Solver for Hydrologic Unstructured Domain (SHUD)

User Guide

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1 Overview

This is a user guide or technical documentation of the SHUD modeling system.

The Solver for Hydrologic Unstructured Domain (SHUD - pronounced "SHOULD") is a multi-process, multi-scale hydrological model where major hydrological processes are fully coupled using the semi-discrete **Finite Volume Method** (FVM).

SHUD-tools is an open-source GIS and hydrological analysis toolkit designed for SHUD modeling system. The SHUD tools provides access to the digital data sets (terrain, forcing and parameters) and tools necessary to drive the model, as well as a collection of GIS-based pre- and post-processing tools.

Collectively the system is referred to as the SHUD Modeling System.

The SHUD and SHUD-tools is an open source software, freely available for download at SHUD website or Github Page along with installation and user guides.

1.1 Standing on the shoulder of giant

SHUD is a descendent of **Penn State Integrated Hydrologic Model (PIHM)**, SHUD inherits the fundamental idea of solving hydrological variables in CVODE, but the model structure, compurational algorithm, programing laguage and input/out files are redesigned. The SHUD is imcompatible to PIHM.

It is our intention (me and previous PIHM group) to begin a debate on the role of Community Models in the hydrologic sciences.

SHUD and PIHM represents our strategy for the synthesis of *multi-state*, *multiscale* distributed hydrologic models using the integral representation of the underlying physical process equations and state variables.

Our interest is in devising a concise representation of watershed and/or river basin hydrodynamics, which allows interactions among major physical processes operating simultaneously, but with the flexibility to add or eliminate states/processes/constitutive relations depending on the objective of the numerical experiment or purpose of the scientific or operational application.

To satisfy the objectives, the SHUD

• is distributed hydrologic model, based on the semi-discrete **Finite Volume**Method (FVM) in which domain discretization is an unstructured triangular

irregular network (e.g. Delaunay triangles) generated with constraints (geometric, and parametric). A local prismatic control volume is formed by the vertical projection of the Delaunay triangles forming each layer of the model. Given a set of constraints (e.g. river network support, watershed boundary, altitude zones, ecological regions, hydraulic properties, climate zones, etc.), an "optimal" mesh is generated. River volume elements are also prismatic, with trapezoidal or rectangular cross-section, and are generated along or cross edges of Delaunay triangles. The local control volume contains all equations to be solved and is referred to as the model kernel.

- is a physically-based model, in which all equations used are describing the physics of the hydrological processes which control the catchment. The physical model is able to predict the water in the ungage water system, to estimate the sediment, pullutants, and vegetation, etc, such that it is practical to be coupled with biochemistry, geomorphology, limnology, and other water-related research. The global ODE system is assembled by combining all local ODE systems throughout the domain and then solved by a state-of-the-art parallel ODE solver known as CVODE developed at the Lawrence Livermore National Laboratory.
- is a fully-coupled hydrologic model, where the state and flux variables in the hydrologic system are solved within the same time step and conserve the mass. The fluxes are infiltration, overland flow, groundwater recharge, lateral groundwater flow, exchange of river and soil/groundwater and river discharge.
- is of an adaptable temporal and spatial resolution. The spatial resolution of the model varies from meters to kilometers based requirement of modeling and computing resources. The internal time step of the iteration step is adjustable; it is able to export the status of the catchment in less 1 second to days. Also, the time interval for exporting results is configured flexibly. The flexible spatial and temporal resolution is rather valuable for community model coupling.
- is an open source model, anyone can access the source code, use and submit their improvement.
- is a long-term yield and single-event flood model.

1.2 Brief History of PIHM system

• 2005 PIHM v1.0

Dr. Yizhong Qu (Qu and Duffy, 2007) developed and verified the first version of PIHM in 2001-2005 during his Ph.D. in Pennsylvania State University, following the blueprint of Freeze and Harlan (1969). This version of PIHM is the soul of the PIHM model.

• 2009 PIHMgis

Dr. Gopal Bhartt (Bhatt, 2012) developed the PIHMgis with support of C++, Qt GUI library, TRIANGLE library, and QGIS developing kit. The development of PIHMgis

makes the learning curve of PIHM moderate and benefits the developing, modeling and coupling.

• 2015 MM-PIHM

Dr. Yuninh Shi led and developed the MM-PIHM (Multi-Module PIHM), which embedded all modules from PIHM family, such as RT-PIHM, LE-PIHM, flux-PIHM, BGC-PIHM, etc. together. The sophisticated design and coupling of the MM-PIHM is the summit of the PIHM as a *Community Model* that combined all water-related modules together.

• 2019 PIHM++

Based on the accumulated contribution of PIHM modeling and coupling with related researches, it is necessary to solve the known bugs and limitations, improve the performance of the model with parallel methods, and adopt new updates from SUNDIALS solver and programming strategy.

Several publications that may helps:

- (Qu, 2004)
- (Qu and Duffy, 2007)
- (Li, 2008)
- (Kumar et al., 2004)
- (Kumar et al., 2009)
- (Yu et al., 2015)
- (Yu et al., 2014)
- (Li and Duffy, 2011)
- (Shi et al., 2015a)
- (Shi et al., 2015b)
- (Bhatt et al., 2014)

1.3 Steps of modeling with SHUD

1.3.1 Essential Terrestrial Variables?

- Atmospheric forcing (precipitation, snow cover, wind, relative humidity, temperature, net radiation, albedo, photosynthetic atmospheric radiation, leaf area index)
- Digital elevation model (DEM)
- River/stream discharge
- Soil (class, hydrologic properties)
- Groundwater (levels, extent, hydro-geologic properties)
- Lake/Reservoir (levels, extent)
- Land cover and land use (biomass, human infrastructure, demography, ecosystem disturbance)

• Water use

Most data reside on federal serversmany petabytes

1.3.2 A-Priori Data Sources

Feature/Tir	ne-	
Series	Property	Source
Soil Porosity; Sand Silt, Clay		CONUS, SSURGO and STATSGO
	Fractions; Bulk	
	Density	_
Geology	Bed Rock	http:
	Depth;	//www.dcnr.state.pa.us/topogeo/,
	Horizontal and	http://www.lias.psu.edu/emsl/
	Vertical	guides/X.html
	Hydraulic	
т 1	Conductivity	IDIC IDAC
Land	LAI	UMC, LDASmapveg;
Cover	3.5	11 1 2000
Land	Manning's	Hernandez et. al., 2000
Cover	Roughness;	(2002)
River	Manning's	Dingman (2002)
D.	Roughness;	
River	Coefficient of	ModHms Manual (Panday and
D.	Discharge	Huyakorn, 2004)
River	Shape and	Derived from regression using depth,
	Dimensions;	width, and discharge data from USGS data
River	Topology:	Derived using PIHMgis (Bhatt et.
	Nodes,	al., 2008)
	Neighboring	, ,
	Elements;	
Forcing	Prec, Temp.	National Land Data Assimilation
	RH, Wind, Rad.	System: NLDAS-2
Topography	DEM	http://seamless.usgs.gov/
Streamflow		http:
		//nwis.waterdata.usgs.gov/nwis/sw
Groundwate	er	http:
		// nwis. water data. usgs. gov/nwis/gw

1.4 Workflow of SHUD Modeling System

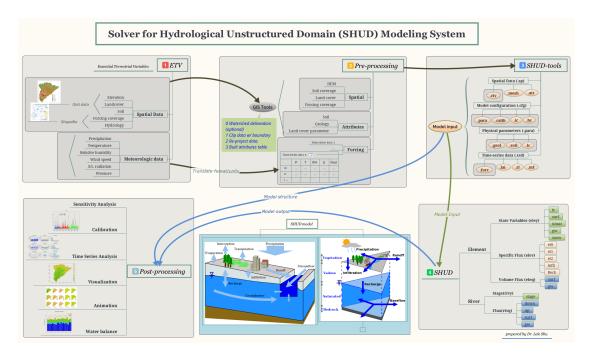


Figure 1.1: The workflow of modeling with SHUD Modeling System $\,$

- 1. Prepare raw Essential Terrestrial Variables (ETV)
- 2. Convert and crop raw data with the research area boundary.
- 3. Build the unstructued modeling domain with SHUD-tools
- 4. Run SHUD on desktop or cluster.
- 5. Analysis the SHUD model results with SHUD-tools or your hydrologic analysis tools.

2 Install SHUD and SHUD-tools

2.1 SUNDIALS/CVODE

The SHUD model requires the support of SUNDIALS or CVODE library. **SUNDIALS** is a SUite of Nonlinear and DIfferential/ALgebraic equation Solvers, consists of six solvers. **CVODE** is a solver for stiff and nonstiff ordinary differential equation (ODE) systems (initial value problem) given in explicit form y' = f(t, y). The methods used in CVODE are variable-order, variable-step multistep methods. You can install the entire SUNDIALS suite or CVODE only.

Since the SUNDIALS/CVODE keeps updating periodically and significantly, the function names and structure are changed accordingly, we suggest to use the specific version of the solver, rather than the latest solver.

 $SUNDIALS/CVODE\ is\ available\ in\ LLNL:\ https://computation.llnl.gov/projects/sundials/sundials-software$

The installation of CVODE v3.x:

- 1. Go to your Command Line and enter your workspace and unzip your CVODE source code here.
- 2. make directories for CVODE, including builddir, instdir and srcdir

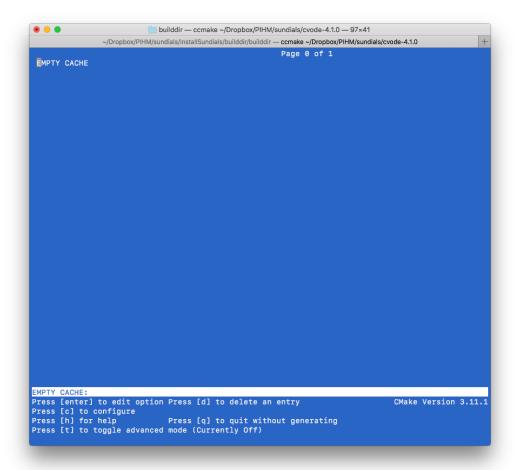
```
mkdir builddir
mkdir instdir
mkdir srcdir
cd builddir/
```

3. Try ccmake. Install cmake if you don't have one.

ccmake

4. Run ccmake to configure your compile environment.

```
ccmake ../sundials/cvode-5.0.0
```



This is an empty configure. Press c to start the configuration.

```
• • •
                               builddir — ccmake ../../sundials-master — 78×42
                ~/Dropbox/SHUD/github/SHUD/InstallSundials/builddir — ccmake ../../sundials-master
                                                                   Page 1 of 2
 BUILD_ARKODE
 BUILD_CVODE
BUILD_CVODES
                                           ON
                                           OFF
 BUILD_IDA
BUILD_IDAS
                                           OFF
OFF
 BUILD_KINSOL
                                           OFF
 BUILD_SHARED_LIBS
 BUILD_STATIC_LIBS
                                           ON
 BUILD_TESTING
CMAKE_BUILD_TYPE
                                           ON
 CMAKE_C_COMPILER
                                           /Applications/Xcode.app/Contents/Develop
 CMAKE_C_FLAGS
 CMAKE_INSTALL_LIBDIR
 CMAKE_INSTALL_PREFIX
CMAKE_OSX_ARCHITECTURES
                                           /Users/leleshu/sundials
 CMAKE_OSX_DEPLOYMENT_TARGET
 CMAKE_OSX_SYSROOT
 CUDA_ENABLE
                                           OFF
 EXAMPLES_ENABLE_C
EXAMPLES_ENABLE_CXX
                                           ON
OFF
                                           ON
 EXAMPLES_INSTALL
 EXAMPLES_INSTALL_PATH F2003_INTERFACE_ENABLE
                                           /Users/leleshu/sundials/example
 F77_INTERFACE_ENABLE
HYPRE_ENABLE
                                           OFF
OFF
 KLU_ENABLE
                                           OFF
 LAPACK_ENABLE
                                           OFF
 MPI_ENABLE
                                           OFF
 OPENMP_DEVICE_ENABLE
OPENMP_ENABLE
                                           OFF
                                           OFF
 PETSC_ENABLE
                                           OFF
 PTHREAD_ENABLE
                                           OFF
 RAJA_ENABLE
                                           OFF
 SUNDIALS_INDEX_SIZE SUNDIALS_PRECISION
                                           64
                                           double
BUILD_ARKODE: Build the ARKODE library
Press [enter] to edit option Press [d] to delete an entry CMake Version 3.11.1
Press [c] to configure
Press [n] for neip Press [q] to quit wi
Press [t] to toggle advanced mode (Currently Off)
                                    Press [q] to quit without generating
```

The default configuration. Make sure the value for three lines:

```
BUILD_CVODE = ON

CMAKE_INSTALL_PREFIX = ~/sundials

EXAMPLES_INSTALL_PATH = ~/sundials/examples
```

After the modification of values, press c to confirm configuration.

```
• • •
                              builddir — ccmake ../../sundials-master — 78×42
                ~/Dropbox/SHUD/github/SHUD/InstallSundials/builddir — ccmake ../../sundials-master
                                                                   Page 1 of 2
 BUILD_ARKODE
 BUILD_CVODE
BUILD_CVODES
                                           ON
                                           OFF
 BUILD_IDA
BUILD_IDAS
                                           0FF
                                           OFF
 BUILD_KINSOL
                                           OFF
 BUILD_SHARED_LIBS
 BUILD_STATIC_LIBS
                                           ON
 BUILD_TESTING
CMAKE_BUILD_TYPE
                                           ON
 CMAKE_C_COMPILER
                                           /Applications/Xcode.app/Contents/Develop
 CMAKE_C_FLAGS
 CMAKE_INSTALL_LIBDIR
 CMAKE_INSTALL_PREFIX
CMAKE_OSX_ARCHITECTURES
                                           /Users/leleshu/sundials
 CMAKE_OSX_DEPLOYMENT_TARGET
 CMAKE_OSX_SYSROOT
 CUDA_ENABLE
                                           OFF
 EXAMPLES_ENABLE_C
EXAMPLES_ENABLE_CXX
                                           ON
                                           OFF
 EXAMPLES_INSTALL
                                           ON
 EXAMPLES_INSTALL_PATH
                                           /Users/leleshu/sundials/example
 F2003_INTERFACE_ENABLE
 F77_INTERFACE_ENABLE
HYPRE_ENABLE
                                           OFF
                                           OFF
 KLU_ENABLE
LAPACK_ENABLE
                                           OFF
                                           OFF
 MPI_ENABLE
                                           OFF
 OPENMP_DEVICE_ENABLE
OPENMP_ENABLE
                                           OFF
                                           OFF
 PETSC_ENABLE
                                           OFF
 PTHREAD_ENABLE
                                           OFF
 RAJA_ENABLE
                                           OFF
 SUNDIALS_INDEX_SIZE SUNDIALS_PRECISION
                                           64
                                           double
BUILD_ARKODE: Build the ARKODE library
Press [enter] to edit option Press [d]
                                                    delete an entry CMake Version 3.11.1
Press [c] to configure
Press [h] for help
                                  Press [g] to generate and exit
Press [g] to quit without generating
Press [t] to toggle advanced mode (Currently Off)
```

The ccmake configures the environment automatically. When the configuration is ready, press g to generate and exit.

1. Then you run commands below:

```
make
make install
```

2.2 SHUD

Configuration in *Makefile*:

- 1. Path of SUNDIALS_DIR. [CRITICAL]. If you install SUNDIALS into ~/sundials, you don't change this line..
- 2. Path of OpenMP if the parallel is preferred.
- 3. Path of SRC_DIR, default is SRC_DIR = .
- 4. Path of BUILT_DIR, default is BUILT_DIR = .

After updating the SUNDIALS path in the Makefile, user can compile the SHUD with:

```
make clean make shud
```

There are more options to compile the SHUD code:

- make all clean, then make both shud and shud_omp
- make help help information
- make SHUD make SHUD executable
- make SHUD_omp make shud_omp with OpenMP support

2.2.1 OpenMP

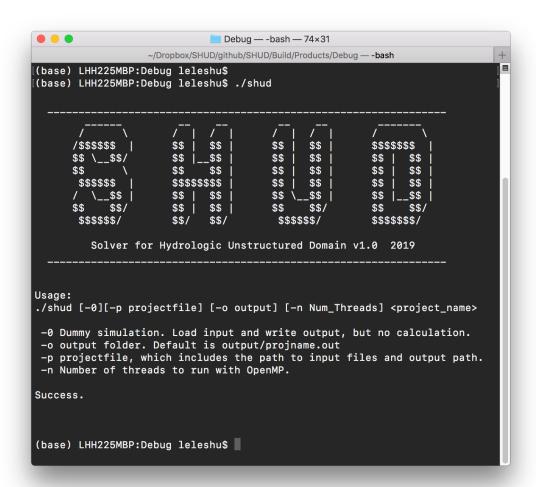
If parallel-computing is prefered, please install OpenMP. For mac:

```
brew install llvm clang
brew install libomp
compile flags for OpenMP:
   -Xpreprocessor -fopenmp -lomp
Library/Include paths:
   -L/usr/local/opt/libomp/lib
   -I/usr/local/opt/libomp/include
```

2.2.2 Run SHUD executables.

After the successful installation and compile, you can run SHUD models using

```
./shud <projectname>
```



Command line pattern is:

./shud [-0][-p projectfile] [-o output] [-n Num_Threads] <project_name>

- -0 Dummy simulation. Load input and write output, but no calculation.
- project name> is the name of the project.
- [-p projectfile] Specify the project file, which includes the path to input files and output path.
- [-o output_folder] Output directory. Default is output/projname.out
- [-n Num_Threads] Number of threads to run with OpenMP, which works with pihm_omp only. Usage:

```
Debug — -
                    ~/Dropbox/SHUD/github/SHUD
(base) LHH225MBP:Debug leleshu$ ./shud
                       $$
                             $$
                             $$
                       $$$$$$$$
                       $$
                             $$
       $$$$$$/
                       $$/
                             $$/
         Solver for Hydrologic Unstruc
                  * openMP disabled.
         Project name: vs
         Project input folder: input/v
         Project output folder: output
         Reading file: input/vs/vs.cfg
2
         Reading file: input/vs/vs.sp.
        The downstream of RIV 10 is ne
         Reading file: input/vs/vs.sp.
        Number of River segmetns: 38
         Reading file: input/vs/vs.sp.
5
6
7
8
         Reading file: input/vs/vs.sp.
         Reading
                  file:
                        input/vs/vs.par
         Reading
                  file: input/vs/vs.par
                  file: input/vs/vs.par
         Reading
         Reading
                  file: input/vs/vs.tsd
10
         Reading
                  file: input/vs/vs.tsd
         Reading file: input/vs/vs.tsd
11
12
         Reading
                  file: input/vs/vs.tsd
13
         Reading file: input/vs/vs.cfg
Initializing data structure ...
openMP disabled
Summary:
        Project name:
                          ٧s
```

When the shud program starts to run, the screen should look like this:

2.3 SHUD-tools

This SHUD-tools is an R package. What you need is to install the package as a source code package. For example:

install_github('SHUD-System/shud-tools')

$2\,$ Install SHUD and SHUD-tools

That is all you need to deploy the SHUD-tools.

3 Input files

List of input files:

File	Category	Comments	Header	# of column
.mesh	sp	Domain element (triangular mesh)	Yes	
.att	sp	Attribute table of triangular elements	Yes	
.riv	sp	Rivers	Yes	
.rivchn	sp	Topologic relation b/w River and Element	Yes	
.calib	cfg	Calibration on physical parameters	Yes	
.para	cfg	Parameters of the model configurature	Yes	
.ic	cfg	Intial conditions	Yes	
.geol	para	Physical parameters for Geology layers	Yes	
.soil	para	Physical parameters for Soil layers	Yes	
.1c	para	Physical parameters for Land cover layers		
. forc	tsd	List of files to the Time-series forcing data		
.csv	tsd	Time-series forcing data	Yes	
.lai	tsd	Time-series LAI data	Yes	
.obs	tsd	Time-series observational data for calibration purpose only	Yes	
$.\mathrm{mf}$	tsd	Time-series Melt Factor data	Yes	
.rl	tsd	Time-series Roughness Length data	Yes	
gis/domain	Shapefile	Shapefile of .mesh file	X	X
gis/river	Shapefile	Shapefile of .riv file	X	X
gis/seg	Shapefile	Shapefile of .rivchn file	X	X

The files in folder gis and fig are not involved in SHUD modeling, but they are very useful for your data pre- and post-processing.

3 Input files

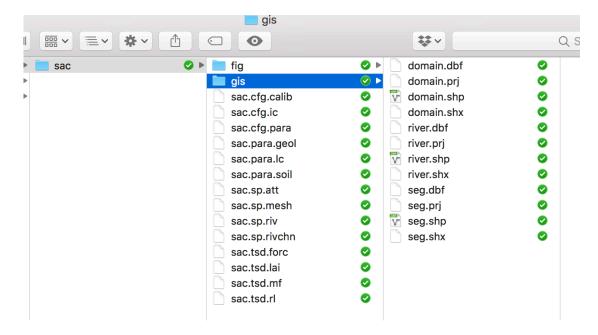


Figure 3.1: The screenshot of input files for SHUD $\,$

3.1 Spatial data

3.1.1 .sp.mesh file

```
Sac.sp.mesh

Sac.
```

There are two tables in the .mesh file, the one is a table of elements and the other is a table of nodes of elements.

- Block 1 (Element information)
- Pre-table

Value1	Value2
Number of rows ($N_{element}$)	Number of columns (8)

• Table

Colname	Meaning	Range	Unit	Comments
ID	Index of element i	$1 \sim N_{element}$	-	
Node1	Node 1 of element i	$1 \sim N_{node}$	-	
Node2	Node 2 of element i	$1 \sim N_{node}$	-	
Node3	Node 3 of element i	$1 \sim N_{node}$	-	
Nabr1	Index of Neighbor 1 of element i	$1 \sim N_{element}$	-	
Nabr2	Index of Neighbor 2 of element i	$1 \sim N_{element}$	-	
Nabr3	Index of Neighbor 3 of element i	$1 \sim N_{element}$	-	
Zmax	Surface elevation of element i	$-9999 \sim +\inf$	m	

- Block 2 (node information)
- Pre-table:

Value1	Value2
Number of rows (N_{node})	Number of columns (5)

• Table

Colname	Meaning	Range	Unit	Comments
ID	Index of node i	$1 \sim N_{element}$	-	
X	X coordinate of node i	$1 \sim N_{node}$	-	
Y	Y coordinate of node i	$1 \sim N_{node}$	-	
AqDepth	Thickness of a quifer i	$0 \sim +\inf$	m	
Elevation	Surface elevation of node i	$-9999 \sim +\inf$	m	

3.1.2 .sp.att file

• Pre-table

Value1	Value2
Number of rows ($N_{element}$)	Number of columns (7)

• Table

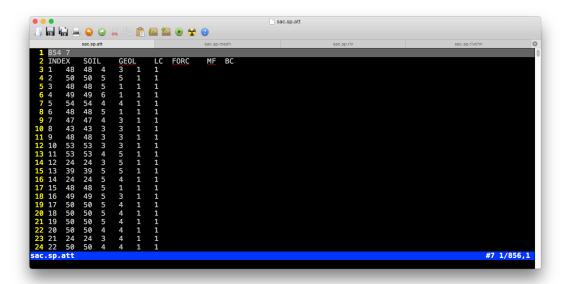


Figure 3.2: Example of .sp.att file

Colname	Meaning	Range	Unit	Comments
ID	Index of element i	$1 \sim N_{element}$	-	
SOIL	Index of soil type	$1 \sim N_{soil}$	-	
GEOL	Index of geology type	$1 \sim N_{qeol}$	-	
LC	Index of land cover type	$1 \sim N_{lc}$	-	$N_{lc} = N_{lai}$
FORC	Index of forcing site	$1 \sim N_{forc}$	-	
MF	Index of melt factor	$1 \sim N_{mf}$	-	
BC	Index of boundary condition	$1 \sim N_{bc}$	-	

3.1.3 .sp.riv file

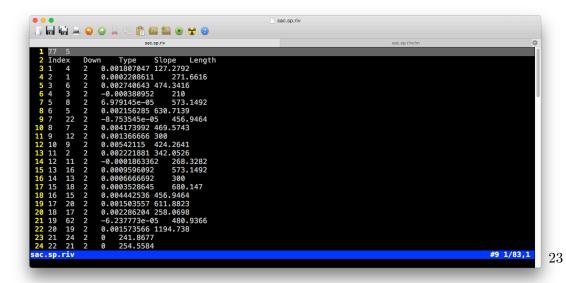


Figure 3.3: Example of .sp.riv file

• Pre-table

Value1	Value2

3 Input files

Colname	Meaning	Range	Unit	Comments
DOWN	Index of downstream	1 ~	-	Negative vlaue indicates
	river	N_{river}		outlet
Type	Index of river	1 ~	-	
	parameters	$N_{rivertype}$		
Slope	Slope of river bed	-10 ~ 10	m/m	${ m Height/Length}$
Length	Length of the river i	$0 \sim \inf$	m	

3.1.4 .sp.rivseg file

• Pre-table

Value1	Value2
Number of rows ($N_{segment}$)	Number of columns (4)

• Table

Colname	Meaning	Range	Unit	Comments
ID	Index of segments i	$1 \sim N_{segment}$	-	
iRiv	Index of river	$1 \sim N_{river}$	-	
iEle	Index of element	$1 \sim N_{element}$	-	
Length	Length of the segments i	$0 \sim \inf$	m	

3.2 Model configuration files

$3.2.1\ .cfg.para\ file$

• Table

Colname	Meaning	Range	Unit	Comments
VERBOSE	Verbose mode	-	-	
DEBUG	Debug mode	-	-	
INIT_MODE	Initial condition	1,2,3	-	1=Dry condition,
	mode			2=Relief condition,
				3=Warm start
ASCII_OUTPUT	ASCII ouput	1/0	-	
Binary_OUTPU	Γ Binary output	1/0	-	
NUM_OPENMP	Number of threads	0 ~	-	
	for OpenMP	$N_{threads}$		

Colname	Meaning	Range	Unit	Comments
ABSTOL	Abosolute tolerance	1e-6 ~	-	
	for CVODE solver	0.1		
RELTOL	Relative tolerance	1e-6 \sim	-	
	for CVODE solver	0.1		
INIT_SOLVER_	_Marker time step for	?	-	
	CVODE solver			
MAX_SOLVER	Maximum time step	?	-	
	for CVODE solver			
ET_STEP	Time step of	$1 \sim 360$	min	
	Evapotranspiration			
START	Start Time	$0 \sim \inf$	day	
END	End Time	-	day	
dt_ye_snow	Time step of output	$0 \sim \inf$	min	
	snow storage			
dt_ye_surf	Time step of output	$0 \sim \inf$	min	
	surface storage			
dt_ye_unsat	Time step of output	$0 \sim \inf$	min	
	unsaturated storage			
dt_ye_gw	Time step of output	$0 \sim \inf$	min	
	groundwater head			
dt_Qe_surf	Time step of output	$0 \sim \inf$	min	
	surface element flux			
dt_Qe_sub	Time step of output	$0 \sim \inf$	min	
	subsurface element			
	flux			
dt_qe_et0	Time step of output	$0 \sim \inf$	min	
	element flux,			
	interception			
dt_qe_et1	Time step of output	$0 \sim \inf$	min	
	element flux,			
	transpiration			
dt_qe_et2	Time step of output	$0 \sim \inf$	min	
	element flux,			
	evaporation			
dt_qe_etp	Time step of output	$0 \sim \inf$	min	
	element flux,			
	potential ET			
dt_qe_prcp	Time step of output	$0 \sim \inf$	min	
	element flux,			
	interception			

3 Input files

Colname	Meaning	Range	Unit	Comments
dt_qe_infil	Time step of output element flux, interception	0 ~ inf	min	
dt_qe_rech	Time step of output element flux, interception	$0 \sim \inf$	min	
dt_yr_stage	Time step of output river stage	$0 \sim \inf$	min	
dt_Qr_down	Time step of output river flux, downstream	$0 \sim \inf$	min	
dt_Qr_surf	Time step of output river flux, surface flow	$0 \sim \inf$	min	
dt_Qr_sub	Time step of output river flux, base flow	$0 \sim \inf$	min	
dt_Qr_up	Time step of output river flux, upstream	0 ~ inf	min	

3.2.2 .cfg.calib file

• Table

Colname	Meaning	Range	Unit	Comments
GEOL_KSATH	Horizontal conductivity of ground water	?	-	
$GEOL_KSATV$	Vertical conductivity of ground water	?	_	
GEOL_KMACSATH	Horizontal conductivity of macropore	?	-	
$GEOL_DMAC$	Macropore depth		-	
$GEOL_THETAS$	Porosity, saturated soil moisture		-	
GEOL_THETAR	Residual soil moisture		-	
$\operatorname{GEOL_MACVF}$	Vertical macropore areal fraction		-	
$SOIL_KINF$	Vertical conductivity of top soil	?	-	
$SOIL_KMACSATV$	Vertical conductivity of soil macropore	?	-	
$SOIL_DINF$	Infiltration depth	?	-	
$SOIL_DROOT$	Root depth		-	
$SOIL_ALPHA$	α value in van Genuchten equation		-	
$SOIL_BETA$	β value in van Genuchten equation		-	
$SOIL_MACHF$	Horizontal macropore areal fraction		-	
$LC_VEGFRAC$	Vegetation fraction		-	
LC_ALBEDO	Emissitive reflection ratio		-	
LC_ROUGH	Manning's roughness of element surface		-	

Colname	Meaning	Range	Unit	Comments
LC_SOILDGD	Soil degradation		-	_
LC_{IMPAF}	Impervious areal fraction		-	
LC_ISMAX	Maximum interception		-	
AQ_DEPTH+	Thichness of aquifer		m	
TS_PRCP	Precipitation		-	
$TS_SFCTMP+$	Temperature		C	
ET_ETP	Transpiration		-	
$\mathrm{ET}_{-}\mathrm{IC}$	Interception		-	
$\mathrm{ET}_{-}\mathrm{TR}$	Evaporation		-	
ET_SOIL	Evaporation		-	
RIV_ROUGH	Manning's roughness of river		-	
RIV_KH	Conductivity of river bed		-	
RIV_DPTH+	Depth of river cross section		m	
RIV_WDTH+	Width of river cross section		m	
RIV_SINU	Sinusity of river path		-	
RIV_CWR	C_{wr} in Chezy equation		-	
RIV_BSLOPE+	Slope of river bed		m/m	
IC_GW+	Initial condition of groundwater		m	
IC_RIV+	Initial condition of river stage		m	

3.2.3 .cfg.ic file

- Block 1 (Element initial condition)
- Pre-table

Value1	Value2
Number of rows ($N_{element}$)	Number of columns (6)

• Table

Colname	Meaning	Range	Unit	Comments
ID	Index of element i	$1 \sim N_{element}$	-	
Canopy	Canopy storage of element i	$0 \sim \inf$	m	
Snow	Snow storage of element i	$0 \sim \inf$	m	
Surface	Surface storage of element i	$0 \sim \inf$	m	
Unsat	Unsaturated storage of element i	$0 \sim \inf$	m	
GW	Groundwater head of element i	$0 \sim \inf$	m	

• Block 2 (river initial condition)

Figure 3.4: Example of .sp.rivseg file

```
| Sac.cfg.para | Sac.para.jc | Sac.para.jc | Sac.para.sol | Sac.pa
```

Figure 3.5: Example of .cfg.para file

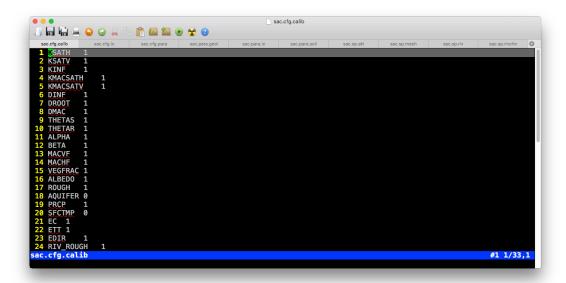


Figure 3.6: Example of .cfg.calib file

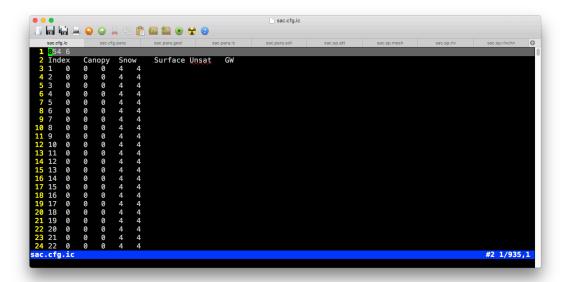


Figure 3.7: Example of .cfg.ic file

3 Input files

• Pre-table:

Value1	Value2
Number of rows (N_{riv})	Number of columns (2)

• Table

Colname Meaning		Meaning	Range	Unit	Comments
	ID	Index of river i	$1 \sim N_{riv}$	-	
	Stage	Stage of river i	$0 \sim \inf$	m	

3.3 Time-series data

3.3.1 .tsd.forc file

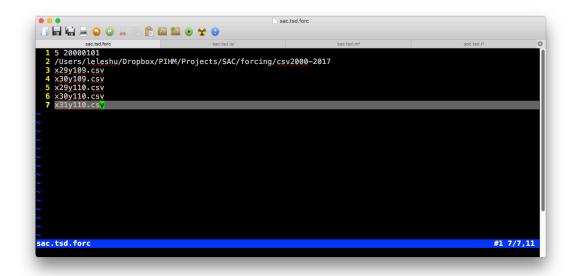


Figure 3.8: Example of .tsd.forc file

- Line 1: Number of forcing sites | Start day (YYYYMMDD)
- Line 2: Directory to the spreadsheet
- $\bullet~$ Line 3~N: Filenames of spreadsheet
- Pre-table:

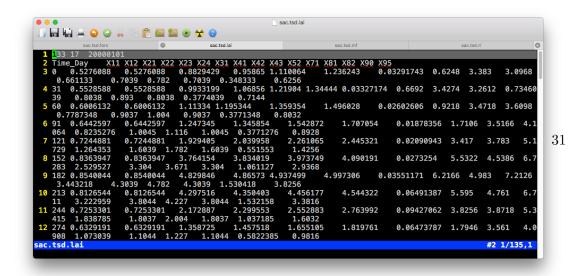
Figure 3.9: Example of .csv forcing file

Value1	Value2
(0)	Number of columns (6)

• Table

Colname	Meaning	Range	Unit	Comments
Day	Time	$0 \sim N_{day}$	day	
PRCP	Precipitation	$0 \sim 1^{\circ}$	m/day	
TEMP	Temperature	$-100 \sim 70$	C	
RH	Relative Humidity	$0 \sim 1$	_	
wind	Wind Speed	$0 \sim \inf$	m/day	
Rn	Solar (shortwave) radiation	?	$J/day/m^2$	

3.3.2 .tsd.lai file



Colname	Meaning	Range	Unit	Comments
TIME	Time	$0 \sim N_{time}$	day	
Column 2	LAI of land cover 1	$0 \sim \inf$	m^2/m^2	
Column i	LAI of land cover $i-1$	$0 \sim \inf$	m^2/m^2	

3.3.3 .tsd.rl file

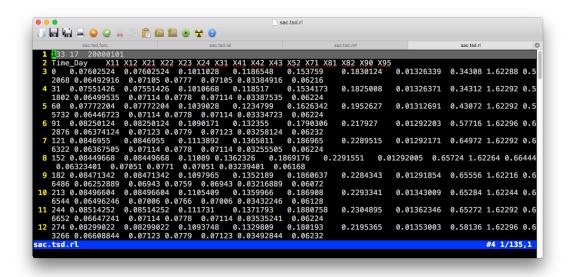


Figure 3.11: Example of .tsd.rl file

• Pre-table:

Value1	Value2	Value3
Number of day (N_{time})	Number of columns (N_{lc})	Start day (YYYYMMDD)

• Table

Colname	Meaning	Range	Unit	Comments
TIME	Time	$0 \sim N_{time}$	day	
Column 2	Roughness length of land cover 1	$0 \sim \inf$	m	
Column i	Roughness length of land cover $i-1$	$0 \sim \inf$	m	
		•••	•••	

3.3.4 .tsd.mf file

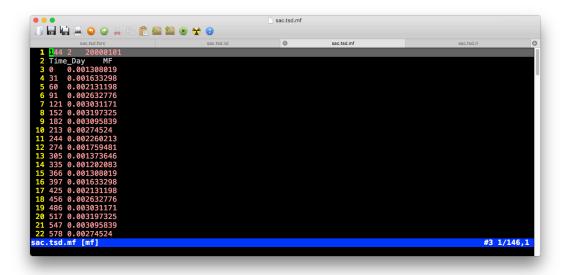


Figure 3.12: Example of .tsd.mf file

• Pre-table:

Value1	Value2	Value3
Number of day (N_{time})	Number of columns (N_{mf})	Start day (YYYYMMDD)

• Table

Colname	Meaning	Range	Unit	Comments
TIME	Time	$0 \sim N_{time}$	day	
Column 2	Melt factor 1	$0 \sim \inf$	-	
Column i	Melt factor $i-1$	$0 \sim \inf$	-	

3.3.5 .tsd.obs file

• Pre-table:

Value1	Value2	Value3
Number of day (N_{time})	Number of columns (N_{obs})	Start day (YYYYMMDD)

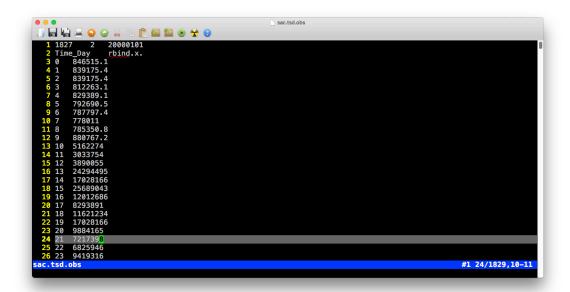


Figure 3.13: Example of .tsd.obs file

• Table

Colname	Meaning	Range	Unit	Comments
TIME	Time	$0 \sim N_{time}$	day	
Column 2	Observational data 1	?	?	
Column i	Observational data $i-1$?	?	
•••		•••		

4 Output files

4.1 Output file names

Format of output file names:

[Project Name].[Identifier].[Format]

-The $[Project\ Name]$ is user defined name of the project, so every input and output files must start with the $[Project\ Name]$. -The [Format] is one of csv or dat. csv is spreadsheet format and dat is bindary format.

The [Identifier] is a combination of variables features, that in format of: [Model Unit][Variable Type][Variable Name]. [Model Unit] is one of three options of ele (elemtns), riv (river) or lak (lake). Variable type includes y, v and q that are state variable (in L), specific flux (in $L^3/L^2/T$) and flux (in L^3/T) respectively.

The list of output files is in following table.

Identifier	Mod unit	Type	Var Name	Meaning	Unit	
.eleyic.	ele	у	ic	Storage of Interception	m	
. eleys now.	ele	y	snow	Storage of snow equivalence	m	
. eley surf.	ele	y	surf	Storage of surface	m	
. eley unsat.	ele	У	unsat	Storage of vados zone	m	
. eley gw.	ele	У	gw	Groundwater head	m	.GW
. elevet p.	ele	\mathbf{v}	etp	Potential ET	$\frac{m^3}{m^2d}$	
. elevet a.	ele	\mathbf{v}	eta	Actual ET	$\frac{m^3}{m^2d}$ $\frac{m^3}{m^2d}$ $\frac{m^3}{m^3}$	
. elevet ic.	ele	\mathbf{v}	etic	Evap of interception	$\frac{m^3}{m^2d}$	
. elevet tr.	ele	\mathbf{v}	ettr	Transpiration	$\frac{\frac{m^2d}{m^2d}}{\frac{m^3}{m^2d}}$	
. elevetev.	ele	\mathbf{v}	etev	Soil Evaporation	$\frac{m^3}{m^2d}$	
. elev prcp.	ele	\mathbf{v}	prcp	Precipitation	$\frac{m^3}{m^2d}$	
. elevnet prcp.	ele	\mathbf{v}	netprcp	Net Precipitation	$\frac{m^3}{m^2d}$	
$. {\it elevinfil}.$	ele	\mathbf{v}	infil	Infiltration Rate	$\frac{m^3}{m^2d}$	
$. {\it elevex fil.}$	ele	\mathbf{v}	infil	Exfiltration Rate	$rac{m^3}{m^2 d}$ $rac{m^2}{m^2 d}$ $rac{m^3}{m^2 d}$ $rac{m^3}{m^2 d}$ $rac{m^3}{m^2 d}$ $rac{m^3}{m^2 d}$	
. elev rech.	ele	\mathbf{v}	rech	Recharge Rate	$\frac{m^3}{m^2d}$	
$. {\it eleq} {\it surf}.$	ele	\mathbf{q}	surf	Overland flow	m^3/d	
. eleq sub.	ele	\mathbf{q}	sub	Subsurface flow	m^3/d	
. rivy stage.	riv	У	stage	River Stage	m	

4 Output files

Identifier	Mod unit	Type	Var Name	Meaning	Unit
.rivqup.	riv	q	up	Flux to upstream	m^3/d
. rivqdown.	riv	\mathbf{q}	down	Flux to downstream	m^3/d
. rivq surf.	riv	q	surf	Flux to landsurface	m^3/d
. rivq sub.	riv	q	sub	Flux to subsurface	m^3/d

4.2 Data format in ASCII (.csv) file

N - Number of column of output data, excluding the time column. m - Number of time-step. StartTime - String of date/time (YYYYMMDD or YYYYMMDD.hhmmss)

N	StartTime			
T_1	$v_{1.1}$	$v_{1.2}$		$v_{1.N}$
T_2	$v_{2.1}$	$v_{2\cdot 2}$		$v_{2\cdot N}$
T_3	$v_{3\cdot 1}$	$v_{3.2}$	•••	$v_{3\cdot N}$
T_m	$v_{m\cdot 1}$	$v_{m\cdot 2}$		$v_{m\cdot N}$

4.3 Data format in binary (.dat) file

The value saved in binary file are identical from ASCII format, but different data structure.

ID	i	Value	Format	Length
1	-	N	double	8
2	-	StartTime	double	8
3	0	T_1	double	8
4	1	$v_{1\cdot 1}$	double	8
5	2	$v_{1\cdot 2}$	double	8
		•••	double	8
(N+1)*(T-1)+i+3	N	$v_{1\cdot N}$	double	8
(N+1)*(T-1)+i+3	0	T_2	double	8
(N+1)*(T-1)+i+3	1	$v_{2\cdot 1}$	double	8
(N+1)*(T-1)+i+3	2	$v_{2\cdot 2}$	double	8
(N+1)*(T-1)+i+3		•••	double	8
(N+1)*(T-1)+i+3	N	$v_{2\cdot N}$	double	8
(N+1)*(T-1)+i+3	0	T_3	double	8
(N+1)*(T-1)+i+3	1	$v_{3\cdot 1}$	double	8
(N+1)*(T-1)+i+3	2	$v_{3\cdot 2}$	double	8

4.3 Data format in binary (.dat) file

ID	i	Value	Format	Length
(N+1)*(T-1)+i+3		•••	double	8
(N+1)*(T-1)+i+3	N	$v_{3\cdot N}$	double	8
(N+1)*(T-1)+i+3		•••	double	8
(N+1)*(T-1)+i+3			double	8
(N+1)*(T-1)+i+3			double	8
(N+1)*(T-1)+i+3			double	8
(N+1)*(m-1)+i+3	0	T_m	double	8
(N+1)*(m-1)+i+3	1	$v_{m\cdot 1}$	double	8
(N+1)*(m-1)+i+3	2	$v_{m\cdot 2}$	double	8
(N+1)*(m-1)+i+3			double	8
(N+1)*(m-1)+i+3	N	$v_{m\cdot N}$	double	8

5 Applications

Some *significant* applications are demonstrated in this chapter.

5.1 Best practice suggestions

- 1. Derive and QC all inputs (time mean, accumulation, screen fo anormalies ...)
- 2. Conduct offline simulations ...
- 3. Start with 'idealized' forcing (Option FORC_debug=1 in .cfg.para file). Which will use uniform forcing data to drive the hydrologic simulations.
- 4. Run with short time period, load the outputs and examine whether results are in expection
- 5. If all above works, then hook all modules and run with your forcing data.

 $This\ chapter\ is\ imcomplete$

- 5.2 Example 1: Vauclin Experiment
- 5.3 Example 2: Shall Hill CZO
- 5.4 Example 3: Conestoga Watershed, Pennsylvanis

6 Calibration

 $This\ chapter\ is\ imcomplete$

File	Comments	Header	# of column
.cfg.cmaes	Configuration of CMA-ES method	No	-

Values in .calib.cmaes file:

Item	Meaning	Default value	Range	Unit
lambda	Number of children in each generation	48		
stopfitness	Threshold to accept the best solution	0.3		-
maxgen	Maximun generations	48		-
$_{ m sigma}$		0.8		-
updateic	Whether to update initial condition after each generation	0	0/1	-
walltime	Walltime to kill the modeling thread	86400	0-inf	second
nspingup	Number of days for spinup	0	0-inf	day
				-

Values in .calib.range file:

Rows: Values in .cfg.calib file. Column: | Item | Meaning | Default value | Range | Unit | |:----:|:-----:|:----:|: | On/off | On or Off | 0 | 0/1 | - | | log | Whether logrithm | 0 | 0/1 | - | | min | Minimun value | - | - | - | | max | Maximun value | - | - | - |

7 Quick, Reproducible and Automatic hydrological modeling

Automatic deployment of SHUD System

8 Source code and program design

The source code of SHUD and SHUD-tool are avaliable via Github: https://github.com/SHUD-System/SHUD and https://github.com/SHUD-System/SHUD-tools.

Bibliography

- Bhatt, G. (2012). A distributed hydrologic modeling system: Framework for discovery and management of water resources. PhD thesis, Pennsylvania State University.
- Bhatt, G., Kumar, M., and Duffy, C. J. (2014). A tightly coupled GIS and distributed hydrologic modeling framework. *Environmental Modelling and Software*, 62:70–84.
- Kumar, M., Bhatt, G., and Duffy, C. J. (2009). An efficient domain decomposition framework for accurate representation of geodata in distributed hydrologic models. *International Journal of Geographical Information Science*, 23(12):1569–1596.
- Kumar, M., Duffy, C. J., and Reed, P. M. (2004). Enhancing the performance of feature selection algorithms for classifying hyperspectral imagery. In Geoscience and Remote Sensing Symposium, 2004. IGARSS '04. Proceedings. 2004 IEEE International, volume 5, pages 3264–3267 vol.5.
- Li, S. (2008). INTEGRATED MODELING OF MULTI-SCALE HYDRODYNAMICS, SEDIMENT AND POLLUTANT TRANSPORT. PhD thesis.
- Li, S. and Duffy, C. J. (2011). Fully coupled approach to modeling shallow water flow, sediment transport, and bed evolution in rivers. Water Resources Research, 47(3):1–20.
- Qu, Y. (2004). An integrated hydrologic model for multi-process simulation using semidiscrete finite volume approach. PhD thesis.
- Qu, Y. and Duffy, C. J. (2007). A semidiscrete finite volume formulation for multiprocess watershed simulation. Water Resources Research, 43(8):1–18.
- Shi, Y., Baldwin, D. C., Davis, K. J., Yu, X., Duffy, C. J., and Lin, H. (2015a). Simulating high-resolution soil moisture patterns in the Shale Hills watershed using a land surface hydrologic model. *Hydrological Processes*, 29(21):4624–4637.
- Shi, Y., Davis, K. J., Zhang, F., Duffy, C. J., and Yu, X. (2015b). Parameter estimation of a physically-based land surface hydrologic model using an ensemble Kalman filter: A multivariate real-data experiment. *Advances in Water Resources*, 83:421–427.
- Yu, X., Duffy, C., Baldwin, D. C., and Lin, H. (2014). The role of macropores and multi-resolution soil survey datasets for distributed surface-subsurface flow modeling. *Journal of Hydrology*, 516:97–106.

Bibliography

Yu, X., Lamačová, A., Duffy, C., Krám, P., and Hruška, J. (2015). Hydrological model uncertainty due to spatial evapotranspiration estimation methods. *Computers & Geosciences*, 90:90–101.