

# Turbulent code in water models

R code

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## Contents

### 1 Close reading 18

```
# PRELIMINARY FUNCTIONS #####

# Load the packages
sensobol::load_packages(c("data.table", "tidyverse", "openxlsx", "tm", "stringr",
                          "pdftools", "tidytext", "scales", "cowplot",
                          "ggrepel", "tidyquant", "text2vec"))
```

```
## Loading required package: text2vec
```

```
##
```

```
## Attaching package: 'text2vec'
```

```
## The following objects are masked from 'package:LSAfun':
```

```
##
```

```
## coherence, normalize
```

```
# Create custom theme
```

```
# Create custom theme
```

```
theme_AP <- function() {
  theme_bw() +
    theme(panel.grid.major = element_blank(),
          panel.grid.minor = element_blank(),
          legend.background = element_rect(fill = "transparent", color = NA),
          legend.key = element_rect(fill = "transparent", color = NA),
          strip.background = element_rect(fill = "white"),
          legend.margin = margin(0.5, 0.1, 0.1, 0.1),
          legend.box.margin = margin(0.2, -4, -7, -7),
          plot.margin = margin(3, 4, 0, 4),
          legend.text = element_text(size = 6),
          axis.title = element_text(size = 10),
          axis.text.x = element_text(size = 7),
          axis.text.y = element_text(size = 7),
          axis.title.x = element_text(size = 7.3),
          axis.title.y = element_text(size = 7.3),
          strip.text.x = element_text(size = 7.4),
```

```

strip.text.y = element_text(size = 7.4),
legend.key.width = unit(0.4, "cm"),
legend.key.height = unit(0.5, "lines"),
legend.title = element_text(size = 7.5))
}

# FUNCTIONS TO CLEAN THE TEXT #####

# Function to remove words from text
removeWords <- function(str, stopwords) {
  x <- unlist(strsplit(str, " "))
  paste(x[!x %in% stopwords], collapse = " ")
}

# Function to remove punctuation, citations, numbers, stopwords in english,
# bring to lowercase and strip whitespace, and especial characters, etc...
clear_text <- function(x, stem = TRUE) {

  y <- tolower(x)
  y <- str_replace_all(y, "[[:punct:]]", " ") # Remove punctuation characters
  y <- tm::removeNumbers(y)
  y <- tm::removeWords(y, stopwords::stopwords(language = "en"))
  y <- str_remove_all(y, "[^\\da-zA-Z ]") # Remove all non-alphanumerical
  y <- gsub("\\s[A-Za-z](?= )", " ", y, perl = TRUE) # Remove isolated letters
  #y <- tm::stripWhitespace(y)
  y <- str_squish(y)

  if (stem == TRUE) {
    y <- stemDocument(y) # Stem the document and keep only the root of the word
  }

  return(y)
}

# READ DATA #####

dt <- data.table(read.xlsx("final.dt.xlsx"))
dt[, keywords.large:= tolower(keywords.large)]
dt[, abstract.cleaned:= clear_text(abstract.large, stem = FALSE)]

# TERMS TO SEARCH #####

keywords <- c("validation", "verification", "calibration", "confirmation", "evaluation",
             "benchmarking")
keywords.stemmed <- stemDocument(keywords)

# keywords.stemmed <- c(

```

```

# "calibration", "verification", "validation", "evaluation",
# "calibrations", "verifications", "validations", "evaluations",
# "calibrated", "verified", "validated", "evaluated",
# "calibrating", "verifying", "validating", "evaluating",
# "calibrative", "verificative", "validative", "evaluative",
# "calibratively", "verificatively", "validatively", "evaluatively"
# )

# SEARCHING FOR TERMS #####

# Check which papers include keywords in abstract, keywords or title -----
selected_cols <- c("title", "abstract", "keywords")
#selected_cols <- c("title.large", "abstract.large", "keywords.large")
out <- list()

for(i in 1:length(keywords.stemmed)) {

  out[[i]] <- dt[, lapply(.SD, function(x)
    str_detect(x, keywords.stemmed[i])), .SDcols = (selected_cols)]
}

# ARRANGE DATA #####

names(out) <- keywords.stemmed

valid.dt <- lapply(out, function(x) rowSums(x, na.rm = TRUE) > 0L) %>%
  do.call(cbind, .) %>%
  data.table() %>%
  .[, any.column:= rowSums(.SD) > 0]

full.dt <- cbind(dt, valid.dt)
full.dt.cols <- data.frame(full.dt[, .SD, .SDcols = keywords.stemmed])

# DESCRIPTIVE STATISTICS #####

full.dt[, lapply(.SD, sum), .SDcols = keywords.stemmed]

##      valid  verif  calibr  confirm  evalu  benchmark
##      <int> <int>   <int>    <int> <int>    <int>
## 1:    536    76    743      74  1065      86

# Count number of papers with mentions to validation, validation + verification,
# validation + calibration, etc -----

# Function to count the number of TRUE values shared between columns
count_shared_true <- function(data, cols) {

```

```

    sum(rowSums(data[, cols]) == length(cols))
  }

  # Create an empty list to store results
  results_list <- list()

  # Loop through all combinations of columns and count shared TRUE values
  for (size in 2:length(keywords.stemmed)) {

    for (cols_combination in combn(ncol(full.dt.cols), size, simplify = FALSE)) {

      shared_true_count <- count_shared_true(data = full.dt.cols, cols = cols_combination)
      col_names <- colnames(full.dt.cols)[cols_combination]

      # Append results to the list
      results_list <- c(results_list, list(data.table(combination = paste(col_names, collapse = " "),
      shared_true_count)))
    }
  }

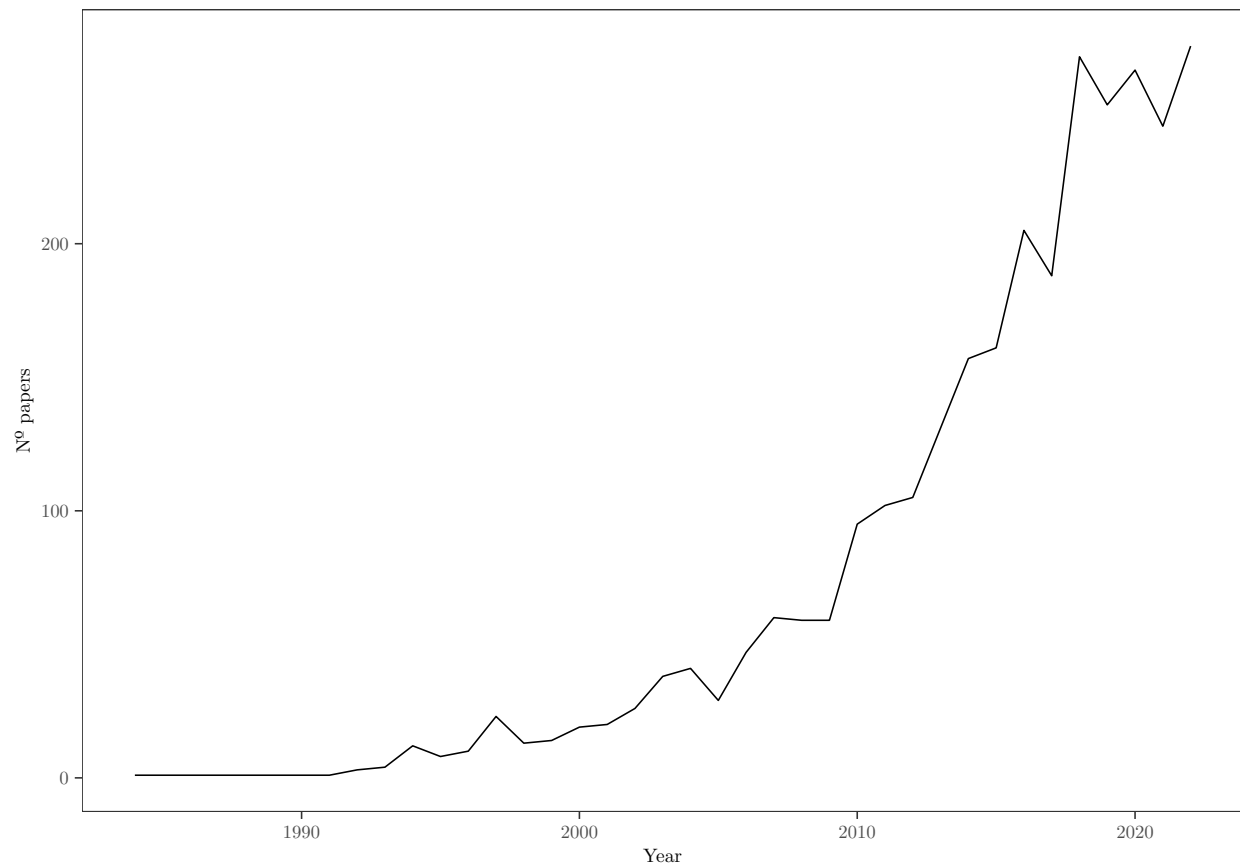
  # Combine the list of data.tables into a single data.table
  comb_dt <- rbindlist(results_list)

  # PLOTS #####

plot.year <- full.dt[, .N, year] %>%
  .[!year == 2023] %>%
  ggplot(., aes(year, N)) +
  geom_line() +
  labs(x = "Year", y = "Nº papers") +
  theme_AP()

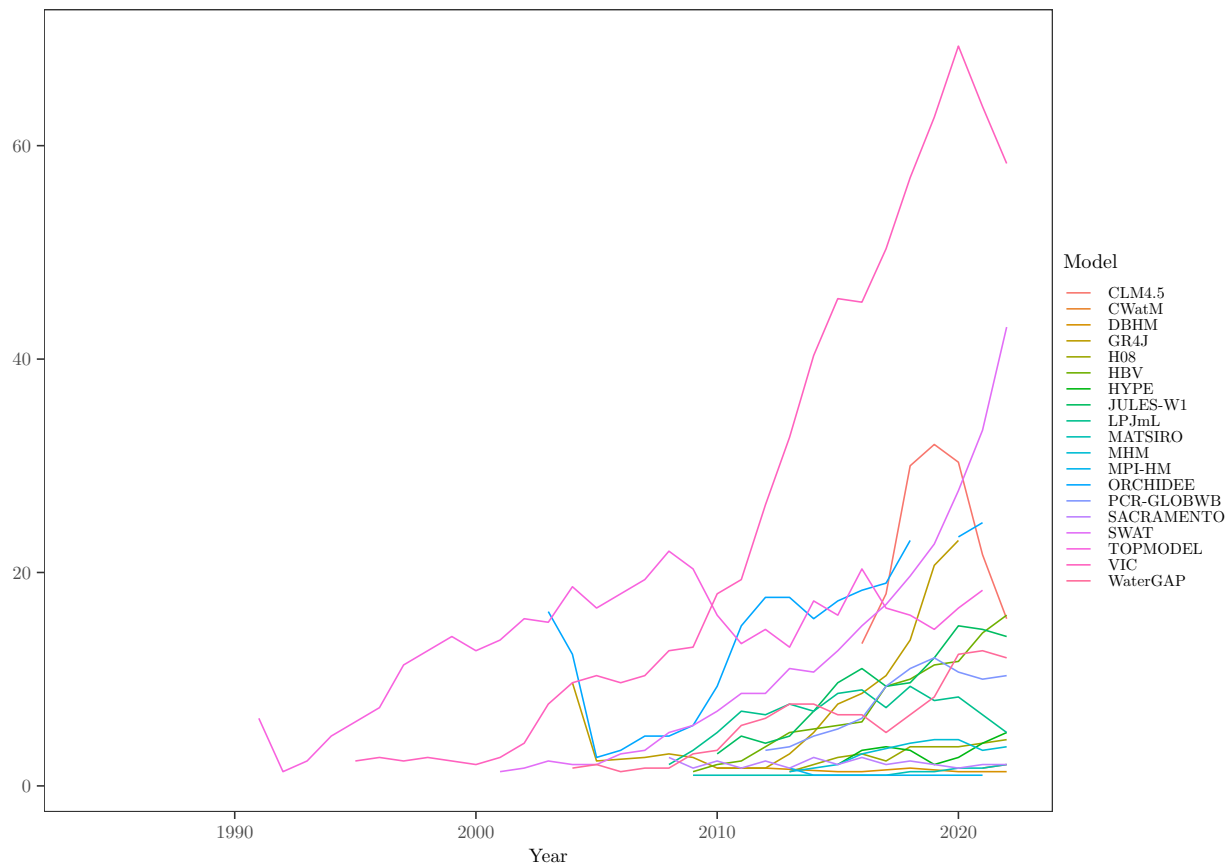
plot.year

```



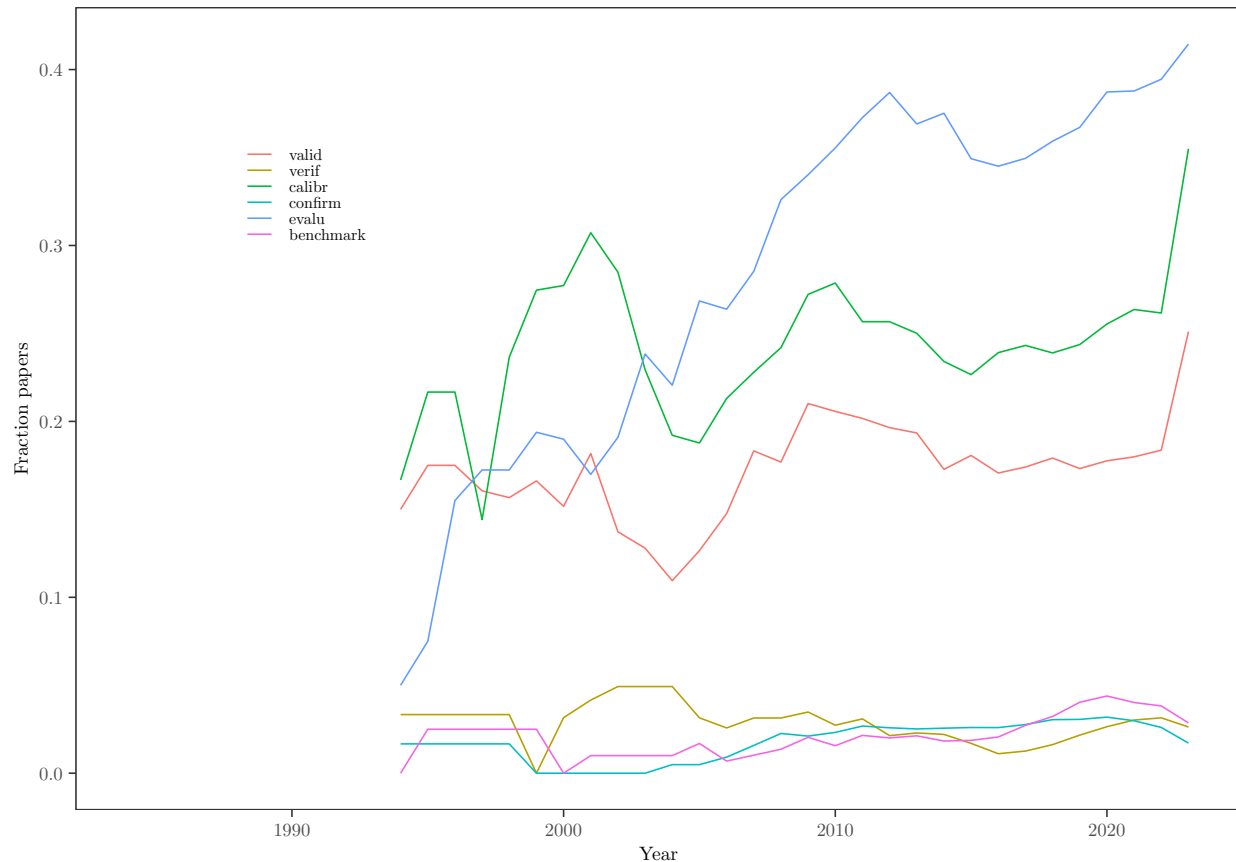
```
plot.model.year <- full.dt[, .N, .(Model, year)] %>%
  .[!year == 2023] %>%
  ggplot(., aes(year, N, color = Model)) +
  geom_ma(ma_fun = SMA, n = 3, lty = 1) +
  labs(x = "Year", y = "") +
  theme_AP()
```

```
plot.model.year
```



```
plot.keywords.time <- merge(full.dt, full.dt[, .(total.papers = .N), year], by = "year") %>%
  melt(., measure.vars = keywords.stemmed) %>%
  .[, sum(value, na.rm = TRUE), .(variable, year, total.papers)] %>%
  .[, fraction:= V1 / total.papers] %>%
  ggplot(., aes(year, fraction, color = variable)) +
  scale_color_discrete(name = "") +
  geom_ma(ma_fun = SMA, n = 5, lty = 1) +
  theme_AP() +
  theme(legend.position = c(0.2, 0.8)) +
  labs(x = "Year", y = "Fraction papers")

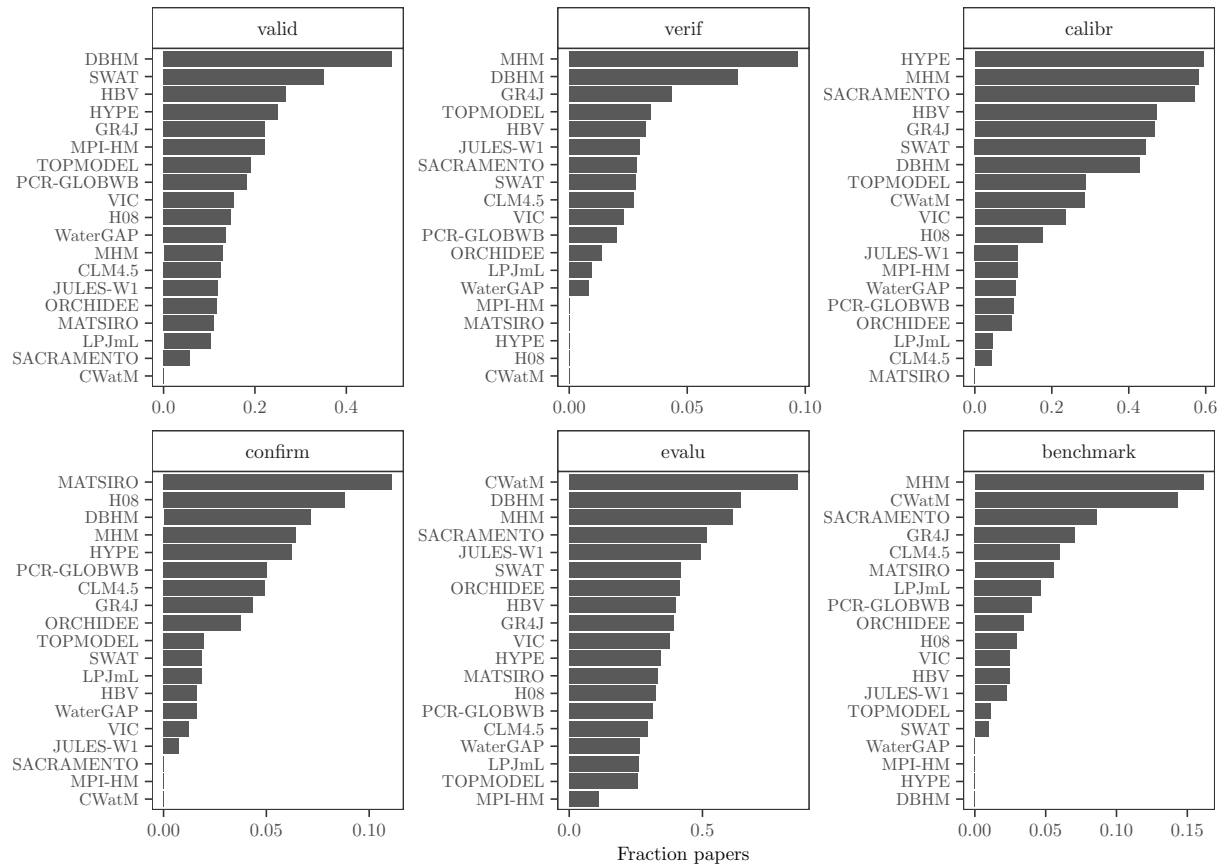
plot.keywords.time
```



```
tmp <- merge(full.dt, full.dt[, .(total.papers = .N), Model], by = "Model") %>%
  melt(., measure.vars = keywords.stemmed) %>%
  .[, sum(value, na.rm = TRUE), .(variable, Model, total.papers)] %>%
  .[, fraction:= V1 / total.papers] %>%
  mutate(variable = as.factor(variable),
         name = reorder_within(Model, fraction, variable))
```

```
plot.keyword.per.model <- tmp %>%
  ggplot(., aes(name, fraction)) +
  geom_bar(stat = "identity") +
  coord_flip() +
  facet_wrap(~variable, scales = "free") +
  scale_x_reordered() +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  theme_AP() +
  labs(x = "", y = "Fraction papers") +
  theme(axis.text.y = element_text(size = 6.5))
```

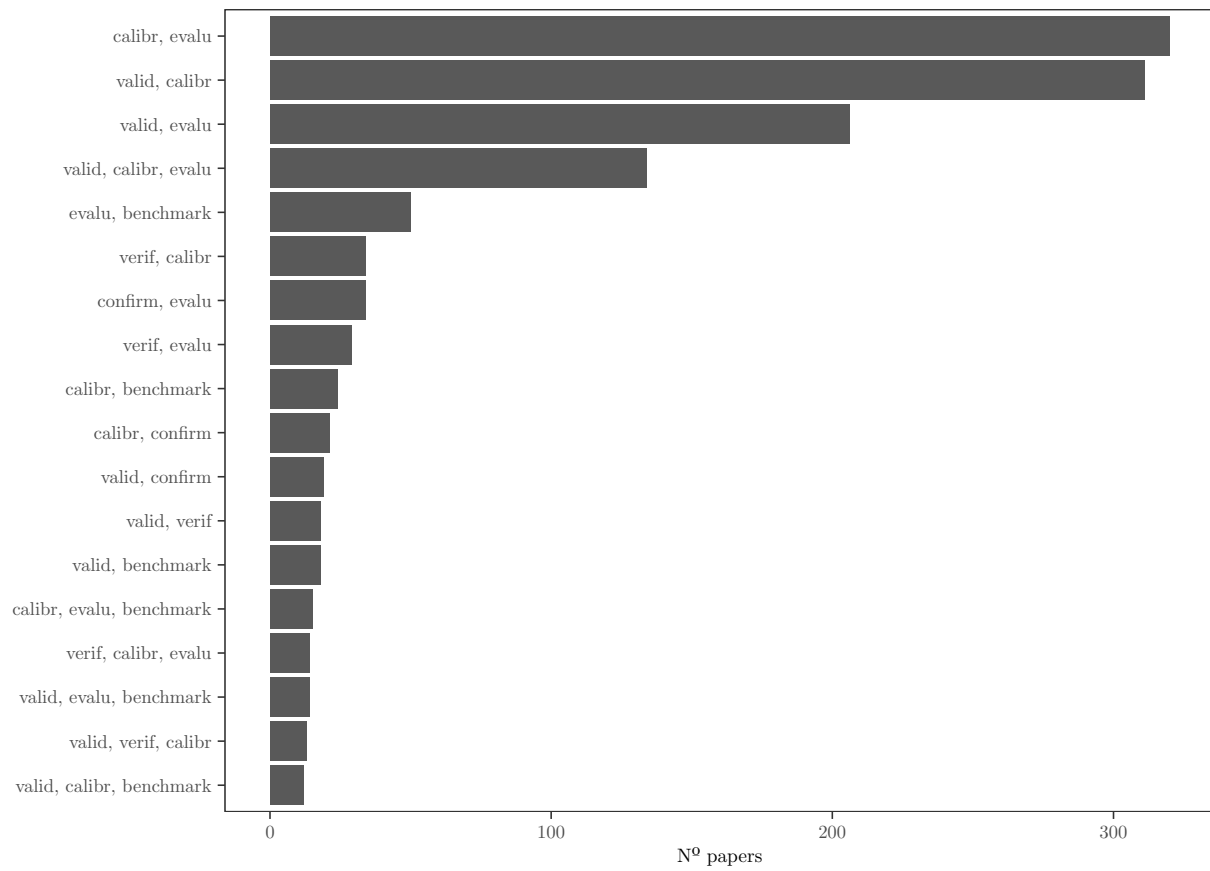
```
plot.keyword.per.model
```



```
plot.keyword.comb <- comb_dt[N > 10] %>%
  ggplot(., aes(reorder(combination, N), N)) +
  geom_bar(stat = "identity") +
  coord_flip() +
  theme_AP() +
  theme(axis.text.y = element_text(size = 7)) +
  labs(x = "", y = "N° papers")

plot.keyword.comb
```

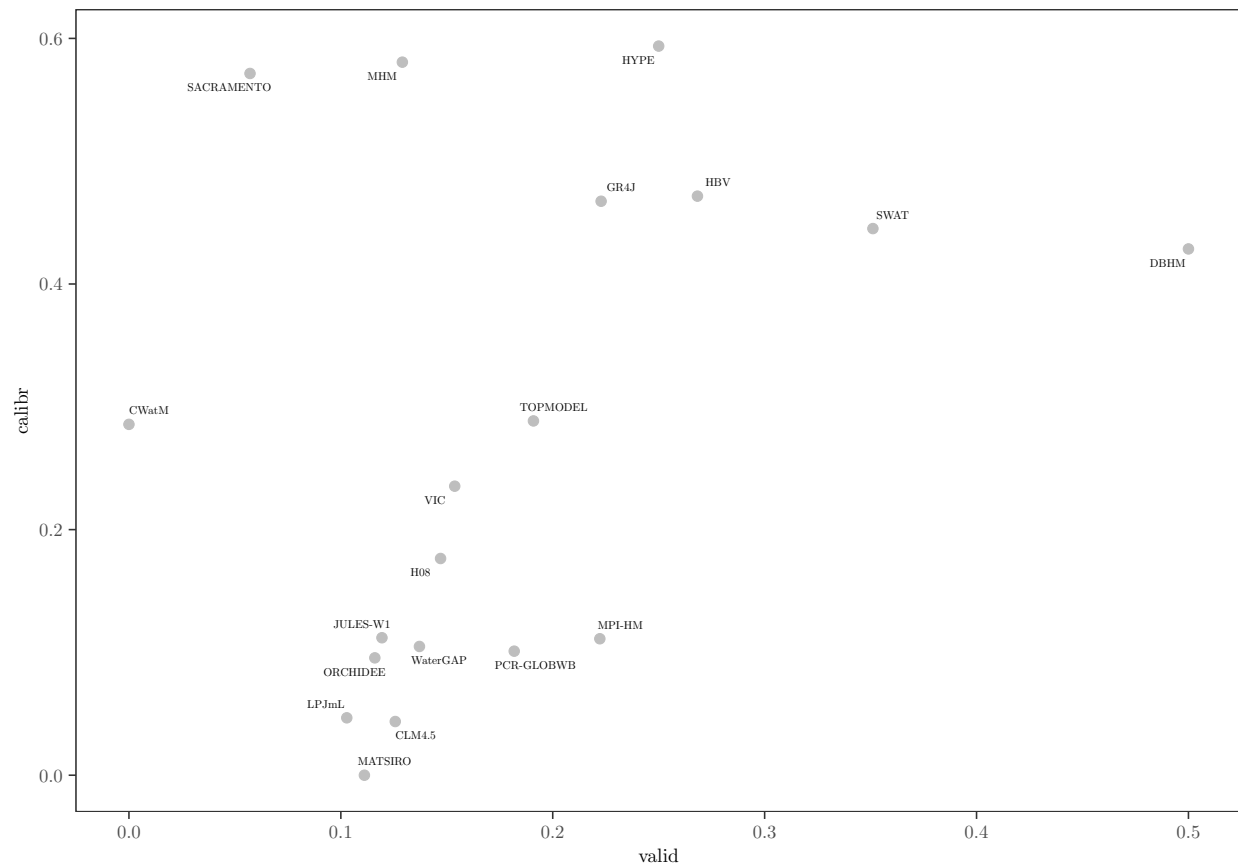




```
total.papers.model <- full.dt[, .N, Model]

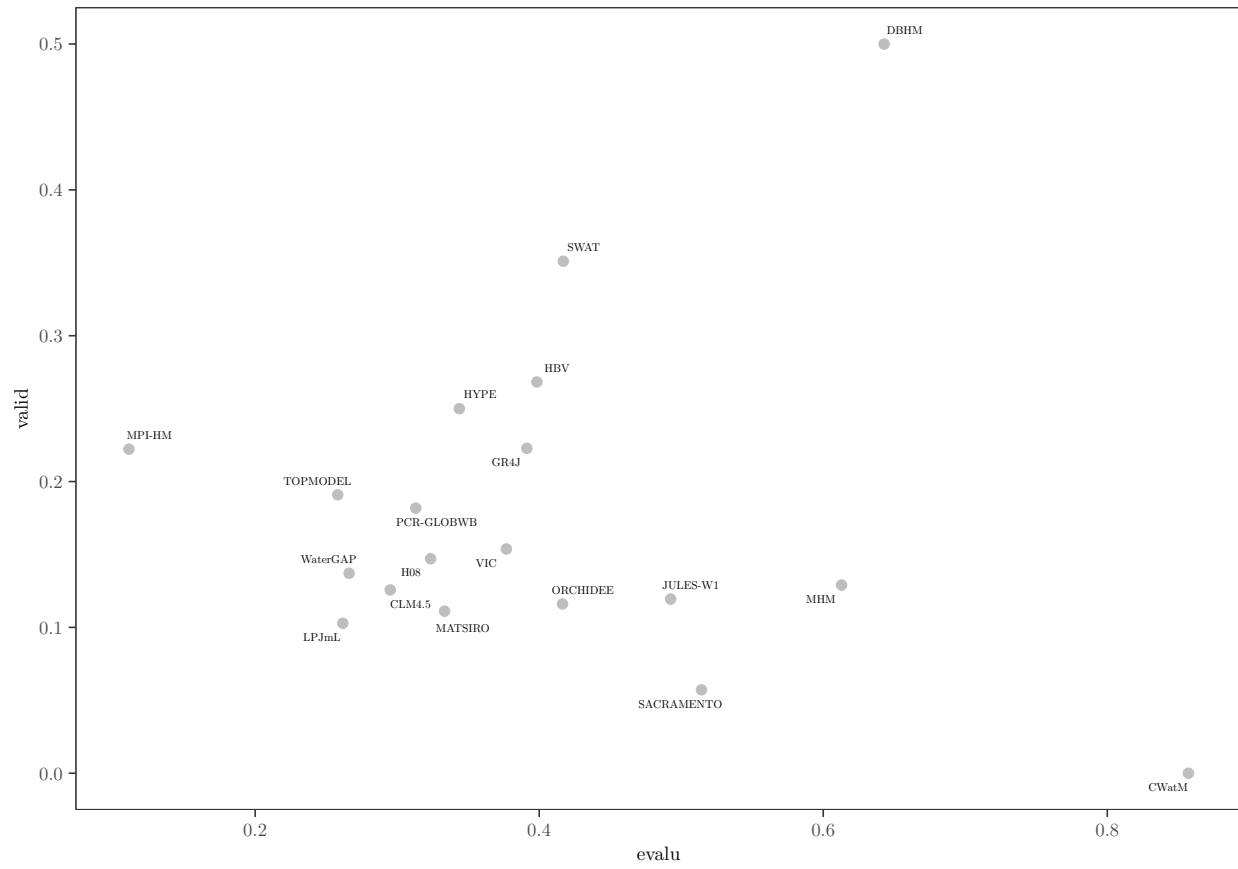
plot.valid.calibr <- tmp %>%
  dcast(., Model ~ variable, value.var = "fraction") %>%
  merge(., total.papers.model, by = "Model") %>%
  ggplot(., aes(valid, calibr, label = Model)) +
  geom_point(color = "grey") +
  geom_text_repel(size = 1.5) +
  theme_AP() +
  theme(legend.position = "none")

plot.valid.calibr
```

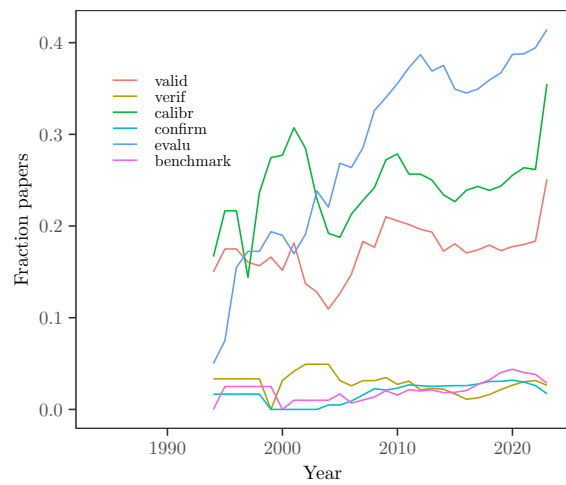


```
plot.eval.valid <- tmp %>%
  dcast(., Model ~ variable, value.var = "fraction") %>%
  merge(., total.papers.model, by = "Model") %>%
  ggplot(., aes(eval, valid, label = Model)) +
  geom_point(color = "grey") +
  geom_text_repel(size = 1.5) +
  theme_AP() +
  theme(legend.position = "right")

plot.eval.valid
```



`plot.keywords.time`

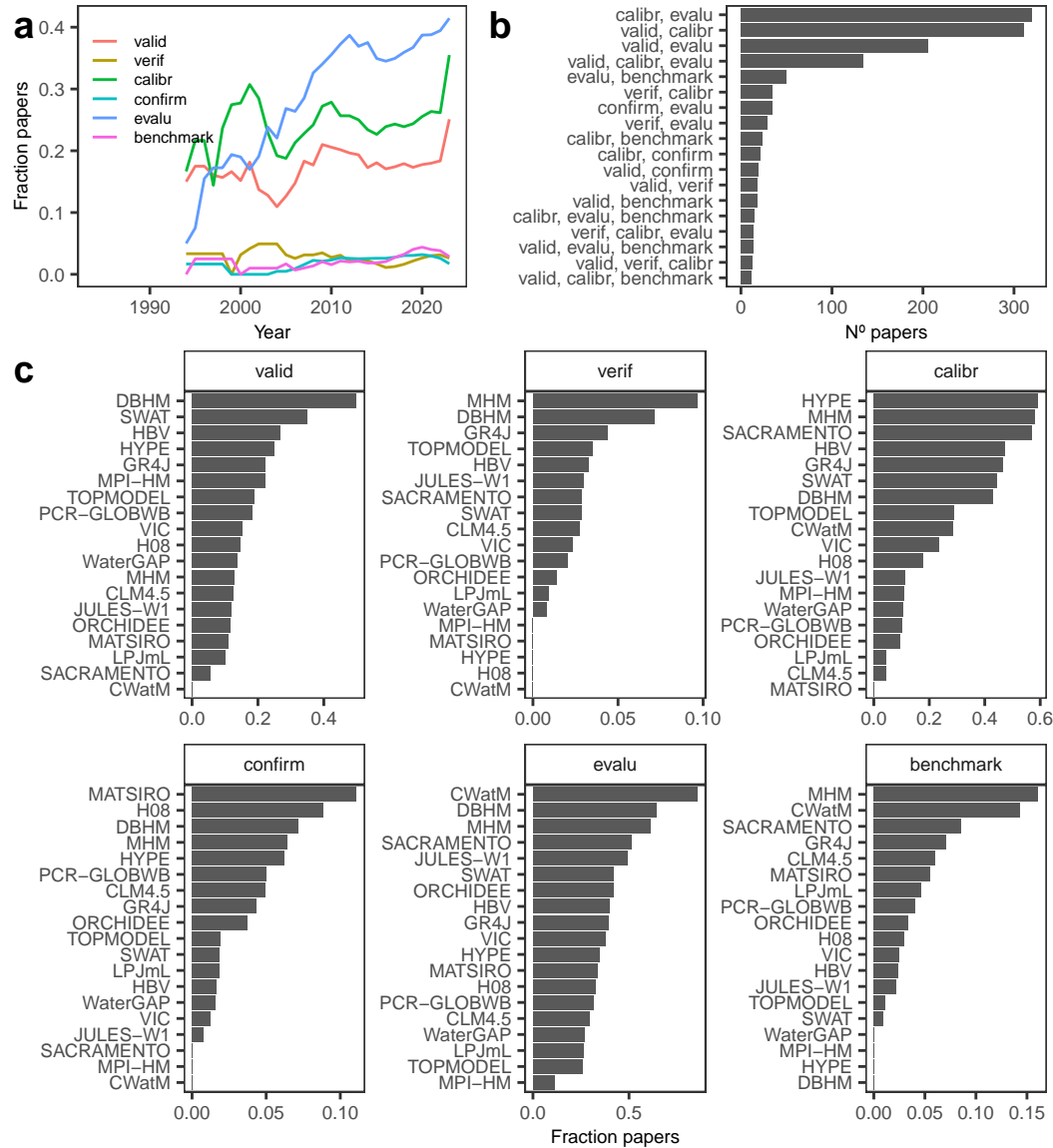


*# MERGE DESCRIPTIVE PLOTS #####*

```
top <- plot_grid(plot.keywords.time, plot.keyword.comb, ncol = 2, labels = "auto",
  rel_widths = c(0.45, 0.55))
```

```
plot.merged <- plot_grid(top, plot.keyword.per.model, ncol = 1,
  labels = c("", "c"), rel_heights = c(0.3, 0.7))
```

plot.merged



```

toppest <- plot_grid(plot.year, plot.model.year, ncol = 2, labels = "auto",
  rel_widths = c(0.4, 0.6))

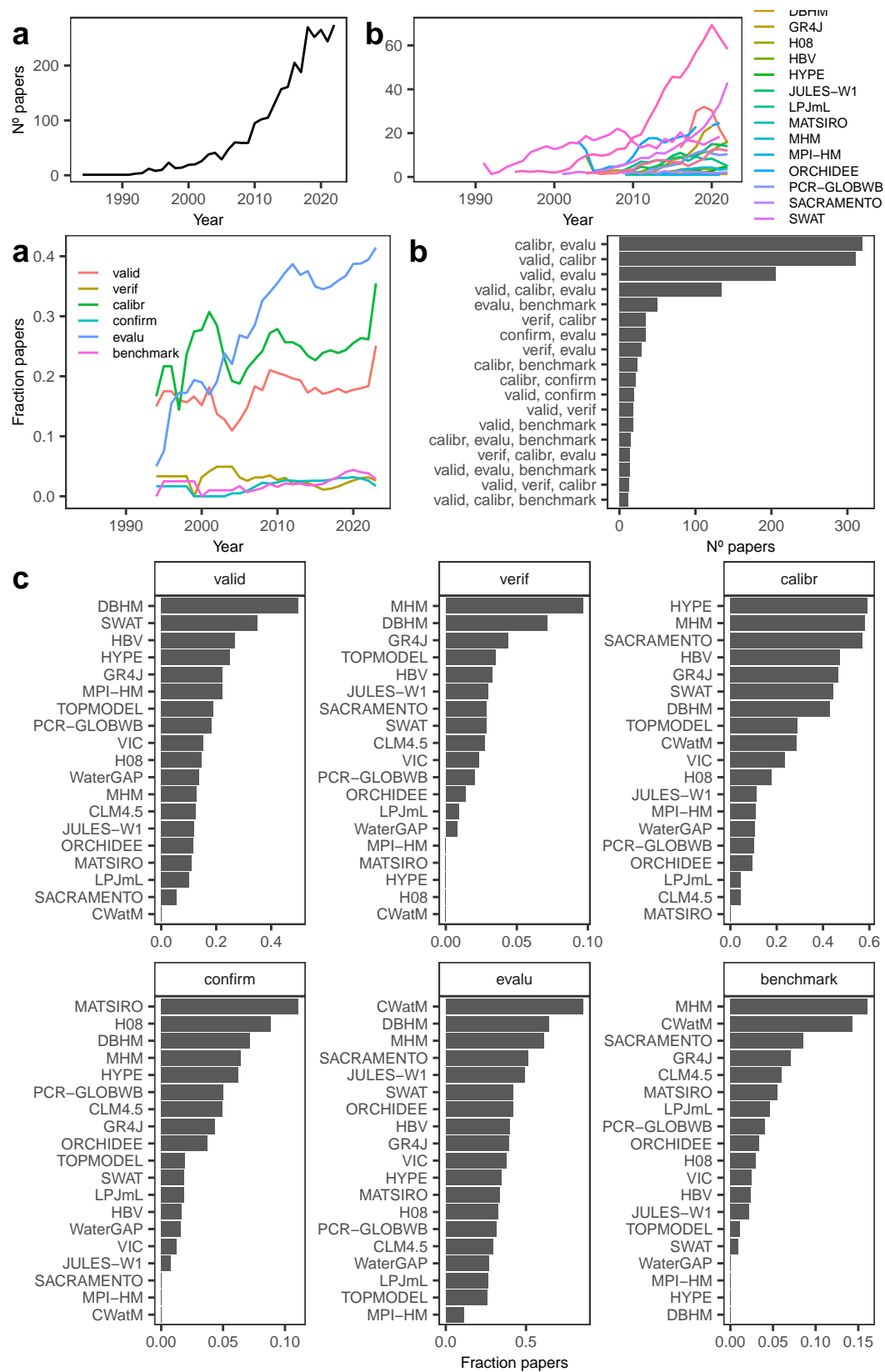
top <- plot_grid(plot.keywords.time, plot.keyword.comb, ncol = 2, labels = "auto",
  rel_widths = c(0.45, 0.55))

both.top <- plot_grid(toppest, top, ncol = 1, rel_heights = c(0.4, 0.6))

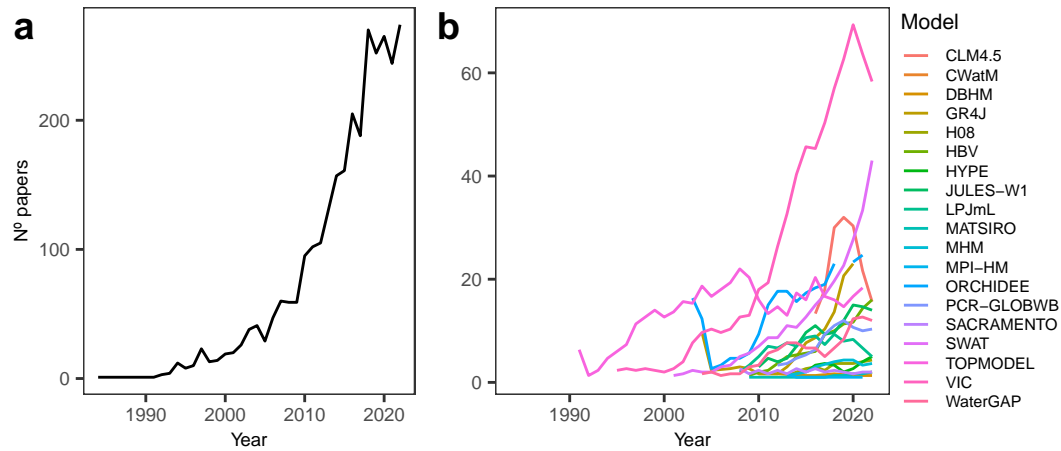
plot.merged <- plot_grid(both.top, plot.keyword.per.model, ncol = 1,
  labels = c("", "c"), rel_heights = c(0.4, 0.6))

plot.merged

```

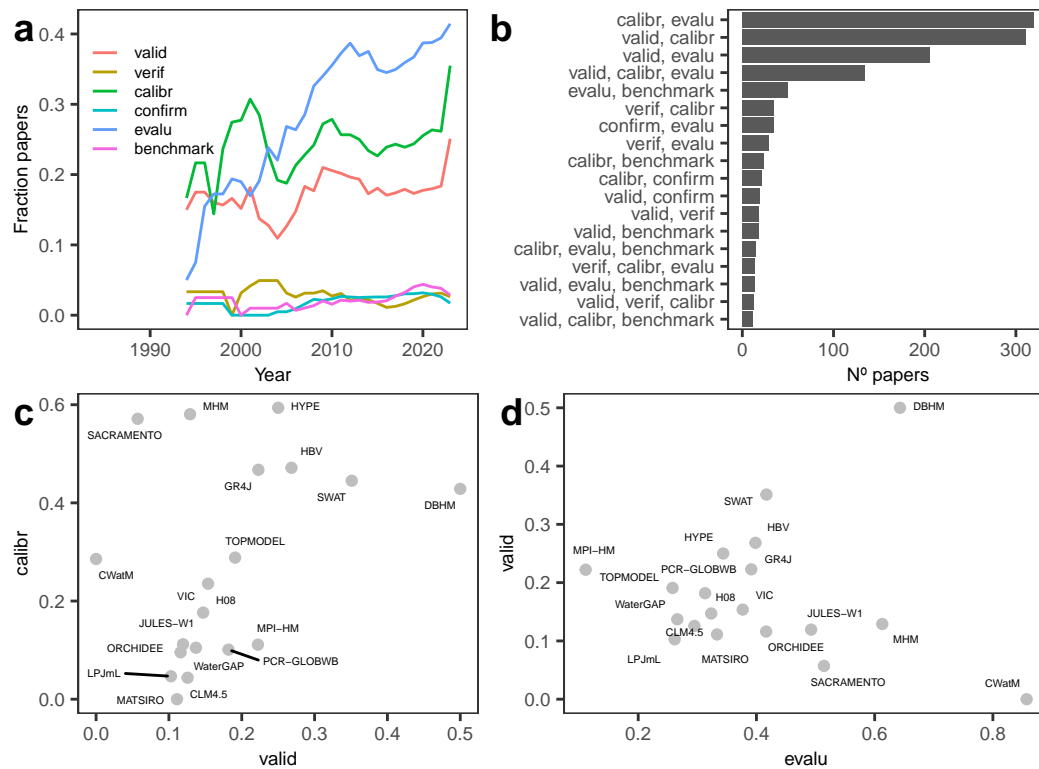


toppest



```
scatter.plots <- plot_grid(plot.valid.calibr, plot.eval.valid, ncol = 2,
                           labels = c("c", "d"), rel_widths = c(0.46, 0.54))

plot_grid(top, scatter.plots, ncol = 1, rel_heights = c(0.5, 0.5))
```



```
# TOKEN ANALYSIS #####

# Create function -----
tokenize_fun <- function(dt, word, keywords, N.tokens) {

  # Create long dataset
  dt <- melt(dt, measure.vars = keywords)
  output <- dt[variable == word & value == TRUE]
```

```

# Token analysis -----
# We count the co-occurrences of words without taking into account their order
# within the n-token
token.analysis <- output %>%
  unnest_tokens(bigram, abstract.cleaned, token = "ngrams", n = N.tokens) %>%
  separate(bigram, into = c("word1", "word2"), sep = " ") %>%
  data.table() %>%
  .[, `:=`(word1= pmin(word1, word2), word2 = pmax(word1, word2))] %>%
  count(word1, word2, sort = TRUE) %>%
  unite(., col = "bigram", c("word1", "word2"), sep = " ") %>%
  data.table()

# Vector to retrieve only the bigrams with uncertainty or sensit
vec <- token.analysis[, str_detect(bigram, word)]

# Final dataset
output.dt <- token.analysis[vec]

# Plot the q0 words most commonly
# associated with uncertainty and sensit -----
plot.token <- output.dt %>%
  .[, sum(n), bigram] %>%
  .[order(-V1)] %>%
  .[, head(.SD, 10)] %>%
  ggplot(., aes(reorder(bigram, V1, sum), V1)) +
  geom_bar(stat = "identity") +
  coord_flip() +
  scale_y_continuous(breaks = pretty_breaks(n = 3)) +
  theme_AP() +
  labs(y = "n", x = "") +
  ggtitle(word) +
  theme(legend.position = "none",
        plot.title = element_text(size = 9),
        axis.text.y = element_text(size = 7))

# Arrange and output -----

out <- list(output.dt, plot.token)
names(out) <- c("data", "token")

return(out)
}

# RUN TOKEN ANALYSIS #####
N.tokens <- 2

```

```

token.dt <- list()

for (j in keywords.stemmed) {

  token.dt[[j]] <- tokenize_fun(dt = full.dt, word = j,
                                keywords = keywords.stemmed,
                                N.tokens = N.tokens)

}

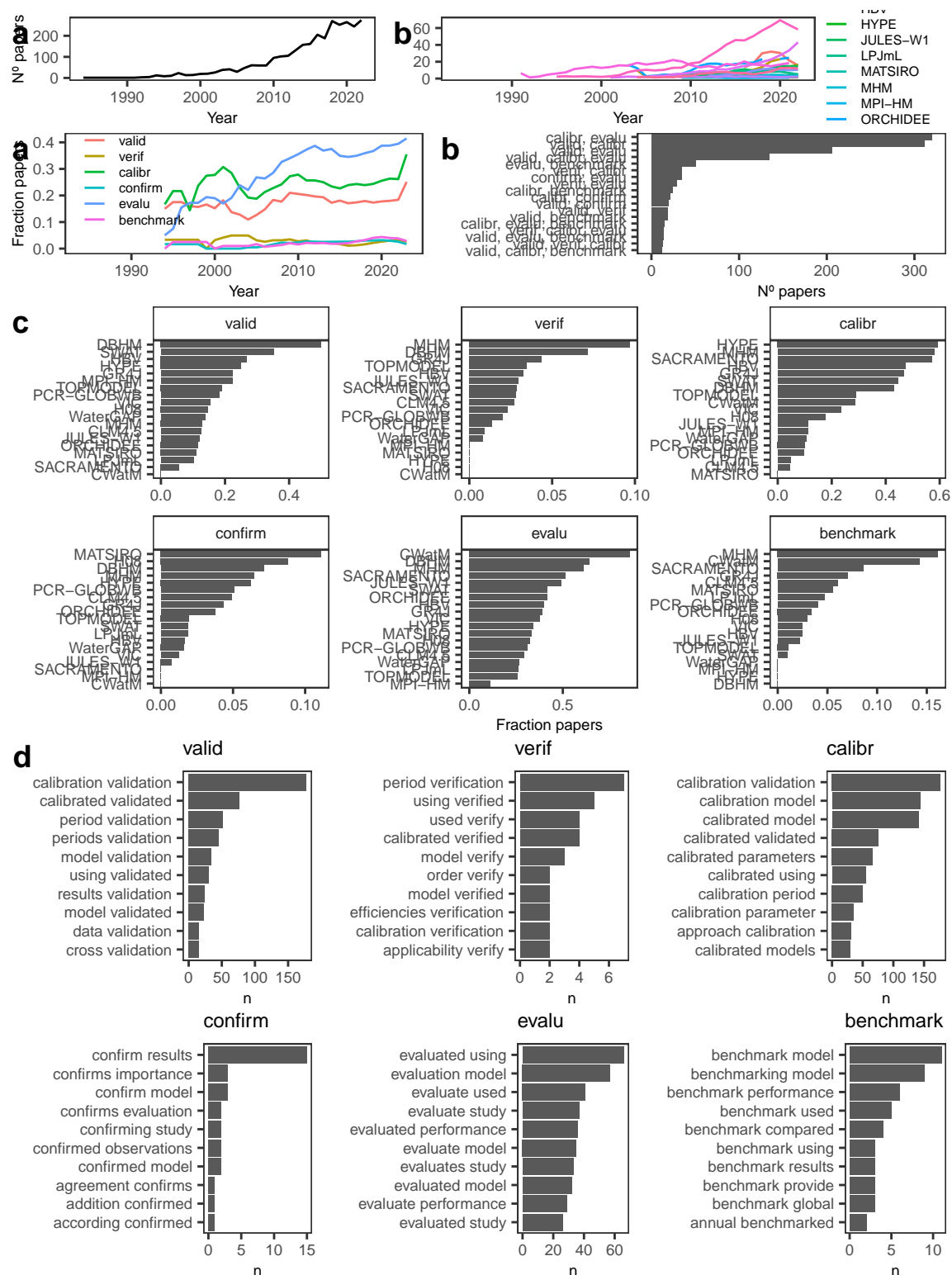
# PLOT RESULTS #####

plot.tokens <- plot_grid(token.dt$valid[[2]], token.dt$verif[[2]], token.dt$calibr[[2]],
                        token.dt$confirm[[2]], token.dt$evalu[[2]], token.dt$benchmark[[2]],
                        ncol = 3)

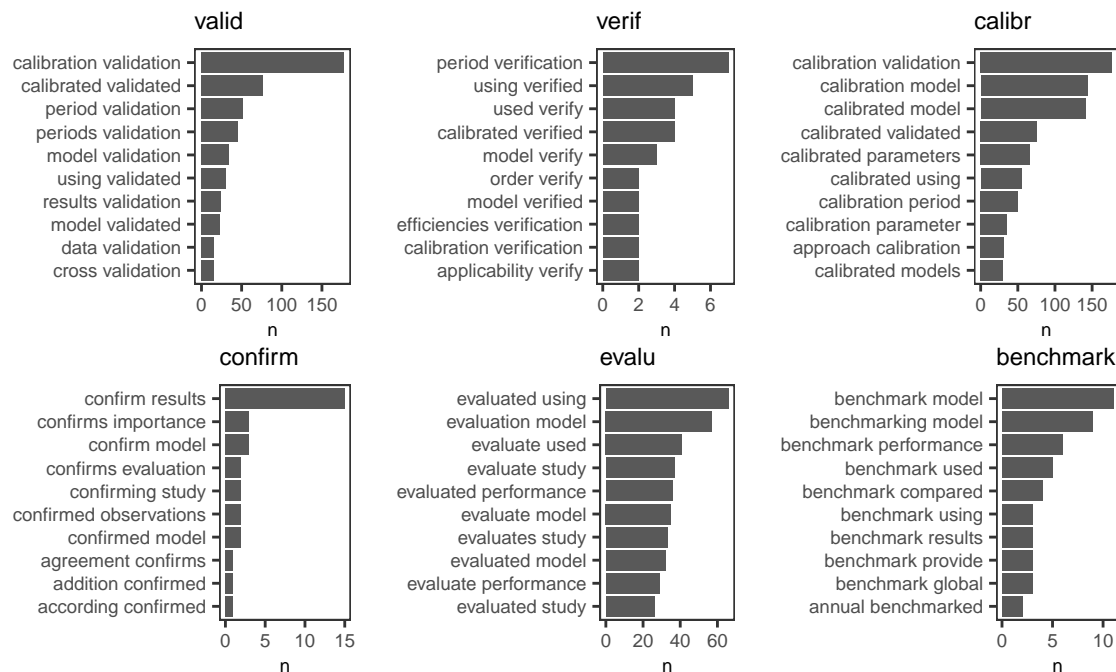
plot_grid(plot.merged, plot.tokens, ncol = 1, labels = c("", "d"),
          rel_heights = c(0.57, 0.43))

```





plot.tokens



# 1 Close reading

```
# KEYWORDS TO LOOK FOR #####

keywords_selected <- c(
  "benchmark", "calibrate", "confirm", "evaluate", "validate", "verify",
  "benchmarks", "calibrates", "confirms", "evaluates", "validates", "verifies",
  "benchmarked", "calibrated", "confirmed", "evaluated", "validated", "verified",
  "benchmarking", "calibrating", "confirming", "evaluating", "validating", "verifying",
  "calibration", "confirmation", "evaluation", "validation", "verification",
  "calibrations", "confirmations", "evaluations", "validations", "verifications",
  "benchmarkable", "calibrative", "confirmative", "evaluative", "validative", "verificative",
  "calibratively", "confirmatively", "evaluatively", "validatively", "verificatively"
)

keywords_selected_stemmed <- unique(stemDocument(keywords_selected))[-c(1, 3, 6)]

# READ IN DATA #####

list.close.reading <- data.table(read.xlsx("dt.papers.close.reading.xlsx"))

dt.students <- data.table(read.xlsx("validation_work_students.xlsx")) %>%
  .[, title.large:= tolower(title)]

dt.close.reading <- merge(list.close.reading[, .(Model, title.large)],
  dt.students[, .(doi, title.large, paragraph)], by = "title.large") %>%
  .[, title.large:= tolower(title.large)] %>%
```

```

[, paragraph.clean:= clear_text(paragraph)]

total.models <- dt.close.reading[, .N, .(Model, title.large)] %>%
  .[, .(Model)] %>%
  .[, .(total.papers = .N), Model]

# COUNT KEYWORDS #####

out <- out.stemmed <- list()

for(i in 1:length(keywords_selected)) {

  pattern <- paste0("\\b", keywords_selected[i], "\\b")

  out[[i]] <- dt.close.reading[, lapply(.SD, function(x)
    str_count(x, pattern)), .SDcols = "paragraph"]

}

for(i in 1:length(keywords_selected_stemmed)) {

  out.stemmed[[i]] <- dt.close.reading[, lapply(.SD, function(x)
    str_count(x, keywords_selected_stemmed[i])), .SDcols = "paragraph"]

}

# ARRANGE DATA #####

dt.keywords <- do.call(cbind, out) %>%
  data.table()

dt.keywords.stemmed <- do.call(cbind, out.stemmed) %>%
  data.table()

colnames(dt.keywords) <- keywords_selected
colnames(dt.keywords.stemmed) <- keywords_selected_stemmed

full.dt.keywords <- cbind(dt.keywords, dt.keywords.stemmed)

vec.columns <- colSums(full.dt.keywords, na.rm = TRUE)

colnames.keywords <- names(vec.columns[!vec.columns == 0])

full.dt.close.reading <- cbind(dt.close.reading, full.dt.keywords) %>%
  merge(., total.models, by = "Model")

```

```

# COSINE ANALYSIS #####

clean_text <- melt(full.dt.close.reading,
                  measure.vars = keywords.stemmed) %>%
  .[!value == 0] %>%
  unnest_tokens(word, paragraph.clean) %>%
  anti_join(stop_words) %>%
  group_by(variable) %>%
  summarize(paragraph.clean = paste(word, collapse = " "))

## Joining with `by = join_by(word)`

# Iterate over the text -----

it <- itoken(clean_text$paragraph.clean, progressbar = FALSE)

# Create vocabulary -----

vocab <- create_vocabulary(it)

# Vectorize text -----

vectorizer <- vocab_vectorizer(vocab)
dtm <- create_dtm(it, vectorizer)

# Apply TF-IDF transformation -----

tfidf <- TfIdf$new()
dtm_tfidf <- tfidf$fit_transform(dtm)

# Compute cosine similarity matrix -----

similarity_matrix <- sim2(dtm_tfidf, method = "cosine", norm = "l2")

# Convert the similarity matrix into a tidy format -----

similarity_df <- as.data.frame(as.table(as.matrix(similarity_matrix)))
colnames(similarity_df) <- c("Paragraph1", "Paragraph2", "Similarity")

# Filter for term-specific comparisons if needed -----

similarity_df <- similarity_df %>%
  filter(Paragraph1 != Paragraph2) %>%
  arrange(desc(Similarity))

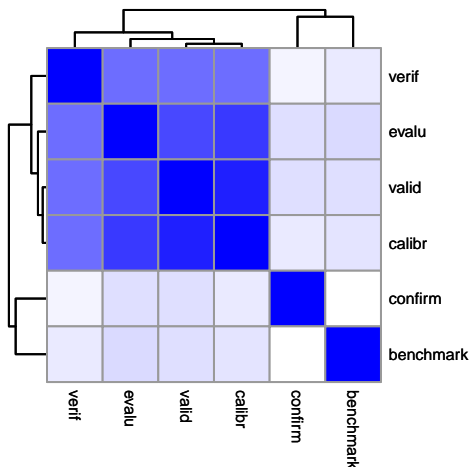
# PLOT #####

```

```
heatmap_data <- similarity_matrix
rownames(heatmap_data) <- clean_text$variable
colnames(heatmap_data) <- clean_text$variable
```

```
plot.heatmap <- pheatmap::pheatmap(as.matrix(heatmap_data),
  color = colorRampPalette(c("white", "blue"))(50),
  fontsize_row = 6,
  fontsize_col = 6,
  treeheight_row = 10,
  treeheight_col = 10,
  legend = FALSE)
```

```
plot.heatmap
```



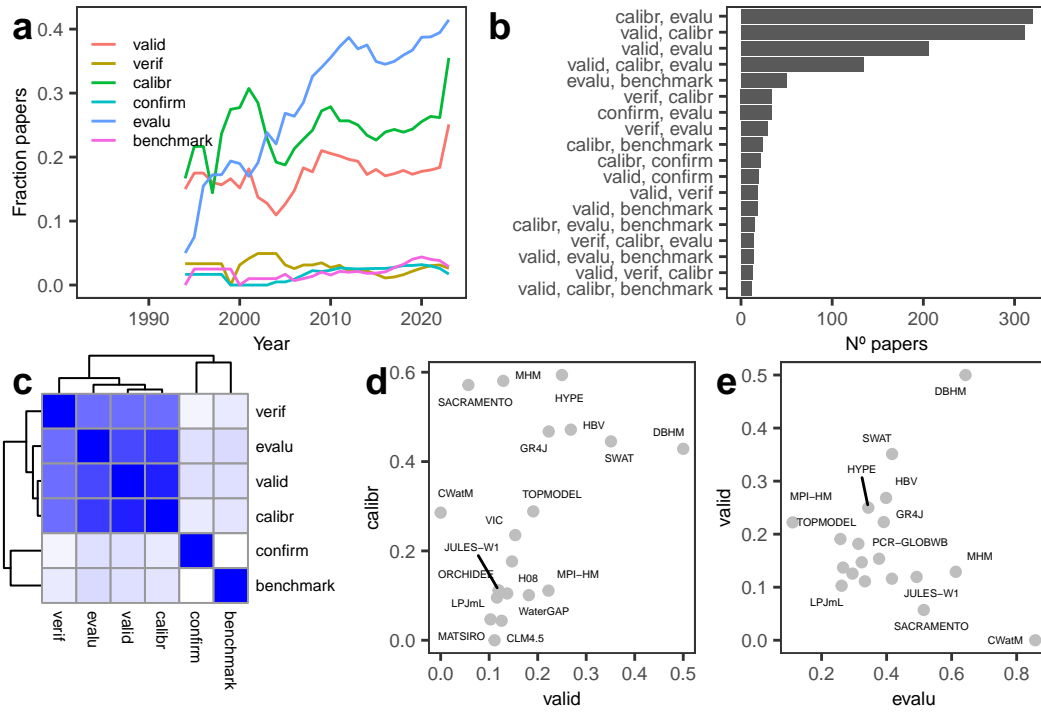
```
grob <- plot.heatmap$gtable
```

```
scatter.plots <- plot_grid(ggdraw(grob), plot.valid.calibr, plot.evalu.valid, ncol = 3,
  labels = c("c", "d", "e"), rel_widths = c(0.33, 0.33, 0.33))
```

```
plot_grid(top, scatter.plots, ncol = 1, rel_heights = c(0.5, 0.5))
```

```
## Warning: ggrepel: 1 unlabeled data points (too many overlaps). Consider
## increasing max.overlaps
```

```
## Warning: ggrepel: 6 unlabeled data points (too many overlaps). Consider
## increasing max.overlaps
```



```
# SESSION INFORMATION #####
```

```
sessionInfo()
```

```
## R version 4.3.2 (2023-10-31)
## Platform: aarch64-apple-darwin20 (64-bit)
## Running under: macOS Sonoma 14.2.1
##
## Matrix products: default
## BLAS: /Library/Frameworks/R.framework/Versions/4.3-arm64/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.3-arm64/Resources/lib/libRlapack.dylib;
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## time zone: Europe/London
## tzcode source: internal
##
## attached base packages:
## [1] parallel stats graphics grDevices utils datasets methods
## [8] base
##
## other attached packages:
## [1] benchmarkme_1.0.8 tidyquant_1.0.7
## [3] quantmod_0.4.25 TTR_0.24.3
## [5] PerformanceAnalytics_2.0.4 xts_0.13.1
## [7] zoo_1.8-12 ggrepel_0.9.5
## [9] LSAfun_0.6.3 rgl_1.1.3
## [11] lsa_0.73.3 SnowballC_0.7.1
## [13] cowplot_1.1.1 scales_1.3.0
## [15] tidytext_0.4.1 pdftools_3.3.3
## [17] tm_0.7-11 NLP_0.2-1
## [19] openxlsx_4.2.5.2 lubridate_1.9.2
## [21] forcats_1.0.0 stringr_1.5.1
## [23] dplyr_1.1.4 purrr_1.0.2
## [25] readr_2.1.4 tidyr_1.3.0
## [27] tibble_3.2.1 ggplot2_3.4.4
## [29] tidyverse_2.0.0 data.table_1.14.99
##
## loaded via a namespace (and not attached):
## [1] tidyselect_1.2.0 filehash_2.4-5 farver_2.1.1
## [4] fastmap_1.1.1 janeaustenr_1.0.0 digest_0.6.34
## [7] timechange_0.2.0 lifecycle_1.0.4 qpdf_1.3.2
## [10] tokenizers_0.3.0 magrittr_2.0.3 compiler_4.3.2
## [13] rlang_1.1.3 tools_4.3.2 utf8_1.2.4
## [16] sensobol_1.1.4 yaml_2.3.7 knitr_1.42
## [19] askpass_1.1 labeling_0.4.3 stopwords_2.3
```

```
## [22] htmlwidgets_1.6.2      curl_5.0.0             xml2_1.3.3
## [25] withr_3.0.0            grid_4.3.2             fansi_1.0.6
## [28] colorspace_2.1-0       iterators_1.0.14       tinytex_0.45
## [31] cli_3.6.2              rmarkdown_2.21         generics_0.1.3
## [34] tikzDevice_0.12.4      rstudioapi_0.15.0     httr_1.4.5
## [37] tzdb_0.3.0             base64enc_0.1-3        vctrs_0.6.5
## [40] Matrix_1.6-1.1         jsonlite_1.8.4         slam_0.1-50
## [43] hms_1.1.3              foreach_1.5.2          glue_1.7.0
## [46] benchmarkmeData_1.0.4  codetools_0.2-19      Quandl_2.11.0
## [49] stringi_1.8.3          gtable_0.3.4           quadprog_1.5-8
## [52] munsell_0.5.0          pillar_1.9.0           htmltools_0.5.5
## [55] R6_2.5.1               Rdpack_2.6             doParallel_1.0.17
## [58] evaluate_0.20          lattice_0.21-9         highr_0.10
## [61] rbibutils_2.2.16       Rcpp_1.0.12            zip_2.3.0
## [64] xfun_0.39              pkgconfig_2.0.3
```

```
## Return the machine CPU
```

```
cat("Machine:      "); print(get_cpu())$model_name)
```

```
## Machine:
```

```
## [1] "Apple M1 Max"
```

```
## Return number of true cores
```

```
cat("Num cores:    "); print(detectCores(logical = FALSE))
```

```
## Num cores:
```

```
## [1] 10
```

```
## Return number of threads
```

```
cat("Num threads: "); print(detectCores(logical = FALSE))
```

```
## Num threads:
```

```
## [1] 10
```