STUDENT SUMMER INTERNSHIP TECHNICAL REPORT

Development of an Integrated Hydrology Spinup Model for the F-Area of Savannah River Site with the ALTEMIS Project

DOE-FIU SCIENCE & TECHNOLOGY WORKFORCE DEVELOPMENT PROGRAM

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EXECUTIVE SUMMARY

This research work has been supported by the DOE-FIU Science & Technology Workforce Development Initiative, an innovative program developed by the U.S. Department of Energy's Office of Environmental Management (DOE-EM) and Florida International University's Applied Research Center (FIU-ARC). During the summer of 2023, a DOE Fellow intern, Aubrey Litzinger, spent ten weeks doing a summer internship at Lawrence Berkeley National Lab (LBNL) under the supervision and guidance of Dr. Zexuan Xu and Dr. Haruko Wainwright. The intern's project was initiated on June 5, 2023, and continued through August 11, 2023, and was focused on working under the ALTEMIS project to develop an understanding of the workflow, input requirements, and tools required to perform hydrology simulations with a new version of ATS, version 1.3, and develop a spinup model for the F-Area of Savannah River Site using high-performance computing.

The Department of Energy (DOE) has identified a knowledge gap in understanding the behavior and movement of pollutants in the surface and subsurface at the various DOE sites across the DOE Complex and their potential consequences for human health and the environment, particularly in the highly braided wetland stream systems characteristic of the Savannah River Site (SRS). To address this concern, the Advanced Long-Term Environmental Monitoring Systems (ALTEMIS) project was created to establish an overarching framework of long-term monitoring at DOE sites by systematically combining state-of-the-art hardware and software technologies. The ALTEMIS project is currently focused on the integration of field observations, AI/ML techniques, and high-resolution modeling to better understand the fate and transport of contaminants and the potential long-term impacts of low-level radioactive waste that was discharged into the SRS F-Area subsurface via a number of seepage basins and is slowly migrating towards the surrounding wetlands and potentially the Fourmile Branch stream system. Understanding the fate and transport of the contaminants within the riverbeds and groundwater of the F-Area is crucial in remediating the area.

The summer internship at LBNL was focused on the high-resolution modeling component of the ALTEMIS project for the F-Area. The intern was able to generate an integrated hydrology spinup model for the F-Area using ATS version 1.3 and achieve steady-state conditions within the model. Constant meteorological forcings and multiple process kernels that control the equations of the model were used and the model was visualized and analyzed using the water balance equation.

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1. INTRODUCTION

The Department of Energy (DOE) has identified a knowledge gap in understanding the behavior and movement of pollutants and their potential consequences for the ecosystem, specifically within DOE's complex. To address the concern, the Advanced Long-Term Environmental Monitoring Systems (ALTEMIS) project was created to establish the overarching framework of long-term monitoring at DOE's legacy sites by systematically combining state-of-art hardware and software technologies. The ALTEMIS project strives to develop an innovative monitoring methodology that combines in-situ observations, artificial intelligence, machine learning techniques (AI/ML), and high-resolution modeling. This integrated approach will yield fresh perspectives that will create an inventive strategy for both remediation and long-term monitoring throughout the DOE Complex.

The DOE's Savannah River Site (SRS) in South Carolina contributed to the production of nuclear weapons material from 1955 and 1988, in which one-third of the weapons-grade plutonium and all the nation's tritium were produced at the site (Savannah River Nuclear Solutions LLC, 2023). During this time, low-level radioactive waste was discharged into three unlined seepage basins within the F-Area, known as the F-Area Seepage Basins (see Figure 1). The waste discarded contained the radioactive contaminants, tritium, uranium, and plutonium isotopes, strontium-90, cesium-137, technetium-99, and iodine-129, while also containing acidic solutions of nitrates, sodium hydroxide (NaOH), and metals. Almost two billion gallons of the waste was discharged into the F-Area Seepage Basins. The goal of the seepage basins was to contain the waste within the soils beneath the basin, yet the radionuclides and heavy metals mobilized through the vadose zone into the groundwater saturated zone. The contaminants have migrated downslope into the braided wetland system of Fourmile Branch watershed. To mitigate the environmental impact of these contaminants, DOE-EM has implemented many remediation methods, for example barrier walls.. However, the contaminants are still present in the groundwater as well as the riverbeds of the braided wetland system, which can potentially be harmful to human health and the environment if released into the Fourmile Branch stream network.

Figure 1. Map of SRS in South Carolina, with the F-Area highlighted in yellow (F) (Savannah River Nuclear Solutions LLC, 2023).

Extreme weather events, like intense precipitation, and long-term changes in climate are anticipated to impact the hydrological exchange between the hillslope, seepage face, and braided riparian wetland system, which may impact the release of contaminants within the F-Area at SRS. Understanding the fate and transport of the containments within the riverbeds and groundwater of the F-Area site is crucial in remediating the area. The ALTEMIS project has focused on addressing the knowledge gap related to the fate and transport containments and the potential long-term impacts of the discarded waste through the integration of field observations, AI/ML techniques, and high-resolution modeling.

During this internship, the focus was on the high-resolution modeling component of the ALTEMIS project for the F-Area for which the Advanced Terrestrial Simulator (ATS) is being used. ATS, developed by the Department of Energy's Office of Biological and Environmental Research (DOE BER), is a fully integrated surface/subsurface hydrological model that analyzes surface and groundwater flows. ATS is an ecosystem-based, integrated, distributed hydrology simulator that is built upon the underlying multi-physics framework provided by Amanzi, the high-performance computing simulator (Coon et al., 2016), and naturally integrates with the Advanced Simulation and Capability for Environmental Management (ASCEM) Program. ATS is used to solve coupled surface and subsurface hydrology problems, which may include surface energy balance, snow processes, freeze/thaw processes, dynamic vegetation, and reactive transport processes. ATS uses a process kernel tree, which is comprised of processes and couplers, to help the user represent the model configuration while providing a rigorous mechanism to capture the relationship of all variables, equations, and predefined fields used in the simulation.

When creating a fully integrated hydrological model, the "spinup" stage is a crucial step. The spinup stage occurs after the data is collected for the model and the mesh is generated. A spinup model is used to establish an equilibrium state so that key hydrological variables, such as soil moisture, groundwater levels, and streamflow, reach a consistent and self-sustaining state. The convergence to a stable state can be quantified by the mass balance equation with the amount of water entering the area equaling the amount of water leaving the area. The discharge, total water content, precipitation, and evapotranspiration are typically used to determine when the model has reached a steady state. The spinup does not include temporal data that varies over time, for example, the precipitation, temperature, and other meteorological features are kept constant with time. In the spinup, the hydrostatic head of the model is kept constant, and the water level is chosen at a value that most closely represents the system. These spinups can be run for as little as a decade, but can also be run for over a thousand years depending on the system. The goal of the spinup is to have the hydrological variables relax to a steady state. The spinup data is used as the initial condition for transient conditions so that the model starts at a steady state. Spinup modeling is critical as it helps minimize the effects of initial conditions and transients in future simulations that assess specific details and accurately represent the long-term behavior of the study site (Jiang et al., 2023).

The internship objective was to work under the ALTEMIS project to develop an understanding of the workflow, input requirements, and tools required to perform hydrology simulations with a new version of ATS, version 1.3. High-performance computing (HPC) is a toolset of ATS as it allows the user to perform complex simulations at high speeds due to the ability to utilize parallel processing techniques. During the internship, HPC fundamentals were learned and applied by developing a spinup model using ATS version 1.3 for the F-Area domain. Previously, research conducted at Florida International University (FIU) under the DOE-FIU Cooperative Agreement utilized ATS version 1.2, a prior version of ATS possessing fewer functionalities compared to the enhanced ATS 1.3.

2. RESEARCH DESCRIPTION

2.1 Site Description

The F-Area has complex hydrology and contaminant transport due to the man-made seepage basins, riparian zone, and wetland system. Figure 2 shows a conceptual cross-section of the F-Area, with the inclusion of the groundwater plume originating from the seepage basins. The plume is widespread and deep, contaminating the groundwater one km^2 below the surface. This plume is seen in yellow in Figure 2, with the highly concentrated areas in red. The plume is believed to be discharging into Fourmile Branch through the groundwater, but currently, research suggests that contaminants may also be entering Fourmile Branch through the riparian zone. In the riparian zone, the contaminants are attenuating within the soil, and being transported during high surface flows due to severe weather events to the Fourmile Branch stream system. The orange color in Figure 2 is the Tan Clay confining zone that is in between the upper and lower aquifers of the site.

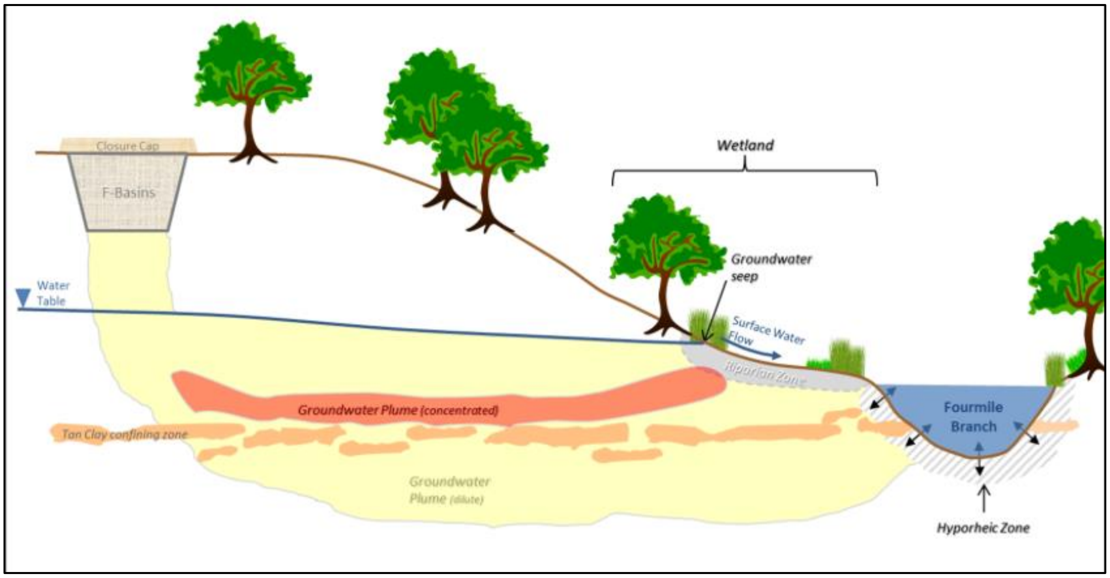

Figure 2. Conceptual cross-section of the F-Area groundwater plume (Eddy-Dilek, C., Kostelnik, K., Denham, M., 2016).

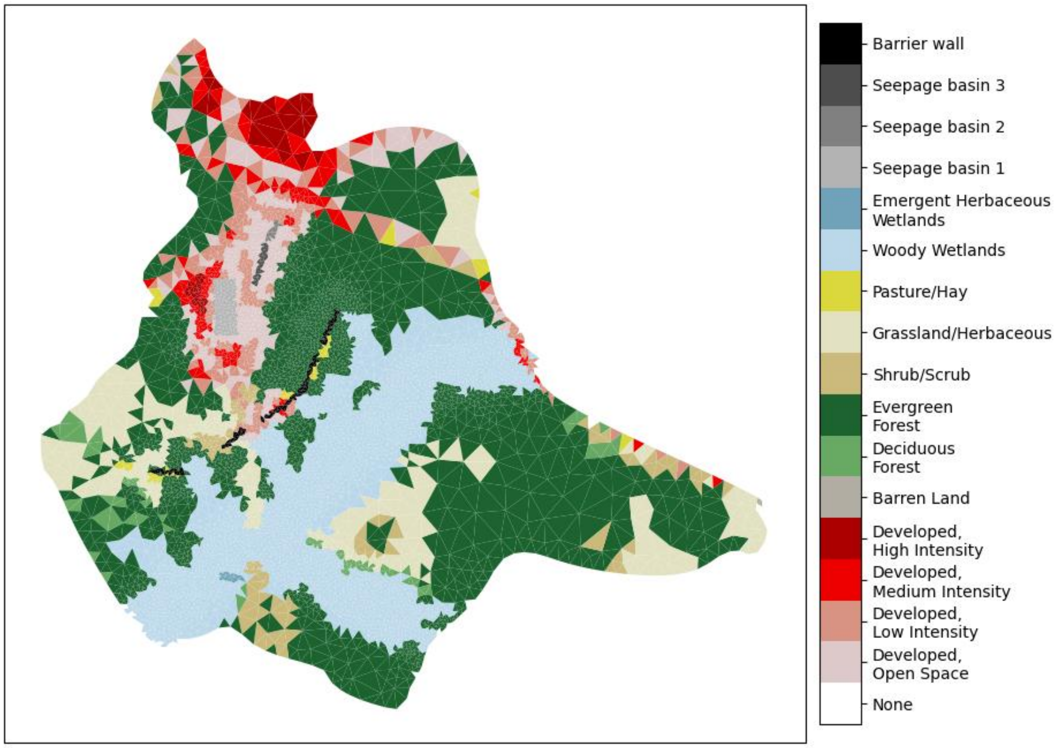

Figure 3. Plot of the F-Area mesh with the national land cover types (NLCD), seepage basins, and the barrier wall displayed.

The F-Area also contains a barrier wall in the upper aquifer of the site, which is not pictured in Figure 2. The subsurface barrier wall is placed before the wetland area displayed in Figure 2. On the surface of the site, there are 13 national land cover types (NLCD), which are displayed in Figure 3. Also included within the same plot are the barrier wall location (black) and the three seepage basins (gray). In addition to the NLCD on the surface, there are soil types provided by SSURGO, which are displayed in Figure 4. Also in Figure 4, are the 3 subsurface layers, the upper and lower aquifer and the tan clay confining zone. These surface and subsurface features were included in the ATS spinup model developed during the summer internship.

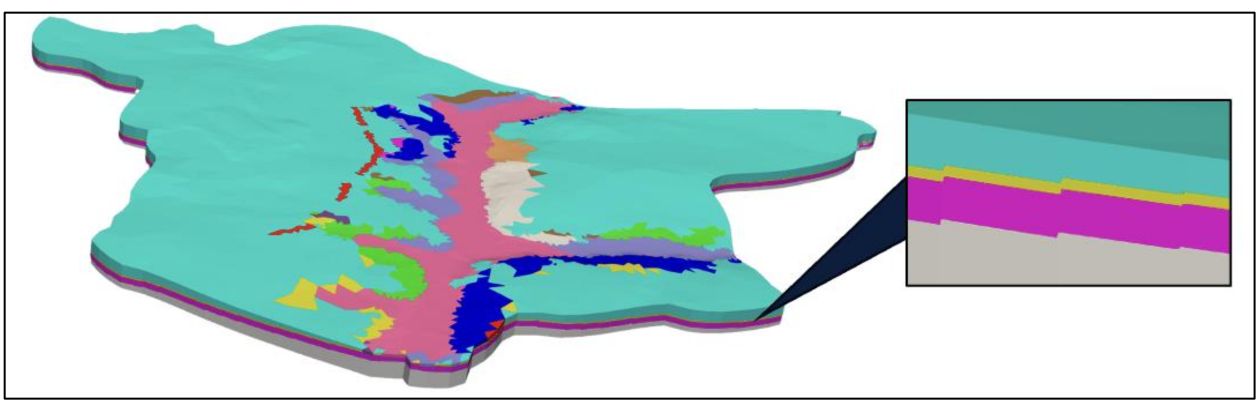

Figure 4. Top: SSURGO soil units, and barrier wall (red). Below SSURGO soil units: upper aquifer (blue), tan clay confining zone (yellow), and lower aquifer (pink) layers, assumed to be rested on top of impermeable layer (gray).

2.2 Workflow for the ATS 1.3 Model Development

The ATS workflow began with the collection and processing of input data. Next, a mesh was generated, followed by an ATS input file. Simulations were then performed using ATS, and the output data visualized and analyzed. This workflow is depicted in Figure 5.

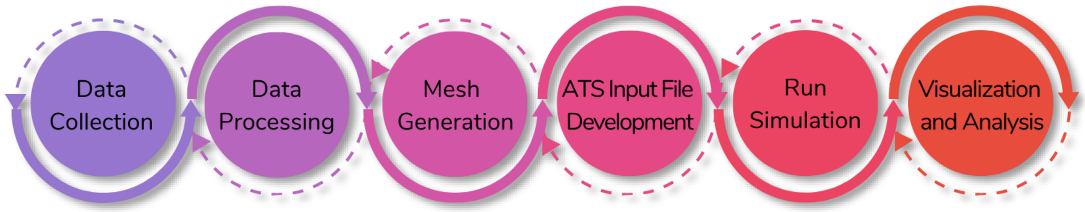

Figure 5. The workflow flows to the right (solid arrows), but issues may arise at any step and result in backtracking to the previous step or require iterations (dashed arrows).

The mesh of the F-Area domain was created with the Python module, Watershed Workflow. Watershed Workflow was developed by Oak Ridge National Lab (ORNL) and was the chosen Python module to create the unstructured, triangulated meshes which were exported as ExodusII files. The ExodusII format allows for geometrical and geophysical information about the site to be encoded into the ATS input file (Livingston, 2020). Watershed Workflow allows for the incorporation of publicly available data into the mesh, like digital elevation maps (DEM), spatial variations in NLCD land cover types, SURRGO soil texture, and GLHYMPS subsurface information. Watershed Workflow also contains a component that allows one to obtain daily atmospheric forcing (precipitation, temperature, radiation) from DayMet, a weather dataset provided by NASA Distributed Active Archive Center (DAAC) at the Oak Ridge National Laboratory. The mesh for the F-Area domain was created at FIU as part of the DOE-FIU Cooperative Agreement prior to the internship, as the objective of the internship was to specifically focus on learning new ATS version 1.3 tools and applications. After the creation of the mesh, an ATS input file was generated. The input file is written in XML format and configures the set of coupled processes for the simulation at run time. This input file also defines all aspects of the hydrological model, such as meteorological data, geometric regions, mathematical equations, boundary conditions, and visualization output. After the simulation was run using the ATS input file described above, visualization files generated during the run were imported into VisIt, a visualization software. VisIt is an open-source, interactive, scalable visualization, animation, and analysis tool developed by the Department of Energy (DOE) Advanced Simulation and Computing Initiative (ASCI). ATS uses unstructured, triangulated meshes to create an integrated hydrology model. The Mimetic Finite Difference (MFD) method accounted for these meshes and couples the surface and subsurface flow. The MFD method is locally conservative and second-order accurate, improving accuracy for local mass conservation. The MFD method aims to maintain elements of the continuum equations within unstructured meshes through discrete approximations. The MFD method uses divergence and gradients to accomplish the goal (Lipnikov et al., 2014).

2.3 F-Area Spinup Model Development

To develop an ATS spinup model for the F-Area, an ATS input file was created during the internship. The goal of the spinup model, as described in the introduction, is to create steady-state conditions within the model. To achieve this goal, a hydrological model was developed using the F-Area mesh shown in Figure 3 and Figure 4, in which the simulation was to model 30 years using constant meteorological forcings like the SRS climate. These meteorological forcings are displayed in Table 1. Meteorological Forcing Parameters for the F-Area Spinup ModelTable 1. Below is an outline of the structure of the ATS input file created for the spinup. The most fundamental component of the ATS input file is the Process Kernel (PK) Tree. The PKs represent a single or system of Partial Differential Equations (PDEs) or Differential Algebraic Equations (DAEs). PKs with singular equations are known as physical PKs and Multi-Process Coordinators (MPCs) are systems of equations that couple other PKs and sometimes other MPCs. The combination of these physical PKs and MPCs creates the PK tree that forms the fundamental definition of the entire system of equations to be solved by ATS. Figure 6 shows the PK tree for the F-Area spinup model (Amanzi, 2023).

The following significant sections of the input file were defined in this model:

1. The mesh in ExodusII format
2. The regions within the mesh:
    a. NLCD
    b. A barrier wall and three seepage basins
    c. SURRGO soil regions
    d. GLHYMPS subsurface layers
3. The cycle driver that determines the simulation time
4. The process kernel tree (PK tree) which details each PK and multi-process coupler (MPC) used, such as:
    a. PK Tree (Weak MPC)
        i. Integrated Hydrology PK (Strong MPC)
            1. Overland Physical PK
            2. Flow Physical PK
        ii. Canopy PK
        iii. Snow PK
5. Some of the state and field evaluators that define variables relating to the area, such as:
    a. Water table level
    b. Water sources (canopy throughfall drainage, snow melt, and surface evaporation)
    c. Surface ponded water depth
    d. Evapotranspiration
    e. Snow melt
    f. Canopy drainage
    g. Precipitation
    h. Surface temperature
    i. Surface overland conductivity
    j. Surface manning coefficient
    k. Van Genuchten parameters, porosity, and permeability for soil types
    l. NLCD parameters
6. Directions for the generation of visualization output files
7. Observations that allow for a more in-depth analysis of variables
8. Checkpoints for status on the simulation run

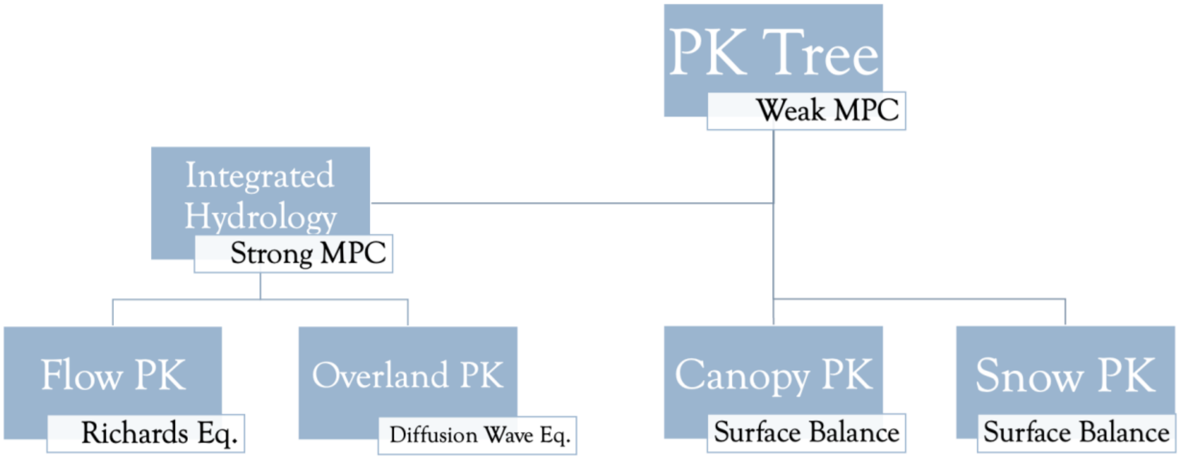

Figure 6. The PK tree for the F-Area spinup input file with the MPCs used and equations present in the PKs.

Figure 6 shows the PK tree that was used in the spinup model for the F-Area. This PK tree uses four physical PKs: Flow PK, Overland PK, Canopy PK, and Snow PK. The overall PK tree couples these equations with a weak MPC, and then the Flow PK and Overland PK are coupled by a strong MPC to create the integrated hydrology model component. The Canopy and Snow PKs add complexity to the integrated hydrology PK by the addition of evapotranspiration and other integral components of a hydrology model. The Canopy PK and Snow PK use a simple vector of ordinary differential equations (ODEs), where the time derivative of a conserved quantity is determined by sources and sinks (Amanzi, 2023).

For the flow PK seen in Figure 6, Richard's equation for variably saturated flow (subsurface) and a diffusion wave approximation for the overland flow PK (surface) are used in ATS. The surface flow (overland PK) uses Equation 1, the conservation of water equation (Coon et al., 2020).

$$\frac{\partial h}{\partial t} + \nabla s \cdot h\vec{q}_s = Q_e + Q_{ss} \qquad \mathbf{(1)}$$

$$h = depth\ of\ ponded\ water\ on\ the\ surface\ (m)$$

$$\nabla s = two\ dimensional\ surface\ gradient\ \left(\frac{1}{m}\right)$$

$$\vec{q}_s = two\ dimensional\ flux\ field\ \left(\frac{m}{s}\right)$$

$$Q_e = rainfall\ (\frac{m}{s})$$

$$Q_{ss} = infiltration\ flux\ from\ subsurface\ (\frac{m}{s})$$

For the subsurface flow, a mixed form of Richard's equation is used to generate robust numerical solutions and maintain mass balance for unsaturated flow problems. Equation 2 shows Richard's equation and Equation 3 shows the Darcy flux equation used within Richard's (Coon et al., 2020).

$$\frac{\partial}{\partial t}(\phi s \eta) + \nabla \cdot (\eta \vec{q}\,) = Q_w \qquad \textbf{(2)}$$

$t = time\ (s)$

$\phi = porosity\ (-)$

$s = water\ saturation\ (\frac{m^3}{m^3})$

$\eta = molar\ water\ density\ (\frac{kmol}{m^3})$

$\vec{q}\ = Darcy\ Flux\ (\frac{m}{s})$

$Q_w = source\ or\ sink\ of\ water\ (\frac{kmol}{m^3 s})$

Below is Equation 3. The Darcy flux found in Equation 2 is calculated with Darcy's Law.

$$-\frac{1}{\mu} K_r K(\nabla p \cdot \rho \vec{g}) = \vec{q} \qquad \textbf{(3)}$$

$\vec{g}\ = vector\ of\ gravity\ (\frac{m}{s^2})$

$\vec{q}\ = darcy\ flux\ (\frac{m}{s})$

$p = water\ pressure\ (Pa)$

$K = absolute\ permeability(\ m^2\ )$

$K_r = relative\ permeability$

$\mu = dynamic\ viscosity\ (Pa \cdot s)$

$\rho = mass\ density\ of\ water\ (\frac{kg}{m^3})$

This version of Richard's equation uses pressure and water content to allow variable density. Some variables within Equation 2 are solved with the standard van Genuchten-Maulem approach. Two MPCs were used in the PK tree, a weak MPC that combines the integrated hydrology PK with the canopy and snow PK. Then a strong MPC was used within the integrated hydrology PK to couple the surface and subsurface equations. The weak MPC is for sequential coupling where noniterative sequential coupling takes place. The strong MPC within the integrated hydrology PK completes globally implicit coupling that solves all PKs as a single system of equations (Amanzi, 2023). When coupling the surface and subsurface equations, pressure and water flux were continuous, and including surface ponded depth was a key factor. Pressure is one of the primary sources to connect the surface and subsurface equations. The coupling of these equations creates a set of nonlinear parabolic equations, in which the MFD method is then used to discretize the equations with the introduction of Lagrange multipliers on the mesh face. An essential component in ATS modeling is the time steps, which are introduced after the MFD method (Coon et al., 2020).

A seepage face boundary condition was added to the surface flow PKs in the input file. This boundary condition allows water (ex. Runoff) to leave the f-area domain when saturation is present. This boundary condition was chosen as it is one of the simpler conditions in the ATS model and is a good starting point for the spinup model.

For the spinup model to reach a steady state, constant meteorological forcings are used, which are written into the ATS input file. Table 1 displays the values used for the spinup model.

Table 1. Meteorological Forcing Parameters for the F-Area Spinup Model

Parameter	Value	Unit
Precipitation: Rain	1.13e-8	m/s
Precipitation: Snow	0	m SWE / s
Air Temperature	290.6	K
Air Vapor Pressure Incoming Shortwave Radiation	1492.43 175.58	Pa W/m^2

3. RESULTS AND ANALYSIS

3.1 Analysis of the Spinup Model

After the input file was developed for the spinup model of the F-Area with the help of the ALTEMIS project work, the simulation was run with ATS version 1.3 on the Lawrence Berkeley National Lab (LBNL) High-Performance Computer (HPC) called the Lawrencium. The ATS input file was uploaded to the Lawrencium, along with the mesh generated by Watershed Workflow and a script was created that allowed ATS version 1.3 to be run using multiple cores in parallel. The result was a spinup model that reached a steady state at approximately 16.5 years (6,000 days), while the entire simulation ran for 30 years. To simplify the spinup, the evapotranspiration was set to zero so it would not interfere with the steady-state water balance as a spinup model is the simplest form of modeling methodology. To determine if the spinup reached a steady state, a global water balance equation was used, as seen in Equation 4.

$$\frac{\partial WC}{\partial t} = P + S - ET - Q \qquad \textbf{(4)}$$

$WC = Total\ global\ water\ content$

$P = Precipitation\ of\ rain$

$S = Precipitation\ of\ snow$

$\mathrm{ET} = Total\ evapotranspiration\ across\ all\ PKs$

$Q = Surface\ water\ runoff$

Since evapotranspiration (ET) and snow (S) were equal to zero in the spinup model, the model converges when rain (P) is equal to surface runoff (Q). The convergence happens around 6,000 days as seen in Figure 7.

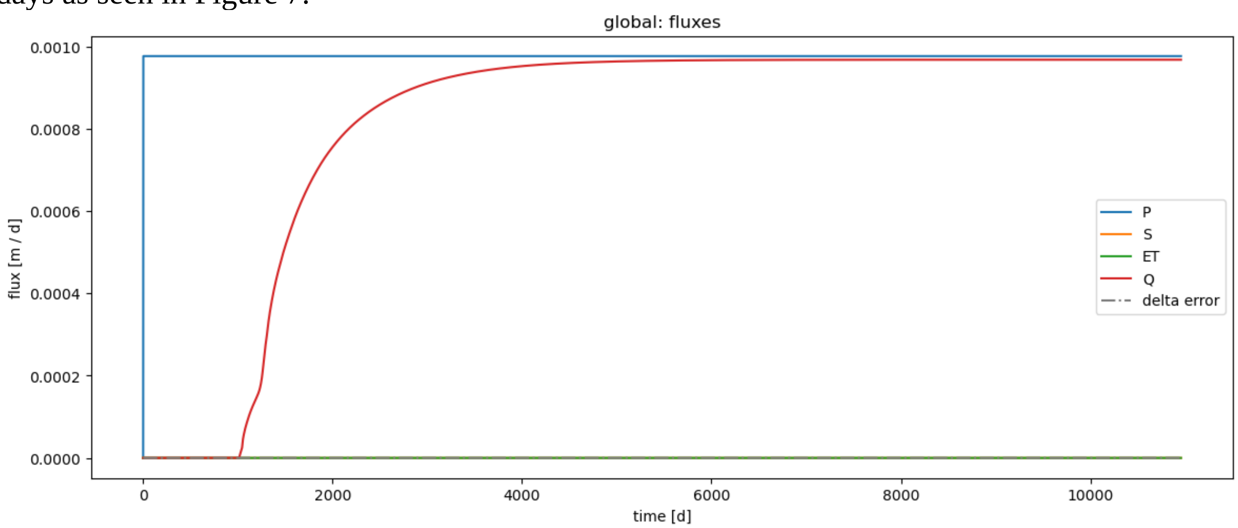

Figure 7. Graph of the water balance from the F-Area spinup model with the flux (m/d) of rain, snow, evapotranspiration, runoff, and the error plotted versus time (d).

The runoff and precipitation converged with a flux of 0.001 meters per day. The cumulative flux for the variables was also calculated and graphed in Figure 8.

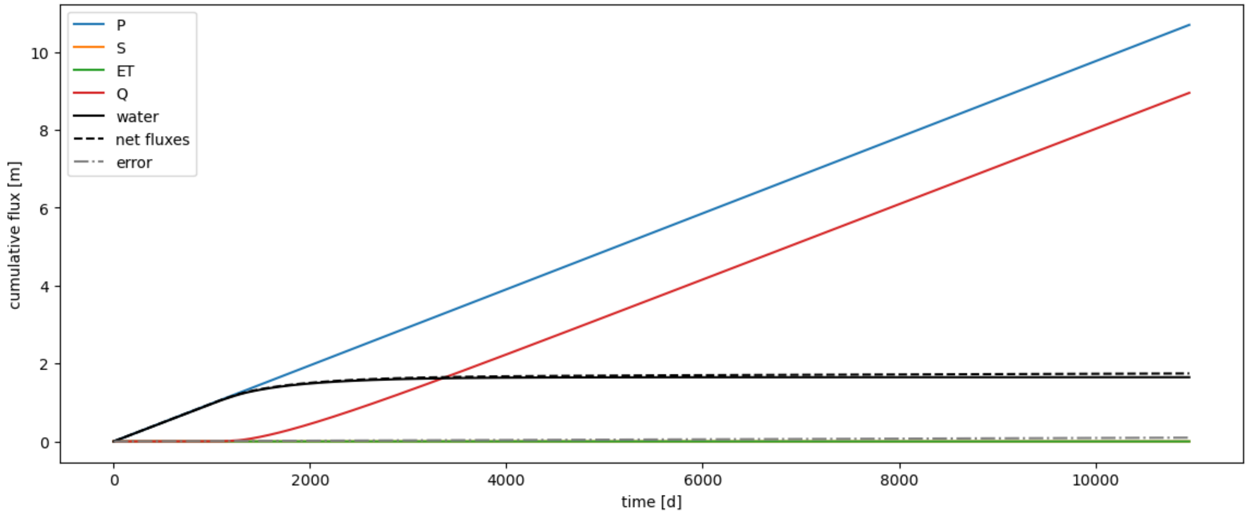

Figure 8. Graph of the water balance from the F-Area spinup model with the cumulative sum of fluxes (m) for rain, snow, evapotranspiration, runoff, and the error plotted versus time (d).

In Figure 8, the cumulative flux in meters was plotted for each of the variables, and since evapotranspiration (ET) and snow (s) were zero in the spinup model they are zero in the graph as seen in Figure 7. The rain and runoff converge around 6,000 days in Figure 7, and in Figure 8 one can see they both steadily increase at the same rate when comparing their cumulative fluxes. The water in Figure 8 stays constant as the amount of water entering and leaving is the same once the spinup reaches a steady state.

3.2 Visualization of the Spinup Model

Visualization occurred after the ATS input file was run in the terminal. ATS generates multiple visualization files that can be opened in VisIt. During the internship, the surface ponded depth and subsurface liquid saturation were the most common fields visualized with these tools. In Figure 9, one can see the F-Area watershed visualized with VisIt. The figure displays an image from a video simulation at the 10th year of the spinup model simulation out of 30 years, with a steady state occurring around the 16th year. The surface layer was given a customized color scheme used by the ALTEMIS group. This color table is used to show the ponded depth of water along the surface after precipitation. The brown represents no ponded water along the surface, and the darker the blue color, the more water is ponded. The surface layer was transformed upward in the z-direction for the visualization to show what is happening in the subsurface for saturation. The subsurface was given a separate custom color scheme used by the ALTEMIS group that displays the level of subsurface liquid saturation. A brown-yellow color resembles no saturation and green-blue shows saturation.

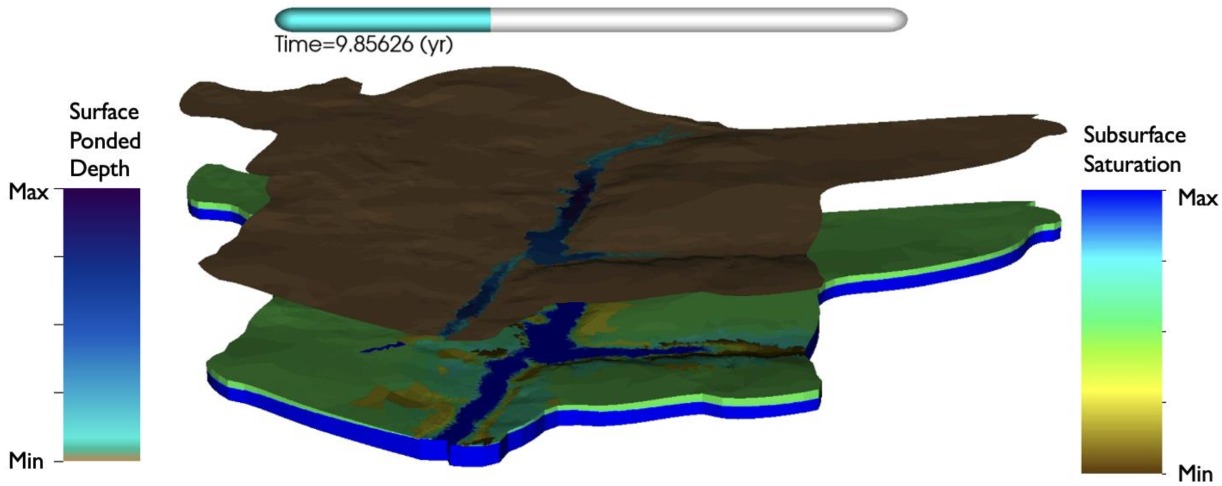

Figure 9. Image from a video simulation of the F-Area spinup model at year 10 in which the surface ponded water depth (top) and the subsurface saturation (bottom) are shown with a color table.

Figure 9 shows that most water ponds and infiltrates the subsurface at the lowest elevation point within the main stream channel of Fourmile Branch near the F-Area. Along the stream, there are soil types that are less saturated than others, potentially due to the different soil characteristics within the area. The steady-state conditions in the spinup model start occurring around year 10 and officially converge around year 16. The visualization shows the beginning of the convergence as there is a clear formation of a stream with consistent runoff and subsurface saturation. The visualization verifies the results from the graphs in Figure 7 and Figure 8.

4. CONCLUSION

In conclusion, the result of this internship at Lawrence Berkeley National Laboratory was the development of a spinup model for the F-Area with guidance from DOE-EM scientists working on the ALTEMIS project and available resources. The DOE Fellow developed a greater understanding of ATS version 1.3, the modeling process, and the purpose of the ALTEMIS project. Knowledge of the fundamentals of hydrology modeling was also gained, such as the importance of a spinup model and the mathematical and hydrological principles behind developing models. The concepts learned while working with the ALTEMIS team during the summer internship will be applied to the work being conducted at Florida International University's Applied Research Center that requires hydrological modeling and the use of High-Performance Computing (HPC) to perform DOE-related research. Figure 10 is a picture of DOE Fellow, Aubrey Litzinger, during her internship at LBNL this summer.

Figure 10. DOE Fellow, Aubrey Litzinger, at LBNL this summer.

5. ACKNOWLEDGEMENTS

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6. REFERENCES

Amanzi. (2023). *GitHub*. Retrieved from https://amanzi.github.io/ats/index.html

Savannah River Nuclear Solutions LLC. "About the Savannah River site." *Savannah River Nuclear Solutions*, 26 May 2023, https://www.savannahrivernuclearsolutions.com/about/about_srs.htm.

Coon, E. T., Moulton, J. D., Kikinzon, E., Berndt, M., Manzini, G., Garimella, R., Lipnikov, K., & Painter, S. L. (2020). Coupling surface flow and subsurface flow in complex soil structures using mimetic finite differences. *Advances in Water Resources*, *144*, 103701. https://doi.org/https://doi.org/10.1016/j.advwatres.2020.103701

Jiang, P., Shuai, P., Sun, A., Mudunuru, M. K., & Chen, X. (2023). Knowledge-informed deep learning for hydrological model calibration: an application to Coal Creek Watershed in Colorado. *Hydrol. Earth Syst. Sci.*, *27*(14), 2621-2644. https://doi.org/10.5194/hess-27-2621-2023

Lipnikov, K., Manzini, G., & Shashkov, M. (2014). Mimetic finite difference method. *Journal of Computational Physics*, *257*, 1163-1227. https://doi.org/https://doi.org/10.1016/j.jcp.2013.07.031

Eddy-Dilek, C., Kostelnik, K., Denham, M., 2016. *The Challenge of Moving Science into Practice: Lessons Learned and New Approaches.* Full paper in the Waste Management Symposia proceedings, Phoenix, Arizona.