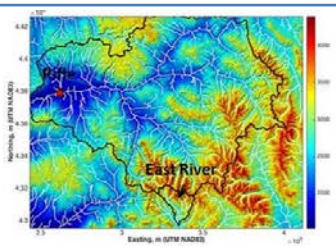
GENOMES TO WATERSHEDS

E-Newsletter for the Berkeley Lab Scientific Focus Area (SFA) 2.0
Issue 3 / Summer 2015



From the Director:

This summer newsletter describes several exciting advances associated with the Genomes to Watershed Scientific Focus Area (SFA) 2.0 Project, which have primarily been carried out at the Rifle CO floodplain located along the Colorado River. Examples include:

- Significant advances in using genomic and metatranscriptimic approaches to reveal the diversity and realized metabolic potential of subsurface microbial communities.
- Successful reactive transport simulations at the Rifle floodplain, performed through inclusion of genome-derived information about chemolithoautrotrophic pathways. Not including genome-based information resulted in an underestimation of dissolved organic carbon exports to the Colorado River by almost 200%.
- New observations of reactive oxygen species (ROS) in the laboratory and Rifle subsurface, which document how ubiquitous dissolved metals (such as Fe) can play an important role in abiotically transforming organic matter in the presence of ROS.
- New capabilities to jointly invert geophysical and other information to autonomously monitor subsurface moisture and temperature that influences microbial activity.

In addition to ongoing research at the Rifle site, we are developing a mountainous headwaters watershed site at the East River of the Upper Colorado River Basin. The Upper Colorado in perhaps the most important Western US River Basin, providing water resources, hydropower, and irrigation for Colorado, California and other Southwestern states. The extension from research on hydrological driven biogeochemical cycling at the Rifle floodplain to the East River watershed represents a transition to increasing spatial scales, terrestrial environment complexity, and societal impact.

Early genome-inspired East River watershed simulation results are also briefly described in this newsletter, which indicate that hyporheic zone flow and reactions lead to lateral redox zonation that may significantly influence the flux of both organic and inorganic carbon into the Colorado fluvial system.

We have developed a series of videos describing some of the SFA 2.0 research, including:

– An overview of the SFA 2.0 project, describing its mission and approach to obtaining a predictive understanding of terrestrial environments, from the genome to the watershed scales.

–Watershed research within the Sustainable Systems SFA 2.0 project—including identification and monitoring of primary factors that control watershed biogeochemical

–Metabolic potential of the subsurface—or how metabolic lifestyles of microbial communities modulate in response to as well as influence environmental change.

–A productive collaboration between the SFA 2.0 and DOE's Joint Genome Institute (JGI), and resulting understanding of the roles microbes play in contamination migration and remediation.

For more information about our project, please visit us at our website.

Susan S. Hubbard

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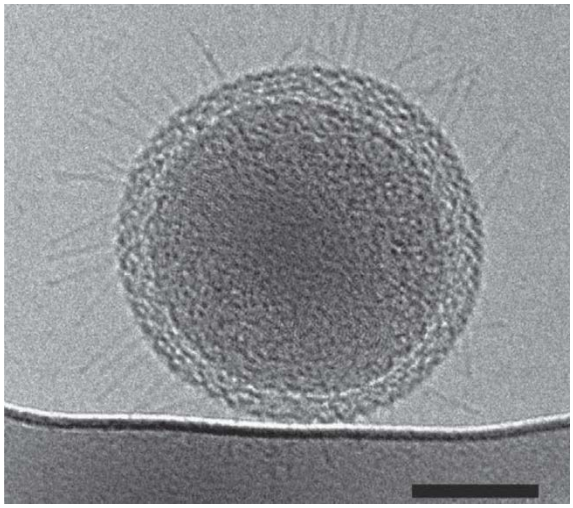
Research Updates

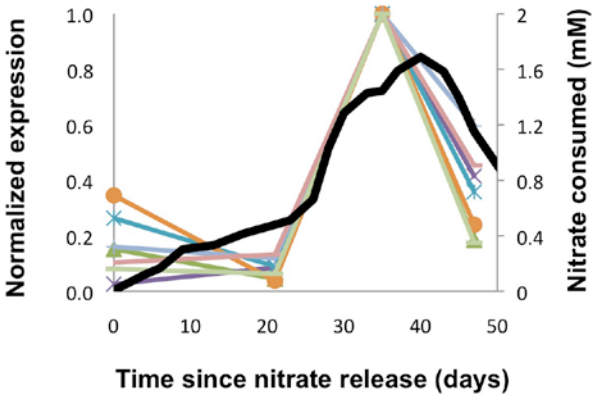
New Genomes Illuminate the metabolic potential of the subsurface: We reconstructed and published genome sequences for over 800 bacteria from a large radiation lacking cultivated organisms (average completeness estimated to be 91%). These bacteria are widespread in the Rifle aquifer subsurface, and also in other subsurface environments. Notably, these organisms consistently have small genomes and, at least in a subset of cases, small cell size. Features of these cells include tightly packed spirals inferred to be DNA, few densely packed ribosomes, and a variety of cellular appendages that might enable inter-organism interactions (Luef et al. 2015 Nature Communications). We designated the large segment of the bacterial domain with which these organisms affiliate as the Candidate Phyla Radiation (CPR; Brown et al. Nature, 2015). In addition to genomic sampling the CPR, we reconstructed and partially curated over 2500 genome sequences for other members of the CPR and other bacterial and archaeal lineages. From the massive genomic dataset we have predicted metabolic capacities and, in some cases, we have integrated the results for specific sample sets or systems to understand which organisms contribute to biogeochemical transformations of interest. An important outcome has been the ability to postulate the metabolic contributions of previously unknown organisms to biogeochemical cycling (Hug et al. Environmental Microbiology, 2015).



A Cryo-TEM image showing the morphology, size and some key features of ultra-small bacteria. The cell envelope includes distinct outer layer (S-layer). Pili-like structures are clearly visible and in some cases these pilin apparently connect adjacent bacteria. Scale bar is 100 nanometers or about 1/500th of the diameter of a human hair. *From Luef et al. 2015, Fig. 4.*

Contributors: **Jill Banfield,** Harry Beller, Chris Brown, Birgit Luef and others.

Metatranscriptomes demonstrate the importance of chemolithoautotrophy in the Rifle subsurface: In a 2-month study of nitrate amendment to the Rifle aquifer, metatranscriptomic (community gene expression) analysis revealed pervasive and diverse chemolithoautotrophic bacterial activity relevant to C, S, N, and Fe cycling (Jewell et al. in prep.). Prior to nitrate injection, anaerobic ammonia-oxidizing (anammox) bacteria accounted for 16% of overall microbial community gene expression, whereas two other groups of chemolithoautotrophic bacteria collectively accounted for 80% of the metatranscriptome during the nitrate release: (1) members of the Fe(II)-oxidizing Gallionellaceae family and (2) strains of the S-oxidizing species, *Sulfurimonas denitrificans*. Notably, the proportion of the metatranscriptome accounted for by these three groups was considerably greater than the proportion of the metagenome coverage that they represented. Transcriptional analysis revealed some unexpected metabolic couplings, most notably, putative nitrate-dependent Fe(II) and S oxidation among nominally microaerophilic Gallionellaceae strains. The three most active groups of chemolithoautotrophic bacteria in this study had overlapping metabolisms that allowed them to occupy different yet related metabolic niches throughout the study. While members of all three groups respired nitrate, they had markedly different temporal expression profiles and activity maxima, even among closely related species/strains within the three groups. Overall, these data provide key insights into the important role of chemolithoautotrophy in the Rifle subsurface and are being used to inform GEWaSC modeling efforts.

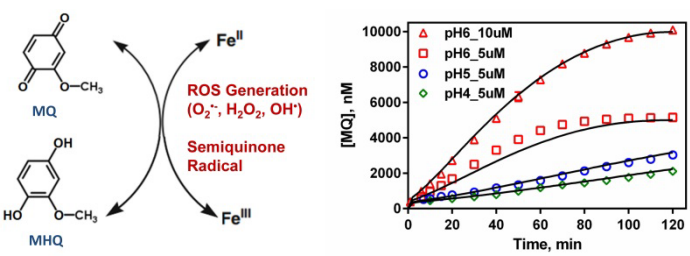


Very strong correspondence between nitrate consumption and expression of selected genes in a Rifle Gallionellaceae strain [including genes for nitrate reduction, Fe(II) oxidation, S oxidation, and CO2 fixation]. All lines are Gallionellaceae transcripts except the thick black line, which represents nitrate added and rapidly consumed (Jewell et al., in prep.).

Contributors: **Harry Beller**, Talia Jewell, Jill Banfield, and others.

Reactive Oxygen Species (ROS) quantified in the lab and the subsurface:

Catalytic activity of a coupled Fe and ROS cycle to catalytically oxidize 'lignin-like' organic functional groups has been documented at the Rifle Site. Results show that in the presence of ROS, ubiquitous dissolved metals (such as Fe) can play an important role in abiotically transforming organic matter, and that reactions with organic matter can maintain steady-state concentrations of Fe(II) in solution in spite of the presence of molecular oxygen. A kinetic model has been built to explain these results (see below). This model can now be used to explore the quantitative importance of this process under different geochemical conditions and can be incorporated into the larger floodplain and watershed modeling effort. In parallel, significant steady-state concentrations of H_2O_2 have been measured along the depth profile of several groundwater wells across the Rifle site. To the best of our knowledge, this is a completely novel observation and will have a dramatic impact on the understanding of the importance of ROS in subsurface systems.

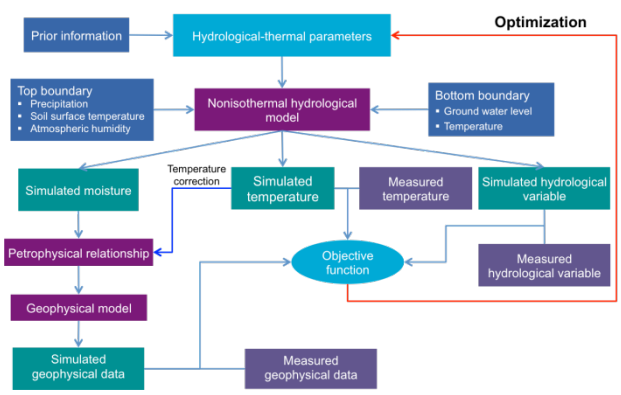


Left: Schematic of Fe catalyzed oxidation of 'lignin-like' methoxy-semiquinone (MHQ) to methoxy-quinone (MQ). Right: Kinetic plots showing that 500 nmol of Fe can catalytically oxidize 10micromol of MBQ within two hours.

Contributors: **Xiu (Joyce) Yuan,** Peter Nico, Ben Gilbert, and others

Temperature-dependent inversion of geophysical data crucial for a thermal-hydrological model of the vadose zone:

Using time-lapse electrical resistivity tomographic (ERT) data and other information, members of the SFA 2.0 team quantified dynamic variations in subsurface moisture content and heat transport important for microbial activity at the Rifle Site. Their investigation was accomplished through development and testing of a coupled hydrological-thermal-geophysical inversion, which was tested on both field-derived and synthetic datasets (Tran et al., submitted). The inversion scheme is based on a non-isothermal hydrological model and simultaneously provided soil moisture and temperature data with a high spatiotemporal resolution, with the model explicitly considering the influence of these two variables on soil electrical conductivity. The model results provide critical information about moisture and heat dynamics as a function of meteorological forcings and infiltration, and as a function of soil and sediment unit. The developed capability permits the use of time-lapse ERT, which is autonomously collected at the Rifle CO site, to estimate thermal and moisture content at fine scales, which can be assimilated into reactive transport models of the site.



Coupled hydrological-thermal-geophysical inversion scheme

Contributors: **Phuong Tran,** Baptiste Dafflon, Ken Williams, Susan Hubbard, Tetsu Tokunaga, Phil Long and others

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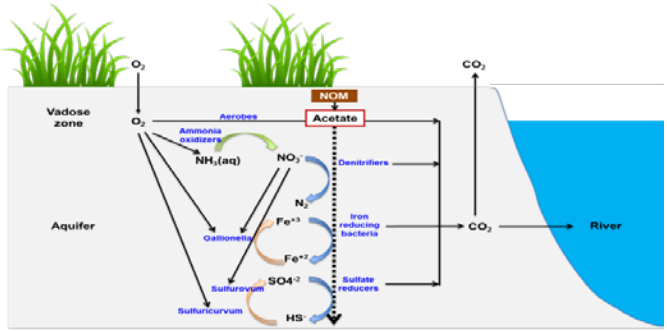
2-D multiphase reactive transport model with hi-fidelity representation of biogeochemical pathways: As part of the SFA 2.0 modeling efforts, a 2-D reactive transport model was developed to investigate the principal controls on subsurface carbon fluxes in the Rifle floodplain. The vertical 2-D (x-z) model was developed using TOUGHREACT along a transect corresponding to the TT series of wells that includes a NRZ location, and incorporates both the unsaturated and saturated zones. The biogeochemical reaction network includes multiple terminal electron acceptors (TEAs), kinetic and equilibrium mineral precipitation and dissolution, as well as spatially distinct pools of Fe and S minerals and functional microbial populations. Simulation results were constrained by measurements of water and carbon fluxes along with water table elevation and by isotope and major element chemistry.

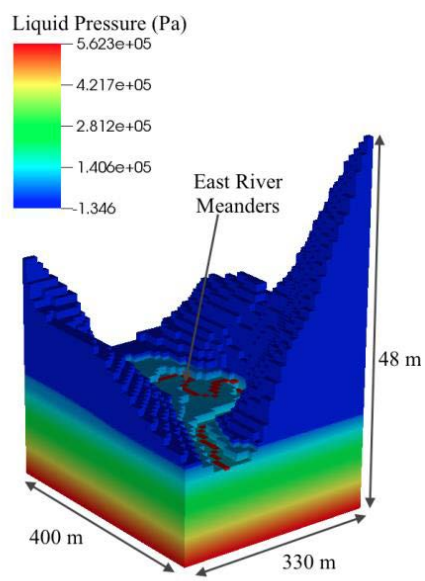
Neglecting the chemolithoautrotrophic pathways associated with reduced zones in the simulations resulted in underestimating dissolved organic carbon exports to the river by almost 200%. Simulated groundwater carbon fluxes to the river decreased when averaged over annual water table variations and increased 180% to 3.3 g m-2 d-1 when averaged over annual temperature fluctuations at the site. Thus incorporation of microbially catalyzed reactions is apparently crucial to accurate prediction of carbon fluxes to rivers.



Schematic representation of the biogeochemical reaction network included in model simulations. In this "reduced-order" model, certain microbial species and their functions are explicitly represented in the reaction network (such as *Sulfuricurvum* as sulfide oxidizer) while the broader diversity of species for other functions (such as sulfate reducers) is modeled by simplified, overall reactions and rates.

Contributors: **Carl Steefel** and others

Simulations of coupled hydrological and biogeochemical interactions at the Watershed Scale: The overarching goal of GEWaSC s to represent heterogeneous hydrological and complex biogeochemical processes in high-resolution, three-dimensional, reactive flow and transport models to predict carbon and nutrient fluxes at the watershed scale. The lower East River system, a high elevation catchment in western Colorado, is rolling-to-mountainous topography with multiple river meanders extending over a distance of 11 km. A hypothesis that we are beginning to test at this new site is that the biogeochemical gradients that exist within the hyporheic zone associated with individual stream meanders significantly impact carbon and nutrient fluxes in the larger East River system, particularly when up-scaled over the entire length of the East River Flood Plain. We used a genome-inspired biogeochemical reaction network, including multiple carbon and nitrogen species and autotrophic, heterotrophic, and chemolithoautotrophic microbial activity, for our preliminary watershed simulations. In the lower East River site, initial results indicate that intra-meander hyporheic zone flow and reaction leads to lateral redox zonation. These redox zones significantly influence the flux of both organic and inorganic carbon into the fluvial system.



Model domain showing meandering lower East River and liquid pressure at steady state. Genome-inspired reaction pathways were used to simulate redox zonation and associated flux of organic and inorganic carbon into the fluvial system.

Contributors: **Dipankar Dwivedi**, Carl Steefel and others

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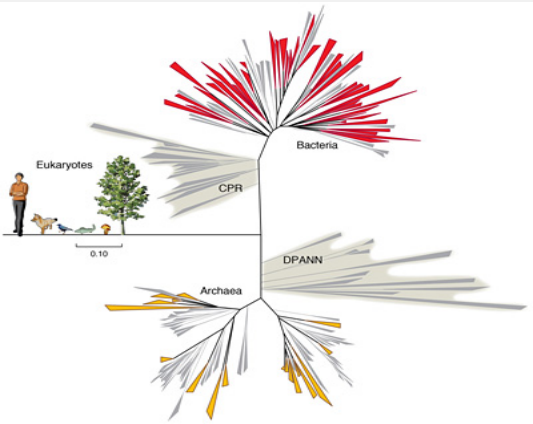
FEATURED PUBLICATIONS:

A few recent publications highlights are provided below associated with SFA 2.0 research; please visit our website to see a full list of our publications

nature International weekly journal of science

Newfound groups of bacteria are mixing up the tree of life: University of California, Berkeley, scientists have identified more than 35 new groups of bacteria, clarifying a mysterious branch of the tree of life that has been hazy because these microbes can't be reared and studied in the lab. The new groups make up more than 15 percent of all known groups or phyla of bacteria, the scientists say, and include the smallest life forms on Earth, microbes a mere 400 nanometers across. The number of new bacterial phyla is equal to all the known animal phyla on Earth. "This is a new view of the tree of life," said lead author Jill Banfield. "These new groups of bacteria and Archaea are changing our understanding of the number and arrangement of branches on the tree of life."
Graduate student Christopher Brown, Banfield and their colleagues reported the discovery online (Monday, June 15, 2015) in the journal *Nature*. Read More



The new groups of bacteria (CPR) greatly expand the known and characterized groups. These and previously reported new groups of Archaea (DSPANN) show that the Tree of Life is more complex than thought. (Banfield group graphic)

The ISME Journal
Multidisciplinary Journal of Microbial Ecology

An article entitled **Aquifer environment selects for microbial species cohorts in sediment and groundwater**, by Laura A. Hug et al., was published in the ISME Journal. They characterized and tracked a sediment community's most abundant 133 organisms across 36 different sediment and groundwater samples, to investigate the biogeography of the Rifle aquifer. Analyses showed that these 133 organisms were more consistently detected in saturated sediments than in samples from the vadose zone, from distant locations, or from groundwater filtrates.

Read-mapping of more than 1.4 terabases of sequence to an assembled metagenome provided detailed detection and abundance estimates for organisms across the sampled environments
Read more

JEQ JOURNAL OF ENVIRONMENTAL QUALITY

Characterization of Chromium Bioremediation Products in Flow-Through Column Sediments Using Micro–X-ray Fluorescence and X-ray Absorption Spectroscopy: by Charuleka Varadharajan, et al..
This study is part of a broader effort investigating the biogeochemical mechanisms for Cr(VI) reduction in Hanford 100H aquifer sediments using flow-through laboratory columns. It had previously been shown that reduced chromium in the solid phase was in the form of freshly precipitated mixed-phase Cr(III)-Fe(III) (hydr)oxides, irrespective of the biogeochemical conditions in the columns. In this study, the reduced Cr phases in the columns were investigated further using spectroscopy to understand the structure and mechanisms involved in the formation of the end products. Read more

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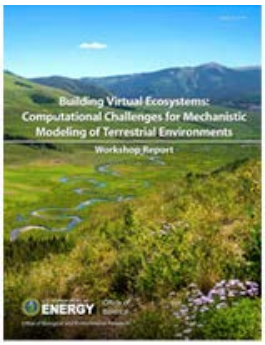
New Projects related to SFA 2.0:

Good IDEAS for Building Virtual Ecosystems: SFA 2.0 members Carl Steefel and Eoin Brodie contributed to a DOE Office of Science workshop report focused on building virtual ecosystems, and in particular, on identifying computational challenges associated with mechanistic modeling of terrestrial environments. The full workshop report is provided **here.**

A recommendation of the workshop was the systematic development of an Interoperable Design of Extreme-Scale Application Software (IDEAS). The DOE Advanced Scientific Computing Research and the Office of Biological and Environmental Research subsequently funded a new IDEAS project (**web link**). Hans Johansen serves as the Focus Lead for Methodologies for Software Predictability, and Carl Steefel is a team member of the Use cases for terrestrial modeling led by David Moulton.

Development of the IDEAS infrastructure will be guided by a number of use-cases, including one that will be carried out at the SFA 2.0's new East River Watershed site, which is shown on the front cover of the workshop report.



Using 'rapid access' support from DOE-BER, Ken Williams initiated sediment and stream water sampling activities at multiple locations along the Animas River corridor impacted by the August 6, 2015 Gold King mine spill near Silverton, Colorado. Samples are to be used as part of a natural tracer study investigating biogeochemical processes that impact the long-term stability of arsenic and other heavy metals within fluvial and riparian systems.

AGU FALL MEETING

San Francisco | 14 – 18 December 2015

The SFA 2.0 project and team members will be active at AGU, as presenters, session chairs and at the Berkeley Lab Earth and Environmental Sciences Booth #1005. We hope to see you there!

Special Sessions that SFA members are co-chairing:

Characterizing Spatial and Temporal Variability of Hydrological and Biogeochemical Processes across Scales. Co-chairs: Bhavna Arora, Haruko Wainwright, and Susan Hubbard

Benchmarking next-generation reactive transport models for predicting watershed biogeochmical cycling. Co-chairs:Dipankar Dwivedi, Sergi Molins, Carl Steefel, and John Moulton.

Biogeochemical cycles across the genomes-to-ecosystems cascade: Observations and computational approaches across scales. Co-chairs: Yiwei Cheng, Eoin Brodie, Jinyun Tang and Haruko Murakami Wainwright.

Biogeochemical hotspots across terrestrial-aquatic ecotones. Co-chairs: Allison A Oliver, Nicholas Bouskill, Carl I Steefel, and David V D'Amore.

Something in the water: measuring coupled geochemical and microbiological processes across hydrologic compartments. Co-chairs: Mike Wilkins, Ken Williams, and Audrey Sawyer.

New paradigms in terrestrial sensing using small unmanned aerial systems. Co-chairs: Baptiste Dafflon, Sebastien Biraud, Shawn Serbin.

SFA 2.0 EARLY CAREER SPOTLIGHT: CHARULEKA VARADHARAJAN

Charu started her career at Lawrence Berkeley Lab's Earth Sciences as a postdoc in 2010, and became a project scientist in 2014. As a biogeochemist, she is interested in studying the nexus of carbon, water and energy in the context of climate change. Her research interests include understanding and predicting carbon fluxes in terrestrial and subsurface environments, monitoring and mitigation of impacts to water from energy production, and informatics for earth sciences.

Charu has worked with a variety of methods that span across a wide range of length and time scales including micro X-ray synchrotron spectroscopy, lab-scale bench experiments, and field-scale sensor-based data collection. She has also used wavelets and statistical data processing to analyze high temporal resolution time-series datasets.

Her research in the SFA 2.0 involves synthesis and management of diverse datasets generated by the project. Her main focus is to develop an interactive portal to search, plot, download and analyze data. She is also exploring relationships between the geochemical, metagenomic and hydrological data.

On a personal note, Charu enjoys classical Indian dancing, traveling and spending time with her family.

RECOGNITIONS, AWARDS & OTHER ACTIVITIES:

Harry Beller appointed as Associate Editor of *BMC Biotechnology*

Susan Hubbard appointed as Associate Lab Director for Earth and Environmental Sciences at Berkeley Lab

David Lesmes, SFA 2.0 Program Manager (DOE-BER SBR) visited the new East River Study site

Jillian Banfield elected to the Australian Academy of Sciences

Haruko Wainwright featured in Savannah River video (starts at 4:30) describing Berkeley Lab's Sustainable Systems SFA 1.0 and ASCEM computational contributions toward developing sustainable remediation strategies for the contaminated Savannah River F-Area. The video also describes a successful humic acid remediation treatment developed by Jiamin Wan and colleagues under the SFA 1.0.

SFA 2.0 KEY COLLABORATORS:

The SFA 2.0 is sponsored by the U.S. Department of Energy, Biological, and Environmental Research, Subsurface Biogeochemical Research Program.

David Lesmes, Program Manager, can be reached at David.Lesmes@science.doe.gov

QUESTIONS/COMMENTS:

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