Water cycle dynamics in a changing environment: Improving predictability through synthesis

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All science is the search for unity in hidden likenesses... The progress of science is the discovery at each step of a new order which gives unity to what had long seemed unlike... For order does not display itself of itself; if it can be said to be there at all, it is not there for the mere looking... order must be discovered and, in a deep sense, it must be created. What we see, as we see it, is mere disorder.

Bronowski [1956, p. 23]

1. Introduction

[1] Many current and widely relied upon hydrologic prediction approaches are founded on the assumption of stationarity [Milly et al., 2008], which permits extrapolation to the future using models that explain historical data. In a changing world, however, neither the structure (e.g., patterns of land use and land cover, connectivity between channels and riparian or wetland environments, or the extent of man-made structures), nor external drivers (e.g., temperature and precipitation forcing) of hydrologic response can be treated as fixed [Wagener et al., 2010]. Instead, changes in structure and drivers create the potential for new dynamics [Kumar, 2011] induced for example by hydrologic systems crossing unknown thresholds [Zehe and Sivapalan, 2009]. The potential for the emergence of such new dynamics poses significant challenges to predictability, especially on decadal or longer time scales.

2. Predictability Under Change

[2] One way to cope with change is to take previously fixed or exogenous factors—such as climate, soil structure, river network topology, vegetation distributions or patterns of human land or water use—and treat them as an endogenous part of the predictive framework. This amounts to an expanded view of hydrology that considers the connections between the water cycle and climatic, ecological, social and earth surface systems. The behavior of the hydrologic system thus emerges from the coevolution of the biotic, physical and

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anthropogenic systems that interact with it. Predictions under change are challenging because in this view, hydrologic predictability means understanding the interactions of multiple complex systems, including systems that are strongly driven by human decision making. These interactions must then be projected forward to make future predictions.

[3] The coevolution of the biotic and abiotic components in any particular ecosystem could (in theory) be simulated from detailed models that include all the relevant system feedbacks and couplings. Recent experience in hydrology has revealed the limits of the usefulness of such mechanistic models, even under the assumptions of stationarity [Blöschl and Montanari, 2010; Montanari, 2011]. The high dimensionality and process complexity of a coevolving system suggests that it may prove even more challenging to describe through detailed models [Strogatz, 1994]. Lower-dimensional approaches are needed [Dooge, 1992]. One possibility is to focus instead on the emergent outcomes of feedbacks and interactions between processes over time, which result in spatial and temporal organization of hydrologic systems: vegetation patterns, river networks and soil catena, or in the time domain, distributions of interevent times and amplitudes of events. These 'patterns' loosely defined as consistent trends of commonality or difference between different places and/or times-contain information on the physical, biotic and socioeconomic mechanisms from which they emerged. Organized patterns not only reduce the dimensionality of the prediction problem but point toward the development of new kinds of understanding, relating for instance to underlying organizing principles or natural laws. Such understanding could lead to entirely new ways of modeling prediction under change [Kleidon and Schymanski, 2008; Schaefli et al., 2011].

3. Role of Synthesis

[4] Given the potential importance of identifying trends, patterns and organization through time and space, classical hydrologic research faces a challenge. Hydrologic research tends to generate knowledge by collecting process- and place-specific data. This can lead to a body of understanding that is detailed and profound, yet fragmented in space and time and constrained by questions that motivated specific process studies. The arguments above suggest that overcoming this fragmentation is an urgent challenge for the field.

[5] Hydrologic synthesis offers one approach toward overcoming this fragmentation of knowledge [*Blöschl*, 2006; *Fogg and LaBolle*, 2006; *Hubbard and Hornberger*, 2006]. The goal of synthesis is to make previously fragmented knowledge and understanding, and different disciplinary

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perspectives of the same phenomenon mutually intelligible across times, places, scales and disciplines [*Blöschl*, 2006], in the sense of *Bronowski* [1956]. Hydrologic synthesis aims to unify existing, diverse pieces of information (data, models and disciplinary theories), to discover unrecognized connections, and to develop scientific understanding that is valid across multiple places, scales and times [*Blöschl*, 2006]. This special section presents results from the NSFfunded University of Illinois (UIUC) Synthesis Project, further details of which are presented by *Wilson et al.* [2010] and *Thompson et al.* [2011a].

4. Focus on Emergent Patterns

[6] An integrating framework for the synthesis approach presented in this series of papers is the focus on emergent patterns. Specifically, the research is aimed to examine if the patterns of hydrologic response found across multiple places correspond with existing hydrologic theory, and whether they could lead to new theories. Once emergent spatiotemporal patterns are identified, a range of questions can be formulated to investigate the nature, generation and consequences of these patterns:

4.1. Investigation of Emergent Patterns: Top-Down Questions

[7] How do we measure and identify patterns and describe them? What can we learn from existing data sets? How should we design new observatories?

4.2. Theoretical Questions: "Deep Why-Type Questions"

[8] Why do these patterns emerge? Under what circumstances do we expect them to occur? What are the underlying principles?

4.3. Bottom-Up Questions

[9] What are the consequences of these patterns (their effects on processes of interest)? How do they scale up in time and space? How does understanding the pattern improve our capacity to make predictions?

4.4. Human Interactions

[10] How do human activities respond to and modify these patterns in time and space? How are the patterns affected by human activities?

The papers appearing in this special section address a range of these questions, which were explored under two different themes, using two different sets of response data and associated patterns (see below). The synthesis project also addressed some of these questions in other, but related contexts as well, and these are reported elsewhere. For example, the synthesis team assisted in the conceptual design of experimental hillslopes aimed at exploring the coevolution of climate, vegetation and soils [*Huxman et al.*, 2009], for instance through modeling the interactions between hydrological, ecologic and pedologic processes in artificial hillslopes [*Dontsova et al.*, 2009; *Hopp et al.*, 2009; *Ivanov et al.*, 2010]. Another component deals with the synthesis of research relating landscape structural features (e.g., channel morphology, sedimentary record, soil heterogeneity) to the stochastic nature of earth surface transport and evolution processes. See *Foufoula-Georgiou* and Stark [2010] for an overview of a special issue of the Journal of Geophysical Research-Earth Surface focused on heavy-tailed stochastic models and fractional partial differential equations.

5. Catchments as a Cascade of Nonlinear Filters

[11] The research presented in this special section is organized under two themes. The first theme involved analysis of interannual variability of water balance and vegetation responses at the catchment scale. The nature of water balance partitioning was explored through recourse to rainfall runoff and vegetation cover data from over 400 catchments across the United States [Sivapalan et al., 2011; *Voepel et al.*, 2011], and independently through the use of remotely sensed data on evapotranspiration at the catchment scale in over 500 catchments [Cheng et al., 2011], in both cases revealing consistent patterns. The second theme involved examination of interannual variability in nutrient delivery at scales ranging from a few hectares to the entire Mississippi Basin. This was also motivated by consistent patterns observed in water quality data in watersheds in both the Mississippi and Baltic Sea Basins.

[12] Both examples share a common conceptualization of the landscape as a cascade of nonlinear filters, which attenuate exogenous forcing (such as climatic drivers or land use inputs). The nature and effect of the filters is determined by the relative roles of transport and reaction time scales, the history and legacy of land use, and the response of ecosystems (e.g., vegetation, microorganisms) to imposed variation. The topographic and geologic template of the landscape and its modification by people determine the sequence in which external inputs pass through these filters, and emerge as signatures of flow or concentration in streams.

[13] The two themes place emphasis on slightly different filters. The first theme primarily considers the role of vegetation activity in the vadose and shallow saturated zones within hillslopes to generate long-term (seasonal, annual and interannual) patterns in water balance. The second theme explicitly considers the interactions of the vadose zone, the shallow saturated zone and the channel network itself in modulating the inputs of rainfall and agricultural chemicals (fertilizer, pesticides), leading to emergent patterns of flow and concentration in stream discharge. A summary of the main research findings encapsulated through the papers in this special issue, under both themes, is presented next.

6. Water Balance at Catchment Scale and Role of Vegetation: Catchment Ecohydrology

[14] This research theme was inspired by Robert Horton's early work on the role of vegetation in growing season catchment water balance. Specifically, *Horton* [1933] observed that the ratio of catchment total vaporization (including interception loss, evaporation and transpiration) to catchment wetting (the fraction of precipitation that is available to plants), hereafter termed the Horton Index, H, was consistent from year to year. Based on his analysis *Horton* [1933, p. 456] hypothesized that the "natural vegetation of a region tends to develop to such an extent that it can

utilize the largest possible proportion of the available soil moisture supplied by infiltration."

[15] Troch et al. [2009] extended Horton's analysis to 90 catchments from the Model Parameter Estimation Experiment (MOPEX) [Duan et al., 2006] database and confirmed Horton's observations for the growing season. When computed for the water year, the mean of H was shown to vary with aridity both within individual catchments and between catchments. In all catchments, H tended to 1 during extremely dry years. Extending this work, Theme 1 aimed to (1) further investigate the physical and climatic controls on mean Horton Index and to (2) explore whether vegetation and water balance dynamics were related in ways that could lead to the consistency in the Horton Index noted in Horton's 1933 study. The study catchments were expanded to include more than 400 MOPEX sites across the continental USA, which were used to explore the relationships between water balance dynamics, vegetation dynamics, and physical features of the catchments.

[16] Inspired by the Horton Index, three models were developed to explore the controls on H: an empirical model, a simple process model and a functional model. The empirical model [Voepel et al., 2011] related the Horton Index statistically to observed climate (i.e., the aridity index) and landscape properties (i.e., slope and elevation). The process-based model by S. Zanardo et al. (Intraannual event rainfall variability controls on interannual variability of catchment water balance: A stochastic analysis, submitted to Water Resources Research, 2011) utilized a stochastic soil moisture balance to derive the probability density function of the annual Horton index analytically. The functional model [Sivapalan et al., 2011], inspired by the work of L'vovich [1979] and Ponce and Shetty [1995], was based on a twostep partitioning of incoming precipitation: (1) at the land surface precipitation is partitioned between quick flow and wetting; and (2) in the subsurface, wetting is partitioned between slow flow and evapotranspiration. This modeling work led to two discoveries: (1) a close symmetry between spatial (regional) variability of mean annual water balances and general trends of temporal (interannual) variability, supporting the potential use of space-time substitution for change prediction, and (2) the empirical and process models confirmed the roles of climatic aridity, within year variability of climatic drivers, drainability (i.e., slope), and soil depth (correlated with vegetation type and potentially related to rooting depth and thus vegetation dynamics) as the dominant drivers of variation in the Horton Index.

[17] The functional model of annual water balance, following L'vovich [1979], also allowed a robust estimation of the sensitivity of annual water balance to changes in annual precipitation, as illustrated by Harman et al. [2011a]. The four parameters of the functional model varied in a spatially coherent manner across the United States. However, they defied simple physical explanations. Further research is needed to link physical and ecological factors (e.g., climate, soils, topography, and vegetation) to these parameterizations of catchment function. In this respect, Brooks et al. [2011] explored the relationship between the variability of the Horton Index and vegetation cover, as measured by Annual Maximum NDVI, and showed that the Horton Index was able to identify differential sensitivity to drying based on vegetation type within catchment ecosystems. In this way catchment-scale partitioning, as measured by the Horton

Index, provided useful information for quantifying regional ecohydrologic response to climate or vegetation change.

[18] Cheng et al. [2011] investigated interannual variability of annual water balance within the alternative Budyko framework [Budyko, 1974] using remotely sensed evapotranspiration (ET) data in over 500 catchments across the United States. They found that the interannual variability of annual evaporation fraction, E/P, can be expressed in terms of a linear relationship with the climatic aridity index, E_p/P . Increasingly, however, the water balance of catchments is affected by human impacts, and there is a real need to separate the effects of climate change from those of direct human impacts. Wang and Hejazi [2011] analyzed data from the same 400 MOPEX catchments as used Sivapalan et al. [2011], also within the Budyko framework. They showed that human impacts were indeed significant over parts of the continent, and worked to separate the relative effects of climate change and direct human impacts, finding interesting regional patterns in their relative effects.

[19] In fact, the simple water balance models reported above could not fully reproduce the interannual variability of Horton Index. This was hypothesized to reflect an inadequate treatment of within-year and within-catchment variability of vegetation response, and to a lesser extent, rainfall runoff processes. To explore the roles of within-year and within-catchment variability, high-resolution flux tower data from 14 Ameriflux sites were also analyzed in a comparative manner [Thompson et al., 2011b]. This analysis highlighted significant differences in the within-year vegetation dynamics and functioning. The analysis highlighted the role of low temperatures in limiting transpiration (presumably due to transport constraints in frozen soils or cold plant conduits [Mellander et al., 2004]), and the role of deep soil moisture reserves or shallow groundwater in sustaining transpiration during periods of atmospheric drought, a characteristic feature highlighted by the analysis of vegetation composition and patterns carried out by Lowry et al. [2010]. The inability to adequately link these patch-scale observations and models to ET dynamics and runoff generation at catchment scales (the 1-D nature of the depiction ignores spatial relationships between hydrology, vegetation and their interactions [Thompson et al., 2010]) meant that it was not generally possible to predict Horton Index based on the tower data.

[20] This scale gap between patch- and catchment-scale estimates of water balance and the Horton Index highlighted the need for a theoretical framework to address spatial scale dependence in water balance prediction. *Thompson et al.* [2011c] explored in a preliminary manner the approach toward such a framework in the form of a simple conceptual model that linked feedbacks between vegetation cover and evapotranspiration along a converging flow path network (similar to a river network). These features resulted in both vegetation cover and water balance self-organizing in space around the imposed network, and naturally resulted in nontrivial spatial scaling of both. This model confirmed that invoking fundamental principles could result in spatial variability of the Horton Index across spatial scales. It also highlighted a set of physical controls on the Horton Index at the catchment scale, expressed in terms of 4 dimensionless similarity variables: (1) an aridity index, (2) a drainage competitiveness index, (3) a vegetation acclimation index, and (4) a network bifurcation index. The conceptual model of vegetation organization and water balances at the catchment scale presented by *Thompson et al.* [2011c] represents the culmination of systematic analysis of catchment water balance data, flux tower data and vegetation cover data, supported by parsimonious models in a top-down manner, all carried out as part of the synthesis project, and can be seen as the beginnings of a catchment scale approach to ecohydrology.

7. Hydrologic and Biogeochemical Filtering of Reactive Solutes: Catchment Biogeochemistry

[21] Theme 2 was motivated by an international study on the patterns of agrochemical export from intensively managed catchments in the United States, Europe and Australia [*Basu et al.*, 2010]. This study revealed strong similarities in the patterns of export from these catchments, specifically showing that annual exported chemical loads scaled linearly with annual discharge, suggesting that flow-weighted concentrations were near constant.

[22] Inspired by these findings, the synthesis effort focused on the Midwestern region of the United States to further investigate these patterns. The results obtained relate to the role of land and water management in generating consistent hydrologic and biogeochemical responses, exploring and defining the nature of biogeochemical exports and their dependence on transport and chemical processes, and to the development of models that can represent these processes in tractable predictive frameworks.

[23] The U.S. Midwest is a highly managed landscape with two important hydrologic features: first, evapotranspiration losses are largely homogeneous due to the expanse of monocultural corn-soybean rotations, and second, runoff processes have been homogenized due to the installation of artificial subsurface drainage (i.e., tile drains). The effects of this management were explored in a frequency domain study of high-resolution streamflow data collected in the Little Vermillion River Watershed (LVRW) [*Guan et al.*, 2011]. This study indicated a strong signature of tile drainage in the streamflow, which persisted across spatial scales ranging from the single tile (~1 ha) to the entire LVRW (~400 km²), and that these transport signatures were also strongly reflected in the patterns of chemical export.

[24] The patterns of chemical export were explored in detail, and two different export patterns were identified. Chemostatic behaviors were exemplified by relatively constant flow-weighted concentrations, and contrasted with episodic behaviors, in which export was intermittent and exhibited high variability in concentrations. Chemostatic export was exhibited by nitrate, while episodic export was demonstrated by atrazine in these managed catchments. Surprisingly, a consistent underlying model can be proposed to explain both models of behavior. This consists of a mass balance for water and solutes in the shallow saturated zone of a tile-drained agricultural field, which is modeled as a well-mixed reactor. Mass balance for water is computed by assuming that the saturated zone acts as a linear reservoir, a reasonable assumption in tile-drained watersheds following the observed exponential behavior of the hydrograph recession [Schilling and Helmers, 2008]. The solute mass balance considers two kinds of inputs: a stochastic forcing associated with recharge from the vadose zone, and a linear release of mass from a chemically recalcitrant store (e.g.,

sorbed P, sorbed herbicides, organic N). Mass degradation is assumed to be linear. Running this model (as illustrated by *Thompson et al.* [2011d]), generates episodic behavior when the rate of degradation is very high or very low compared to the rate of mass input from storage. When degradation rates are comparable to rates of mass input, however, chemostatic export dynamics result.

[25] These two different patterns of export suggest different hydrologic and biogeochemical controls on solute behavior. Episodic exports require an explicit treatment of the stochastic drivers of export. Chemostatic exports, by contrast, can be predicted on the basis of annual discharge provided the flow-weighted mean concentration is known. Stochastic inputs of water and chemicals to the vadose zone were the explicit focus of the Hydrologic Event-Based Infiltration and Solute Transport (HEIST) model [Harman et al., 2011b]. HEIST accounts for hydrological and biogeochemical interactions within the vadose zone by explicitly simulating evapotranspiration (ET), retardation and degradation, and also allows a probabilistic treatment of the solute delivery ratio to be analytically or semianalytically derived. The analytical solutions made the links between solute dynamics and water balance explicit. Solute transit times through the vadose zone – which fundamentally determine the amount of degradation that a solute, such as a pesticide, experiences on its way to the water table – were shown to vary with the Horton Index H as $(1-H)^{-1/2}$ [*Troch et al.*, 2009]. This probabilistic approach allows the effects of land management and climate on solute delivery to the water table to be treated within a risk assessment framework.

[26] In-stream dynamics provide important controls on delivery of reactive solutes over large spatial scales. The effect of the stochasticity of the climate on the solute "Delivery Ratio," $DR = \exp(-k\tau)$, where τ [T] is residence time and k [T⁻¹] is in-stream removal rate constant, was explored by Basu et al. [2011a] by extending the formulation of Botter et al. [2010] to develop the probability density function (pdf) of DR. Model results indicated that the efficiency of in-stream solute removal increased with increasing variability in the discharge, primarily due to greater net processing during periods of low discharge. Surprisingly, the pdf of Mississippi scale processing efficiency was adequately described by this reach scale model indicating the existence of scale independence [Basu et al., 2011a]. Indeed, the functional form of the inverse relationship between k and the stream stage was independent of spatial and temporal averaging at scales as large as the Mississippi Basin. The scale independence was further explored by adding biogeochemical components to the existing Representative Elementary Watershed (REW) stream network model by Li and Sivapalan [2011] and Reggiani et al. [2001], as shown by S. Ye et al. (Dissolved nutrient retention dynamics in river networks: A modeling investigation of transient flows and scale effects, submitted to Water Resources Research, 2011). The stream network model has two compartments: a main channel and a hyporheic transient storage zone. The results of this modeling study are consistent with the observations of Stewart et al. [2011] that although a surface transient storage zone with greater exchange rates might exist at the reach scale, its relative importance in solute processing is less at the network scale due to longer residence times. The model results revealed that the functional dependence of k on the flow properties of the river (e.g., stream stage) was scaleinvariant in humid catchments, while strong nonlinearities arose in arid watersheds.

[27] Finally, the role of land use and land management was considered by a data analysis that considered gradients of external chemical impact associated with direct management (e.g., fertilization or road salting for de-icing), air pollution (e.g., acid rain inputs), or natural fluctuations (e.g., sea salt episodes). Surprisingly, for several of the chemicals studied, there appeared to be a trend, with "low impact" catchments tending to exhibit episodic export patterns, and "high impact" catchments behaving more chemostatically [Thompson et al., 2011d]. An important example is nitrate, which exhibited significantly greater variability in concentrations in pristine catchments compared to natural catchments [Thompson et al., 2011d]. These results were interpreted in terms of the conceptual model described above, and specifically the role of the recalcitrant mass store. Such stores are known to build up in response to prolonged periods of high loading (e.g., "saturation" effects in nitrogen, sulfur and phosphorus processing). In the absence of such a store, episodic exports were shown to be probable outcomes of the simple mass balance model, while in the presence of such a store, chemostatic exports were [Thompson et al., 2011d].

[28] As outlined by *Basu et al.* [2011b], these synthesis findings have implications for land and water management and restoration of intensively managed catchments. If large recalcitrant mass stores are indeed responsible for chemostatic export patterns, then the ubiquity of such export patterns for environmental pollutants such as nitrate is deeply concerning. Available studies suggest that there may be time lags of several decades between ending external nitrogen inputs and significant reductions in the nitrogen concentrations [*Meals et al.*, 2010]. Understanding the time scales of such lags, and their links to the history and spatial patterns of land use would prove valuable for designing restoration or mitigation programs.

8. A Synthesis of Newtonian and Darwinian Approaches

[29] There have been several calls to reexamine the fundamental approaches used in hydrologic science [Dooge, 1986, 1988; Gupta et al., 2000; Hooper, 2009; Torgersen, 2006]. Harte [2002] contrasted a physics-like "Newtonian" approach with the ecology-like "Darwinian" approach, and suggested that contemporary challenges in the earth sciences, such as dealing with environmental change, require a synthesis between the two. The Newtonian approach is exemplified in hydrology by detailed process-based models. This approach builds understanding from universal laws that govern the individual parts of the system. A Newtonian objective in hydrology is the mechanistic characterization of how water, energy and mass fluxes and transformations occur in the various parts of the landscape in the form of a boundary value problem. Even though the laws employed are taken to be universal, and not tied to a particular landscape, their solution depends strongly on the boundary and initial conditions, which must be characterized for a given landscape.

[30] The Darwinian approach values holistic understanding of the behavior of the given landscape. It embraces the history of a given place, including those features that are relics of historical events, as central to understanding both its present and its future. The Darwinian approach gains predictive power by connecting a given site to several sites located along critical gradients. Laws in the Darwinian approach will seek to explain patterns of variability and commonality across several sites, as exemplified by the work of Kumar and Ruddell [2010] who used ecohydrologic data taken from several flux towers to discover underlying organizing principles. As previously argued by McDonnell et al. [2007] and Kumar [2011], the synthesis between the Newtonian and Darwinian approaches in hydrology thus offers the possibility for combining predictive understanding of the mechanisms of change with an explanatory understanding of the patterns that emerge when these mechanisms interact in real landscapes. This synthesis ensues when advances are made across the divide from both sides: when Newtonian process descriptions are used to develop explanatory hypotheses for variations between places, and when the particularities of many places, when viewed together at a certain distance, reveal commonalities that can help develop new process descriptions at large scales. The latter approach stands in contrast to the traditional reductionist approach where new process descriptions are developed through the treatment of phenomena at finer and finer scales.

[31] The work represented in the papers appearing in this special section offers examples of both approaches. Newtonian process descriptions (necessarily simplified) were used in the works of Harman et al. [2011b], Thompson et al. [2011d, 2011b], and S. Zanardo et al. (submitted manuscript, 2011), respectively, to develop parsimonious insights and explanations for the variations of vadose zone travel times, solute delivery and transformation, and differences in water balance between places with different climates and landscapes. In none of these cases would the models used be called "state of the art" in terms of the details of their Newtonian process descriptions, but each provided fundamental insights that a more sophisticated model run in one place for one time would not. In the other direction, the motivating works of Troch et al. [2009], Brooks et al. [2011], and Basu et al. [2010], each used large data sets to reveal intriguing patterns of commonality that cried out for explanation. These patterns were used by Voepel et al. [2011], Sivapalan et al. [2011], and Harman et al. [2011a] to develop new predictive relationships for spatial and temporal variations in water balance and by Thompson et al. [2011d] and Basu et al. [2011a] to develop predictive models of reach and catchment-scale solute transformations. These process models rely on the emergence of ordered behavior at larger scales as a result of the evolutionary history of the systems, though the models do not (and need not) express that evolutionary process explicitly.

[32] In conclusion, the work reported in this special section can therefore be seen as tentative first steps toward a new approach to hydrologic science based on a synthesis of the Newtonian and Darwinian approaches. While significant breakthroughs are yet to be fully realized, it is our belief that if hydrologic synthesis as outlined in this paper is vigorously pursued it has the potential to generate transformative outcomes for hydrologic science.

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