Releasing Scientific Software in GitHub: A Case Study on SWMM2PEST

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SE4Science, May 28, 2019

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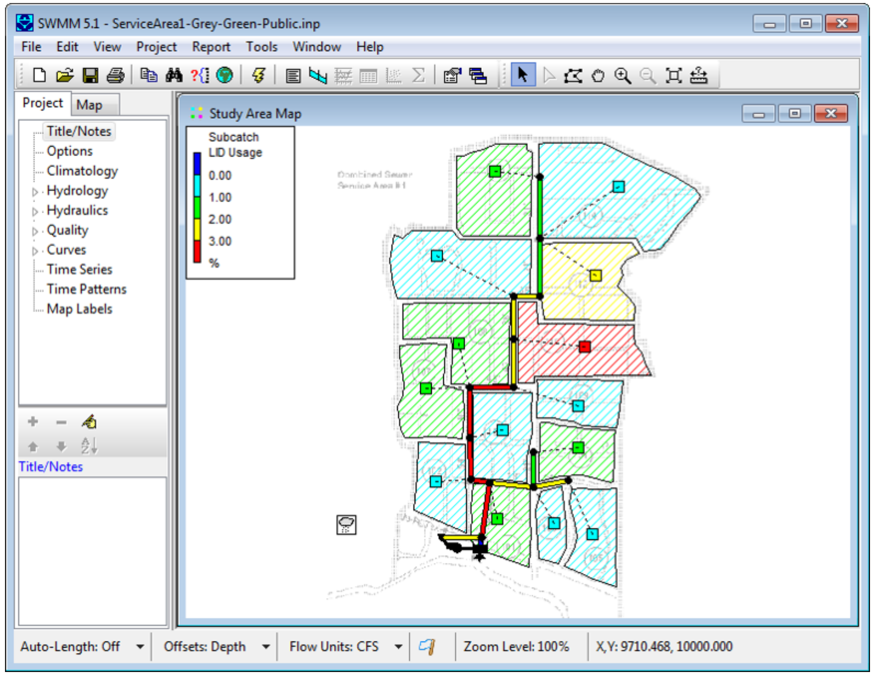
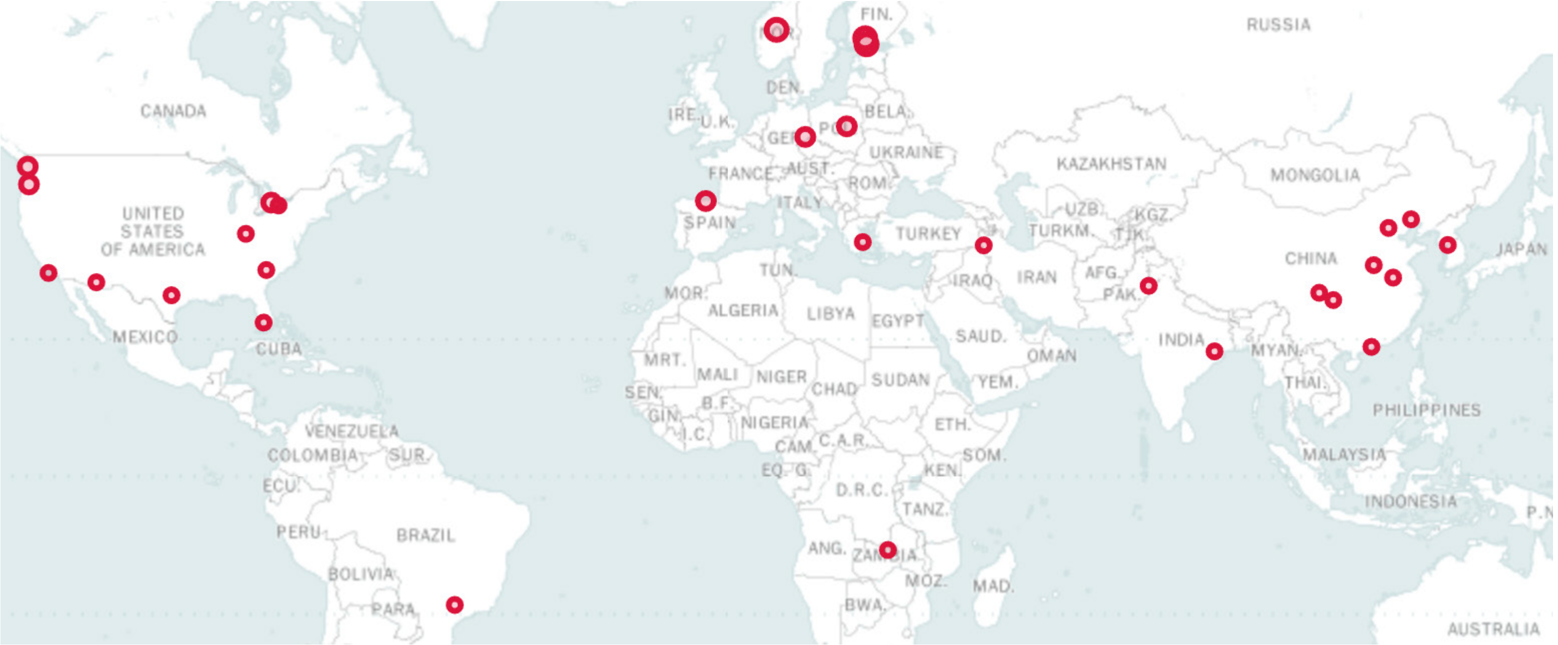
Storm Water Management Model (SWMM)



Auto-Length: Off | Offsets: Depth | Flow Units: CFS | Zoom Level: 100% | X,Y: 9710.468, 10000.000



United States Environmental Protection Agency

EPA

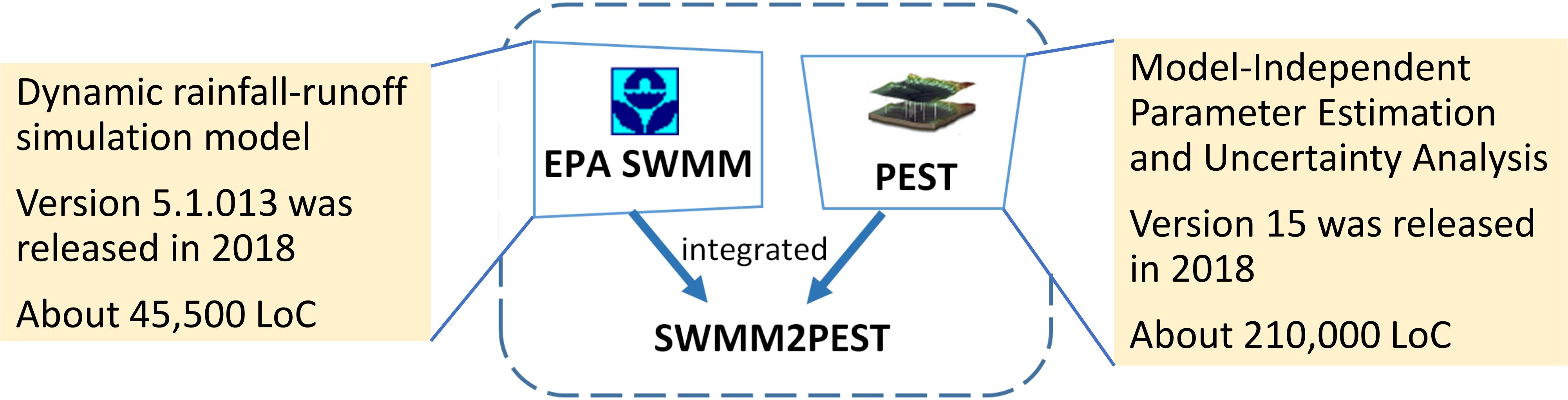
https://www.epa.gov/water-research/storm-water-management-model-swmm

Partial statistics on using SWMM for research in 2018 based on Google Scholar

The scientific software we are releasing

SWMM2PEST

An integration of the SWMM and PEST scientific programs



Dynamic rainfall-runoff simulation model

Version 5.1.013 was released in 2018

About 45,500 LoC

EPA SWMM

PEST

integrated

SWMM2PEST

Model-Independent Parameter Estimation and Uncertainty Analysis

Version 15 was released in 2018

About 210,000 LoC

Characteristics of scientific software

- Highly specialized: 1,000 to 100,000 LoC
- People: A few scientists-developers

Scientists often develop their own software for research for a relatively small user set, which may not be well documented and debugged for general use of others.

GitHub

helps

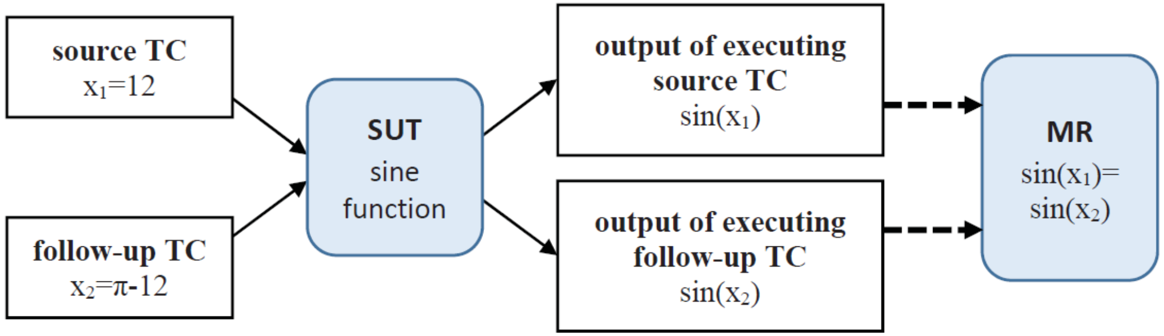
Release engineering

- Help accelerate software development and delivery
- Increase customer trust and satisfaction
- Provide faster feedback to developers
- Enhance the communication of integration systems
- Improve software quality
- …

How to release **scientific software** by applying release engineering

Metamorphic testing

Alleviate the oracle problem



source TC
$x_1=12$

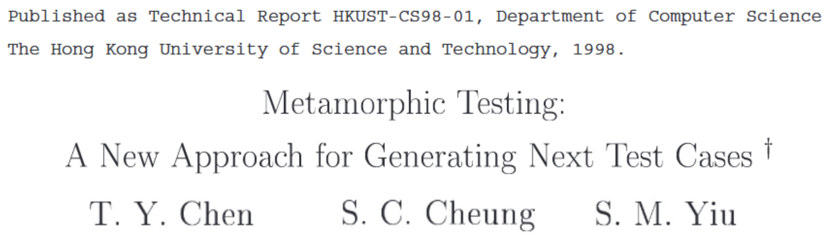
follow-up TC
$x_2=\pi-12$

SUT
sine
function

output of executing
source TC
$\sin(x_1)$

output of executing
follow-up TC
$\sin(x_2)$

MR
$\sin(x_1)=$
$\sin(x_2)$

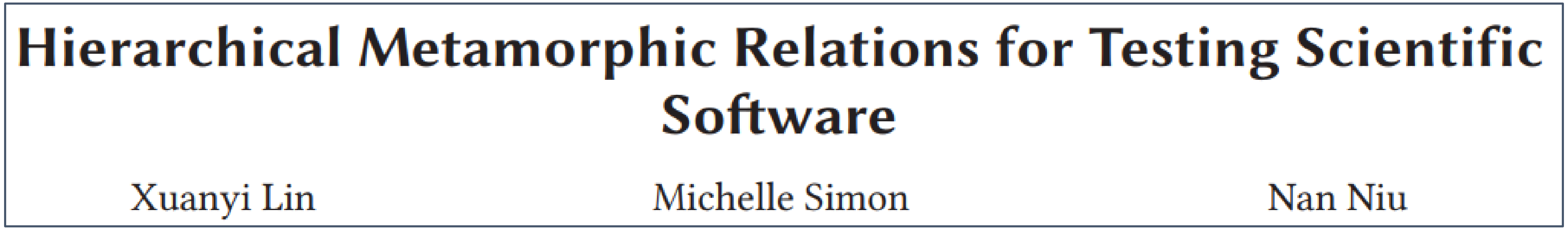


Published as Technical Report HKUST-CS98-01, Department of Computer Science
The Hong Kong University of Science and Technology, 1998.

Metamorphic Testing:
A New Approach for Generating Next Test Cases [†]

T. Y. Chen S. C. Cheung S. M. Yiu

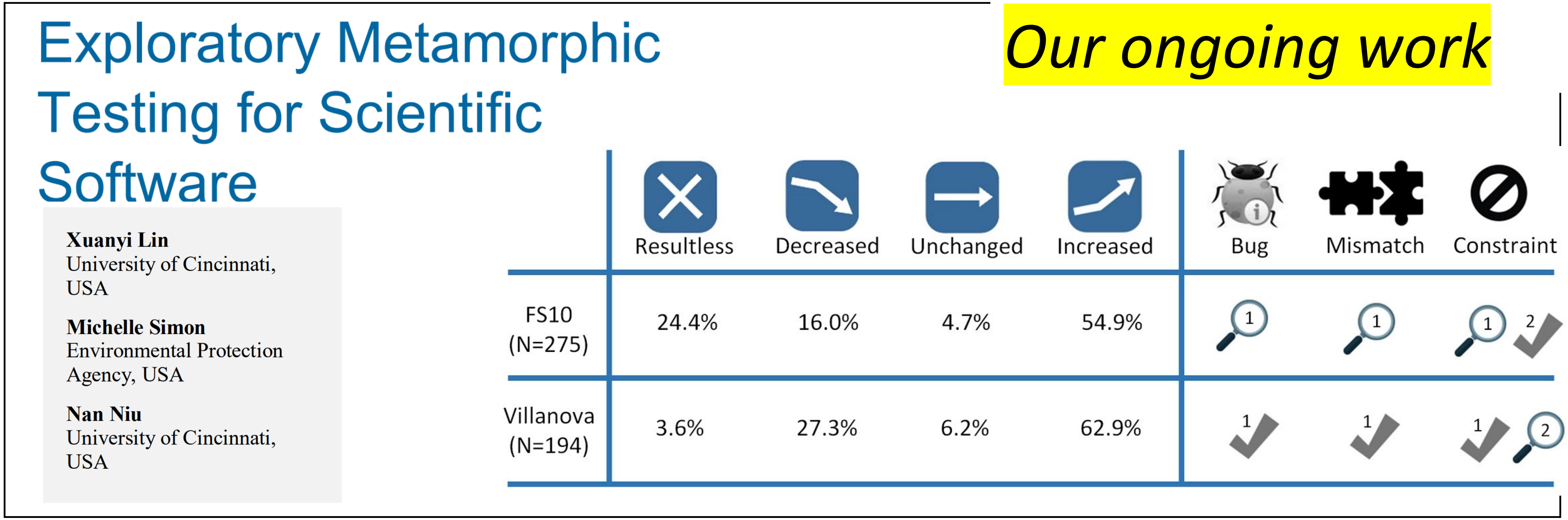
Metamorphic testing on SWMM2PEST



Hierarchical Metamorphic Relations for Testing Scientific Software

Xuanyi Lin Michelle Simon Nan Niu

Our ongoing work



Exploratory Metamorphic Testing for Scientific Software

Xuanyi Lin
University of Cincinnati,
USA

Michelle Simon
Environmental Protection
Agency, USA

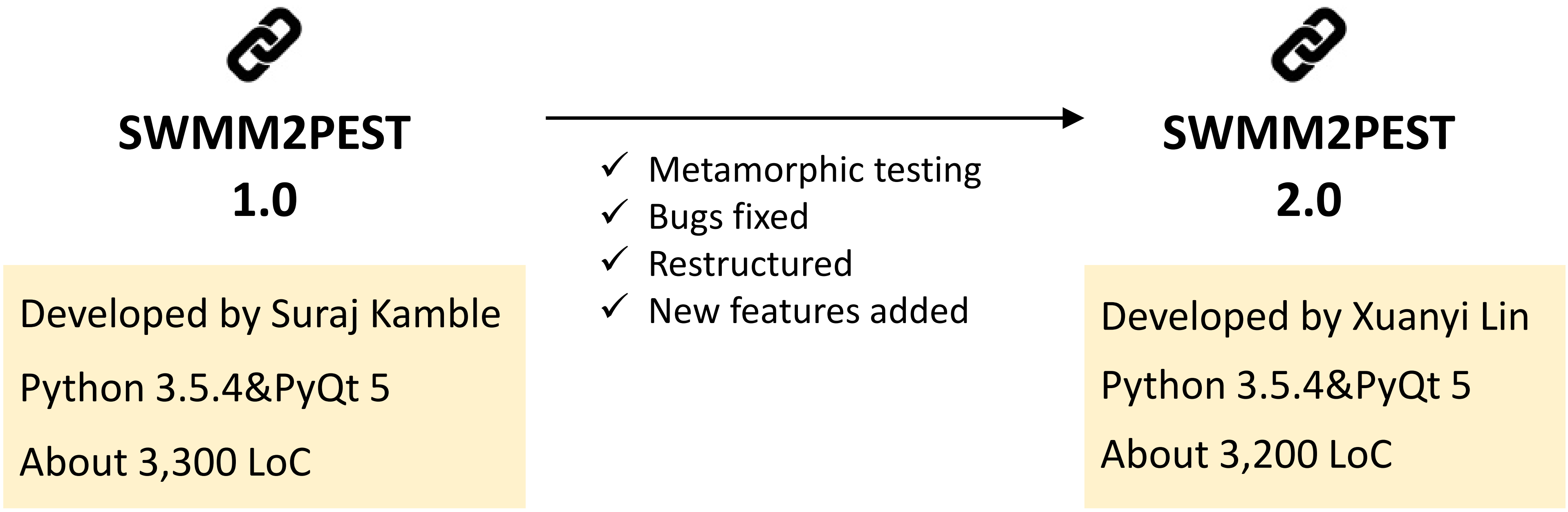
Nan Niu
University of Cincinnati,
USA

	✗ Resultless	↘ Decreased	→ Unchanged	↗ Increased	Bug	Mismatch	⊘ Constraint
FS10 (N=275)	24.4%	16.0%	4.7%	54.9%	🔍1	🔍1	🔍1 ✓2
Villanova (N=194)	3.6%	27.3%	6.2%	62.9%	✓1	✓1	✓1 🔍2

SWMM2PEST 1.0 to 2.0

Changes

Added & modified lines (source code)	Deleted lines (source code)	Added & modified UI files	Deleted UI files
1029	696	5	2



SWMM2PEST 1.0

Developed by Suraj Kamble

Python 3.5.4&PyQt 5

About 3,300 LoC

- ✓ Metamorphic testing
- ✓ Bugs fixed
- ✓ Restructured
- ✓ New features added

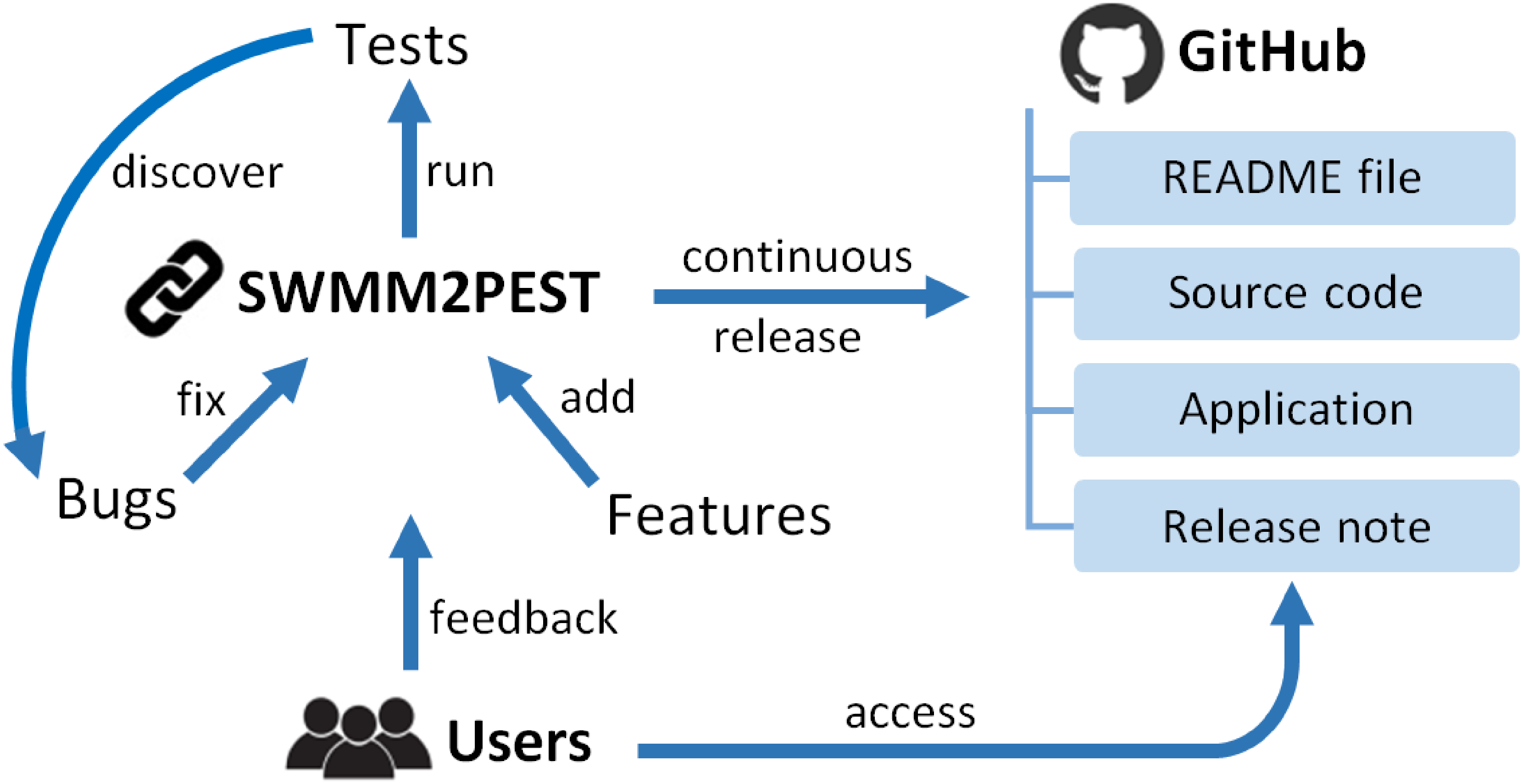
SWMM2PEST 2.0

Developed by Xuanyi Lin

Python 3.5.4&PyQt 5

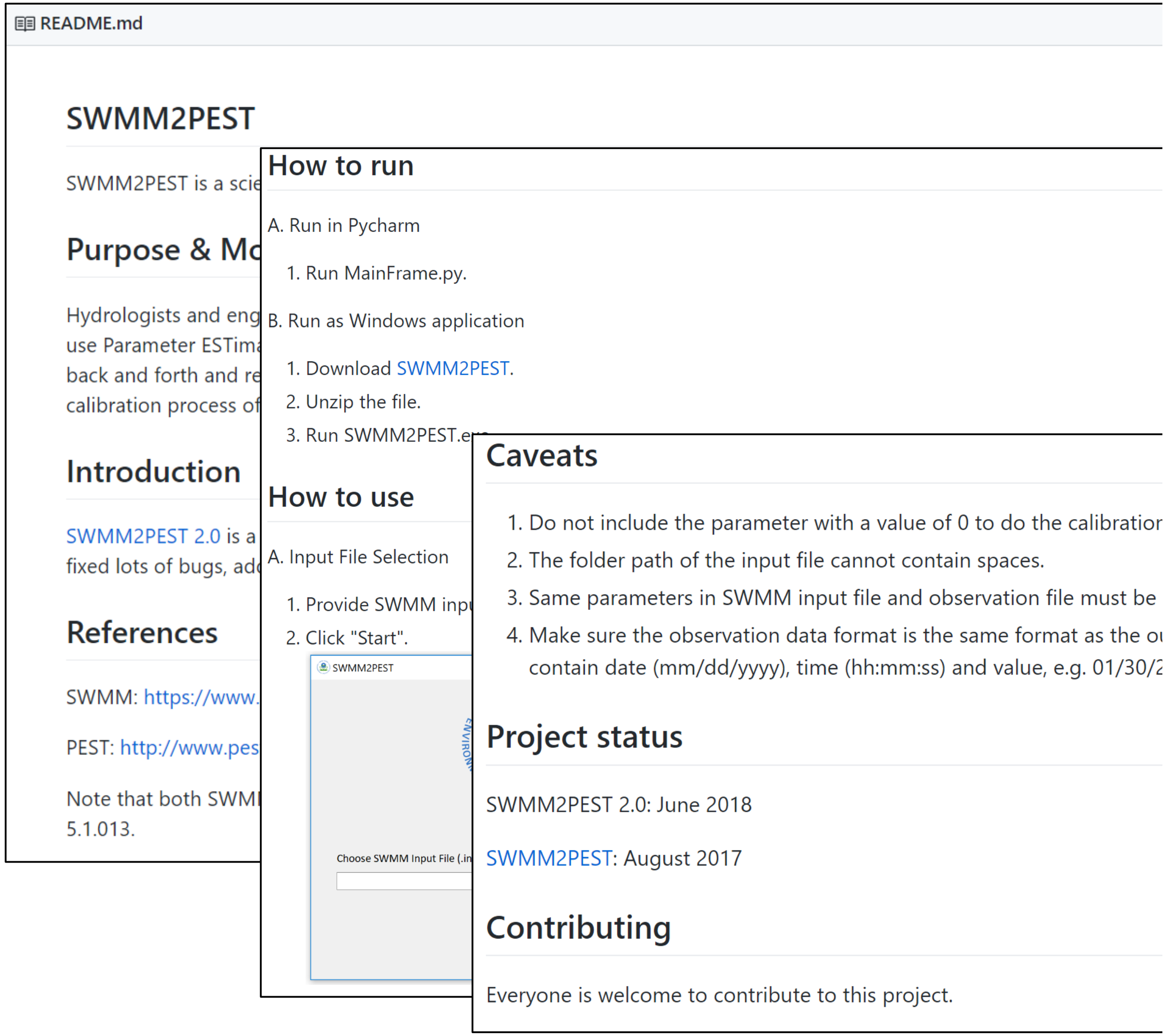
About 3,200 LoC

Release workflow



GitHub-driven release process

Releasing in GitHub



README.md

SWMM2PEST

SWMM2PEST is a scie

Purpose & Mo

Hydrologists and eng
use Parameter ESTima
back and forth and re
calibration process of

Introduction

SWMM2PEST 2.0 is a
fixed lots of bugs, ad

References

SWMM: https://www.

PEST: http://www.pes

Note that both SWM
5.1.013.

How to run

A. Run in Pycharm

1. Run MainFrame.py.

B. Run as Windows application

1. Download SWMM2PEST.
2. Unzip the file.
3. Run SWMM2PEST.e

How to use

A. Input File Selection

1. Provide SWMM inp
2. Click "Start".

Caveats

1. Do not include the parameter with a value of 0 to do the calibratior
2. The folder path of the input file cannot contain spaces.
3. Same parameters in SWMM input file and observation file must be
4. Make sure the observation data format is the same format as the o contain date (mm/dd/yyyy), time (hh:mm:ss) and value, e.g. 01/30/2

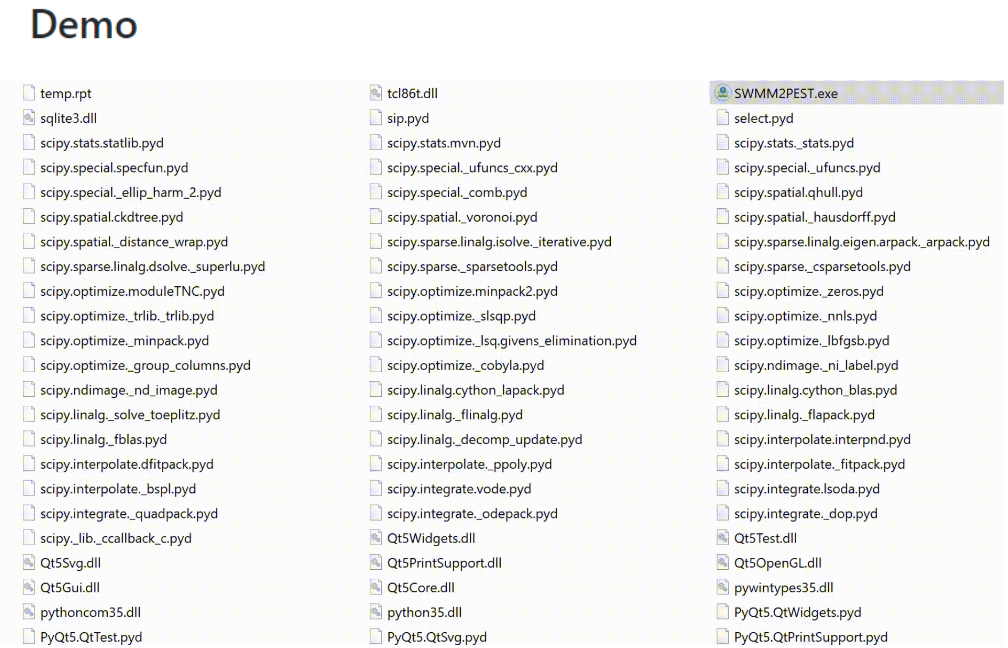
Project status

SWMM2PEST 2.0: June 2018

SWMM2PEST: August 2017

Contributing

Everyone is welcome to contribute to this project.



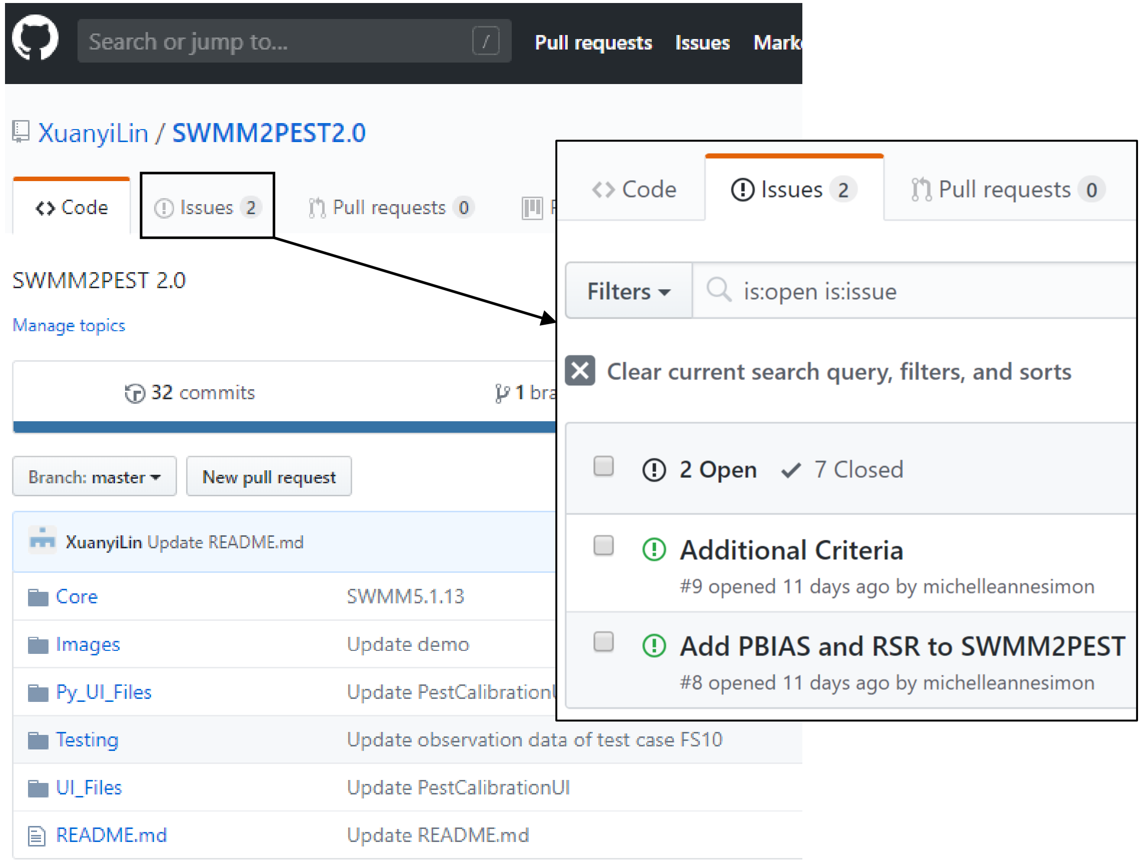
Demo

temp.rpt
sqlite3.dll
scipy.stats.statlib.pyd
scipy.special.specfun.pyd
scipy.special._ellip_harm_2.pyd
scipy.spatial.ckdtree.pyd
scipy.spatial._distance_wrap.pyd
scipy.sparse.linalg.dsolve._superlu.pyd
scipy.optimize.moduleTNC.pyd
scipy.optimize._trlib._trlib.pyd
scipy.optimize._minpack.pyd
scipy.optimize._group_columns.pyd
scipy.ndimage._nd_image.pyd
scipy.linalg._solve_toeplitz.pyd
scipy.linalg._fblas.pyd
scipy.interpolate.dfitpack.pyd
scipy.interpolate._bspl.pyd
scipy.integrate._quadpack.pyd
scipy._lib._ccallback_c.pyd
Qt5Svg.dll
Qt5Gui.dll
pythoncom35.dll
PyQt5.QtTest.pyd
tcl86t.dll
sip.pyd
scipy.stats.mvn.pyd
scipy.special._ufuncs_cxx.pyd
scipy.special._comb.pyd
scipy.spatial._voronoi.pyd
scipy.sparse.linalg.isolve._iterative.pyd
scipy.sparse._sparsetools.pyd
scipy.optimize.minpack2.pyd
scipy.optimize._slsqp.pyd
scipy.optimize._lsq.givens_elimination.pyd
scipy.optimize._cobyla.pyd
scipy.linalg.cython_lapack.pyd
scipy.linalg._flinalg.pyd
scipy.linalg._decomp_update.pyd
scipy.interpolate._ppoly.pyd
scipy.integrate.vode.pyd
scipy.integrate._odepack.pyd
Qt5Widgets.dll
Qt5PrintSupport.dll
Qt5Core.dll
python35.dll
PyQt5.QtSvg.pyd
SWMM2PEST.exe
select.pyd
scipy.stats._stats.pyd
scipy.special._ufuncs.pyd
scipy.spatial.qhull.pyd
scipy.spatial._hausdorff.pyd
scipy.sparse.linalg.eigen.arpack._arpack.pyd
scipy.sparse._csparsetools.pyd
scipy.optimize._zeros.pyd
scipy.optimize._nnls.pyd
scipy.optimize._lbfgsb.pyd
scipy.ndimage._ni_label.pyd
scipy.linalg.cython_blas.pyd
scipy.linalg._flapack.pyd
scipy.interpolate.interpnd.pyd
scipy.interpolate._fitpack.pyd
scipy.integrate.lsoda.pyd
scipy.integrate._dop.pyd
Qt5Test.dll
Qt5OpenGL.dll
pywintypes35.dll
PyQt5.QtWidgets.pyd
PyQt5.QtPrintSupport.pyd

Categorizing the Content of GitHub README Files

Gede Artha Azriadi Prana[1] · Christoph Treude[2] · Ferdian Thung[1] ·
Thushari Atapattu[2] · David Lo[1]

Releasing in GitHub



SWMM2PEST 2.0

XuanyiLin Update README.md

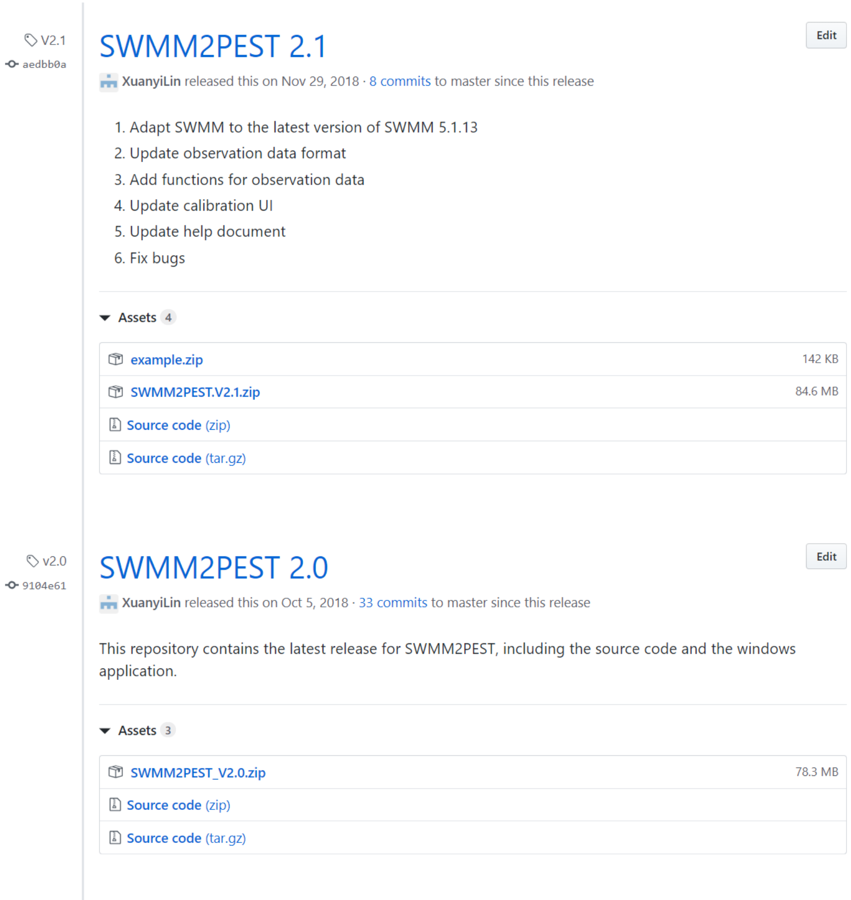
Core	SWMM5.1.13
Images	Update demo
Py_UI_Files	Update PestCalibrationI
Testing	Update observation data of test case FS10
UI_Files	Update PestCalibrationUI
README.md	Update README.md

□ 2 Open ✓ 7 Closed

□ Additional Criteria
#9 opened 11 days ago by michelleannesimon

□ Add PBIAS and RSR to SWMM2PEST
#8 opened 11 days ago by michelleannesimon

Source Code



SWMM2PEST 2.1

XuanyiLin released this on Nov 29, 2018 · 8 commits to master since this release

1. Adapt SWMM to the latest version of SWMM 5.1.13
2. Update observation data format
3. Add functions for observation data
4. Update calibration UI
5. Update help document
6. Fix bugs

Assets 4

example.zip	142 KB
SWMM2PEST.V2.1.zip	84.6 MB
Source code (zip)	
Source code (tar.gz)	

SWMM2PEST 2.0

XuanyiLin released this on Oct 5, 2018 · 33 commits to master since this release

This repository contains the latest release for SWMM2PEST, including the source code and the windows application.

Assets 3

SWMM2PEST_V2.0.zip	78.3 MB
Source code (zip)	
Source code (tar.gz)	

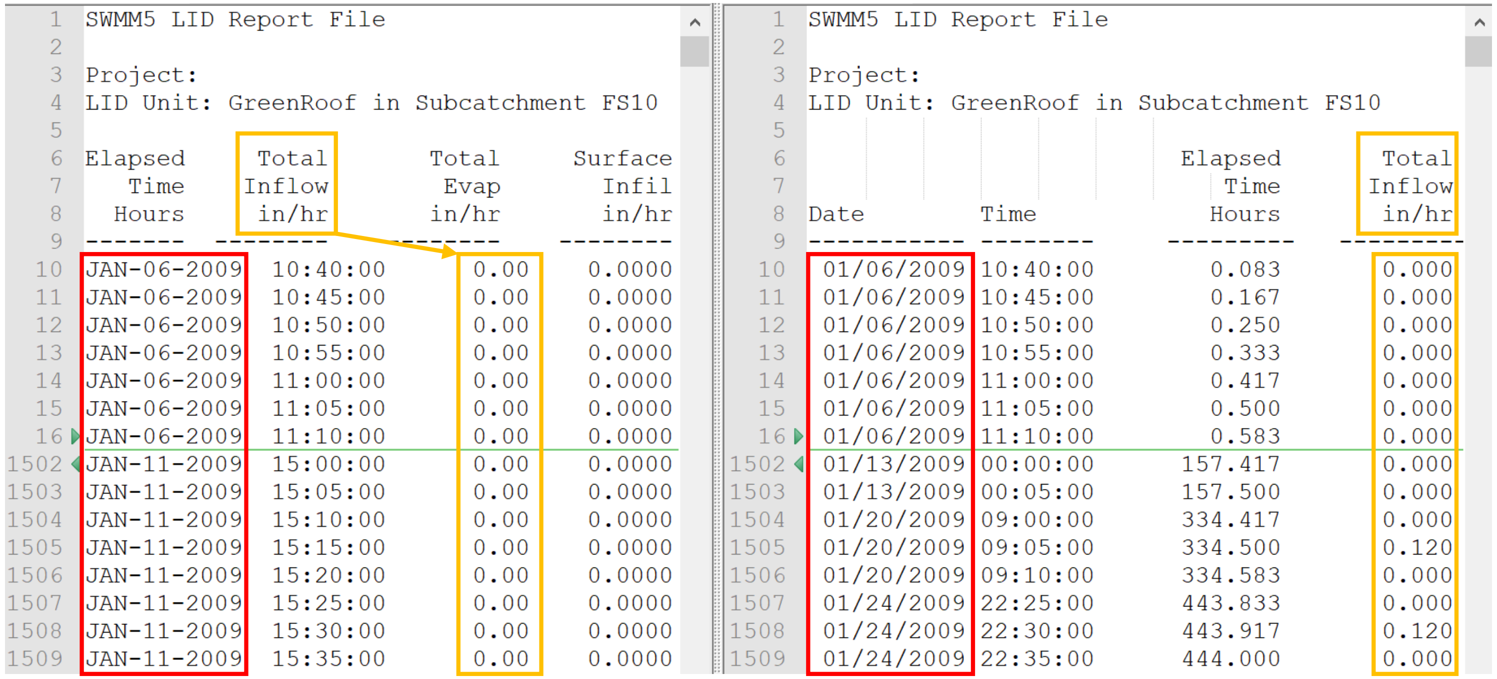
Release software

Changes between versions

SWMM2PEST

	SWMM2PEST 1.0	SWMM2PEST 2.0	SWMM2PEST 2.1
SWMM	5.1.10	5.1.10	5.1.13
PEST	13.3	14.2	14.2

SWMM 5.1.10



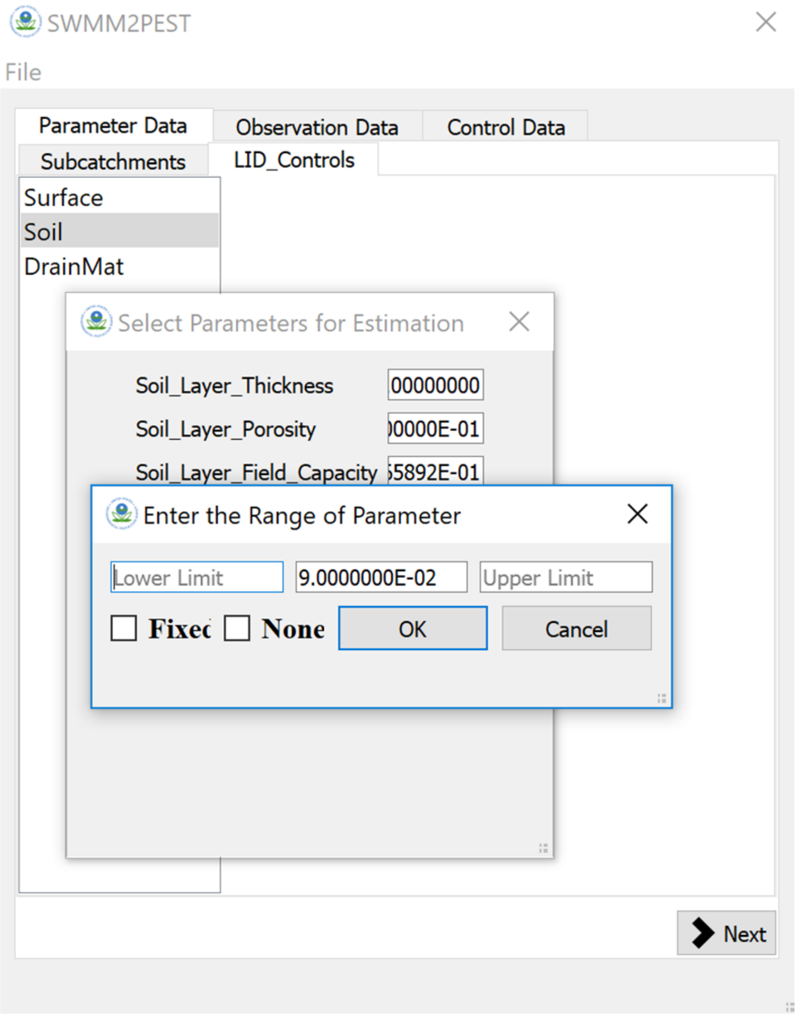
```
SWMM5 LID Report File

Project:
LID Unit: GreenRoof in Subcatchment FS10

Elapsed    Total          Total    Surface
   Time   Inflow           Evap      Infil
  Hours    in/hr          in/hr      in/hr
-------  --------      --------   --------
JAN-06-2009  10:40:00      0.00     0.0000
JAN-06-2009  10:45:00      0.00     0.0000
JAN-06-2009  10:50:00      0.00     0.0000
JAN-06-2009  10:55:00      0.00     0.0000
JAN-06-2009  11:00:00      0.00     0.0000
JAN-06-2009  11:05:00      0.00     0.0000
JAN-06-2009  11:10:00      0.00     0.0000
JAN-11-2009  15:00:00      0.00     0.0000
JAN-11-2009  15:05:00      0.00     0.0000
JAN-11-2009  15:10:00      0.00     0.0000
JAN-11-2009  15:15:00      0.00     0.0000
JAN-11-2009  15:20:00      0.00     0.0000
JAN-11-2009  15:25:00      0.00     0.0000
JAN-11-2009  15:30:00      0.00     0.0000
JAN-11-2009  15:35:00      0.00     0.0000
```

```
SWMM5 LID Report File

Project:
LID Unit: GreenRoof in Subcatchment FS10

                            Elapsed      Total
                               Time     Inflow
Date          Time            Hours      in/hr
-----------  --------     ---------  ---------
 01/06/2009  10:40:00         0.083      0.000
 01/06/2009  10:45:00         0.167      0.000
 01/06/2009  10:50:00         0.250      0.000
 01/06/2009  10:55:00         0.333      0.000
 01/06/2009  11:00:00         0.417      0.000
 01/06/2009  11:05:00         0.500      0.000
 01/06/2009  11:10:00         0.583      0.000
 01/13/2009  00:00:00       157.417      0.000
 01/13/2009  00:05:00       157.500      0.000
 01/20/2009  09:00:00       334.417      0.000
 01/20/2009  09:05:00       334.500      0.120
 01/20/2009  09:10:00       334.583      0.000
 01/24/2009  22:25:00       443.833      0.000
 01/24/2009  22:30:00       443.917      0.120
 01/24/2009  22:35:00       444.000      0.000
```

SWMM 5.1.13

Improvements as requirements change

SWMM2PEST 1.0 UI



Soil_Layer_Thickness 00000000

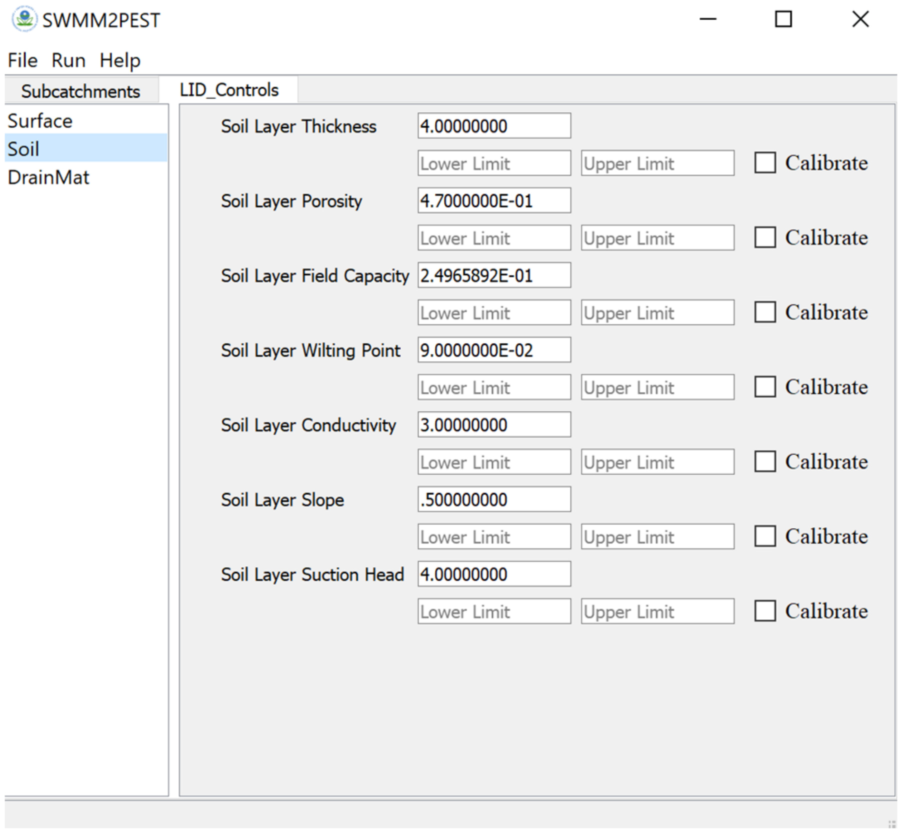
Soil_Layer_Porosity)0000E-01

Soil_Layer_Field_Capacity ;5892E-01

Lower Limit 9.0000000E-02 Upper Limit

□ Fixec □ None

SWMM2PEST 2.0 UI



Soil Layer Thickness	4.00000000	Lower Limit	Upper Limit	□ Calibrate
Soil Layer Porosity	4.7000000E-01	Lower Limit	Upper Limit	□ Calibrate
Soil Layer Field Capacity	2.4965892E-01	Lower Limit	Upper Limit	□ Calibrate
Soil Layer Wilting Point	9.0000000E-02	Lower Limit	Upper Limit	□ Calibrate
Soil Layer Conductivity	3.00000000	Lower Limit	Upper Limit	□ Calibrate
Soil Layer Slope	.500000000	Lower Limit	Upper Limit	□ Calibrate
Soil Layer Suction Head	4.00000000	Lower Limit	Upper Limit	□ Calibrate

Insights

- Release as ***required***
- ***Connector*** versus ***connectee*** release
- Release to help automated ***testing***

Future work

- Investigate other repositories
- Continuous release with more comprehensive user feedback and other developers' opinions

Thank you

Releasing Scientific Software in GitHub:
A Case Study on SWMM2PEST

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UNIVERSITY OF Cincinnati