Reservoir Modeling Working Group Meeting Information
2012 Geothermal Technologies Program Peer Review
Westminster, Colorado, May 10, 2012

Discussion on a Code Comparison Effort for the Geothermal Technologies Program

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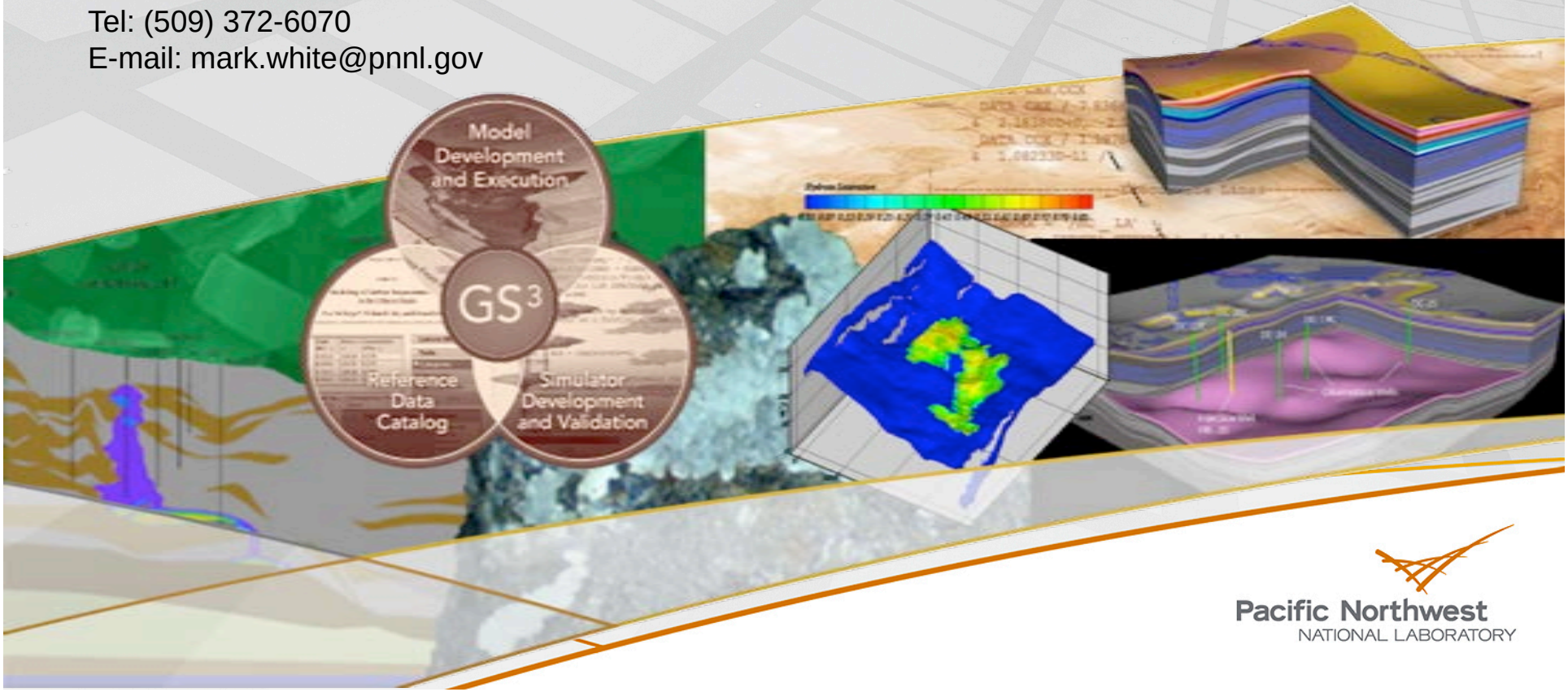

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Colleague

Dr. Timothy D. (Tim) Scheibe was selected as the 2010 Henry Darcy Distinguished Lecturer in Ground Water Science. Scheibe, a staff scientist at Pacific Northwest National Laboratory, was invited by the National Ground Water Research and Educational Foundation to spend next year lecturing at colleges and universities to educate and create interest in groundwater science and technology.

- Lectures and faculty/student meetings
- Roughly 40 host institutions across the United States and internationally
- Beyond the Black Box: Integrating Advanced Characterization of Microbial Processes with Subsurface Reactive Transport Models
- Quantifying Flow and Reactive Transport in the Heterogeneous Subsurface Environment: From Pores to Porous Media and Facies to Aquifers

E-mail: tim.scheibe@pnnl.gov

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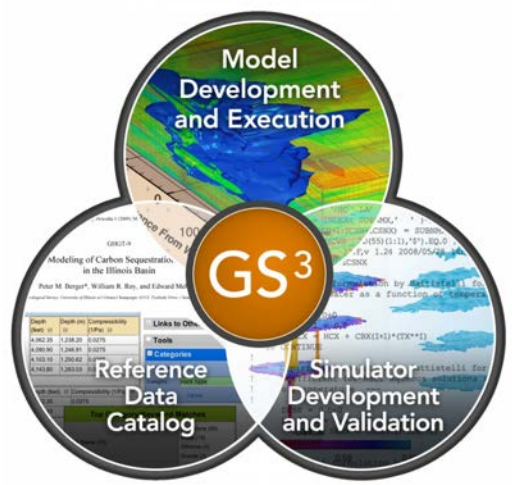
Topics

- PNNL's Participation in Code Comparisons
- Code Comparison Observations
- Preliminaries for a Geothermal Reservoir Code Comparison
- VELO: Knowledge Management Framework for Modeling and Simulation
- STOMP: PNNL's Subsurface Flow and Transport Simulator



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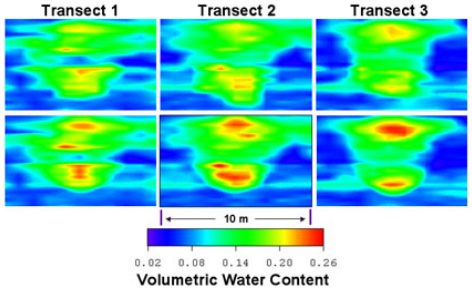
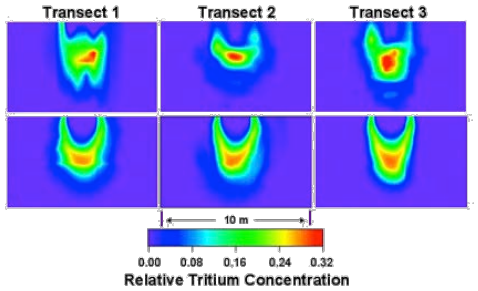
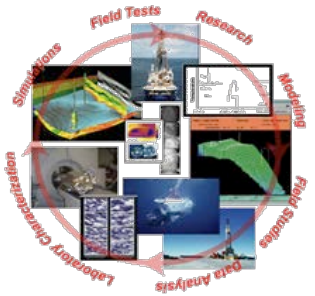
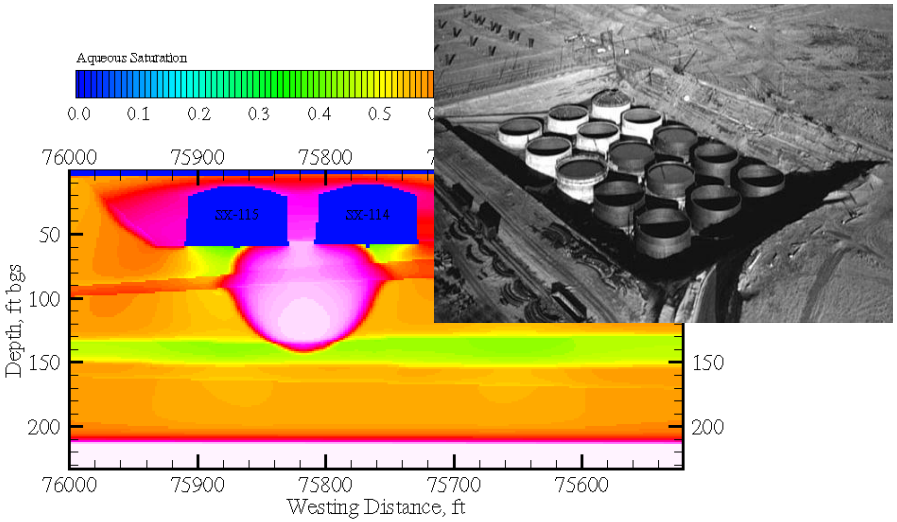
Code Comparisons

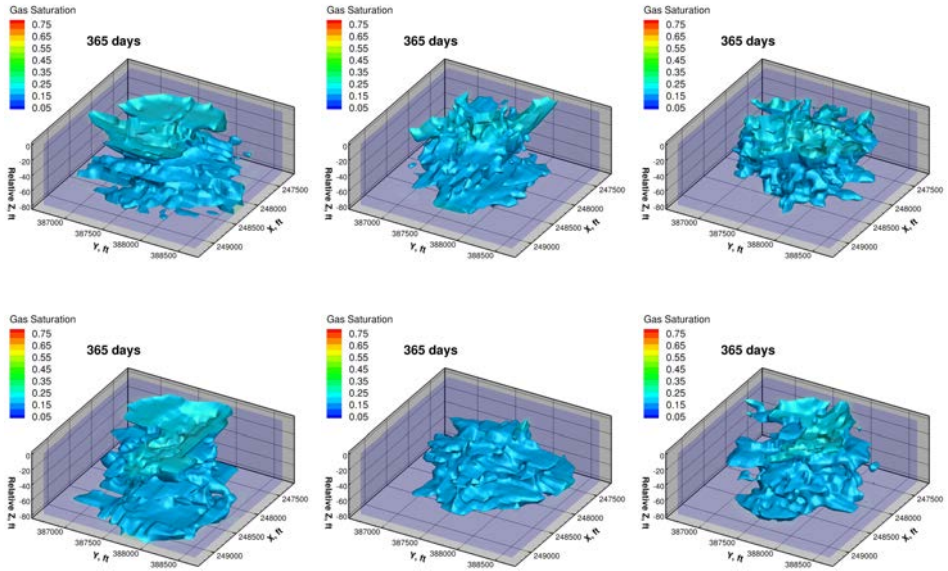
- Las Cruces Trench (1993)
- Yucca Mountain (1994)
- Hanford Site (1999)
- GeoSeq (2002)
- International Hydrate Code Comparison (2007)
- Sim-SEQ (2011)





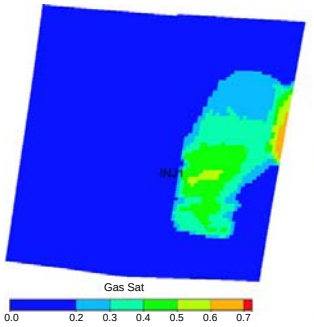




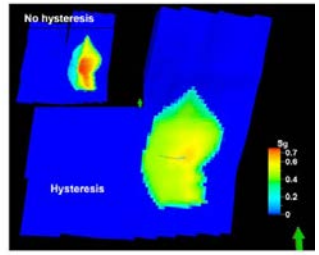


Observations

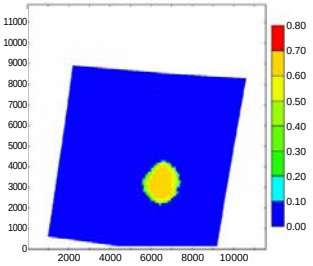
- Blind comparisons
  - Detract from open scientific exchanges
  - Emphasis on coding errors
  - Daunting for new modeling groups
  - Reminiscent of looking up posted grades
- Problem Complexity
  - Core benchmarking problems are essential
  - Early comparisons bond the modeling groups
  - Legacy of increasing problem complexity invites future teams
  - Complex problems will generate differences in results



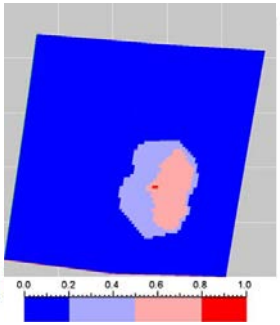
(a) ECLIPSE (Heriot Watt)



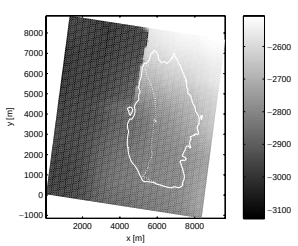
(b) ECLIPSE (Schlumberger)



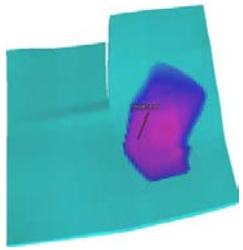
(c) GEM (Heriot Watt)



(d) GPRS (Stanford Uni)



(e) VESA (Princeton Uni)



(f) MoReS (Shell)

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Observations

- Problem Definitions
  - Collective agreement on problem types increases participation
  - Single author problem descriptions were generally more complete and more comprehensible
  - Collective review of the problem descriptions diminishes differences in code capabilities
  - Data collection details need to be included for field data comparisons
- Participants
  - Diversity is an asset.
  - Kickoff workshop promotes collaborative discourse in future conference calls
  - Rotating conference call times encourages international participation

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Observations

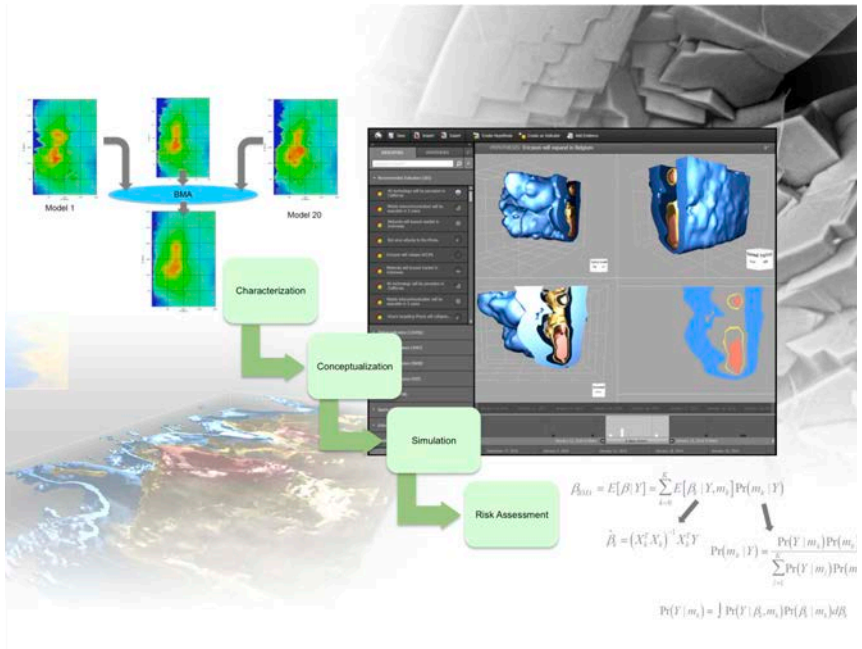
- Simulators
  - Research codes have the greatest flexibility for change.
  - Industrial codes need financial motivation to change.
  - Commercial codes are generally the least flexible and least open with respect to details and numerical schemes.
  - Flexible commercial codes allow for diverse modeling approaches.
  - Academic licenses for commercial codes are considerably less than their profession equivalents
- Technology Transfer
  - Public website invites interest and new modeling teams
  - Combined joint and individual publications are effective
  - Special edition publications motivate modeling teams

Perspective

- International community with governmental agency, national laboratory, independent research, industrial, and academic representation.
- Kickoff workshop.
- Repository of progressively more complex EGS problems.
- Simple problems isolate thermodynamics, hydrodynamics, rock mechanics, and geochemistry.
- Analytical, code inter-comparison, laboratory data, field data.
- Collaborative but secure computational framework.
- Public access to problems and simulation results.
- Publication of findings.

Preliminaries

- Soliticiting national and international participation
- Developing a set of protocols and comparison procedures
- Planning a kick-off workshop
- Creating an instance of VELO for the Geothermal Technologies Program

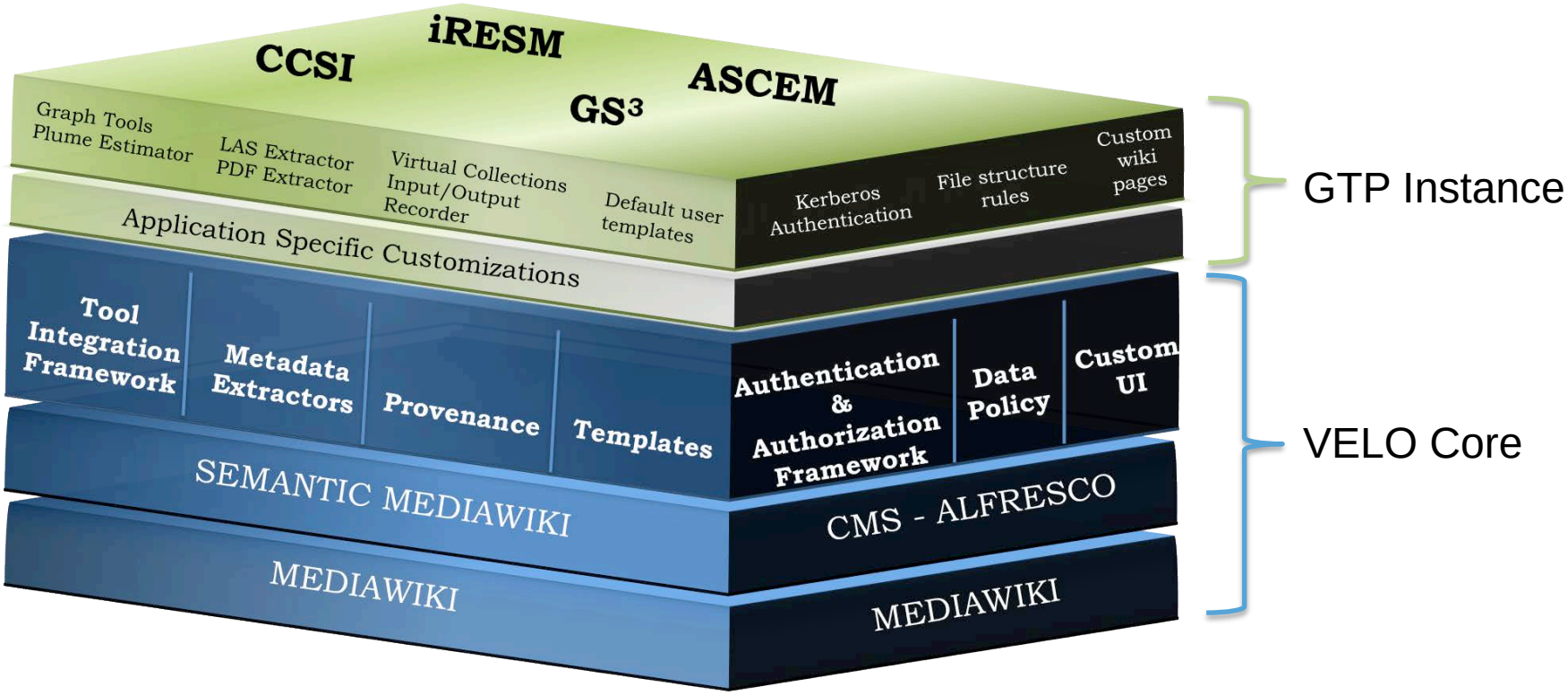


VELO

A flexible, foundational, collaborative technology that can be used in modeling and simulation projects to

- capture, organize, query, and share experimental and observational data, along with the scientific processes and reasoning that are used to develop computational models
- provide versioning of model inputs for specific projects and provenance for simulation results
- enable simulations to be launched on remote computational platforms
- support both tight and loose integration of third-party tools to facilitate various modeling activities, such as model development and visualization

VELO Architecture



- **MEDIAWIKI**: provides a collaborative and extensible user environment
- **ALFRESCO**: manages complex, large data sets used in scientific modeling
- **SEMANTIC MEDIAWIKI**: provides semantic markup and search capabilities

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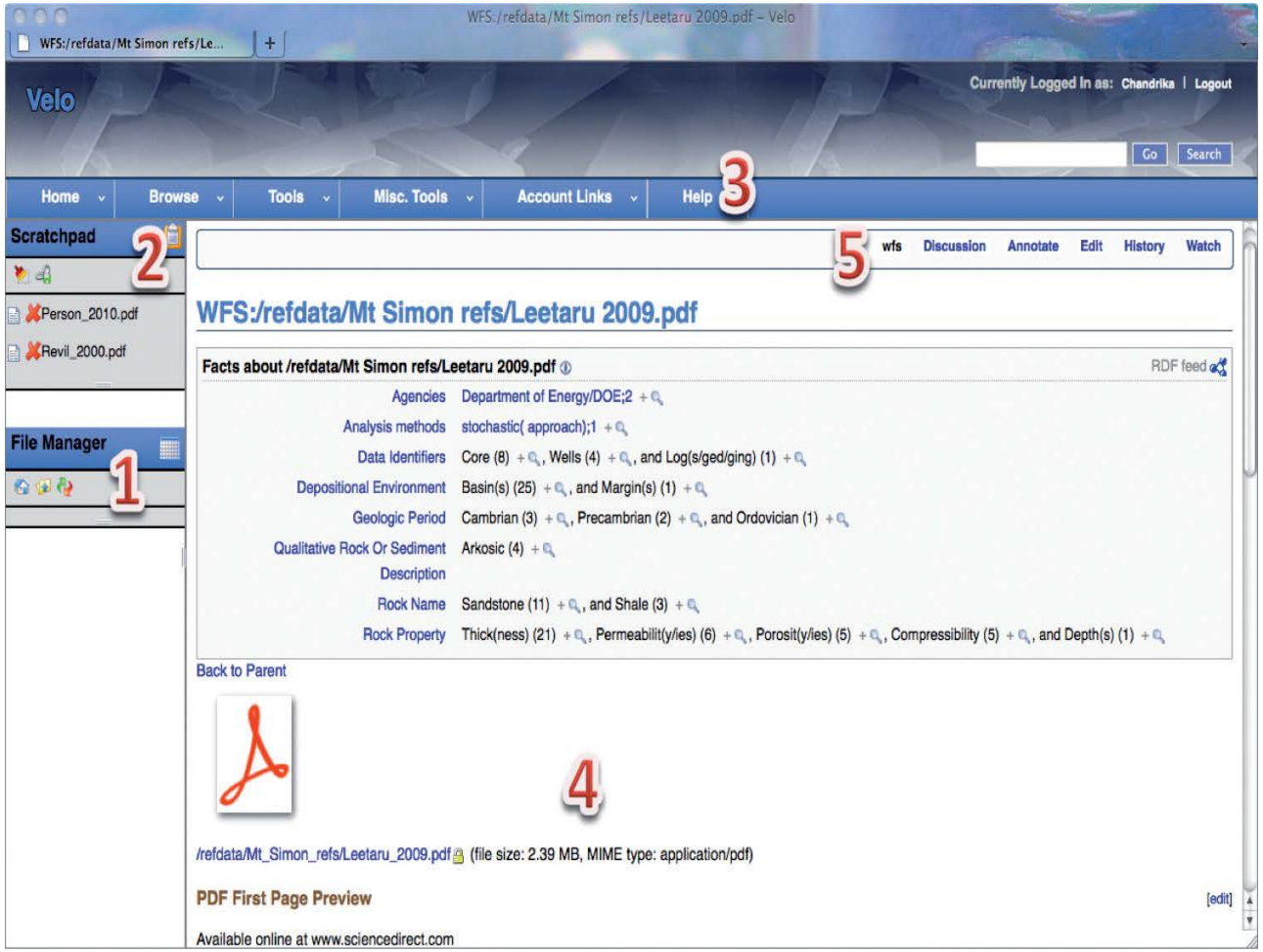
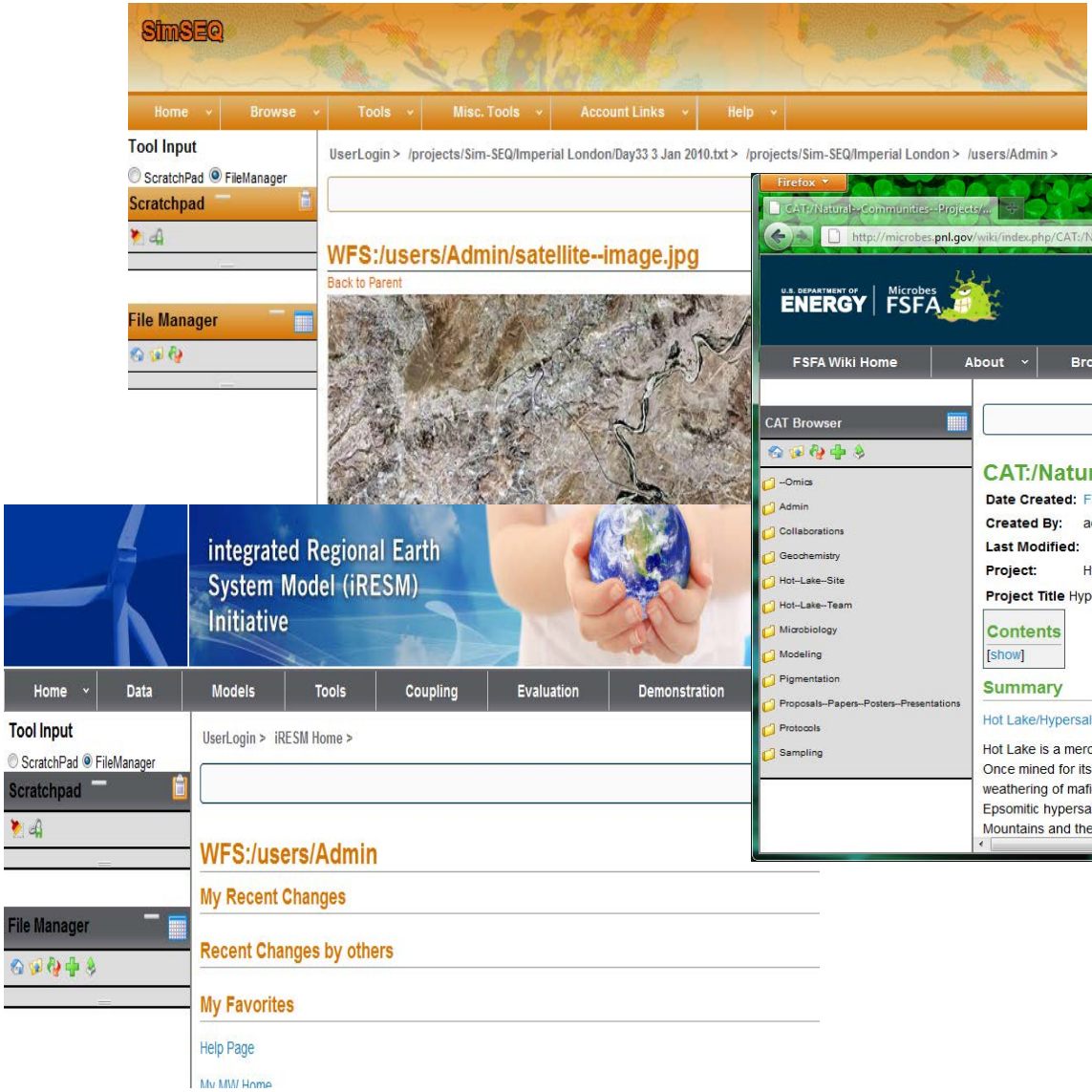
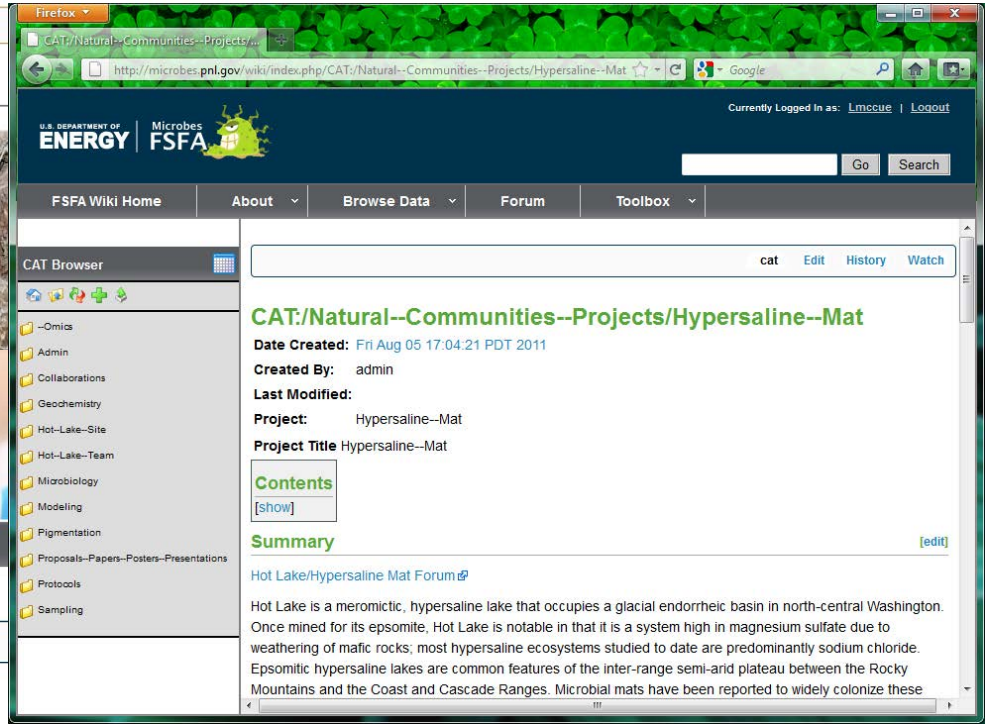
VELO Page

1. File Manager
2. Scratchpad
3. Tool Access and Navigation
4. Content Area
5. Wiki Functions



VELO Instances





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STOMP at a Glance

Subsurface Transport Over Multiple Phases (STOMP) is a numerical simulator, developed at PNNL, for modeling multifluid flow and reactive transport through geologic media.

- STOMP - sequential implementation (Fortran)
- eSTOMP - scalable implementation (Fortran/Global Arrays/MPI)
- Phases - aqueous, gas, nonaqueous phase liquid, ice, hydrate, solid
- Components - water, air, oil, salt, CO_2, CH_4, noncondensible gases, heavy oils, light oils, dilute solutes, reactive species (ECKEChem)
- Thermal Environments - isothermal, nonisothermal
- Saturation Functions - nonhysteretic, entrapment, residual
- Gridding - structured (Cartesian, cylindrical, boundary fitted)
- Numerical Solvers - banded, conjugate gradient (SPLIB, Indiana University), parallel (PETSc, Argonne National Lab)
- Website - http://stomp.pnl.gov

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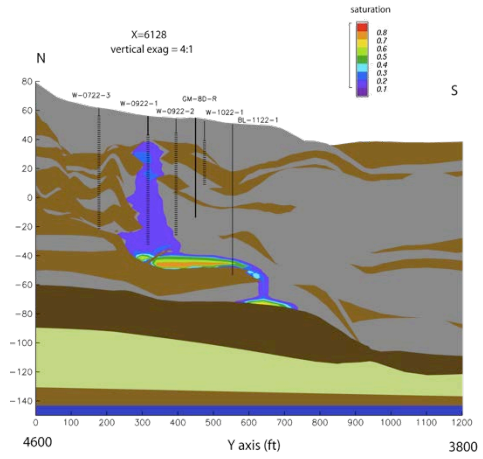
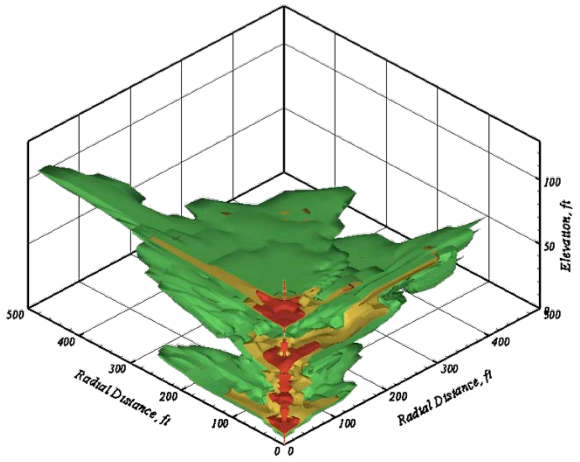
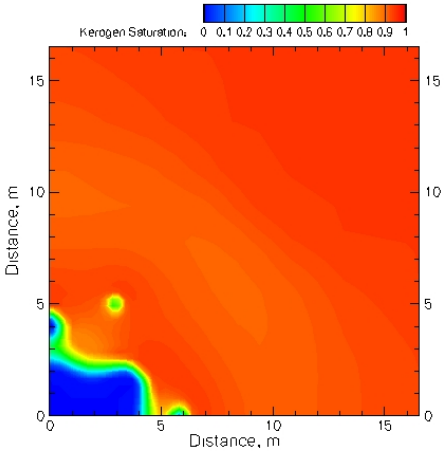


Base Case 2500





Environmental Stewardship

U.S. Department of Energy legacy waste from the nuclear weapons material production era:

- Radionuclide migration and remediation
- Nuclear waste tank leakage
- Vegetated surface barrier design
- Freeze-wall technology

Environmental Remediation

U.S. Department of Energy, U.S. Department of defense, and Superfund site remediation:

- Carbon tetrachloride in deep vadose zone environment
- Trichloroethylene in arid climate
- Petrol-processing waste in shallow water table environment

Geologic CO_2 Sequestration

Industrial, U.S. Department of Energy, and regional partnership projects:

- Deep sedimentary saline formations
- Deep basaltic saline formations
- Methane hydrate formations with co-production

Hydrocarbon Production

Industrial, U.S. Department of Energy, Indian Governmental and Korean Governmental projects:

- Alaska Northslope gas hydrate accumulations
- Suboceanic gas hydrate accumulations
- Piceance Basin oil shale
- Enhanced oil recovery technologies

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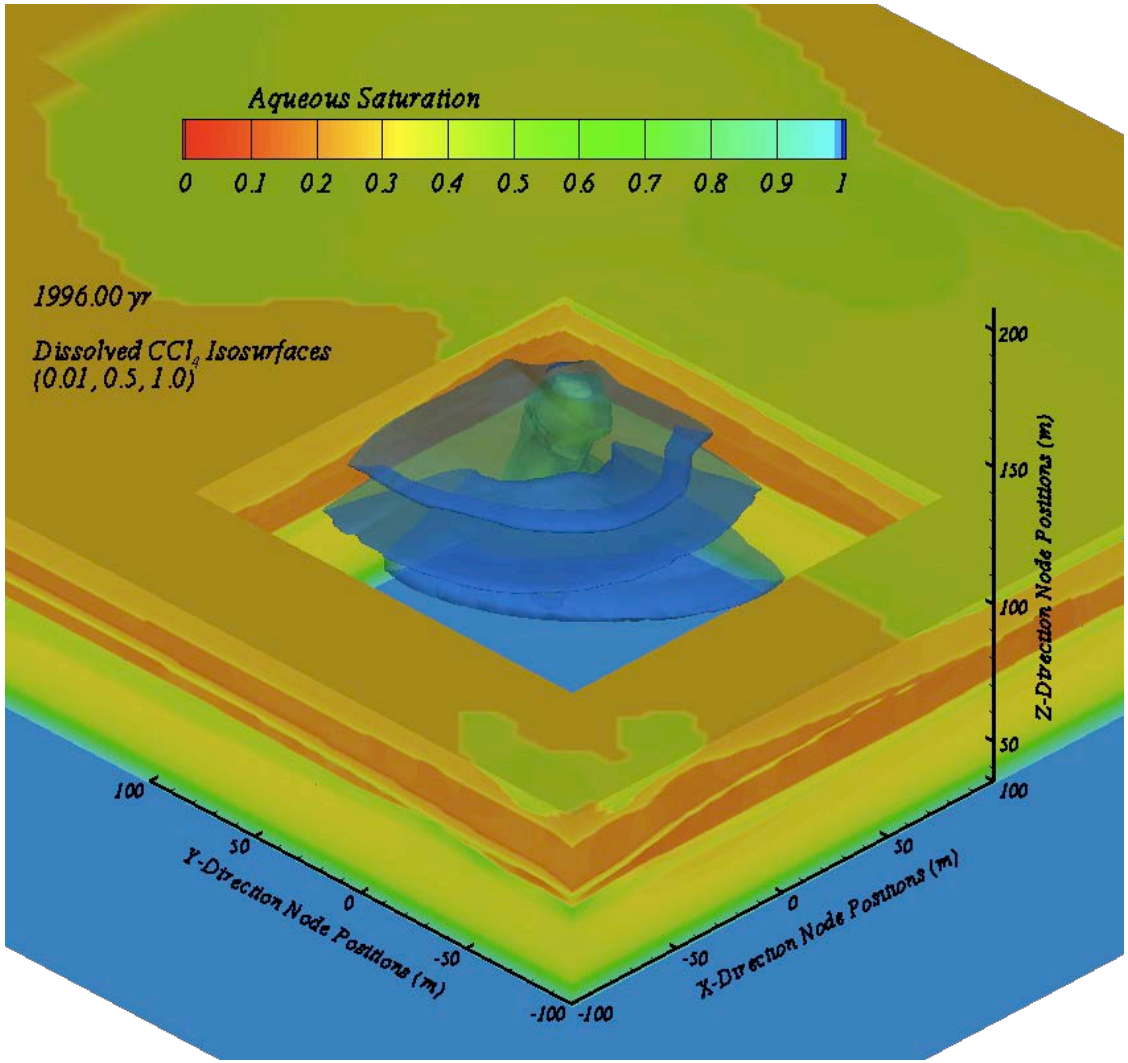
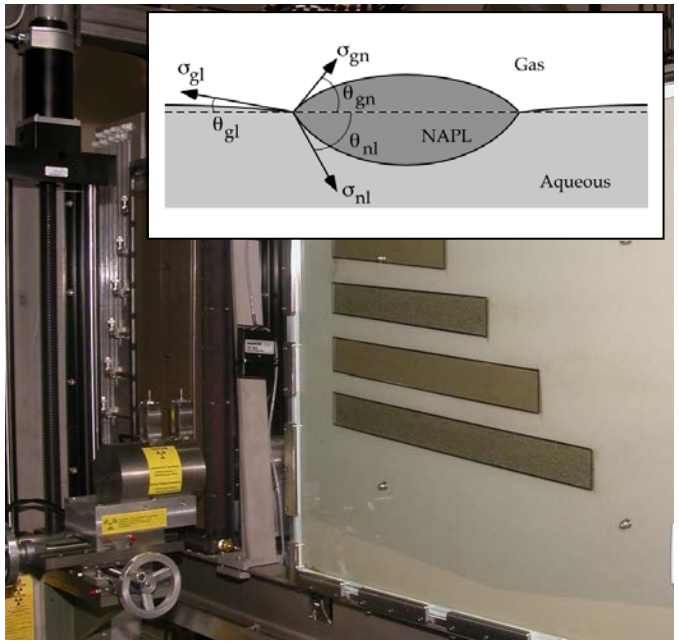
Experimental Links

- CCl_4 Migration and Remediation
- Z-9 Crib, Hanford Site, Washington, United States





Technology Transfer

KIGAM Korea Institute of Geoscience and Mineral Resources

Masdar INSTITUTE

UAF UNIVERSITY OF ALASKA FAIRBANKS

SCHOOL OF MINES 1874 COLORADO

Battelle
The Business of Innovation

Colorado State University

OSU Oregon State University

Universität Stuttgart

TU Delft
Delft University of Technology

THE UNIVERSITY OF UTAH

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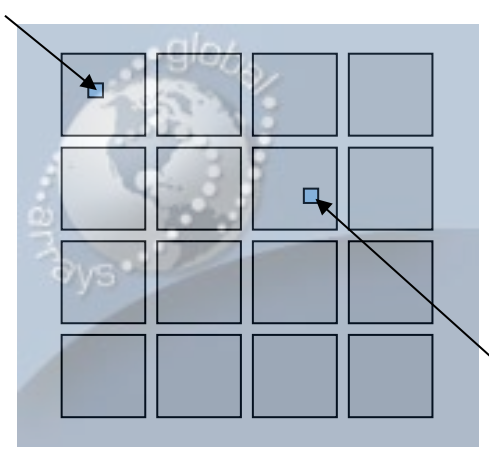
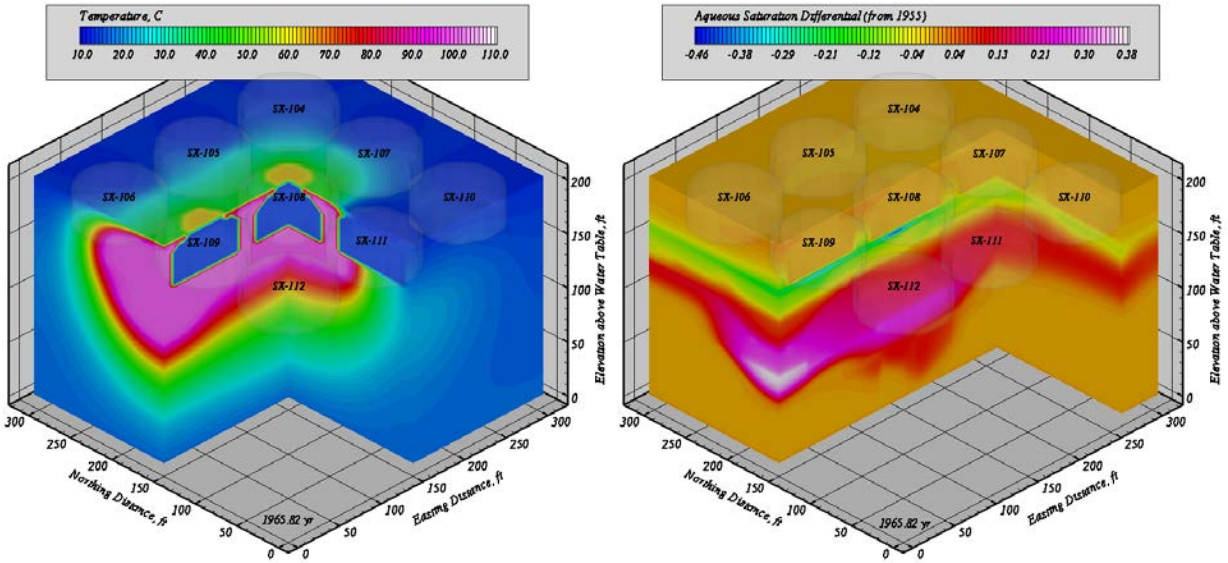
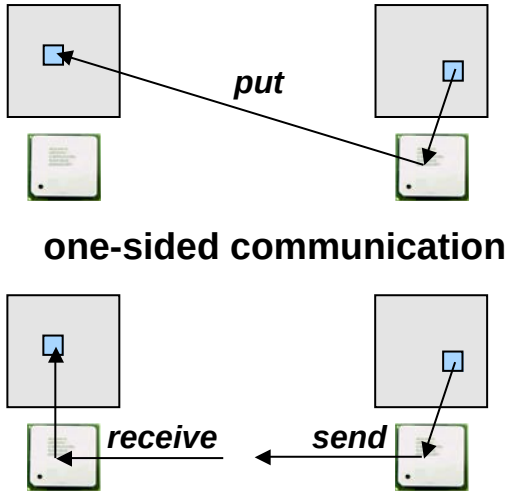
Scalable Computing

- Global Arrays
- Implicit Solve on 1G Unknowns
- 1.4K Processors







SX Tank Farm, Hanford Site, Washington

Temperature and Aqueous Saturation: 1965.82 yr

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