Reproducible research in computational subsurface hydrology

First steps in R with RMODFLOW and RMT3DMS

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We need to work on reproducibility in computational hydrology!

- “Most computational hydrology is not reproducible, so is it really science?”
  Hutton et al. 2016

- “Repeatable research: What hydrologists can learn from the Duke cancer research scandal.”
  Fienen & Bakker 2016

- “Reproducible Research in Vadose Zone Sciences.”
  Skaggs et al. 2015
R offers great tools and community!

https://www.jasondavies.com/wordcloud/
https://cran.r-project.org/web/views/ReproducibleResearch.html
Subsurface hydrology R community is small however, although R has great potential!

R and subsurface hydrology
- specific types of plots (hydrogeo)
- very specific purposes (quarrint, kwb.hantush)

R and hydrology
- hydrological time series analysis packages (hydroTSM, waterData, ...)
- lumped conceptual rainfall-runoff models (hydromad, TUWmodel, RHydro, ...)
- distributed hydrological models (topmodel, ...)
- weather generators or related packages (RMAWGEN, SPEI, ...)
- soil water packages (soiltexture, soilwaterfun, soilwaterptf, soilwater, HydroMe, ...)

Other useful things available in R
- mapping (OpenStreetMap, ggmap, rgdal, sp, sf, mapview, leaflet, ...)
- 3d viewing (rgl, plot3D, plot3Drgl, ...)
- geostatistics (gstat, RandomFields, geoR, ...)
- machine learning (CARET, ...)
- reproducible research (knitr, rmarkdown, xtable, ...)
- time series analysis (TSA, ...)
- spreadsheet & data base access (read_excel, xlsx, DBI, ...)
- data science (tidyverse)
- calibration & uncertainty estimation (hydroPSO, dream, DEoptim, ...)
- solving partial differential equations (deSolve, ReacTran, ...)
- ...
MODFLOW (groundwater flow) and MT3DMS (solute transport) codes are widely used in subsurface hydrology


R interfaces to MODFLOW and MT3DMS would be great!

- Alternative to mflab\(^1\) and flopy\(^2,3\) for the R user
- State-of-the-art static visualization of model input and output with ggplot2\(^2\)
- Interactive visualization with htmlwidgets
- Enables customizable interaction of stakeholders with developed models, through the use of shiny\(^4\)
- Brings R’s reproducible research capabilities to computational subsurface hydrology
- Would stimulate the development of an R subsurface hydrology community

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\(^1\) [https://code.google.com/archive/p/mflab/](https://code.google.com/archive/p/mflab/)

\(^2\) [https://github.com/modflowpy/flopy](https://github.com/modflowpy/flopy)


\(^4\) [e.g. http://www.it.ethz.ch/projects/china-groundwater-management/project/research/ียง.html](http://www.it.ethz.ch/projects/china-groundwater-management/project/research/ียง.html)
The RMODFLOW package

- pre- and post-processing of MODFLOW files
- read_* functions
- write_* functions
- create_* functions
- S3 methods for 2D, 3D and 4D arrays
  - ggplot2 plotting for maps, cross-sections
  - rgl for 3D visualization
  - export
    - shapefiles
    - animations
- basic model running, calibration and sensitivity analysis support

https://water.usgs.gov/nrp/geoheritage/ModModelingHelp/index.htm?example_model.htm


The RMT3DMS package

- pre- and post-processing of MT3DMS files
- read_* functions
- write_* functions
- imports RMODFLOW S3 methods
- basic model running support
MODFLOW or MT3DMS useR? Please do contribute!

Current coverage of MODFLOW\textsuperscript{1} packages:

BAS6, DIS, MULT, ZONE, PVAL, BCF6, LPF, HUF2, KDEF, LVDA, UPW, HFB6, UZF, SWI2, BFH, CHD, FHB, RCH, WEL, DRN, DRT, ETS, EVT, GHG, LAK, MNW1, MNW2, RES, RIP, RIV, SFR, STR, UZF, DE4, GMG, PCG, PCGN, SIP, NWT, GAGE, HYD, LMT6, MNWI, OC, IBS, SUB, SWT, CHOB, DROB, GBOB, HOB, RVOB, STOB, SWR1, CFP, CRCH, COC, FMP

Current coverage of MT3DMS\textsuperscript{2} packages:

BTN, ADV, DSP, SSM, RCT, GCG, FMI, UTL, TOB

\textsuperscript{1} MODFLOW-2005 and derived versions.
\textsuperscript{2} In future, the MT3D-USGS might be supported.
Real-life .Rnw example of reproducible research with RMODFLOW and RMT3DMS

1. Maps
2. Cross-sections
3. Post-processed data

Specify material properties & boundary conditions
Create different MT3DMS input files
Run MT3DMS
Check simulation properties
Check convergence
Visualize results:

For more information

Visit the pkgdown websites:

https://rogiersbart.github.io/RMODFLOW/
https://rogiersbart.github.io/RMT3DMS/