AMANZI ATS

Short Course – Sept 1&2, 2021

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Special Acknowledgement: Daniel Livingston

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National Laboratory

Los Alamos
NATIONAL LABORATORY

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Pacific Northwest
NATIONAL LABORATORY

OAK RIDGE National Laboratory

Program Development Funding

U.S. DEPARTMENT OF ENERGY

Office of Science

ExaSheds

IDEAS WATERSHEDS

Technical Support

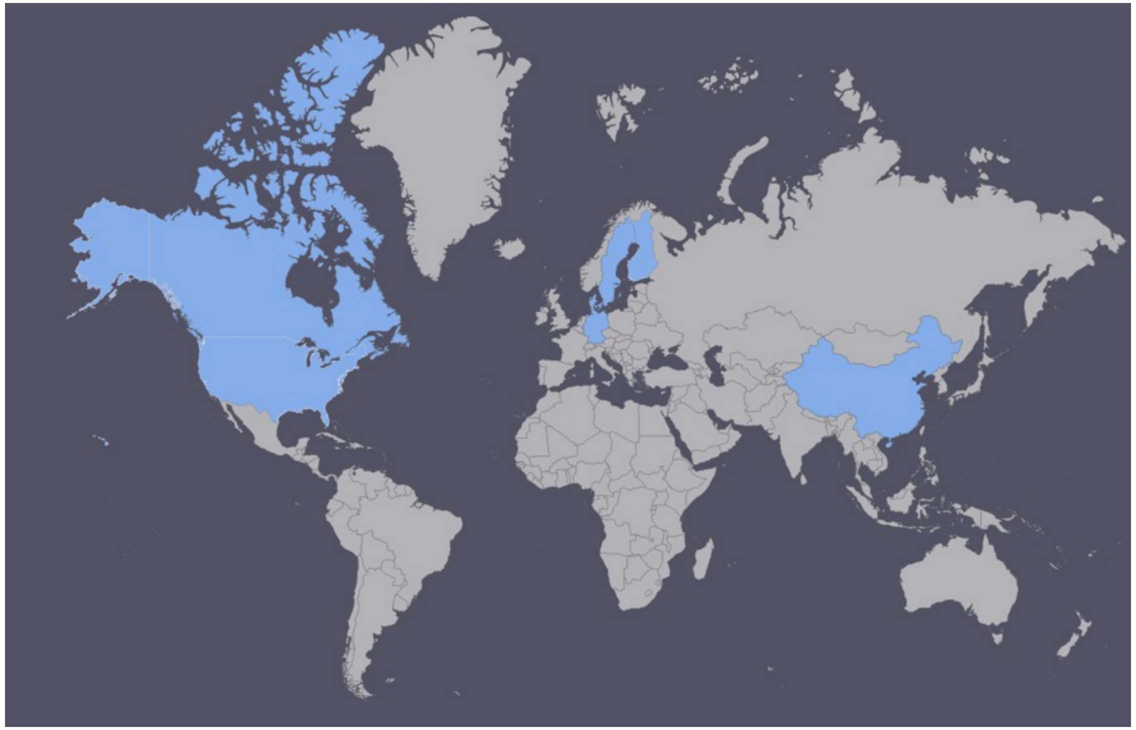
Zoom Connection Difficulties

Josh Smith

Amanzi–ATS/Docker Difficulties

Daniel Livingston, David Moulton

Thank You!



- 70+ attendees
- 7 countries
- 7 time zones around the world

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

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	Salinity Intrusion	D. Svyatsky

Goals for this Short Course

Expectations of Attendees:

- Understand the fundamentals of hydrologic modeling
  water cycle + calculus & differential equations
- Understand the basics of computing
  navigating a command line prompt, basic scripting
- Fundamentals of modeling science
  hypothesis-driven science; numerical experiments
- *Willingness to learn, ask questions, and engage*

Goals for this Short Course

Attendees will leave this short course with:

- The ability to set up and and run basic problems in ATS by following the pattern of demo problems.
- Understand the basics of how to modify problems to address scientific hypotheses on synthetic and real-world modeling domains
- Knowledge of how to get help to do more
- Knowledge of how they can give back to the community

Goals for this Short Course

Interactive and Collaborative

- Please use chat for questions
- Demos are intended to be interactive – break things and ask questions!

Not to be covered...

- Code installation
  - Feel free to use the Docker container beyond this short course
  - Installation isn't hard and is getting easier
    (at least on laptops and workstations)
  - See Github page or user guide for more
- Mathematics (discretizations, solvers, time integration) beyond the defaults.
- Problem optimization and knob tweaking for best performance (beyond a few gotchas)

Amanzi–ATS is a research code!

- There will be bugs (report them);
  be curious and think critically.
- We do not try very hard to prevent you from trying to do something that is not very smart (ask the user's group).
- Developers are researchers too!
  - Cite the code, cite the paper
  - Acknowledge the community if it helped you
  - We are always happy to collaborate in exchange for co-authorship!
- If it hasn't been done before, don't be afraid to ask!

Connect and Contribute

Amanzi–ATS Users Group: ats-users@googlegroups.com

- https://groups.google.com/g/ats-users

Source code, Wiki, Issue tracking

- https://github.com/amanzi/amanzi
- https://github.com/amanzi/ats

Demos, Example problems, Tests

- https://github.com/amanzi/ats-demos
- https://github.com/amanzi/ats-regression-tests

Users' Guide, FAQs

- https://amanzi.github.io/ats
- https://github.com/amanzi/ats/wiki/FAQs

A short history of Amanzi and ATS

Ethan Coon[1], J. David Moulton[2], Scott Painter[1]*

[1]Oak Ridge National Laboratory

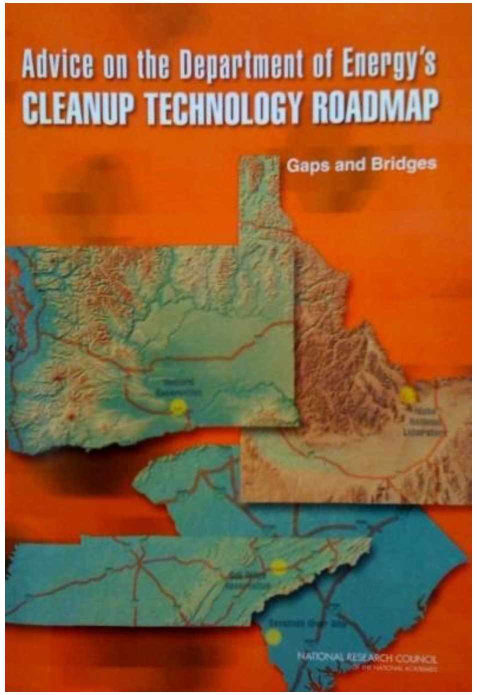
[2]Los Alamos National Laboratory

Amanzi was motivated by the DOE's environmental management mission

NAS : Need for Advanced Subsurface Modeling and Simulation within EM cleanup mission

National Academies of Science: 2009

…..'***Modern computing power*** *can help ensure that more sophisticated numerical models are* ***<u>well integrated </u>with the biochemical, ecological, and geochemical sciences*** *sufficiently to provide the resolution needed to improve the accuracy of model simulations and predictions needed to advance cleanup, remediation, and risk reduction.'*

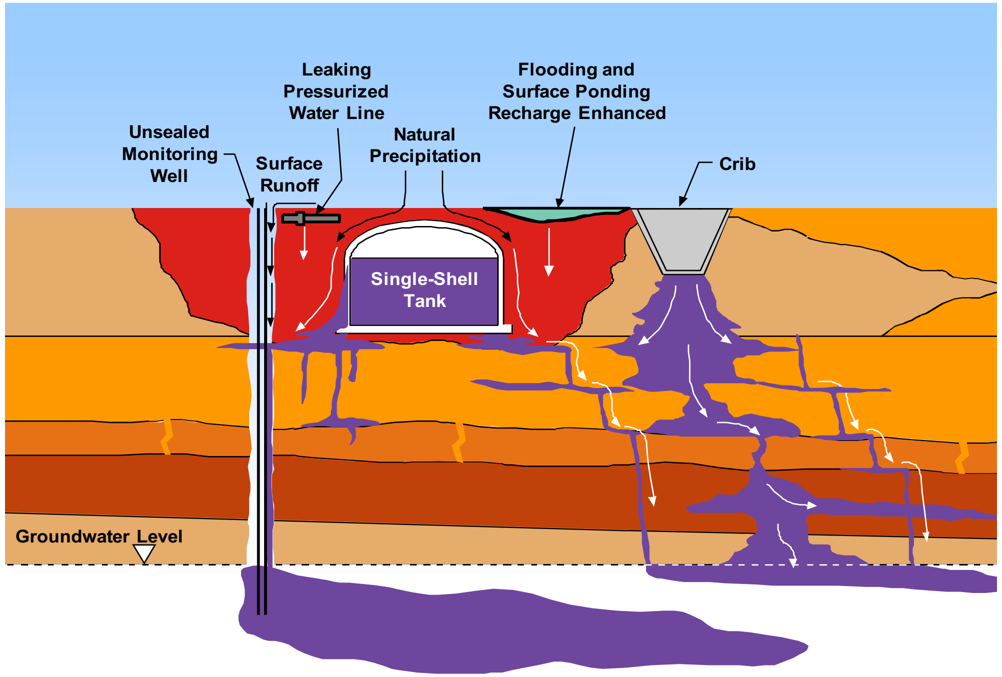


THE NATIONAL ACADEMIES
Advisers to the Nation on Science, Engineering, and Medicine

Science and technology for DOE Site cleanup: Nuclear and Radiation Studies Board Workshop Summary, NRC 2010

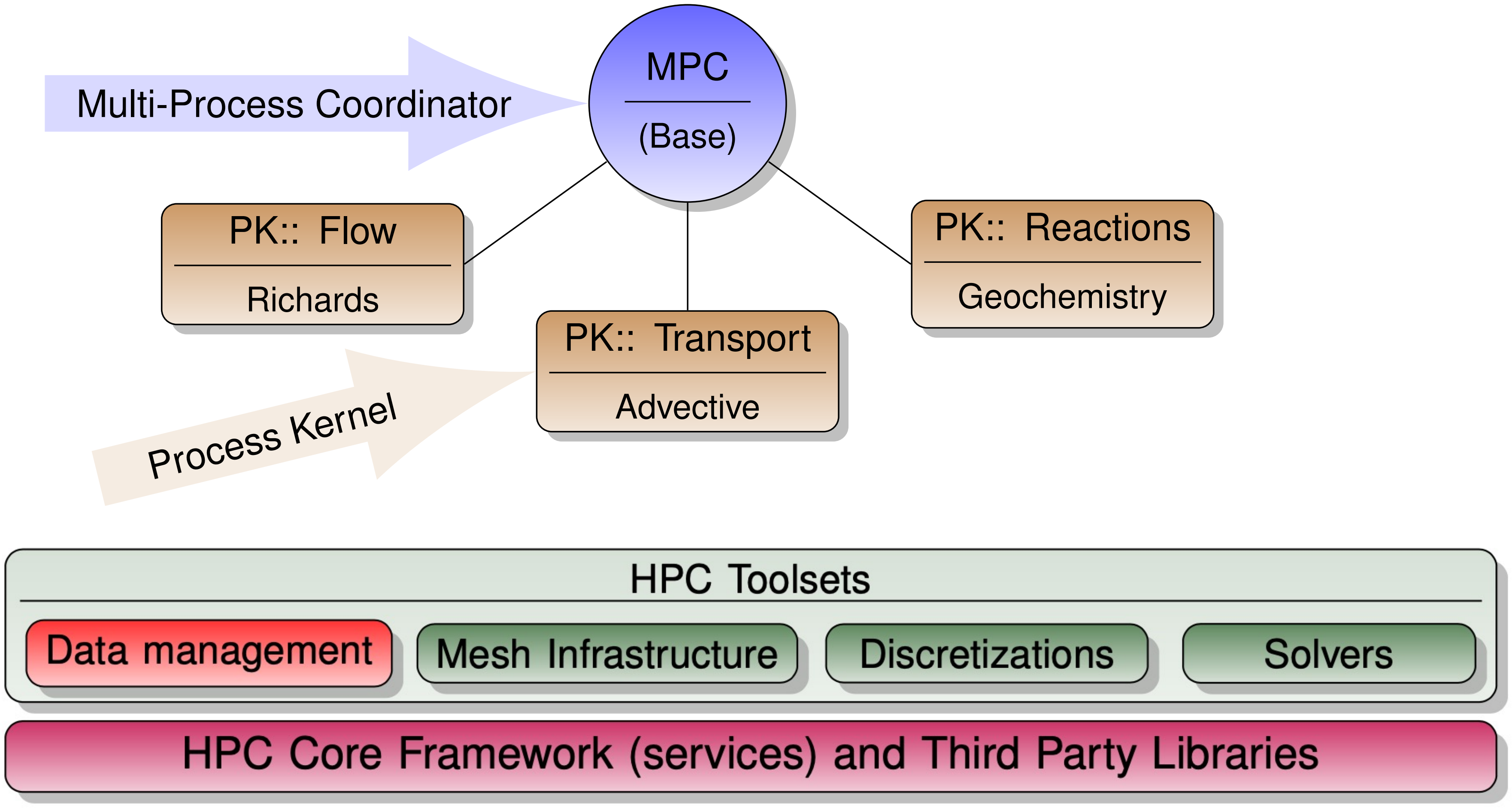
Amanzi: flexible and extensible HPC toolset with multiple process models

- Multilab project led by David Moulton (LANL)
- Transient unsaturated flow with reactive transport on unstructured meshes with general polyhedral cells
- Parallel by domain decomposition with parallel i/o
- **Modular, extensible and open source**
- Leverages existing capabilities from decades of DOE investments in computing, computational science, and environmental science
  - Trilinos : Parallel programming services
  - PETsc: Portable, Extensible Toolkit for Scientific Computation
  - Unstructured meshing and spatial discretization capabilities
  - Geochemistry and reactive transport simulation expertise
- A **community platform** for testing and integrating new process-based understanding

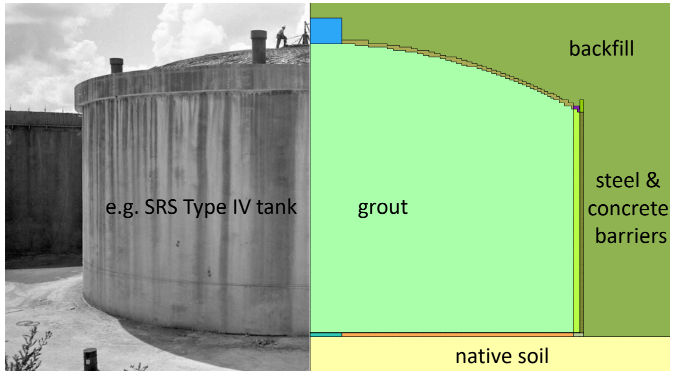


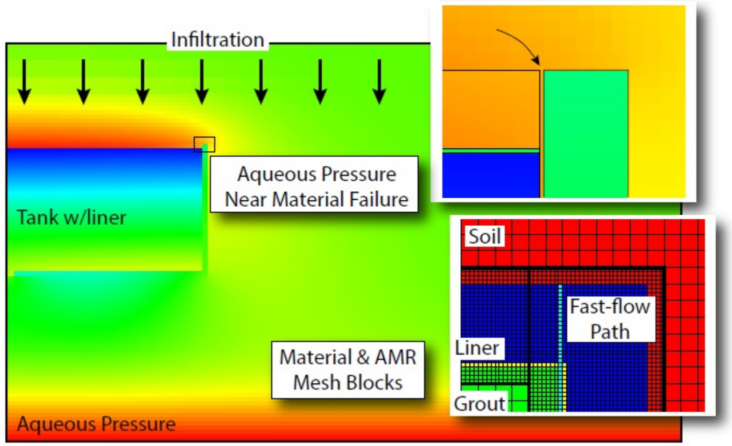
Wide Range of Platforms

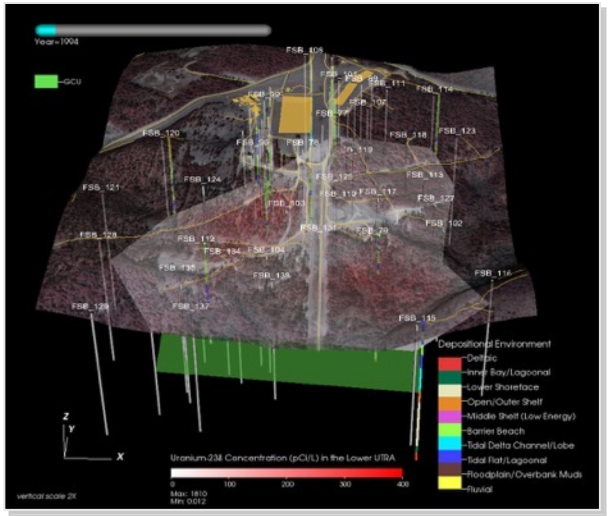
Amanzi: Application-Centric High-Level Design

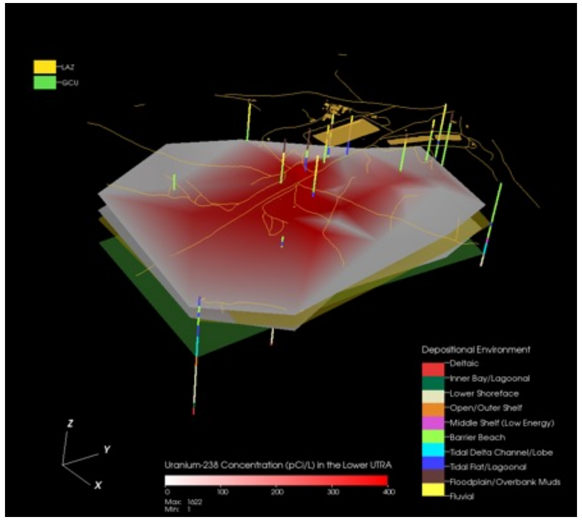


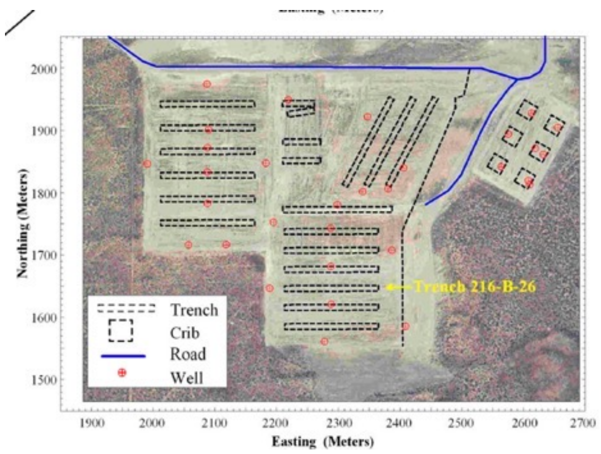
Amanzi was designed for real-world complexities of environmental management applications

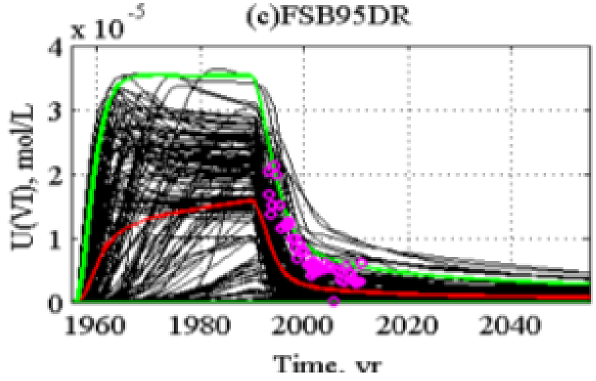




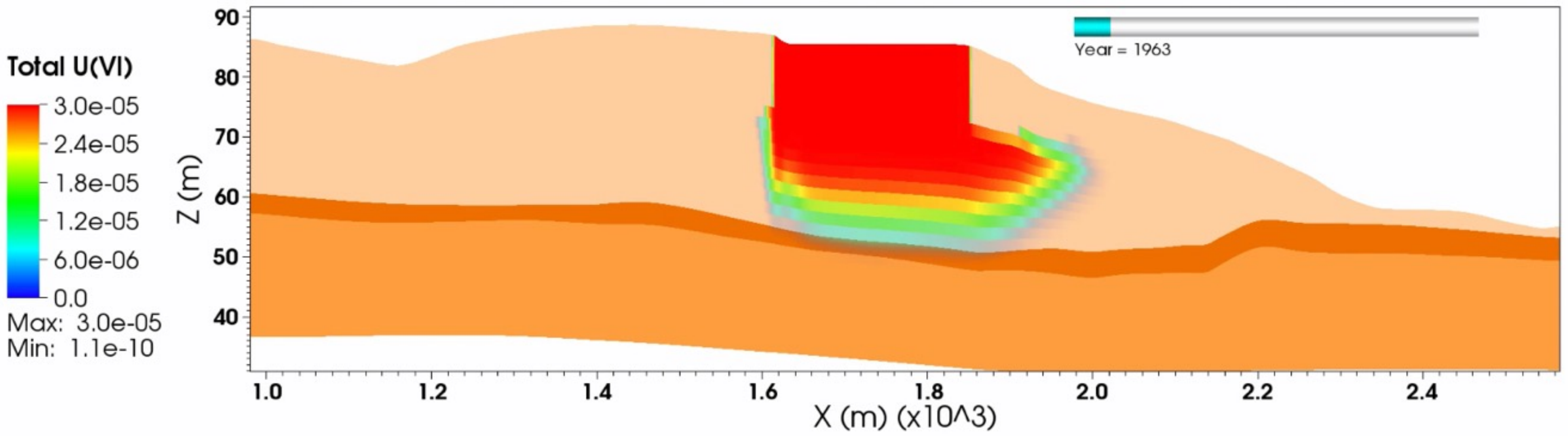


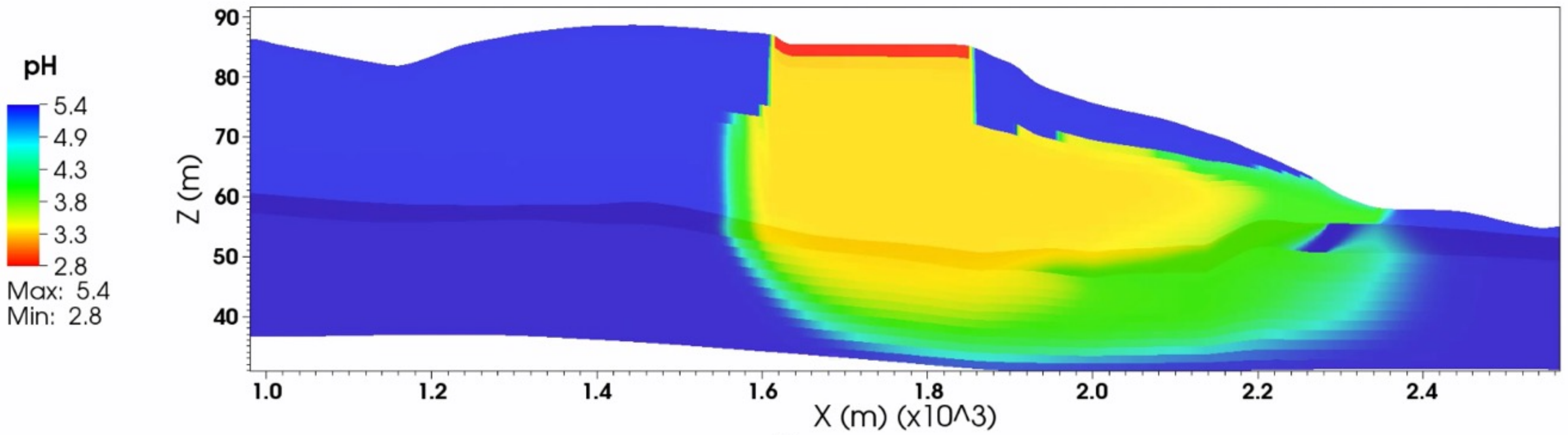






Amanzi Simulation of Uranium Mobility



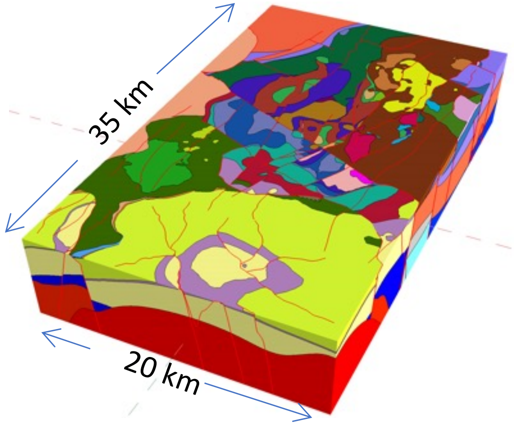


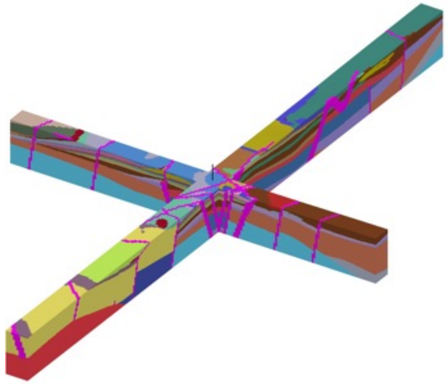
Geochemically complex,

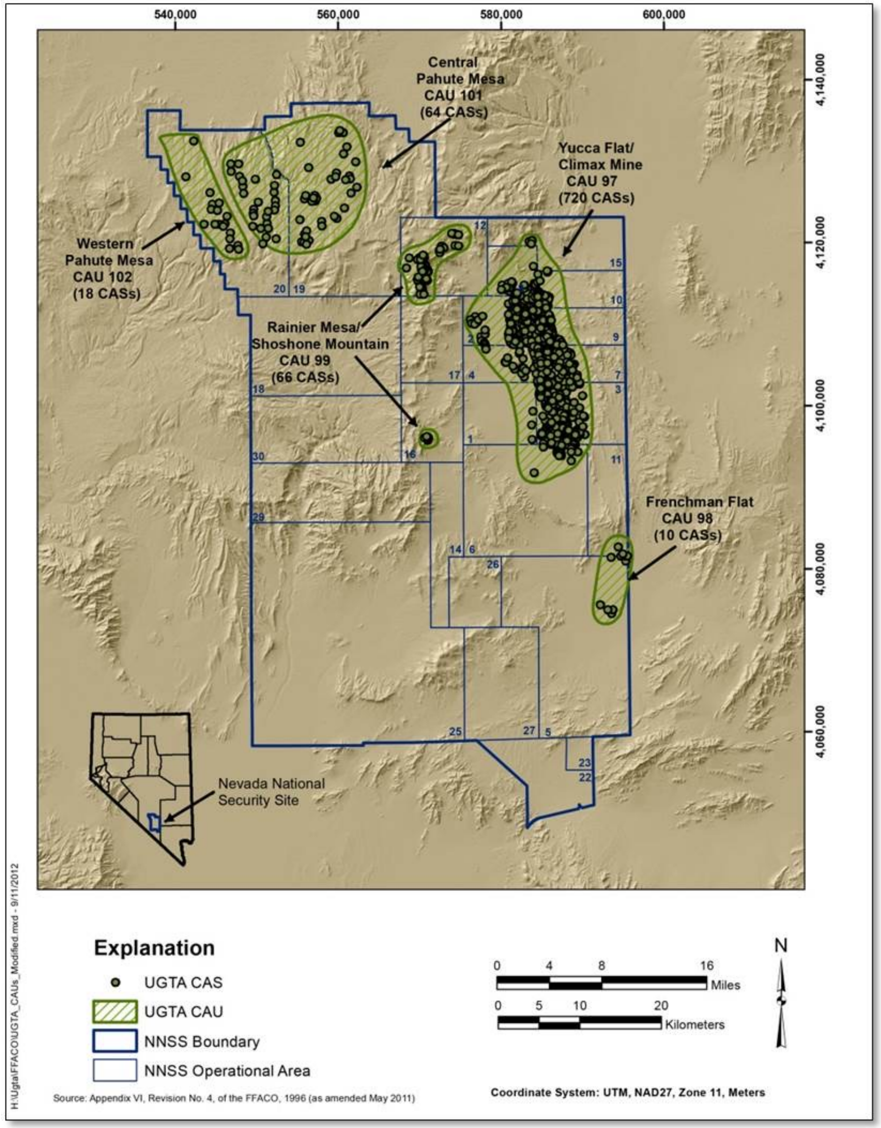
- 13 primary species,
- 8 minerals
- Uranium sorbed via a pH-dependent surface complexation reaction
- pH controlled by mineral reactions and ion exchange

Flow and Transport at the NNSS

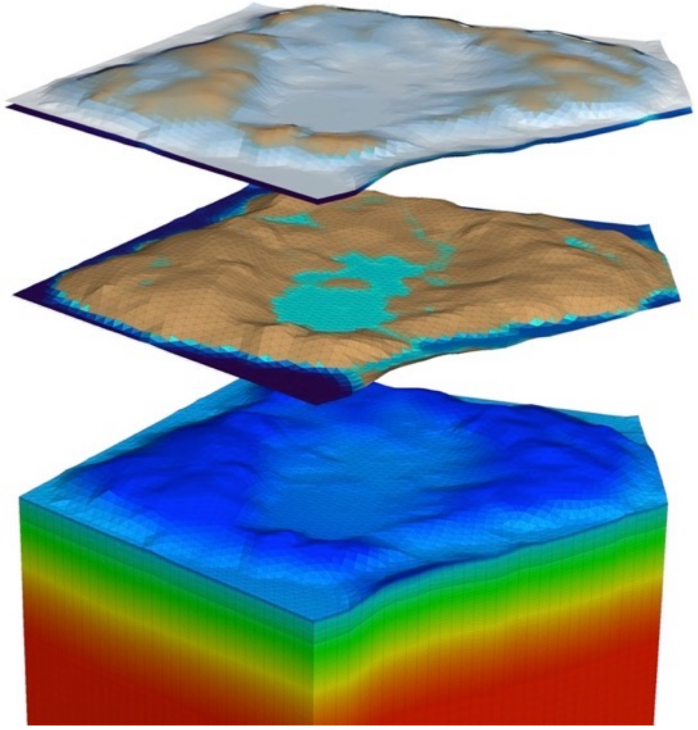
NNSS (former NTS) has groundwater contamination from 828 underground nuclear tests conducted between 1957 and 1992





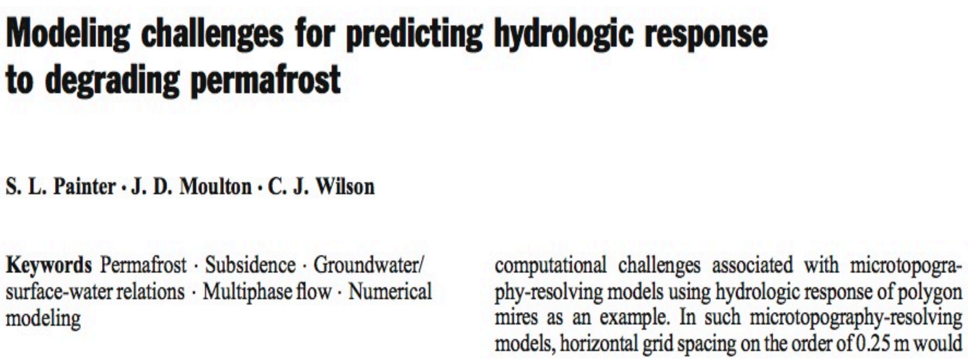


The Arctic Terrestrial Simulator



- Circa 2012-2015
- Ethan Coon, lead developer
- LANL internal project led by Scott Painter and David Moulton and NGEE-Arctic project
- Leverages Amanzi for advanced discretizations, mesh infrastructure, nonlinear solvers
- xSDK libraries provide scalability (e.g., Trilinos, PETSc, Hypre)
- Introduced Arcos flexible fine-grained multiphysics framework
- Extended Amanzi's mesh infrastructure to represent multiple spatial domains

Hydrogeology Journal, 2013



Modeling challenges for predicting hydrologic response to degrading permafrost

S. L. Painter · J. D. Moulton · C. J. Wilson

Keywords Permafrost · Subsidence · Groundwater/surface-water relations · Multiphase flow · Numerical modeling

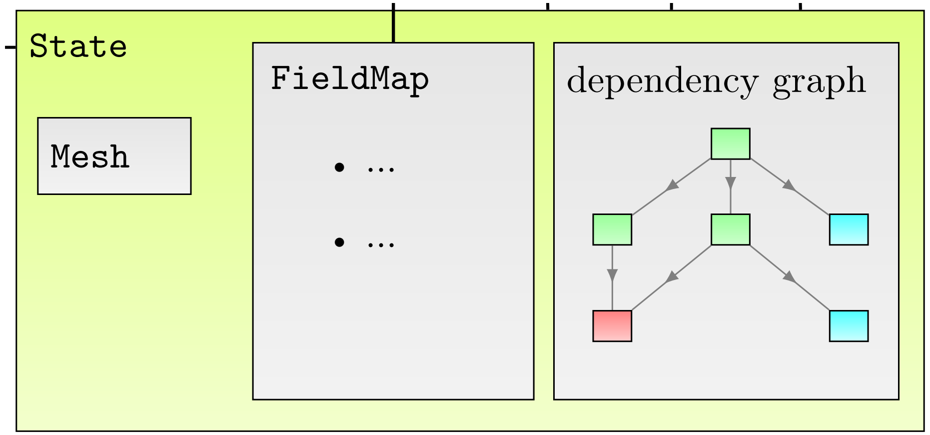
computational challenges associated with microtopography-resolving models using hydrologic response of polygon mires as an example. In such microtopography-resolving models, horizontal grid spacing on the order of 0.25 m would

Arcos Multiphysics Framework

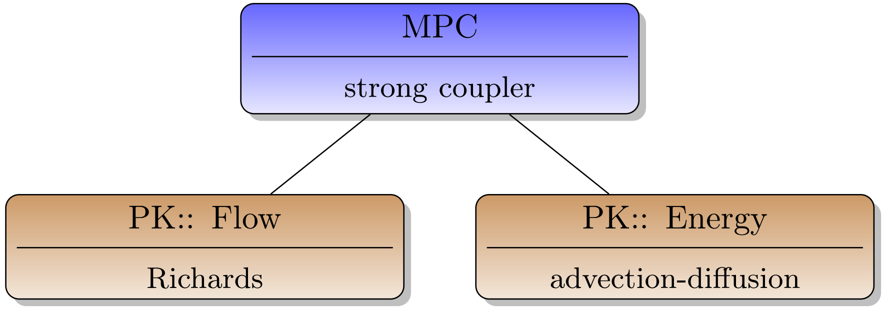
Environmental Modelling & Software
Volume 78, April 2016, Pages 134-149

Managing complexity in simulations of land surface and near-surface processes

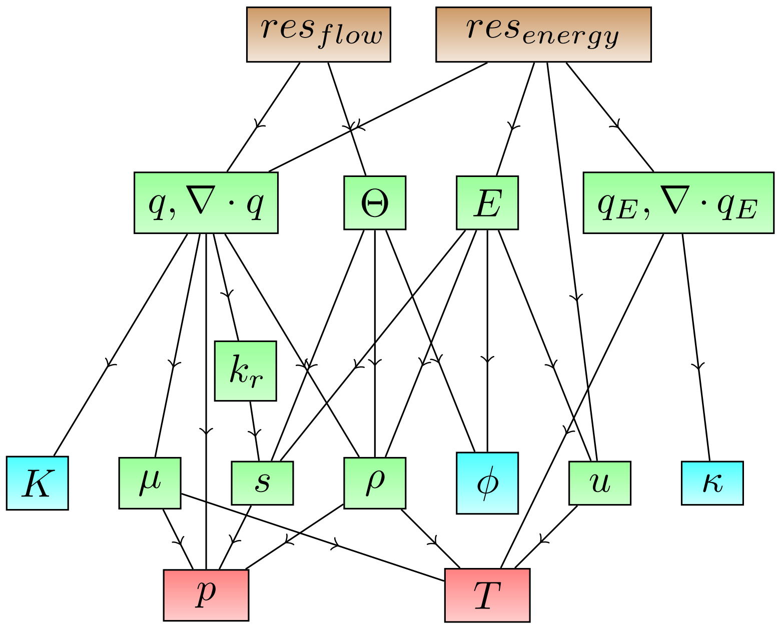
Ethan T. Coon [a], J. David Moulton [b], Scott L. Painter [c]



Dynamic Data Manager



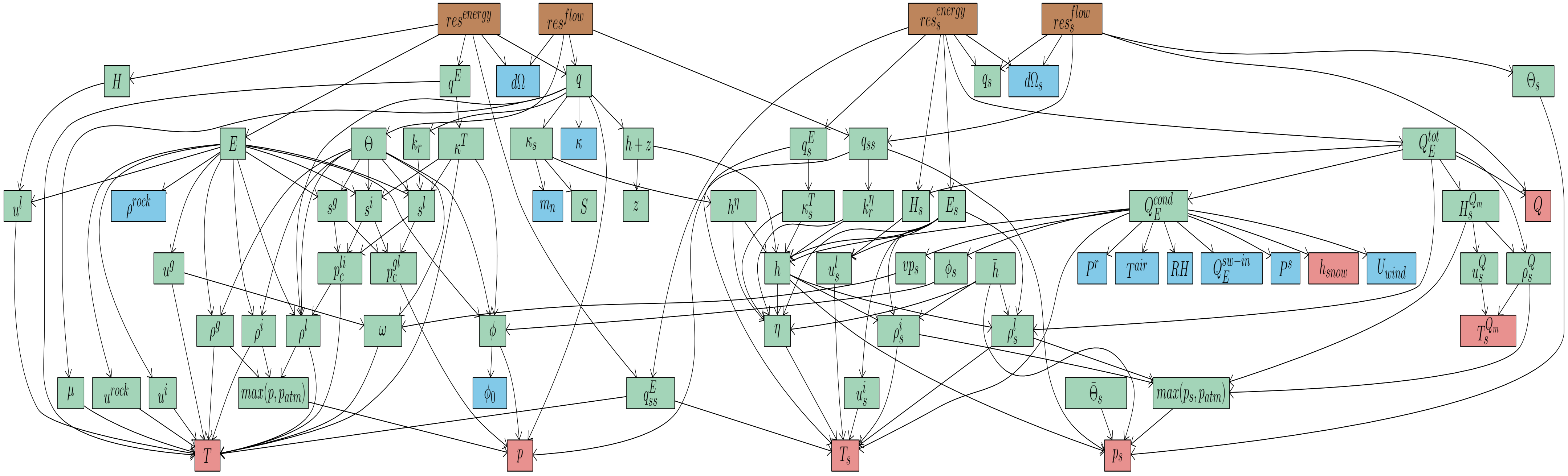
Process Kernel Tree



Dependency Graph

Automated Graph Construction is Necessary to Manage Complexity in Multi-Process Models

Consider the graph of surface/subsurface flow with thermal dependence and surface energy balance for the Arctic Terrestrial Simulator …



- Pink: Primary variables in a process kernel or evaluator
- Green: Dependent variables in the system (e.g., relative permeability)
- Blue: Input data (e.g., density of the medium)

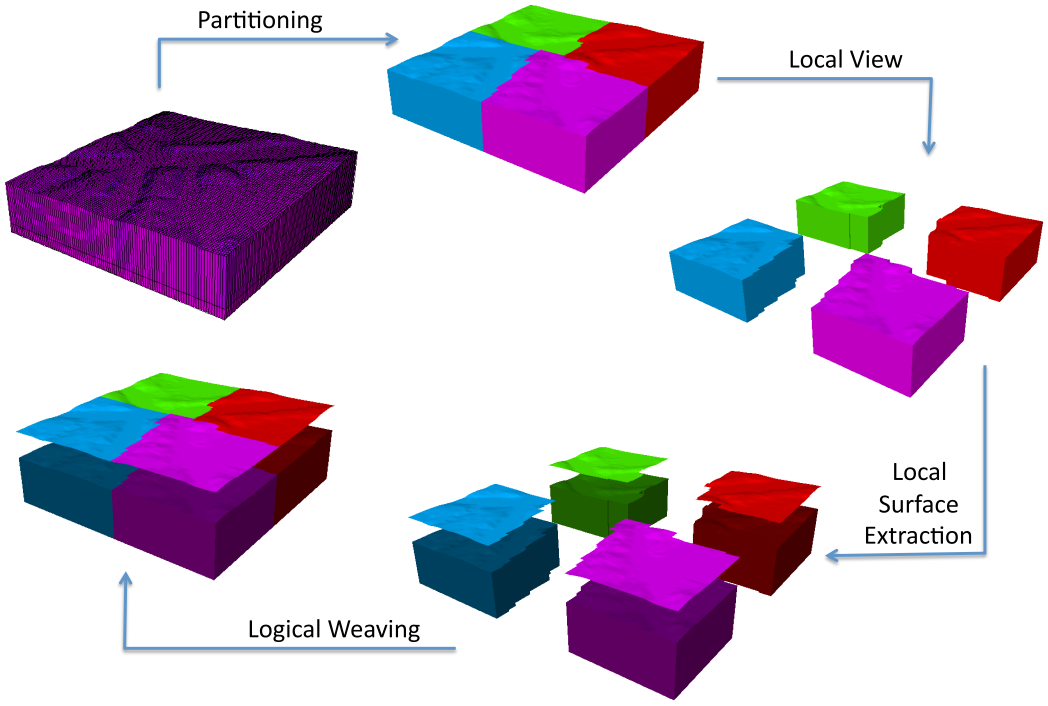
AMANZI ATS

Flexible Parallel Unstructured Mesh Workflow

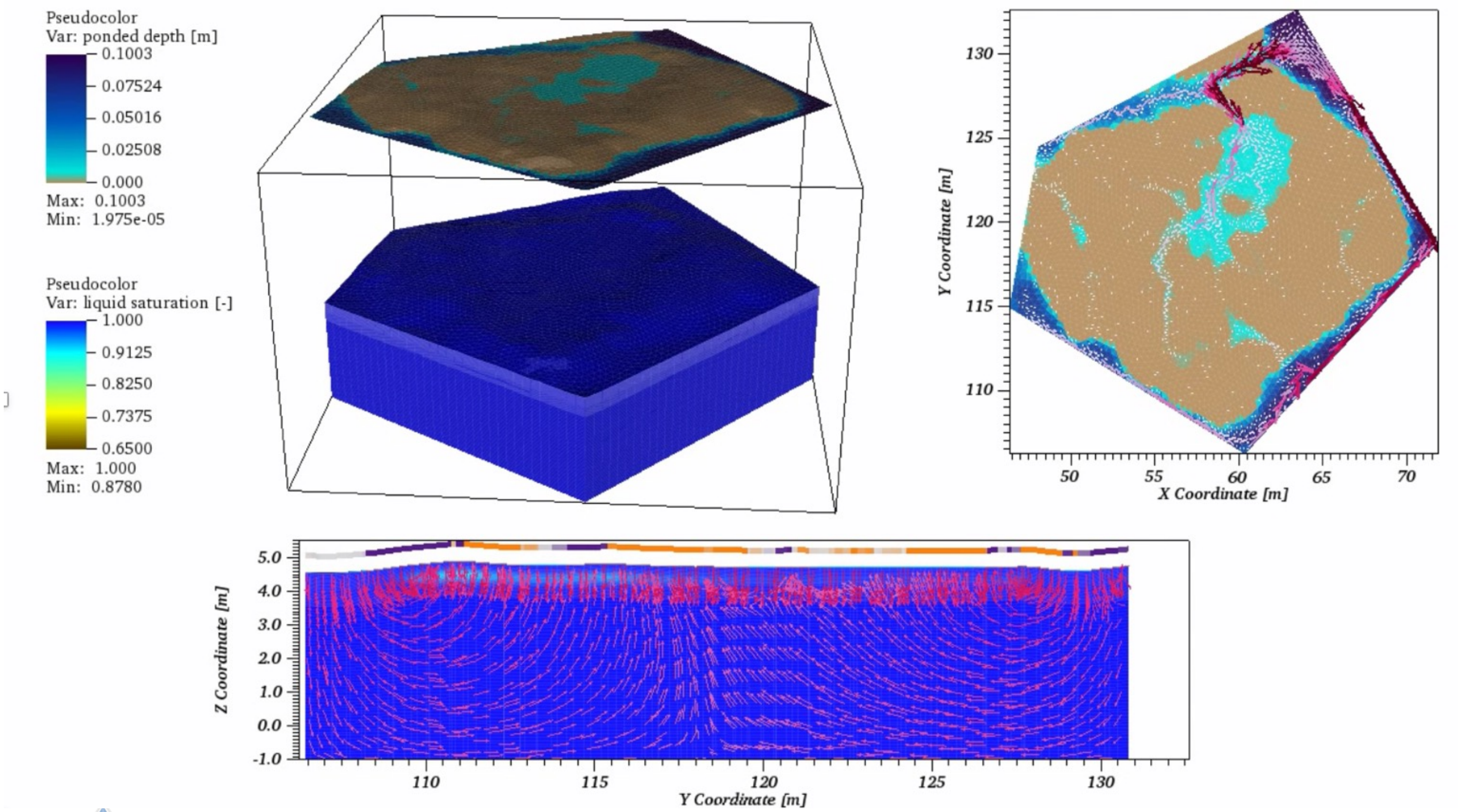
Amanzi provides an extensible unstructured mesh infrastructure for parallel distributed meshes with polyhedral cells.

New meshing capabilities developed for the ATS include

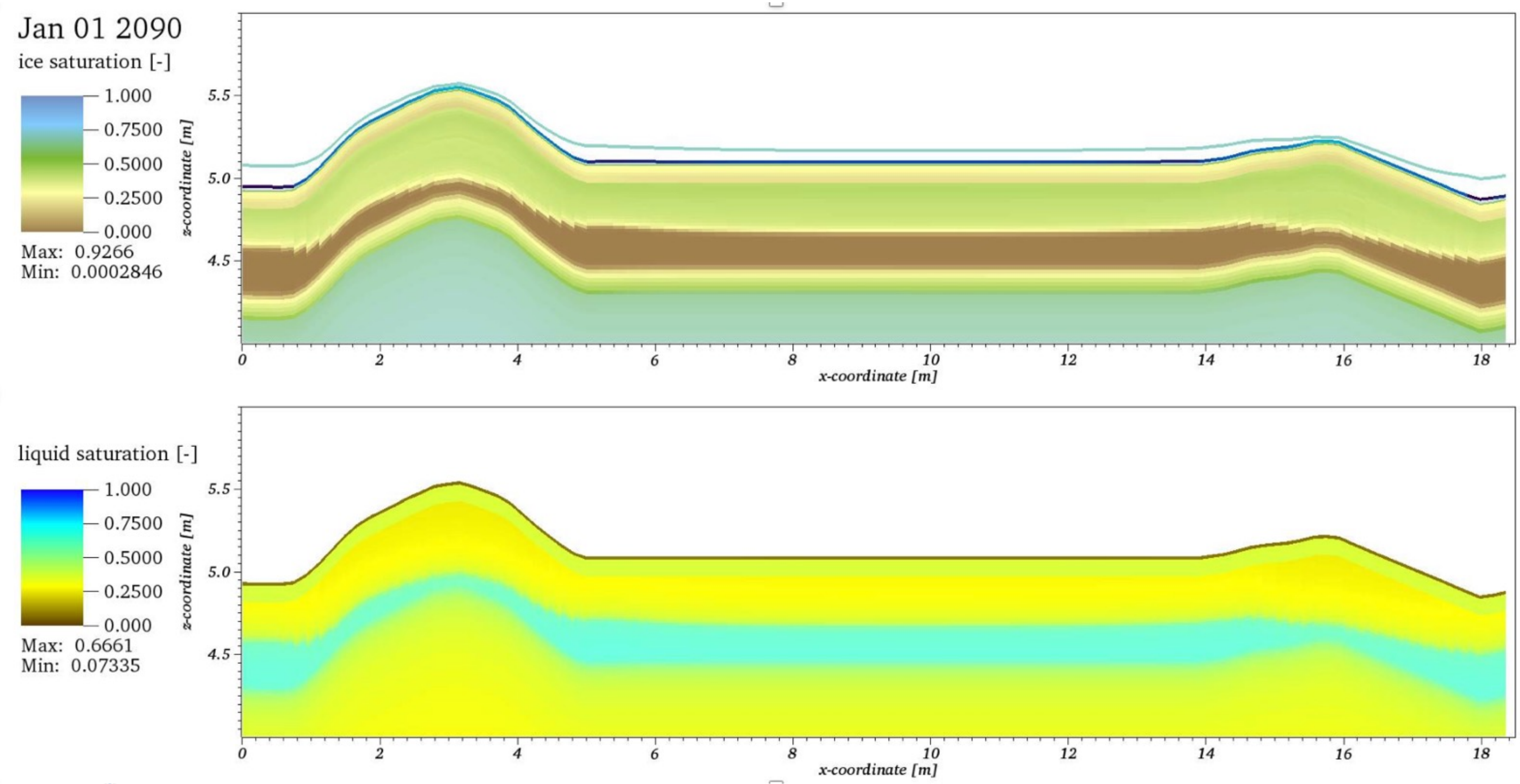
- Parallel creation of a surface mesh from a volume mesh
- Multiple meshes or sub-meshes, with run-time association of processes.
- Dynamically evolving meshes (support permafrost deformation).



Coupling Surface/Subsurface Flow

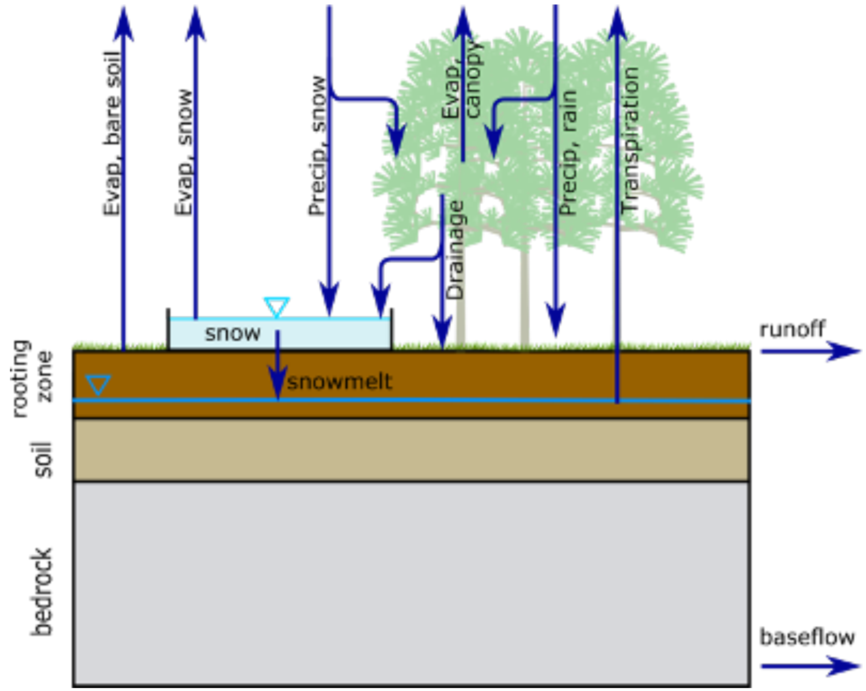


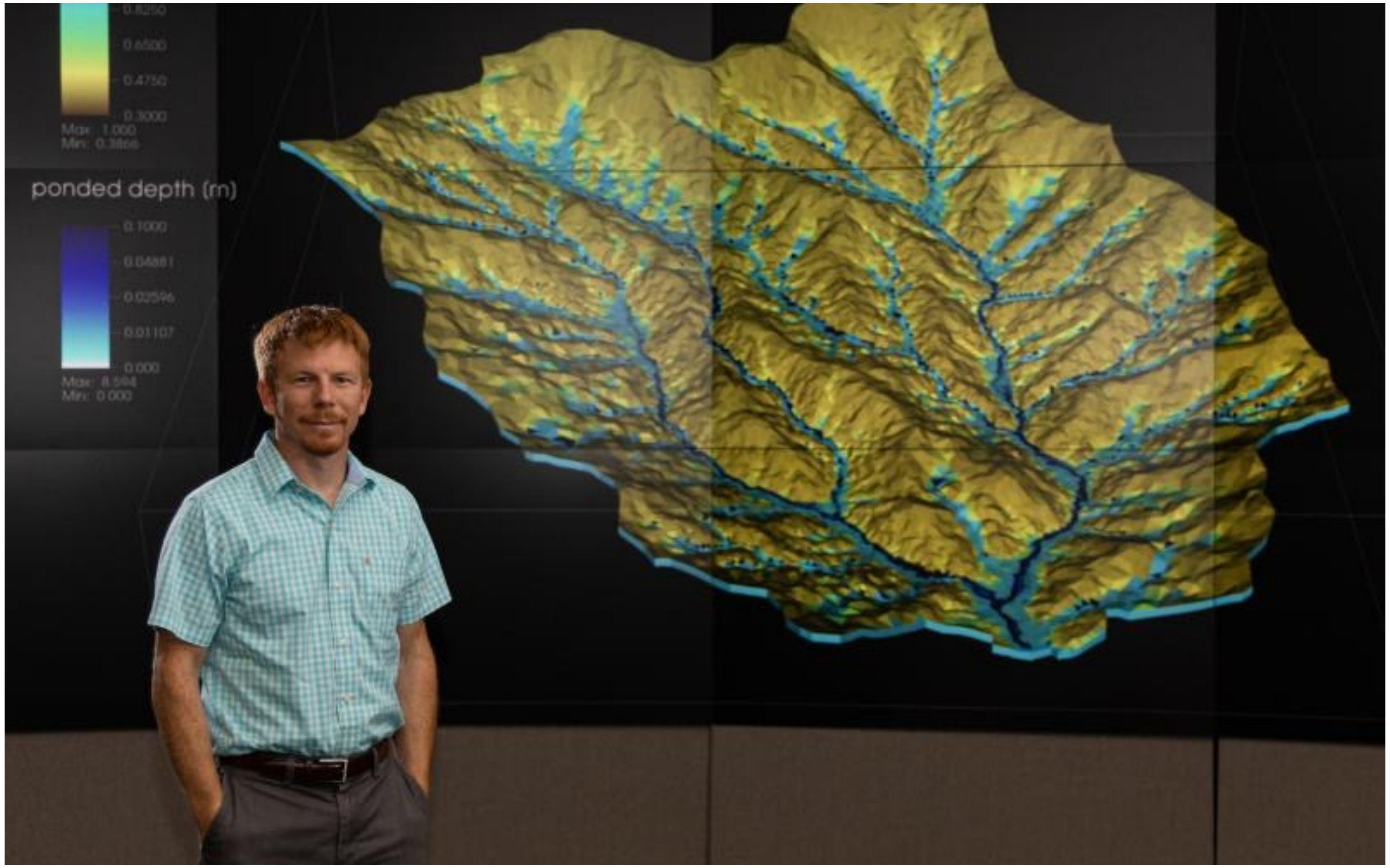
Low Center Polygon: 2080 to 2100



~~Arctic~~ Advanced Terrestrial Simulator

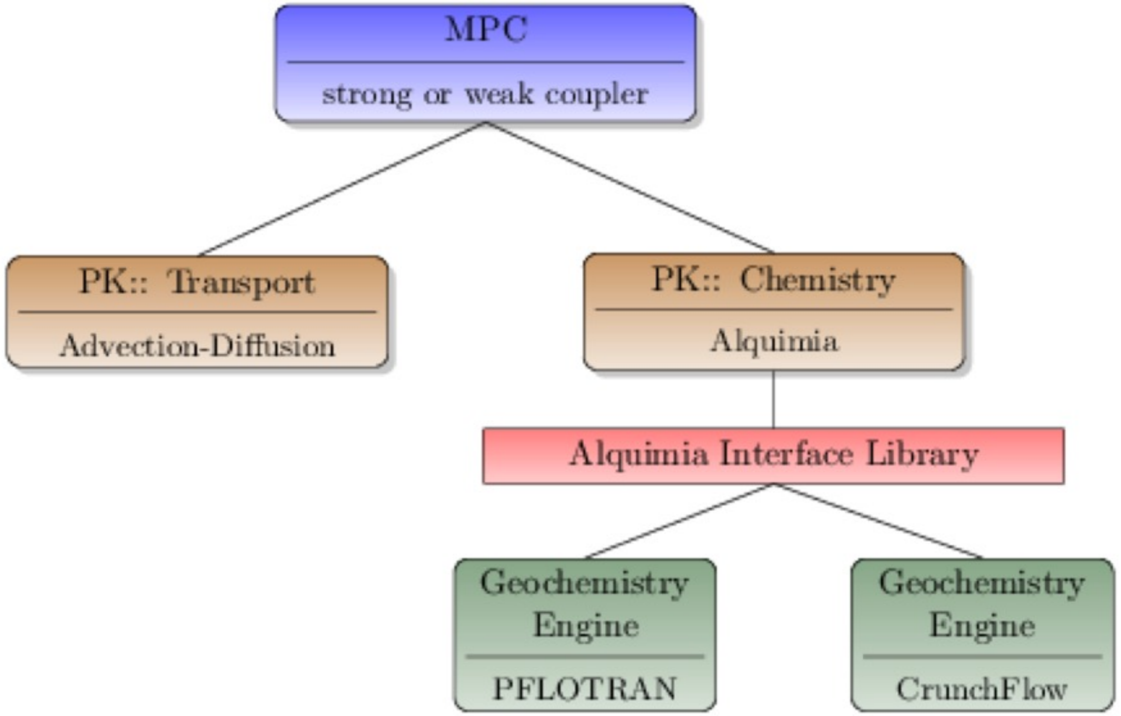
Circa 2015





Alquimia: A geochemistry interface library

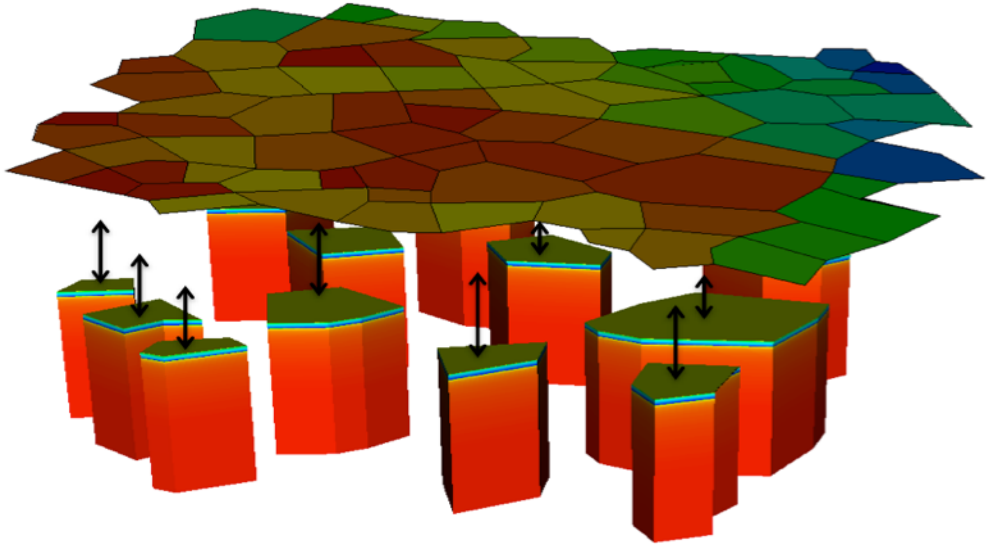
- Alquimia currently assumes that reactive transport uses operator-splitting.
- Assists in enforcing geochemical conditions (speciation) for transport boundary conditions
- Alquimia can facilitate benchmarking of geochemical capabilities in existing codes
- Geochemistry libraries, such as PFLOTRAN and CrunchFlow, have implemented interfaces to Alquimia.



Alquimia is open source, https://bitbucket.org/berkeleylab/alquimia

Extensions to enable multiscale simulations

- Circa 2016-2018
- Mesh infrastructure extended to allow
- Hierarchical model design and sub-cycling control
- Process kernels (PKs) are reused, instantiated on meshes as needed

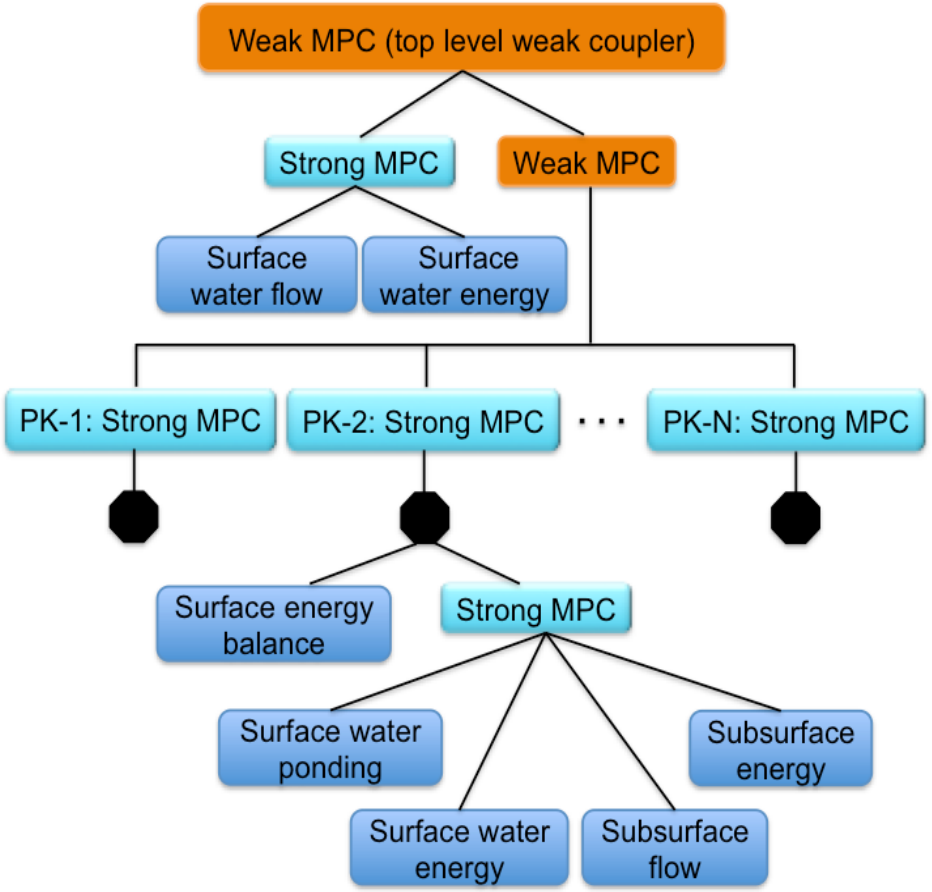


Comput Geosci (2018) 22:163–177
DOI 10.1007/s10596-017-9679-3

ORIGINAL PAPER

An intermediate-scale model for thermal hydrology in low-relief permafrost-affected landscapes

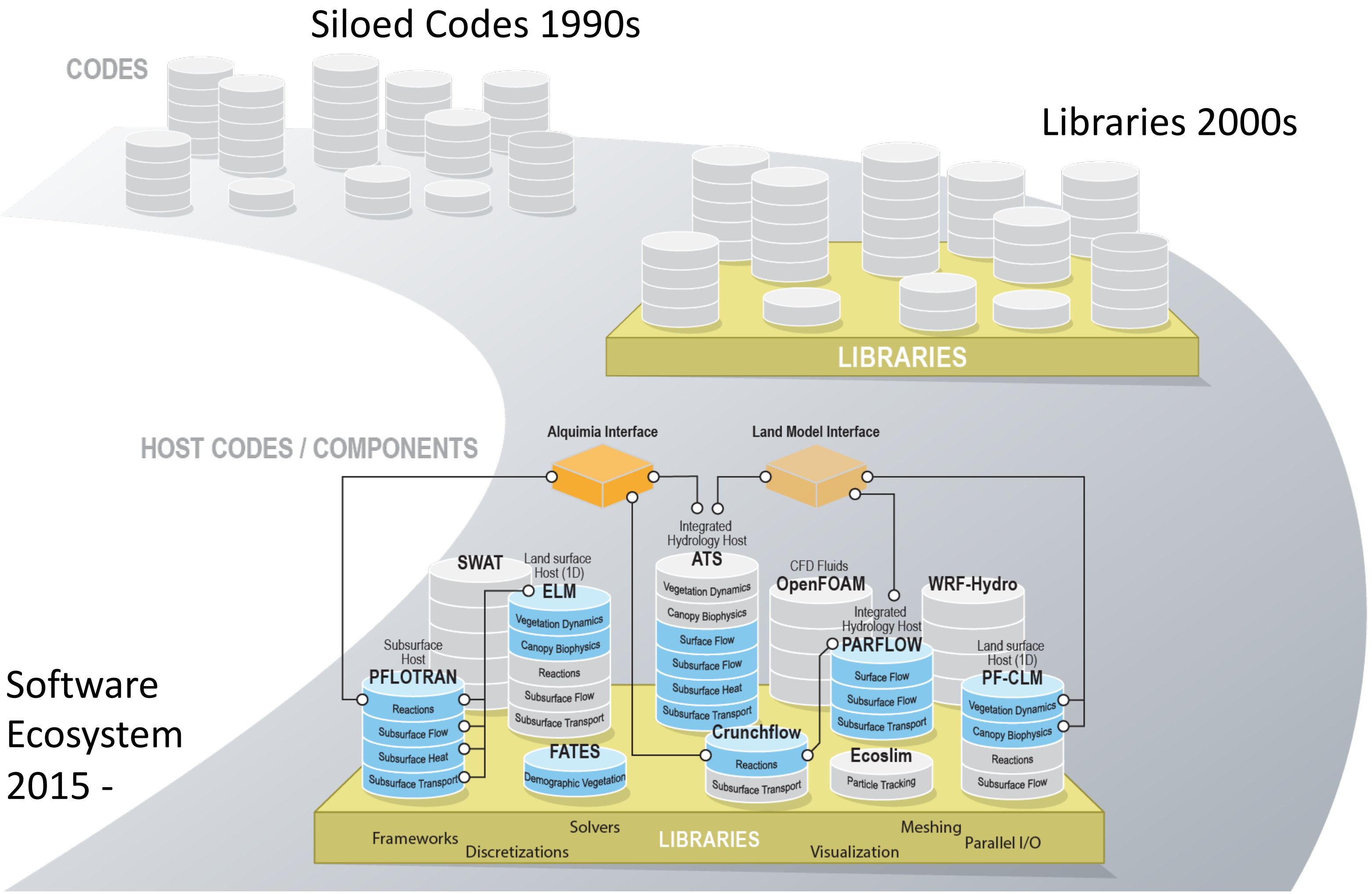
Ahmad Jan[1] · Ethan T. Coon[1,2] · Scott L. Painter[1] · Rao Garimella[3] · J. David Moulton[3]



AMANZI ATS

ATS becomes a cornerstone in DOE's Environmental System Science Software Ecosystem

From Silos to an Ecosystem

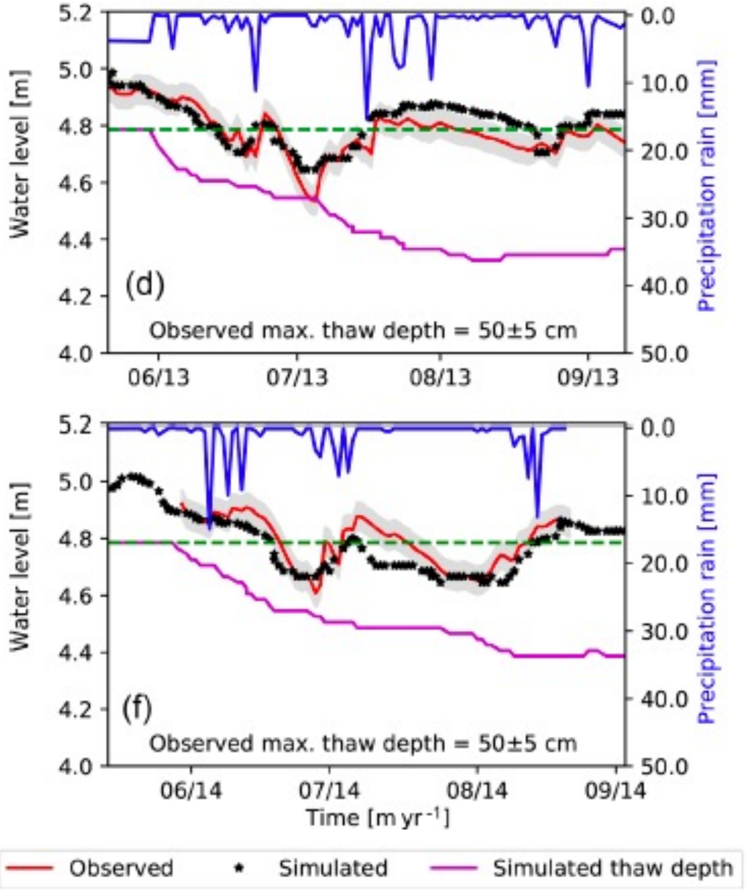


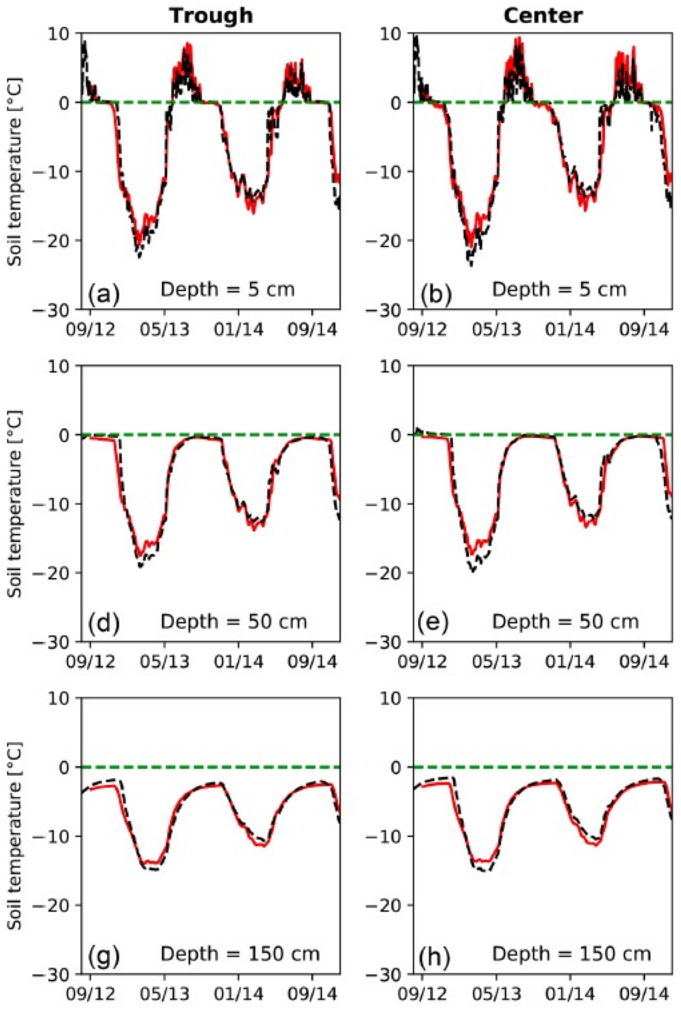
Software Ecosystem 2015 -

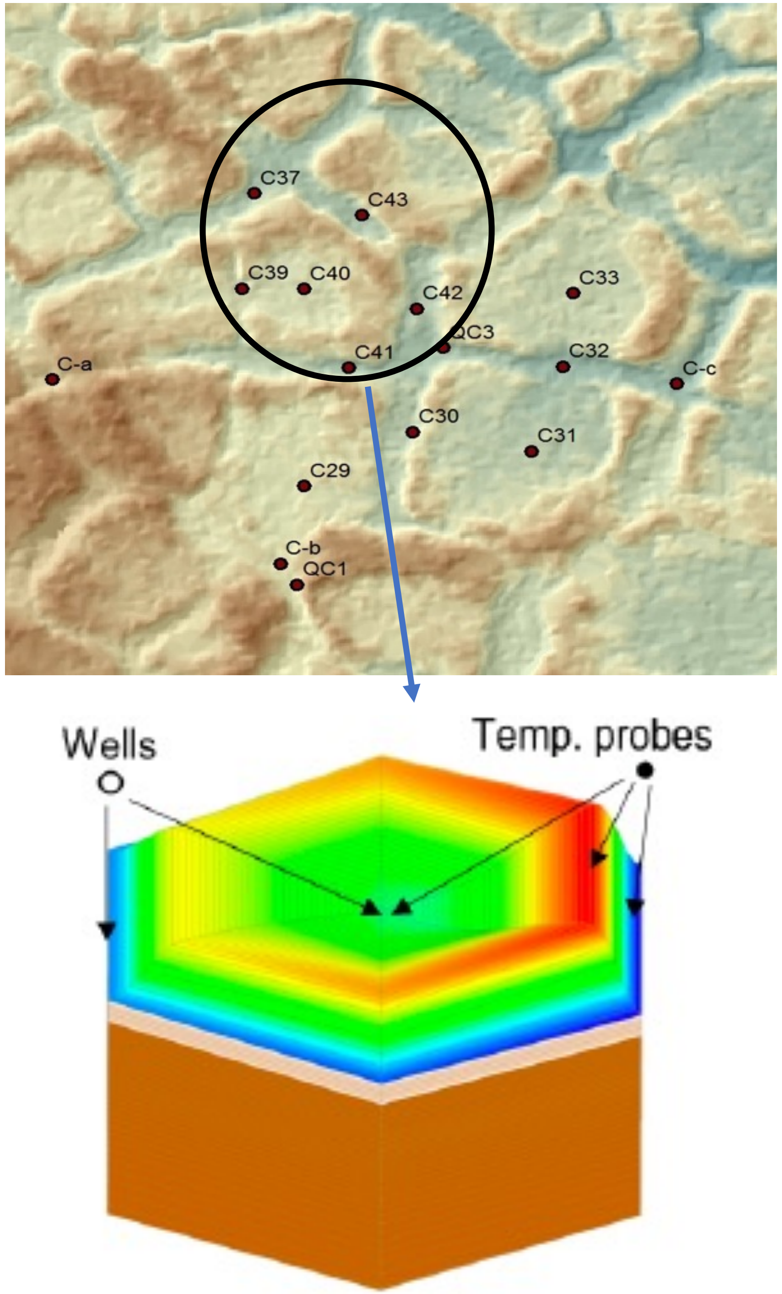
AMANZI ATS

Comparisons to field observations

Jan et al. 2020







2020 R&D 100 Award

Amanzi–ATS: Modeling Environmental Systems across Scales

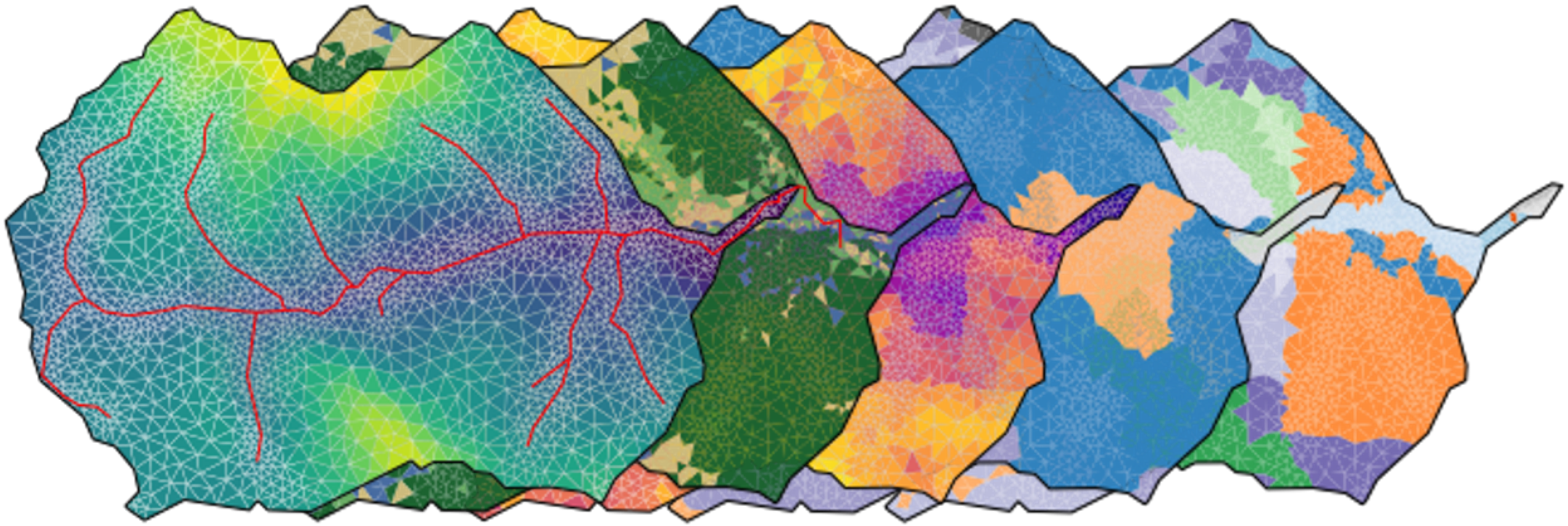
Established in 1963, the R&D 100 Awards is the only S&T (science and technology) awards competition that recognizes new commercial products, technologies and materials for their technological significance that are available for sale or license. The R&D 100 Awards have long been a benchmark of excellence for industry sectors as diverse as telecommunications, high-energy physics, software, manufacturing, and biotechnology. This year's R&D 100 2020 winner is listed below in their respective category.

R&D 100 AWARDS

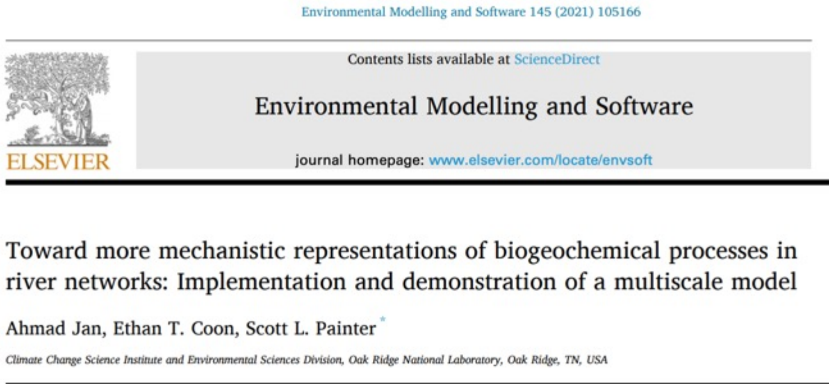
Watershed Workflow

Greatly accelerates construction of ATS input by pulling from multiple national data products

2019-2021

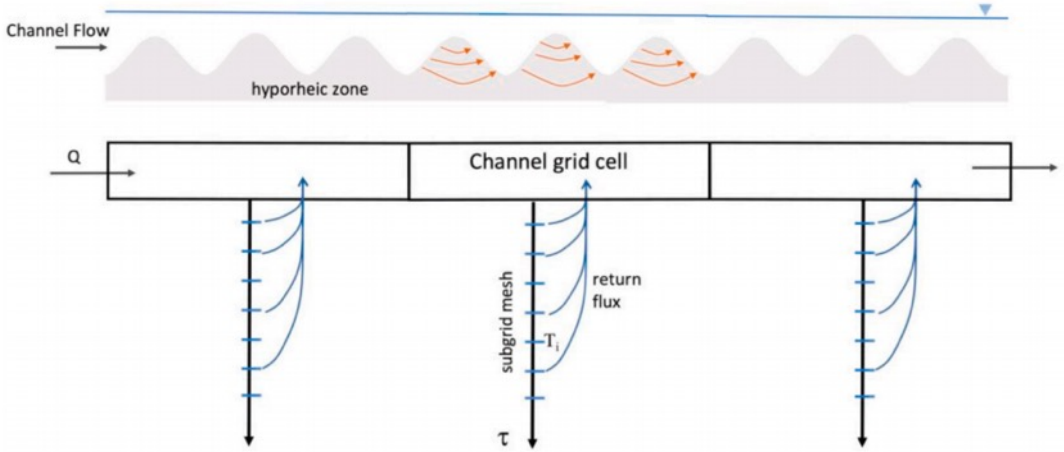


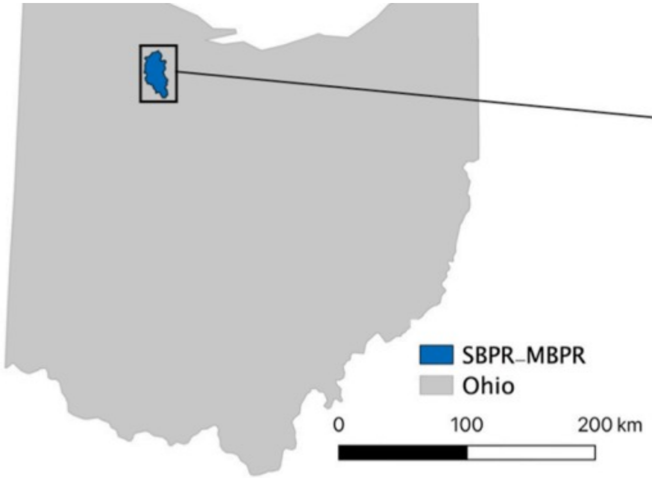
Multiscale model for reactive transport in river networks

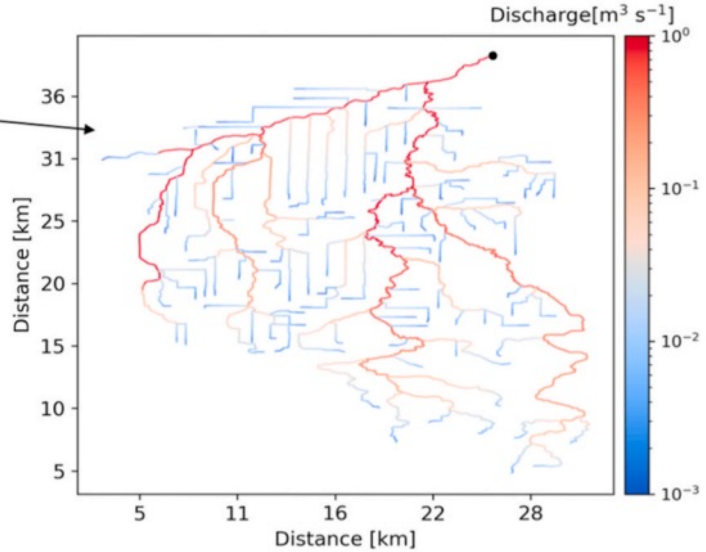

Environmental Modelling and Software 145 (2021) 105166
Contents lists available at ScienceDirect
Environmental Modelling and Software
journal homepage: www.elsevier.com/locate/envsoft
ELSEVIER

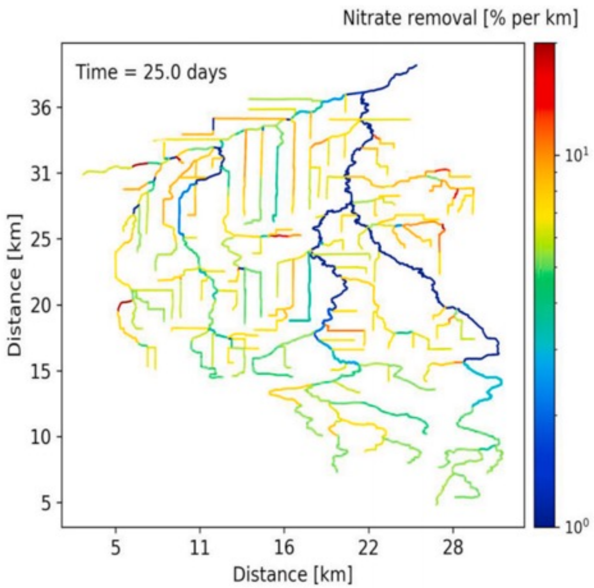
Toward more mechanistic representations of biogeochemical processes in river networks: Implementation and demonstration of a multiscale model

Ahmad Jan, Ethan T. Coon, Scott L. Painter *
Climate Change Science Institute and Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA





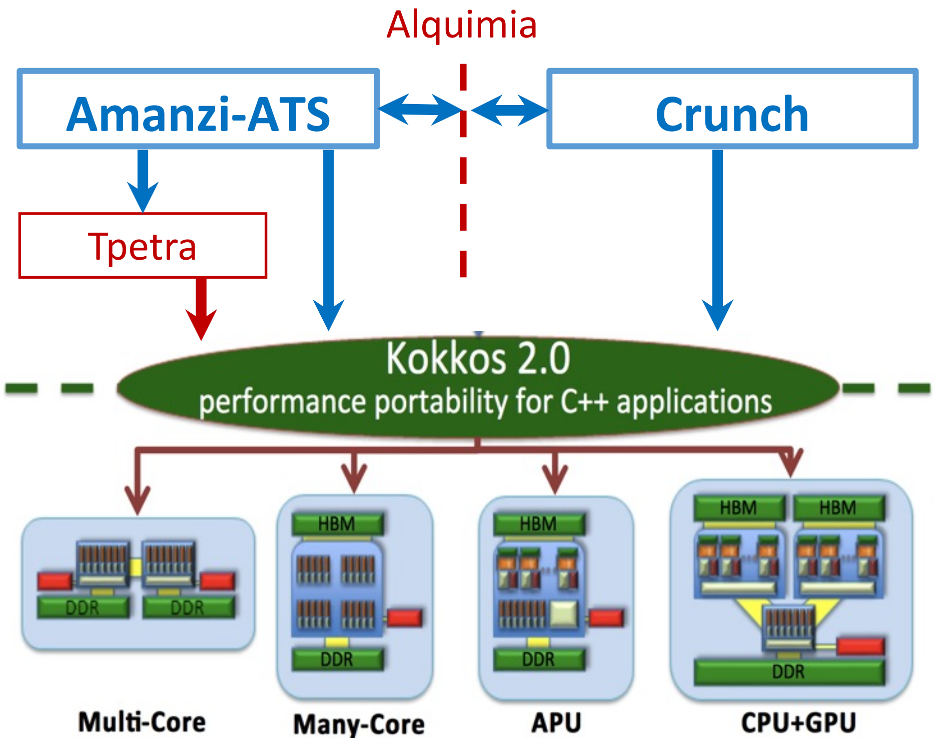




AMANZI ATS

Ongoing development

- Improved canopy biophysics
- Salinity transport and density driven flow
- Sediment transport
- Improvements to multiscale reactive transport
- Support for heterogeneous architectures GPU/CPU
- Watershed-based hybrid parallelization strategy



How to cite

Amanzi

Moulton, J. D., et al. "High-level design of Amanzi, the multi-process high performance computing simulator." *Office of Environmental Management, United States Department of Energy, Washington DC* 495 (2012).

https://github.com/amanzi/amanzi

ATS

E.T. Coon, M. Berndt, A. Jan, D. Svyatsky, A.L. Atchley, E. Kikinzon, D.R. Harp, G. Manzini, E. Shelef, K. Lipnikov, R. Garimella, C. Xu, J.D. Moulton, S. Karra, S.L. Painter, E. Jafarov, and S. Molins. 2020. Advanced Terrestrial Simulator. U.S. Department of Energy, USA. Version 1.0. DOI: 10.11578/dc.20190911.1

Citing key capability

Multiphysics. Coon et al. 2016. Managing complexity in simulations of land surface and near-surface processes. Environmental Modelling and Software

Mesh infrastructure. Garimella et al. 2014. Mesh Infrastructure for Coupled Multiprocess Geophysical Simulations. Procedia Engineering. 82. 10.1016/j.proeng.2014.10.371.

Integrated surface/subsurface flow. Coon et al. 2020. Coupling surface flow and subsurface flow in complex soil structures using mimetic finite differences. Advances in Water Resources

Permafrost and freeze/thaw. Painter et al. 2016. Integrated surface/subsurface permafrost thermal hydrology: Model formulation and proof-of-concept simulations. Water Resources Research

Multiscale Arctic and multiscale in general. Jan et al. 2018. An intermediate-scale model for thermal hydrology in low-relief permafrost landscapes. Computational Geosciences

Comparisons to observations. Jan et al. 2020. Evaluating integrated surface/subsurface permafrost thermal hydrology models in ATS (v0. 88) against observations from a polygonal tundra site. Geoscientific Model Development

Multiscale reactive transport. Jan et al. 2021. Toward more mechanistic representations of biogeochemical processes in river networks: Implementation and demonstration of a multiscale model. Environmental Modelling and Software

Alquimia. https://bitbucket.org/berkeleylab/alquimia

Integrated surface/subsurface reactive transport. In prep.

See https://amanzi.github.io/references for complete list

Opportunities to join the ATS development team at ORNL

Computational scientist/hydrologist

https://career-hcm20.ns2cloud.com/sfcareer/jobreqcareer?jobId=6403&company=utbattelleP

Postdoctoral researcher in computational watershed science

paintersl@ornl.gov

Concepts & Fundamentals

Ethan Coon
Oak Ridge National Laboratory

Amanzi–ATS is a Multiphysics Model

(not a *hydrologic model* or *reactive transport* model)

Rarely is the process certain.

There is no “best model.”

*Alan Kay

ATS is a Multiphysics Model

*"Simple things should be simple;
complex things should be possible."*

- An extremely customizable set of tools for combining components to form environmental models.
- A rich set of demos illustrating commonly used models.

ATS is a Multiphysics Model

(not a *hydrologic model* or *reactive transport* model)

No "modes" – models are assembled from components

- Representing almost any model concept is possible
- Input files are verbose and buggy

Process Kernel (PK)

A single differential equation, on a single domain,

(subsurface, surface, fractures, canopy)

often representing conservation of a single quantity.

(mass, energy, chemical component C)

- Subsurface flow (conservation of water in the soil)
- Surface transport (conservation of C in the stream)
- Snow (conservation of water in the snowpack)

Process Kernel (PK)

Implement an interface related to time integration

- Setup()
- Initialize()
- while not done:
  - get_dt()
  - AdvanceStep()
  - CommitStep()

Multi-Process Couplers (MPCs)

PKs are coupled together via MPCs.

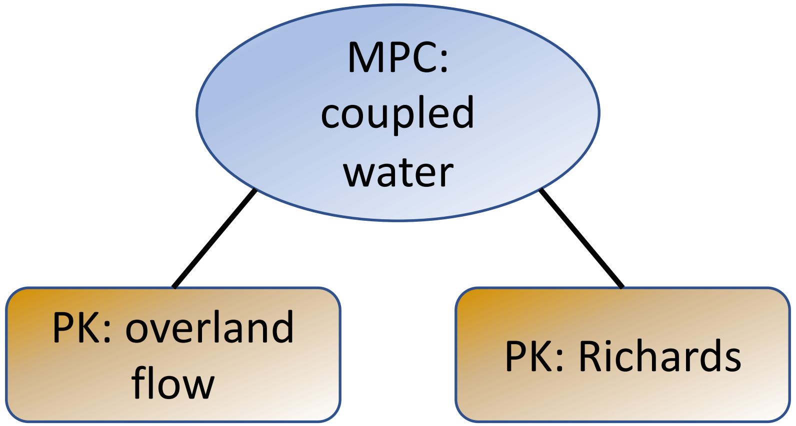
- MPCs *are* PKs themselves
- MPCs can couple other MPCs
- *Abstract* MPCs
  - *weak* MPC: sequential, noniterative
  - *strong* MPC: globally implicit
  - *Subcycling* MPC: subcycle one PK relative to another
- *Custom* MPCs: know about the physics of their PKs

Process Kernel Tree

PK: Richards

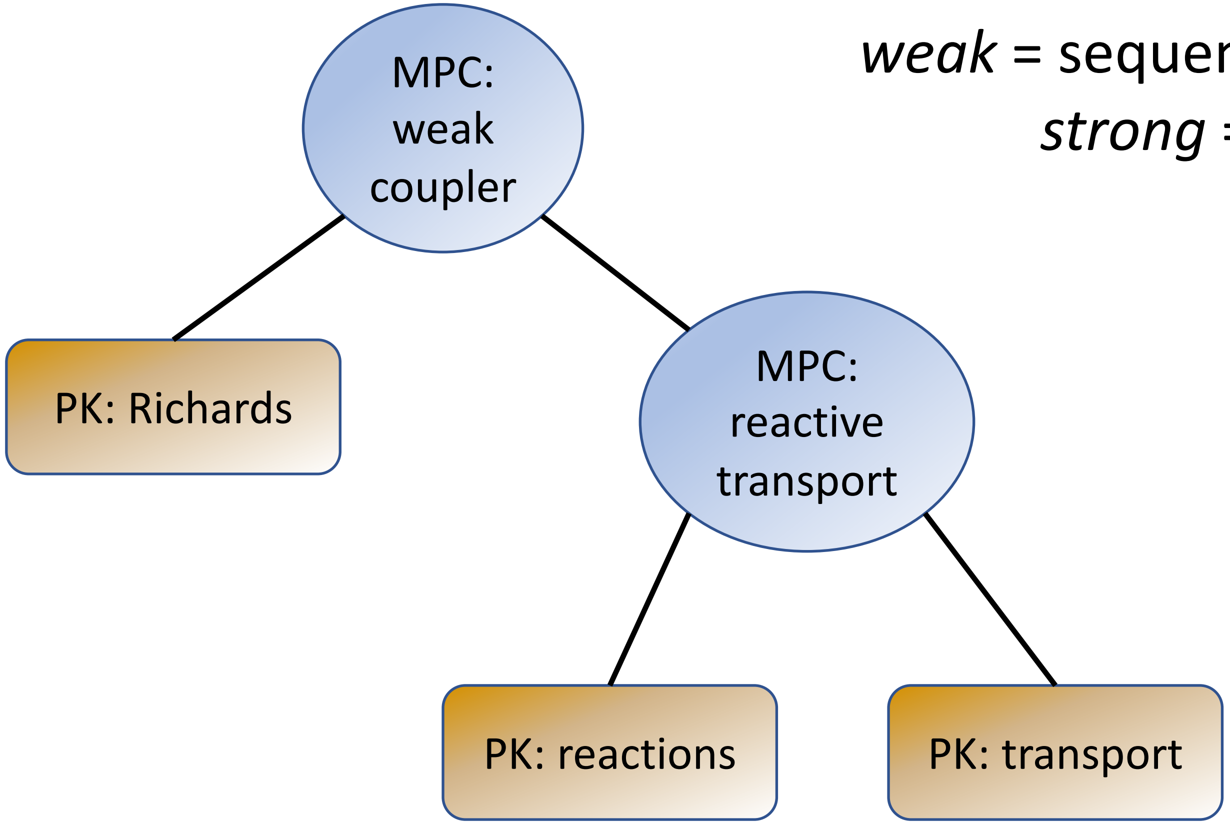
Process Kernel Tree

Integrated Hydrology

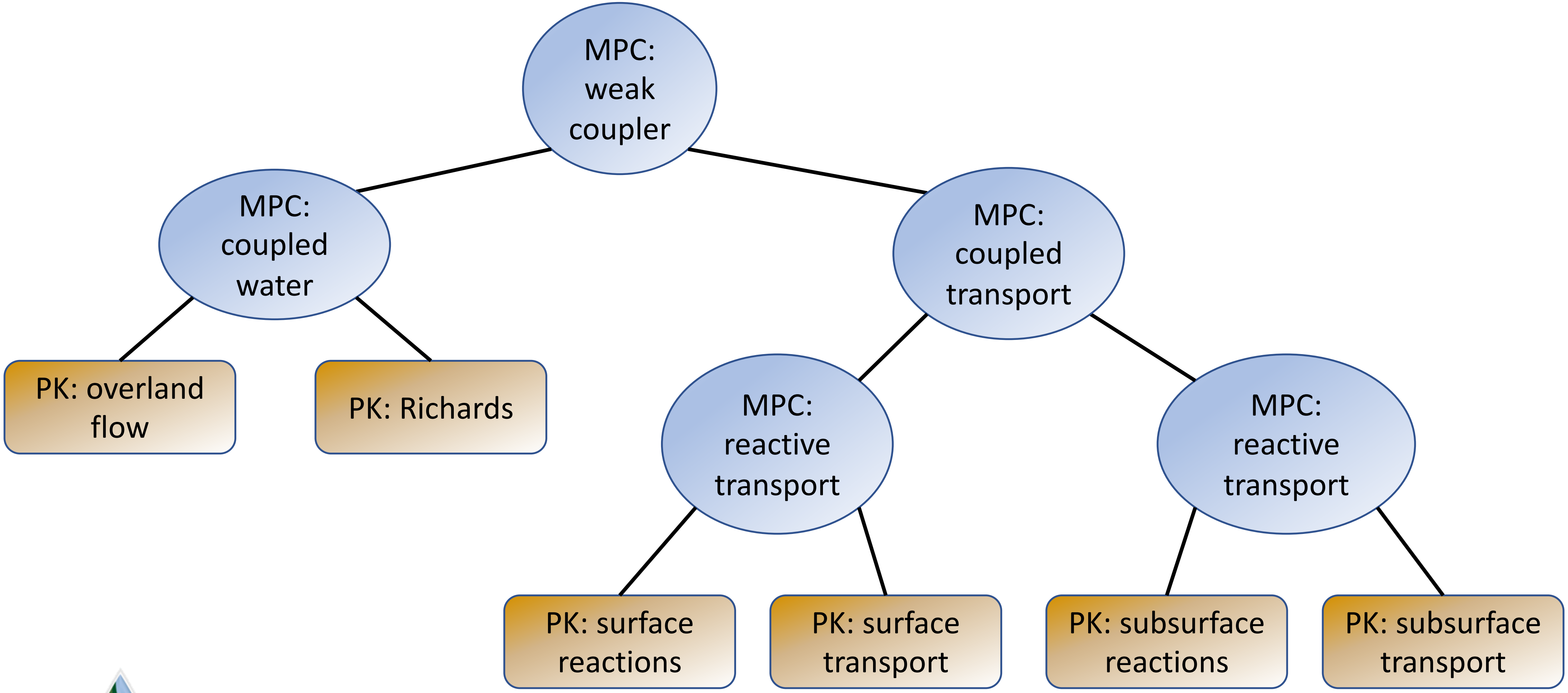


Process Kernel Tree Subsurface Flow + Reactive Transport

weak = sequential, noniterative
strong = globally implicit

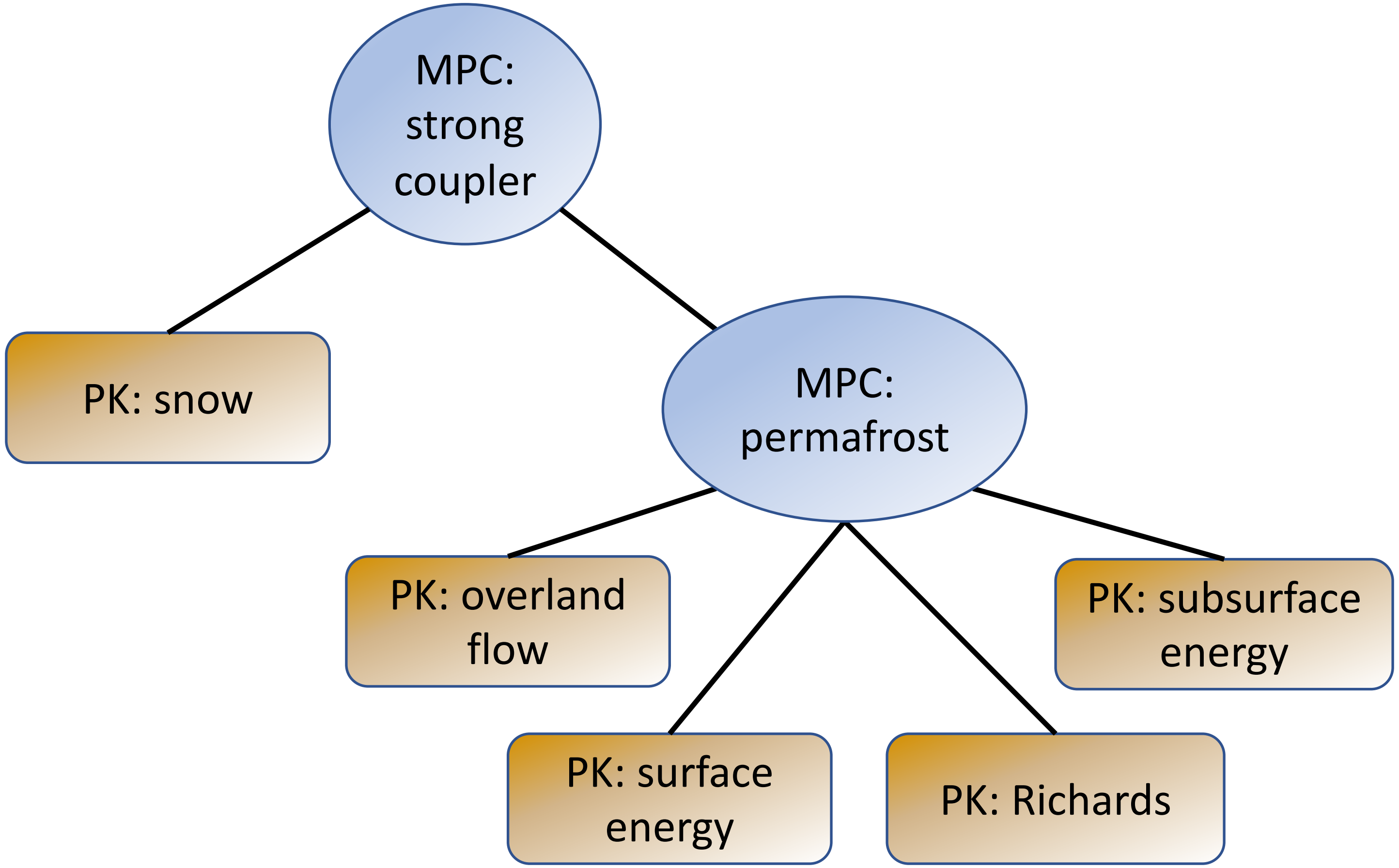


Process Kernel Tree Integrated Flow + Reactive Transport

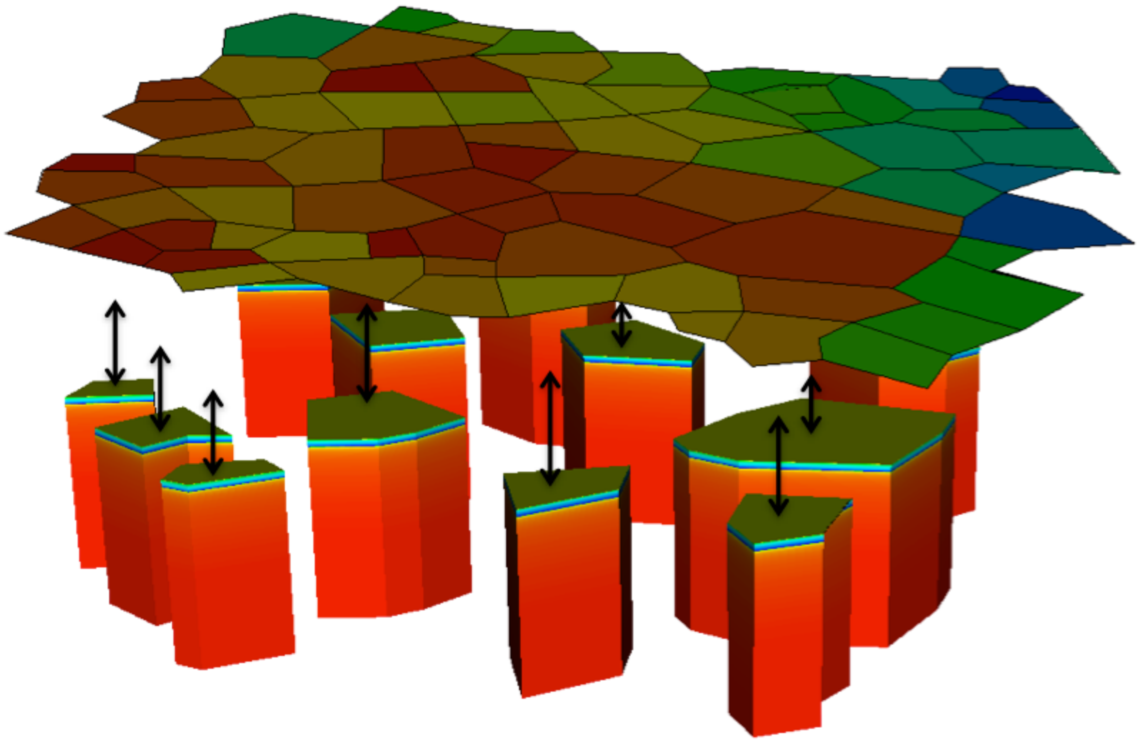


Process Kernel Tree

Arctic Hydrology



Process Kernel Tree



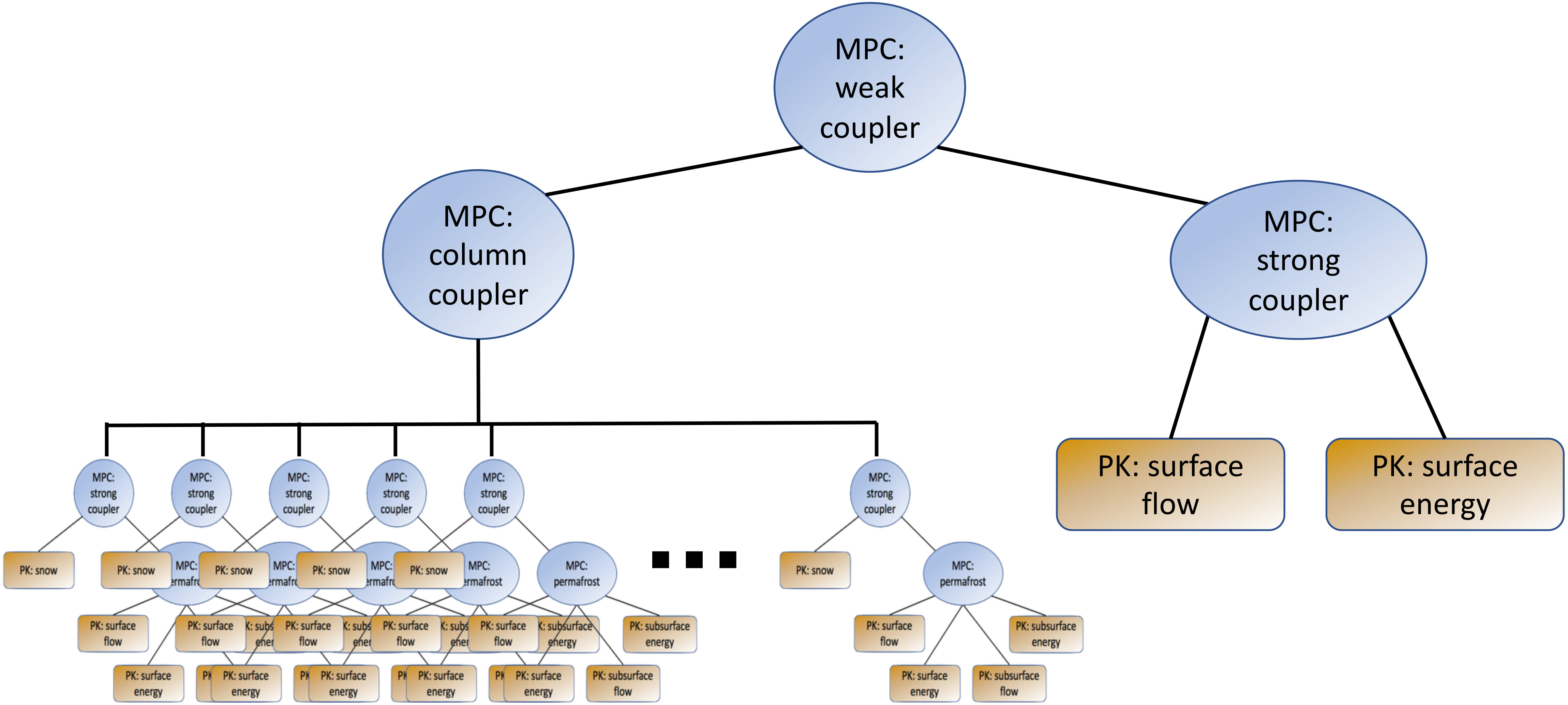
Polygonal Tundra Model

Ina Timling, North Slope, Alaska

Konstanze Piel, Lina River Delta, Siberia

Process Kernel Tree

Polygonal Tundra Model



Process Kernels & Multi-Process Couplers

Why?

- *Flexibility & Rapid development*
  Create new models from existing parts by writing custom couplers.
- *Code Reuse*
  One PK means one place to add features and fix bugs.
- *Better Testing*
  Test in isolation, then test while coupled.

Dependency Graph

- PKs are made up of many *terms* or *variables* in an equation
- Each term is a point of customization or process uncertainty.
- Conceptually, each term in an equation is one of:
  - Primary variable – the variable to be solved
  - Independent variable – data provided by the user
  - Secondary variable – a function of other variables
  - Residual – a secondary variable representing the misfit or error of an equation, given a value of the primary variables.

Dependency Graph

Richards' Equation

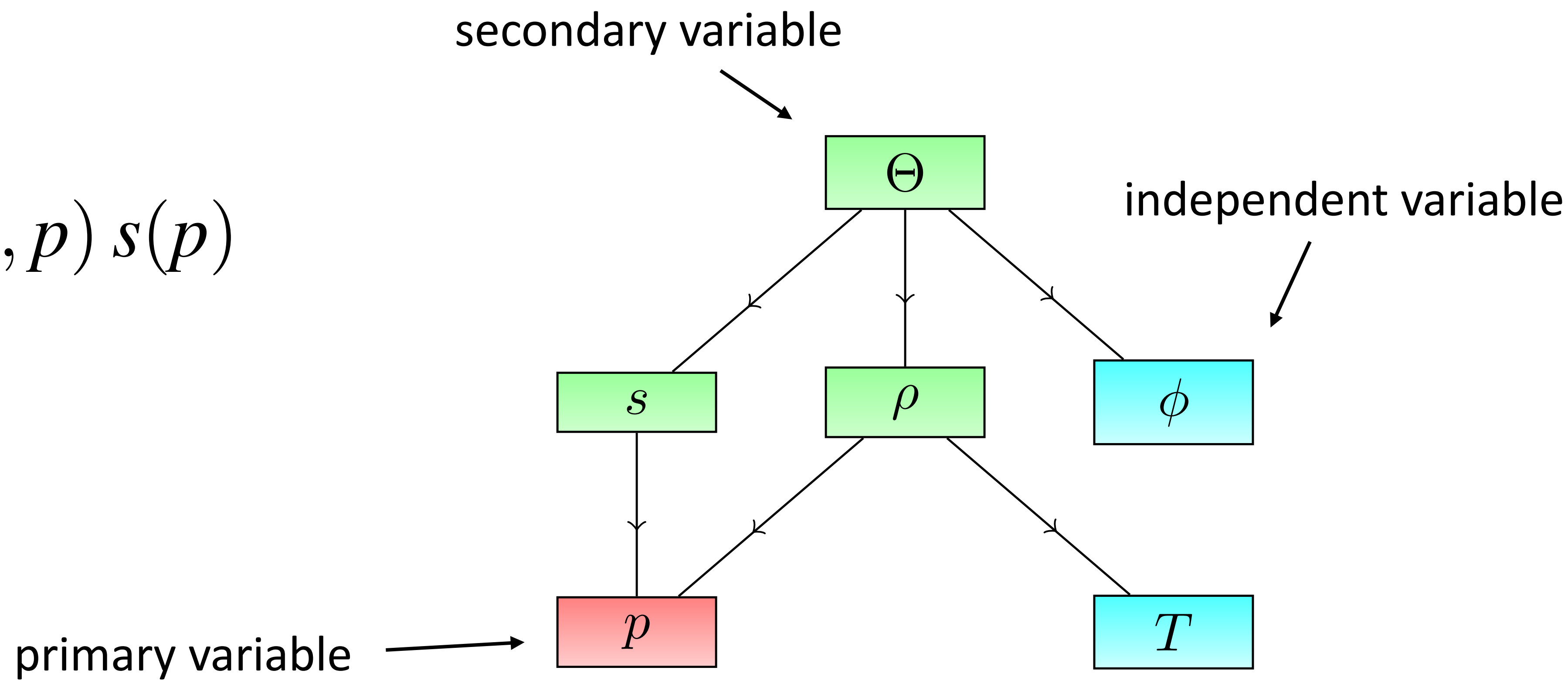
$$\frac{\partial \Theta}{\partial t} = -\nabla \cdot q + Q$$

Constitutive Equation

$$\Theta = ?$$

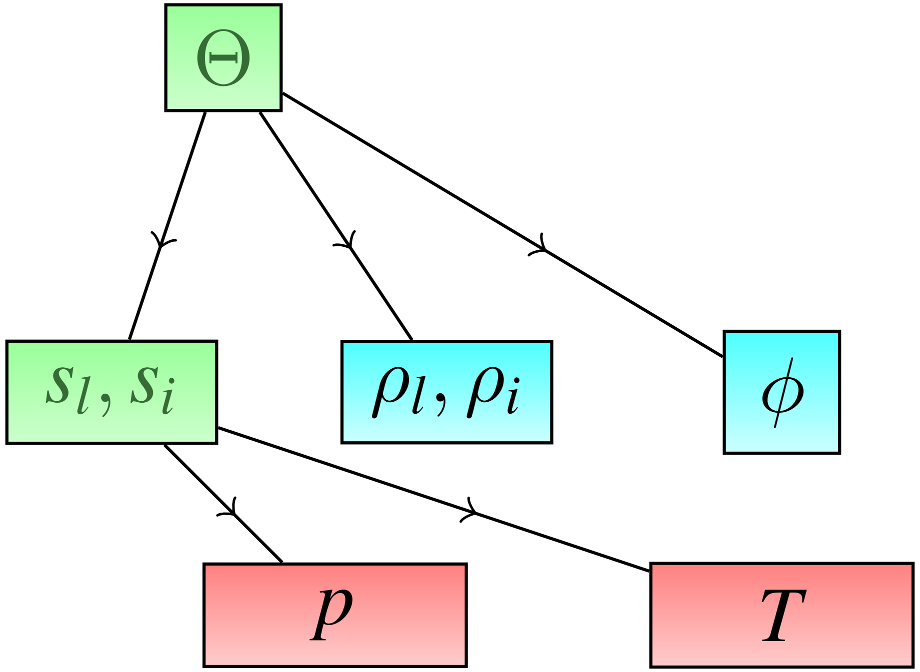
Dependency Graph

$$\Theta = \phi\, \rho(T,p)\, s(p)$$



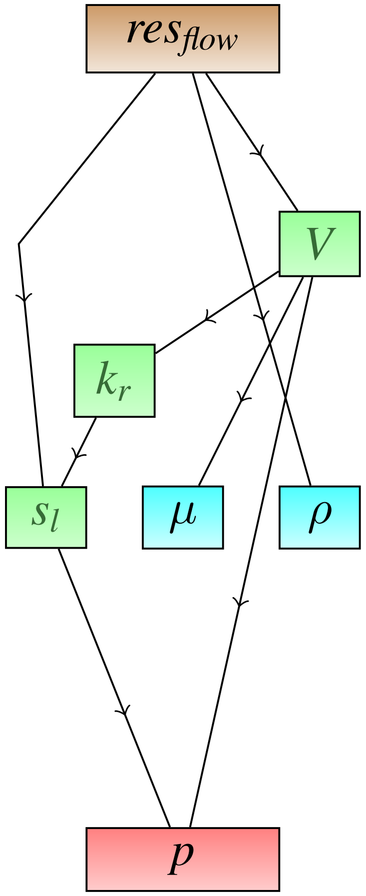
Dependency Graph

$$\Theta = \phi \left[\rho_l \, s_l(p,T) \; + \rho_i \, s_i(p,T)\right]$$

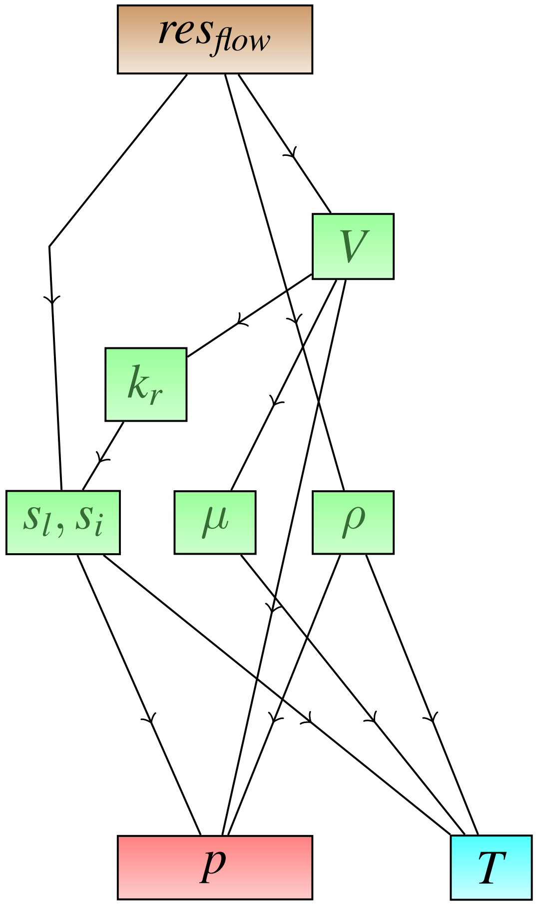


Dependency Graph

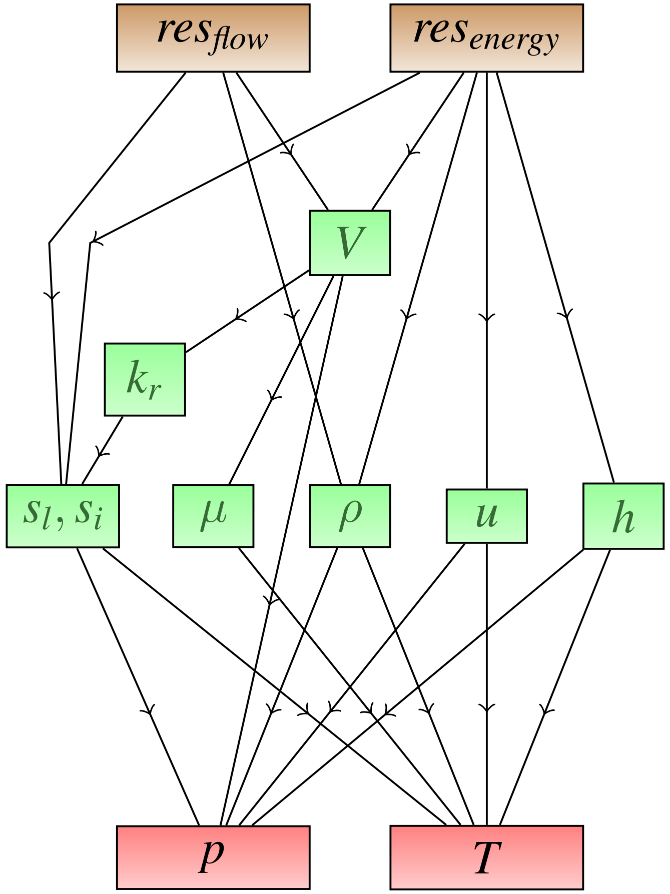
Richards' equation



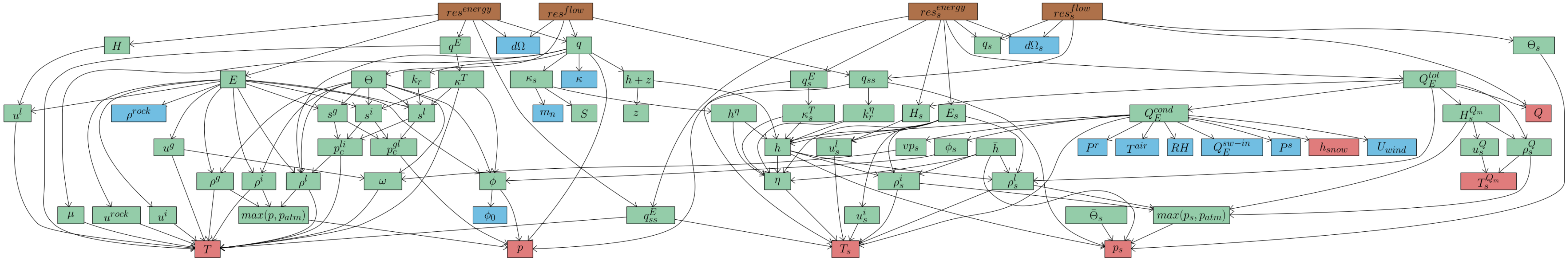
Nonisothermal Richards' equation



Richards' + Energy equations



Dependency Graph: Evaluators



- *Evaluator*: A class representing one node in the dependency graph.
- Each evaluator only knows about its direct children.
- A dependency graph is *directed* and *acyclic.*

*Coon et al, Env. Model. Soft 2016

Dependency Graph

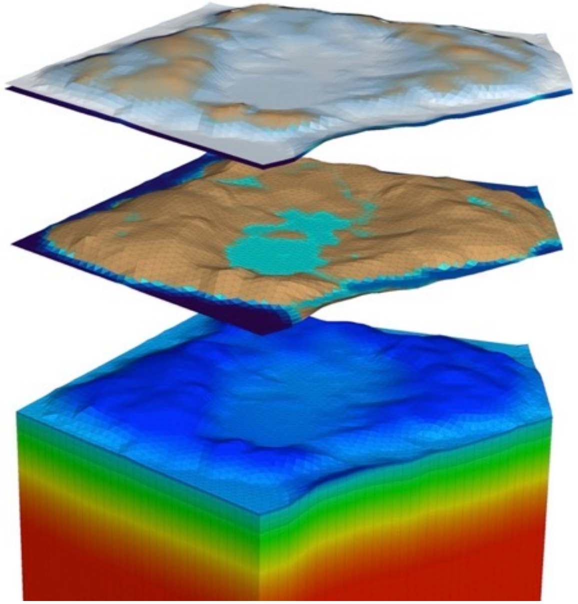
Why?

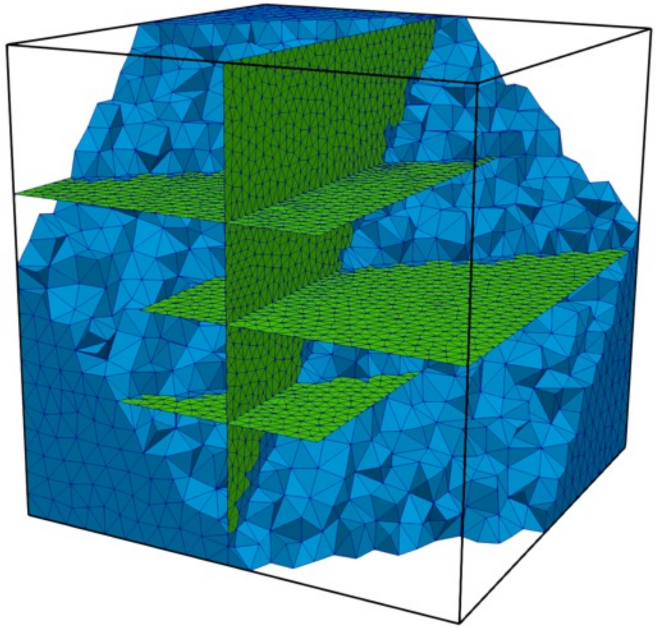
- *Flexibility & Rapid development*
  Create new models from existing parts by adding new evaluators.
- *Code Reuse*
  Multiple PKs may reuse the same evaluator.
  (density of water on the surface vs density of water in the subsurface)
- *Better Testing*
  Test in isolation, then test as a part of PKs.
- Potential for *task-based parallelism*.

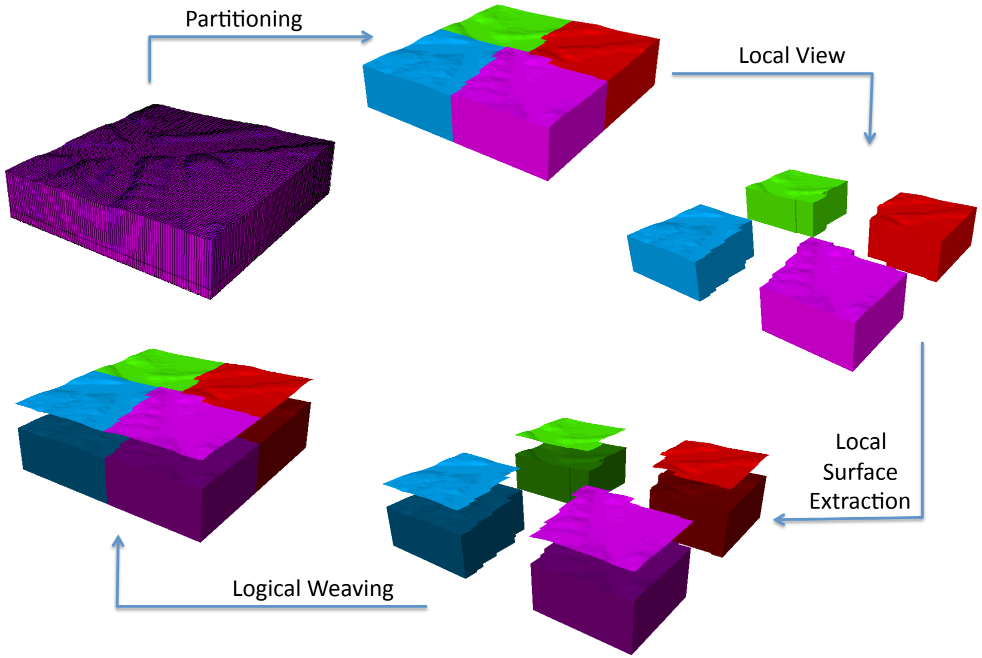
Model Domain: Mesh

*Garimella et al, Procedia Eng. 2014

- Domain = conceptual, Mesh = concrete, discrete representation
- Unstructured meshes (though often "extruded, terrain following")
- Arbitrary polyhedra, pinch-outs, co-planar faces, etc.
- Derived meshes (extracted columns, surface meshes)







Model Domain: Regions

- Geometric subsets of the domain (point, plane, box, boundary, labeled set)
- Used to specify materials/model parameters, initial and boundary conditions, etc.
- Region + Mesh + Entity type → Set of Entities

Simulation Control: Cycle Driver

- ***Cycle***: a single timestep that advances all PKs in time by a uniform step size dt.
- ATS typically uses a variable timestep size
  - Often controlled by nonlinear solver performance
  - "Failure" of the code: time step size → 0
- Cycle driver controls the simulation:
  - begin and end time
  - end cycle, end wallclock duration
  - Ensures vis, checkpoint, observations happen as required
- Includes the PK tree

Model I/O: Checkpoint/Restart

- Checkpoint:
  - Files that contain all needed information to continue a simulation
  - Read by the code, not by the user
  - HDF5 file format
- Restart:
  - In the "cycle driver" list, set the option:
    `"restart from checkpoint file"="/path/to/checkpoint.h5"`
  - No other changes to the input file – ATS reads the time, timestep size, etc from the checkpoint file and continues the run.
  - *Nearly* identically to how your run stopped (identically is WIP)

Model I/O: Visualization

- Sparse in time, dense in space
- Store all variables (by default) on time slices
- Store values at all cells (but only cells) so can be big
- XDMF + HDF5:
  - read natively by VisIt or ParaView
    ats_vis_data.VisIt.xmf or ats_vis_DOMAIN_data.VisIt.xmf
  - Python reader: $ATS_SRC_DIR/tools/utils/ats_xdmf.py
- Silo:
  - read natively by VisIt or Paraview
  - Required for arbitrary polyhedral meshes

Model I/O: Observations

- Dense in time, sparse in space
- Selected by the variable name, a region, and time slices
- Accumulated on regions: average, min, max, integral, extensive integral (sum)
- "time integrated" option allows for better tracking of fluxes
- CSV text files read via pandas, Excel, others.

Input File

- xml – intended to be read by machines, not people
- Nested `ParameterList` correspond to classes in the code
- Input parameters are [documented]()
  - Reasonably well, getting better all the time…
  - Converters between release versions at: `$ATS_SRC_DIR/tools/input_converters`
- Never written from scratch – start from a demo or test
- Learn your tools: fold and manipulate as XML (not text)

Input File

```xml
<ParameterList name="Main" type="ParameterList">
  <ParameterList name="mesh" type="ParameterList">...</ParameterList>
  <ParameterList name="regions" type="ParameterList">...</ParameterList>

  <ParameterList name="cycle driver" type="ParameterList">...</ParameterList>

  <ParameterList name="PKs" type="ParameterList">
    <ParameterList name="water balance" type="ParameterList">...</ParameterList>
    <ParameterList name="snow storage" type="ParameterList">...</ParameterList>
    <ParameterList name="surface-subsurface coupler" type="ParameterList">...</ParameterList>
    <ParameterList name="flow" type="ParameterList">...</ParameterList>
    <ParameterList name="overland flow" type="ParameterList">...</ParameterList>
  </ParameterList>

  <ParameterList name="state" type="ParameterList">
    <ParameterList name="field evaluators" type="ParameterList">...</ParameterList>
    <ParameterList name="initial conditions" type="ParameterList">...</ParameterList>
  </ParameterList>

  <ParameterList name="checkpoint">...</ParameterList>
  <ParameterList name="visualization">...</ParameterList>
  <ParameterList name="observations" type="ParameterList">...</ParameterList>
</ParameterList>
```

Variable Naming (in Vis, Obs)

Template for variable names:

<DOMAIN>-<VARIABLE>.<COMPONENT>.<DoF>

Examples:

- pressure.cell.0
- surface-ponded_depth.face.0
- surface-total_component_concentration.cell.NO3-

Units

- By default, all units are SI and, when they appear in documentation or the input spec, appear in brackets: [m], [s], [mol], [kg], [K], [Pa], [J], [W]
- Derived units are spelled out without division, e.g. [mol s^-3] NOT [mol / m^3]
- Exceptions: Energy [MJ]
- Amanzi–ATS includes processes for density-driven flows (ice vs water, salinity):
  - pressure (not head)
  - water content in mols of H2O (not m^3)
  - permeability (not hydraulic conductivity)
- Concentration in mol ratio [$mol_C \, mol_{H20}^{-1}$], similar to molality