***PFLOTRAN-E4D: A parallel open source PFLOTRAN module for
simulating time-lapse electrical resistivity data***

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Abstract

Time-lapse electrical resistivity tomography (ERT) is finding increased application for remotely monitoring processes occurring in the near subsurface in three-dimensions (i.e. 4D monitoring). However, there are few codes capable of simulating the evolution of subsurface resistivity and corresponding tomographic measurements arising from a particular process, particularly in parallel and with an open source license. Herein we describe and demonstrate an electrical resistivity tomography module for the PFLOTRAN subsurface flow and reactive transport simulation code, named PFLOTRAN-E4D. The PFLOTRAN-E4D module operates in parallel using a dedicated set of compute cores in a master-slave configuration. At each time step, the master processes receives subsurface states from PFLOTRAN, converts those states to bulk electrical conductivity, and instructs the slave processes to simulate a tomographic data set. The resulting multi-physics simulation capability enables accurate feasibility studies for ERT imaging, the identification of the ERT signatures that are unique to a given process, and facilitates the joint inversion of ERT data with hydrogeological data for subsurface characterization. PFLOTRAN-E4D is demonstrated herein using a field study of stage-driven groundwater/river water interaction ERT monitoring along the Columbia River, Washington, USA. Results demonstrate the complex nature of subsurface electrical conductivity changes, in both the saturated and unsaturated zones, arising from river stage fluctuations and associated river water intrusion into the aquifer. The results also demonstrate the sensitivity of surface based ERT measurements to those changes over time. PFLOTRAN-E4D is available with the PFLOTRAN development version with an open-source license at <https://bitbucket.org/pflotran/pflotran-dev> .

1. *Key Words*

hydrogeophysics, time-lapse geophysics, electrical resistivity tomography, groundwater, simulation, multi-physics, parallel, open-source

2. *Introduction*

Electrical Resistivity Tomography (ERT) is a geophysical imaging application whereby the bulk electrical conductivity (i.e. the reciprocal of resistivity) distribution of the subsurface is remotely estimated. ERT has found wide application for understanding the near subsurface because bulk conductivity is governed by both the structural and geochemical properties that characterize subsurface interactions [e.g. *Revil et al.*, 2012]. More recently, time-lapse ERT developments have enabled subsurface processes to be monitored in terms of spatial and temporal changes in bulk conductivity [*Binley et al.*, 2015; *Kemna et al.*, 2006; *Singha et al.*, 2015]. Time-lapse imaging allows the static contributions of bulk conductivity to be removed, thereby revealing the temporal evolution of spatial changes in bulk conductivity. These changes can often be uniquely related to some subsurface process (e.g. fluid transport, geochemical alteration etc.), thereby providing the capability to remotely monitor that process in space and time (see previous references for examples).

Despite the growing popularity of time-lapse ERT imaging, multi-physical simulation codes designed specifically to simulate changes in subsurface bulk conductivity arising from some subsurface process, and then to simulate the corresponding time-lapse ERT data arising from that process, are lacking. Because of this, ERT practitioners have limited tools for investigating the feasibility or performance of a time-lapse ERT imaging campaign for a particular subsurface process prior to field trial. The resulting uncertainty raises the risk of failure and reduces the overall utility of ERT imaging. In addition, ERT survey design, which comprises both electrode layout and measurement sequence, is typically based on standardized applications, as opposed

to being customized to a particular anticipated subsurface process. The capability to accurately simulate the ERT data arising from that process given multiple survey design scenarios would facilitate customized survey designs to improve imaging resolution in both space and time. It would also enable the discovery of critical electrical signatures associated with some processes of interest, and the exploitation of that signature for effective process monitoring. Such a simulator would also facilitate the use of time-lapse ERT data in hydrogeological parameter estimation (deterministic and stochastic) algorithms [Commer *et al.*, 2014; Linde *et al.*, 2006; Rings *et al.*, 2010]. Given the recent advancements in understanding the mechanistic relationships between bulk conductivity and subsurface structural and geochemical states [Revil, 2013; Slater, 2007 and references therein], the capability to accurately derive bulk conductivity from existing subsurface simulators is within reach.

In this work we describe a parallel ERT computing module for PFLOTRAN [Hammond *et al.*, 2014], a massively parallel reactive flow and transport model for simulating surface and subsurface processes. Using Message Passing Interface (MPI) libraries [Gropp *et al.*, 1999], a group of processors is created exclusively to accommodate ERT forward modeling. After each time step, PFLOTRAN passes relevant simulation results to this group of modules, which are then transformed to subsurface bulk conductivity, and used to compute a simulated ERT survey for that time step. We demonstrate the code using a groundwater/surface water interaction simulation based upon actual field data. The results show the complex nature of the changes in bulk conductivity arising from stage-driven changes in water table elevation and groundwater/surface water interaction. The results also demonstrate the sensitivity of the ERT data to these processes, thereby validating the capability to monitor them at the field scale. The code and user documentation are available with the PFLOTRAN distribution and associated open source license (<https://bitbucket.org/pflotran/pflotran-dev>).

3. Methods

3.1. E4D (background, capabilities, parallel structure)

E4D is a parallel ERT forward modeling and inversion code available with a Berkeley Software Distribution open source license [Johnson and Wellman, 2015a; Johnson et al., 2010] (see <https://e4d.pnnl.gov>). The ERT method uses hardware and software to image the bulk electrical conductivity of the subsurface. Bulk electrical conductivity is influenced by physical, biological, and geochemical interactions, making time-lapse images of changes in bulk conductivity useful for monitoring subsurface processes. Measurements are collected using a four-electrode configuration, whereby current is injected between a source and a sink electrode, and the resulting electrical potential is measured between a positive and negative potential electrode. The ratio of the observed potential to the current injected (or some transform thereof) is called the transfer resistance, and constitutes the primary ERT measurement [Daily and Owen, 1991]. In a typical ERT survey, hundreds to tens of thousands of such measurements are strategically collected using array of static electrodes deployed along the surface and/or within boreholes. Time-lapse data sets consist of many identical ERT surveys collected over time to monitor the changes in transfer resistance associated with some subsurface process of interest. Forward modeling is the process whereby the transfer resistance measurements are simulated, given the subsurface bulk conductivity distribution in space and time.

ERT imaging involves inverting the transfer resistance measurements to estimate the bulk conductivity distribution that gave rise the measurements. In comparison to forward modeling, the inversion process is computationally demanding in terms of both CPU load and memory requirements. Details concerning the parallel inversion may be found in Johnson et al. (2010). The work herein focuses on forward modeling, where the subsurface bulk conductivity distribution is generated by converting subsurface states simulated by PFLOTTRAN to bulk

conductivity using a petrophysical transform. The petrophysical transform is defined herein as the relationship between hydrogeological properties and states, and the corresponding subsurface bulk conductivity.

The direct-current electrical potential arising from a given current source is given by the Poisson equation

$$\nabla \cdot \sigma_b(\mathbf{r}) \nabla \phi(\mathbf{r}) = -\nabla \cdot \mathbf{J}(\mathbf{r})$$

eq. 1

where $\mathbf{r}$ is a position vector, σ_b is effective bulk electrical conductivity, ϕ is electrical potential, and $\mathbf{J}$ is the source current density. Given σ , $\mathbf{J}$, and appropriate boundary conditions, the objective of the forward model is to solve eq. **Error! Reference source not found.** for ϕ , which is measured during an ERT experiment. Because potential is a linear function of current density, equation 1 can be solved by superimposing solutions with different current source terms. A pole solution is a solution to equation 1 for a given point source of current with a current sink at infinite distance from the source. Because there are typically many more current source injections than electrodes for a given ERT survey, it is generally more efficient to model the pole solutions for each electrode, and then subtract the pole solution for the sink electrode from the pole solution for the source electrode to simulate the potential field generated by a particular source sink pair. In this way, the number of solutions to equation 1 required to simulate an ERT survey is equal to the number of electrodes instead of the number of measurements.

We use the forward modeling capabilities of E4D to simulate time-lapse ERT surveys in this paper. E4D solves equation 1 using the finite element method on an unstructured tetrahedral mesh. Details concerning numerical aspects of the forward solution can be found in Rucker et al. (2006) and Johnson et al., (2010). Details concerning the parallelization are found in Johnson et al. (2010), and the forward computations are summarized by the flow diagram in

Figure 1. Numerous aspects of Figure 1 are discussed in the forthcoming sections, including the PFLOTTRAN-E4D coupling, mesh interpolation and petrophysical transformation. Of note here are the master-slave configuration of E4D and the highly parallel nature of the E4D forward computations. In particular, E4D has one master process that provides the communication link to PFLOTTRAN and orchestrates all E4D computations. Slave nodes accommodate the primary computational burdens and memory requirements, and communicate only with the master node during pre and post solution phases through MPI broadcast calls, making the forward modeling highly scalable.

3.2.PFLOTTRAN (background, capabilities, parallel structure)

PFLOTTRAN is a massively-parallel multi-physics simulator [Hammond et al., 2014] developed and distributed under an open source GNU Lesser General Public License license. It is written in object oriented FORTRAN 2003/2008 and founded upon the PETSc framework [Balay et al., 2015], which provides the underlying parallel data structures and solvers for scalable high performance computing

Although PFLOTTRAN is designed for massively parallel computation, the same single code base can run on a single process without recompilation, though available memory may be a limitation. PFLOTTRAN's object oriented design facilitates the incorporation of new process models within the code and/or coupling with code developed externally (e.g. E4D). Lichtner et al. (2015) provides a comprehensive overview of PFLOTTRAN capability.

For the demonstration in this paper, PFLOTTRAN simulated single phase variably saturated flow and solute transport . Single-phase variably saturated flow is based on the Richards' equation with the form

$$\frac{\partial}{\partial t}(\phi s \rho) + \nabla \cdot \rho \mathbf{q} = 0,$$

eq. 2

142 with water density ρ , porosity φ , and saturation s . The Darcy velocity $\mathbf{q}$ is given by

143
$$\mathbf{q} = -\frac{kk_r}{\mu} \nabla(p - \rho g z),$$

144 eq. 3

145 with water pressure p , viscosity μ , acceleration of gravity g , intrinsic permeability k , relative
146 permeability k_r . Conservative solute transport in the liquid phase is based on the advection-
147 dispersion equation

148
$$\frac{\partial}{\partial t}(\varphi s C) + \nabla \cdot (\mathbf{q} - \varphi s D \nabla) C = 0,$$

149 eq. 4

150 with solute concentration C and dispersion coefficient D . PFLOTRAN employs backward Euler
151 time discretization and the Newton-Raphson method (where necessary) to solve for flow and
152 transport state variables over time.

153

154 ***3.3. PFLOTRAN-E4D coupling***

155 The PFLOTRAN workflow is factored into a tree structure of hierarchical process models
156 (multiphysics processes coupled to numerical methods). As process models are added to
157 PFLOTRAN, factories are adapted or created to accommodate these new process models
158 classes. During simulation initialization, these factories set up process models and link them
159 within a tree data structure (tree graph theory). Each process model has two pointers: one to a
160 child and another to a peer process model as shown in Figure 2. Peer process models
161 synchronize at specified times while descendants play catch up at their own pace . Therefore,

for the process model tree shown in Figure 3, the master process model A executes first taking as many time steps as necessary to reach a synchronization point. For each A time step, B takes as many time steps as necessary to catch up to A. Once A (and its child B) have reached the synchronization point, C time steps until it reaches the same point in time. Key state variables and parameters are updated between A and C at the synchronization point and between A and B before and after each of A's time steps.

For the PFLOTTRAN-E4D coupling, flow serves as the master process model with solute transport as its child, and E4D is the descendant of solute transport as shown in Figure 4. During the initialization, PFLOTTRAN sends E4D the porosity distribution, and E4D reads the static Archie's Law (Archie, 1942) parameter distributions (tortuosity factor, cementation factor, and saturation exponent) from a user supplied text file. After each transport step, fluid conductivity and water saturation is passed to E4D, thereby enabling E4D to determine the bulk conductivity distribution at each time step using Archie's Law. If PFLOTTRAN is simulating temperature, the temperature distribution is also passed to E4D at each time step. E4D then adjusts the bulk conductivity using a linear transform specified by a user supplied input file. Note that E4D's execution is non-blocking. Once PFLOTTRAN hands off the state variables the flow and transport process models can proceed with their execution before E4D has completed its step.

3.4. Initialization

Inter-process communications in both PFLOTTRAN and E4D are governed using direct MPI calls. Upon initialization, PFLOTTRAN divides the available compute cores between PFLOTTRAN and E4D as directed by user input. Once the E4D module is initialized, both PFLOTTRAN and E4D proceed to read their respective input files and execute pre-simulation setup. This includes generation of the PFLOTTRAN-to-E4D mesh interpolation matrix generated by E4D as described

in section 4.7. The mesh interpolation matrix is used to accurately transfer PFLOTTRAN state simulations from the PFLOTTRAN mesh to the E4D mesh.

3.5. PFLOTTRAN->E4D data transfer

Once setup computations are complete, PFLOTTRAN begins the subsurface simulation. Upon completion of each time step, PFLOTTRAN passes relevant states (e.g. fluid conductivity, saturation, temperature) to the E4D master node and proceeds to the next time step. The E4D master node then determines whether an E4D simulation is required for the current time step, as specified by user input. If a forward simulation is required, the PFLOTTRAN states are converted to bulk conductivity and mapped to the E4D mesh by the E4D master node as described in sections 4.6 and 4.7 (Figure 1B). The master node then broadcasts the bulk conductivity distribution to the E4D slave nodes and instructs them to execute a forward run as described in section 4.8. In terms of timing, E4D follows behind PFLOTTRAN, executing a forward simulation for the current time step while PFLOTTRAN proceeds to simulate the subsurface states for the next time step.

3.6. Petrophysical Transform

On its own, bulk electrical conductivity is generally not considered a property of primary importance. However, bulk conductivity is governed by variables that are often considered primary, and are therefore directly simulated by subsurface simulation codes. The direct relationship between these primary variables and bulk conductivity enables spatial and temporal changes in bulk conductivity to be interpreted in terms of corresponding primary properties and processes. The petrophysical transform provides the mathematical link for transforming relevant states simulated by PFLOTTRAN to bulk electrical conductivity.

PFLOTTRAN-E4D uses Archie's Law [Archie, 1942], which is given by

$$\sigma_b = \frac{1}{a} \Phi^m s_w^n \sigma_w, \quad \text{eq. 5}$$

where a is the tortuosity factor, Φ is porosity, m is the cementation exponent, s_w is fluid saturation, n is the saturation exponent, σ_w is the fluid conductivity.. With the exception of a , m and n , PFLOTRAN is capable of simulating the state of each parameter on the right hand side of equation 5. Each of these parameters are passed to E4D by PFLOTRAN in order to compute the bulk conductivity distribution. PFLOTRAN is also capable of simulating temperature, which, when simulated, is passed to E4D and used to correct the bulk conductivity estimated using equation 5, using a user-provide linear transform.. Once the relevant parameters and state variables are passed to E4D by PFLOTRAN, the E4D master node uses equation 5 and the temperature correction to determine bulk conductivity on the PFLOTRAN mesh, and then interpolates those results to the E4D mesh using the approach described in the next section.

3.7. Mesh interpolation matrix

Once simulated states are transferred from PFLOTRAN to E4D at a given time step, those states must be transformed to bulk conductivity and mapped to the E4D mesh before a forward run is executed. In addition to the incongruent alignment of the structured mesh used by PFLOTRAN and the unstructured mesh used by E4D, each mesh will typically differ in scale in different regions of the model domain in order to accurately model the differing physics relevant to subsurface fluid flow and electrical current flow from point sources. In order to address these conditions, we integrate the bulk conductivity of the PFLOTRAN mesh over each E4D mesh element. The bulk conductivity is provided at any point in the PFLOTRAN modeling domain using a tri-linear interpolation of the value at the eight PFLOTRAN cell centers surrounding that

231 point. Figure 5 illustrates the general approach. Let m_i^e be the bulk conductivity of element i in
 232 the E4D mesh. Then

$$233 \quad m_i^e = \frac{1}{V_i} \int_{V_i} m^c(\mathbf{r}) dV \approx \frac{1}{n_k} \sum_{k=1}^{n_k} m_{i,k}^c \quad \text{eq. 6}$$

234 where V_i is the volume of E4D mesh element i , $\mathbf{r}$ is a position vector, m^c is the bulk conductivity
 235 on the PFLOTRAN mesh, n_k is the number of subdivisions by which E4D element i is divided
 236 for the integral approximation, and $m_{i,k}^c$ is the bulk conductivity within element i and subdivision
 237 k . The value of $m_{i,k}^c$ is determined using a tri-linear interpolation of the values of m^c at each of
 238 the eight PFLOTRAN cell centers surrounding point i,k .. This gives

$$239 \quad m_{i,k}^c = \sum_{j=1}^{n_c} m_j^c W_{i,j,k} \quad \text{eq. 7}$$

240 where n_c is the number of elements in the PFLOTRAN mesh, m_j^c is the bulk conductivity of
 241 element j in the PFLOTRAN mesh, and $W_{i,j,k}$ is the weight given to m_j^c in determining the value
 242 of sub-element k within mesh element i of the E4D mesh.

243 Combining equations 6 and 7 gives the interpolation equation for an E4D mesh element i ,

$$244 \quad m_i^e = \frac{1}{n_k} \sum_{k=1}^{n_k} \sum_{j=1}^{n_c} m_j^c W_{i,j,k} \quad \text{eq. 8}$$

245 Equation 8 is expressed in matrix form as

$$246 \quad \mathbf{m}^e = \mathbf{M} \mathbf{m}^c \quad \text{eq. 9}$$

where $\mathbf{m}^c$ is an n_c length vector containing the bulk conductivity values on the PFLOTRAN mesh, $\mathbf{m}^e$ is a n_e length vector containing the bulk conductivity values on the E4D mesh, n_e is the number of elements in the E4D mesh, and $\mathbf{M}$ is the $n_e \times n_c$ mesh interpolation matrix. Although $\mathbf{M}$ is sparse, its computation is somewhat demanding. However, $\mathbf{M}$ only needs to be computed once, and its computation is highly parallelizable. As shown in figure 1A, $\mathbf{M}$ is computed in parallel by the E4D slave processes during the setup phase. After each slave computes its assigned rows of $\mathbf{M}$, it returns the results to the master process, which assembles the matrix in a sparse format. As shown in figure 1B, the master process is also responsible for conducting the mesh interpolation multiplication represented by equation 9, and transferring the resulting $\mathbf{m}^e$ vector of bulk conductivity values to the slave processes in preparation for a forward run.

3.8. PFLOTRAN-E4D forward modeling

This section summarizes the forward modeling operations of the PFLOTRAN-E4D module discussed in previous sections. Upon initialization, PFLOTRAN assigns E4D a user specified number of processors. E4D then assigns one processor to be the master process, and the remaining processes as slave processes. The master process reads the E4D input files, passes relevant information to the slave processes, and instructs the slaves to construct and return the mesh interpolation matrix. The master node then instructs the slaves to build the finite element coupling matrix in preparation to solve equation 1 given the bulk conductivity supplied by PFLOTRAN at each user-specified time step.

At each PFLOTRAN time-step, PFLOTRAN sends E4D the simulated subsurface states necessary to derive bulk conductivity using the petrophysical transform given by equation 5. If user input specifies that an ERT survey should be simulated for the current time step, these states are converted to bulk conductivity and mapped to the E4D mesh by the E4D master

node. The E4D master process then broadcasts the bulk conductivity distribution for the current time step to the slave processes, and instructs the slave processes to compute the solutions for each electrode assigned. The slave processes then extract the relevant electrode potentials from their respective solutions and send them to the master where they are assembled and output to a text file.

4. Groundwater/Surface water interaction monitoring simulation

We simulated ERT monitoring of a groundwater/surface-water interaction system along the Columbia River at the Hanford Site 300 Area in south-central WA, USA (Figure 6). Aquifer sediments bounding the Columbia River are generally coarse grained and highly permeable [Hammond and Lichtner, 2010; Williams et al., 2008]. Coupled with dynamic stage variations, the resulting system is characterized by active stage driven intrusion and retreat of river water into the adjacent unconfined aquifer system.

During baseline, low-stage conditions (October-February), the Columbia River is a gaining stream, and the aquifer pore space is occupied by groundwater. As stage levels rise, two processes induce opposing changes in the bulk electrical conductivity of the aquifer (Johnson et al., 2015b). First, the rising water table causes previously unsaturated sediments to become saturated, resulting in an increase in bulk conductivity near the water table (see equation 5). The second change originates in the contrast between lower conductivity river water, and higher conductivity groundwater. As river stage rises river water is driven into the inland aquifer, displacing higher conductivity groundwater, and decreasing bulk conductivity within the saturated zone.

Computational meshes

Changes in bulk conductivity caused by stage-driven water table fluctuations and river water

intrusion were monitored over time in three-dimensions using ERT with a surface array of 352 electrodes (Johnson et al., 2015b). In this example we use PLOTTRAN with the E4D module to simulate river water intrusion and the corresponding time-lapse ERT surveys over the first 30 days of the experiment. The PFLOTTRAN mesh is shown in Figure 7A. Each mesh element is 2m by 2m wide in the horizontal direction, and 0.5 m in the vertical direction, giving 1.6 million elements in total. The mesh is divided into a background host sediment and a higher permeability paleochannel as shown, meant to mimic the paleochannel structures known to govern fluid flow in the 300 Area. The E4D mesh is shown in Figure 7B. The mesh was created to conform to the surface topography and riverbed bathymetry. The boundaries are placed far from electrodes to reduce the effects of the zero-potential subsurface boundary conditions used to solve equation 1. In total, the E4D mesh contains 905,185 elements.

To illustrate the alignment between the two meshes, Figure 7C shows the PFLOTTRAN mesh superimposed on a transparency of the E4D mesh. Note that the maximum elevation of the water table is 106.7 m, and the PFLOTTRAN mesh extends to 110 m to enable simulation of stage-driven changes in saturation and pore water conductivity in both the saturated and unsaturated zones. PFLOTTRAN elements located above the river channel (figure 7C) are inactive in the simulation, such that the PFLOTTRAN mesh conforms to the river bathymetry (not shown).

Material Properties

The hydrogeologic properties of the host material and paleochannel used for the PFLOTTRAN simulation were selected to provide realistic estimates of field conditions (Lichtner et al., 2010; Williams et al., 2008), and are shown in table 1 below. The unsaturated hydraulic conductivity is computed using the Van Genuchten water retention function [*Vangenuchten*, 1980] and the Burdine permeability relationship [*Burdine*, 1953].

318 **Table 1. Hydrogeologic material properties of host material and channel shown in Figure 7.**

Material	Porosity	Permeability (m ²)	Van Genuchten/Burdine Parameters		
			Residual Saturation	m	λ
Host	0.30	1.05e-9	0.13	0.748	1.43E-4
Channel	0.20	4.39e-9	0.16	0.340	7.27E-4

319

320 **Boundary and Initial Conditions**

321 Both pressure and solute concentration boundary and initial conditions are required for the
 322 PFLOTRAN simulation. At the northern, western, and southern boundaries, transient
 323 (hydrostatic) head conditions were applied using hourly water table elevation measurements
 324 [Chen et al. (2013)]. At the eastern boundary transient head boundary conditions are described
 325 using river stage measured by a pressure transducer. A conductance value of 10^{-12} m was
 326 applied to the eastern boundary to mimic the damping effect of low-permeability material on the
 327 river bed, (Williams et al., 2008, Hammond et al., 2010). A no-flow boundary condition was
 328 specified at the bottom of the domain since the domain is underlain by low permeability Ringold
 329 Formation materials.

330 River water intrusion was tracked by introducing a conservative tracer at the river boundary.
 331 The concentration boundary conditions for the tracer were set to be free outflow at the northern,
 332 western, and southern boundaries, while a constant concentration was maintained at the river
 333 boundary. A zero-flux tracer boundary condition was applied at the lower no flow boundary. The

initial flow condition was a hydrostatic pressure distribution based on the water table. The initial conservative tracer concentration was set to be zero over the entire model domain.

As previously described, zero potential boundary conditions are specified on the subsurface boundaries of the E4D mesh. Zero current flux boundary conditions are specified normal to the surface boundary. The E4D elements outside of the PFLOTRAN domain assume a user specified bulk conductivity provided at each time, which is in this case the bulk conductivity provided by the equation 5 at time zero.

Petrophysical Transformation

We assume for the simulation that each variable in equation 5 is known and constant through time, except for fluid conductivity and saturation. . PFLOTRAN simulates saturation and river water concentration in terms of fluid conductivity, and sends each to E4D at each time step. The end-member fluid conductivities are 0.040 S/m for river water, and 0.015 S/m for groundwater, which were determined by direct measurement. Upon receipt from PFLOTRAN, E4D constructs the bulk conductivity field according to equation 5, maps the field to the E4D mesh, and executes the forward run. For the simulation, we assumed $a = 1$, $m=1.3$, and $n=2.0$ for the Archies parameters.

All files required to execute the simulation and reproduce the results given in the next section may be downloaded at (pnnl_sfa_website_address to be placed here upon acceptance).

5. Results

The simulation was executed with 128 processors allocated to PFLOTRAN and 353 processors allocated to the E4D module (1 master and 352 slaves, one for each electrode). With this allocation, E4D was able to complete a forward simulation (from mesh interpolation

through output) within the time required for a single PFLOTTRAN time-step, so there was no additional computation time required beyond that required for PFLOTTRAN alone. The entire simulation required approximately 3 hours. Given the high permeability of sediments in the simulation, the groundwater table is at all times near the river stage elevation. With this in mind, we demonstrate the results of the PFLOTTRAN simulation, petrophysical transformation, and mesh interpolation at two times (5 days and 15 days) and at two elevations, one below the water table (105 m), and one above the water table (107 m). At 5 and 15 days the river stage is at approximately 105.8 m and 106.4 m respectively (Figure 8). Figure 9 shows the change in saturation and river water fraction from baseline conditions at 105 m and 107 m simulated by PFLOTTRAN, and on the PFLOTTRAN mesh (upper panels). The lower panels show the corresponding changes in bulk conductivity derived from the petrophysical transform, interpolated onto to the E4D mesh.

The performance of the mesh interpolation scheme is evident by comparing the change in river water fraction (PFLOTTRAN mesh) to the change in bulk conductivity (E4D mesh) at 105 m for each time shown. Since the subsurface is fully saturated at 105 m, the relationship between a change in fluid conductivity and a change in bulk conductivity is linear, meaning the spatial distribution of the changes should be identical at this elevation. The 105 m images in Figure 9 show this to be the case, and demonstrate the performance of the mesh interpolation scheme. The same images show the expected behavior of river water intrusion to flow preferentially into the high permeability paleochannel, and the corresponding decrease in bulk conductivity as river water replaces groundwater in the pore space. The uneven river water/groundwater front within the host material (i.e. outside of the channel) is caused by variability in the river bottom bathymetry incorporated into the PFLOTTRAN mesh.

The effects of the differing material properties shown in table 1 are highlighted by the change in saturation plots at the 107 m elevation. At both 5 and 15 days, saturation at 107 m

increases within the host material as the water table rises, but saturation increase within the channel is relatively minor. The river water fraction plots show that pore water moving upward into the unsaturated zone is primarily groundwater at 5 days, suggesting the corresponding change in bulk conductivity at 5 days and 107 m elevation is caused primarily by an increase in saturation with groundwater. Conversely, the change in conductivity at 15 days and 107 m elevation bares the imprint of the river water intrusion within the saturated zone. The conductivity increase within the vadose zone above the river water intrusion zone is subdued as lower conductivity river water moves into the unsaturated zone through capillary action. Overall, the simulation demonstrates the complex nature of stage driven changes in bulk conductivity associated with this relatively simple synthetic representation of the 300 Area, including complex patterns of conductivity increase within the vadose zone, underlain by decreases in conductivity within the saturated, river water intrusion zone.

Figure 10 shows the E4D-simulated change in electrical potential on the surface from conditions at time zero, and for three different current injection points. The current electrodes for each of the three measurement configurations (M1, M2, and M3) are arranged in a Wenner Alpha array, whereby the two potential measurement electrodes are placed in between the current electrodes, with equal spacing between any two adjacent electrodes. In each case that spacing is 20m. The locations of each measurement are shown in Figure 10A. M1 is located near the shoreline directly over the paleochannel. M2 is located outside of paleochannel and near the shoreline. M3 is located within the paleochannel, far from the shoreline. For each measurement, the positive current electrode is to the south, the negative current electrode is to the north. Figure 10B shows the change in potential on the ground surface for each measurement, normalized to 1 ampere of injected current, at 5 and 15 days. At 5 days measurements M2 and M3 show similar patterns of potential difference that are caused primarily by the rising water table, because M2 and M3 do not overlie the river water intrusion

zone at 5 days (see Figure 9). Contrast this to M1, which does overlie the intrusion zone at 5 days, and displays a significantly different potential difference pattern compared to M2 and M3. At 15 days, the potential difference distributions for all measurements have changed significantly compared to 5 days. This demonstrates the sensitivity of the ERT measurements to stage driven hydrodynamics, and verifies the corresponding opportunity to image stage-driven changes in electrical conductivity using time-lapse ERT.

To further illustrate this point, Figure 11 shows the time series for the potentials measured at M1, M2, and M3 superimposed on the river stage elevation shown in figure 8. Note that the simulated potentials are normalized by the injected current to give the transfer resistance. If the support volume for a given measurement becomes less conductive (more resistive), then the transfer resistance will increase, and vice versa. The transfer resistance time series are informative in this regard. M1 displays an increasing trend in transfer resistance, indicating that the subsurface within the support volume for M1 is becoming more resistive, on average. This is consistent with the location of M1, directly over the channel and near the shoreline, where the measurement support volume is primarily influenced by more resistive river water. Note however the influences of water table variations are not lost on the same time series. When river stage (and thus water table) drop, the M1 time series displays a corresponding increase in transfer resistance correspond to the decrease in saturation associated with the falling water table, and vice versa. The same can be observed for M2 and M3. Measurements M2 and M3 are primarily influenced by the river stage-driven increase in water table elevation up to about day 10. The rising water table causes an increase in saturation and corresponding decrease in resistivity, as evidenced by the decreasing transfer resistance over that period. After day 10 the transfer resistance begins to increase in M2 and M2 as more resistive river water begins to enter support volume of each measurement.

6. Discussion

In the introduction we stated that a multi-physics simulator capable of modeling the bulk electrical conductivity evolution arising from a given subsurface processes would, among other things, 1) enable practitioners to investigate the feasibility of monitoring that process using ERT, and 2) enable the discovery of critical electrical signatures associated with the process, and the exploitation of that signature for effective process monitoring. The groundwater/surface water interaction simulation presented in sections 5 and 6 is illustrative in this regard. First, the simulation demonstrated that contrasts in bulk conductivity originating from stage-driven river water intrusion provide ERT measurements with adequate sensitivity for monitoring (Figure 11), thereby demonstrating the feasibility of 4D ERT monitoring of river water intrusion and retreat. Second, the simulation revealed the contrasting influences of water table fluctuations and river water intrusion on the bulk conductivity distribution along with the relative magnitudes of those influences in terms of the corresponding ERT measurements (Figure 11). In terms of electrical signatures, those measurements that are not influenced by river water intrusion are characterized by a decrease in transfer resistance with respect to baseline conditions associated with the rising water table. Only measurements that are influenced by river water intrusion experience an increase in transfer resistance compared to baseline conditions. As shown by Wallin et al. (2013) and Johnson et al. (2015b), the ERT data alone do not provide sufficient information to resolve between these competing influences using standard ERT inversion algorithms. Recognition of this fact enabled the development of customized constraints that allowed only increase in bulk conductivity within the vadose zone, and decreases in conductivity within the saturated zone, in relation to baseline conditions (Figure 9). These constraints provided the imaging algorithm with the information necessary to delineate between the influences of water table fluctuations and river water intrusion, thereby enabling effective imaging of the river water intrusion zone. We expect the coupled PFLOTRAN-E4D

modeling demonstrated here will provide similar utility in other ERT monitoring applications of complex systems.

Conclusion

It is well recognized that geophysical data, particularly time-lapse geophysical data, have the potential to significantly reduce uncertainty in hydrogeologic parameter estimations [Dafflon *et al.*, 2011; Jardani *et al.*, 2013; Linde *et al.*, 2006; Pollock and Cirpka, 2012]. Progress toward informing hydrogeologic inversions with geophysical data is complicated by the general requirement for an accurate field scale petrophysical transform, and by the computational demands of simulating both the hydrological and geophysical observations. The latter can be addressed in part through high performance computing and suitable codes such as PFLOTRAN-E4D. We also note the many advantages of the open source license provided by PFLOTRAN-E4D, which facilitates transparency and collaboration, and enables users to modify the code as needed for custom applications.

7. Acknowledgements

This research was supported by the U.S. Department of Energy (DOE), Office of Biological and Environmental Research (BER), as part of BER's Subsurface Biogeochemistry Research Program (SBR). This contribution originates from the SBR Scientific Focus Area (SFA) at the Pacific Northwest National Laboratory (PNNL).

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543

544 *Figures*

545

A) Setup phase

B) Run phase

Figure 1. Flow diagram showing the setup and run phases of the E4D module. A) In the setup phase, E4D is initialized by PFLOTRAN. The master node receives setup and instructs

549 the slave nodes to construct the PFLOTRAN-E4D mesh interpolation matrix. B) At each time
550 step, the E4D master node receives subsurface state information from PFLOTRAN, converts
551 that information to bulk conductivity with a user supplied petrophysical transform, maps the bulk
552 conductivity to the E4D mesh, and transfers the results to the slave nodes. The slave nodes
553 compute pole solutions for assigned electrodes, and transfer the relevant potentials to the
554 master node for assembly. The master node assembles the potentials to create the simulated
555 measurements, and writes the results to a file.

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PFLOTRAN Process Model

559 Figure 2. The PFLOTRAN process model class coupling physics/chemistry to numerical
560 methods for their solution. Each process model has a pointer to a neighboring peer and child,
561 which enables linkage between process models through a tree data structure (tree graph
562 theory). Here a peer is another process model, which may or may not have one or more child
563 processes.

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566 Figure 3. Example process model tree with master process model A linked to child B and
567 peer C. Process model B follows A's time stepping (either lock step or through sub-steps) while
568 A and C are synchronized at specified points in time.

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571 Figure 4. The process model tree for PFLOTTRAN-E4D coupling where single-phase
572 variably saturated flow is the master process model with solute transport as its child and
573 geophysics is the child of transport. In most cases, all three process models proceed lock step
574 with each other (flow → transport → geophysics).

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578 **Figure 5. Components used to interpolate bulk conductivity from the PFLOTRAN mesh to the E4D mesh.**

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581 Figure 6. Location of simulated study area along the Columbia River at the Hanford 300
582 Area in south-central WA, USA.

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Figure 7. A) PFLOTRAN computational mesh showing a high permeability paleochannel embedded in a lower permeability host sediment. B) Interior E4D mesh showing surface topography and mesh refinement at electrode locations. C) PFLOTRAN mesh (blue channel

588 and red host material) superimposed on a transparent view of the E4D mesh.

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591 Figure 8. River stage during simulation period (April 1 – April 28, 2013).

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Figure 9. (Top Row) Simulated change in saturation and river water fraction from baseline conditions on the PFLOTRAN mesh at 5 and 15 days, and at 105 m and 107 m elevation. (Bottom Row) Simulated change in bulk electrical conductivity from baseline conditions at 5 and 15 days, and at 105 m and 107 m elevation.

601 Figure 10. A) Locations of the three (M1-M3) 4-electrode Wenner measurements
602 demonstrated in (B) and in figure 8. B) Change in surface potential per ampere of current
603 injected for measurements M1-M3, at 5 and 15 days.

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Figure 11. Transfer resistance time series for measurements M1-M3 (see figure 7)

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superimposed on the river stage elevation.

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