AMANZI ATS

Short Course – Sept 1&2, 2021

Ethan Coon
Daniil Svyatsky
Bo Gao

J. David Moulton
Sergi Molins
Zexuan Xu

Scott Painter
Saubhagya Rathore
Pin Shuai

Special Acknowledgement: Daniel Livingston

Agenda: Day 1

UTC	*US Eastern*	*Topic*	*Speaker*
1500	**11:00**	**Introduction**	**E. Coon**
1515	11:15	History of Amanzi & ATS	S. Painter
1545	11:45	Concepts & Fundamentals	E. Coon
1615	12:15	Technical Logistics	D. Moulton
1630	12:30	Break & Technical Support	
1650	12:50	*Lightning Talks Session 1*	A. Hamm; S. Rathore
1700	1:00	Demo 1: Flow	D. Svyatsky, D. Moulton
1800	2:00	*Lightning Talks Session 2*	Y. Zhang; B. Gao
1810	2:10	Break	
1820	2:20	Demo 2: Model Setup	P. Shuai, E. Coon
1920	3:20	*Lightning Talks Session 3*	D. Livingston; P. Shuai
1930	3:30	Discussion: Future Directions	S. Painter
2000	4:00	Optional: Collaboration Time	

Agenda: Day 2

UTC	*US Eastern*	*Topic*	*Speaker*
1500	11:00	Recap & Welcome Back	E. Coon
1515	11:15	Demo 3: Reactive Transport	S. Molins, S. Rathore, Z. Xu
1645	12:45	Break	
1705	1:05	*Lightning Talks Session 4*	Z. Xu, J. Beisman
1715	1:15	Demo 4: Arctic Hydrology	S. Painter, B. Gao, E. Coon
1845	2:40	Break	
1855	2:55	*Lightning Talks Session 5*	Y. Sjöberg; D. Svyatsky
1905	3:05	Debugging and Getting Help	E. Coon
1950	3:50	Closing and Wrap-Up	E. Coon
2000	4:00	Optional: Collaboration Time	

Lightning Talks

Session	Topic	Speaker
1	Arctic hydrologic modeling	A. Hamm
	Multi-model ensembles	S. Rathore
2	Coastal modeling of sediment transport	Y. Zhang
	Arctic process uncertainty	B. Gao
3	Tinerator, PyLaGrit for complex meshing	D. Livingston
	Watershed modeling	P. Shuai
4	Watershed reactive transport	Z. Xu
	Land surface modeling	J. Beisman
5	Groundwater temperature, permafrost, & fish.	Y. Sjöberg
	Salinity Intrusion	D. Svyatsky

Lightning Talks

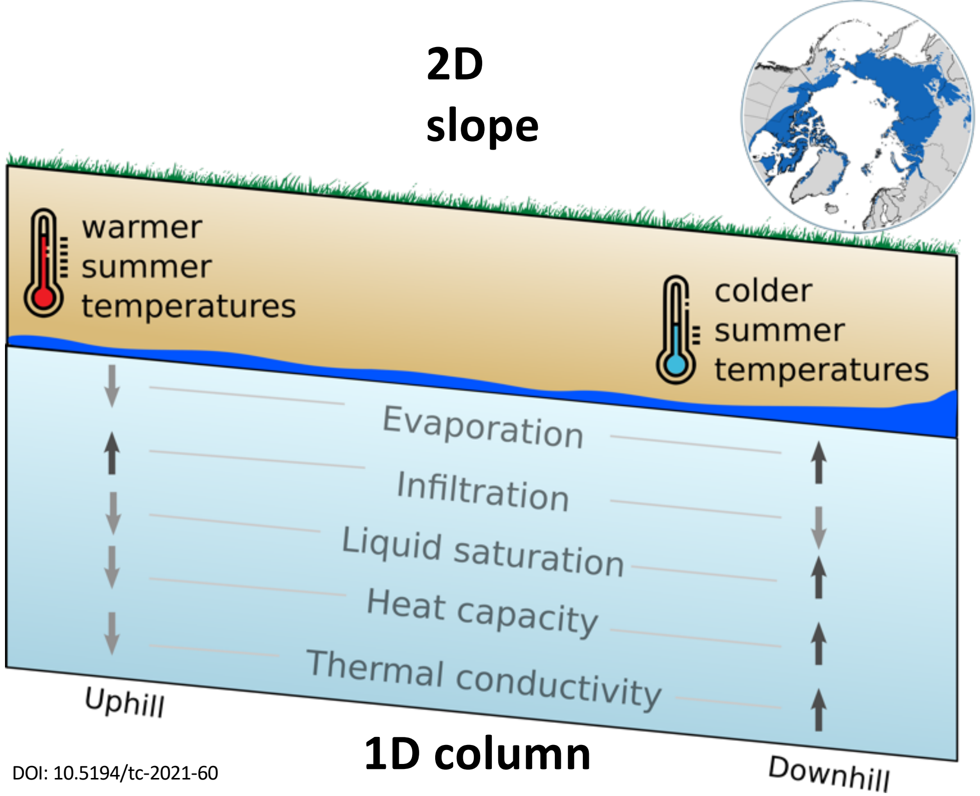
Alexandra Hamm, Univ. of Stockholm

Saubhagya Rathore, Oak Ridge National Laboratory

High Arctic Hillslope Hydrology

Alexandra Hamm, Univ. of Stockholm

Alexandra Hamm
Stockholm Univ.



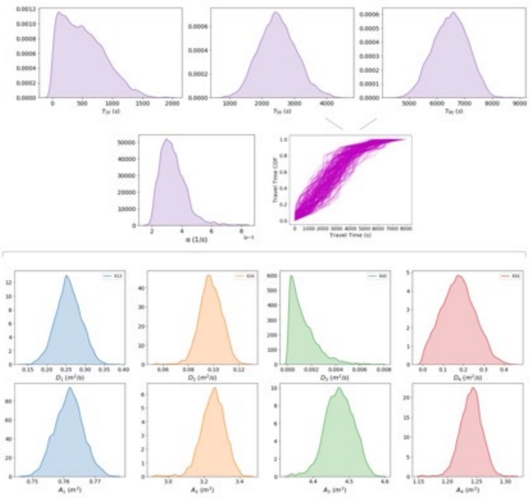
DOI: 10.5194/tc-2021-60

Workflows for ATS Ensembles

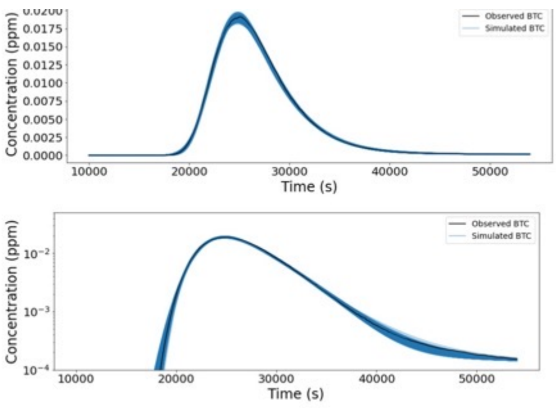
Saubhagya Rathore, Oak Ridge National Laboratory

Ensemble ATS Runs

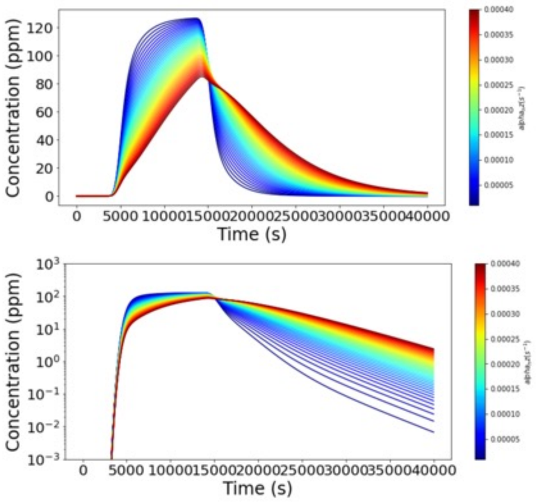
Parameter estimation/MCMC



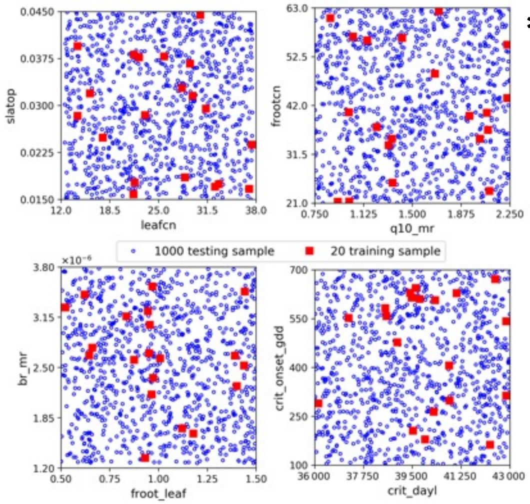
Predictive uncertainty



Parameter sensitivity



Meta/surrogate-modeling



*

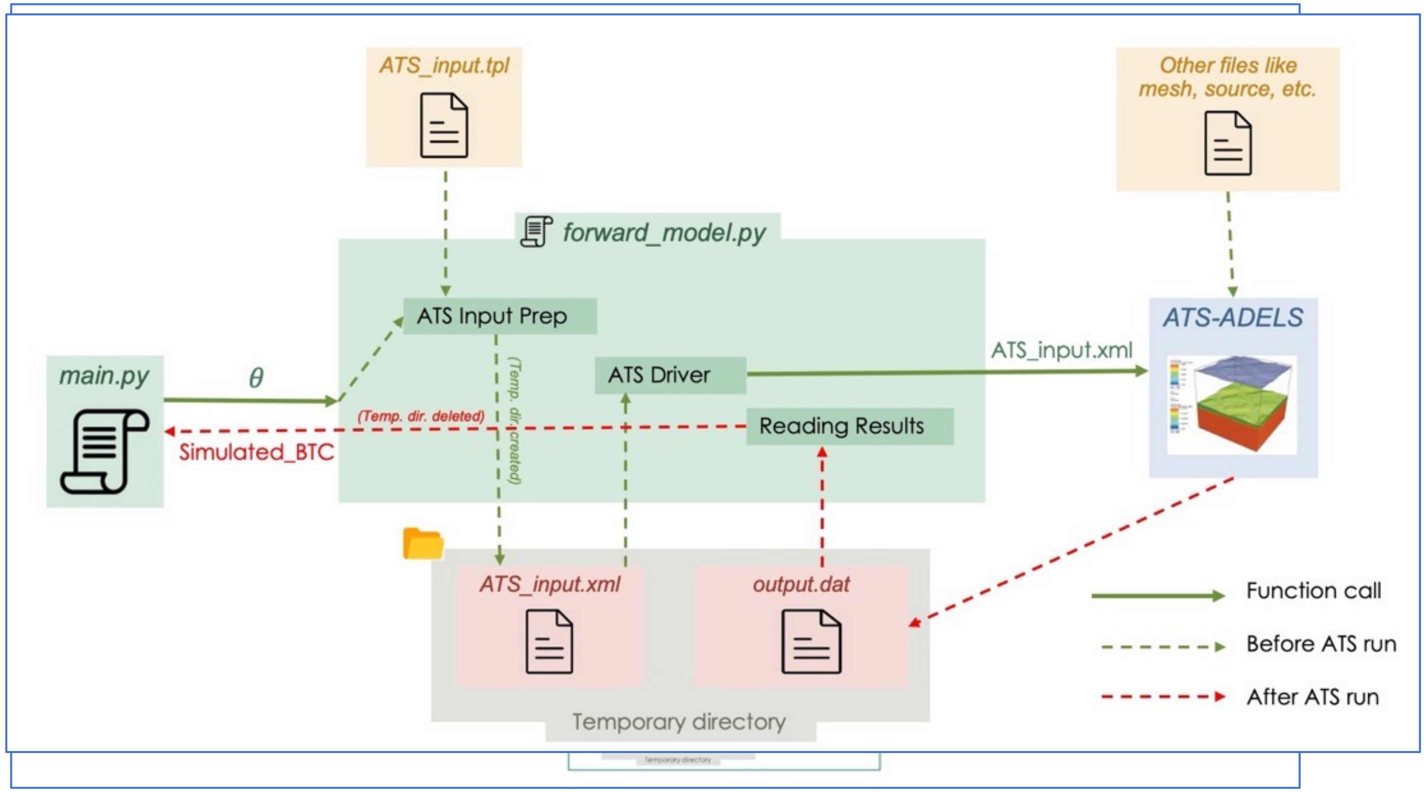
Common requirement: Running ATS with different parameter sets in <u>parallel</u>

Figures: Rathore et al., (WRR, 2021); Lu and Ricciuto, (GMD, 2019)

** Not an ATS example*

Workflow

Example of MCMC for stream tracer test analysis



- Input files specific to proposed parameter set accessed by ATS
- ATS result files not overwritten
- Unnecessary files gets deleted

Terminal snippets

```
error.txt
11c79742e1074a7884489a326229405c
26f8adc26e714c1a9ca443732cc53292
b3016830c4574175a070031477941191
c1e0e92aa2e44a52a40aef898f857df3
cf76594c3b864ee5a37e7828893028a2
screen_out.log
2faf489c46ea4741be14aff364fc817c
5609a4f61963435e9b5a32ac73006c9a
6197c4c62a9f423393e446c474a2247f
9a891a4d17c14054a02ea7b651c801bc
c8c9d4f34a22458a9854536754d194ae
Python_ouput.txt
45b059de380248228b1bb50dde4b4f5f
5a9316683d564f67ba39deedad9be2ac
b7557529a00348bca3649445db417c91
d0c83a0788a44c5391bab663b2f3c692
__pycache__
output.txt
BTC_observed.csv
decay_ingrowth_sz.tpl
decay_ingrowth_hz.tpl
mcmc_run.py
decay_ingrowth.tpl
forward_model.py
hanford.dat
multisubgrid.tpl
```

```
outlet.dat
ats_out.log
decay_ingrowth_sz.in.out.alquimia
decay_ingrowth_hz.in.out.alquimia
decay_ingrowth.in.out.alquimia
decay_ingrowth_hz.in
decay_ingrowth.in
decay_ingrowth_sz.in
multisubgrid.xml
```

MATK + amanzi_xml *packages are used to write input files using template files*

Lightning Talks

Yu Zhang, Los Alamos National Laboratory

Bo Gao, Oak Ridge National Laboratory

Coastal wetland eco-geomorphological modeling

Yu Zhang, Daniil Svyatsky, J. David Moulton, & Joel Rowland
Los Alamos National Laboratory

Motivation

What will be the “fate” of future coastal wetlands?

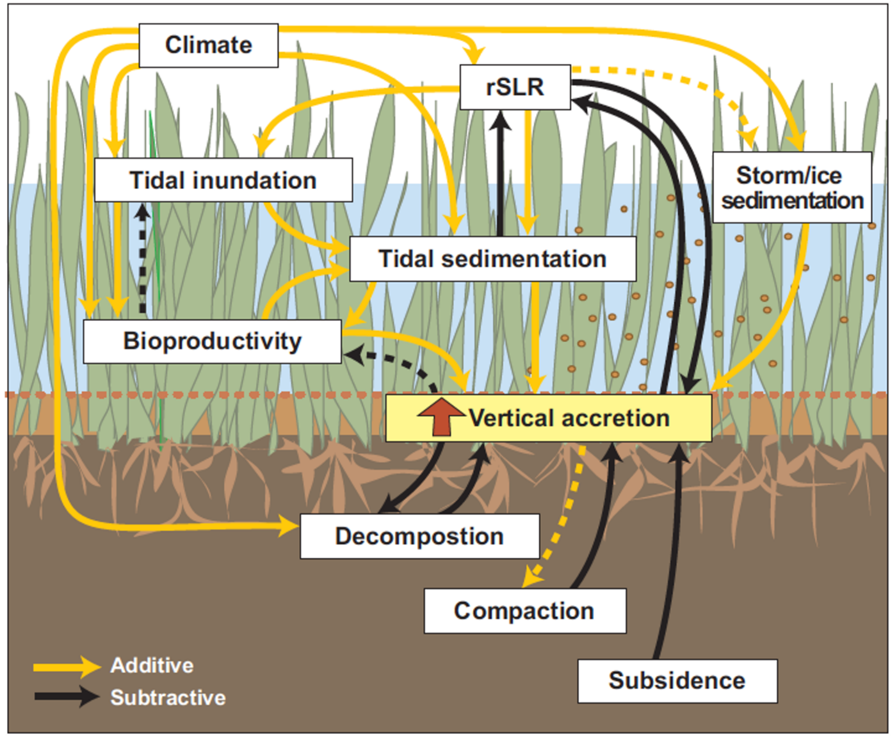
Future

Now

SLR

Modeling the hydro-eco-geomorphological feedbacks facing sea level rise

Eco-geomorphologic processes



(Argow & Fitzgerald, 2006)

The governing equation for coastal landscape evolution

$$\frac{dz}{dt} = \frac{1}{1-p}(-E + D)$$

Erosion

Sedimentation

$$E = \underline{E_{shear}} + \underline{E_{break}}$$

Bed erosion due to current

Erosion due to wave breaking

$$D = \underline{D_s} + \underline{D_t} + \underline{D_o}$$

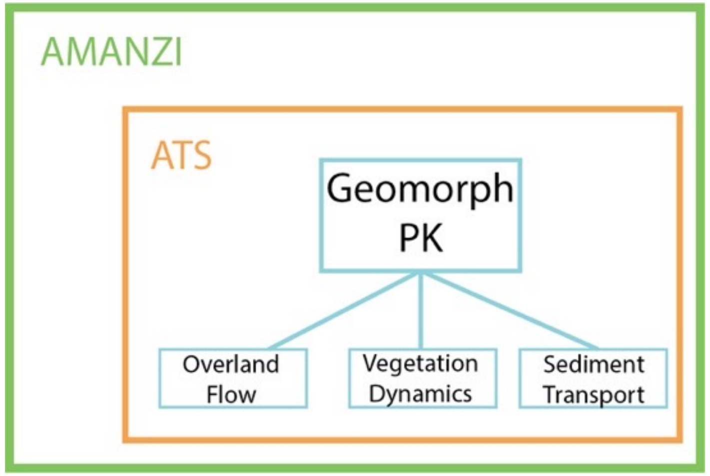
Sediment settling

Sediment trapping

Organic soil production

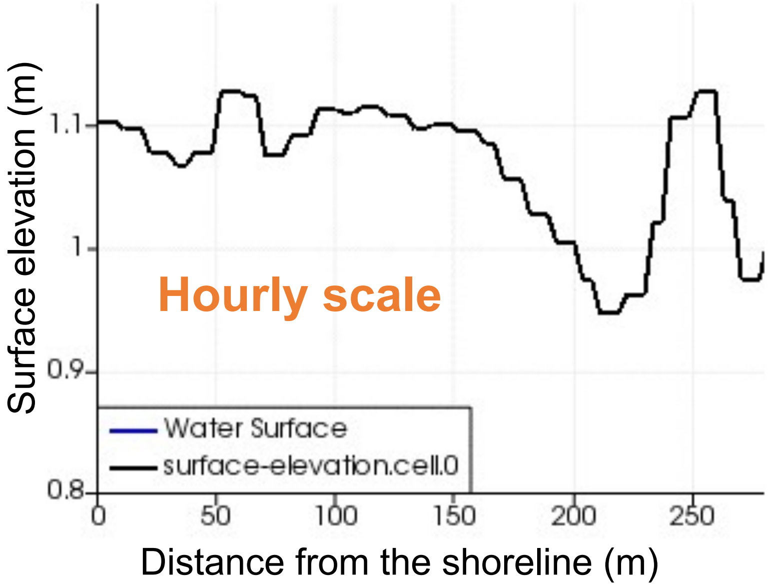
Modeling the hydro-eco-geomorphological feedbacks facing sea level rise

ATS hydro-eco-geomorphologic module

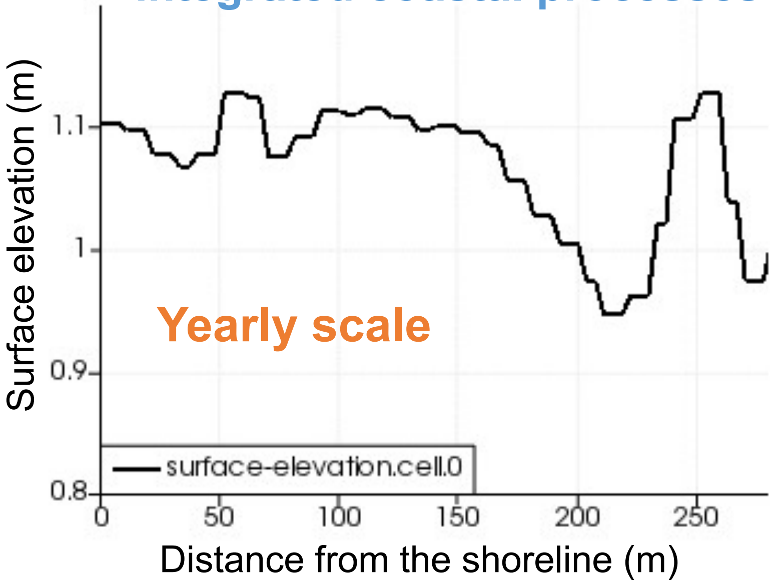


Hydrodynamics: Shallow water scheme
Veg dynamics: Single species linear scheme
Organic soil production/trapping
Sed transport: Sediment settling
Current erosion
Subsurface hydrology: 3-D density-dependent groundwater flow

Improved representation of hydrodynamics on complex terrain

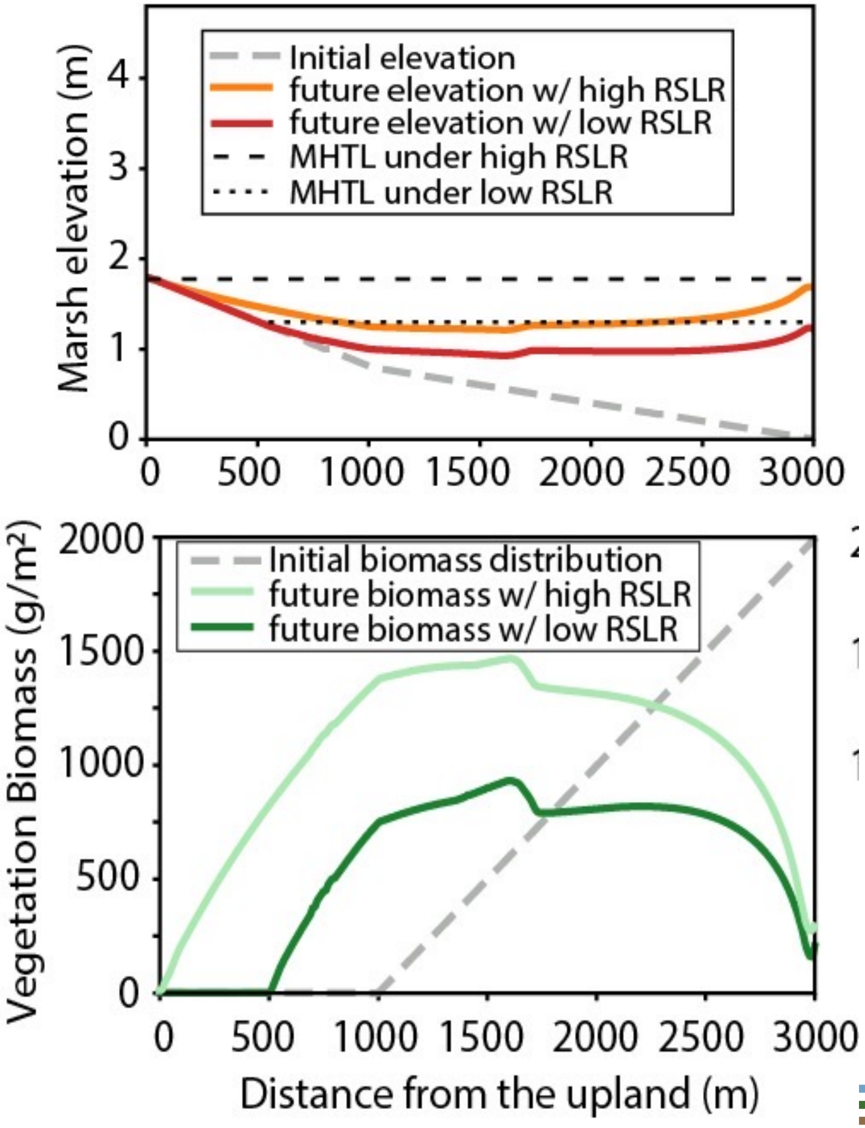


Topographic change driven by integrated coastal processes

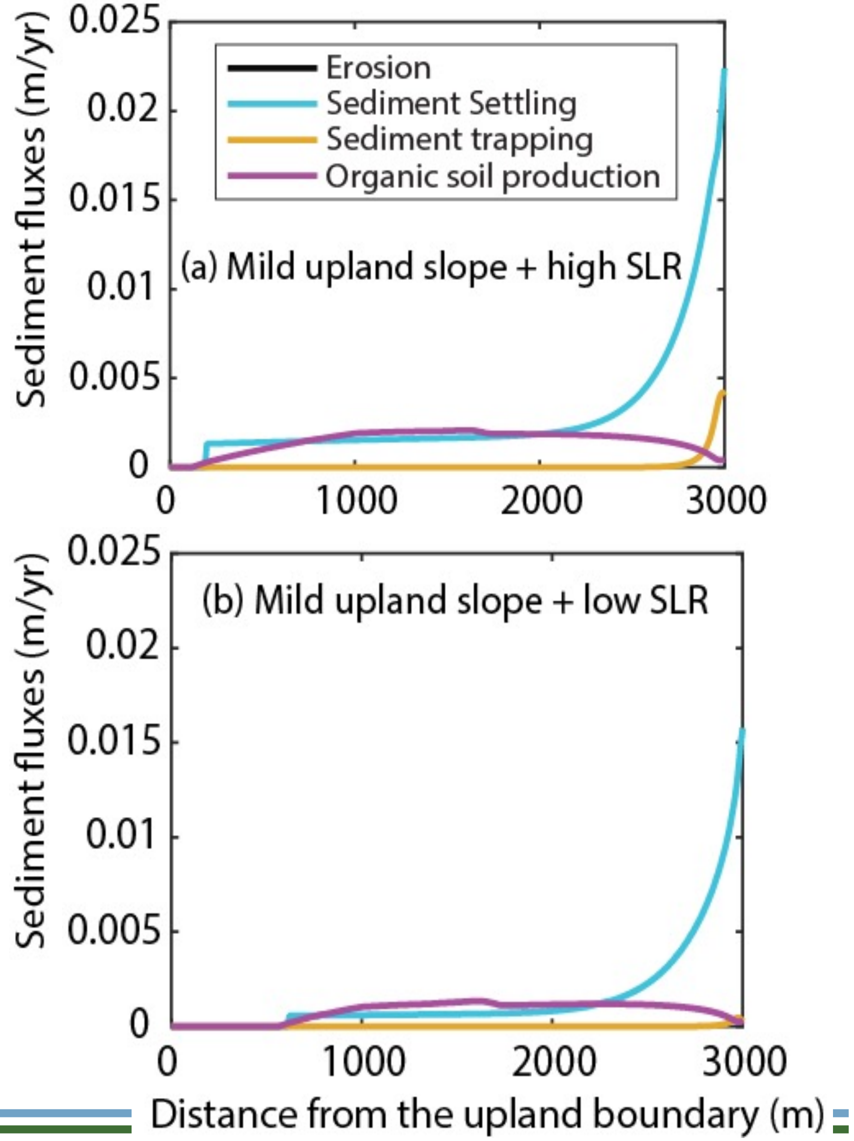


Modeling the hydro-eco-geomorphological feedbacks facing sea level rise

Marsh evolution in 100 years



Sediment fluxes at different location



AMANZI

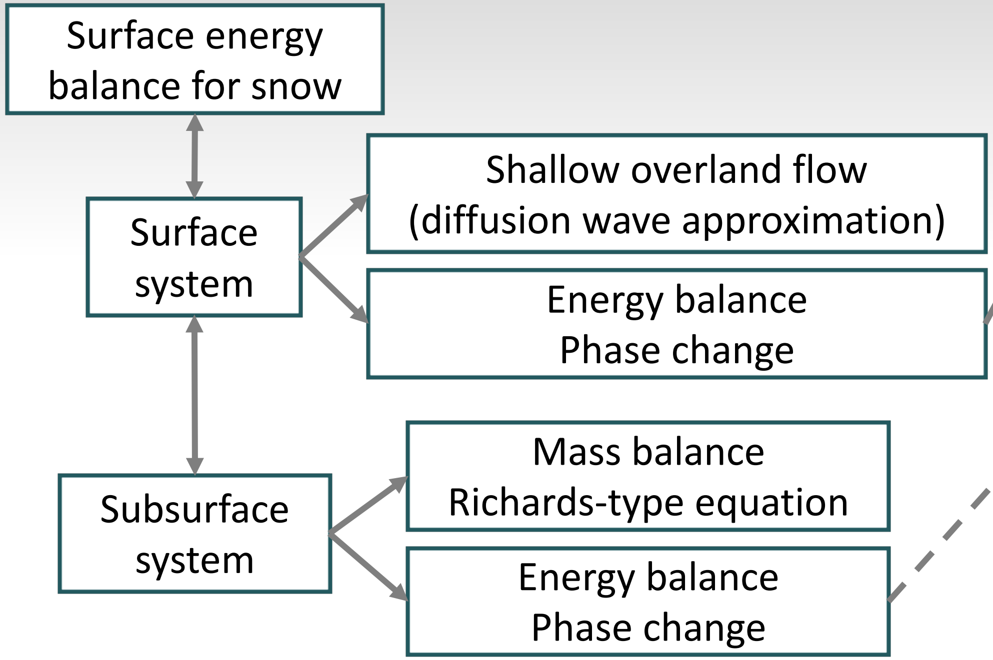
Permafrost Process Uncertainty

Bo Gao, Oak Ridge National Laboratory

Oak Ridge National Laboratory

Understanding the impact of physics representation on permafrost modeling

Permafrost Process



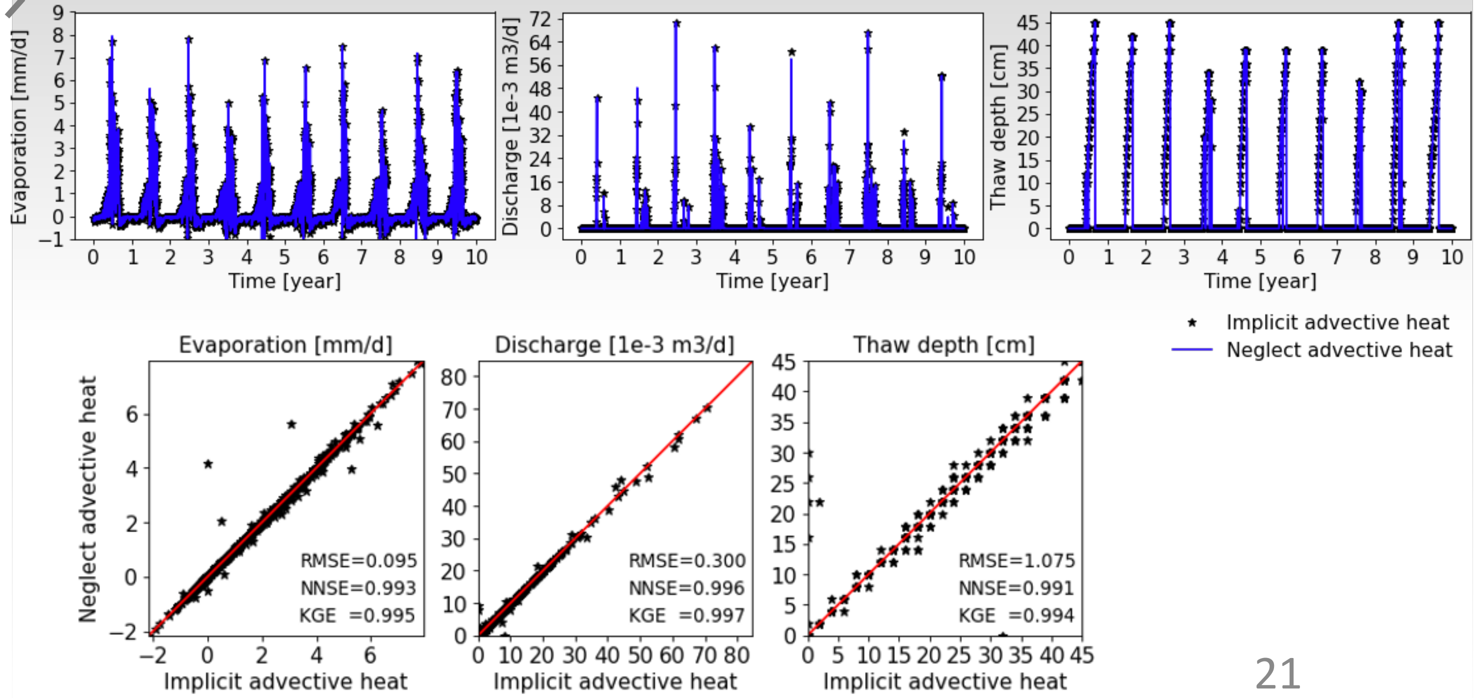
Energy balance equations

Bo Gao

$$\frac{\partial}{\partial t}\{[\chi\rho_l u_l + (1-\chi)\rho_i u_i]\delta_w\} + \underbrace{\nabla\cdot(h_l\chi\rho_l\delta_w \mathbf{U}_w)}_{\text{advective heat}} \underbrace{-\nabla\cdot\{[\chi\kappa_l + (1-\chi)\kappa_i]\delta_w\nabla T\}}_{\text{conductive heat}} = Q_{in} - Q_{out}$$

$$\frac{\partial}{\partial t}\left[\phi\sum_{n=l,i,g}(\rho_n s_n u_n) + (1-\phi)c_{v,soil}T\right] + \underbrace{\nabla\cdot(\rho_l h_l \mathbf{V}_l)}_{\text{advective heat}} \underbrace{-\nabla\cdot(\kappa_e\nabla T)}_{\text{conductive heat}} = Q_E$$

Does advective heat transport affect hydrological output?



My questions

- Can we neglect advective heat transport?
- Can we assume equal density between ice and liquid?
- Can we neglect the change of matric suction due to soil freezing (cryosuction)?

Lightning Talks

Daniel Livingston (Los Alamos National Laboratory)

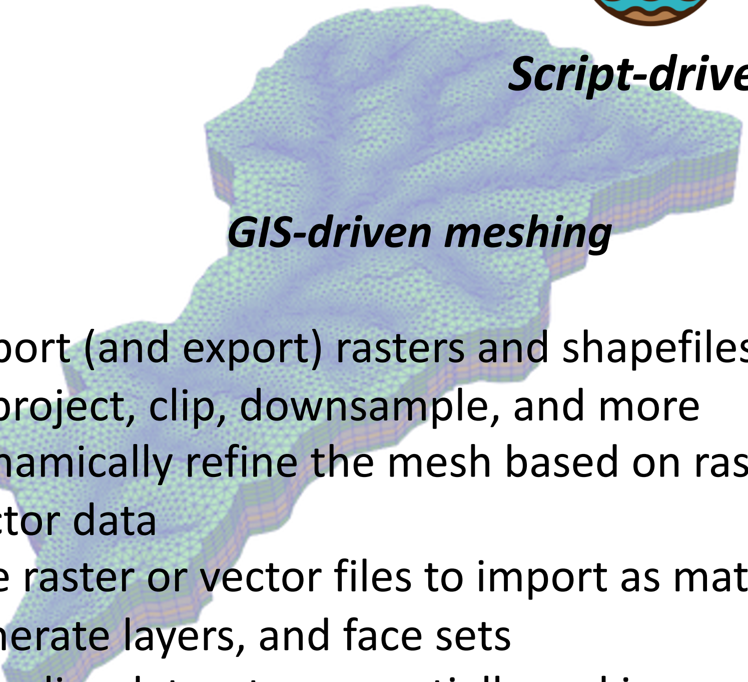
Pin Shuai (Pacific Northwest National Laboratory)

Daniel Livingston
Computational Earth Science group
Los Alamos National Laboratory

AMANZI ATS

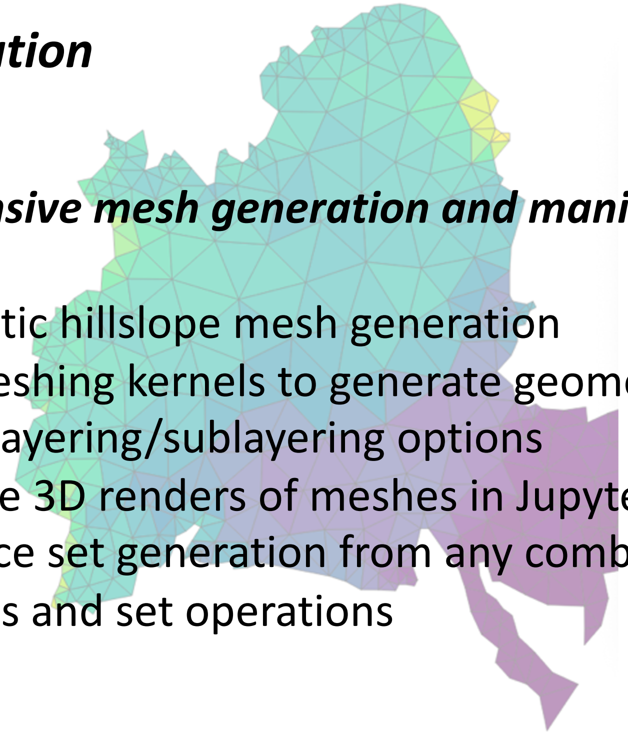
tinerator

Script-driven geospatial mesh generation



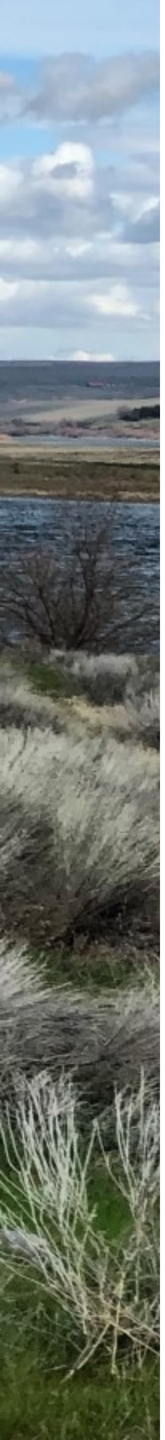
GIS-driven meshing

- Import (and export) rasters and shapefiles
- Reproject, clip, downsample, and more
- Dynamically refine the mesh based on raster or vector data
- Use raster or vector files to import as materials, generate layers, and face sets
- Visualize datasets geospatially and in any CRS



Comprehensive mesh generation and manipulation

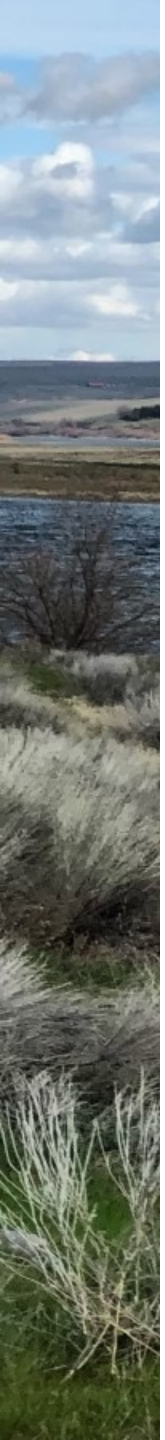
- Programmatic hillslope mesh generation
- Multiple meshing kernels to generate geometry
- Numerous layering/sublayering options
- Visualize live 3D renders of meshes in Jupyter
- Complex face set generation from any combination of data sources and set operations



Pacific Northwest
NATIONAL LABORATORY

Watershed Model Intercomparison between ATS, SWAT and NWM: an example with the American River Watershed

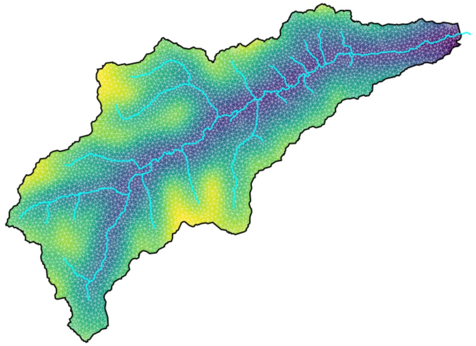
Xingyuan Chen, Kyongho Son,
Peishi Jiang, and Pin Shuai

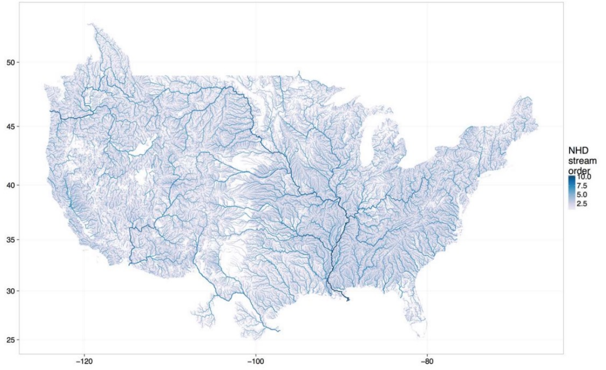


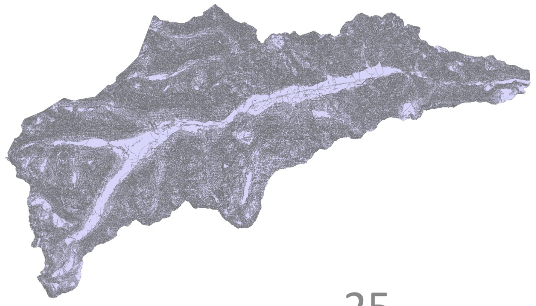
Pacific Northwest NATIONAL LABORATORY

Model summary

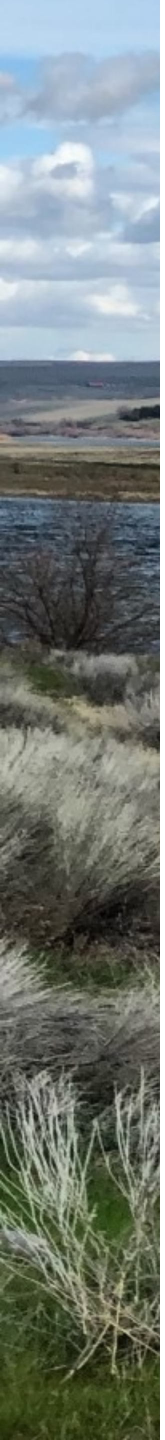
	Advanced Terrestrial Simulator (ATS)	National Water Model (NWM)	Soil & Water Assessment Tool (SWAT)
Capability	• Land surface processes • Integrated hydrology • Integrated transport • Reactive transport coupled with PFLOTRAN/CrunchFlow	• Land surface processes • Integrated hydrology	• Land surface processes • Integrated hydrology • Nutrient loading
Model characteristic	• Fully distributed • Structured/unstructured	• Fully distributed • Structured	• Semi-distributed • HRU based







HRUs: hydrologic response units

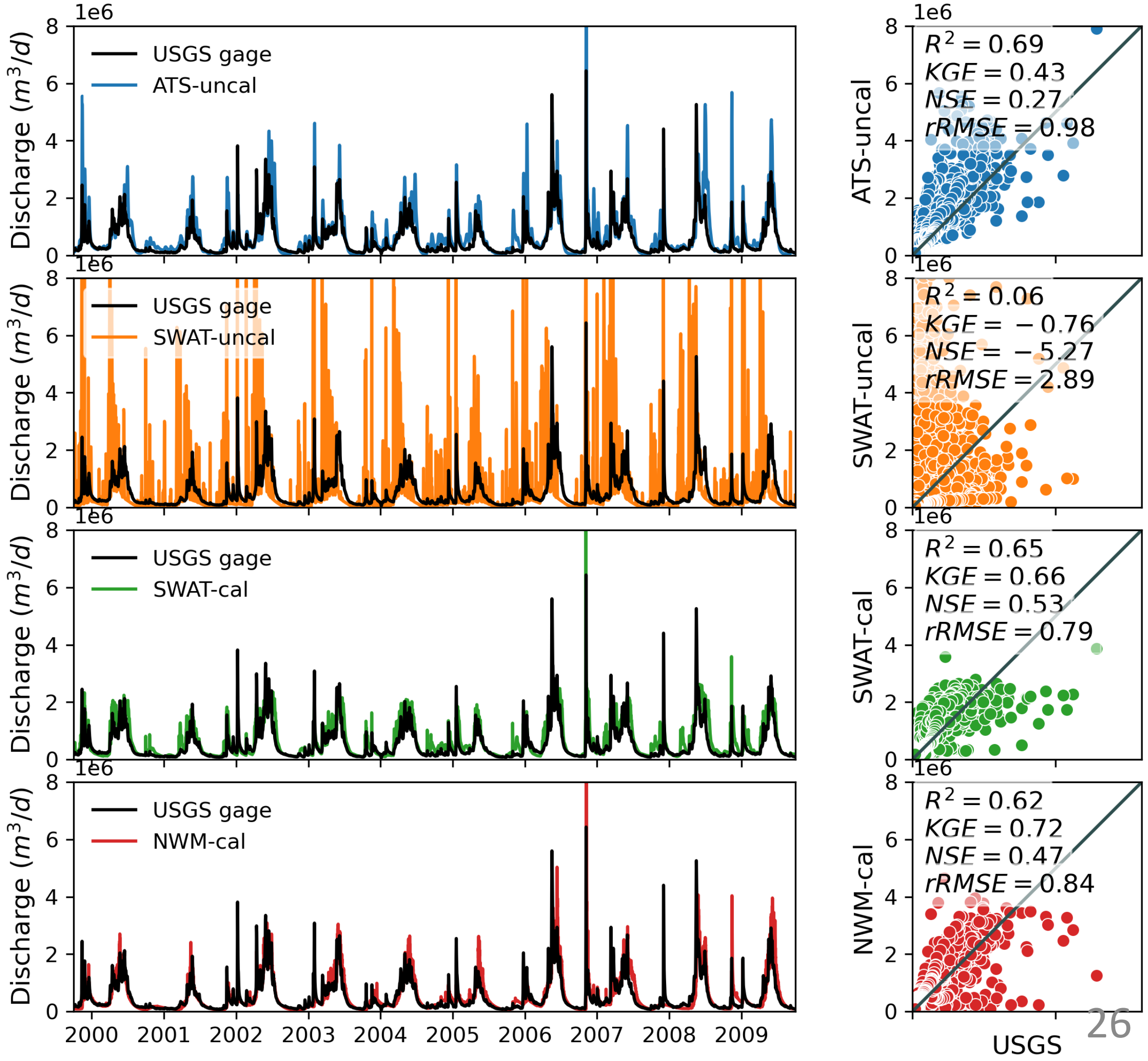


Pacific Northwest NATIONAL LABORATORY

Watershed discharge comparison

- Without any calibration, ATS can simulate streamflow reasonably well
- ATS outperforms uncalibrated SWAT, and is closely behind calibrated SWAT and NWM

	R^2	KGE	NSE	rRMSE
ATS-uncal	0.69	0.43	0.27	0.98
SWAT-uncal	0.06	-0.76	-5.27	2.89
SWAT-cal	0.65	0.66	0.53	0.79
NWM-cal	0.62	0.72	0.47	0.84



Lightning Talks

Zexuan Xu, Berkeley National Laboratory

Joe Beisman, Oak Ridge National Laboratory

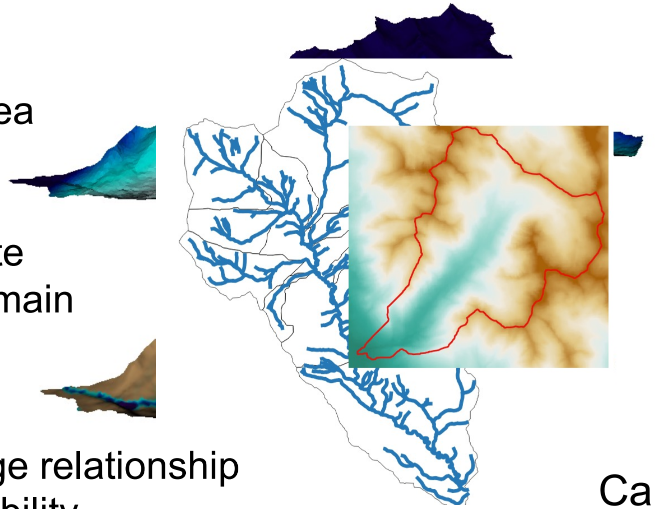
Zexuan Xu

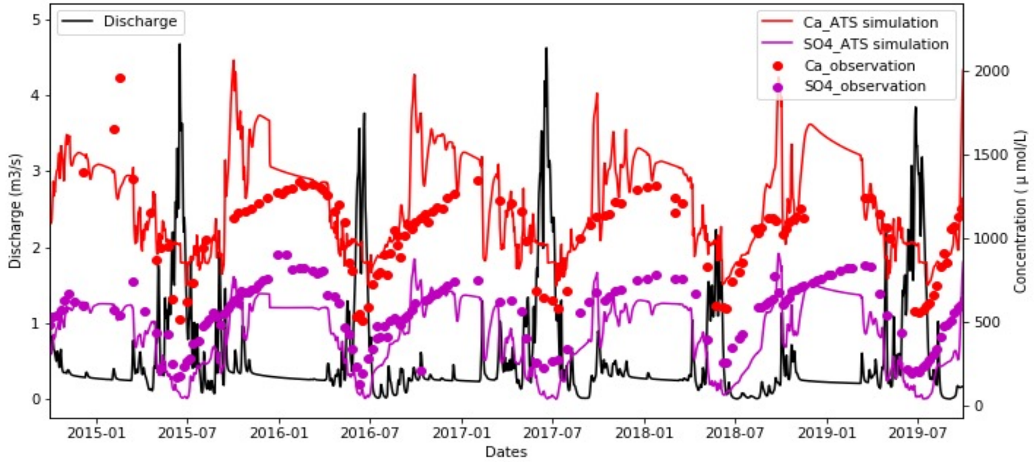
Integrated Hydrology and Reactive Transport Modeling in Mountainous Watersheds

A 3D case study at Copper Creek in the East River, Colorado

Tech Details

- Domain: 30-m deep, 23 km^2 total area
- Mesh: 5-layer, 50-m resolution,
- Met forcing: ten-year Daymet
- Reactive transport: Calcite and Pyrite
- Snow distribution on the surface domain
- >192 processors on NERSC



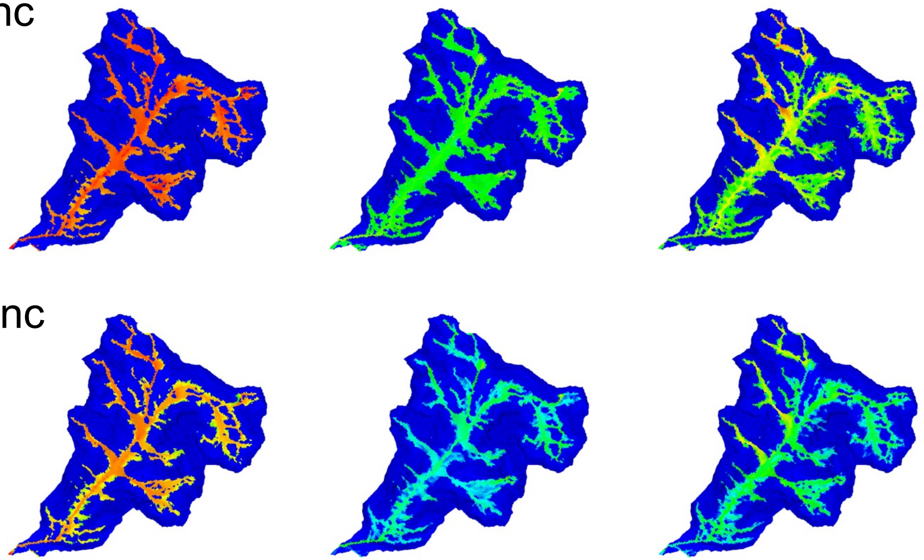


Application

- Understand Concentration-Discharge relationship
- Evaluate responses to climate variability
- Investigate contribution of mineral weathering to chemical exports

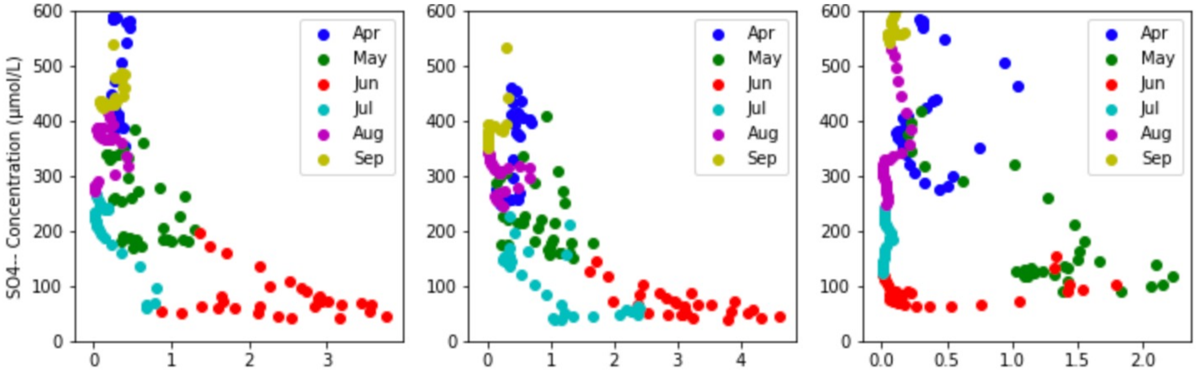
Ca conc

SO_4 conc



Jan 2017 May 2017 July 2017

Average WY2016 Wet WY2017 Dry WY2018

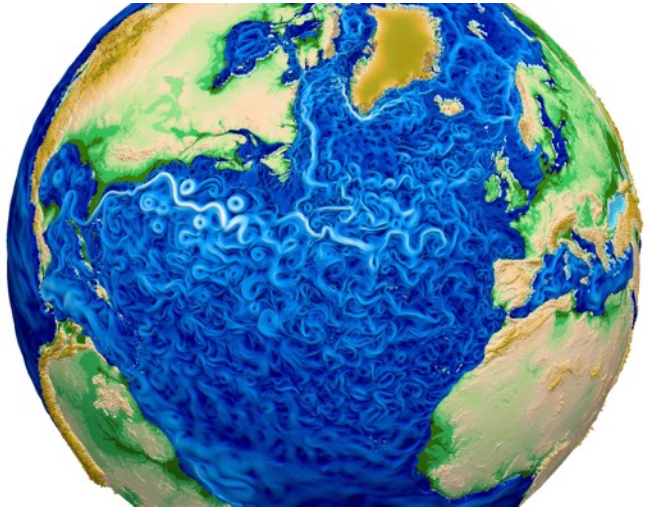


ATS Land Surface Modeling

¡Future Capability!

Refactoring E3SM Land Model (ELM) for use with ATS

Joe Beisman

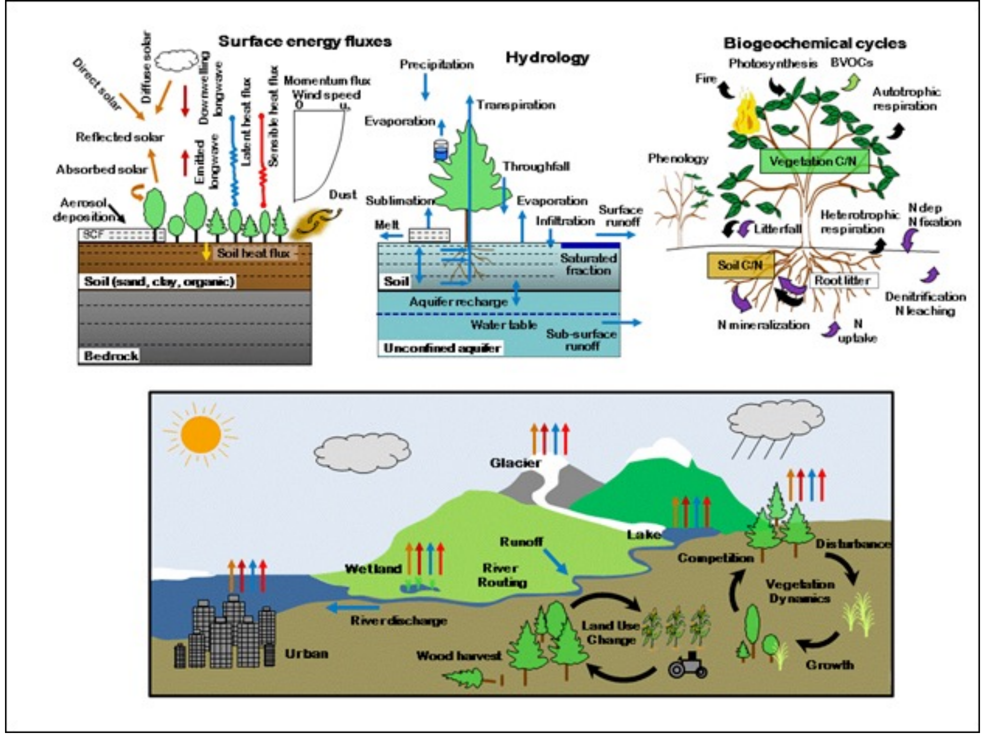


Energy Exascale Earth System Model (E3SM) (Golaz et al 2018)

LSMs don't include lateral subsurface flow; hydrology models have incomplete surface representations

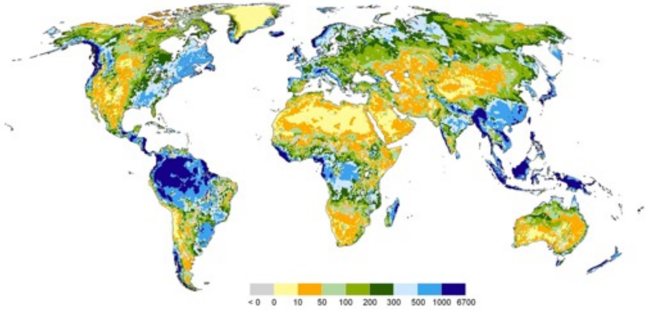
Disruptive hardware changes force software to adapt

Let's modernize ELM and use it to improve ATS!
- "kernelization" of ELM will allow task parallelism on modern HPC resources
- Portable across architectures
- Physics-based kernel design allows easy experimentation with new models of physical processes

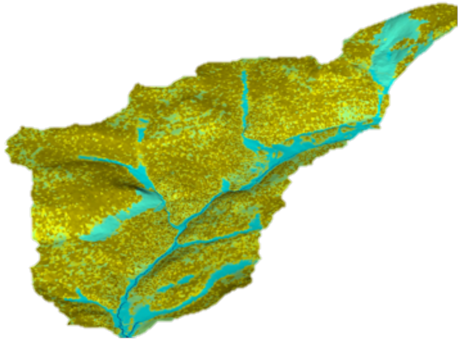


CLM 4.5 Technical Note

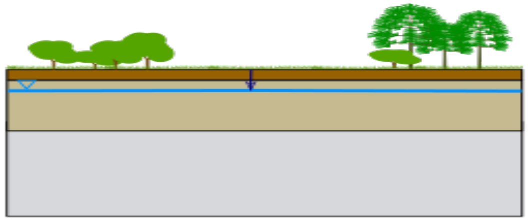
Current work – prescribed phenology biophysics
Improve fidelity of terrestrial surface representation in ATS:
- Surface water and energy balance
- Canopy hydrology
- Photosynthesis and transpiration
- Root function
- Snow model
- Albedo and surface radiation



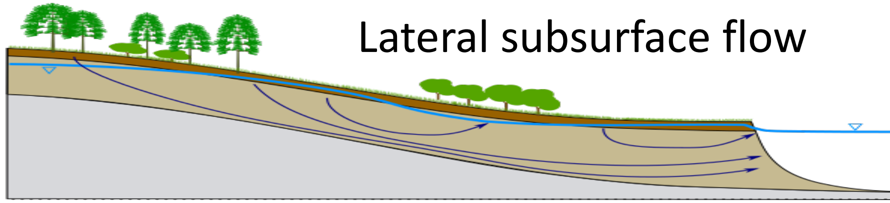
km -> m resolution



Next phase?:
- Vegetation dynamics and competition?
- Biogeochemistry?



->



Lateral subsurface flow

AMANZI ATS

Lightning Talks

Ylva Sjöberg, Univ. of Copenhagen

Daniil Svyatsky, Los Alamos National Laboratory

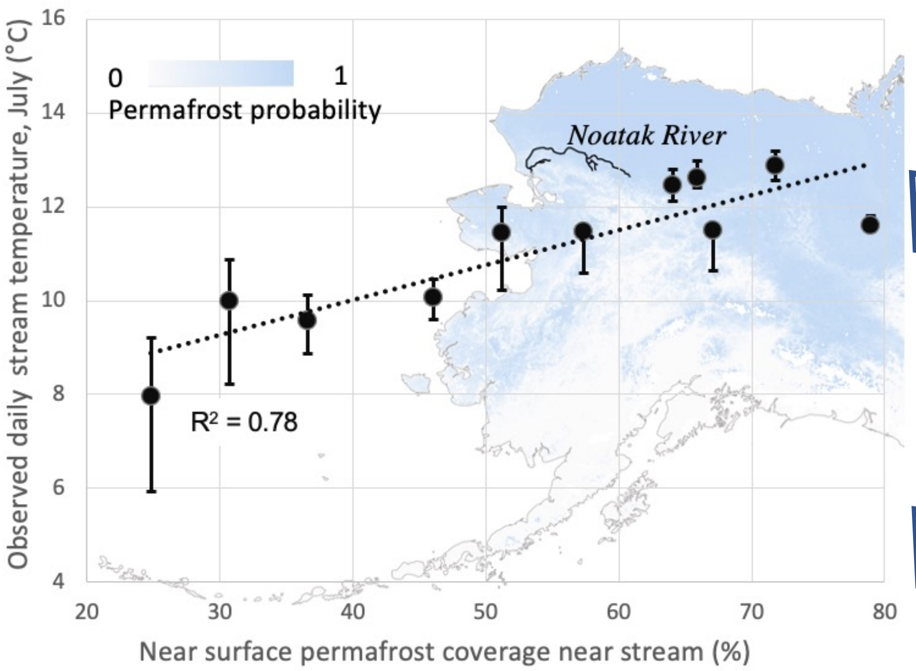
Lightning Talks

Ylva Sjöberg, Univ. of Copenhagen

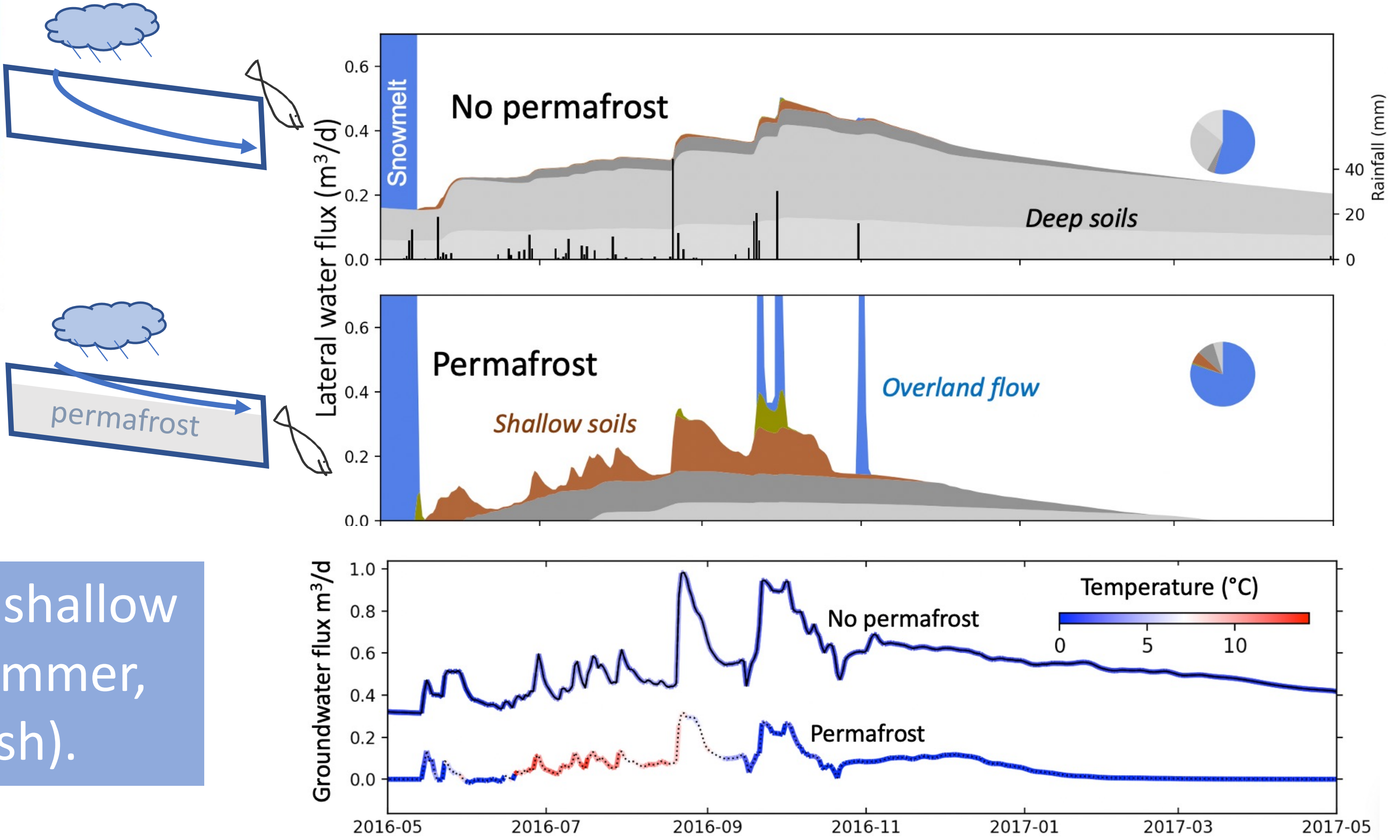
Groundwater temperatures, permafrost, and fish

Y. *Sjöberg[1], A. Jan[2], S. L. Painter[2], E. T. Coon[2], M. P. Carey[3], J. A. O'Donnell[4], and J. C. Koch[3]*
1 Uni. of Copenhagen, 2 Oak Ridge Nat. Lab., 3 U.S. Geol. Survey, 4 Nat. Parks Service

Observations



Hillslope model



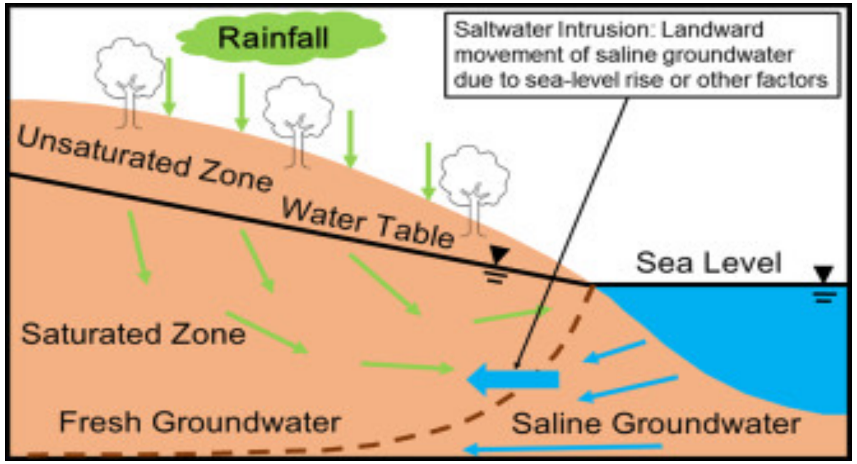
Permafrost promotes flow through shallow soils, which warm quickly during summer, resulting in warmer streams (and fish).

WRR: https://doi.org/10.1029/2020WR027463

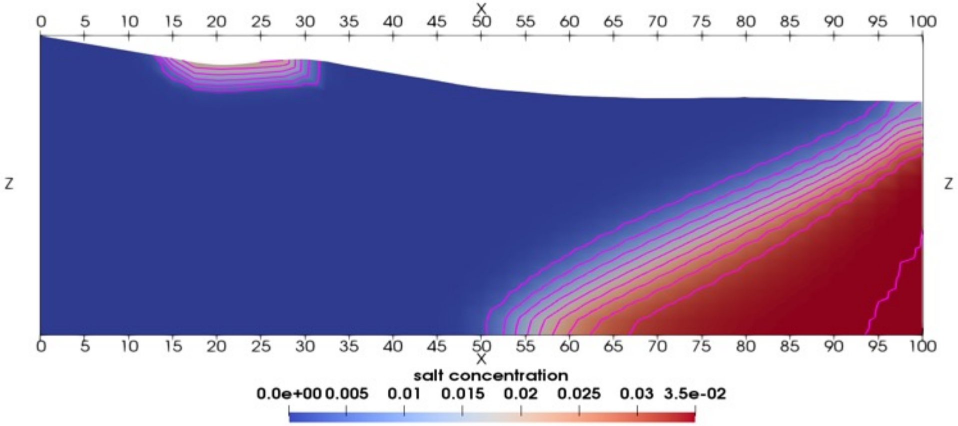
Saltwater intrusion

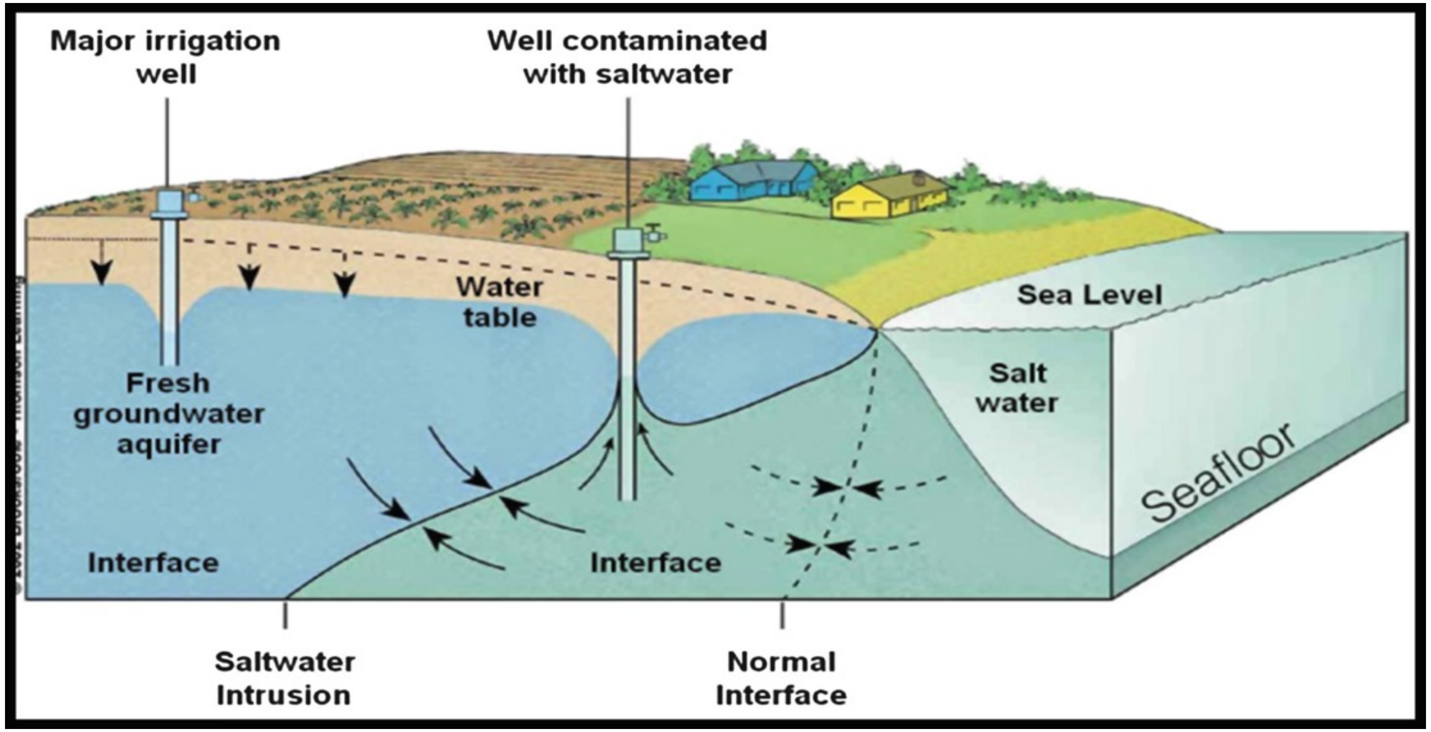
Daniil Svyatsky, Yu Zhang, J. David Moulton
Los Alamos National Laboratory

Salt water intrusion on coastal aquifers



https://doi.org/10.1016/j.scitotenv.2018.02.184





Salt water intrusion model in ATS

$$\frac{\partial \phi s n_w}{\partial t} + \nabla \cdot \mathbf{q} = Q_w^s + \Gamma_i \qquad \mathbf{q} = -n_w \frac{k k_r}{\mu}(\nabla p + \rho_w g)$$

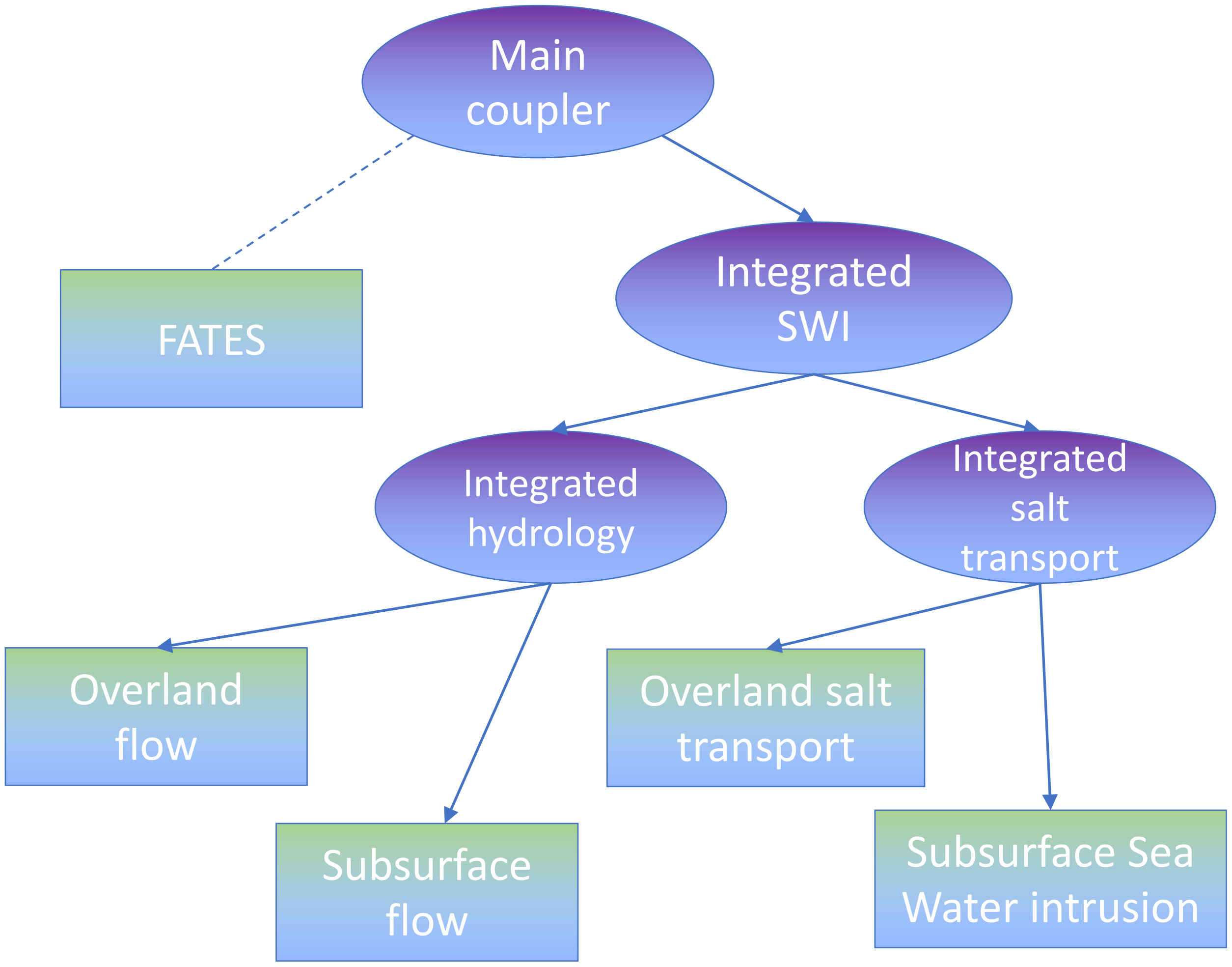
$$\frac{\partial h n_w}{\partial t} + \nabla \cdot \mathbf{u} = Q_w^o - \Gamma_i \qquad \mathbf{u} = -n_w h \frac{h^{2/3}}{n_{mann}\sqrt{|\nabla_S Z_s| + \varepsilon}} \nabla_s (h + Z_s)$$

$$\frac{\partial C \phi s n_w}{\partial t} + \nabla \cdot C\mathbf{q} - \nabla \cdot D_s^* \nabla C = Q_{int}(C)$$

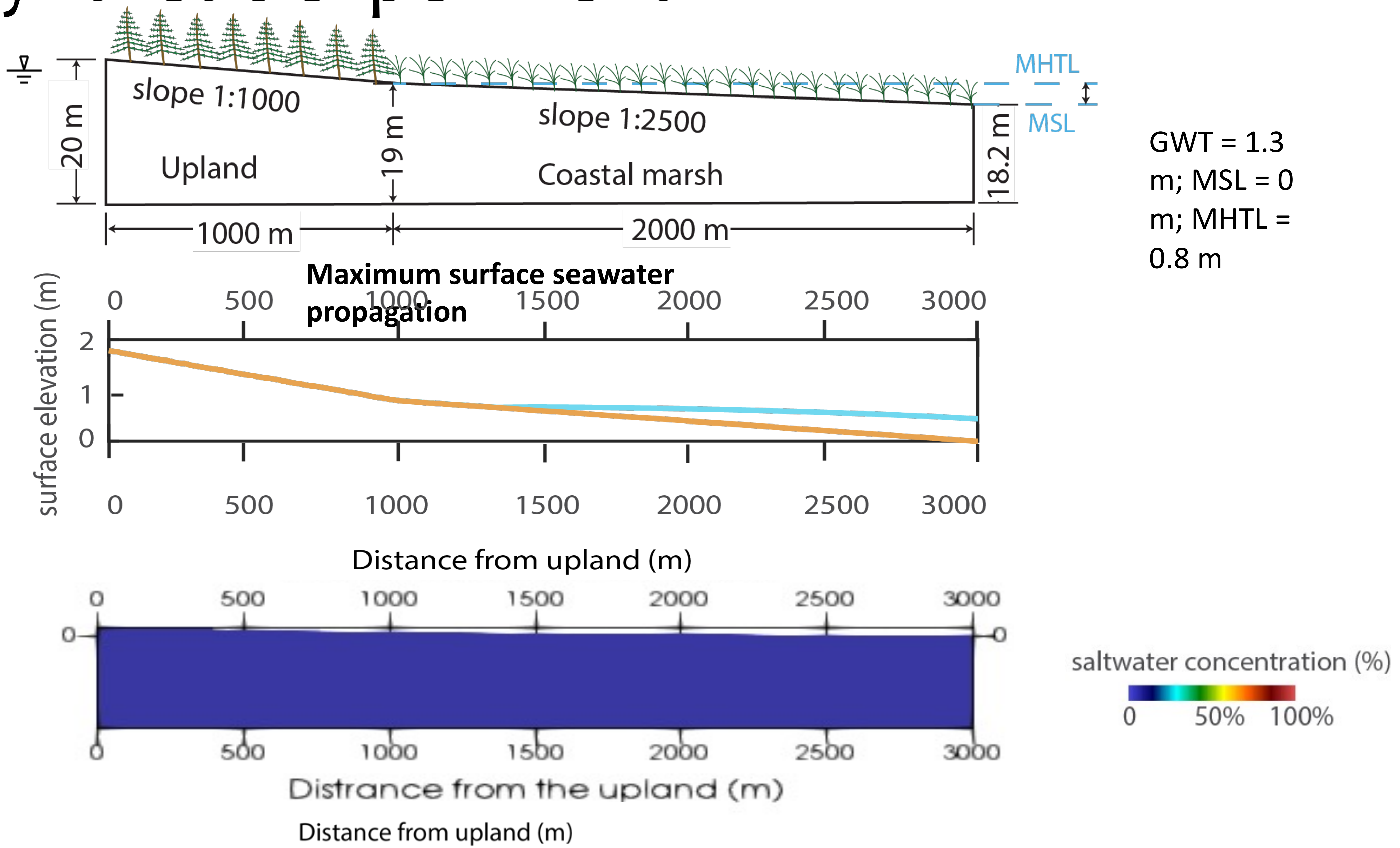
$$\frac{\partial C \phi s n_w}{\partial t} + \nabla \cdot C\mathbf{u} - \nabla \cdot D_o^* \nabla C = -Q_{int}(C)$$

$$\rho_w = \rho_w + \alpha(C - C_0)$$

ATS PK Tree



A synthetic experiment

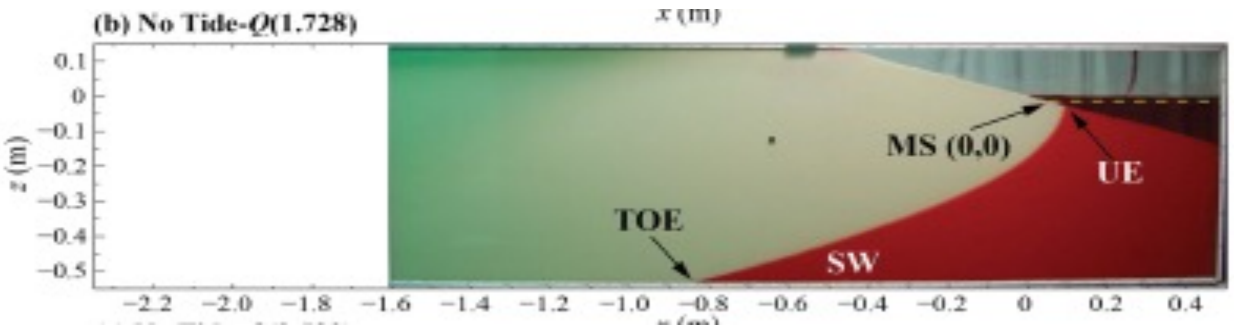


GWT = 1.3 m; MSL = 0 m; MHTL = 0.8 m

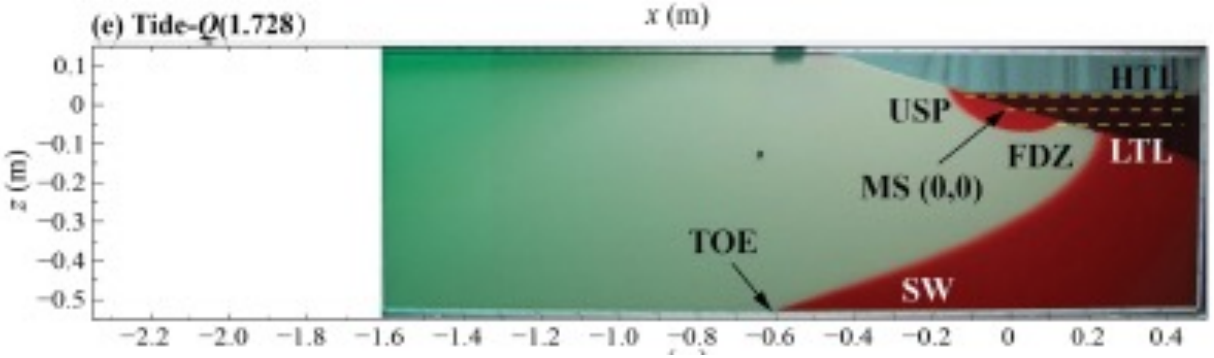
Benchmark simulation of saltwater intrusion

Zhang et al. 2021 WRR (in review)

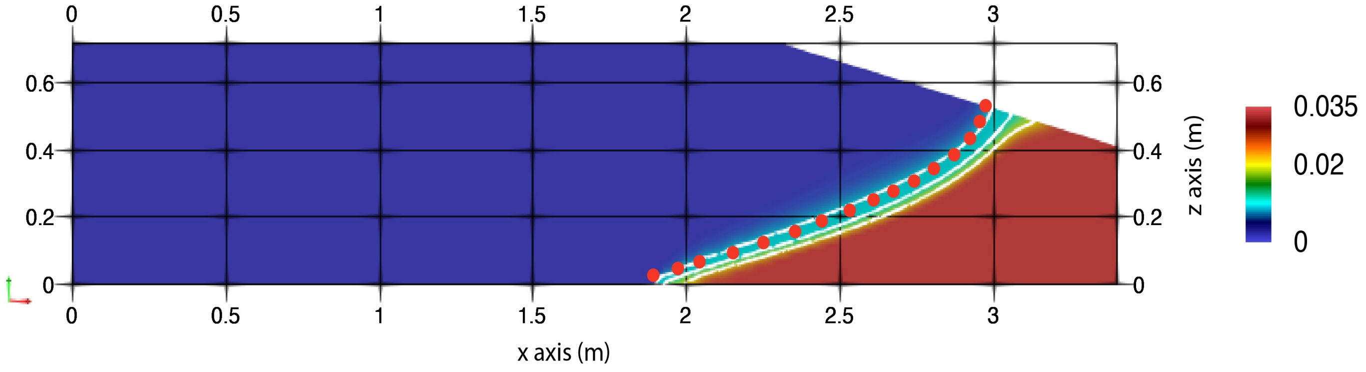
Lab experiment of the steady state saltwater profile driven by constant sea level from Kuai et al. 2019



Lab experiment of the steady state saltwater profile driven by constant sea level + tidal variation from Kuai et al. 2019



ATS simulated steady state saltwater profile driven by constant sea level (red dots indicates the interface location in the lab experiment above)



ATS simulated steady state saltwater profile driven by constant sea level + tidal variation (white dashed line indicates the interface location in the lab experiment above)