tiledb-user2021/",
           "https://cloud.r-project.org")
install.packages("tiledb.user2021", repos=repos)
```

Loading the package will show where the example files are located.

The conference slack channel for the tutorial is `#tut_tiledb`.

Introductory Example

```r
# if needed: install.packages("tiledb")      # installation from CRAN
library(tiledb)                               # load the package
library(palmerpenguins)                       # example data
setwd("/tmp")                                 # or other scratch space

# create array from data frame with default settings
fromDataFrame(penguins, "penguins")

# read array as data.frame and without (default, added) row index
arr <- tiledb_array("penguins", as.data.frame=TRUE, extended=FALSE)
show(arr)                                     # some array information
```

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Introductory Example (cont.)

```
> df <- arr[]
> str(df)
'data.frame':	344 obs. of  8 variables:
 $ species          : chr  "Adelie" "Adelie" "Adelie" "Adelie" ...
 $ island           : chr  "Torgersen" "Torgersen" "Torgersen" "Torgersen" ...
 $ bill_length_mm   : num  39.1 39.5 40.3 NA 36.7 39.3 38.9 39.2 34.1 42 ...
 $ bill_depth_mm    : num  18.7 17.4 18 NA 19.3 20.6 17.8 19.6 18.1 20.2 ...
 $ flipper_length_mm: int  181 186 195 NA 193 190 181 195 193 190 ...
 $ body_mass_g      : int  3750 3800 3250 NA 3450 3650 3625 4675 3475 4250 ...
 $ sex              : chr  "male" "female" "female" NA ...
 $ year             : int  2007 2007 2007 2007 2007 2007 2007 2007 2007 2007 ...
>
```

Introductory Example (cont.)

Key Features

- We will discuss available options to create arrays
  - dense arrays versus sparse arrays
  - one or multiple indices (on sparse arrays)
  - options for creating and accessing arrays
  - but we mention tuning (tile extent, tile layout, ...) only in passing
- We will show different ways to read arrays back into R

Dense Arrays

Dense Data

The introductory example `quickstart_dense.R` creates an array with two integer domains and a single integer attribute:

```
# The array will be 4x4 with dims "rows" and "cols" and domain [1,4]
dom <- tiledb_domain(dims = c(tiledb_dim("rows", c(1L, 4L), 4L, "INT32"),
                              tiledb_dim("cols", c(1L, 4L), 4L, "INT32")))
# The array will be dense with a single attribute "a" so
# each cell (i,j) cell can store an integer.
schema <- tiledb_array_schema(dom, attrs=c(tiledb_attr("a", type="INT32")))
# Create the (empty) array on disk.
uri <- "quickstart_dense"
tiledb_array_create(uri, schema)
```

Dense Data (cont.)

Having created the array we can now open it for writing and add data.

```
# equivalent to matrix(1:16, 4, 4, byrow=TRUE)
data <- array(c(c(1L, 5L, 9L, 13L),
                c(2L, 6L, 10L, 14L),
                c(3L, 7L, 11L, 15L),
                c(4L, 8L, 12L, 16L)), dim = c(4,4))
# Open the array and write to it.
A <- tiledb_array(uri = uri)
A[] <- data
```

Dense Data (cont.)

Data can be read back with different convenience wrappers:

```
arr <- tiledb_array(uri); arr[]                              # list of columns

arr <- tiledb_array(uri, as.data.frame=TRUE); arr[] # a data.frame

arr <- tiledb_array(uri, as.matrix=TRUE); arr[]     # a matrix

arr <- tiledb_array(uri, as.array=TRUE); arr[]      # an array
```

Dense Data (cont.)

A data.frame example for dense arrays:

```
library(tiledb)              # load our package
uri <- tempfile()            # any local directory, more later on cloud access

## any data.frame, data.table, tibble ...; here we use penguins_raw
fromDataFrame(palmerpenguins::penguins_raw,  uri)

# we want a data.frame, and we skip the implicit row numbers added as index
x <- tiledb_array(uri, as.data.frame = TRUE, extended = FALSE)

newdf <- x[]                 # full array (we can index rows and/or cols too)
```

Dense Data (cont.)

```
> str(newdf[, 1:14])   # omitting last three cols for brevity
'data.frame':   344 obs. of  17 variables:
 $ studyName           : chr  "PAL0708" "PAL0708" "PAL0708" "PAL0708" ...
 $ Sample Number       : num  1 2 3 4 5 6 7 8 9 10 ...
 $ Species             : chr  "Adelie Penguin (Pygoscelis adeliae)"  ...
 $ Region              : chr  "Anvers" "Anvers" "Anvers" "Anvers" ...
 $ Island              : chr  "Torgersen" "Torgersen" "Torgersen" "Torgersen" ...
 $ Stage               : chr  "Adult, 1 Egg Stage" "Adult, 1 Egg Stage" ...
 $ Individual ID       : chr  "N1A1" "N1A2" "N2A1" "N2A2" ...
 $ Clutch Completion   : chr  "Yes" "Yes" "Yes" "Yes" ...
 $ Date Egg            : Date, format: "2007-11-11" ...
 $ Culmen Length (mm) : num  39.1 39.5 40.3 NA 36.7 39.3 38.9 39.2 34.1 42 ...
 $ Culmen Depth (mm)  : num  18.7 17.4 18 NA 19.3 20.6 17.8 19.6 18.1 20.2 ...
 $ Flipper Length (mm): num  181 186 195 NA 193 190 181 195 193 190 ...
 $ Body Mass (g)       : num  3750 3800 3250 NA 3450 ...
 $ Sex                 : chr  "MALE" "FEMALE" "FEMALE" NA ...
```

Sparse Arrays

Sparse Array: Numeric

```
library(tiledb)                       # TileDB package
library(Matrix)                       # for sparse matrix functionality
uri <- tempfile()                     # array location
set.seed(123)                         # fix RNG seed

mat <- matrix(0, nrow=8, ncol=20)
mat[sample(seq_len(8*20), 15)] <- seq(1, 15)
spmat <- as(mat, "dgTMatrix")         # new sparse 'dgTMatrix'

fromSparseMatrix(spmat, uri)          # store the sparse matrix in TileDB
chk <- toSparseMatrix(uri)            # and retrieve it to check
```

Sparse Array: Numeric (cont.)

```
> chk      # to check retrieved sparse matrix
8 x 20 sparse Matrix of class "dgTMatrix"

[1,] . . . . . . . .  . . .  .  . . . . . 13  . 8
[2,] . . . . . . 3 .  . . .  9  . . . . .  .  . .
[3,] . . . . . 5 . .  . . . 10 14 . . . .  .  . .
[4,] . . . . . . . .  . . . 12  . . . . .  .  . .
[5,] . . . . . . . .  . . .  .  . . . . .  .  . 7
[6,] . 2 . . . . . .  . . .  .  . . 4 . .  .  . .
[7,] . . . . . . . .  . . .  .  . . . . .  . 11 1
[8,] . . . . . . . . 15 . .  .  . . . . .  .  . 6
>
```

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Sparse Array: Data Frame

```r
library(tiledb)              # load our package
uri <- tempfile()            # any local directory, more later on cloud access
## now sparse with a character and integer ('year') index colum
## with wider range than seen in the data for year we allow appending
fromDataFrame(palmerpenguins::penguins,  uri, sparse = TRUE,
              col_index = c("species", "year"),
              tile_domain=list(year=c(2000L, 2021L)))

x <- tiledb_array(uri, as.data.frame = TRUE, extended = FALSE)
newdf <- x[]                 # full array (we can index rows and/or cols too)
```

Sparse Array: Data Frame (cont.)

```
x <- tiledb_array(uri, as.data.frame = TRUE, extended = FALSE)
selected_ranges(x) <- list(year=cbind(2007L, 2008L),
                           species=cbind("Gentoo", "Gentoo"))
newdf <- x[]
```

Now we retrieve with two constraints: ‘years’ from 2007 to 2008 (both included), and ‘species’ equal to “Gentoo” (given as lower and upper range which implies equality). Note that both are *dimension* columns.

Sparse Array: Data Frame (cont.)

```
qc <- tiledb_query_condition_init("body_mass_g", 6000, "INT32", "GE")
query_condition(x) <- qc
newdf <- x[]
```

This selects rows based on the given attribute value, here `body_mass_g` which is required to be greater or equal to 6000 (grams).

Query conditions on attributes can also be combined (via standard Boolean operators).

Also (but not on CRAN yet): `qc <- parse_query_condition(body_mass_g >= 6000)`

Sparse Array: Select Attribute Columns

```r
x <- tiledb_array(uri, as.data.frame = TRUE, extended = FALSE)
attrs(x) <- c("island", "sex")
```

This results in just the two selected attribute columns being returned (along with the two dimension columns).

Column selections can be combined with row selections.

Sparse Array: Incremental Writes

Setting the initial *domain* of the dimension columns (to ranges that accomodate future writes) allows incremental writes in batches.

As TileDB is serverless and inherently parallel, multiple writes can be made at the same time.

fromDataFrame & tiledb_array

fromDataFrame

High-level Array Writer

- Helper function to *create* arrays from existing data.frame data in R
- Can write dense arrays as well as sparse arrays
  - can add ad-hoc row-indices (dense and sparse)
  - or can use multiple index colums (sparse)
  - these can use int, numeric, or char data
- Defaults to using a ZStd compression filter
- Can set different TileDB array attributes and parameters
- Can support *append* mode via explicit dimension domain values
- We will see some examples later

tiledb_array

High-level Array Reader

- General array accessor for both dense and sparse arrays
- Supports multiple options to return as
    - data.frame
    - matrix
    - array
- Supports selection of row ranges (via dimension constraint)
- Supports selection of returned columns

Full TileDB API

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Full API

```r
dims <- c(tiledb_dim("rows", c(1L, 4L), 4L, "INT32"),
          tiledb_dim("cols", c(1L, 4L), 4L, "INT32"))
attrs <- tiledb_attr("a", type = "INT32")
schema <- tiledb_array_schema(tiledb_domain(dims), attrs)
tiledb_array_create(uri, schema)
data <- 1:16
arr <- tiledb_array(uri = uri)
qry <- tiledb_query(arr, "WRITE")
qry <- tiledb_query_set_layout(qry, "ROW_MAJOR")
qry <- tiledb_query_set_buffer(qry, "a", data)
qry <- tiledb_query_submit(qry)
qry <- tiledb_query_finalize(qry)
stopifnot(tiledb_query_status(qry)=="COMPLETE")
```

This example shows "quickstart_dense"

Each key function in the underlying TileDB Embedded (C++) API has been wrapped and is accessible directly.

This is useful when the higher-level functions need to be tweaked or customized.

Full API (using R 4.1.0 pipe)

```r
dims <- c(tiledb_dim("rows", c(1L, 4L), 4L, "INT32"),
          tiledb_dim("cols", c(1L, 4L), 4L, "INT32"))
attrs <- tiledb_attr("a", type = "INT32")
schema <- tiledb_array_schema(tiledb_domain(dims), attrs)
tiledb_array_create(uri, schema)
data <- 1:16
tiledb_array(uri = uri) |>
    tiledb_query("WRITE") |>
    tiledb_query_set_layout("ROW_MAJOR") |>
    tiledb_query_set_buffer("a", data) |>
    tiledb_query_submit() |>
    tiledb_query_finalize()
stopifnot(tiledb_query_status(qry)=="COMPLETE")
```

This example shows "quickstart_dense" with the native pipe.

As many of the TileDB APi functions operate on the query type argument and return it, this style is easily supported.

Full API

Another example: retrieve the default configuration, overriden number of threads and asking for fragment meta-data consolitation (useful after many chunks have been written):

```
cfg <- tiledb_config()
cfg["sm.num_reader_threads"] <- 8
cfg["sm.num_writer_threads"] <- 8
cfg["vfs.num_threads"] <- 8
cfg["sm.consolidation.mode"] <- "fragment_meta"
ctx <- tiledb_ctx(cfg)
array_consolidate(uri=uri, cfg=cfg)
```

S3

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S3

```r
uri <- "s3://namespace/bucket"          # change URI as needed

## you need either these two environment variables
##   AWS_SECRET_ACCESS_KEY
##   AWS_ACCESS_KEY_ID
## or set this in the TileDB config object

fromSparseMatrix(spmat, uri)     # stored
chk <- toSparseMatrix(uri)       # retrieved

## lazy eval: e.g. for subsets only requested data transferred to client
```

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S3 (cont.)

```
> pp <- tiledb_array("s3://tiledb-conferences/useR-2021/palmer_penguins", as.data.frame=TRUE)
> dat <- pp[]
> head(dat)
  species year    island bill_length_mm bill_depth_mm flipper_length_mm body_mass_g    sex
1  Adelie 2007     Dream           36.0          17.9               190        3450 female
2  Adelie 2007     Dream           42.3          21.2               191        4150   male
3  Adelie 2007 Torgersen           40.3          18.0               195        3250 female
4  Adelie 2007 Torgersen           34.6          21.1               198        4400   male
5  Adelie 2007 Torgersen           36.6          17.8               185        3700 female
6  Adelie 2007 Torgersen           36.7          19.3               193        3450 female
>
```

Arrow

Arrow

```r
suppressMessages( { library(tiledb); library(arrow) } )
val <- 1:3      # arbitrary, could be rnorm() too
typ <- int8()  # any Arrow type
vec <- Array$create(val, typ)           # Arrow vector

aa <- tiledb_arrow_array_ptr()
as <- tiledb_arrow_schema_ptr()
on.exit( { tiledb_arrow_array_del(aa); tiledb_arrow_schema_del(as) } )
arrow::ExportArray(vec, aa, as)  # export Arrow to TileDB

newvec <- arrow::Array$create(arrow::ImportArray(aa, as))
stopifnot(all.equal(vec, newvec))
print(newvec)   # show round-turn
```

Arrow (cont.)

```
> print(newvec)   # show round-turn
Array
<int8>
[
  1,
  2,
  3
]
>
```

Additional examples demonstrate zero-copy transfer from Arrow into TileDB Arrays, and the inverse from TileDB to Arrow.

Additional higher-level functions will likely get added soon.

Time Travel

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Time Travel

```
uri <- "... some uri, either local or on s3 or ..."

arr <- tiledb_array(uri,
                    as.data.frame = TRUE,   # convenient format
                    timestamp = as.POSIXct("2021-01-02 03:04:05"))
## standard access to 'arr' as before
```

TileDB Arrays add content in immutable “layers” (or fragments).

We can access their content at points in time!

Time Travel (cont.)

```
D <- data.frame(key=1:10, value=1:10)
uri <- tempfile()

fromDataFrame(D, uri, col_index="key",
              sparse=TRUE, allows_dups=FALSE)
now <- Sys.time()

Sys.sleep(60)                              # one minute
arr <- tiledb_array(uri)
D$value <- 100 + D$value
arr[] <- D
then <- Sys.time()
```

Time Travel (cont.)

```
## we have written twice
show(arr[])

arrEarlier <- tiledb_array(uri, timestamp=now)
show(arrEarlier[])

arrLater <- tiledb_array(uri, timestamp=then)
show(arrLater[])
```

Encryption

Encryption

```
uri <- "... some uri, either local or on s3 or ..."

arr <- tiledb_array(uri,
                    as.data.frame = TRUE,   # convenient format
                    encryption_key = "...an AES-256 key here...")
## standard access to 'arr' as before
```

TileDB Arrays support encryption. The underlying files are controlled by standard filesystem access control layers, and additionally the content can be encrypted using standard AES-256 technology.

Encryption (cont.)

```r
dom <- tiledb_domain(dims = tiledb_dim("rows", c(1L, 4L), 4L, "INT32"))
schema <- tiledb_array_schema(dom, attrs=tiledb_attr("a", type = "INT32"),
                              sparse = TRUE)
uri <- tempfile()
enckey <- "0123456789abcdef0123456789ABCDEF"
invisible( tiledb_array_create(uri, schema, enckey) ) # schema with key

arr <- tiledb_array(uri, encryption_key = enckey)     # open with key to
arr[] <- data.frame(rows=1:4, a=101:104)              # write and read

chk <- tiledb_array(uri, encryption_key = enckey, as.data.frame=TRUE)
chk[]
```

Applications

SQL

SQL

Setup

- TileDB integrates with different frontends as well as languages
- One example: MariaDB with TileDB accessed via a 'storage plugin'
- Due to architectural choices at MariaDB, plugins
    - have to be compiled with the exact configuration as the server itself
    - we need to consistently build MariaDB, TileDB plugin ... and TileDB
- One easy way to do this is via Docker container `tiledb-mariadb-r`
- See `https://hub.docker.com/r/tiledb/tiledb-mariadb-r/`

SQL (cont.)

Setup (cont.)

We launch the container as a daemon, allow MariaDB to accept empty password, and name the running image 'tiledb-mariadb-r':

```
## line break for display here
docker run --name tiledb-mariadb-r -it -d --rm \
   -e MYSQL_ALLOW_EMPTY_PASSWORD=1 tiledb/tiledb-mariadb-r
```

If desired, we can mount local directories via the standard Docker option `-v local:container` to access host data in container.

SQL (cont.)

We then start R via Docker connecting to this session:

```
docker exec -it -u root tiledb-mariadb-r R
```

and in R write

```
library(tiledb)
fromDataFrame(palmerpenguins::penguins_raw, "/tmp/penguinsraw")
```

to create a TileDB Array in the context of the container.

SQL (cont.)

We then start R again via the same command for another R shell but now access the data.

Note that per standard semantics this query did *not* yet materialize.

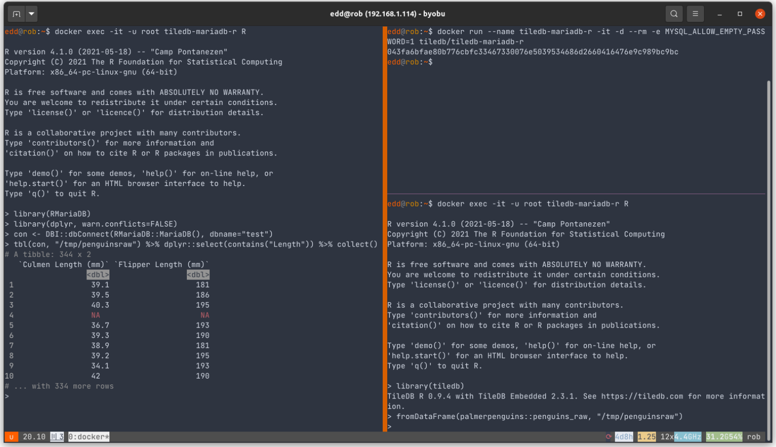
```
> library(RMariaDB)
> library(dplyr, warn.conflicts=FALSE)
> con <- DBI::dbConnect(RMariaDB::MariaDB(), dbname="test")
> tbl(con, "/tmp/penguinsraw") |> dplyr::select(contains("Length"))
# Source:   lazy query [?? x 2]
# Database: mysql [@localhost:NA/test]
   `Culmen Length (mm)` `Flipper Length (mm)`
                  <dbl>                 <dbl>
 1                 39.1                   181
 2                 39.5                   186
 3                 40.3                   195
 4                 NA                      NA
 5                 36.7                   193
 6                 39.3                   190
 7                 38.9                   181
 8                 39.2                   195
 9                 34.1                   193
10                 42                     190
# ... with more rows
>
```

SQL (cont.)

By adding `collect()` to the pipeline we ensure an actual retrieval of the data.

```
> tbl(con, "/tmp/penguinsraw") |>
+     dplyr::select(contains("Length")) |>
+     collect()
# A tibble: 344 x 2
   `Culmen Length (mm)` `Flipper Length (mm)`
                  <dbl>                 <dbl>
 1                 39.1                   181
 2                 39.5                   186
 3                 40.3                   195
 4                 NA                      NA
 5                 36.7                   193
 6                 39.3                   190
 7                 38.9                   181
 8                 39.2                   195
 9                 34.1                   193
10                 42                     190
# ... with 334 more rows
>
```

SQL (cont.)



Start with top right to launch container ad daemon.

Next bottom right to create an array.

Finally left pane to access it.

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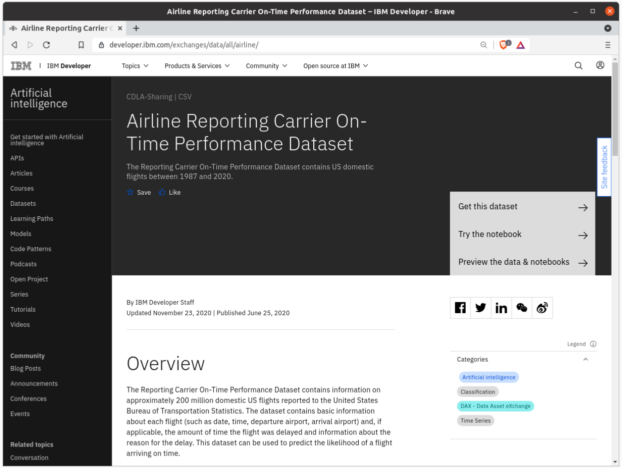
Data Science with Flights Data

Data Science Example: Large Data Frame

We have already seen several examples for data.frames. The ability to index on different column types maps well with data.frame objects.

This example uses the well known flights data set.

Data Science Example: Large Data Frame



We use the full 'flights' data set (available under a permissible data license at the IBM site shown on the left.

It is available as both the full data set with 194 million rows, as well as in a 2 million row subset.

Large Data Frame (cont.)

Creating the TileDB Array

The data comes as `tar.gz` containing a compressed csv file.

We cannot efficiently read all of the csv so we wrap a loop around, extracting chunks (via `sed`) which `data.table::fread()` can ingest. (We also skip a number of uninformative extra columns.)

We select four index columns. Three of these are character based and automatically obtain a `<null,null>` domain which we can append to.

For the fourth, we explicitly set an earlier start data and later (current) end date.

Large Data Frame (cont.)

```r
createIteratively <- function(csvxzfile, uri, n=100000, N=2000000) {
    stopifnot(`no csv.xz`=file.exists(csvxzfile))

    cmd <- paste0("xz -c -d ", csvxzfile, "| sed -n -e'1,", format(n+1, scientific=FALSE), "'p")
    cat(cmd, "\n")
    D <- fread(cmd=cmd, drop=c(48,57:109))
    cn <- colnames(D)   # used below
    D <- filterData(D)  # helper converting a few columns: utf8 char, bool to int, factor to char
    if (tiledb_vfs_is_dir(uri)) tiledb_vfs_remove_dir(uri)
    fromDataFrame(D, uri, sparse=TRUE,
                  col_index = c("FlightDate", "Reporting_Airline", "Origin", "Dest"),
                  tile_domain=list(FlightDate=c(as.Date("1970-01-01"), Sys.Date())))
    written <- n        # keep track of data written

    ## remainder on next slide
```

Large Data Frame (cont.)

```r
    ## continued from previous slide

    arr <- tiledb_array(uri)
    while (written < N) {
        cmd <- paste0("xz -c -d ", csvxzfile, "| sed -n -e'1d' -e'",
                      format(written+1+1, scientific=FALSE), ",",
                      format(min(written+n+1, N+1), scientific=FALSE), "'p")
        cat(cmd, "\n")
        D <- fread(cmd=cmd, drop=c(48,57:109))
        colnames(D) <- cn                    # assign colnames from first chunk
        D <- filterData(D)
        arr[] <- D                           # append chunk to TileDB array
        written <- written + n
    }
    invisible(NULL)
}
```

Large Data Frame (cont.)

Operating on the full dataset–but selecting *by dimensions* 'FlightDate' and 'Reporting_Airline':

```
arr <- tiledb_array(uri, as.data.frame=TRUE)
fromD <- as.Date("2000-01-01")
toD <- as.Date("2000-12-31")
selected_ranges(arr) <- list(FlightDate=cbind(fromD, toD),
                             Reporting_Airline=cbind("UA", "UA"))
res <- arr[]
print(dim(res)) ## 776559 x 55
```

Large Data Frame (cont.)

We we add additional conditions on attributes:

```
## as before
qc1 <- tiledb_query_condition_init("ArrDelay", 120, "FLOAT64", "GE")
qc2 <- tiledb_query_condition_init("DepDelay", 120, "FLOAT64", "GE")
query_condition(arr) <- tiledb_query_condition_combine(qc1, qc2, "AND")
res <- arr[]
print(dim(res))  ## now 21893 x 55
```

Large Data Frame (cont.)

With not-yet-on-CRAN-but-at-GitHub current version can use a more direct approach:

```
qc <- parse_query_condition(ArrDelay >= 120.001 && DepDelay >= 120.001)
query_condition(arr) <- qc
res <- arr[]
print(dim(res))  ## now 21893 x 55
```

(The query condition parsing is independent of the array and does not know the underlying types which is why we used 120.001 to provide a hint that the delay columns are FLOAT64.)

Large Data Frame (cont.)

Not that this is fully remote evaluation: we transmit the request including the selection constraints, and only the requested data is returned: here 22k rows out of 194 million.

Large Data Frame and SQL

We combine the two previous applications! Launching first in the directory above the 'flights' array:

```
docker run --name tiledb-mariadb-r -it -d --rm \
       -e MYSQL_ALLOW_EMPTY_PASSWORD=1 \
       -v $PWD:/mnt tiledb/tiledb-mariadb-r
```

to make the current ("outer") directory (accessed via shell variable `$PWD`) in the container a path `/mnt`. Then we launch `R` in the container via

```
docker exec -it -u root tiledb-mariadb-r R
```

Large Data Frame and SQL

```
> library(RMariaDB); library(dplyr, warn.conflicts=FALSE)
> con <- DBI::dbConnect(RMariaDB::MariaDB(), dbname="test")
> tbl(con, "/mnt/airline") |> dplyr::select(contains("Dep"))
# Source:   lazy query [?? x 7]
# Database: mysql [@localhost:NA/test]
   DepartureDelayGroups DepDel15 DepTime DepTimeBlk DepDelay DepDelayMinutes
                  <int>    <dbl>   <int> <chr>         <dbl>           <dbl>
 1                    0        0    1402 1400-1459         1               1
 2                    0        0    1750 1700-1759         0               0
 3                    0        0    1108 1100-1159         0               0
 4                    0        0     511 0001-0559         0               0
 5                    0        0     928 0900-0959         1               1
 6                    0        0    1631 1600-1659         1               1
 7           2147483647        0    2111 2100-2159        -3               0
 8           2147483647        0    1305 1300-1359        -1               0
 9                    0        0     858 0800-0859         3               3
10                    0        0     648 0600-0659         2               2
# ... with more rows, and 1 more variable: CRSDepTime <int>
>
```

[tile]DB

LiDAR

LiDAR

- LiDAR stands for Light Detection and Ranging
- It is a method for determining ranges (often using lasers)
- Used in spatial analysis, forestry, or even autonomous driving
- Many (public) data sets via LAS or LAZ (compressed) files
- As these are multidimensional arrays use maps well to TileDB

Lidar Ingest

The PDAL (Point Data Abstraction Library) is central, and the `pdal` binary can be built with TileDB support.

We use a Docker container tiledb-geospatial to read LAS (or LAZ) files and create an array as described on the TileDB docs website.

Command:

```
pdal pipeline -i pipeline.json
```

where `pdal` may come from the tiledb-geospatial container, and the JSON control file shown to the right might control *reading* and *writing* steps.

```
[
    {
    "type": "readers.las",
    "filename": "autzen.laz"
    },
    {
    "type": "writers.tiledb",
    "array_name": "autzen_tiledb",
    "chunk_size": 10000000
    }
]
```

LiDAR

```r
lasfile <- "LAS_17258975.las"
if (!file.exists(lasfile)) {
    ## note: the file is 451 mb
    op <- options()                        # store
    options(timeout=3600)                  # (much) more patience downloading
    lasfileurl <- file.path("https://clearinghouse.isgs.illinois.edu/las-east/cook/las/", lasfile)
    download.file(lasfileurl,lasfile)
    options(op)                            # reset
}

if (!dir.exists("las_array")) {
    wd <- getwd()
    cmd <- paste0("docker run --rm -ti -u 1000:1000 -v ", wd, ":/data ",
                  "-w /data tiledb/tiledb-geospatial pdal pipeline -i pipeline.json")
    system(cmd)                            # fancier return code check possible
}
```

LiDAR (cont.)

Note that we can loop similarly over many LAS or LAZ files, and can also inject them in parallel. The JSON file needs `"append": true` to append; this way we can store *many* LAS or LAZ files in a single TileDB Array, locally or in the cloud.

Being able to store many such files in a single (cloud-hosted or local) array shows one of the strengths of TileDB. And data requests will transfer only the requested subset.

LiDAR (cont)

We can then read from the LiDAR array. The following extracts just 100k rows of points from a well-known building:

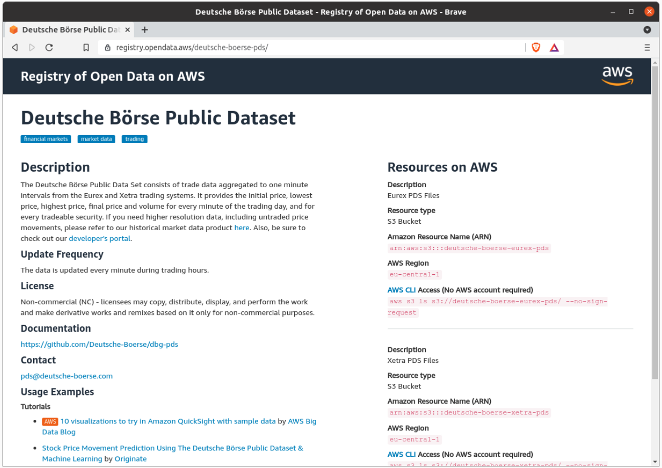
```
library(tiledb)
arr <- tiledb_array("las_array", as.data.frame=TRUE)
selected_ranges(arr) <- list(X = cbind(1174100, 1174400),  Y = cbind(1899125, 1899250))
L <- arr[]
## print(dim(L))    # 108655 x 15

library(lidR)
L$ScanAngleRank <- as.integer(L$ScanAngleRank)
LL <- LAS(L)
plot(LL)                                  # open rgl device
## plot(LL, backend="lidRviewer")         # if lidRviewer is installed
```

Finance / Time Series

Time Series

TileDB can also be used for financial data such as transactions data from an exchange, times and sales data from trades, or aggregates. In this example we will look at a data set provided (and regularly updated) by Deutsche Boerse covering one-minute bars of each stock and etf (for the stock exchanges) and each future (for the Eurex sister exchange focussing on derivatives).

Time Series



Provided by the exchange via AWS

"[...] provides the initial price, lowest price, highest price, final price and volume for every minute of the trading day, and for every tradeable security."

"If you need higher resolution data, including untraded price movements, please refer to our historical market data product here."

Time Series

List the files (here a small demo sample).

Helper function to construct datetime column, and remove date and time columns.

Simple injection loop. First file creates the array and defines the schema. We set minimum amd maximum time values.

Injection could run in parallel, or an automated script appending new data.

```
uri <- "dboerse"
files <- list.files(pattern="2020-.*\\.csv") # files retrieved Fall of 2020

readAndAddDatetime <- function(file) {  # simple helper
    D <- fread(file)
    setDT(D)
    D[, Datetime := as.POSIXct(paste(Date, Time))]
    D[, `:=`(Date = NULL, Time = NULL)]
    invisible(D)
}

n <- length(files)
for (i in seq_len(n)) {
    D <- readAndAddDatetime(files[i])
    if (i == 1) {
        fromDataFrame(D, uri, sparse = TRUE,
                      col_index=c("Mnemonic","Datetime"),
                      tile_domain=list(Datetime=c(as.POSIXct("1970-01-01 00:00:00"), Sys.time())))
    } else {
        arr <- tiledb_array(uri, as.data.frame = TRUE)
        arr[] <- D
        tiledb_array_close(arr)
    }
}
```

Time Series

Simple usage example: one hour of BMW trades in one-minute bars

```
arr <- tiledb_array(uri, as.data.frame = TRUE)
selected_ranges(arr) <- list(Mnemonic=cbind("BMW", "BMW"),
                             Datetime=cbind(as.POSIXct("2020-11-04 09:00"),
                                            as.POSIXct("2020-11-04 10:00")))
BMW <- arr[]
```

Time Series

```r
suppressMessages({
    library(rtsplot)                          # for nicer financial plot
    library(xts)                              # used by rtsplot
})
setDT(BMW)
symbol <- ”BMW”
rt <- as.xts(BMW[Mnemonic==symbol,
                 .(Datetime, Open=StartPrice, High=MaxPrice,
                   Low=MinPrice, Close=EndPrice, Volume=TradedVolume)])

cols <- rtsplot.colors(2)
layout(c(1,1,1,1,2))
rtsplot(rt, type=”n”)
rtsplot.ohlc(rt, col=rtsplot.candle.col(rt))
rtsplot.legend(symbol, cols[1], list(rt))
rt <- rtsplot.scale.volume(rt)
rtsplot(rt, type = 'volume', plotX = FALSE, col = 'darkgray')
rtsplot.legend('Volume', 'darkgray', quantmod::Vo(rt))
```

GWAS

What *is* a GWAS?

Overview

- *GWAS*: Genome-wide Association Study
- Used to identify regions of the genome that are associated with a particular trait (e.g., hair color)
- Requires:
    1) sequencing data on a large population of samples to identify genetic variants
    2) measurements for the trait of interest across the same samples

GWAS Results Example

variant	beta	se	tstat	pval
1:15791:C:T	-1.70174e+01	5.66755e+01	-3.00260e-01	7.63979e-01
1:69487:G:A	-5.70053e-02	1.11014e-01	-5.13496e-01	6.07605e-01
1:69569:T:C	-2.30684e-03	1.99098e-02	-1.15865e-01	9.07760e-01
1:139853:C:T	-5.62416e-02	1.11017e-01	-5.06603e-01	6.12434e-01
1:692794:CA:C	7.72562e-04	9.22074e-04	8.37852e-01	4.02114e-01
1:693731:A:G	1.31202e-03	8.71218e-04	1.50596e+00	1.32078e-01
1:707522:G:C	8.77269e-04	9.79498e-04	8.95631e-01	3.70450e-01
1:717587:G:A	-8.32431e-05	2.33724e-03	-3.56160e-02	9.71589e-01
1:723329:A:T	-1.15975e-02	6.88597e-03	-1.68422e+00	9.21406e-02
1:730087:T:C	4.23934e-05	1.21371e-03	3.49286e-02	9.72137e-01

Data source: UK Biobank

About

Provides an incredibly rich source of biomedical data collected from hundred of thousands of volunteers in the United Kingdom.

UK Biobank GWAS Dataset Stats

- Contains ~12,000 GWAS results files
- Analyzed over >4,000 traits across >350,000 individuals
- Also includes different versions of each analysis (e.g., sex-specific results)
- Each file:
  - contains ~10 million rows
  - ~500Mb gzipped (1.7Gb uncompressed)

UK Biobank announcement:

`http://www.nealelab.is/uk-biobank/ukbround2announcement`

Data Accessibility Goals

- Available on a remote cloud bucket
- Facilitate comparisons across phenotypes
- Query variants by their genomic location
- Query traits by their descriptive names

Tutorial Files

Copy GWAS tutorial to your working directory

```
# library(tiledb.user2021)
file.copy(
  from = system.file("examples/exGWAS.R", package = "tiledb.user2021"),
  to = "exGWAS.R"
)
```

Download GWAS results files

```
dir.create("gwas-tutorial/data", recursive = TRUE)
download_gwas_files("gwas-tutorial/data")
```

Extracting Genomic Location Data

variant
1:15791:C:T
1:69487:G:A
1:69569:T:C
1:139853:C:T
1:692794:CA:C
1:693731:A:G
1:707522:G:C
1:717587:G:A

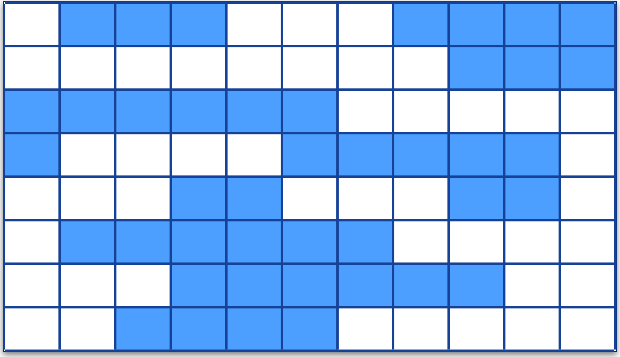
becomes

chr	pos	ref	alt
1	15791	C	T
1	69487	G	A
1	69569	T	C
1	139853	C	T
1	692794	CA	C
1	693731	A	G
1	707522	G	C
1	717587	G	A

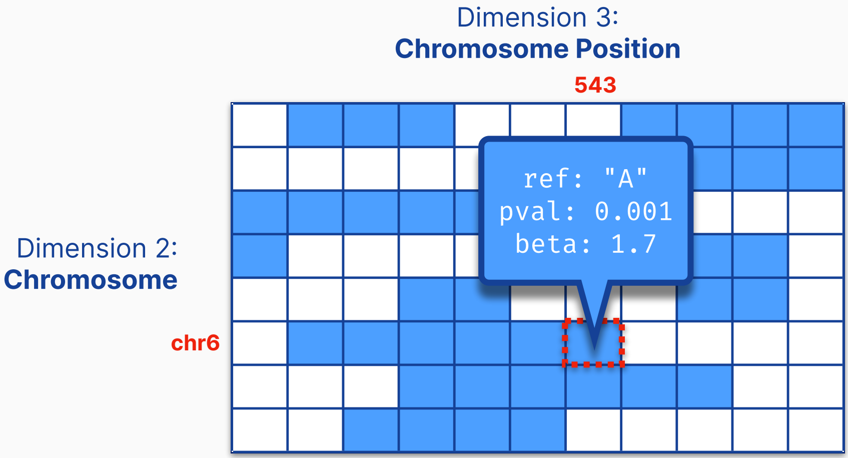
GWAS Array Layout

Dimension 3:
Chromosome Position

Dimension 2:
Chromosome

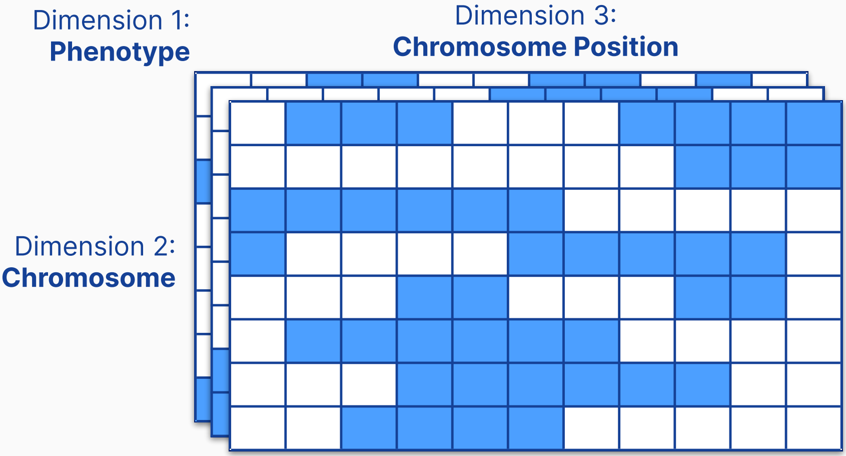


GWAS Array Layout

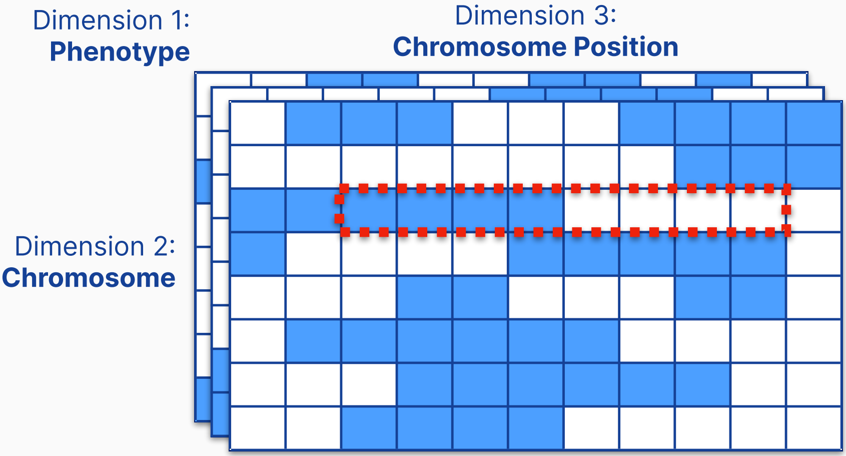


[tile]DB

GWAS Array Layout



GWAS Array Layout



[tile]DB

Array Dimensions

1. GWAS `phenotype` (e.g., *Ventricular rate*)
2. Variant `chr`omosome (e.g., *chromosome 1*)
3. Chromosome `pos`ition (e.g., 43,113,410 bp)

See our docs for more information about choosing/ordering dimensions.

GWAS Array Dimension 1

Phenotype (the descriptive name for each analyzed trait)

```r
dim_pheno <- tiledb_dim(
  name = ”phenotype”,
  domain = NULL,
  tile = NULL,
  type = ”ASCII”
)
```

GWAS Array Dimension 2

Chromosome labels

```r
dim_chr <- tiledb_dim(
    name = ”chr”,
    domain = NULL,
    tile = NULL,
    type = ”ASCII”
  )
```

GWAS Array Dimension 3

Chromosome position

```r
dim_pos <- tiledb_dim(
  name = ”pos”,
  domain = c(1L, 249250621L),
  tile = 1e5L,
  type = ”UINT32”
)
```

GWAS Array Attributes

```r
attr_filters <- tiledb_filter_list(tiledb_filter("ZSTD"))

all_attrs <- list(
  ref = tiledb_attr("ref", type = "CHAR", filter_list = attr_filters),
  alt = tiledb_attr("alt", type = "CHAR", filter_list = attr_filters),
  minor_AF = tiledb_attr("minor_AF", type = "FLOAT64", filter_list = attr_filters),
  pval =  tiledb_attr("pval", type = "FLOAT64", filter_list = attr_filters),
  tstat = tiledb_attr("tstat", type = "FLOAT64", filter_list = attr_filters),
  se   =  tiledb_attr("se", type = "FLOAT64", filter_list = attr_filters),
  beta =  tiledb_attr("beta", type = "FLOAT64", filter_list = attr_filters)
)
```

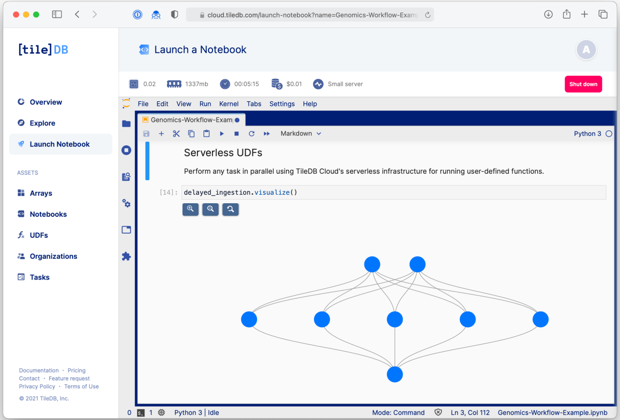
GWAS Array Creation

```r
# assemble the schema
gwas_schema <- tiledb_array_schema(
  domain = tiledb_domain(dims = c(dim_pheno, dim_chr, dim_pos)),
  attrs = all_attrs,
  sparse = TRUE,
  allows_dups = TRUE
)

# create the array
gwasdb_uri <- "data/ukbiobank-gwasdb"
tiledb_array_create(gwasdb_uri, schema = gwas_schema)
```

Ingest GWAS Results

```r
# Open the array in WRITE mode
gwasdb <- tiledb_array(gwasdb_uri, "WRITE", as.data.frame = TRUE)

# load and ingest each gwas file
gwas_files <- dir("gwas-tutorial/data", full.names = TRUE)

for (i in seq_along(gwas_files)) {
  tbl_gwas <- vroom(gwas_files[i], col_types = cols(chr = col_character
  gwasdb[] <- tbl_gwas
}
```

Parallel Ingestion



TileDB supports parallel reads and writes, so data ingestion could easily be distributed across nodes using *e.g.* HPCs or severless UDFs on TileDB Cloud.

Query the GWAS Array

Let's return the results as a `data.frame` that includes the subset of attributes we're interested in.

```
gwasdb <- tiledb_array(
  gwasdb_uri,
  is.sparse = TRUE,
  as.data.frame = TRUE,
  attrs = c("beta", "se", "tstat", "pval")
)
```

GWAS Query #1

Use `[]` indexing to query the first 2 dimensions (e.g., `phenotype` and `chr`).

```
gwasdb["Water intake", "20"]
```

```
# A tibble: 295,761 x 7
  phenotype     chr     pos       beta      se  tstat  pval
  <chr>         <chr> <int>      <dbl>   <dbl>  <dbl> <dbl>
1 Water intake 20     61098  0.00199   0.00246  0.812  0.417
2 Water intake 20     61270 -0.00113   0.00719 -0.157  0.876
3 Water intake 20     61795  0.000381  0.00218  0.175  0.861
4 Water intake 20     62731 -0.00200   0.00328 -0.611  0.541
5 Water intake 20     63231  0.00219   0.00683  0.320  0.749
```

GWAS Query #2

Use `selected_ranges` to query all 3-dimensions and extract data for a specific genomic region.

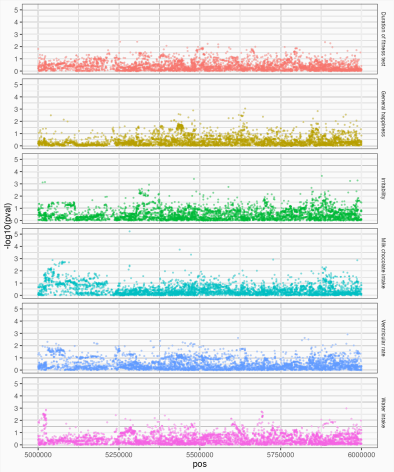
```r
selected_ranges(gwasdb) <- list(
  phenotype = cbind("Water intake", "Water intake"),
  chr = cbind("20", "20"),
  pos = cbind(5e6, 6e6)
)
gwasdb[]
```

```
# A tibble: 5,198 x 7
  phenotype    chr       pos     beta      se  tstat   pval
  <chr>        <chr>   <int>    <dbl>   <dbl>  <dbl>  <dbl>
1 Water intake 20    5000142  0.0138  0.0103   1.34  0.180
2 Water intake 20    5000146 -0.00457 0.00529 -0.864 0.388
3 Water intake 20    5000279  0.00523 0.0181   0.288 0.773
4 Water intake 20    5000280 -0.00605 0.00246 -2.46  0.0139
5 Water intake 20    5000337 -0.00459 0.00529 -0.867 0.386
```

GWAS Query #3

Examine p-values across all phenotypes for the same genomic region.

```
selected_ranges(gwasdb) <- list(
  phenotype = NULL,
  chr = cbind(”20”, ”20”),
  pos = cbind(5e6, 6e6)
)
gwas_results <- gwasdb[]
manhattan_plot(gwas_results)
```



GWAS Resources

1. UK Biobank (`https://www.ukbiobank.ac.uk`)
2. Neale Lab UK Biobank GWAS results (`https://www.nealelab.is/uk-biobank`)
3. GWAS Results Manifest

[tile]DB

Wrap-Up

In Summary

TileDB

- an open-source embeddable storage engine
- an open-source format for modeling any type of data
- fully cloud-native on AWS, GCS, Azure
- limitless scalability
- offers time travel
- offers Encryption

In Summary

TileDB R Package

- available on CRAN, and already used by Bioconductor
- high-level R-friendly interface for creating/query TileDB arrays
- also includes low-level access to the full TileDB API
- fully interoperable with DBI, Arrow, ...

In Summary

Use cases

- limitless 😉 – just get in touch with TileDB for a demo

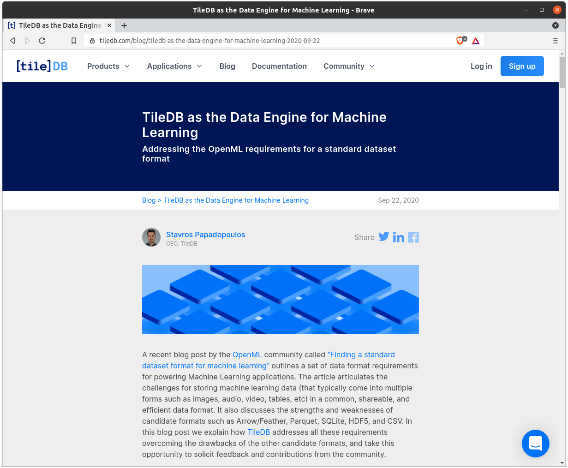
Use cases covered today

- Data Frames
- LiDAR and Geospatial uses
- Finance and Time Series
- Population Genomics and GWAS

Further Resources

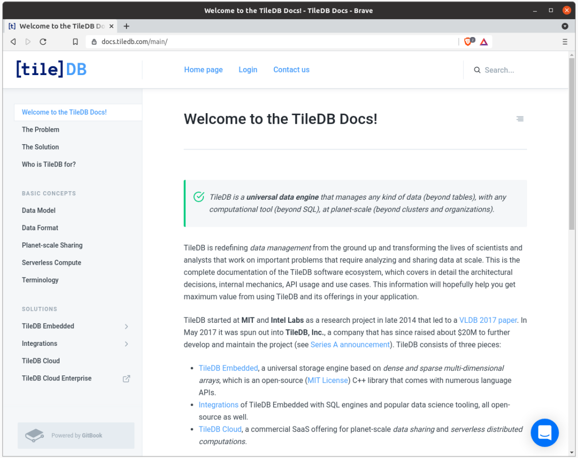
[tile]DB

Resources



Blog post describing how TileDB answers the data format requirements for scientific data as layed out in an earlier post by the OpenML team.

Documentation



Extensive documentation on TileDB, APIs, Usage, and more

`docs.tiledb.com`

`github.com/TileDB-Inc/TileDB-R`

`github.com/TileDB-Inc/TileDB`

[tile]DB

Talk to TileDB

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