Response to editorial and reviewer Comments for "Simulating Coupled Surface-Subsurface Flows with ParFlow v3.5.0: Capabilities, applications, and ongoing development of an open-source, massively parallel, integrated hydrologic model"

On behalf of my co-authors and myself, we'd like to thank you, the Executive Editor, the Handling Topical Editor, and the referees for carefully considered evaluation of our revised manuscript. We were happy to see the revision was well-received and that our intended message was clear. The minor comments provided by the referees were particularly helpful in bettering specific sections of the manuscript, including word omissions and typographical errors, which can be difficult to spot in one's own manuscript. The revised manuscript addresses the concerns raised by the referee and the Handling Topical Editor and we are glad the Editor found it suitable for publication without major external review.

Please find below our revision, which includes detailed point-by-point response to all referee comments. The response to the referee comments are structured as follows: (1) comments from referees, (2) author's response, and (3) author's changes in a marked-up manuscript version showing all the changes made. We are glad to discuss any aspect of the revision with you, the handling topical editor, or the referees if questions arise. The original text of the comments is below in plain face font and our responses are given in bold face italic font for maximum clarity. We have included references to specific line numbers regarding all changes and these line numbers refer to the "tracked changes" version to make it as simple as possible to evaluate the changes in the context of the previous submission.

The Handling Topical Editor's Comments:

Comments to the Author:

Dear Benjamin,

Thank you for your revised manuscript.

Reviewer 1 has provided a few technical corrections but is otherwise very happy with the paper. Could you check equation 18 prior to publication.

Reviewer 2 was unavailable, however I believe the revisions made given this reviewers comments have significantly improved the manuscript and added clarity in a number of areas. The are some remaining differences over what I believe are fair points to debate. For example, the choice of which details to include in the title, the need for a section on development history, and issues around completeness and coverage. However, in my view a compelling case is put forward for the decisions taken in compiling the revised version. Furthermore, issues of scientific substance have been amended to address the reviewers concerns.

Finally, I'd like to thank both reviewers for taking the time to read the manuscript and provide constructive and detailed feedback.

Bets wishes,

Jeff

Authors Response

We greatly appreciate the Handling Topical Editor for his comments. The Handling Editor's direction to check equation 18 has been considered, and relevant changes have been made. See Lines 354 in the revised manuscript.

Anonymous Referee #1 Comments

Authors have done an excellent job incorporating reviewers' comments. I added 3 minor comments below that can be addressed during the copy editing process:
Line numbering is based on the tracked version of the paper:

Line 76 –I understand that you removed unsaturated based on reviewer 2 comments. However, the sentence is more correct if you keep "unsaturated"

Authors Response

We agree with the reviewer that keeping the word "unsaturated" makes the sentence more correct. We have revised the text to maintain "unsaturated" in the sentence. See Line 75 in the revised manuscript.

Line 84 – Add "using" before the Richards'

Authors Response

The manuscript has been revised to include "using" before the Richards'. See Line 83 in the revised manuscript.

Line 356 – In the first equation, changes in pressure head should be relative to dx not dy.

Authors Response

We have revised equation 18 to reflect reviewer's concern that changes in pressure head should be relative to dx not dy. See Line 354 in the revised manuscript.

Simulating Coupled Surface-Subsurface Flows with ParFlow v3.5.0: Capabilities, applications, and ongoing development of an open-source, massively parallel, integrated hydrologic model

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Abstract

Surface and subsurface flow constitute a naturally linked hydrologic continuum that has not traditionally been simulated in an integrated fashion. Recognizing the interactions between these systems has encouraged the development of integrated hydrologic models (IHMs) capable of treating surface and subsurface systems as a single integrated resource. IHMs is dynamically evolving with improvement in technology and the extent of their current capabilities are often only known to the developers and not general users. This article provides an overview of the core functionality, capability, applications, and ongoing development of one open-source IHM, ParFlow. ParFlow is a parallel, integrated, hydrologic model that simulates surface and subsurface flows. ParFlow solves Richards' equation for three-dimensional variably saturated groundwater flow and the two-dimensional kinematic wave approximation of the shallow water equations for overland flow. The model employs a conservative centered finite difference scheme and a conservative finite volume method for subsurface flow and transport, respectively. ParFlow uses multigrid preconditioned Krylov and Newton-Krylov methods to solve the linear and nonlinear systems within each time step of the flow simulations. The code has demonstrated very efficient parallel solution capabilities. ParFlow has been coupled to geochemical reaction, land surface (e.g. Common Land Model), and atmospheric models to study the interactions among the subsurface, land surface, and the atmosphere systems across different spatial scales. This overview focuses on the current capabilities of the code, the core simulation engine, and the primary couplings of the subsurface model to other codes, taking a high-level perspective.

1. Introduction

Surface and subsurface (unsaturated and saturated zones) water are connected components of a hydrologic continuum (Kumar et al., 2009) . The recognition that flow systems (i.e. surface and subsurface) are a single integrated resource has stimulated the development of integrated hydrologic models (IHMs), which include codes like ParFlow (Ashby and Falgout, 1996; Kollet and Maxwell, 2006) , HydroGeoSphere (Therrien and Sudicky, 1996), PIHM (Kumar, 2009), and CATHY (Camporese et al., 2010) . These codes explicitly simulate different hydrological processes such as feedbacks between processes that affect the timing and rates of evapotranspiration, vadose zone flow, surface runoff and groundwater interactions. That is, IHMs are designed specifically to include the interactions between traditionally incompatible flow domains (e.g. groundwater and land surface flow) (Engdahl and Maxwell, 2015) . Most IHMs adopt a similar, physically-based approach to describe watershed dynamics where the governing equations of three–dimensional variably saturated subsurface flow are coupled to shallow water equations for surface runoff. The advantage of the coupled approach is that it allows hydraulically-connected groundwater–surface water systems to evolve dynamically, and for natural feedbacks between the systems to develop (Sulis et al., 2010; Maxwell et al., 2011; Weill et al., 2011; Williams and Maxwell, 2011; Simmer et al., 2015). A large body of literature now exists presenting applications of the various IHMs to solve hydrologic questions. Each model has its own technical documentation, but the individual development, maintenance, and sustainability efforts differ between tools. Some IHMs represent commercial investments and others are community,

69 open-sourced projects, but all are dynamically evolving as technology improves and new features
70 are added. Consequently, it can be difficult to answer the question of "what exactly can this IHM
71 do today" without navigating dense user documentation. The purpose of this manuscript is to
72 provide a current review of the functions, capabilities, and ongoing development of one of the
73 open-source integrated models, ParFlow, in a format that is more accessible to a broad audience
74 than a user manual or articles detailing specific applications of the model.

75 ParFlow is a parallel integrated hydrologic model that simulates surface, unsaturated, and
76 groundwater flow (Maxwell et al., 2016). ParFlow computes fluxes through the subsurface, as well
77 as interactions with aboveground or surface (overland) flow: all driven by gradients in hydraulic
78 head. Richards' equation is employed to simulate variably saturated three-dimensional
79 groundwater flow (Richards, 1931). Overland flow can be generated by saturation or infiltration
80 excess using a free overland flow boundary condition combined with Manning's equation and the
81 kinematic wave formulations of the dynamic wave equation (Kollet and Maxwell, 2006). ParFlow
82 solves these governing equations employing either a fully coupled or integrated approach where
83 surface and subsurface flows are solved simultaneously using the Richards' equation in three-
84 dimensional form (Gilbert and Maxwell, 2016) , or an indirect approach where the different
85 components can be partitioned and flows in only one of the systems (surface or subsurface flows)
86 is solved. The integrated approach allows for dynamic evolution of the interconnectivity between
87 the surface water and groundwater systems. This interconnection depends only on the properties
88 of the physical system and governing equations. An indirect approach permits partitioning of the
89 flow components i.e. water and mass fluxes between surface and subsurface systems. The flow

components can be solved sequentially. For the groundwater flow solution, ParFlow makes use of an implicit backward Euler scheme in time, and a cell-centered finite-difference scheme in space (Woodward, 1998). An upwind finite-volume scheme in space and an implicit backward Euler scheme in time is used for the overland flow component (Maxwell et al., 2007). ParFlow uses Krylov linear solvers with multigrid preconditioners for the flow equations along with a Newton method for the nonlinearities in the variably saturated flow system (Ashby and Falgout, 1996; Jones and Woodward, 2001). ParFlow's physically based approach requires a number of parameterizations e.g. subsurface hydraulic properties, such as porosity, the saturated hydraulic conductivity, and the pressure-saturation relationship parameters (relative permeability), etc. (Kollet and Maxwell, 2008a).

ParFlow is well documented and has been applied to surface and subsurface flow problems including simulating the dynamic nature of groundwater and surface-subsurface interconnectivity in large domains (e.g. over 600 km^2) (Kollet and Maxwell, 2008; Ferguson and Maxwell, 2012; Condon et al., 2013; Condon and Maxwell, 2014), small catchments (e.g. approximately 30 km^2) (Ashby et al., 1994; Kollet and Maxwell, 2006; Engdahl et al., 2016), complex terrain with highly heterogenous subsurface permeability such as the Rocky Mountain National Park, Colorado, United States (Engdahl and Maxwell, 2015; Kollet et al., 2017), large watersheds (Abu-El-Sha'r and Rihani, 2007; Kollet et al., 2010), continental scale flows (Condon et al., 2015; Maxwell et al., 2015) and even subsurface–surface and –atmospheric coupling (Maxwell et al., 2011; Williams and Maxwell, 2011; Williams et al., 2013; Gasper et al., 2014; Shrestha et al., 2015). Evidences from these studies suggest ParFlow produce accurate results in simulating flows in

surface-subsurface systems in watersheds i.e. the code possesses the capability of performing simulations that accurately represent the behaviors of natural systems on which models are based. The rest of the paper is organized as follows: We provide a brief history of ParFlow's development in Sect. 1.1. In Sect. 2, we describe the core functionality of the code, i.e. the primary functions and the model equations and grid type used by ParFlow. Sect. 3 covers equation discretization and solvers (e.g. inexact Newton-Krylov, the ParFlow Multigrid (PFMG) preconditioner, and the Multigrid-Preconditioned Conjugate Gradient (MGCG) method) used in ParFlow. Examples of parallel scaling and performance efficiency of ParFlow are revisited in Sect. 4. The coupling capabilities of ParFlow, with other atmospheric, land surface, and subsurface models are shown in Sect. 5. We provide a summary and discussion, future directions to the development of ParFlow, and give some concluding remarks in Sect. 6.

1.1 Development History

ParFlow development commenced as part of an effort to develop an open–source, object–oriented, parallel watershed flow model initiated by scientists from the Center for Applied Scientific Computing (CASC), Environmental Programs, and the Environmental Protection Department at the Lawrence Livermore National Laboratory (LLNL) in the mid–1990s. ParFlow was born out of this effort to address the need for a code that combines fast, nonlinear solution schemes with massively parallel processing power, and its development continues today (e.g. Ashby et al., 1993; Smith et al., 1995; Woodward, 1998; Maxwell and Miller, 2005; Kollet and Maxwell, 2008; Rihani et al., 2010; Simmer et al., 2015). ParFlow, is now a collaborative effort

between numerous institutions including Colorado School of Mines, Research Center Jülich, University of Bonn, Washington State University, the University of Arizona, and Lawrence Livermore National Laboratory, and its working base and development community continues to expand.

ParFlow was originally developed for modeling saturated fluid flow and chemical transport in three-dimensional heterogeneous media. Over the past few decades, ParFlow underwent several modifications and expansions (i.e. additional features and capabilities have been implemented) and has seen an exponential growth of applications. For example, a two-dimensional distributed overland flow simulator (surface water component) was implemented into ParFlow (Kollet and Maxwell, 2006) to simulate interaction between surface and subsurface flows. Such additional implementations have resulted in improved numerical methods in the code. The code's applicability continues to evolve, for example, in recent times, ParFlow has been used in several coupling studies, with subsurface, land surface, and atmospheric models to include physical processes at the land surface (Maxwell and Miller, 2005; Maxwell et al., 2007, 2011; Kollet, 2009; Williams and Maxwell, 2011; Valcke et al., 2012; Valcke, 2013; Shrestha et al., 2014; Beisman et al., 2015) across different spatial scales and resolutions (Kollet and Maxwell, 2008; Condon and Maxwell, 2015; Maxwell et al., 2015). Also, a terrain following mesh formulation has been implemented (Maxwell, 2013) that allows ParFlow to handle problems with fine space discretization near the ground surface that comes with variable vertical discretization flexibility

which offer modelers the advantage to increase the resolution of the shallow soil layers (these are discussed in detail below).

2. Core Functionality of ParFlow

The core functionality of the ParFlow model is the solution of three-dimensional variably saturated groundwater flow in heterogeneous porous media ranging from simple domains with minimal topography and/or heterogeneity to highly resolved continental-scale catchments (Jones and Woodward, 2001; Maxwell and Miller, 2005; Kollet and Maxwell, 2008; Maxwell, 2013). Within this range of complexity, the ParFlow model can operate in three different modes: 1). variably saturated; 2). steady–state saturated; and 3). integrated–watershed flows; however, all these modes share a common sparse coefficient matrix solution framework.

2.1 Variably Saturated Flow

ParFlow can operate in variably saturated mode using the well-known, mixed form of Richards' equation (Celia et al., 1990). The mixed form of Richards' equation implemented in ParFlow is:

$$S_s S_w(p) \frac{\partial p}{\partial t} + \phi \frac{\partial (S_w(p))}{\partial t} = \nabla . \boldsymbol{q} + q_s, \qquad (1)$$

$$\boldsymbol{q} = -k_s k_r(p) \nabla (p - z), \qquad (2)$$

where S_s is the specific storage coefficient [L^{-1}], S_w is the relative saturation [$-$] as a function of pressure head p of the fluid/water [L], t is time [T], ϕ is the porosity of the medium [$-$], $\boldsymbol{q}$ is the

specific volumetric (Darcy) flux [LT^{-1}], k_s is the saturated hydraulic conductivity tensor [LT^{-1}], k_r is the relative permeability [–] which is a function of pressure head, q_s is the general source/sink term [T^{-1}] (includes wells and surface fluxes e.g. evaporation and transpiration), and z is depth below the surface [L]. The Richards' equation assumes that the air phase is infinitely mobile (Richards, 1931). ParFlow has been used to numerically simulate river-aquifer exchange (free-surface flow and subsurface flow), (Frei et al., 2009), and highly heterogenous problems under variably-saturated flow conditions (Woodward, 1998; Jones and Woodward, 2001; Kollet et al., 2010). Under saturated conditions e.g. simulating linear groundwater movement under assumed predevelopment conditions, the steady-state saturated mode can be used.

2.2 Steady–State Saturated Flow

The most basic operational mode is the solution of the steady state, fully saturated groundwater flow equation:

$$\nabla . \boldsymbol{q} - q_s = 0, \tag{3}$$

where q_s represents a general source/sink term e.g. wells [T^{-1}], $\boldsymbol{q}$ is the Darcy' flux [LT^{-1}] which is usually written as:

$$\boldsymbol{q} = -k_s \nabla P \tag{4}$$

where k_s is the saturated hydraulic conductivity [LT^{-1}] and P represents the 3-D hydraulic head-potential [L]. ParFlow does include a direct solution option for the steady state saturated flow that is distinct from the transient solver. For example, ParFlow uses the solver "impes" under single-phase, fully saturated steady state condition relative to the variably saturated, transient mode where

190 Richards' equation solver is used (Maxwell et al., 2016). When studying sophisticated or complex
191 phenomena e.g. simulating fully coupled system (i.e. surface and subsurface flow), an overland
192 flow boundary condition is employed.
193
194 2.3 Overland Flow
195 Surface water systems are connected to the subsurface, and these interactions are
196 particularly important for rivers. However, these connections have been historically difficult to
197 represent explicitly in numerical simulations. A common approach has been to use river routing
198 codes, like HEC, and MODFLOW and its River Package to determine head in the river, which is
199 then used as a boundary condition for the subsurface model. This approach prevents feedbacks
200 between the two models, and a better representation of the physical processes in these kinds of
201 problems is one of the motivations for IHMs. Overland flow is implemented in ParFlow as a two–
202 dimensional kinematic wave equation approximation of the shallow water equations. The
203 continuity equation for two-dimensional shallow overland flow is given as;
204 $$\frac{\partial \psi_s}{\partial t} = \nabla . (\vec{v}\psi_s) + q_s, \quad (5)$$
205 where $\vec{v}$ is the depth averaged velocity vector [LT^{-1}], ψ_s is the surface ponding depth [L], t is time
206 [T], and q_s is a general source/sink (e.g. precipitation rate) [T^{-1}]. Ignoring the dynamic and
207 diffusion terms results in the momentum equation
208 $$S_{f,i} = S_{o,i}, \quad (6)$$

209 which is known as the kinematic wave approximation. The $S_{f,i}$ and $S_{o,i}$ represent the friction $[-]$
210 and bed slopes (gravity forcing term) $[-]$ respectively, where i indicates $x-$ and $y-$ directions
211 (also shown in Eq. (7) and Eq. (8)) (Maxwell et al., 2015). Manning's equation is used to generate
212 a flow depth–discharge relationship:

213 $$v_x = \frac{\sqrt{S_{f,x}}}{n}\psi_s^{2/3}, \text{ and} \quad (7)$$

214 $$v_y = \frac{\sqrt{S_{f,y}}}{n}\psi_s^{2/3} \quad (8)$$

215 where n is the Manning's roughness coefficient $\left[\mathrm{TL}^{-1/3}\right]$. Flow of water out of overland flow
216 simulation domain only occurs horizontally at an outlet which is controlled by specifying a type
217 of boundary condition at the edge of the simulation domain. In a natural system, the outlet is
218 usually taken as the region where a river enters another water body such as stream or a lake.
219 ParFlow determines overland flow direction through the D4 flow routing approach. In a simulation
220 domain, the D4 flow routing approach allows for flow to be assigned from a focal cell to only one
221 neighboring cell accessed via the steepest or most vertical slope. The shallow overland flow
222 formulation (Eq. (9)) assumes that the flow depth is averaged-vertically and neglects a vertical
223 change in momentum in the column of surface water. To account for vertical flow (from the surface
224 to the subsurface or subsurface to the surface), a formulation that couples the system of equations
225 through a boundary condition at the land surface becomes necessary. Equation (5) can be modified
226 to include an exchange rate with the subsurface, q_e, as:

227 $$\frac{\partial \psi_s}{\partial t} = \nabla.(\vec{v}\psi_s) + q_s + q_e \quad (9)$$

which is common in other IHMs. In ParFlow, the overland flow equations are coupled directly to Richards' equation at the top boundary cell under saturated conditions. Conditions of continuity of pressure (i.e. the pressures of the subsurface and surface domains are equal right at the ground surface) and flux at the top cell of the boundary between the subsurface and surface systems are assigned Fig. 1 is provided demonstrating continuity of pressure at the ground surface for flow from the surface into the subsurface. This assignment is done by setting pressure–head, in Eq. (1) equal to the vertically–averaged surface pressure, ψ_s;

$$p = \psi_s = \psi, \tag{10}$$

and the flux, q_e equal to the specified boundary conditions (e.g. Neumann or Dirichlet type). For example, if Neumann type boundary conditions are specified, which are given as;

$$q_{BC} = -k_s k_r \nabla(\psi - z) \tag{11}$$

and one solves for the flux term in Eq. (10), the result is;

$$q_e = \frac{\partial \|\psi,0\|}{\partial t} - \nabla\vec{v}\|\psi,0\| - q_s \tag{12}$$

where the $\|\psi,0\|$ operator is defined as the greater of the quantities, ψ and 0. Substituting Eq. (12) for the boundary condition in Eq. (11), requiring the aforementioned flux continuity $q_{BC} = q_e$, leads to

$$-k_s k_r \nabla(\psi - z) = \frac{\partial \|\psi,0\|}{\partial t} - \nabla.(\vec{v}\|\psi,0\|) - q_s \tag{13}$$

Equation (13) shows that the surface water equations are represented as a boundary condition to the Richards' equation. That is, the boundary condition links flow processes in the subsurface with those at the land surface. This boundary condition eliminates the exchange flux and accounts for

the movement of the free surface of ponded water at the land surface (Kollet and Maxwell, 2006; Williams and Maxwell, 2011).

Many IHMs couple subsurface and surface flows making use of the exchange flux, q_e model. The exchange flux between the domains (the surface and the subsurface) depends on hydraulic conductivity and the gradient across some interface where indirect coupling is used (VanderKwaak, 1999; Panday and Huyakorn, 2004). The exchange flux concept gives a general formulation of a single set of coupled surface-subsurface equations. The exchange flux term, q_e may be included in the shallow overland flow continuity equation as the exchange rate term with the subsurface (Eq. (9)) in a coupled system (Kollet and Maxwell, 2006).

Figure. 1 Caption: Coupled surface and subsurface flow systems. Note in this figure the physical system is represented on the left and a schematic of the overland flow boundary condition (continuity of pressure and flux at the ground surface) is on the right. The equation, $p = \psi_s = \psi$ in Fig. 1 signifies that the vertically averaged surface pressure and subsurface pressure head are equal right at the land surface.

2.4 Multi-Phase Flow and Transport Equations

Most applications of the code have reflected ParFlow's core functionality as a single-phase flow solver, but there are also embedded capabilities for multi-phase flow of immiscible fluids and solute transport. Multi–phase systems are distinguished from single–phase systems by the presence of one or more interfaces separating the phases, with moving boundaries between phases. The flow

equations that are solved in multi–phase systems in a porous medium comprise a set of mass balance and momentum equations. The equations are given by:

$$\frac{\partial}{\partial t}(\phi \rho_i S_i) + \nabla.(\phi \rho_i S_i \vec{v}_i) - \rho_i Q_i = 0, \quad (14)$$

$$\phi S_i \vec{v}_i + \lambda_i.(\nabla p_i - \rho_i \vec{g}) = 0, \quad (15)$$

where $i = 1, \ldots, n$ denotes a given phase (such as air or water). In these equations, ϕ is the porosity of the medium [–] which explains the fluid capacity of the porous medium, and for each phase, i, $S_i(\vec{x}, t)$ is the relative saturation [–] which indicates the content of phase i in the porous medium, $\vec{v}_i(\vec{x}, t)$ represent Darcy velocity vector [LT^{-1}], $Q_i(\vec{x}, t)$ stands for source/sink term [T^{-1}], $p_i(\vec{x}, t)$ is the average pressure [$\mathrm{ML}^{-1}\mathrm{T}^{-2}$], $\rho_i(\vec{x}, t)$ is the mass density [ML^{-3}], λ_i is the mobility [$\mathrm{L}^3\mathrm{TM}^{-1}$], $\vec{g}$ is the gravity vector [LT^{-2}], $\vec{x}$ and t represent space vector and time respectively. ParFlow solves for the pressures on a discrete mesh and uses a time-stepping algorithm based on a mass conservative backward Euler scheme and spatial discretization (a finite volume method). ParFlow's multi–phase flow capability has not been applied in major studies, however, this capability is also available for testing (Ashby et al., 1993; Tompson et al., 1994; Falgout et al., 1999; Maxwell et al., 2016).

The transport equations included in the ParFlow package describe mass conservation in a convective flow (no diffusion) with degradation effects and adsorption included along with extraction and injection wells (Beisman et al., 2015; Maxwell et al., 2016). The transport equation is defined as follows:

$$\left(\frac{\partial}{\partial t}\left(\phi c_{i,j}\right)+\lambda_j \phi c_{i,j}\right)+\nabla.\left(c_{i,j}\vec{v}\right)=-\left(\frac{\partial}{\partial t}\left((1-\phi)\rho_s F_{i,j}\right)+\lambda_i(1-\phi)\rho_s F_{i,j}\right)+$$

$$\sum_k^{nI}\gamma_k^{I;i}\,\chi\Omega_k^I\left(c_{i,j}-c_{i,j}^{-k}\right)-\sum_k^{nE}\gamma_k^{E;i}\,\chi\Omega_k^E c_{i,j} \qquad (16)$$

where $c_{i,j}(\vec{x},t)$ represents concentration fraction of contaminant $[-]$, , λ_i is degradation rate $[\mathrm{T}^{-1}]$, $F_i(\vec{x},t)$ is the mass concentration $[\mathrm{L}^3\mathrm{M}^{-1}]$, $\rho_s(\vec{x})$ is the density of the solid mass $[ML^{-3}]$, n_I is injection wells $[-]$, $\gamma_k^{I;i}(t)$ is injection rate $[\mathrm{T}^{-1}]$, $\Omega_k^I(\vec{x})$ represent the area of the injection well $[-]$, $c_{i,j}^{-k}(\vec{x},t)$ is the injected concentration fraction $[-]$, n_E is the extraction wells $[-]$, $\gamma_k^{E;i}(t)$ is extraction rate $[\mathrm{T}^{-1}]$, $\Omega_k^E(\vec{x})$ is an extraction well area $[-]$, $i=0,\dots,n_{p-1}$ $\left(n_p\,\epsilon\{1,2,3\}\right)$ is the number of phases, $j=0,\dots,n_c-1$ represents the number of contaminants, $c_{i,j}$ is the concentration of contaminant j in phase i, k is hydraulic conductivity $[\mathrm{LT}^{-1}]$, $\chi\Omega_k^I$ is the characteristic function of an injection well region, and $\chi\Omega_k^E$ is the characteristic function of an extraction well region. The mass concentration term, $F_{i,j}$ is taken to be instantaneous in time and a linear function of contaminant concentration:

$$F_{i,j}=K_{d;j}c_{i,j} \qquad (17)$$

where $K_{d;j}$ is the distribution coefficient of the component $[\mathrm{L}^3\mathrm{M}^{-1}]$. The transport/advection equation or convective flow calculation performed by ParFlow offers a choice of a first-order explicit upwind scheme or a second-order explicit Godunov scheme. The advection calculations are discretized as boundary value problems for each primary dimension over each compute cell. The discretization is a fully-explicit, forward Euler first-order accurate in time approach. The implementation of a second-order explicit Godunov scheme (second-order advection scheme) minimizes numerical dispersion and presents accurate computational process at these time scales

than either an implicit or lower-order explicit scheme. Stability issue here is that the simulation timestep is restricted via the courant-Friedrichs-Lewy (CFL) condition, which demands that time steps are chosen small enough to ensure that mass not be transported more than one grid cell in a single timestep in order to maintain stability (Beisman, 2007).

2.5 Computational Grids

An accurate numerical approximation of a set of partial differential equations is strongly dependent on the simulation grid. Integrated hydrologic models can use unstructured or structured meshes for the discretization of the governing equations. The choice of grid type to adopt is problem-specific and often a subjective choice since the same domain can be represented in many ways, but there are some clear tradeoffs. For example, structured grid models, such as ParFlow, may be preferred to unstructured grid models because structured grids provide significant advantages in computational simplicity and speed, and are amenable to efficient parallelization (Durbin, 2002; Kumar et al., 2009; Osei-Kuffuor et al., 2014). ParFlow adopts a regular, structured grid specifically for its parallel performance. There are currently two regular grid formulations included in ParFlow, an orthogonal grid and a terrain-following formulation (TFG); both allow for variable vertical discretization (thickness over an entire layer) over the domain.

2.5.1 Orthogonal Grid

Orthogonal grids have many advantages, and many approaches are available to transform an irregular grid into an orthogonal grid such as conformal mapping. This mapping defines a transformed set of partial differential equations using an elliptical system with “control functions”

328 determined in such a way that the generated grid would be either orthogonal or nearly orthogonal.
329 However, conformal mapping may not allow flexibility in the control of the grid node distribution,
330 which diminishes its usefulness with complex geometries (Mobley and Stewart, 1980; Haussling
331 and Coleman, 1981; Visbal and Knight, 1982; Ryskin and Leal, 1983; Allievi and Calisal, 1992;
332 Eca, 1996).

333 A Cartesian, regular, orthogonal grid formulation is implemented by default in ParFlow,
334 though some adaptive meshing capabilities are still included in the source code. For example,
335 layers within a simulation domain can be made to have varying thickness. The upper portion of
336 Fig. 2 shows the standard way topography or any other non-rectangular domain boundaries are
337 represented in ParFlow. The domain limits, and any other internal boundaries, can be defined using
338 grid-independent triangulated irregular network (TIN) files that define a geometry, or a gridded
339 indicator file can be used to define geometric elements. ParFlow uses octree space partitioning
340 algorithm (a grid-based algorithm or mesh generators filled with structured grids) (Maxwell, 2013)
341 to depict complex structures/land surface representations (e.g. topography, watershed boundaries,
342 and different hydrologic facies) in three-dimensional space (Kollet et al., 2010). These land surface
343 features are mapped onto the orthogonal grid, and looping structures that encompass these irregular
344 shapes are constructed (Ashby et al., 1997). The grid cells above ground surface are inactive
345 (shown in upper region of Fig. 2) and are stored in the solution vector but not included in the
346 solution.

347 2.5.2 Terrain Following Grid

348 The inactive portion of a watershed defined with an orthogonal grid can be quite large in
349 complex watersheds with high-relief. In these cases, it is advantageous to use a grid that allows
350 these regions to be omitted. ParFlow's structured grid conforms to the topography via
351 transformation by the terrain following grid formulation. This transform alters the form of Darcy's
352 law to incorporate a topographic slope component. For example, subsurface fluxes are computed
353 separately in both x and y directions making use of the terrain following grid transform as:

354 $$q_x = K\sin(\theta_x) + K\frac{\partial p}{\partial x}\cos(\theta_x), \text{ and}$$

355 $$q_y = K\sin(\theta_y) + K\frac{\partial p}{\partial y}\cos(\theta_y) \qquad (18)$$

356 where q_x and q_y represent source/sink terms, such as fluxes, that include potential recharge flux
357 at the ground surface $[\mathrm{LT}^{-1}]$, p is the pressure head [L]; K is the saturated hydraulic conductivity
358 tensor , $[\mathrm{LT}^{-1}]$, θ is the local angle $[-]$ of topographic slope, S_x and S_y in the x and y directions
359 and may be presented as $\theta_x = \tan^{-1} S_x$ and $\theta_y = \tan^{-1} S_y$ respectively (Weill et al., 2009). The
360 terrain following grid formulation comes handy when solving coupled surface and subsurface
361 flows (Maxwell, 2013). The terrain following grid formulation uses the same surface slopes
362 specified for overland flow to transform the grid, whereas the slopes specified in the orthogonal
363 grid are only used for 2-D overland flow routing and do not impact the subsurface formulation
364 (see Fig. 2). Note that TIN files can still be used to deactivate portions of the transformed domain.
365

Figure 2 Caption: Representation of orthogonal (upper) and the terrain following (lower) grid formulations and schematics of the related finite difference dependences (left). The *i*, *j*, and *k* are the *x*, *y*, and *z* cell indices

3. Equation Discretization and Solvers

The core of the ParFlow code is its library of numerical solvers. As noted above, in most cases, the temporal discretization of the governing equations uses an implicit (backward Euler) scheme; with cell-centered finite differences in spatial dimensions. Different components of this solution framework have been developed for the various operational modes of ParFlow including an inexact Newton-Krylov nonlinear solver (Sect. 3.1), a multigrid algorithm (Sect. 3.2), and a multigrid-preconditioned conjugate gradient (MGCG) solver in (Sect. 3.3). The conditions, requirements, and constraints on the solvers depend on the specifics of the problem being solved, and some solvers tend to be more efficient (faster overall convergence) than others for a given problem. The core structure of these solvers and some of their implementation details are given below, with an emphasis on the main concepts behind each solver.

3.1 Newton–Krylov solver for Variably Saturated Flow

The cell-centered fully-implicit discretization scheme applied to Richards' equation leads to a set of coupled discrete nonlinear equations that need to be solved at each time step, and, for variably saturated subsurface flow, ParFlow does this with the inexact Newton-Krylov method

386 implemented in the KINSOL package (Hindmarsh et al., 2005; Collier et al., 2015). Newton-
387 Krylov methods were initially utilized in the context of partial differential equations by (Brown
388 and Saad, 1990). In the approach, coupled nonlinear system as a result of discretization of the
389 partial differential equation is solved iteratively. Within each iteration, the nonlinear system is
390 linearized via a Taylor expansion. After linearization, an iterative Krylov method is used to solve
391 the resulting linear Jacobian system (Woodward, 1998; Osei-Kuffuor et al., 2014). For variably
392 saturated subsurface flow, ParFlow uses the GMRES Krylov method (Saad and Schultz, 1986).
393 Figure 3 is a flow chart of the solution technique ParFlow uses to provide approximate solutions
394 to systems of nonlinear equations.
395
396 Figure 3 caption: Working flow chart of ParFlow's solver for linear and non-linear system solution
397
398 The benefit of this Newton-Krylov method is that the Krylov linear solver requires only
399 matrix-vector products. Because the system matrix is the Jacobian of the nonlinear function, these
400 matrix-vector products may be approximated by taking directional derivatives of the nonlinear
401 function in the direction of the vector to be multiplied. This approximation is the main advantage
402 of the Newton-Krylov approach as it removes the requirement for matrix entries in the linear
403 solver. An inexact Newton method is derived from a Newton method by using an approximate
404 linear solver at each nonlinear iteration, as is done in the Newton-Krylov method (Dembo et al.,
405 1982; Dennis and Schabel, 1996). This approach takes advantage of the fact that when the
406 nonlinear system is far from converged, the linear model used to update the solution is a poor

approximation. Thus, the convergence criteria of early linear system solve is relaxed. The tolerance required for solution of the linear system is decreased as the nonlinear function residuals approach zero. The convergence rate of the resulting nonlinear solver can be linear or quadratic, depending on the algorithm used. Through the KINSOL package, ParFlow can either use a constant tolerance factor or ones from (Eisenstat and Walker, 1996). Krylov methods can be very robust, but they can be slow to converge. As a result, it is often necessary to implement a preconditioner, or accelerator, for these solvers.

3.2 Multigrid Solver

Multigrid (MG) methods constitute a class of techniques or algorithms for solving differential equations (system of equations) using a hierarchy of discretization (Volker, 1987; Briggs et al., 2000). Multigrid algorithms are applied primarily to solve linear and nonlinear boundary value problems and can be used as either preconditioners or solvers. The most efficient method for preconditioning the linear systems in ParFlow is the ParFlow Multigrid algorithm (PFMG) (Ashby and Falgout, 1996; Jones and Woodward, 2001). Multigrid algorithms arise from discretization of elliptic partial differential equations (Briggs et al., 2000), and, in ideal cases, have convergence rates that do not depend on the problem size. In these cases, the number of iterations remains constant even as problems sizes grow large. Thus, the algorithm is algorithmically scalable. However, it may take longer to evaluate each iteration as problem sizes increase. As a result, ParFlow utilizes the highly efficient implementation of PFMG in the hypre library (Falgout and Yang, 2002).

For variably saturated subsurface flow, ParFlow uses the Newton-Krylov method coupled with a multigrid preconditioner to accurately solve for the water pressure (hydraulic head) in the subsurface and diagnoses the saturation field (which is used in determining the water table). (Woodward, 1998; Jones and Woodward, 2000, 2001; Kollet et al., 2010). The water table is calculated for computational cells having hydraulic heads above the bottom of the cells. Generally, a cell is saturated if the hydraulic head in the cell is above the node elevation (cell center) or the cell is unsaturated if the hydraulic head in the cell is below the node elevation. For saturated flow, ParFlow uses the conjugate gradient method also coupled with a multigrid method. It is important to note that subsurface flow systems are usually much larger radially than they are thick, so it is common for the computational grids to have highly anisotropic cell aspect ratios to balance the lateral and vertical discretization. Combined with anisotropy in the permeability field, these high aspect ratios produce numerical anisotropy in the problem, which can cause the multigrid algorithms to converge slowly (Jones and Woodward, 2001). To correct this problem, a semicoarsening strategy or algorithm is employed, where the grid is coarsened in one direction at a time. The direction chosen is the one with the smallest grid spacing i.e. the tightest coupling. In an instance where more than one direction has the same minimum spacing, then the algorithm chooses the direction in the order of x, followed by y, and then in z. To decide on how and when to terminate the coarsening algorithm, Ashby and Falgout (1996) determined that a semicoarsening down to a $(1 \times 1 \times 1)$ grid is ideal for groundwater problems.

3.3 Multigrid-Preconditioned Conjugate Gradient (MGCG)

ParFlow uses the multigrid-preconditioned conjugate gradient (CG) solver to solve the groundwater equations under steady-state, and fully saturated flow conditions (Ashby and Falgout, 1996). These problems are symmetric and positive definite, two properties for which the CG method was designed to target. While CG lends itself to efficient implementations, the number of iterations required to solve a system such as results from discretization of the saturated flow equation increases as the problem size grows. The PFMG multigrid algorithm is used as a preconditioner to combat this growth and results in an algorithm for which the number of iterations required to solve the system grows only minimally. See Ashby and Falgout (1996) for a detailed description of these solvers and the parallel implementation of the multigrid preconditioned CG method in ParFlow (Gasper et al., 2014; Osei-Kuffuor et al., 2014).

3.4 Preconditioned Newton-Krylov for Coupled Subsurface – Surface Flows

As discussed above, coupling between subsurface and surface or overland flow in ParFlow is activated by specifying an overland boundary condition at the top surface of the computational domain, but this mode of coupling allows for activation and deactivation of the overland boundary condition during simulations where ponding or drying occur. Thus, surface-subsurface coupling can occur anywhere in the domain during a simulation and it can change dynamically during the simulation. Overland flow may occur by the Dunne or Horton mechanism depending on local dynamics. Overland flow routing is enabled when the subsurface cells are fully saturated. In ParFlow the coupling between the subsurface and surface flows is handled implicitly. ParFlow solves this implicit system with the inexact Newton-Krylov method described above.

However, in this case, the preconditioning matrix is adjusted to include terms from the surface coupling. In the standard saturated or variably saturated case, the multigrid method is given the linear system matrix, or a symmetric version, resulting from discretization of the subsurface model. Because ParFlow uses a structured mesh, these matrices have a defined structure making their evaluation and application of multigrid straightforward. Due to varying topographic height of the surface boundary, where the surface coupling is enforced, the surface effects add non-structured entries in the linear system matrices. These entries increase complexity of the matrix entry evaluations and reduce effectiveness of the multigrid preconditioner. In this case, the matrix-vector products are most effectively performed through computation of the linear system entries, rather than the finite difference approximation to the directional derivative. For the preconditioning, surface couplings are only included if they model flow between cells at the same vertical height i.e. in situations where overland flow boundary conditions are imposed or activated. This restriction maintains the structured property of the preconditioning matrix while still including much of the surface coupling in the preconditioner. Both these adjustments led to considerable speedup in coupled simulations (Osei-Kuffuor et al., 2014).

4. Parallel Performance Efficiency

Scaling efficiency metrics offer a quantitative method for evaluating the performance of any parallel model. Good scaling generally means that the efficiency of the code is maintained as the solution of the system of equations is distributed onto more processors or as the problem resolution is refined and processing resources are added. Scalability can depend on the problem

size, the processor number, the computing environment, and the inherent capabilities of the computational platform used e.g. choice of a solver. The performance of ParFlow (or any parallel code) is typically determined through weak and strong scaling (Gustafson, 1988). Weak scaling involves the measurement of code's efficiency in solving problems of increasing size (i.e. describes how the solution time change with change in the number of processors for a fixed problem size per processor). In weak scaling, the simulation time should remain constant, as the size of the problem and number of processing elements grow such that the same amount of work is conducted on each processing element. Following Gustafson (1988), scaled parallel efficiency is given by:

$$E(n,p) = \frac{T(n,1)}{T(pn,p)} \tag{19}$$

where $E(n,p)$ denotes parallel efficiency, T represents the run time as a function of the problem size n, which is spread across several processors p. Parallel code is said to be perfectly efficient if $E(n,p) = 1$, and the efficiency decreases as $E(n,p)$ approaches 0. Generally, parallel efficiency decreases with increasing processor number as communication overhead between nodes/processors becomes the limiting factor.

Strong scaling describes the measurement of how much the simulation or solution time changes with the number of processors for a given problem of fixed total size (Amdahl, 1967). In strong scaling, a fixed size task is solved on a growing number of processors, and the associated time needed for the model to compute the solution is determined (Woodward, 1998; Jones and Woodward, 2000). If the computational time decreases linearly with the processor number, a

perfect parallel efficiency, (E = 1) results. The value of E is determined using Eq. (19). ParFlow has been shown to have excellent parallel performance efficiency, even for large problem sizes and processor counts (see Table 1) (Ashby and Falgout, 1996; Kollet and Maxwell, 2006). In situations where ParFlow works in conjunction with or coupled to other subsurface, land surface or atmospheric models (see Sect. 5) i.e. increased computational complexity by adding different components or processes, improved computational time may not only depend on ParFlow. The computational cost of such an integrated model is extremely difficult to predict because of the nonlinear nature of the system. The solution time may depend on number of factors including the number of degrees of freedom, the heterogeneity of the parameters, which processes are active (e.g. snow accumulation compared to nonlinear snowmelt processes in land surface model or the switching on or off of the overland flow routing in ParFlow). The only way to know how fast a specific problem will run is to try that problem. Many of the studies presented in Table 1 include computational times for problems with different complexities where ParFlow was used. In a scaling study with ParFlow, Maxwell (2013) examined the relative performance of preconditioning the coupled variably saturated subsurface and surface flow system with the symmetric portion or full matrix for the system. Both options use ParFlow's multigrid preconditioner. Solver performance was demonstrated by combining the analytical Jacobian and the non-symmetric linear preconditioner. The study showed that the non-symmetric linear preconditioner presents faster computational times and efficient scaling . A section of the study results is reproduced in Table 1, in addition to other scaling studies demonstrating ParFlow's parallel efficiency. This tradeoff was also examined in Jones and Woodward (2000).

It is worth noting that large and/or complex problem sizes (e.g. simulating a large heterogenous domain size with over 8.1 billion unknowns) will always take time to solve directly, but the approach for setting up a problem depends on the specific problem being modeled. Even for one specific kind of model there may be multiple workflows and how to model such complexity becomes sole responsibility of the modeler. The studies involving ParFlow outlined in Table 1 provide a wealth of knowledge regarding domain setup for problems of different complexities. Since these are all specific applications, their information will likely be very useful to modelers trying to build a new domain during the setup and planning phases.

Table 1: Details for the various parallel scaling studies conducted using ParFlow.

5. Coupling

Different integrated models including atmospheric or weather prediction models (e.g. Weather Research Forecasting Model, Advanced Regional Prediction System, Consortium for Small-Scale Modeling), land surface models (e.g. Common Land Model, Noah Land Surface Model), and a subsurface model (e.g. CruchFlow) have been coupled with ParFlow to simulate a variety of coupled earth system effects (see Figure 4(a)). Coupling between ParFlow and other integrated models was performed to better understand the physical processes that occur at the interfaces between the deeper subsurface and ground surface, and between the ground surface and the atmosphere. None of the individual models can achieve this on their own because ParFlow cannot

552 account for land surface processes (e.g. evaporation), and atmospheric and land surface models
553 generally do not simulate deeper subsurface flows (Ren and Xue, 2004; Chow et al., 2006;
554 Beisman, 2007; Maxwell et al., 2007; Shi et al., 2014). Model coupling can be achieved either via
555 "offline coupling" where models involved in the coupling process are run sequentially and
556 interactions between them is one–way (i.e. information is only transmitted from one model to the
557 other) or "online" where they interact and feedback mechanisms among components are
558 represented (Meehl et al., 2005; Valcke et al., 2009). Each of the coupled models uses its own
559 solver for the physical system it is solving, then information is passed between the models. As
560 long as each model exhibits good parallel performance, this approach still allows for simulations
561 at very high resolution, with a large number of processes (Beven, 2004; Ferguson and Maxwell,
562 2010; Shen and Phanikumar, 2010; Shi et al., 2014). This section focuses on the major couplings
563 between ParFlow and other codes. We point out specific functions of the individual models as
564 stand–alone codes that are relevant to the coupling process. In addition, information about the role
565 or contribution of each model at the coupling interface (see Fig. 4(b)) that connects with ParFlow
566 are presented (Fig. 5 shows the communication network of the coupled models). We discuss
567 couplings between ParFlow and its land surface model (a modified version of the original Common
568 Land Model introduced by Dai et al., (2003)), Consortium for Small-Scale Modeling (COSMO),
569 Weather Research Forecasting Model, Advanced Regional Prediction System, and CruchFlow in
570 sections 5.1, 5.2, 5.3, 5.4, and 5.5 respectively.

571 Figure 4(a) Caption: A pictorial description of the relevant physical environmental features and
572 model coupling. CLM represents the Community Land Model, a stand-alone Land Surface Model

573 (LSM) via which ParFlow couples' COSMO. The modified version of CLM by Dai et al., (2003)
574 and is not shown in Fig. 4(a) because it is a module only for ParFlow, not really a stand-alone
575 LSM any longer.
576
577 Figure 4(b) Caption: Schematic showing information transmission at the coupling interface. PF,
578 LSM, and ATM indicate the portions of the physical system simulated by ParFlow, Land Surface
579 Models, and Atmospheric Models respectively. The downward and upward arrows indicate the
580 directions of information transmission between adjacent models. Note: Coupling between ParFlow
581 and CrunchFlow (not shown) occur within the subsurface.

582 5.1 ParFlow–Common Land Model (PF.CLM)

583 The Common Land Model (CLM) is a land surface model designed to complete land-
584 water-energy balance at the land surface (Dai et al., 2003). CLM parameterizes the moisture,
585 energy and momentum balances at the land surface and includes a variety of customizable land
586 surface characteristics and modules, including land surface type (land cover type, soil texture, and
587 soil color), vegetation and soil properties (e.g. canopy roughness, zero-plane displacement, leaf
588 dimension, rooting depths, specific heat capacity of dry soil, thermal conductivity of dry soil,
589 porosity), optical properties (e.g. albedos of thick canopy), and physiological properties related to
590 the functioning of the photosynthesis-conductance model (e.g. green leaf area, dead leaf, and stem
591 area indices). A combination of numerical schemes is employed to solve the governing equations.
592 CLM uses a time integration scheme which proceeds by a split-hybrid approach, where the solution
593 procedure is split into "energy balance" and "water balance" phases in a very modularized structure

(Mikkelson et al., 2013; Steiner et al., 2005, 2009). The CLM described here and as incorporated in ParFlow is a modified version of the original CLM introduced by Dai et al., (2003), though the original version was coupled to ParFlow in previous model applications (e.g. Maxwell and Miller, 2005). The current coupled model, PF.CLM consist of ParFlow incorporated with land surface model Jefferson et al., (2015), (2017), and Jefferson and Maxwell, (2015). The modified CLM is composed of a series of land surface modules that are called as a subroutine within ParFlow to compute energy and water fluxes (e.g. evaporation and transpiration) to and out of the soil. For example, the modified CLM computes bare ground surface evaporative flux, E_{gr} as

$$E_{gr} = -\beta \rho_a u_* q_* \tag{20}$$

where β (dimensionless) denotes soil resistance factor, ρ_a represents air density [ML^{-3}], u_* represents friction velocity [LT^{-1}], and q_* (dimensionless) stands for humidity scaling parameter (Jefferson and Maxwell, 2015). Evapotranspiration for vegetated land surface, E_{veg} is computed as

$$E_{veg} = \left[R_{pp,dry} + L_w\right] L_{SAI} \left[\frac{\rho_a}{r_b}\left(q_{sat} - q_{af}\right)\right] \tag{21}$$

where r_b is the air density boundary resistance factor [LT^{-1}], q_{sat} (dimensionless) is saturated humidity at the land surface, and q_{af} (dimensionless) is the canopy humidity. Combination of q_{sat} and q_{af} forms the potential evapotranspiration. The potential evapotranspiration is divided into transpiration $R_{pp,dry}$ (dimensionless) which depends on the dry fraction of the canopy, and evaporation from foliage covered by water L_w (dimensionless). L_{SAI} (dimensionless) is summation of the leaf and stem area indices which estimates the total surface from which evaporation can

occur. A detailed description of the equations CLM of PF.CLM uses can be found in Jefferson et al., (2015), (2017), and Jefferson and Maxwell, (2015).

PF.CLM simulates variably saturated subsurface flow, surface or overland flow, and above-ground processes. PF.CLM was developed prior to the current community land model (see Sect. 5.2), and the module structure of the current and early versions are different. PF.CLM has been updated over the years to improve its capabilities. PF.CLM was first done in the early 2000's, as an undiversified, a column proof-of-concept model, where data or message was transmitted between the coupled models via input/output files (Maxwell and Miller, 2005). Later, PF.CLM was presented in a distributed or diversified approach with a parallel input/output file structure where CLM is called as a set sequence of steps within ParFlow (Kollet and Maxwell, 2008a). These modifications, for example, were done to incorporate subsurface pressure values from ParFlow into chosen computations (Jefferson and Maxwell, 2015). These, to some extent differentiate the modified version (PF.CLM) from the original CLM by Dai et al., (2003). Within the coupled PF.CLM, ParFlow solves the governing equations for overland and subsurface flow systems and the CLM modules add the energy balance and mass fluxes from the soil, canopy, and root zone that can occur (i.e. interception, evapotranspiration etc.) (Jefferson and Maxwell, 2015).

At the coupling interface where the models overlap and undergo online communication (Fig. 4(b)), ParFlow calculates and passes soil moisture as well as pressure heads of the subsurface to CLM, and CLM calculates and transmits transpiration from plants, canopy and ground surface evaporation, snow accumulation and melt, and infiltration from precipitation to ParFlow (Ferguson et al., 2016). In short, CLM does all canopy water balances and snow, but once the water through

falls to the ground, or snow melts, ParFlow takes over and estimates the water balances via the nonlinear Richards' equation. The coupled model, PF.CLM, has been shown to more accurately predict root-depth soil moisture compared to the uncoupled model i.e. stand-alone land surface model (CLM) with capability of computing near surface soil moisture. This increased accuracy results from the coupling of soil saturations determined by ParFlow and their impacts on other processes including runoff and infiltration (Kollet, 2009; Shrestha et al., 2014; Gebler et al., 2015; Gilbert and Maxwell, 2016). For example, (Maxwell and Miller, 2005) found that simulations of deeper soil saturation (more than 40cm) vary between PF.CLM and uncoupled models, with PF.CLM simulations closely matching the observed data. Table 2 contains summaries of studies conducted with ParFlow coupled to either the original version of CLM by (Dai et al., 2003) or modified CLM (ParFlow with land surface model).

5.1.1. ParFlowE–Common Land Model (ParFlowE[CLM])

It is well established that ParFlow in conjunction with CLM does perform well in estimating all canopy water and subsurface water balances (Maxwell and Miller, 2005; Mikkelson et al., 2013; Ferguson et al., 2016). ParFlow, as a component of the coupled model has been modified into a new parallel numerical model, ParFlowE to incorporate the more complete heat equation coupled to variably saturated flow. ParFlowE simulates coupling of terrestrial hydrologic and energy cycles i.e. coupled moisture, heat, and vapor transport in the subsurface. ParFlowE is based on the original version of ParFlow having identical solution schemes and coupling approach with CLM. A coupled three-dimensional subsurface heat transport equation is implemented in ParFlowE using a cell-centered finite difference scheme in space and an implicit backward Euler

differencing scheme in time. However, the solution algorithm employed in ParFlow is fully exploited in ParFlowE where the solution vector of the Newton-Krylov method was extended to two dimensions (Kollet et al., 2009). In some integrated and climate models, the convection term of subsurface heat flux and the effect of soil moisture on energy transport is neglected due to simplified parameterizations and computational limitations. However, both convection and conduction terms are considered in ParFlowE (Khorsandi et al., 2014). In ParFlowE, functional relationships (i.e. equations of state) are performed to relate density and viscosity to temperature and pressure, and thermal conductivity to saturation. That is, modeling thermal flows by relating these parameterizations in simulating heat flow is an essential component of ParFlowE. In coupling between ParFlowE and CLM, ParFlowE[CLM], the one-dimensional subsurface heat transport in the CLM is replaced by the three-dimensional heat transport equation including the process of convection of ParFlowE. CLM computes mass and energy balances at ground surface that lead to moisture fluxes and pass these fluxes to the subsurface moisture algorithm of ParFlowE[CLM]. These fluxes are used in computing subsurface moisture and temperature fields which are then passed back to the CLM.

5.2 ParFlow in the Terrestrial Systems Modeling Platform, TerrSysMP

ParFlow is part of the Terrestrial System Modeling Platform TerrSysMP, which comprise the nonhydrostatic fully compressible limited-area atmospheric prediction model, COSMO, designed for both operational numerical weather prediction and various scientific applications on the meso–β (horizontal scales of 20–200km) and meso–γ (horizontal scales of 2–20km) (Duniec

and Mazur, 2011; Levis and Jaeger, 2011; Bettems et al., 2015), and the Community Land Model version 3.5 (CLM3.5). Currently, it is used in direct simulations of severe weather events triggered by deep moist convection, including intense mesoscale convective complexes, prefrontal squall–line storms, supercell thunderstorms, and heavy snowfall from wintertime mesocyclones. COSMO solves nonhydrostatic, fully compressible hydro–thermodynamical equations in advection form using the traditional finite difference method (Vogel et al., 2009; Mironov et al., 2010; Baldauf et el., 2011; Wagner et al., 2016).

An online coupling between ParFlow and the COSMO model is performed via CLM3.5 (Gasper et al., 2014; Shrestha et al., 2014; Keune et al., 2016). Similar to the Common Land Model (by (Dai et al., 2003)), CLM3.5 module accounts for surface moisture, carbon, and energy fluxes between the shallow or near-surface soil (discretized/specified top soil layer), snow, and the atmosphere (Oleson et al., 2008). The model components of a fully coupled system consisting of COSMO, CLM3.5, and ParFlow are assembled by making use of the multiple–executable approach (e.g. with OASIS3-MCT model coupler). The OASIS3-MCT coupler employs communication strategies based on the message passing interface standards, MPI1/MPI2 and the Project for Integrated Earth System Modeling, PRISM, Model Interface Library (PSMILe) for parallel communication of two–dimensional arrays between OASIS3-MCT coupler and the coupling models (Valcke et al., 2012; Valcke, 2013). The OASIS3-MCT specifies the series of coupling, frequency of the couplings, the coupling fields, the spatial grid of the coupling fields, transformation type of the (two–dimensional) coupled fields, and simulation time management and integration.

At the coupling interface, the OASIS3-MCT interface interchanges the atmospheric forcing terms and the surface fluxes in serial mode. The lowest level and current time step of the atmospheric state of COSMO is used as the forcing term for CLM3.5. CLM3.5 then computes and returns the surface energy and momentum fluxes, outgoing longwave radiation, and albedo to COSMO (Baldauf et al., 2011). The air temperature, wind speed, specific humidity, convective and grid-scale precipitation, pressure, incoming shortwave (direct and diffuse) and longwave radiation, and measurement height are sent from COSMO to CLM3.5. In CLM3.5, a mosaic/tilling approach may be used to represent the subgrid-scale variability of land surface characteristics, which considers a certain number of patches/tiles within a grid cell. The surface fluxes and surface state variables are first calculated for each tile and then spatially averaged over the whole grid cell (Shrestha et al., 2014) . As with PF.CLM3.5, the one–dimensional soil column moisture predicted by CLM3.5 gets replaced by ParFlow's variably saturated flow solver, so ParFlow is responsible for all calculations relating soil moisture redistribution and groundwater flow. Within the OASIS3-MCT ParFlow sends the calculated pressure and relative saturation for the coupled region soil layers to CLM3.5. The CLM3.5 also transmits depth-differentiated source and sink terms for soil moisture including soil moisture flux e.g. precipitation, and soil evapotranspiration for the coupled region soil layers to ParFlow. Applications of TerrSysMP in fully coupled mode from saturated subsurface across the ground surface into the atmosphere include a study on the impact of groundwater on the European heat wave 2003 and the influence of anthropogenic water use on the robustness of the continental sink for atmospheric moisture content (Keune et al., 2016).

5.3 ParFlow–Weather Research Forecasting models (PF.WRF)

719 The Weather Research and Forecast (WRF) is a mesoscale numerical weather prediction
720 system designed to be flexible and efficient in a massively parallel computing architecture. WRF
721 is a widely used model that provides a common framework for idealized dynamical studies, full
722 physics numerical weather prediction, air-quality simulations, and regional climate simulations
723 (Michalakes et al., 1999, 2001; Skamarock et al., 2005). The model contains numerous mesoscale
724 physics options such as microphysics parameterizations (including explicitly resolved water vapor,
725 cloud, and precipitation processes), surface layer physics, shortwave radiation, longwave
726 radiation, land surface, planetary boundary layer, data assimilation, and other physics and
727 dynamics alternatives suitable for both large-eddy and global-scale simulations. Similar to
728 COSMO, the WRF model is a fully compressible, conservative-form, non-hydrostatic atmospheric
729 model which uses time-splitting integration techniques (discussed below) to efficiently integrate
730 the Euler equations (Skamarock and Klemp, 2007).
731 The online ParFlow WRF coupling (PF.WRF) extends the WRF platform down to bedrock
732 by including highly resolved three-dimensional groundwater and variably saturated shallow or
733 deep vadose zone flows, and a fully integrated lateral flow above ground surface (Molders and
734 Ruhaak, 2002; Seuffert et al., 2002; Anyah et al., 2008; Maxwell et al., 2011). The land surface
735 model portion that links ParFlow to WRF is supplied by WRF through its land surface component,
736 the Noah Land Surface Model (Ek et al., 2003); the standalone version of WRF has no explicit
737 model of subsurface flow. Energy and moisture fluxes from the land surface are transmitted
738 between the two models via the Noah LSM which accounts for the coupling interface, and which
739 is conceptually identical to the coupling in PF-COSMO. The three-dimensional variably saturated

subsurface and two-dimensional overland flow equations, and the three-dimensional atmospheric equations given by ParFlow and WRF are simultaneously solved by the individual model solvers. Land surface processes, such as evapotranspiration, are determined in the Noah LSM as a function of potential evaporation and vegetation fraction. This effect is calculated with the formulation:

$$E(x) = F^{fx}(1 - f_{avg})E_{pot} \quad (22)$$

where $E(x)$ stands for rate of soil evapotranspiration (length per unit time), fx represents empirical coefficient, f_{avg} denotes vegetation fraction, and E_{pot} is potential evaporation, determined that depends on atmospheric conditions from the WRF boundary layer parameterization (Ek et al., 2003). The vegetation fraction is zero over bare soils (i.e. only soil evaporation), so Eq. 22 becomes:

$$E(x) = F^{fx}E_{pot} \quad (23)$$

The quantity F is parameterized as follows:

$$F = \frac{\phi S_w - \phi S_{res}}{\phi - \phi S_{res}}, \quad (24)$$

where ϕ is the porosity of the medium, S_w and S_{res} are relative saturation and residual saturation respectively, from vanGenuchten relationships (VanGenuchten, 1980; Williams and Maxwell, 2011). Basically, F refers to the parameterization of the interrelationship between evaporation and near-ground soil water content and provides one of the connections between Noah LSM and ParFlow, and thus WRF.

In the presence of a vegetation layer, plant transpiration (length per unit time) is determined as follows:

$$T = G(z)C_{plant}f_{veg}E_{pot}, \quad (25)$$

where $C_{plant}(-)$ represents a constant coefficient between 0 and 1, which depends on vegetation species, and the $G(z)$ function represents soil moisture which provides other connection between the coupled models (i.e. ParFlow, Noah, and WRF). The solution procedure of PF.WRF uses an operator–splitting approach where both model components use the same time step. WRF soil moisture information including runoff, surface ponding effects, unsaturated and saturated flow, which includes an explicitly resolved water table are calculated and sent directly to the Noah LSM within WRF by ParFlow and utilized by the Noah LSM in the next time step. WRF supplies ParFlow with evapotranspiration rates and precipitation via the Noah LSM (Jiang et al., 2009). The interdependence between energy and land balance of the subsurface, ground surface, and lower atmosphere can fully be studied with this coupling approach. The coupled PF.WRF via the Noah-LSM has been used to simulate explicit water storage and precipitation within basins, to simulate surface runoffs and to simulate the land-atmosphere feedbacks and wind patterns as a results of subsurface heterogeneity (Maxwell et al., 2011; Williams and Maxwell, 2011). Studies with coupled model PF.WRF are highlighted in Table 2.

5.4 ParFlow–Advanced Regional Prediction System (PF. ARPS).

The Advanced Regional Prediction System (ARPS) composed of a parallel mesoscale atmospheric model created to explicitly predict convective storms and weather systems. The ARPS platform aids in effectively investigating the changes and predictability of storm-scale weather in both idealized and more realistic settings. The model deals with the three dimensional, fully compressible, non-hydrostatic, spatially filtered Navier-Stokes equations (Rihani et al., 2015). The

781 governing equations include conservation of momentum, mass, water, heat or thermodynamic,
782 turbulent kinetic energy, and the equation of state of moist air making use of a terrain-following
783 curvilinear coordinate system (Xue et al., 2000). The governing equations presented in a
784 coordinate system with z as the vertical coordinate are given as

785 $$\frac{dv}{dt} = -2\Omega \times v - \frac{1}{\rho}\nabla P + g + F \quad (26)$$

786 $$\frac{d\rho}{dt} = -\rho\nabla . v \quad (27)$$

787 $$\frac{dT}{dt} = -\frac{RT}{C_v}\nabla . v + \frac{Q}{C_v} \quad (28)$$

788 $$P = \rho RT \quad (29)$$

789 Equations (26) to (29) are momentum, continuity, thermodynamic and equation of state,
790 respectively. The material (total) derivative d/dt is defined as

791 $$\frac{d}{dt} = \frac{\partial}{\partial t} + \nabla . v \quad (30)$$

792 The variables v, ρ, T, P, g, F, Q in Eq. (26) to (29) represent velocity [LT^{-1}], density [ML^{-3}],
793 temperature [K], pressure [$ML^{-1}T^{-2}$], gravity [LT^{-2}], frictional force [MLT^{-2}], and the diabatic
794 heat source [$ML^{-2}T^{-2}$], respectively (Xu et al., 1991). The ARPS model employs high-order
795 monotonic advection technique for scalar transport and fourth-order advection for other variables
796 e.g. mass density and mass mixing ratio. A split-explicit time advancement scheme is utilized with
797 leapfrog on the large time steps, and an explicit and implicit scheme for the smaller time steps is
798 used to inculcate the acoustic terms in the equations (Rihani et al., 2015).

The PF.ARPS forms a fully–coupled model that simulates spatial variations in above ground processes and feedbacks, forced by physical processes in the atmosphere and the below the ground surface. In the online coupling process, ARPS land surface model forms the interface between ParFlow and ARPS to transmit information (i.e. surface moisture fluxes) between the coupled models. ParFlow as a component of the coupled model replaces the subsurface hydrology in the ARPS land surface model. Thus, ARPS is integrated into ParFlow as a subroutine to create a numerical overlay at the coupling interphase (specified layers of soil within the land surface model in ARPS) with the same number of soil layers at the ground surface within ParFlow. The solution approach employed is an operator-splitting that allows ParFlow to match the ARPS internal timesteps. ParFlow calculates the subsurface moisture field at each timestep of a simulation and passes the information to ARPS land surface model, which is used in each subsequent timestep. At the beginning of each time step, the surface fluxes from ARPS that are important to ParFlow include evapotranspiration rate and spatially–variable precipitation (Maxwell et al., 2007). PF. ARPS has been applied to investigate the effects of soil moisture heterogeneity on atmospheric boundary layer processes. PF.ARPS keeps a realistic soil moisture that is topographically-driven distribution and shows spatiotemporal relationship between water depth, land surface and lower atmospheric variables (Maxwell et al., 2007; Rihani et al., 2015). A summary of current studies involving PF. ARPS is included in Table 2.

5.5 ParFlow–CrunchFlow (ParCrunchFlow)

CrunchFlow is a software package developed to simulate multicomponent multi-dimensional reactive flow and transport in porous and/or fluid media (Steefel, 2009). Systems of chemical reactions that can be solved by the code include kinetically controlled homogenous and heterogeneous mineral dissolution reactions, equilibrium–controlled homogeneous reactions, thermodynamically controlled reactions, and biologically–mediated reactions (Steefel and Lasaga, 1994; Steefel and Yabusaki, 2000). In CrunchFlow, discretization of the governing coupled partial differential equations which connect subsurface kinetic reactions and multicomponent equilibrium, flow and solute transport is based on finite volume. (Li et al., 2007; Li et al., 2010). Coupling of reactions and transport in CrunchFlow that are available at runtimes are performed using two approaches. These are briefly discussed below.

First, a global implicit or one–step method approach is based on a backwards Euler time discretization, with a global solution of the coupled reactive transport equations using Newton's method. This global implicit scheme solves the transport and reaction terms simultaneously (up to two-dimensional) (Kirkner and Reeves, 1988; Steefel, 2009). Second, a time or operator splitting of the reaction and transport terms which is based on an explicit forward Euler method; the sequential non-iterative approach, SNIA (in which the transport and reaction terms are solved) (Steefel and Van Cappellen, 1990; Navarre-Sitchler et al., 2011). The stability criteria associated with the explicit approach is that the simulation timestep is restricted via the courant-Friedrichs-Lewy (CFL) condition, under the circumstance that the transportation of mass does not occur over multiple grid cell, but a single grid cell in a timestep. Thus, a small-time step must be used to ensure this condition holds. This small step size may lead to simulations that will demand much

time to solve Beisman, (2007), so more processors are used, in order to decrease the processor workload and decrease solution time of the simulation. Coupling of fully saturated flow to the reactive transport calculations and coupling between a partially saturated flow and transport (flow and diffusion) can be done successively. However, these simulations require calculations of the flow and liquid saturation fields with a different model.

ParCrunchFlow is a parallel reactive transport model developed by combining ParFlow with CrunchFlow. ParCrunchFlow was designed to be only applicable for subsurface simulation. The coupled model relies on ParFlow's robustness ability to efficiently represent heterogeneous domains and simulate complex flow to provide a more realistic representation of the interactions between biogeochemical processes and non-uniform flow fields in the subsurface than the uncoupled model. ParFlow provides solution of Richards' equation to ParCrunchFlow, which is not present in the biogeochemical code CrunchFlow. ParCrunchFlow employs operator-splitting method to reactive transport, in which the transport and reaction terms are decoupled and calculated independently. Online coupling between the models is achieved through a sequential non-iterative approach, where the reaction terms in CrunchFlow's operator-splitting solver gets connected to ParFlow's advection terms. ParCrunchFlow takes advanatage of multidimensional advection capability of ParFlow instead of CrunchFlow's advective-dispersive transport capabilities (up to two-dimensional). A steady state governing differential equation for reaction and advection (with no dispersion and diffusion terms) in a single-phase system is given by

$$\frac{\partial C_i}{\partial t} + \nabla.(vC_i) - R_i = 0\,, \quad (i = 1,\, N_{tot}\ ) \tag{31}$$

where C_i is the concentration of species i, v represents velocity of flow, R_i indicates total reaction rate of species i, and N_{tot} represents total species number. In the coupling process, the advection terms are calculated by ParFlow's transport solver through a first-order explicit upwind scheme or a second-order explicit Godunov scheme. Low-order upwind weighting schemes can introduce numerical dispersion, which can impact the simulated reactions, and a comparison of several upwinding schemes can be found in (Benson et al., 2017). CrunchFlow calculates the reaction terms using the Newton-Raphson method. For example, in the coupled–model ParCrunchFlow, ParFlow code assigns all hydrological parameters, undertakes the functions relating to parallelization including domain decomposition and message transmission, and solves for pressure and flow fields. The CrunchFlow module is then used to evaluate all reaction terms and conversions between mobile and immobile concentrations. Sequence of simulations of a floodplain aquifer, comprising biologically mediated reduction of nitrate have been performed with ParCrunchFlow. The simulations demonstrate that ParCrunchFlow realistically represents the changes in chemical concentrations seen in most field scale systems than CrunchFlow alone (summarized in Table 2) (Beisman, 2007; Beisman et al., 2015).

Figure 5 Caption: Schematic of the communication structure of the coupled models. Note: CLM represents a stand-alone Community Land Model. The modified version of CLM by Dai et al., (2003) is not shown here because it is a module only for ParFlow, not really a stand-alone LSM any longer.

6. Discussion and Summary

IHMs constitute classes of simulation tools ranging from simple lumped parameter models to comprehensive deterministic, distributed and physically based modeling systems for simulation of multiple hydrological processes (LaBolle et al., 2003; Castronova et al., 2013). They are indispensable in studying the interactions between surface and subsurface systems. IHMs that calculate surface and subsurface flow equations in a single matrix (Maxwell et al., 2015), scaling from the beginning parts to the mouth of continental river basins at high-resolutions are essential (Wood, 2009) in understanding and modeling surface-subsurface systems. IHMs have been used to address surface and subsurface science and applied questions. For example, evaluating the effects of groundwater pumping on streamflow and groundwater resources (Markstrom et al., 2008), evaluating relationship between topography and groundwater (Condon and Maxwell, 2015), coupling water flow and transport (Sudicky et al., 2008; Weill et al., 2011) and assessing the resilience of water resources to human stressors or interventions and the variations in the (Maxwell et al., 2015) over large spatial extents at high resolution. Modeling or simulation at large spatial extents e.g. regional and continental scales and resolution e.g. $1km^2$ (Fig. 6), and even small spatial scale (Fig. 7) comes with the associated computational load even on massively parallel computing architectures. IHMs, such as ParFlow have overcome the computational burden of simulating or resolving questions (e.g. involving approximating variably saturated and overland flow equations) beyond such levels of higher spatial scales and resolutions. This capability may not be associated with more conceptually based models which, for example, may not simulate lateral groundwater flow or resolve surface and subsurface flow by specifying zones of

groundwater network of stream before performing a simulation (Maxwell et al., 2015) For cross-comparison of ParFlow with other contemporary IHMs, a more comprehensive model testing and analyses have recently been done and readers can access these resources at Maxwell et al., (2014), Koch et al., (2016) and Kollet et al., (2017).

Figure 6 Caption: Map of water table depth (m) over the simulation domain with two insets zooming into the North and South Platte River basin, headwaters to the Mississippi River. Colors represent depth in log scale (from 0.01 to 100 m) (Maxwell et al., 2015).

Figure 7 Caption: Map of hydraulic conductivity (K) and stream depth in the East Inlet watershed in Colorado (Engdahl and Maxwell, 2015). This domain covers 30km^2 using 3.1 million lateral grid cells. The springs emanating from within the hillslopes highlight the realism afforded by integrated modeling at small scales.

ParFlow is based on efficient parallelism (high performance efficiency) and robust hydrologic capabilities. The model solvers and numerical methods used are powerful, fast, robust, and stable, which has contributed to the code's excellent parallel efficiency. As stated earlier, ParFlow is very capable of simulating flows under saturated and variably saturated conditions i.e. surface, vadose, and groundwater flows, even in highly heterogeneous environments. For example, in simulation of surface flows (i.e. solving the kinematic wave overland flow equations), ParFlow possess the ability to accurately solve streamflow (channelized flow) by using parameterized river routing subroutines (Maxwell and Miller, 2005; Maxwell et al., 2007, 2011). ParFlow includes

coupling capabilities with a flexible coupling interface which has been utilized extensively in resolving many hydrologic problems. The interface-based and process-level coupling used by ParFlow is an example for enabling high-resolution, realistic modeling. However, based on the applications, it would be worthwhile to create one, or several, generic coupling interfaces within ParFlow to make it easier to use its surface/subsurface capabilities in other simulations. Nonetheless, ParFlow has been used in coupling studies in simulating different processes and/or systems including simulating energy and water budgets of the surface and subsurface (Rihani et al., 2010; Mikkelson et al., 2013), surface water and groundwater flows and transport (Kollet and Maxwell, 2006; Beisman, 2007; Beisman et al., 2015; Maxwell et al., 2015), and subsurface, surface, and atmospheric mass and energy balance (Maxwell and Miller, 2005; Maxwell et al., 2011; Shrestha et al., 2014; Sulis et al., 2017). Undoubtedly, such coupled-model simulations come with computational burden and ParFlow performs well in overcoming such problems, even at high spatial scale and resolutions. This capability of ParFlow (coupling with other models) is continuously being exploited by hydrologic modelers, and new couplings are consistently being established. For example, via model coupling, the entire transpiration process could be investigated i.e. from carbon dioxide sequestration from the atmosphere by plants, subsurface moisture dynamics and impacts, to oxygen production by plants. Likewise, land cover change effects on mountain pine beetles may be investigated via coupling of integrated models. But these projected research advances can only be achieved if the scientific community keeps advancing code performance by developing, revising, updating, and rigorously testing these models' capabilities.

Presently, ParFlow's open source model and open developer community is fully transparent, and this openness is a major difference between it and other models that has enabled ParFlow to continue evolving. The user community is growing daily across the globe. Code developers have made available, aside from the ParFlow working manual, an active and frequently-updated blog (current blog: "http://parflow.blogspot.com/") and other sources including "https://www.parflow.org" and "https://github.com/parflow" where code developers and experienced users provide great information and suggestions that help in fixing bugs and ease frustrations of other users. Over the years, these easily accessible resources have proven to be helpful. The code is constantly updated through release of new versions with modifications designed to meet varying hydrologic challenges and directions for applications across different scales and fields. Each ParFlow package (version) comes with verified simulation test cases with directions that simulate different real systems and idealized cases. These serve as great resource where additional code modifications have been tested in every release of the code. ParFlow has a clear, rigorous verification procedure to make sure that any changes checked in do not "break" previous developments. This ensures numerical accuracy and backwards compatibility. Moreover, the full suite of test cases is automatically re-run before any submitted change can even be considered for merging with the master branch of the code. The number of branches/forks cannot be controlled in any open source (or community) code, but any contributions to the master branch are exhaustively vetted before being pushed out to users. Further, there is a software development and sustainability plan to improve the capabilities of ParFlow such as incorporation of new formulations of both kinematic and diffusive wave approximations, and advanced parallelization

support (GPU's and heterogeneous compute architectures). ParFlow works very well on different computing architectures and operating systems from "Laptops to Supercomputers" (single CPU, Linux clusters, highly scalable systems including IBM Blue Gene) with the same source code and input on all platforms. The code can use significant computational power and runs efficiently on supercomputing environments (e.g. Edison, Cori, JUQUEEN, and Yellowstone). Through ParFlow hydrologic modelers have available a very efficient yet still growing integrated hydrologic model to simulate and understand surface-subsurface flows.

Code availability

ParFlow is an open–source, object–oriented, parallel watershed flow model developed by community of scientists from the Environmental Protection Department at the Lawrence Livermore National Laboratory (LLNL), Colorado School of Mines and F-Z Jülich with supporting scientists from several other institutions. The current version of ParFlow is available at: https://github.com/parflow/parflow/releases/tag/v3.6.0. The version of ParFlow described in this manuscript is archived on zenodo: https://doi.org/10.5281/zenodo.3555297.

Author Contribution

Section 3 of the manuscript was written by Carol S. Woodward. Benjamin N. O. Kuffour and Nicholas B. Engdahl wrote the other Sections, and the entire manuscript was edited by Laura E. Condon, Stefan Kollet, and Reed M. Maxwell.

Competing Interest

We declare that no conflict of interest exist whatsoever between any of the authors and the editors or the referees.

Acknowledgement

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FIGURES

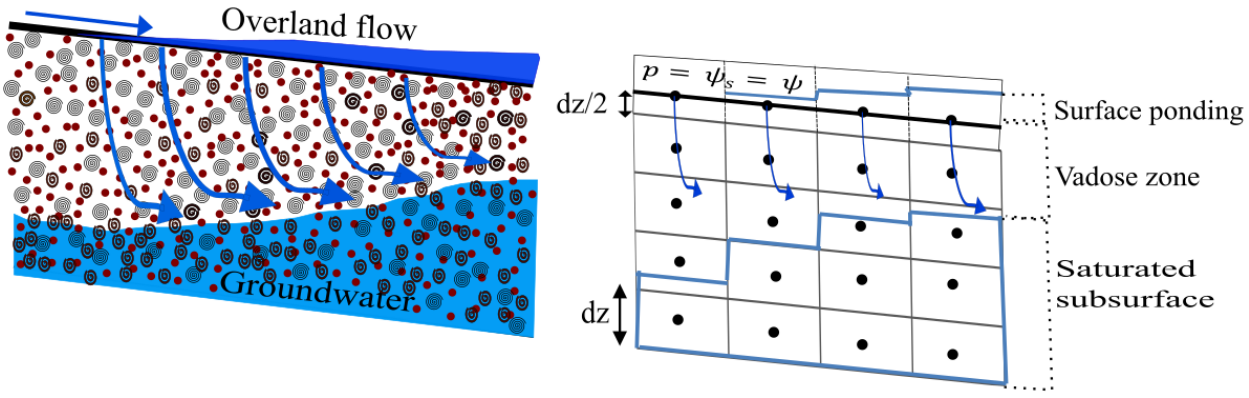

Figure 1: Coupled surface and subsurface flow systems. The physical system is represented on the left and a schematic of the overland flow boundary condition (continuity of pressure and flux at the ground surface) is on the right. The equation, $p = \psi_s = \psi$ in Fig. 1 signifies that at the ground surface, the vertically averaged surface pressure and subsurface pressure head are equal, which is the unique overland flow boundary used by ParFlow.

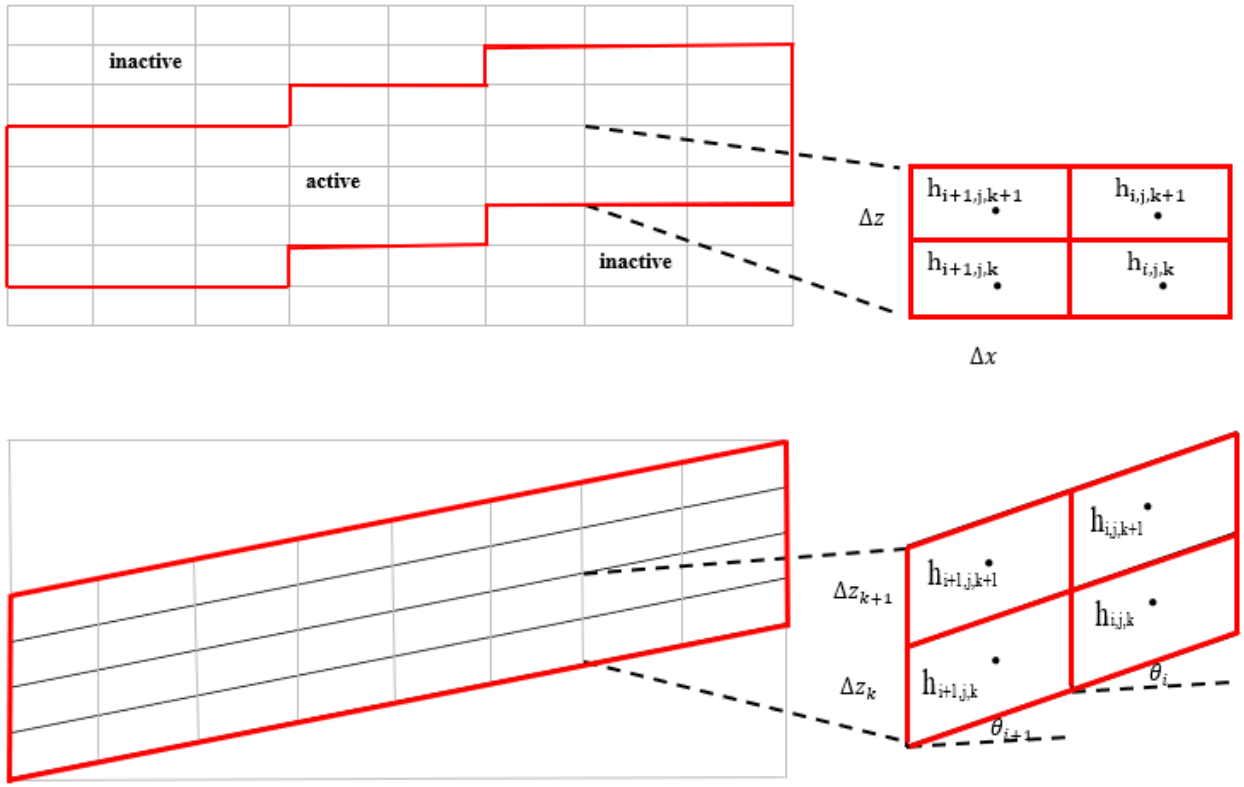

Figure 2: Representation of orthogonal (upper) and the terrain following (lower) grid formulations and schematics of the associated finite difference dependences (right). The i, j, and k are the x, y, and z cell indices

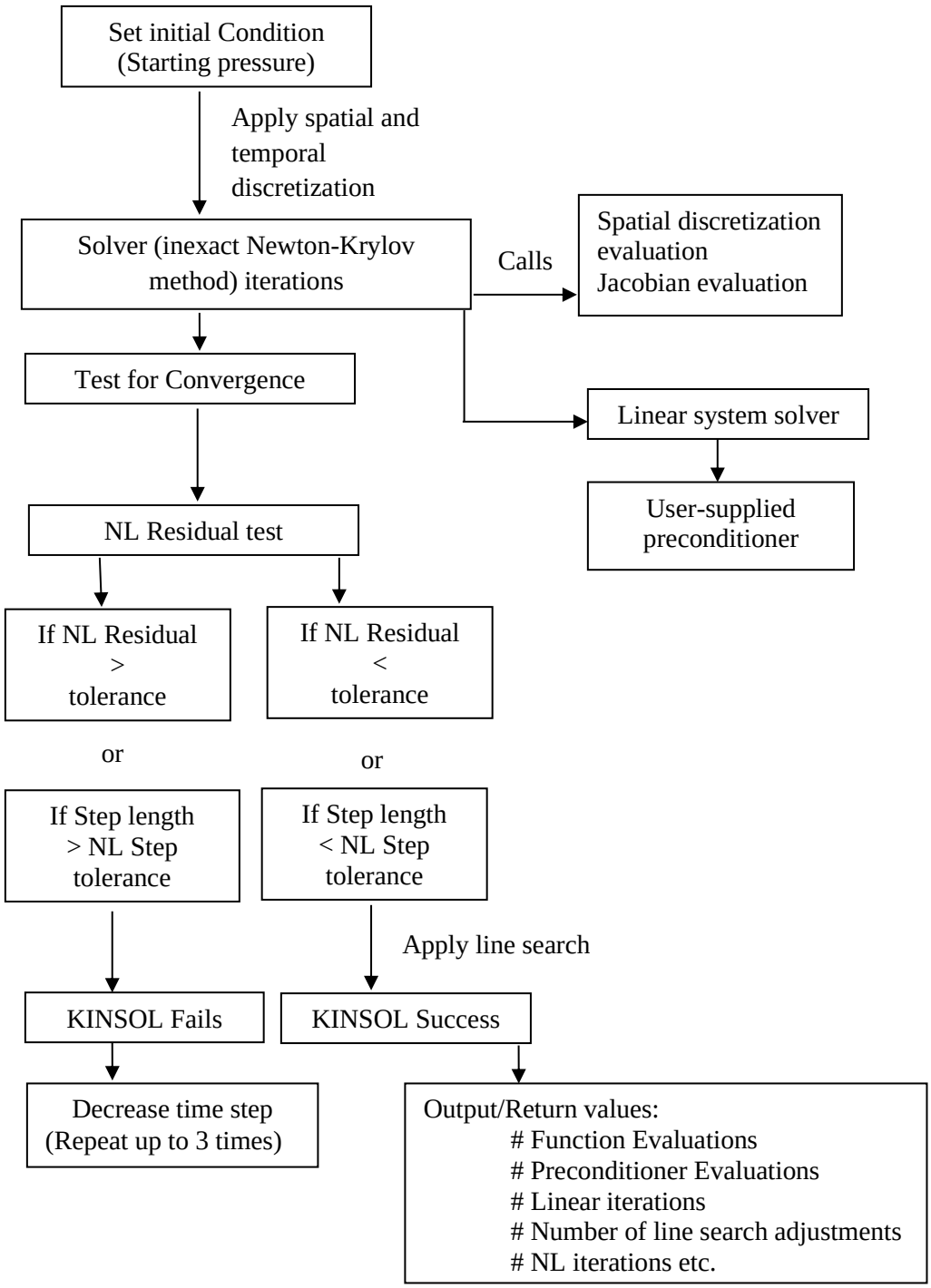

Figure 3: Working flow chart of ParFlow's solver for linear and non-linear system solution

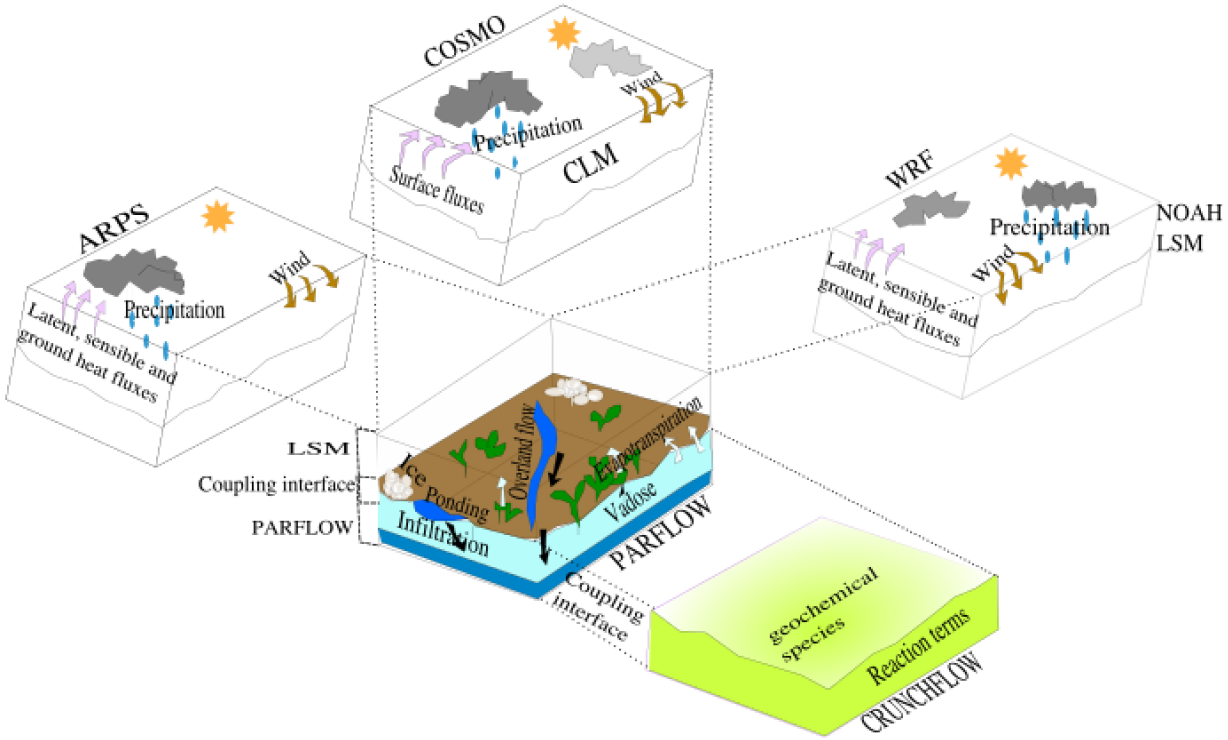

Figure 4(a): A pictorial description of the relevant physical environmental features and model coupling. CLM represents the Community Land Model, a stand-alone Land Surface Model (LSM) via which ParFlow couples' COSMO. The modified version of CLM by Dai et al., (2003) and is not shown in Fig. 4(a) because it is a module only for ParFlow, not really a stand-alone LSM any longer. The core model (ParFlow) always solves the variably saturated 3-D groundwater flow problem but the various couplings add additional capabilities.

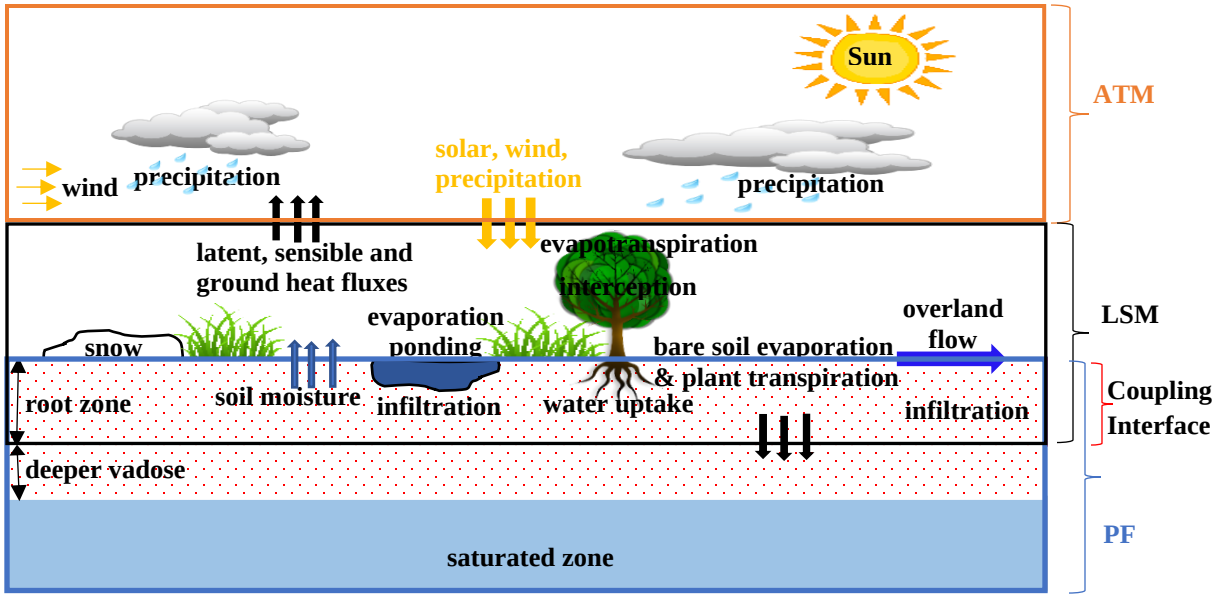

Figure 4(b): Schematic showing information transmission at the coupling interface. PF, LSM, and ATM indicate the portions of the physical system simulated by ParFlow, Land Surface Models, and Atmospheric Models respectively. The downward and upward arrows indicate the directions of information transmission between adjacent models. Note: Coupling between ParFlow and CrunchFlow (not shown) occur within the subsurface.

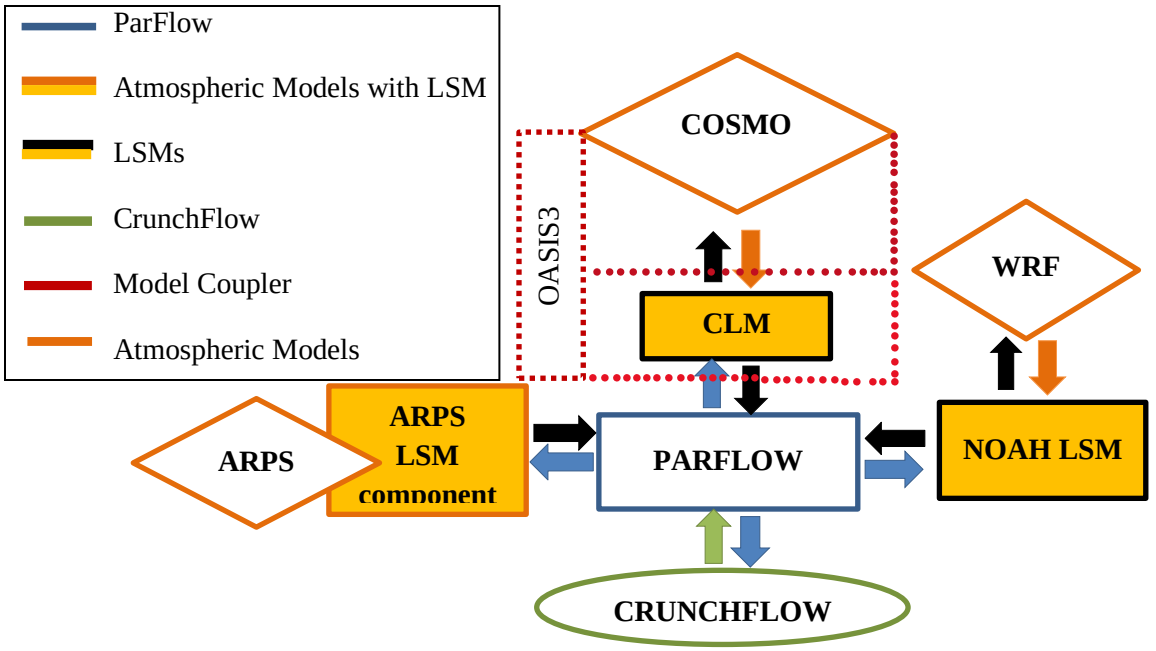

Figure 5: Schematic of the communication structure of the coupled models. Note: CLM represents a stand-alone Community Land Model. The modified version of Common Land Model by Dai et al., (2003) is not shown here because it is a module only for ParFlow, not really a stand-alone LSM any longer.

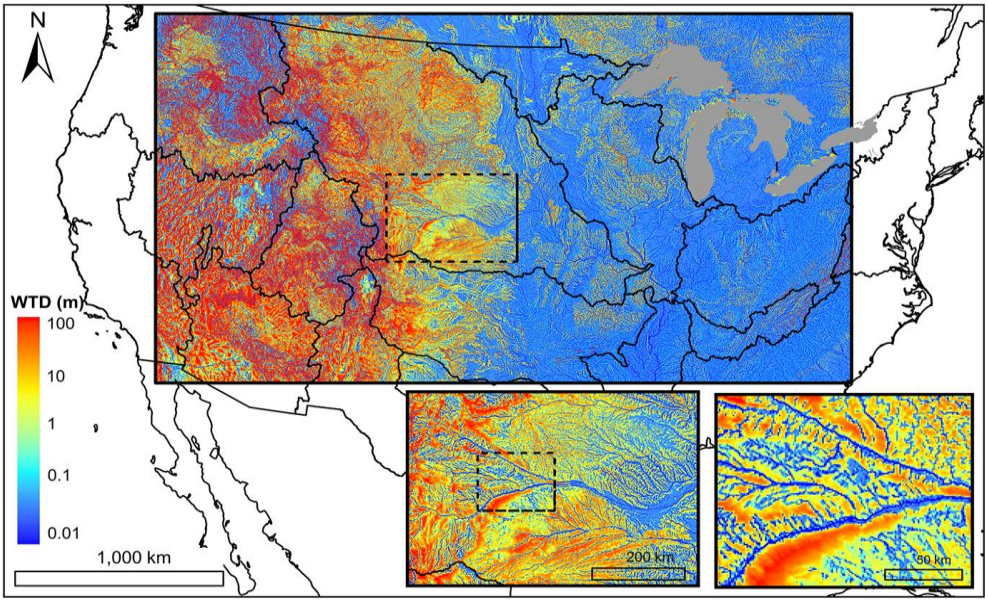

Figure 6: Map of water table depth (m) over the simulation domain with two insets zooming into the North and South Platte River basin, headwaters to the Mississippi River. Colors represent depth in log scale (from 0.01 to 100 m) (reproduced from Maxwell et al., 2015). The domain uses 1km^2 grid cells and represents one of the largest, and highest resolution domains simulated by integrated models to date.

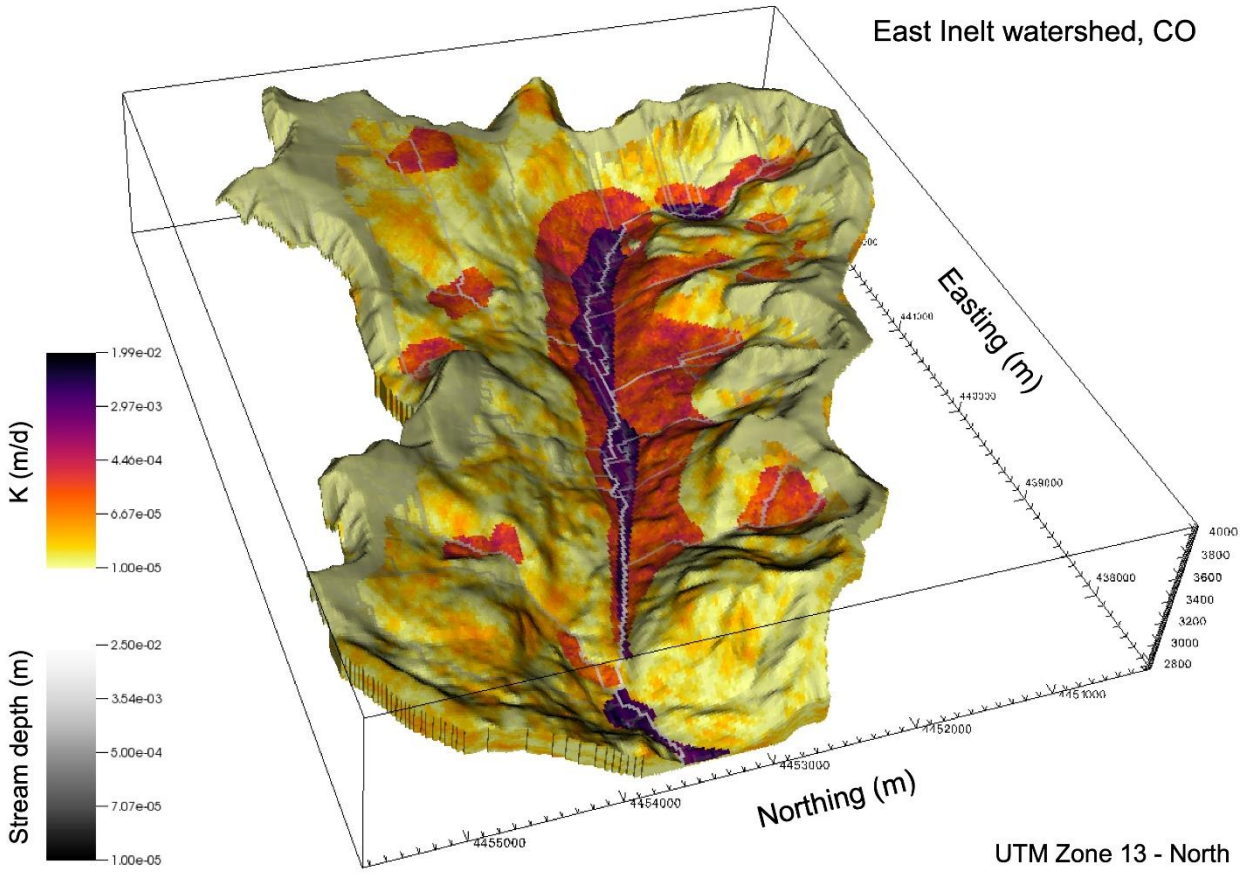

Figure 7: Map of hydraulic conductivity (K) and stream depth in the East Inlet watershed in Colorado (Engdahl and Maxwell, 2015). This domain covers 30km^2 using 3.1 million lateral grid cells. The springs emanating from within the hillslopes highlight the realism afforded by integrated modeling at small scales.

1098 Table 1: Details for the various scaling studies conducted using ParFlow

Simulation Case	Computer System	Processor Number	Jacobian/ Numerical Method	Preconditioner	Computation time (seconds)	Problem Size (cell Number)	Parallel Efficiency (%)	Study
Surface processes and variably saturated flow (ParFlow and CLM)	JUGENE (IBM Blue-Gene Super-computer)	16,384	Finite difference	ParFlow Multigrid	10,920	486,000	58.00	(Kollet et al., 2010)
Terrain Following Grid	JUGENE (IBM Blue-Gene Super-computer)	4,096	Analytical	Non-Symmetric	1,130.50	2,048,000,000	80.91	(Maxwell, 2013)
Overland flow	Intel Xeon Tightly coupled Linux Cluster	100	Finite difference	–	10,800	50,000	82.00	(Kollet and Maxwell, 2006)
Excess infiltration produced runoff	Intel Xeon Tightly coupled Linux Cluster	100	Finite difference	–	10,800	50,000	72.00	(Kollet and Maxwell, 2006)
Terrain Following Grid	JUGENE (IBM Blue-Gene Super-computer)	16,384	Finite difference	Symmetric	2,100.81	8,192,000,000	50.60	(Maxwell, 2013)
Subsurface and Overland flow coupling	IBM BGQ architecture	1,024	Analytical /Finite difference	ParFlow Multigrid	7,200	150,000	50.00	(Osei-Kuffuor et al., 2014)
Fully coupling terrestrial systems modeling platform	IBM BGQ system JUQUEEN	4,096	–	–	–	38,880	82.00	(Gasper et al., 2014)
Performance evaluation of ParFlow code (modified version of ParFlow)	(IBM Blue-Gene Super-computer) JUQUEEN	458,752	Finite difference	–	–	10,569,646,080	–	(Burstedde et al., 2018)

1099 a: The hyphen "– "shows that information was not provided by the appropriate study

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1101 Table 2: Selected coupling studies involving application of ParFlow and atmospheric, land surface, and subsurface models

Application	**Coupled Model**	**Simulation Scale and Size (*x*, *y*, and *z* dimensions)**	**Model Development**	**Model Calibration**	**Study**
Surface heterogeneity, surface energy budget	CLM	Watershed (30m x 30m x 84m)			(Reyes et al., 2016)
Sensitivity analysis (evaporation parameterization)	CLM (modified)	Column (1m x 1m x 10m)			(Jefferson and Maxwell, 2015)
Sensitivity of photosynthesis and stomatal resistivity parameters	CLM (modified)	Column (2m x 2m x 10m)			(Jefferson et al., 2017)
Active subspaces; dimension reduction; energy fluxes	CLM (modified)	Hillslope (300m x 300m x 10m)			(Jefferson et al., 2015)
Spin-up behavior; initial conditions watershed	CLM	Regional (75km x 75km x 200m)			(Seck et al., 2015)
Urban processes	CLM	Regional (500m x 500m x 5m)		Yes	(Bhaskar et al., 2015)
Global sensitivity	CLM	Watershed (84km x 75km x 144m)		Yes	(Srivastava et al., 2014)
Entropy production optimization and inference principles	CLM	Hillslope (100m x 100m x 5m)			(Kollet, 2015)
Soil moisture dynamics	CLM	Catchment (1180m x 74m x 1.6m)		Yes	(Zhufeng et al., 2015)
Dual-boundary forcing concept	CLM	Catchment (49km x 49km x 50m)			(Rahman et al., 2015)
Initial conditions; Spin-up	CLM	Catchment; Watershed (28km x 20km x 400m)			(Ajami et al., 2014, 2015)
Groundwater-fed irrigation impacts of natural systems; optimization water allocation algorithm	CLM	Watershed; Sub-watershed (41km x 41km x 100m)			(Condon and Maxwell, 2013, 2014)
Subsurface heterogeneity (land surface fluxes)	CLM	Watershed (209km x 268km x 3502m)			(Condon et al., 2013)
Mountain Pine Beetle	CLM	Hillslope (500m x 1000m x 12.5m)			(Mikkelson et al., 2013)
Groundwater-land surface-atmosphere feedbacks	CLM	Watershed (32km x 45km x 128m)			(Ferguson and Maxwell, 2010, 2011, 2012)
Subsurface heterogeneity (land surface processes)	CLM	Hillslope (250m x 250m x 4.5m)			(Atchley and Maxwell, 2011)
Computational scaling	CLM	Hillslope (150m x 150m x 240m)			(Kollet et al., 2010)

Subsurface heterogeneity (infiltration in arid environment)	CLM	Hillslope (32km x 45km x 128m)			(Maxwell, 2010)
Subsurface heterogeneity (land energy fluxes)	CLM	Hillslope (5km x 0.1km x 310m)			(Rihani et al., 2010)
Heat and subsurface energy transport (ParFlowE)	CLM	Column (1m x 1m x 10m)	Yes		(Kollet et al., 2009)
Subsurface heterogeneity on evapotranspiration	CLM	Column, Hillslope (32m x 45m x 128m)			(Kollet, 2009)
Subsurface heterogeneity (land-energy fluxes; runoff)	CLM	Watershed; Hillslope (3km x 3km x 30m)			(Kollet and Maxwell, 2008)
Climate change (land-energy feedbacks to groundwater)	CLM	Watershed (3000m x 3000m x 30m)			(Maxwell and Kollet, 2008)
Model development experiment	CLM	Column	Yes		(Maxwell and Miller, 2005)
Subsurface transport	CLM	Aquifer (30m x 15m x 0.6m)			(Tompson et al., 1998, 1999; Maxwell et al., 2003)
Model development (TerrSysMP)	COSMO	Watershed (64km x 64km x 30m)	Yes		(Shrestha et al., 2014)
Implementation and Scaling (TerrSysMP)	COSMO	Continental	Yes		(Gasper et al., 2014)
Groundwater response to ground surface-atmosphere feedbacks	COSMO	Continental (436m x 424m x 103m)	Yes		(Keune et al., 2016)
Atmosphere, DART, data assimilation	WRF	Watershed (15km x 15km x 5m)	Yes		(Williams et al., 2013)
Coupled model development (Atmosphere)	WRF	Watershed (15km x 15km x 5m)	Yes		(Maxwell et al., 2011)
Subsurface heterogeneity (runoff generation)	WRF	Hillslope (3km x 3km x 30m)			(Meyerhoff and Maxwell, 2010)
Subsurface uncertainty to the atmosphere	WRF	Watershed (15km x 15km x 5m)	Yes		(Williams and Maxwell, 2011)
Subsurface transport	ARPS	Watershed (17m x 10.2m x 3.8m)		Yes	(Maxwell et al., 2007)
Terrain and soil moisture heterogeneity on atmosphere	ARPS	Hillslope (5km x 2.5km x 80m)			(Rihani et al., 2015)
Risk Assessment of CO leakage	CRUNCHFLOW	Aquifer (84km x 75km x 144m)		Yes	(Atchley et al., 2013)
Reactive transport heterogeneous saturated subsurface environment	CRUNCHFLOW	Aquifer (120m x 120m x 120m)			(Beisman et al., 2015)

b: "CLM" show that coupling with ParFlow was by the original Common Land Model or Community Land Model. "CLM (modified)" show that the modified version of Common Land Model by (Dai et al., 2003) was a module for ParFlow.

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