

A semidiscrete finite volume formulation for multiprocess watershed simulation

4 Yizhong Qu¹ and Christopher J. Duffy¹

5 Received 26 November 2006; revised 30 April 2007; accepted 9 May 2007; published XX Month 2007.

[1] Hydrological processes within the terrestrial water cycle operate over a wide range of 6 time and space scales, and with governing equations that may be a mixture of ordinary 7 differential equations (ODEs) and partial differential equations (PDEs). In this paper we 8 propose a unified strategy for the formulation and solution of fully coupled process 9 equations at the watershed and river basin scale. The strategy shows how a system of 10mixed equations can be locally reduced to ordinary differential equations using the 11 semidiscrete finite volume method (FVM). Domain decomposition partitions the 12 13 watershed surface onto an unstructured grid, and vertical projection of each element forms a finite volume on which all physical process equations are formed. The projected 14volume or prism is partitioned into surface and subsurface layers, leading to a fully 15 coupled, local ODE system, referred to as the model "kernel." The global ODE system is 16 assembled by combining the local ODE system over the domain, and is then solved by a 17 state-of-the-art ODE solver. The unstructured grid, based on Delaunay triangulation, is 18 19generated with constraints related to the river network, watershed boundary, elevation contours, vegetation, geology, etc. The underlying geometry and parameter fields are then 20projected onto the irregular network. The kernel-based formulation simplifies the process 21of adding or eliminating states, constitutive laws, or closure relations. The strategy is 22demonstrated for the Shale Hills experimental watershed in central Pennsylvania, and 23 24several phenomena are observed: (1) The enslaving principle is shown to be a useful approximation for soil moisture-water table dynamics for shallow soils in upland 25watersheds; (2) the coupling shows how antecedent moisture (i.e., initial conditions) can 26amplify peak flows; (3) the coupled equations predict the onset or threshold for upland 27ephemeral channel flow; and (4) the model shows how microtopographic information 2829 controls surface saturation and connectivity of overland flow paths for the Shale Hills site. The open-source code developed in this research is referred to as the Penn State Integrated 30 Hydrologic Model (PIHM). 31

33 **Citation:** Qu, Y., and C. J. Duffy (2007), A semidiscrete finite volume formulation for multiprocess watershed simulation, *Water* 34 *Resour. Res.*, *43*, XXXXXX, doi:10.1029/2006WR005752.

36 1. Introduction

[2] In this paper we address the problem of process 37 integration for hydrologic prediction in watersheds and river 38 basins. Simulation is now widely utilized as a complemen-39 tary research methodology to theory and experiment [Post 40 and Votta, 2005]. However, the grid resolution, scale of the 41 model, and range of hydrologic processes operating in 42watersheds and river basins offer the dilemma of what is 43necessary to predict hydrologic response or to simulate 44 45certain behaviors of the coupled system. In this paper we 46 formulate a multiscale strategy that incorporates constitutive relationships representing volume-average state variables. 47 For small watersheds and fine numerical grids, local contin-48

49 uum relationships (e.g., Darcy's law) lead to a fully coupled,

physics-based, distributed model. At larger scales and coarse 50 grids, empirical relationships with large-scale volume aver-51 ages are applied, and the model becomes a semidistributed 52 model. A brief review of hydrologic modeling strategies 53 demonstrates the issues involved with integration and cou-54 pling of multiple processes and clarifies the purpose of this 55 paper. 56

[3] Current hydrologic models may be described from 57 two perspectives: physically based, spatially distributed 58 models, and lumped conceptual models. *Freeze and Harlan* 59 [1969] developed the first blueprint for numerical solutions 60 to physically based, distributed watershed models starting 61 from a continuum perspective (i.e., Richards' equations for 62 subsurface flow, Saint Venant equations for surface flow and 63 channel routing). It was some years before the SHE model 64 [*Abbott et al.*, 1986a, 1986b] and its variants produced a 65 second generation where the coupled physical equations are 66 actually solved on a regular grid, with coupling handled 67 through a sophisticated control algorithm that passes information between processes (e.g., surface water–groundwater 69 exchange). 70

¹Department of Civil and Environmental Engineering, Pennsylvania State University, University Park, Pennsylvania, USA.

Copyright 2007 by the American Geophysical Union. 0043-1397/07/2006WR005752\$09.00

[4] The approach of coupling multiple processes through 71time-lagging and iterative coupling through boundary 72conditions is generally considered a weak form of coupling, 73 in that it may lead to significant instability and errors 74[LaBolle et al., 2003]. The approach also requires consider-7576able reprogramming if changes are made to the physical equations for a specific application. More recently, Panday 77 and Huyakorn [2004] have developed an approach where all 78 equations in the model are of the diffusive type, which are 79 solved in a single system on a regular grid (e.g., Richard's 80 equation and diffusive wave equation), while equations for 81 other processes (vegetation, energy, snow) are dealt with 82 separately (iteratively). Yeh et al. [1998] have used a similar 83 approach but with finite elements. As will be described later, 84 our approach couples all dynamical equations within the 85 same prismatic volume (a prism is defined by a triangle 86 projected from the canopy, through the land surface to the 87 lower boundary of groundwater flow); and all equations are 88 solved simultaneously, eliminating the need for a controller, 89 90 delayed, or off-line process equations.

91 [5] Lumped or spatially integrated models are widely used today, where the goal of the prediction is outflow 92 from forcing (e.g., rainfall-runoff, recharge-baseflow, 93 precipitation-infiltration). Lumped systems are low-94dimensional and conveniently solved, but still require an 95empirical relationship for flux discharge that is generally 96 assumed to be linear or weakly nonlinear and fitted or 97 calibrated to the data. The reduced parameter set of this 98 approach can resolve the overall mass balance but cannot by 99 definition inform the internal space-time variation of phys-100ical processes. The Stanford watershed model is an early 101 example of the lumped model that includes watershed 102processes [Crawford and Linsley, 1966]. There have been 103efforts to try to bridge these two approaches. Duffy [1996] 104 describes a two-state model by integrating Richards' equa-105tion over a hillslope into saturated and unsaturated states, 106107and later extended this approach to the problem of mountain-front recharge using hypsometry to partition the upland, 108 transition, and flood plain zones into a intermediate-109 dimensional system [Duffy, 2004]. Reggiani et al. [1998, 110 1999] proposed a comprehensive semidistributed frame-111 work in which integrated conservation equations of mass, 112momentum, and energy are solved over a representative 113elementary watershed (REW). They discuss the issues 114 involved in parameterizing the integral flux-storage relation 115at the REW scale, and refer to this as hydrologic closure. 116

[6] The decision of using a lumped, distributed, or semi-117 distributed approach to model watershed systems ultimately 118 depends on the purpose of the model, and each has its 119120advantages and disadvantages. For the distributed case, the governing equations are derived from local constitutive 121relationships. For instance, the Darcy equation is applicable 122at the plot or perhaps hillslope scale, but it is not clear what 123should be the effective relation of flux-to-state variable 124when integrated over larger scales where semidistributed 125or lumped models are used (e.g., the hydrologic closure 126 problem discussed by Beven [2006]). At present there is 127 considerable discussion in the literature about the relation of 128 data needs and predictive models, including the issues of 129model type (lumped, semidistributed, distributed), unique-130ness, and the appropriate scales of integration [Sivapalan et 131al., 2002]. 132

[7] In the present paper a new strategy for integrated 133 hydrologic modeling is proposed that naturally handles 134 physical processes of mixed partial differential equations 135 (PDEs) and ordinary differential equations (ODEs) as a 136 fully coupled system. The model formulates the local 137 physical equations via the finite volume method, using 138 geographic information systems (GIS) tools to decompose 139 the model domain on an unstructured grid, as well s 140 distributing a priori parameter estimates to each grid cell. 141 In the limit of small-scale numerical grids, the finite volume 142 method implements classical (e.g., contiuum) constitutive 143 relationships. For larger grid scales the method reflects the 144 assumptions of the semidistributed approach described 145 above, but with full coupling of all elements. The process 146 of altering the physical model to accommodate effective 147 parameterizations or new equations is a relatively simple 148 process, since all equations reside in the same location in 149 the code (i.e., the kernel). In this approach, the interactions 150 are assembled on the right-hand side of the global ODE 151 system, which is then solved with a state-of-the-art solver 152 designed for stiff, nonlinear systems. The approach utilizes 153 a triangular irregular grid that covers the domain with the 154 fewest number of triangles [Palacios-Velez and Duevas- 155 Renaud, 1986; Polis and McKeown, 1993] subject to 156 constraints as defined by the particular problem. 157

Modeling Approach 158

2.1. Semidiscrete FVM Approach

[8] In this section we develop the finite volume approx- 160 imation for an arbitrary physical process operating on an 161 unstructured grid cell. A general form of the mass conser- 162 vation equation for an arbitrary scalar state variable χ can 163 be written 164

$$\frac{\partial \chi}{\partial t} + \nabla \cdot \chi \mathbf{V} + \frac{\partial \chi}{\partial z} = \Omega_{\chi}, \tag{1}$$

where χ represents mass fraction of storage (dimension- 166 less). For convenience, the velocity vector in (1) is divided 167 into horizontal (V = {u, v}) and vertical components {w}, 168 and Ω_{χ} is a local source/sink term for the process 169 represented by χ . Volume integration of (1) proceeds in 170 two steps: First, we integrate over the depth of the layer and 171 then over the area. For a single layer of thickness $z_a \leq z \leq z_b$ 172 containing the scalar χ , the integral over the depth takes the 173 form 174

$$\frac{\partial}{\partial t} \int_{z_a}^{z_b} \chi dz - \chi_{z_b} \frac{\partial z_b}{\partial t} + \chi_{z_a} \frac{\partial z_a}{\partial t} + \nabla \int_{z_a}^{z_b} \chi V dz - (V\chi)_{z_b} \nabla z_b$$
$$+ (V\chi)_{z_a} \nabla z_a + (w\chi)_{z_a} - (w\chi)_{z_b} = \int_{z_a}^{z_b} \Omega_{\chi} dz$$
(2)

We can evaluate the boundary terms, by rewriting 176 equation (2) for a small layer about the boundary itself, 177 $z_b^- \leq z_b \leq z_b^+$, where $z_b^- = z_b - \varepsilon$ and $z_b^+ = z_b + \varepsilon$. Letting the 178 layer thickness approach zero, $z_b^+ - z_b^- \rightarrow 0$, the integral 179 terms are eliminated and the remaining terms must balance 180

(5)

220

as we approach the interface from both sides, leading to adefinition of the net interface flux:

$$\chi_{b^+} \frac{\partial z_{b^+}}{\partial t} + (\nabla \chi)_{b^+} \nabla z_{b^+} - (w\chi)_{b^+} = \chi_{b^-} \frac{\partial z_{b^-}}{\partial t} + (\nabla \chi)_{b^-} \nabla z_{b^-} - (w\chi)_{b^-} = Q_b,$$
(3)

where Q_b is the net flux across $z = z_b$. A similar expression is found for Q_a at $z = z_a$. Equation (2) is now written in terms of vertically integrated storage in the layer:

$$\frac{\partial \overline{\chi}}{\partial t} + \nabla (\mathbf{V} \overline{\chi}) = Q_b - Q_a + \omega, \tag{4}$$

where $\overline{\chi}$ is the volumetric storage per unit area (L) in the layer defined by

$$\overline{\chi} = \int\limits_{z_a}^{z_b} \chi dz,$$

191 and ω is the vertically integrated source/sink term

$$\omega = \int_{z_q}^{z_b} \Omega_{\chi} dz.$$

193 To complete the volume integration, equation (4) is now 194 written

$$\frac{\partial}{\partial t} \int_{A} \overline{\chi} dA + \int_{\Gamma} N(\nabla \overline{\chi}) d\Gamma = \int_{A} (Q_b - Q_a + \omega) dA, \qquad (7)$$

where the divergence theorem was applied to the second term, Γ is the perimeter of *A*, and *N* is the unit normal vector on Γ . Writing (7) in semidiscrete finite volume form [*Leveque*, 2002] yields

$$\frac{\mathrm{d}\overline{\chi}}{\mathrm{d}t} = \sum_{k=1}^{2} \mathcal{Q}_k - \sum_{i=1}^{m} \mathcal{Q}_i, \qquad (8)$$

where $\overline{\chi}$ is now interpreted as the volumetric storage (L³) of 201 202 χ in the control volume (incompressible fluid), Q_i is net 203volumetric flux through the sides i = 1, 2, 3 of the control volume, and Q_k is the net volumetric flux across the upper 204205and lower boundaries k = 1, 2. Later it will be convenient to 206divide (8) by the projected horizontal surface area of the finite volume such that storage is an equivalent depth, and 207volumetric flux terms are normalized to a unit horizontal 208 surface area. 209

[9] The vector form of equation (8) represents all pro-210cesses $\overline{\chi} = \{\chi_1, \chi_2, \dots, \chi_k\}$ within the control volume and 211forms a fully coupled local ODE system. The fluxes across 212the sides of the control volume are evaluated by appropriate 213constitutive (or closure) relationships for specific processes 214 and applications. We note again that the finite volume 215method guarantees mass conservation for each control 216volume [Leveque, 2002], and that the semidiscrete repre-217218 sentation reduces all equations to a standard form. 219

2.2. Multiscale, Multiprocess Formulation

[10] The next step in developing the multiprocess system 221 is domain decomposition. The horizontal projection of the 222 watershed area is decomposed into Delauney triangles. Each 223 triangle is projected vertically to span the "active flow 224 volume" forming a prismatic volume which is further 225 subdivided into layers to account for the physical process 226 equations and material layers. When governing equations 227 are a mix of ODEs (e.g., vegetation interception) and PDEs 228 (e.g., overland flow, groundwater flow), the PDEs are first 229 reduced to ODEs by applying the semidiscrete finite volume 230 method (FVM) approach described above, and then all 231 ODEs are associated with a layer within the prism. The 232 prism is where all physical equations (and thus all time- 233 scales of the problem) reside, and we refer to this local 234 system as the kernel. Assembling the local ODE system 235 over the watershed domain, a global system is formed 236 which is then solved with an efficient ODE solver. This 237 solution method is also known as the "method of lines" 238 [Madsen, 1975], here applied to a system of differential 239 equations. For the multiple processes encountered in water- 240 shed research, the approach has several advantages. First, 241 the model kernel representing all physical processes oper- 242 ating within the prismatic control volume can be easily 243 modified for different applications or processes without 244 altering the solver or even the domain decomposition. Since 245 all physical equations are in a single subroutine, adding or 246 omitting processes, material properties, or forcing makes 247 modifications to the program quite simple. Second, the 248 ODE is solved as a "fully coupled" system, with no time 249 lagging or iterative linking of processes. Third, alternative 250 constitutive or closure relationships are also easily imple- 251 mented and tested in this strategy. The constitutive relation- 252 ship might come from conceptual models, numerical 253 experiments [Duffy, 1996], or theoretical derivation 254 [Reggiani et al., 1999; Reggiani and Rientjes, 2005]. It is 255 noted that constitutive relationships are sensitive to the scale 256 of volume integration [Beven, 2006], a feature that is natural 257 to the semidiscrete approach used here. 258

[11] In this research we are developing an open-source 259 community code for the simulation of watersheds and river 260 basins, and we refer to this code as PIHM: Penn State 261 Integrated Hydrologic Model. In this first generation of 262 PIHM, we consider the following processes and dimen- 263 sions: one-dimensional (1-D) channel routing, 2-D overland 264 flow, and 2-D subsurface flow are governed by PDEs, while 265 canopy interception, evapotranspiration, and snowmelt are 266 described by ODEs. Each process is assigned to a layer 267 within the kernel with overland flow and channel flow 268 assigned to the surface layer, and the channel centered on 269 any edge of the element. Prior to domain decomposition, the 270 river network, hydraulic structures, or other devices, such as 271 dams, gages, weirs, etc., are identified as special points used 272 to constrain the decomposition. Although it imposes some 273 computational burden to the grid generation, this idea 274 simplifies the geometry of the decomposed region, which 275 in turn facilitates assembling the global ODE system. For 276 example, this step will guarantee that no channel intersects 277 the control volume interior, or the channel segments are 278 always centered on the boundary between two watershed 279 elements. It also locates gages (stage, well level, climate 280 station) at vertices of elements where desired, simplifying 281



Figure 1. Schematic view of domain decomposition for hillslopes and stream reach. The finite control volumes, elements, are prisms projected from the triangular irregular grid also referred to as a TIN (triangular irregular network). The TIN is generated with channels as constraints, which will guarantee that the channel is along the element boundary. In the upper part of the figure, the basic element is shown to the left with multiple hydrological processes. A channel segment for a triangle bounded by a stream is shown to the right.

postprocessing. Figure 1 illustrates the decomposition and kernel for the system to be studied here.

285 3. Building the Local ODE System

[12] The choice of equations in any situation is a practical 286balance of the most important physical processes assumed 287to operate on a watershed (Shale Hills, in our case), the 288assumptions made about these processes in a particular 289290 representation, and the scale of computation. We note that there are no intrinsic limitations to more complex (or 291simpler) equations/processes. Those presented here are 292 sufficient to characterize the physics of the particular 293294physical setting we have chosen to demonstrate.

3.1. Processes Governed by PDEs 296

3.1.1. Surface Overland Flow

[13] The governing equations for surface flow are the 2-D 298 St. Venant equations. *Sleigh et al.* [1998] have developed a 299 numerical algorithm solving the full St. Venant equations 300 using the finite volume method for predicting flow in rivers 301 and estuaries, where the normal flux vector is calculated 302 using Riemann approach [*Leveque*, 2002], and we follow 303 their approach here. Letting $\overline{\chi} \rightarrow h_o(x, y, t)$, the vertically 304 integrated form of the continuity equation (4) is given by 305

$$\frac{\partial h_o}{\partial t} + \frac{\partial (uh_o)}{\partial x} + \frac{\partial (vh_o)}{\partial y} = \sum_{k=1}^2 q_k, \tag{9}$$

297

triangular element of $D_4D_7D_8$ is identical. The plane is then 352 defined by (see Figure 2) 353

$$\begin{vmatrix} x & y & H & 1 \\ x_2 & y_2 & H_2 & 1 \\ x_3 & y_3 & H_3 & 1 \\ x_4 & y_4 & H_4 & 1 \end{vmatrix} = 0.$$
 (12)

Note that

355

and thus the hydraulic head gradient along the maximum 357 slope direction of element $D_4D_7D_8$ is given by 358

 ∇H

$$\frac{\partial H}{\partial s} = \sqrt{\left(\frac{(y_3 - y_2)(H_4 - H_2)}{(x_2 - x_3)(H_4 - H_2)}\right)^2 + \left(\frac{(x_4 - x_2)(H_3 - H_2)}{(x_3 - x_2)(H_4 - H_2)}\right)^2}.$$
(13)

For elements that border a channel, special handling is 360 required, and we discuss this in section 3.1.3. For the 361 diffusion wave approximation, the surface flux per unit 362 width of flow is given by

$$Q_s = h_o k_s \frac{\partial H}{\partial s}, \qquad s = s(x, y)$$
 (14)

using (11) and (13). Applying the semidiscrete approach 365 discussed above to equation (10) and normalizing by the 366 surface area of the element yields the semidiscrete 367 approximation for overland flow 368

$$\left(\frac{dh_o}{dt} = p - q^+ - e + \sum_{j=1}^3 q_j^s\right)_i,$$
 (15)

where q_j^s is the normalized lateral flow rate from element *i* 369 to its neighbor *j*. The terms *p*, q^+ , and *e* are throughfall 371 precipitation, infiltration, and evaporation, respectively. 372 **3.1.2.** Subsurface Flow 373

[15] For subsurface flow we start again from (1) and let 374 our scalar be the moisture content (volume water/void 375 volume), $\chi \rightarrow \theta$, which we write (1) as 376

$$\frac{\partial\theta}{\partial t} + \nabla\theta V + \frac{\partial(w\theta)}{\partial z} = +S_{\theta},\tag{16}$$

where once again the divergence terms are separated into 378 vertical (*w*) and horizontal or V = (u, v) components. Flow 379 within the subsurface layer is complicated by the existence 380 of a free surface boundary or water table within the layer. 381 The layer is partitioned into two parts, where the soil above 382 the water table (z^+) is governed by gravitational and surface 383

Figure 2. Delaunay triangulation and Voronoi diagram. The solid lines form Delanunay triangles, and the dashed lines form Voronoi polygons. The circumcenter V_i is the vertex of the perpendicular bisectors of the triangle, and is used to represent the triangle for the volume average of the state variable.

331 where $h_o(x, y, t)$ is the local water depth. Here u and v are velocities in the plane x, y; q_k are the surface flux terms 332 normalized by surface area. Note that there are three 333 unknowns, h_o , u, and v, for each element. To reduce the 334 complexity of solving the full St. Venant equations, we 335 336 neglect inertia terms in the momentum equation, and 337 Manning's formula is used to close equation (9), which 338 yields the diffusion wave approximation [Gottardi and 339 Venutelli, 1993]

$$\frac{\partial h_o}{\partial t} = \frac{\partial}{\partial x} \left(h_o k_s \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial x} \left(h_o k_s \frac{\partial H}{\partial x} \right) + \sum_k q_k \qquad (10)$$

341 with

$$k_s = \frac{h_o^2}{n_s} \frac{1}{|\partial H/\partial s|^2},$$
 (11)

where H(x, y, t) is the water surface elevation above an horizontal datum, *n* is Manning roughness coefficients, s =s(x, y) is the vector direction of maximum slope, and q_k are the layer top and bottom input/output.

[14] Since the basic element in our implementation is a vertically projected prism (Figure 1), the evaluation for k_s is slightly complicated. Let (x_i, y_i, H_i) be the local coordinates of the free water surface at vertex V_i . Assume the free surface plane is determined by vertex V_2 , V_3 , V_4 and that the



tension forces, while gravity alone governs below the water table (z^-). Using (2) and (3) and integrating over the depth of the layer yields

$$\theta_s \frac{\partial h_u}{\partial t} + \nabla(\theta V h_u) = q^+ - q^o$$

$$\theta_s \frac{\partial h_g}{\partial t} + \nabla(\theta V h_g) = q^o - q^-.$$
(17)

The divergence terms in (17) represent horizontal flow in the unsaturated (plus sign) and saturated (minus sign) parts of the layer, θ_s is the moisture content at saturation, h_u is the equivalent depth of moisture storage above the water table, and h_g is the depth of saturation below the water table defined by

$$h_{u} = \int_{z_{o}^{+}}^{z_{b}} \frac{\theta}{\theta_{s}} dz, \qquad h_{g} = \int_{z_{a}}^{z_{o}} \frac{\theta_{s}}{\theta_{s}} dz, \qquad (18)$$

where the layer is now defined with two complementary 394 zones above $(z_a \leq z \leq z_o^+)$ and below the water table $(z_a \leq z_o^+)$ 396 $z \leq z_o^{-}$). The flux terms or source terms to the soil 397 moisture zone $(q^+ \text{ and } q^o)$ are defined respectively as 398 infiltration/exfiltration through the soil surface, and recharge 399 to and from the water table. The flux q^{-} admits an exchange 400with a deeper groundwater layer. The divergence terms for 401lateral flow are evaluated by integrating (17) over the 402projected surface area of the control volume (Figure 1). 403Applying the Reynolds transport theorem [Slattery, 1978] 404and the divergence theorem yields equations for flow above 405406 and below the water table, respectively:

$$\frac{1}{A} \iint_{A} \nabla(\theta V h_{u}) dA = \frac{1}{A} \iint_{B} (\theta V h_{u}) n dB \simeq \sum_{j=1}^{3} q_{j}^{u}$$

$$\frac{1}{A} \iint_{A} \nabla(\theta V h_{g}) dA = \frac{1}{A} \iint_{B} (\theta V h_{g}) n dB \simeq \sum_{j=1}^{3} q_{j}^{g}.$$
(19)

408 See *Duffy* [1996] for details. Finally, the balance equations 409 are formed for a fully coupled unsaturated-saturated flow 410 within the layer,

$$\theta_{s} \frac{dh_{u}}{dt} = q^{+} - q^{o} + \sum_{j=1}^{3} q_{j}^{u}$$

$$\theta_{s} \frac{dh_{g}}{dt} = q^{o} - q^{-} + \sum_{j=1}^{3} q_{j}^{g},$$
(20)

where the unsaturated and saturated depth of storage (h_u, h_g) are now interpreted as volume averages per unit projected horizontal surface area. The divergence terms in (20) define the net lateral soil moisture flux and net lateral groundwater exchange with adjacent elements. From this point we will assume that the flow is vertical in the unsaturated zone, but that lateral saturated groundwater flow is

$$\sum_{j=1}^3 q_j^g \neq 0$$

420 We note that this term also represents stream-aquifer 421 interaction for elements adjacent to a channel. The net flux to/from the water table $q^0(h_u, h_g)$ represents the integral 422 properties of unsaturated flow and recharge to/from the 423 water table, as well as the effect of water table fluctuations. 424 Again, in the governing ODEs all fluxes are normalized by 425 projected horizontal surface area of the element with units 426 [L/T]. 427

[16] For applications where the Darcy relationship is 428 appropriate, lateral groundwater fluxes are evaluated using 429 its volume-average form [*Duffy*, 2004] given by 430

$$q_{ij}^{g} = B_{ij}K_{eff} \frac{(H_{g})_{i} - (H_{g})_{j}}{D_{ij}} \frac{(h_{g})_{i} + (h_{g})_{j}}{2}, \qquad (21)$$

where B_{ij} is length of common boundary and D_{ij} is distance 432 between the circumcenters of elements *i* and *j*. $(H_g = h_g + z)_i$ 433 is hydraulic head where z_i is elevation of datum of element 434 *i*. The effective hydraulic conductivity K_{eff} is the harmonic 435 mean of the hydraulic conductivity in element *i* and *j*. The 436 storage-discharge relation in equation (21) is nonlinear 437 due to vertical integration. *Brandes* [1998] also shows, by 438 way of numerical experiments, that the integral storagedischarge or "effective" constitutive relationship is a 440 nonlinear function of hydraulic head at the hillslope scale. 441 Flexible constitutive relationships from conceptual models, 442 numerical experiments, and theoretical derivations can be 443 introduced where deemed appropriate. 444

[17] The approach used here assumes that each subsur- 445 face layer in the model can have both saturated and 446 unsaturated storage components. The interaction or cou- 447 pling term between the unsaturated and saturated storage is 448 defined by q^0 , the recharge or water table flux in equation 449 (20). *Duffy* [2004] developed a simplified analytic expression for the flux of recharge to/from a water table based on 451 integration over the unsaturated portion of the layer using a 452 simple exponential-type soil characteristic [*Gardner*, 1958], 453 which has the form 454

$$q^{0}(h_{u},h_{g}) = K_{s} \frac{1 - e^{-\alpha(z_{s} - h_{g})} - \alpha h_{u}}{\alpha(z_{s} - h_{g}) - \left(1 - e^{-\alpha(z_{s} - h_{g})}\right)},$$
(22)

where K_s is saturated hydraulic conductivity. The α is a soil 456 texture parameter for the exponential soil model; z_s is total 457 layer thickness. The integrated internal flux at the water 458 table q^o is a nonlinear function of the water table position 459 and the depth of soil moisture storage above the water table. 460 Equation (22) is shown for a clay loam soil in Figure 3 after 461 *Duffy* [2004]. It is noted that although *van Genuchten* 462 [1980] or *Brooks and Corey* [1964] formulations are more 463 generally used in discretized form, the recharge function 464 (22) has the advantage of simplicity and computation speed. 465

[18] The general point is that the kernel is easily edited 466 for the desired constitutive or closure relation, with proper 467 care taken for new parameters required by the formulation. 468 A special situation occurs under shallow water table con- 469 ditions, where unsaturated storage is approximated by a 470 simple function of the saturated storage and the system (20) 471 can be reduced. This idea is developed for a particular case 472 in section 6. 473



Figure 3. Illustration of the theoretical recharge $q^o [LT^{-1}]$ or flux of water to/from a water table within a partially saturated layer based on equation (22). The figure shows the relationship of unsaturated and saturated storage with recharge, and is based on a solution to Richard's equation for an exponential-type soil characteristic [*Duffy*, 2004]. For this example we neglect lateral flow in the unsaturated zone.

474 3.1.3. Channel Routing

⁴⁷⁵ [19] For channel routing, applying the semidiscrete ap-476 proach to the 1-D Saint Venant equations with the same 477 assumptions as overland flow yields

$$\left(\frac{dh_c}{dt} = p - e + \sum_{l=1}^{2} \left(q_l^s + q_l^g\right) + q_{in}^c - q_{out}^c\right)_i, \quad (23)$$

479 where h_c is depth of water in the channel, p and e are precipitation and evaporation for the channel segment, and 480 q_l^g and q_l^s are the lateral interaction terms for the aquifer and 481surface flow from each side of the channel. The upstream 482and downstream channel segments are q_{in}^c and q_{out}^c , 483 respectively. The volumetric fluxes are normalized by the 484 horizontally projected surface area of the channel segment, 485where the channel is a 1-D prismatic volume with a 486 trapezoidal or other cross section. As in the case of overland 487 flow, the diffusion wave approximation is applied to the 488 upstream and downstream channel flux terms. 489

[20] The interaction of surface overland flow and channel 490routing, q_I^s in equation (15) and (23), is controlled by a weir-491type equation following Panday and Huyakorn [2004]. For 492the case of channel flooding (i.e., the channel depth exceeds 493critical depth), the condition becomes a submerged weir 494where the discharge is a function of flow depth in surface 495496 overland flow and the channel segment. The interaction between the saturated groundwater flow and channel rout-497 ing q_1^g in equation (20) and (23) is governed by the discrete 498 form of the Darcy equation as in (21) where the adjacent 499head is the depth of the channel. 500

[21] The interaction between the surface flow and sub- 501 surface flow is controlled by two runoff generation mech- 502 anisms. When there is ponding on the surface, the 503 infiltration rate in equation (15) and (20) is a function of 504 the soil moisture, with the upper bound the max infiltra- 505 tion capacity (e.g., a bounded linear relation). If the layer 506 is fully saturated, then the runoff is generated by subsur- 507 face saturation (Dunne runoff generation mechanism), and 508 the precipitation is rejected within that time step. 509

3.2. Processes Governed by ODEs 511

3.2.1. Interception Process

[22] In the presence of vegetation and canopy cover, a 513 fraction of precipitation is intercepted and temporally stored 514 until it returns to the atmosphere as evaporation, or passes 515 through the canopy as throughfall or stemflow. In this case 516 the conservation equations are directly written as balance 517 equations in ODE form. Assuming that spatial interactions 518 of canopy storages among elements are insignificant, the 519 governing equation has the form 520

$$\left(\frac{\mathrm{d}h_{v}}{\mathrm{d}t}=p_{v}-e_{v}-p\right)_{i},$$
(24)

512

where h_v is vegetation interception storage. Here p_v is total 522 water equivalent precipitation, e_v represents evaporation 523 from surface vegetation, and p is throughfall and stemflow 524 or effective precipitation to surface storage in equation (15). 525 The upper bound of h_v is a function of vegetation type, 526 canopy density, and even the precipitation intensity 527

528 [*Dingman*, 1994]. When the canopy reaches the upper 529 threshold, all precipitation becomes throughfall.

530 3.2.2. Snowmelt Process

[23] The accumulation and melting process of snow is a 531cold-season counterpart to interception. Although a more 532comprehensive physics of snow could be applied, here we 533534use a simple index approach to snow accumulation and melt [Dingman, 1994]. Assuming that vegetation is dormant 535during the snow season, and while air temperature is below 536snow-melting temperature T_m , the snowpack will accumu-537 late during precipitation, and if air temperature exceeds the 538melting temperature the snowpack melts. The dynamic 539snowmelt conservation equation is given by 540

$$\left(\frac{\mathrm{d}\mathbf{h}_s}{\mathrm{d}t} = p_s - e_s - \Delta w\right)_i,\tag{25}$$

542 where Δw is snow melting rate, which is also an input to 543 overland flow. It can be calculated by the air temperature 544 with

$$\Delta w = \begin{cases} M(T_a - T_m), & T_a > T_m \\ 0, & T_a \le T_m, \end{cases}$$
(26)

546 where *M* is melt factor, which can be estimated from 547 empirical formulas [*Dingman*, 1994], and e_s is evaporation 548 directly from snow.

549 3.2.3. Evaporation and Evapotranspiration

Evaporation from vegetation interception, overland flow, and snow and river surfaces is estimated using the Pennman equation [*Bras*, 1990], which represents a com-

553 bined mass-transfer and energy method:

$$\left(e = \frac{\Delta(R_n - G) + \rho_a C_p(\varepsilon_s - \varepsilon_a)}{\Delta + \gamma}\right)_i.$$
 (27)

Potential evapotranspiration from soil and plant is estimatedusing Pennman-Monteith equation

$$\left(et_{0} = \frac{\Delta(R_{n} - G) + \rho_{a}C_{p}\frac{(\varepsilon_{s} - \varepsilon_{a})}{r_{a}}}{\Delta + \gamma\left(1 + \frac{r_{s}}{r_{a}}\right)}\right)_{i}.$$
(28)

Here et_0 refers to potential evapotranspiration, R_n is net 558 radiation at the vegetation surface, G is soil heat flux 559density, $\varepsilon_s - \varepsilon_a$ represents the air vapor pressure deficit, and 560 ρ_a is the air density, C_p is specific heat of the air. Δ is slope 561of the saturation vapor pressure-temperature relationship, γ 562is the psychometric constant, and r_s , r_a are the surface and 563aerodynamic resistances. Actual evapotranspiration is a 564function of potential eto and current plant, climatic, and 565566 hydrologic conditions, such as soil moisture. In the implementation, coefficients are introduced to calculate 567actual ET from potential following Kristensen and Jensen 568[1975]. Allen et al. [1998] provides guidelines used here for 569computing those coefficients for different vegetation. 570

571 [25] Combining equations (15), (20), (23), (24), and (25) 572 leads to a local system of ODEs representing multiple 573 hydrological processes within the prism or kernel element *i*. 574 Spatial interactions are evaluated with appropriate constitutive or closure relationships for (14), (21), (22), (26), 575 and (27). 576

[26] A central feature of the integrated model PIHM is 577 that all processes are fully coupled, first through the local 578 kernel, and then in the global ODE system. Here we have 579 outlined the interactions between major hydrologic processes, 580 e.g., surface overland flow, unsaturated subsurface flow, 581 saturated subsurface flow, and channel routing. More details 582 can be found in the dissertation by Qu [2005]. 583

4. Assemble Global ODE System

[27] The global ODE system is formed by assembling the 586 local system of equations (e.g., the kernel) and assigning 587 cell-to-cell connections over the watershed domain. Gener-588 ation of the unstructured grid involves domain decomposi-589 tion into prismatic volumes. The unstructured grid 590 generation attempts to achieve the fewest number of cells 591 to cover the region, while satisfying specific constraints 592 (e.g., rivers form along the edge of a cell, cells should be as 593 close to equilateral as possible for a quality grid, etc.). 594

[28] We apply Delaunay triangulation [Delanunay, 1934; 595 Voronoi, 1907; Du et al., 1999] to form an orthogonal 596 triangular unstructured grid [see Palacios-Velez and Duevas- 597 Renaud, 1986; Polis and McKeown, 1993; Vivoni et al., 598 2004]. The grid is optimal in the sense that each triangle is as 599 close to equilateral as possible, for a given set of constraints. 600 The constraints can include watershed boundaries, the 601 stream network, geologic boundaries, elevation contours, 602 or hydraulic structures. After completion of the domain 603 decomposition, the triangular irregular network (TIN) need 604 def is projected vertically downward to form prismatic 605 volume elements, as shown in Figures 1 and 2. Using the 606 circumcenter as the node defining each triangle instead of 607 the centroid of the cell assures that the flux across any edge 608 with its neighbor is normal to the common boundary. For 609 instance, V_1V_2 is normal to D_4D_7 in Figure 2. This sim- 610 plifies evaluation of the flux across each boundary. How- 611 ever, it has the restriction that the circumcenter must remain 612 within the triangle under all circumstances. Shewchuk 613 [1997] has developed an algorithm that computes the 614 Delaunay triangulation satisfying the above requirement 615 from a set of points and constraints, in principle, and we 616 adopt this algorithm here. 617

[29] Grid generation for the watershed domain starts from 618 a set of defined control points. In general, the goal is to 619 represent the terrain with a minimum of triangles and 620 special constraints, such as hydrographic points (e.g., gaged 621 sites, dams etc.), and other specified critical terrain points 622 (e.g., local topographic maximum/minimum, convexity/ 623 concavity, or saddle points). These special points are se- 624 lected using terrain analysis tools. Once selected, they are 625 honored for any subsequent grid generation. In addition to 626 special points, we can also use line segments from catch- 627 ment boundaries such as the stream network, elevation 628 contours, vegetation polygons, etc., as constraints in the 629 grid generation. This preserves certain natural boundaries in 630 the domain decomposition for a particular problem. Usually 631 the goal is to generate a mesh having as small a number of 632 elements as possible while still satisfying all requirements 633 of the Delauney triangle (minimum angle, maximum area, 634 and constraints, etc.), and meeting the goals of the hydro- 635



Figure 4. Schematic view of the steps in domain decomposition. During the disaggregating process, catchments boundary, river network, and critical terrain points, etc., are introduced as constraints for generation of the TIN. GIS tools along with soil survey and/or gelogic maps are utilized to assign a priori hydraulic properties for each model element.

logic simulation (minimum support for the river network,minimum channel length increment, etc.).

638 [30] Figure 4 illustrates the sequence of procedures used to generate the grid and estimate parameters for each 639 element in a river basin. The decomposition process 640 involves delineation of the catchments boundary and river 641network at the desired resolution (support), given the 642 constraint framework. The constraints, often delineated 643 from digital elevation data or other related coverages 644 [Tarboton et al., 1991; Palacios-Velez et al., 1998; 645 Maidment, 2002], clearly play a very important role in 646 domain decomposition. 647

[31] Careful matching of the special point and line constraints including the channel network, with the choice of minimum area support (resolution), will assure that the domain boundaries are consistent before domain decomposition. Once the grid is generated, a priori parameter fields from the GIS (soil and geologic hydraulic properties, 653 vegetation parameters, etc.) are projected onto the grid. 654

5. Solving the Global ODE System 655

[32] Combining the local ODE system across the solution 656 domain yields a global ODE system in form 657

$$My' = f(t, y; x), \tag{29}$$

where M is the identity matrix, y is an n by 1 vector of state 659 variables, and x is the forcing. The unknown states are fully 660 coupled on the right-hand side of equation (29). 661

[33] An explicit solver is always preferred if an accept- 662 able solution can be achieved, since within each time step, 663 an explicit solver requires fewer evaluations of the right- 664 hand side. However, the multiple timescales arising from 665



Figure 5. The Shale Hills watershed and measurement locations. It consists of 44 wells, 44 neutron probes, and four weirs distributed over the 19-acre watershed.

watershed processes typically make (29) a highly stiff 666 system [Ascher and Petzold, 1998]. For stiff problems, the 667 overall computational cost of an explicit solution may 668 actually be higher than an implicit solver due to stability 669 670 concerns. The implicit sequential solver used here is the SUNDIALS package (suite of nonlinear and differential/ 671 algebraic equation solvers), developed at the Lawrence 672 Livermore National Laboratory. The code has been widely 673 applied, with extensive testing, and with excellent support. 674[34] For the initial condition $y(t_0) = y_0$, a multistep 675 formula is written 676

$$\sum_{i=0}^{K_1} \alpha_{n,i} y_{n-i} + h_n \sum_{i=0}^{K_2} \beta_{n,i} y'_{n-i} = 0,$$
(30)

where α and β are coefficients. For stiff ODEs, CVODE [*Cohen and Hindmarsh*, 1994] in the SUNDIAL package applies the backward differentiation formula (BDF) with an adaptive time step and method order varying between 1 and 5. Applying (30) to (29) yields a nonlinear system of the form

$$G(y_n) \equiv y_n - h_n \beta_{n,0} f(t_n, y_n) - a_n = 0$$
(31)

684 with

$$a_n \equiv \sum_{i>0} \left(\alpha_{n,i} y_{n-i} + h_n \beta_{n,i} y'_{n-i} \right).$$
(32)

Numerically solving equation (31), with some variant of Newton iteration, is equivalent to iteratively solving a linear system of the form

$$M(y_{n(m+1)} - y_{n(m)}) = -G(y_{n(m)}),$$
(33)

691 where M is $I - h\beta_{n,0}J$ with $J = \partial f/\partial y$.

[35] The GMRES (generalized minimal residual) iterative 692 linear solver in SUNDIAL makes the computational cost of 693 solving the global ODE system very competitive when 694 compared with other open-source solvers. 695

6. The Shale Hills Field Experiment

[36] The Shale Hills hydrologic experiment was con- 697 ducted on a 19.8-acre watershed in the Valley and Ridge 698 physiographic province of central Pennsylvania in 1974 by 699 the Forest Hydrology group at the Pennsylvania State 700 University [*Lynch and Corbett*, 1985; *Lynch*, 1976]. The 701 objectives of the experiment were to determine the physical 702 mechanisms of runoff and strea-flow generation at the 703 upland forested watershed, and to evaluate the effects of 704 antecedent soil moisture on the runoff peak and timing. The 705 fully coupled numerical model PIHM described earlier is 706 now applied to the Shale Hills site. The goal is to generally 707 explore the questions of the original field experiment using 708 an integrated model. Specifically these include the follow- 709 ing: (1) What is the impact of groundwater flow and soil 710 moisture on stream runoff and peakflow generation? (2) What 711



Figure 6. Spray irrigation devices are regulated to control the rate of irrigation under the tree canopy during the Shale Hills experiment.



Figure 7. The six artificial rainfall events of equal magnitude and duration and the corresponding runoff at the outlet weir for the Shale Hills experiment.

712 is the role of complex topography in producing runoff at 713 Shale Hills? (3) Can fully coupled models improve the 714 ability to simulate catchments that have ephemeral and/or

715 intermittent channels?

717 6.1. Experimental Design and Data

[37] The design consisted of a comprehensive network of 718 40 piezometers, 40 neutron access tubes for soil moisture, 719and four weirs. The distribution of sampling sites is shown 720 in Figure 5. The upper part of the channel is ephemeral or 721 intermittent, flowing during large storms or during the 722 seasonal snowmelt period. The watershed was implemented 723 with a spray irrigation network, shown in Figure 6, to 724 precisely control the amount of artificial rainfall over the 725entire watershed. The irrigation was applied below the tree 726 canopy and above forest litter, eliminating canopy intercep-727 tion storage during irrigation events. The watershed has a 728 mixed deciduous and coniferous canopy, with a relatively 729 thick forest litter. The soil profile at Shale Hills is typically a 730 silt loam, ranging from 0.6-m thickness at the ridge top, to 731 2.5 m deep near the channel. Three soil types are identified 732 733as Ashby, a shaley-silt loam in the upland portion of the 734 watershed; the Blairton silt loam on the intermediate elevation slopes; and the Ernest silt loam in the lower region 735 along the channel. Underlying the soil is the Rose Hill Shale, 736 which is thought to have a relatively low permeability 737 [Lynch, 1976] and acts as an effective barrier to deeper flow. 738 The bedrock topography was estimated by the limit of hand 739augering through the soil profile to bedrock. 740

[38] From July to September 1974, a series of six equal artificial rainfall events (0.64 cm/h for 6 hours) were applied to the entire watershed [*Lynch*, 1976]. The events were timed such that the antecedent moisture gradually increased from very dry in the first storm, to near saturation after the last event. Along with the artificial rainfall, a few natural 746 rainfall events also occurred. We note that the experiment 747 was conducted in late summer through the fall season when 748 evapotranspiration is small, and when the snow and frost 749 could be neglected. Many irrigation treatments were con-750 ducted during this experiment. The data chosen here spe-751 cifically reflect an experiment to test the effect of antecedent 752 moisture on peak runoff by sequential storm events of the 753 same rate and duration. 754

6.2. Water Budget

[39] Figure 7 illustrates the forcing and runoff data mea-757 sured at 15-min intervals from late July to early September. 758 Note the six artificial rainfall (irrigation) events, as well as 759 natural rainfall. Natural rainfall would of course be applied 760 to the top of the canopy. Nonetheless, during the late season 761 we assume interception storage to be small and can be 762 neglected. 763

[40] From the field data, the runoff/precipitation ratio is 764 calculated for each rainfall event and the results are given in 765 Table 1. A mass balance including change in storage shows 766

 Table 1. Observed Cumulative Input/Output and Runoff Ratio t1.1

 for the 1974 Rainfall-Runoff Experiment at Shale Hills

Event	Duration	Irrigation, m	Input, m ³	Output, m ³	Runoff/Precipitation Ratio, %	t1.
1	1-7 Aug	0.04318	3355.236	407.4109	12.1	t1.
2	7-14 Aug	0.045974	3572.339	998.8983	279	t1.
3	14-19 Aug	0.038608	2999.975	1287.057	42.9	t1.
4	19-23 Aug	0.038862	3019.712	1340.731	44.4	t1.
5	23-27 Aug	0.04064	3157.869	1839.37	58.2	t1.
6	27-31 Aug	0.071628	5565.744	3530.845	63.4	t1.
Total	1-31 Aug	0.2789	21670.88	9404.31	43.4	t1.



Figure 8. The unstructured grid used to simulate the watershed response for the Shale Hills watershed.

that 4.2% of total rainfall could not be accounted for in the
balance. This "error" may be due to insufficient density of
measurements, missing processes, or parameters (i.e., interception or deep loss to bedrock).

772 6.3. Antecedent Soil Moisture Effect

[41] By conducting the experiment with equal rainfall 773 events (0.64 cm/h for 6 hours), it is possible to test the effect 774 of initial condition or antecedent moisture on runoff yield. 775 We note that there was no significant infiltration-excess 776 overland flow observed during the experiment. Apparently 777 the infiltration capacity is large enough to accommodate the 778 rainfall rate without producing overland flow. However, the 779 deep forest litter makes this observation problematic. 780 Figure 7 and Table 1 both indicate that as the antecedent 781 moisture increases from a very dry to a very wet pre-event 782condition, the peak flow and total runoff increases as well, 783 with only 12% of rainfall becoming runoff for the first storm 784(very dry), and 63% runoff ratio for very wet conditions. 785 The relaxation for the sixth event in Figure 7 and the runoff 786 ratio in Table 1 clearly suggest the significance of soil 787 moisture and groundwater storage on the changing moisture 788 threshold for rainfall-runoff generation. This is examined in 789 more detail with the integrated model implementation next. 790

792 6.4. Model Domain and a Priori Data

[42] The surface terrain at Shale Hills is represented by a 793 1-m resolution digital elevation modedl (DEM) digitized 794795 from a detailed topographic survey of the watershed. There 796 were 44 monitoring wells/neutron probes covering the domain as shown in Figure 5. The bedrock elevation was 797 measured at piezometer locations and then interpolated 798 to the whole domain. The domain is decomposed into 799 800 566 triangle elements with 315 nodes (Figure 8). The 801 channel is delineated from the DEM with 21 segments, including both ephemeral and permanent reaches. Surface 802 infiltration capacity is set to be the same as saturated 803 hydraulic conductivity. Surface roughness varies with flow 804 depth and surface obstacles [Hauser, 2003]. In this case, an effective surface roughness was estimated (trial and error) to 806 be 0.83 min $m^{-1/3}$. The precipitation/irrigation forcing was 807 shown in Figure 7. Only daily temperature was available 808 near the site, so daily data were used to get a rough estimate 809 of evapotranspiration. The channel was assumed to be 810

rectangular, 1.5 m wide and 0.5 m deep. The hydraulic 811 roughness for the channel is set to 0.5 min $m^{-1/3}$. The 812 watershed boundary condition was assumed no flow for 813 surface and groundwater, and at the outlet of the catchment 814 the channel was assumed to be at critical depth. All initial 815 conditions were estimated by interpolation of neutron probe 816 and observation well data to the value just prior to the first 817 irrigation.

[43] The vertical profiles of soil moisture and saturated 819 thickness with locations shown in Figure 5 were measured 820 just before and after each irrigation and again at intervals 821 between irrigations in the experiment. The spatial average 822 depth of soil moisture storage (\overline{h}_u) across the entire site was 823 calculated and plotted against the spatial average saturated 824 groundwater storage (\overline{h}_g) and is shown in Figure 9. It 825 reveals a strong correlation between saturated and unsaturated storage. Soil hydraulic properties were estimated from 827 this information, and the procedure is described in the next section. 829



Figure 9. The saturated-unsaturated soil moisture storage for the spatially averaged Shale Hills data (dots) during the experiment. The solid lines represent the theoretical "steady state" saturated-unsaturated storage relationship for the shallow groundwater assumption based on the van Genuchten and the exponential soil characteristic. See section 6.5 for specific parameters. Note that $h_s = h_g - z_b$ and the height of saturation above bedrock is plotted in this case, where z_b is the elevation of the shale bedrock.



Figure 10. Observed and model groundwater levels for 1 August, 16 August, and 29 August. The fit is not significantly different from a slope of 1.

6.5. Simpified Shale Hills Model

[44] The system of equations developed in section 3 was 832 used to model the Shale Hills site. However, it was 833 determined that a simplification was possible as a result 834 of the shallow soil at the site. Duffy [2004] developed a 835 theoretical argument, that where the groundwater table is 836 near the land surface, the governing equations for subsur- 837 face flow can be simplified into a single state by applying 838 the "enslaving principal." That is, the water table enslaves 839 the soil moisture such that 840

$$\frac{dh_u}{dt} = G(h_g) \frac{dh_g}{dt}$$
(34)
$$G(h_g) = \frac{dh_u}{dh},$$
(35)

where $G(h_g)$ can be thought of as the integrated form of the 844 soil characteristic function (see Duffy [2004] for details). 845 This argument is essentially what was done by Bierkens 846 [1998] in an earlier paper. The coupled two-state subsurface 847 model (20) can now be reduced to 848

dho

$$G(h_g)\frac{dh_g}{dt} = p + q^+ - et + \sum_{j=1}^3 q_j^g.$$
 (36)



Figure 11. Observed (blue) versus model (red) runoff simulation for Shale Hills experiment. Note that the coupled model successfully simulates the internal runoff at each weir, including the upper ephemeral part of the channel.



Figure 12. The simulated surface saturation area immediately after each of the six rainfall events. Note that the saturation area is patchy and unconnected after the first two events, with little connectivity to the channel. The patches of saturation occur at a local break in slope or within topographic depressions. For later events, the connectivity increases as the water table rises and saturation overland flow occurs. It is noted that the saturation values were interpolated to 1-m resolution using inverse distance weighting from the triangle elements.

Bierkens [1998] uses the van Genuchten soil characteristic function to derive a form for $G(h_g)$ in (34) given by A similar expression can be developed for the exponential 861 soil characteristic (22) shown earlier which is given by 862

$$G(h_g) = \varepsilon_0 + (\theta_s - \theta_r) \Big(1 - (1 + (\alpha(z_s - h))^n)^{-((n+1)/n)} \Big), \quad (37)$$

where h_g and z_s are height of phreatic surface and surface elevation of the layer relative to some reference. The ε_0 is a small parameter to handle the singularity in the function $G(h_g)^{-1}$ when $h_g \rightarrow z_s$. The θ_s and θ_r are saturated and residual moisture content, and α and n are soil parameters. Substituting (18) and (35) into (37), and performing the integration yields an expression for h_u as a function of h_g :

$$h_{u} = \frac{1}{\alpha} \left[1 + \left(\alpha \left(z_{s} - h_{g} \right) \right)^{-n} \right]^{-\frac{1}{n}}.$$
 (38)

$$h_u = \frac{1}{\alpha} \left(1 - e^{-\alpha \left(z_x - h_g \right)} \right). \tag{39}$$

873

Using the site averaged data for h_u and h_g , the parameters in 864 (38) and (39) were estimated and the results shown in 865 Figure 9. The mean data from Figure 9 were used together 866 with the soil survey information to estimate van Genuchten 867 parameters used in the simulation: $\theta_s = 0.40$, $\theta_r = 0.05$, $\alpha = 868 2.0$ L/m, n = 1.8, $0.6 \le z_s \le 2.5$ m, and $K_s = 1 \times 10^{-5}$ m/s. 869 Also note in Figure 9 that the height of saturation above the 870 shale bedrock elevation is plotted using $h_s = h_g - z_b$.

6.6. Model Results

[45] For the domain, forcing, and a priori parameters 874 described above, the simulation was carried out on a dual- 875 processor desktop machine, completing the simulation in a 876



Figure 13. The flow depth along the channel for the third irrigation event. The solid lines show the distribution of flow depth during the event and immediately after the event (600 min). The dashed lines show the flow depth during the relaxation or recession period. The outlet weir is located on the right side of the graph.

few seconds. Because of the relatively small scale of the 877 simulation, computational efficiency is not an issue in this 878 problem. Figure 10 compares modeled and observed 879 880 groundwater depth for three days during the experiment, 1 August, 16 August, and 30 August, respectively, with an 881 overall regression slope of 1.05, and R = 0.965. Figure 11 882 illustrates simulated and observed runoff data at all four 883 weirs. The first event does not match as well as others, 884 due possibly to errors in the initial conditions, and this is 885 discussed below. The sixth event also shows some depar-886 ture, which might be related to our assumption to neglect 887 canopy interception. It is interesting that both the obser-888 vations and the model display a double peak in the 889 hydrograph for each single rainfall event (Figure 11). This 890 seems to be caused by a complex interaction of surface 891 runoff controlled by small-scale topography and near-892 channel surface runoff, with subsurface flow. Additional 893 experiments are necessary to partition the precise effects, 894 but it is clear that the fully coupled distributed model can 895 capture this kind of behavior. For the Shale Hills field 896 897 experiment the rainfall-runoff generation mechanisms assumed in the model include Hortonian overland flow due 898 to precipitation excess, and saturation overland flow. During 899 most of the numerical experiment, the soil infiltration capac-900 ity is large enough to accommodate rainfall, and Hortonian 901 flow is of limited importance except in the upland regions 902during the fifth and sixth events. Saturation overland flow 903 occurs at locations where water table saturates the land 904 surface from below. In Figure 12, the simulated regions of 905 surface saturation after each rainfall event are plotted. Note 906 that the saturation area is patchy and unconnected during the 907 first two events with little connectivity to the channel. The 908 patches of saturation occur at a local break in slope or in 909

topographic depressions. Recall that the hydraulic properties 910 of the soil and the forcing in the watershed are homogeneous, 911 and thus local variability is largely the result of topography. 912 The impact of noncontiguous temporary patches of saturation 913 is that the water reinfiltrates locally since it does not have a 914 path to the channel. This threshold for surface flow due to 915 local topography is discussed by *VanderKwaak and Loague* 916 [2001], and they introduce a subgrid parameterization to 917 resolve it. 918

[46] For later rainfall events (3–6), the connectivity of 919 surface saturation increases as the water table rises and 920 saturation overland flow connects the patches with the 921 channel. Rejected rainfall during the later events also 922 contributes to an increase in saturated area. In this analysis, 923 the surface and bedrock topography exert a strong control 924 on saturation overland flow, and thus have a dominant 925 impact on surface runoff in Shale Hills experiment. This 926 is similar to observations of *Amerman* [1965] and *Dunne* 927 and Black [1970a, 1970b] at other northeastern watersheds. 928

[47] Another aspect of the simulation observed in 929 Figure 11 is the onset of streamflow in the upper ephemeral 930 channel reach. Channel flow in the upper part of the 931 watershed is only observed during years with heavy snow 932 or after very large fall storms. Figure 13 shows the inte- 933 grated model result for flow depth along the channel in 934 response to the third rainfall event. The beginning of the 935 third rainfall is identified as 0 min and most of the channel 936 is dry (not shown). During the event (200 min) the length of 937 flowing channel has grown considerably. After 400 min the 938 event is over, and the channel continues to grow until about 939 10 hours, when it reaches a maximum and begins to relax. 940 After 3000 min the channel reach is largely dry again. The 941 ability to examine the internal details of the flow is an 942



Figure 14. Simulation of the effect of a dry initial condition (drought persistence) on runoff at the outlet. The initial condition for soil moisture and groundwater level was set to very low values and then the experimental forcing was applied to the model. Note that the recovery is complete at approximately 333 hours.

943 important aspect of the fully coupled approach, including 944 thresholds of wet and dry channels.

946 6.7. Sensitivity to Initial Conditions

[48] Next we simulate the impact of very dry antecedent 947 soil moisture and low water table conditions to get some 948 idea of the time it takes the watershed to recover from a 949 major drought. The model is run with the same forcing 950 sequence except that the initial states (groundwater and soil 951moisture) are reduced to the minimum possible values. The 952 response at the outlet weir is shown in Figure 14. Note that 953 954it takes a relatively short time for a complete recovery of 955peak flow as compared with the previous simulation (third event or 333 hours). This simple result offers a clue that 956 there is some problem with our assumptions in the model, 957since it has been subsequently observed during the 1990's 958 drought, that the outlet weir completely dried up and did not 959 recover for several years. This suggests that there might be a 960 slower and deeper flow component (e.g., a multivear 961 timescale) within the underlying less permeable shale rego-962 lith. This might also explain the missing mass described 963earlier, and this study is currently under way. 964

966 7. Conclusions

[49] In this paper we describe a semidiscrete finite volume strategy for fully coupled integrated hydrologic model
that is efficient for adding and subtracting processes and for
constructing the discrete solution domain. We demonstrate

the strategy by coupling equations for a mixed PDE-ODE 971 system that includes 2-D overland flow, 1-D channel flow, 972 1-D unsaturated flow, and 2-D groundwater flow, canopy 973 interception, and snowmelt. The complete system of equa- 974 tions including constitutive or closure relations is coupled 975 directly within a local kernel for a single prismatic element. 976 GIS tools are used to decompose the domain into an 977 unstructured grid, and the kernel is distributed over the grid 978 and assembled to form the global ODE system. The global 979 ODE system is solved with a state-of-the-art ODE solver. 980 The strategy provides an efficient and flexible way to 981 couple multiple distributed processes that can capture 982 detailed dynamics with a minimum of elements. The FVM 983 guarantees mass conservation during simulation at all cells. 984 The model is referred to as the Penn State Integrated 985 Hydrologic Model (PIHM). 986

[50] The approach has been implemented at the Shale 987 Hills field experiment in central Pennsylvania. Model 988 results show that it can successfully simulate observed 989 groundwater levels, as well as runoff at the outlet and at 990 internal points within the watershed using a priori param- 991 eters. The simulation is used to identify the important runoff 992 generation mechanisms, and to illustrate the impact of 993 antecedent soil moisture and groundwater level for ampli- 994 fying the volume and peak runoff in the watershed. The 995 effect of complex topography is shown to be a very 996 important control on infiltration/reinfiltration areas within 997 the watershed. The coupled model is able to simulate the 998 onset and relaxation of ephemeral streamflow in the upland 1000 part of the watershed. The processes and components of the 1001 model have been individually tested, and these results are 1002 given by Qu [2005]. A complete GIS interface for PIHM is 1003 currently being finalized for Web posting as a flexible and 1004 easily implemented open-source community modeling 1005 resource.

1006 [51] Acknowledgments. This research was funded by grants from the 1007 National Science Foundation (Science and Technology Center for Sustain-1008 ability of Water Resources in Semi-Arid Regions, NSF EAR 9876800; 1009 Integrated modeling of precipitation-recharge-runoff at the river basin scale: 1010 The Susquehanna, NSF ER030030), the National Oceanic and Atmospheric 1011 Administration (Modeling seasonal to decadal oscillations in closed basins, 1012 NICAA CARP Depresent NACAA PAA10055), and the National Armorek

1012 NOAA_GAPP Program, NA04OAR4310085), and the National Aeronau-1013 tics and Space Administration (The role of soil moisture and water table

- 1014 dynamics in ungaged runoff prediction in mountain-front systems, NASA
- 1015 GAPP Program, ER020059). This support is kindly acknowledged.

1016 **References**

- 1017 Abbott, M. B., J. A. Bathurst, and P. E. Cunge (1986a), An introduction to
- 1018 the European Hydrological System-Systeme Hydrologicque Europeen
- "SHE": part 1. History and philosophy of a physically based distributed modeling system, J. Hydrol., 87, 45–59.
- 1021 Abbott, M. B., J. A. Bathurst, and P. E. Cunge (1986b), An introduction to
- 1022 the European Hydrological System-Systeme Hydrologicque Europeen
- 1023 "SHE": part 2. Structure of a physically based distributed modeling 1024 system, *J. Hydrol.*, *87*, 61–77.
- 1025 Allen, R. G., L. S. Pereira, D. Raes, and M. Smith (1998), Crop evapotranspiration, *FAO Irrig. Drain. Pap. 56*, United Nations Food and Agric.
 1027 Organ., Rome.
- 1028 Amerman, C. R. (1965), The use of unit-source watershed data for runoff 1029 prediction, *Water Resour. Res.*, 1(4), 499–508.
- 1030 Ascher, U. M., and L. R. Petzold (1998), Computer Methods for Ordinary 1031 Differential Equations and Differential Algebraic Equations, Soc. for
- 1032 Ind. and Appl. Math., Philadelphia, Pa.
- 1033 Beven, K. (2006), Searching for the holy grail of scientific hydrology: Qt = 1034 H(SR)A as closure, *Hydrol. Earth Syst. Sci. Discuss.*, 3, 769–792.
- 1035 Bierkens, M. F. P. (1998), Modeling water table fluctuations by means of a
- 1036 stochastic differential equation, Water Resour. Res., 34(10), 2485-2499.
- 1037 Brandes, D. (1998), A low-dimensional dynamical model of hillslope soil
- moisture, with application to a semiarid field site, Ph.D. thesis, Pa. StateUniv., University Park.
- Bras, R. L. (1990), Hydrology: An Introduction to Hydrologic Science,
 Addison-Wesley, Boston, Mass.
- 1042 Brooks, R. H., and A. T. Corey (1964), Hydraulic properties of porous 1043 media, *Hydrol. Pap. 3*, Colo. State Univ., Fort Collins.
- 1044 Cohen, S. D., and A. C. Hindmarsh (1994), CVODE user guide, *Rep.*1045 UCRL-MA-118618, Numer. Math. Group, Lawrence Livermore Natl.
 1046 Lab., Livermore, Calif.
- 1047 Crawford, N. H., and R. K. Linsley (1966), Digital simulation on hydrology:
 1048 Stanford Watershed Model IV. *Stanford Univ. Tech. Rep.* 39, Stanford
- 1049 Univ., Palo Alto, Calif.1050 Delanunay, B. (1934), Sur la sphere vide, *Bull. Acad. Sci. USSR Class Sci.*
- 1051 Math. Nat., 7(6), 793-800. 1052 Dingman, S. L. (1994), Physical Hydrology, Prentice-Hall, Upper Saddle
- 1052 Dingman, S. E. (1994), *Thysical Hydrology*, Flende-Han, Opper Sadde
- 1054 Du, Q., V. Faber, and M. Gunzburger (1999), Centroidal Voronoi tessala-1055 tions: Applications and algorithms, *SIAM Rev.*, *41*(4), 637–676.
- 1056 Duffy, C. J. (1996), A two-state integral-balance model for soil moisture
 and groundwater dynamics in complex terrain, *Water Resour. Res.*, 32(8),
 2421–2434.
- 1059 Duffy, C. J. (2004), Semi-discrete dynamical model for mountain-front
- 1060 recharge and water balance estimation, Rio Grande of southern Colorado 1061 and New Mexico, in *Groundwater Recharge in a Desert Environment:*
- 1062 The Southwestern United States, Water Sci. Appl. Ser., vol. 9, edited by
- 1063 J. F. Hogan et al., pp. 255-271, AGU, Washington, D. C.
- 1064 Dunne, T., and R. D. Black (1970a), An experimental investigation of
- 1065 runoff production in permeable soils, *Water Resour. Res.*, 6(2), 478–490.
- 1066 Dunne, T., and R. D. Black (1970b), Partial area contributions to storm 1067 runoff in a small New England watershed, *Water Resour. Res.*, *6*(5),
- 1068 1296–1311.
- 1069 Freeze, R. A., and R. L. Harlan (1969), Blueprint for a physically-based, 1070 digitally-simulated hydrologic response model, *J. Hydrol.*, *9*, 237–258.

- Gardner, W. R. (1958), Some steady-state solutions of the unsaturated 1071 moisture flow equation with application to evaporation from a water 1072 table, *Soil Sci.*, 85, 228–232. 1073
- Gottardi, G., and M. Venutelli (1993), A control-volume finite-element 1074 model for two-dimensional overland flow, *Adv. Water Resour.*, *16*, 1075 277–284. 1076
- Hauser, G. E. (2003), River modeling system user guide and technical 1077 reference, report, Tenn. Valley Auth., Norris, Tenn. 1078
- Kristensen, K. J., and S. E. Jensen (1975), A model for estimating actual 1079 evapotranspiration from potential evapotranspiration, *Nord. Hydrol.*, 6, 1080 170–188.
- LaBolle, E. M., A. A. Ayman, and E. F. Graham (2003), Review of the 1082 integrated groundwater and surface-water model (IGSM), *Ground Water*, 1083 41(2), 238–246. 1084
- Leveque, R. J. (2002), *Finite Volume Methods for Hyperbolic Problems*, 1085 Cambridge Univ. Press, New York. 1086
- Lynch, J. A. (1976), Effects of antecedent moisture on storage hydrographs, 1087 Ph.D. thesis, 192 pp., Dep. of Forestry, Pa. State Univ., University Park. 1088
- Lynch, J. A., and W. Corbett (1985), Source-area variability during peakflow, 1089 in watershed management in the 80's, J. Irrig. Drain. Eng., 300–307. 1090
- Madsen, N. K. (1975), The method of lines for the numerical solution of 1091 partial differential equations, in *Proceedings of the SIGNUM Meeting on Software for Partial Differential Equations*, pp. 5–7, ACM Press, New 1093 York.
- Maidment, D. R. (2002), Arc Hydro: GIS for Water Resources, 140 pp., 1095 ESRI Press, Redlands, Calif. 1096
- Palacios-Velez, O. L., and B. Duevas-Renaud (1986), Automated rivercourse, ridge and basin delineation from digital elevation data, *J. Hydrol.*, 1098 86, 299–314.
- Palacios-Velez, O., W. Gandoy-Bernasconi, and B. Cuevas-Renaud (1998), 1100 Geometric analysis of surface runoff and the computation order of unit 1101 elements in distributed hydrological models, *J. Hydrol.*, 211, 266–274. 1102
- Panday, S., and P. S. Huyakorn (2004), A fully coupled physically-based 1103 spatially-distributed model for evaluating surface/subsurface flow, Adv. 1104 Water Resour., 27, 361–382. 1105
- Polis, M. F., and D. M. McKeown (1993), Issues in iterative TIN generation 1106 to support large scale simulations, paper presented at 11th International 1107 Symposium on Computer Assisted Cartography (AUTOCARTO11), 1108 Minneapolis, Minn. 1109
- Post, D. E., and L. G. Votta (2005), Computational science demands a new 1110 paradigm, *Phys. Today*, 58(1), 35–41. 1111
- Qu, Y. (2005), An integrated hydrologic model for multi-process simulation 1112 using semi-discrete finite volume approach, Ph.D. thesis, 136 pp., Civ. 1113 and Environ. Eng. Dep., Pa. State Univ., Univ. Park. 1114
- Reggiani, P., and T. H. M. Rientjes (2005), Flux parameterization in the 1115 representative elementary watershed approach: Application to a natural 1116 basin, *Water Resour. Res.*, 41, W04013, doi:10.1029/2004WR003693. 1117
- Reggiani, P., M. Sivapalan, and M. Hassanizadeh (1998), A unifying frame-1118 work for watershed thermodynamics: Balance equations for mass, 1119 momentum, energy and entropy, and the second law of thermodynamics, 1120 Adv. Water Res., 22, 367–398. 1121
- Reggiani, P., M. Hassanizadeh, M. Sivapalan, and W. G. Gray (1999), A 1122 unifying framework for watershed thermodynamics: Constitutive relationships, *Adv. Water Res.*, 23, 15–39. 1124
- Shewchuk, J. R. (1997), Delaunay refinement mesh generation, Ph.D. 1125 thesis, Carnegie Mellon Univ., Pittsburgh, Pa. 1126
- Sivapalan, M., C. Jothityangkoon, and M. Menabde (2002), Linearity and 1127 non-linearity of basin response as a function of scale: Discussion of 1128 alternative definitions, *Water Resour. Res.*, 38(2), 1012, doi:10.1029/ 1129 2001WR000482. 1130
- Slattery, J. (1978), Momentum, Energy, and Mass Transfer in Continua, 1131 Krieger, Melbourne, Fla. 1132
- Sleigh, P. A., P. H. Gaskell, M. Berzins, and N. G. Wright (1998), An 1133 unstructured finite-volume algorithm for predicting flow in rivers and 1134 estuaries, *Comput. Fluids*, 27(4), 479–508. 1135
- Tarboton, D. G., R. L. Bras, and I. Rodriguez-Iturbe (1991), On the extraction of channel networks from digital elevation data, *Hydrol. Processes*, 1137 5, 81–100. 1138
- VanderKwaak, J. E., and K. Loague (2001), Hydrologic response simulations for the R-5 catchment with a comprehensive physics-based model, 1140 *Water Resour. Res.*, 37(4), 999–1013. 1141
- van Genuchten, M. T. (1980), A closed form equation for predicting the 1142 hydraulic conductivity of unsaturated soils, *Soil Sci. Soc. Am. J.*, 44, 1143 892–898. 1144
- Vivoni, E. R., V. Y. Ivanov, R. L. Bras, and D. Entekhabi (2004), Generation of triangulated irregular networks based on hydrological similarity, 1146 *J. Hydrol. Eng.*, 9(4), 288–302. 1147

- 1148 Voronoi, G. (1907), Nouvelles applications des paramètres continus à la
- 1149 théorie des formes quadratiques, J. Reine Angewandte Math., 133, 97-
- 1150 178.
- 1151 Yeh, G. T., H. P. Cheng, J. R. Cheng, H. C. Lin, and W. D. Martin (1998), A
- 1152 numerical model simulating water flow, contaminant and sediment trans-
- 1153 port in a watershed systems of 1-D stream-river network, 2-D overland

regime, and 3-D subsurface media (WASH123D: Version 1.0), Tech. 1154 Rep. CHL-98-19, U. S. Environ. Prot. Agency Environ. Res. Lab., 1155 Athens, Ga. 1156

C. Duffy and Y. Qu, Department of Civil and Environmental 1158 Engineering, Pennsylvania State University, 212 Sackett Building, 1159 University Park, PA 16802, USA. (cxd11@psu.edu) 1160