eSTOMP: Extreme-Scale Computing for Subsurface Science and Engineering

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XSCI Brown Bag, April 15, 2011

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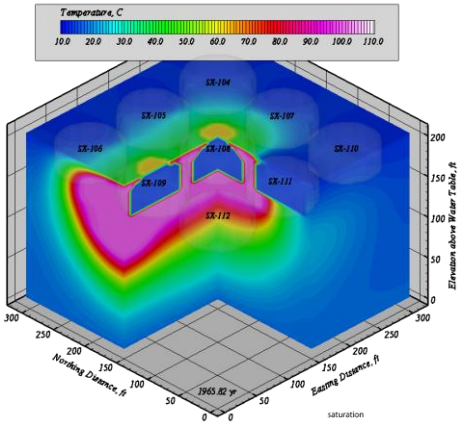
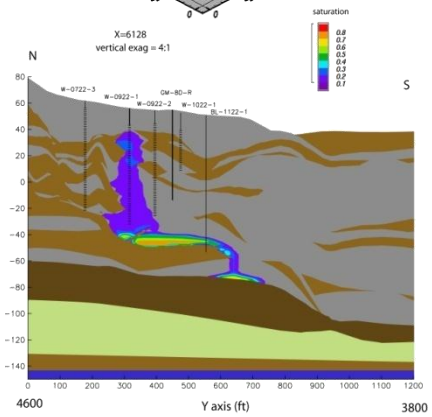
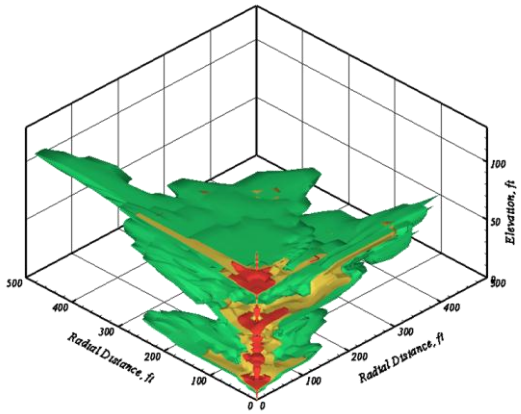




Base Case 2500



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 EPA 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

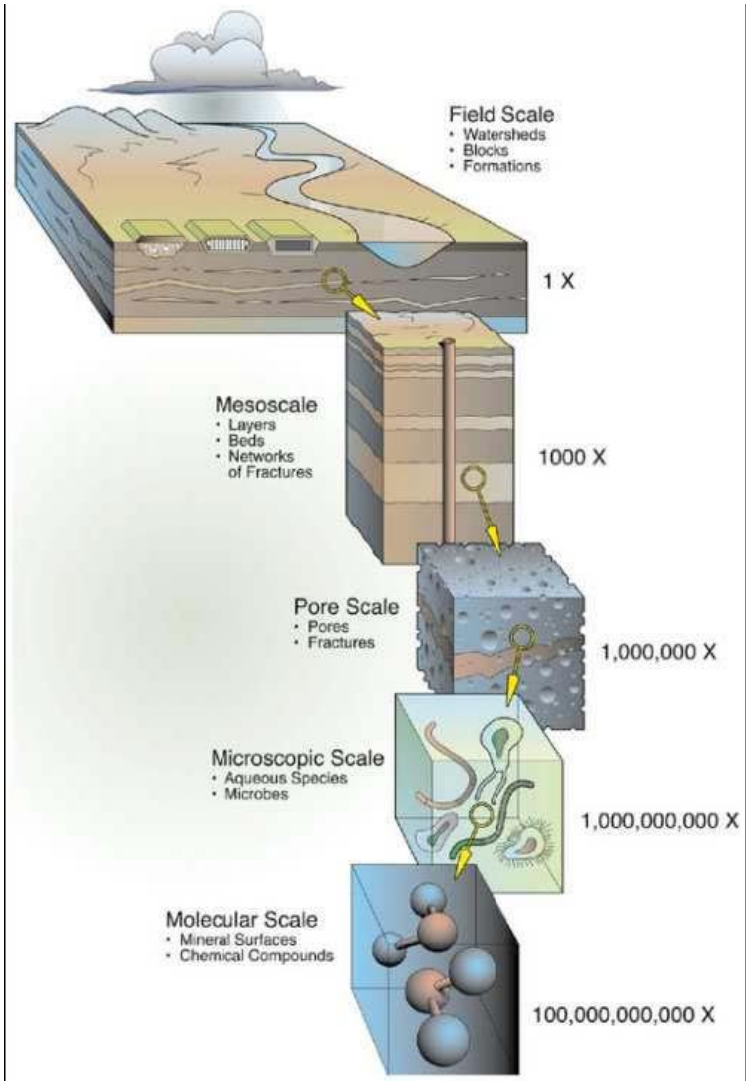
Hydrocarbon Production

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

Critical Science Need for Highly Scalable Subsurface Codes

- High spatial resolution
  - to capture effects of multi-scale heterogeneity
  - Highly localized processes
- Extreme degrees of freedom
  - Multi-dimensional, multidomain, multifluid, multiphase, multicomponent
  - Tightly coupled hydrology, geology, geochemistry, microbiology
- Large numbers of realizations
  - Uncertainty quantification
  - Inverse modeling



Subsurface Transport Over Multiple Phases (STOMP)

Operational Modes

- STOMP-W, -WA, WAE -- Water-Air-Energy Operational Modes
- STOMP-WO, -WOA, WOAE -- Water-Oil-Air-Energy Operational Modes
- STOMP-WS, -WSA, WSAE -- Water-Salt-Air-Energy Operational Modes
- STOMP-WCS, -WCSE -- Water-CO2-Salt-Energy Operational Modes
- STOMP-WCMSE -- Water-CO2-CH4-Salt-Energy Operational Modes

Implementations

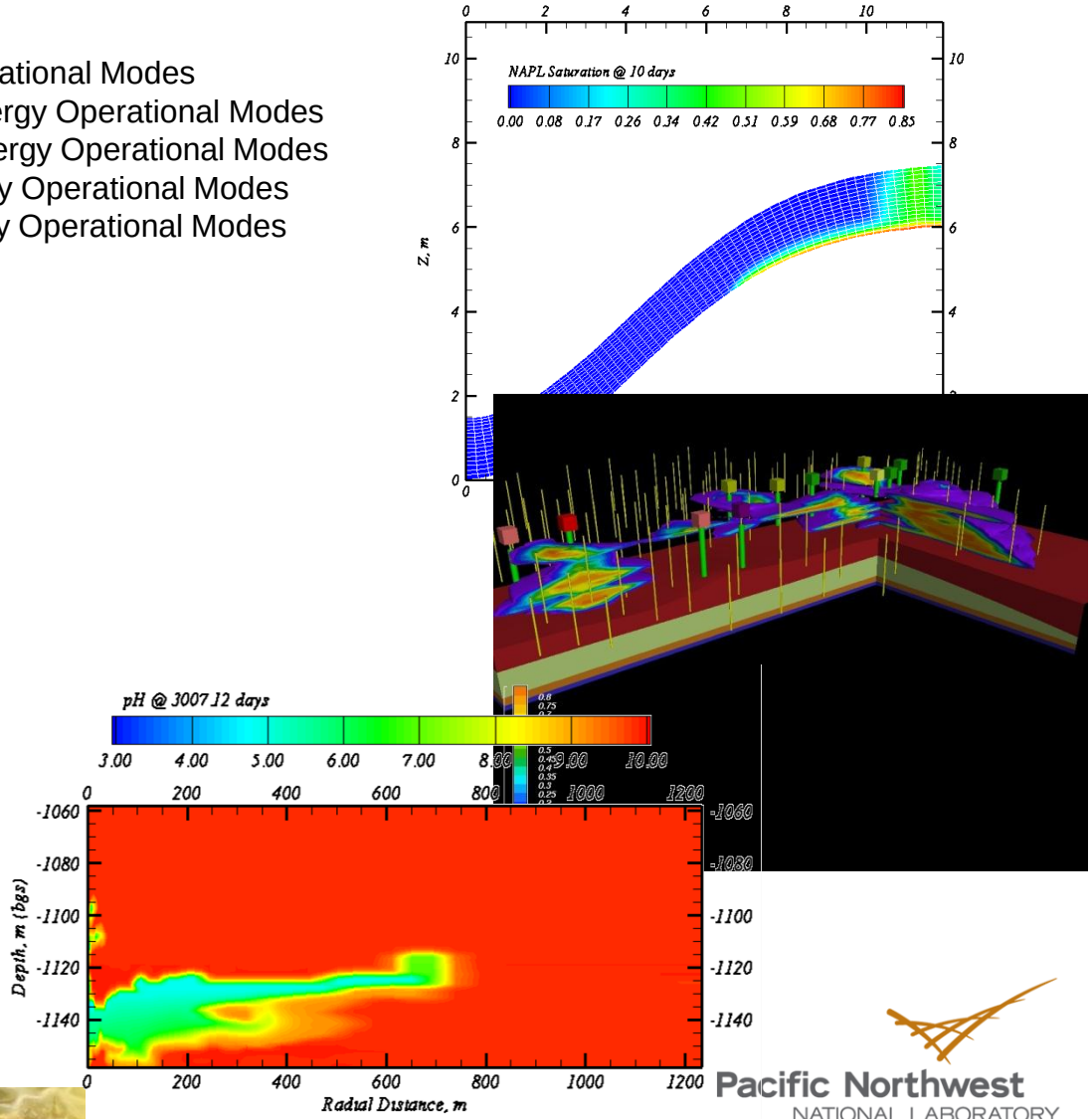
- Original development in 1992
- > 800K lines of Fortran Code
- Fortran, MPI, PETSc

Licensing and Quality Assurance

- Academic, U.S. Gov., Foreign Gov., Industrial
- Documentation (Guides, Website, Publications)
- Short Courses (University Sponsored)
- DOE Order 414.1C (System Safety Software)

Applications

- Nuclear waste disposal and migration
- Environmental remediation and stewardship
- Natural gas hydrate production
- Oil shale production
- Geothermal
- Oil sand production
- Geologic CO_2 sequestration
- Enhanced Hydrocarbon production



STOMP Subsurface Transport Over Multiple Phases

http://stomp.pnl.gov

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Project Goal

- Develop a highly-scalable version of the STOMP code for subsurface characterization and modeling with extremely high resolution of the model parameters and processes.
- The next generation code that results from this project will provide a key capability needed for PNNL to perform computationally-based research on critical subsurface science issues.

Related Projects

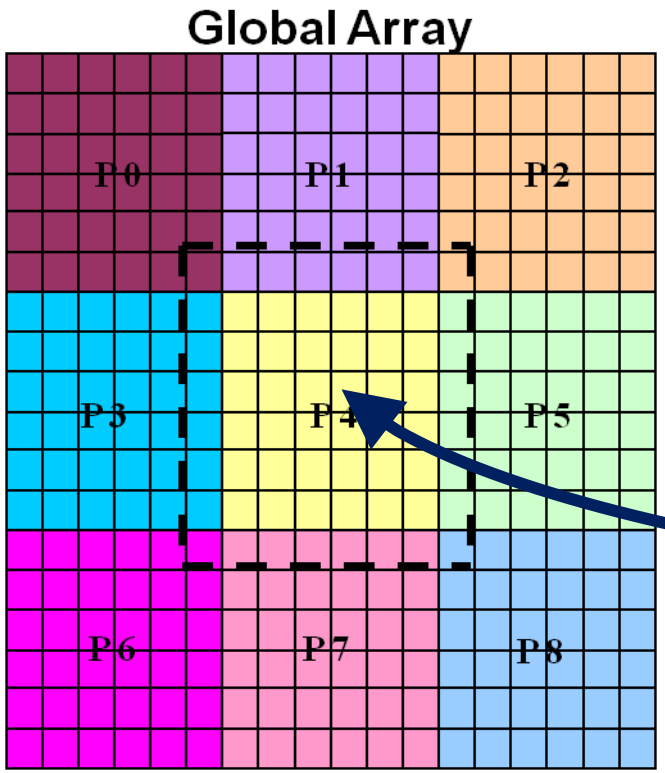
- PNNL Carbon Sequestration Initiative (Alain Bonneville)
  - Advanced scientific simulation capability for PNNL's Carbon Sequestration Initiative
- PNNL Groundwater SciDAC (Tim Scheibe)
  - CCA implementation of STOMP (Bruce Palmer / Yilin Fang)
  - Scientific workflow and data management environment (Karen Schuchardt)
- LANL Groundwater SciDAC (Peter Lichtner)
  - PFLOTRAN Development (Glenn Hammond)
- Advanced Subsurface Computing for Environmental Management
  - 5 yr DOE/EM project (FY2011 PNNL: $3.5M)
  - Platform to support scientifically defensible predictions of engineering remediation and waste management performance
  - Full-featured community model that runs on desktop to leadership class computers
  - DOE/SC: SBR Science + ASCR Computing technology

eSTOMP

- Developed from STOMP full-featured serial source code
- Staged development began with single-phase water flow in porous media
  - Subsequent addition of transport and biogeochemistry
  - Testbed for scaling assessment and restructuring
- Re-engineering
  - Structured grid code removed from main computational kernel routines
  - Implementation of one-sided communication paradigm
  - Componentization of key parts of the code
- Performance with ease of use
  - Insulate domain scientists from low-level communication details
  - Easy to run and enhance code capabilities by those familiar with the original STOMP code.

Global Array Toolkit (GA) Implementation

- One-sided communication provides efficient and flexible message passing
- Supports global shared memory programming paradigm
  - Encapsulates and hides process-to-process communication
  - Shared data looks like an array



- Local data placed in the GA, using

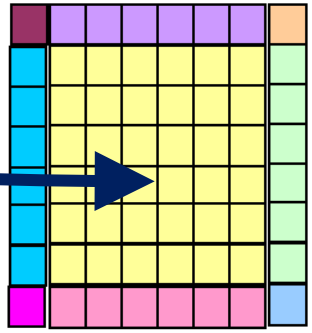
  `GA::GlobalArray::put()`

- Processes sync'd, using

  `GA::GAServices::sync()`

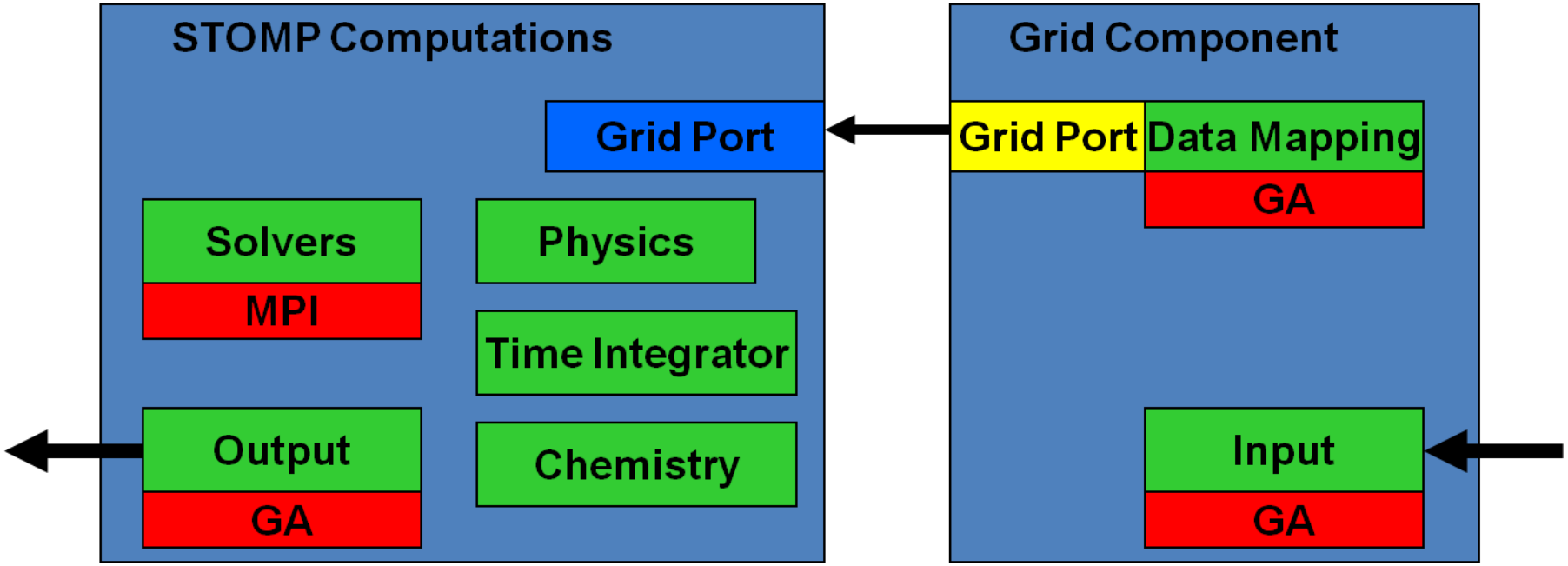
- Local ghost cells filled with data from the appropriate donor cell, using

  `GA::GlobalArray::get()`



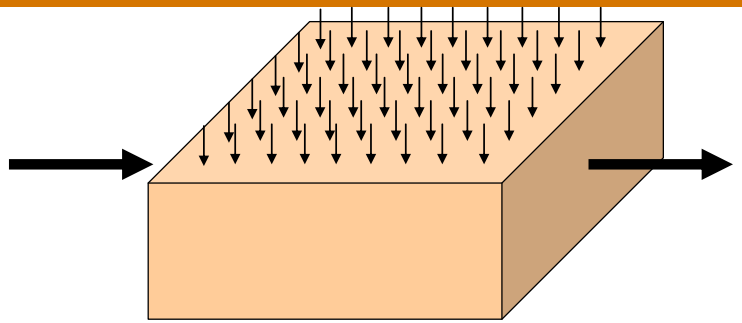
Local data & ghost cells on processor

Grid Component



- Grid interface insulates the principal science routines from the lower level details of distributing the global arrays.
  - supports easy addition of extra fields to the grid,
  - allows for upgrades to more complicated grids
  - enabled the general re-use of serial STOMP calculational routines and modules
  - small GA footprint in the STOMP computations

Scaling Studies

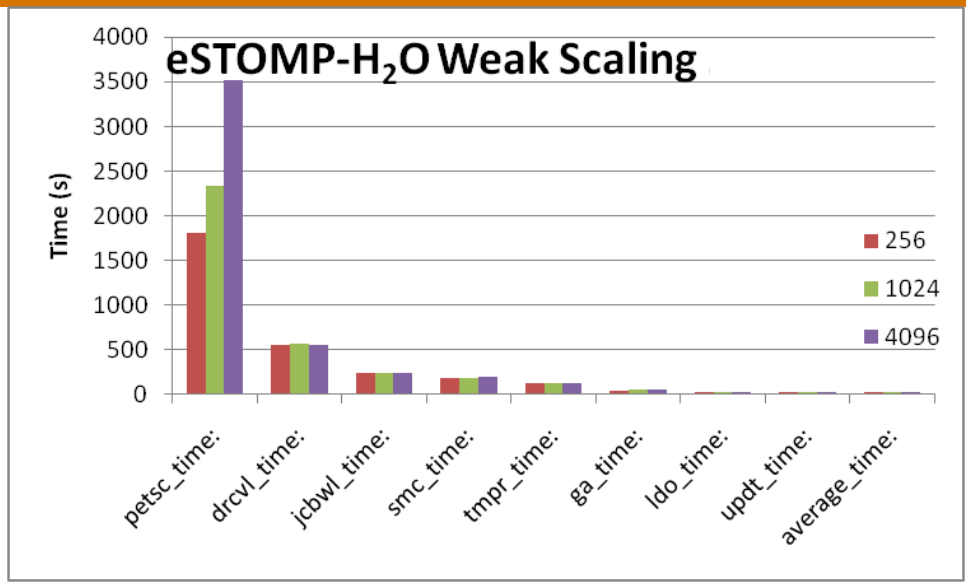


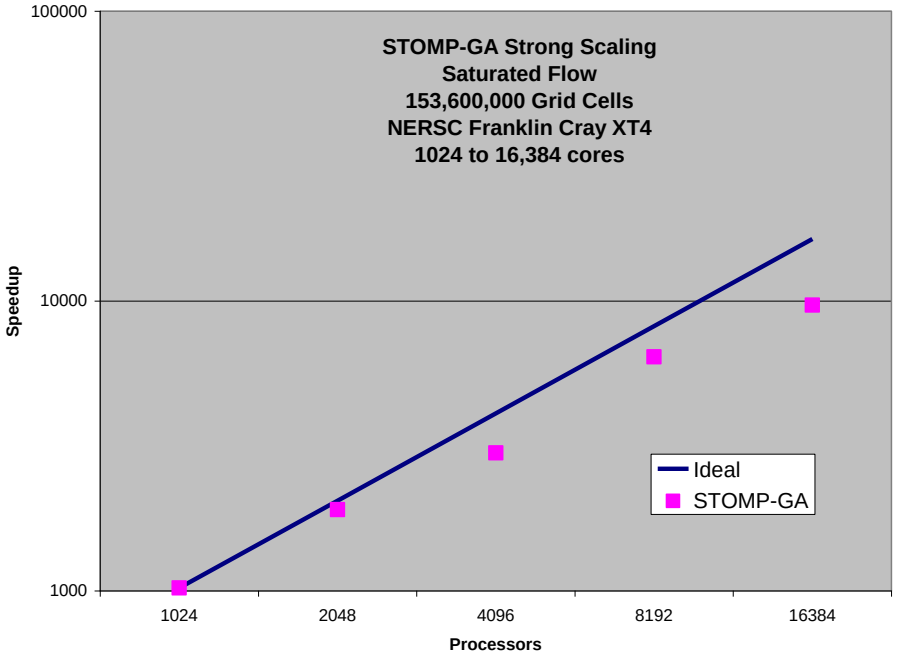
- Uniform grid: $\Delta x = \Delta y = \Delta z = 1$ m
- saturated case
  - top recharge: 1.6428×10^{-4} m/d
  - west and east hydraulic gradient, with pressure gradient of 0.005
- Strong scaling: 125x125x75 grid (1,171,875 cells)
- Weak scaling:

# processors	problem size	#x_grid	#y_grid	#z_grid
1	9,375	25	25	15
4	37,500	50	50	15
16	150,000	100	100	15
64	600,000	200	200	15
256	2,400,000	400	400	15
1024	9,600,000	800	800	15

eSTOMP-H_2O

- Efficient scaling for single phase flow and transport
  - Removal of STOMP scaling bottlenecks
  - Remaining scaling issues are due to third party solver
- Demonstrated on multiple architectures
  - Chinook
  - Franklin

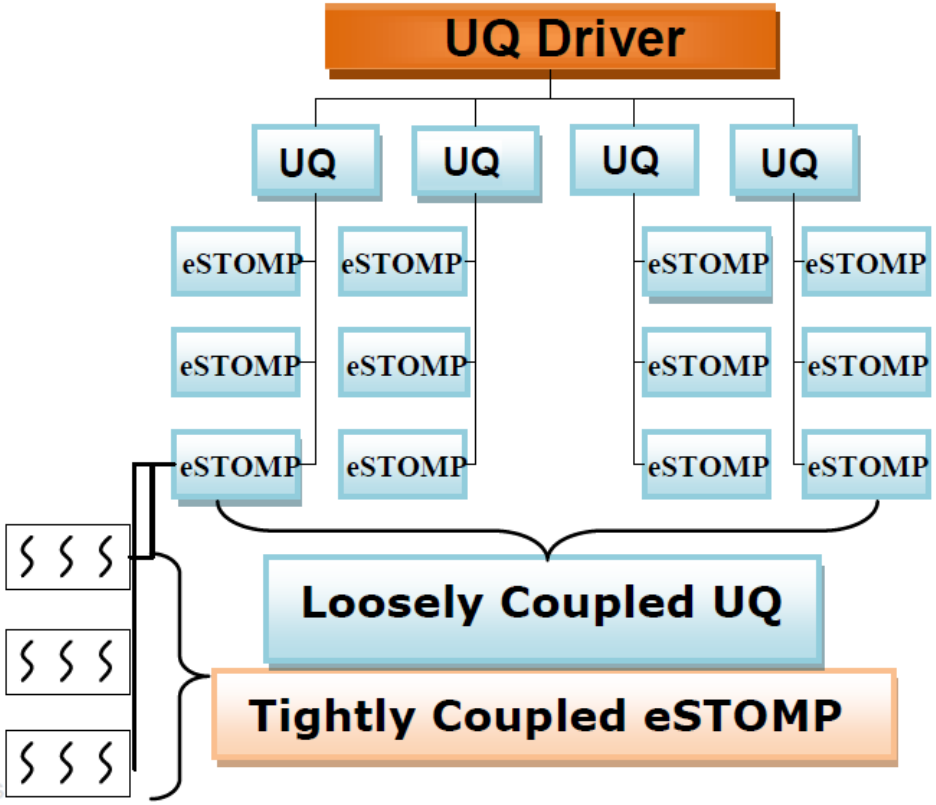




eSTOMP-PG: Multilevel Parallelism

GA Processor Groups

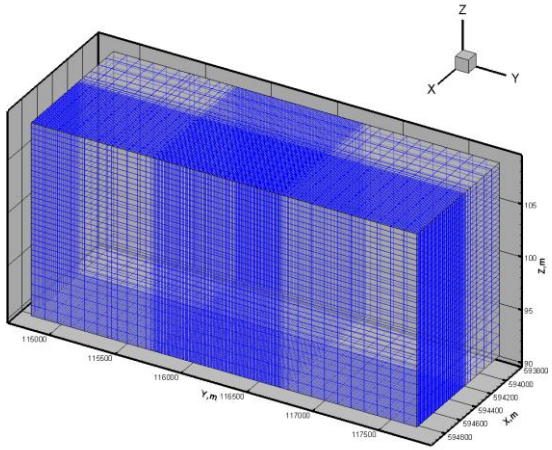
- Uncertainty Quantification
- Multivariate Joint Inversion

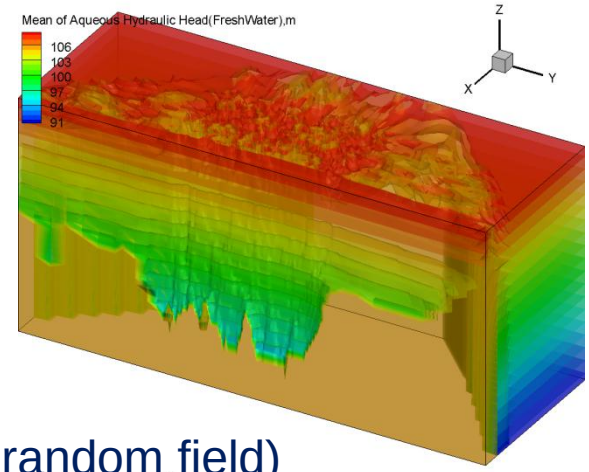


Hanford 300 Area

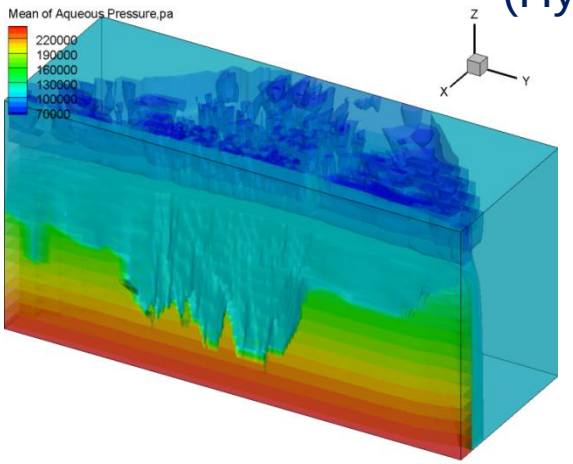
Uncertainty Quantification of 3D Subsurface Flow in the Hanford 300 Area

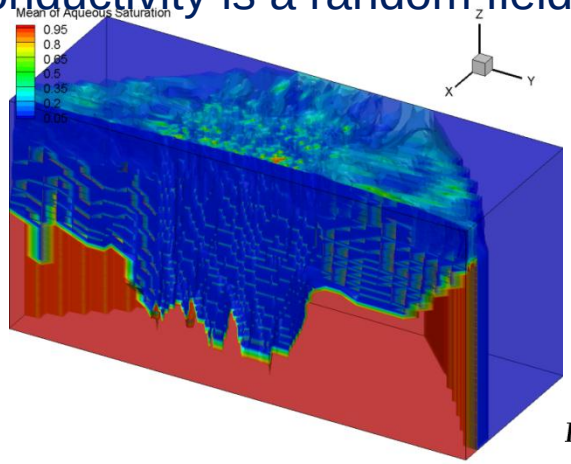
- Total 317 Collocation points - running 10 tasks/PG on 32 PG (4096 cores) in 23 hours
- Single desktop simulation: 1 week





(Hydraulic Conductivity is a random field)





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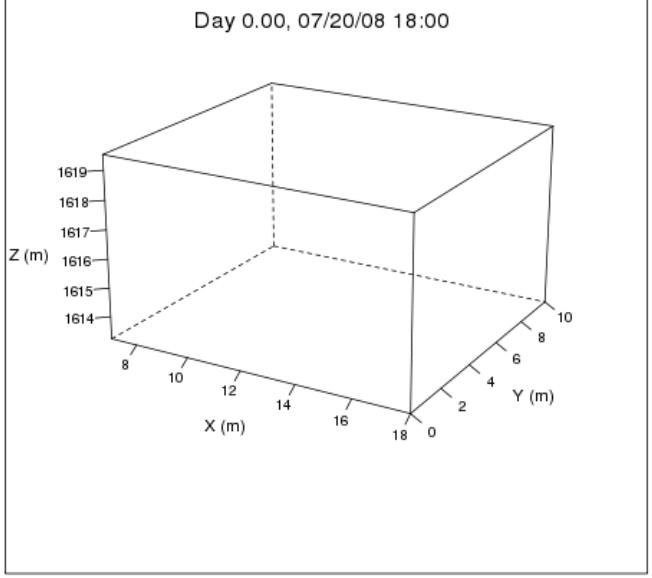
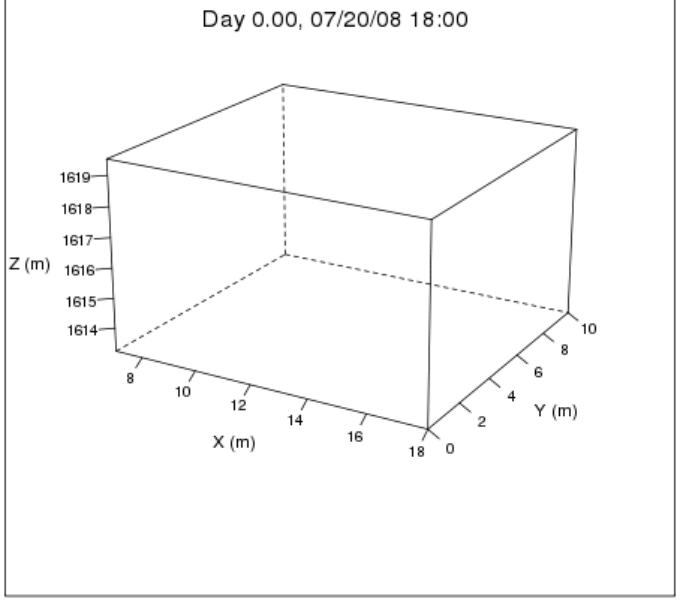
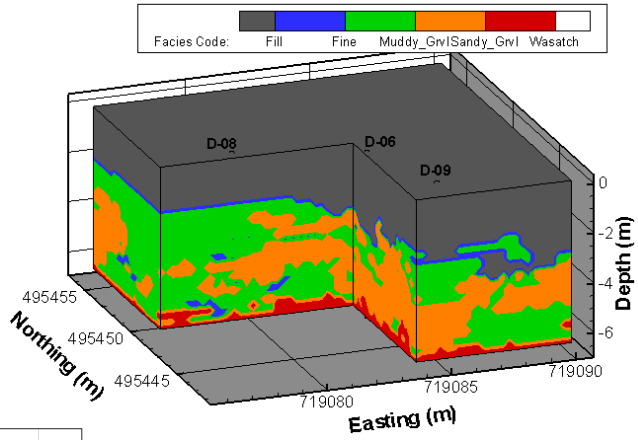
Rifle IFRC: In Situ Uranium Bioremediation

Acetate (5 mM)

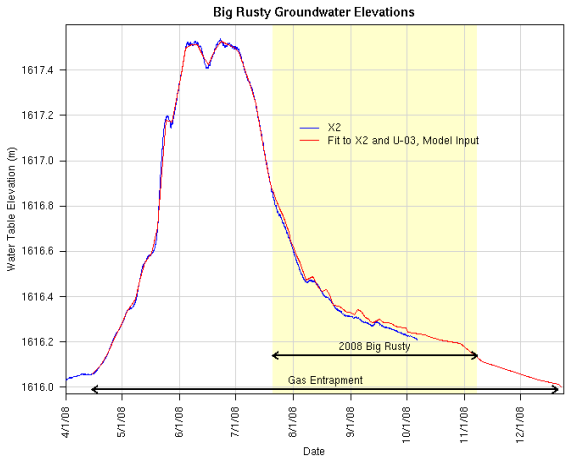


U(VI) (aq) (0.4 μM)

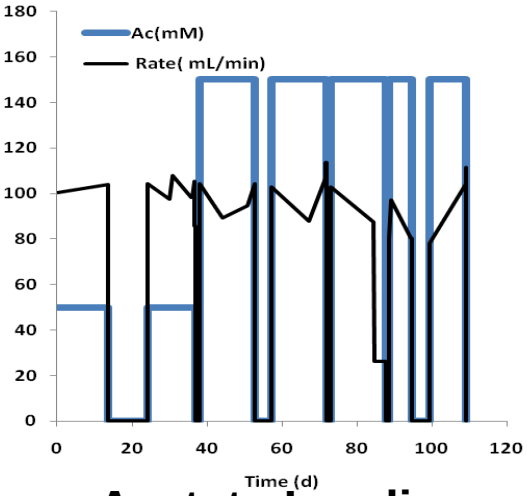




Heterogeneity



Seasonal Water Table



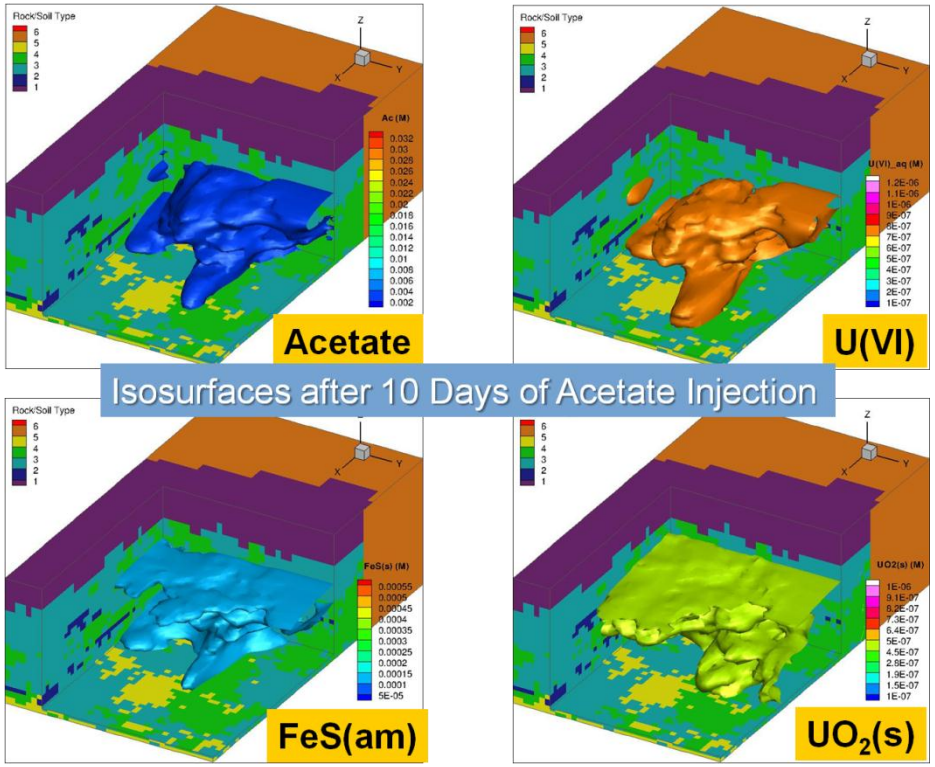
Acetate Loading

Scientific Productivity

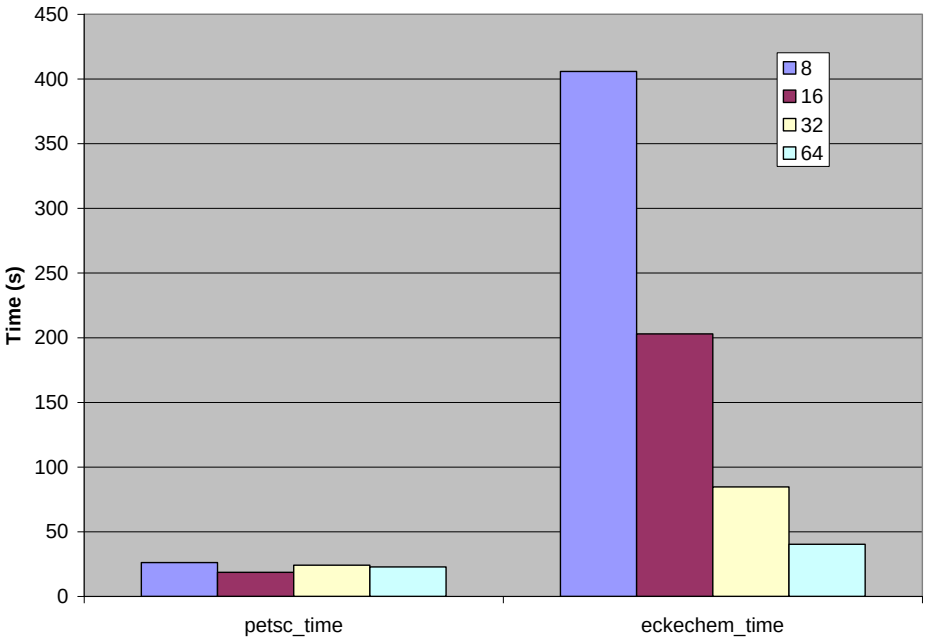
- Computationally demanding simulations
  - transient variably saturated flow
  - multi-component biogeochemical reactive transport
    - 102 biogeochemical species
    - 7 minerals
  - 3-D physically and chemically heterogeneous sediments
    - Hydraulic conductivity, porosity
    - Reactive surface area for surface complexation models
    - 96,320 grid cells with variable spacing from 0.15 m, 0.25 m, 0.10 m in the x, y, z directions, respectively
    - Multiple realizations
- Scientific efficiency
  - 160 day simulation at high resolution: **12 hours** using 128 processor cores (EMSL Chinook)
  - Equivalent simulation without parallel processing would have taken **60 days**, assuming sufficient memory was available

Reaction Solver

- Issues
  - Chemistry computational effort is 30X flow and transport
  - 8-64 processors more than sufficient for flow + transport, insufficient for chemistry
  - Load imbalance
    - inactive cells
    - reaction fronts



Isosurfaces after 10 Days of Acetate Injection



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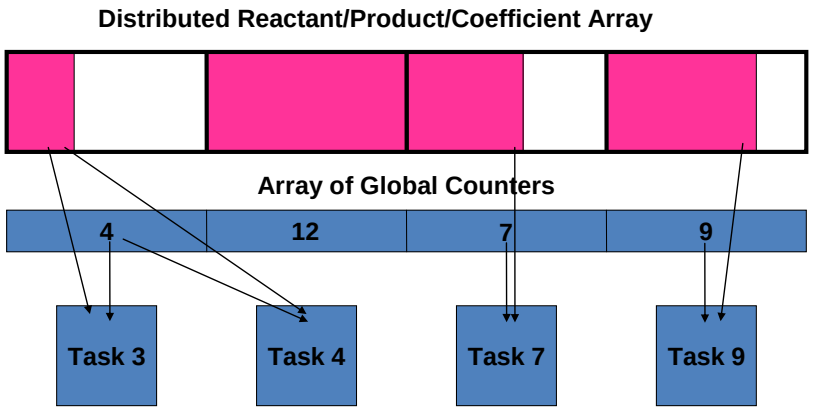
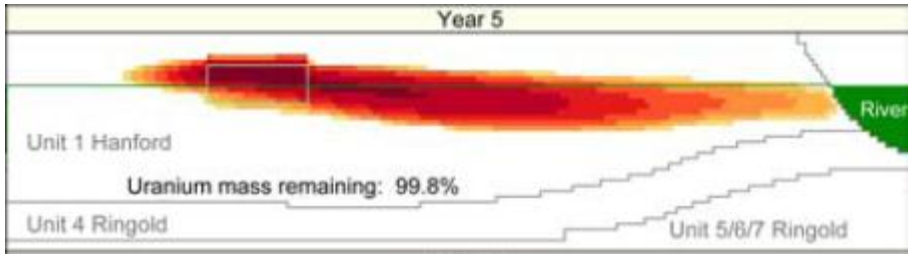
Load Balancing

- Work stealing scheme using GA counters for load balancing
  - Chemical reactions
  - Multiphase update of secondary variables
- Time reduction on Hanford 300 Area uranium geochemistry
  - 16 processors
  - With counters: 86.0 seconds
  - Without counters: 96.8 seconds

Load Balancing Scheme for Chemical Reactions based on Global Counters





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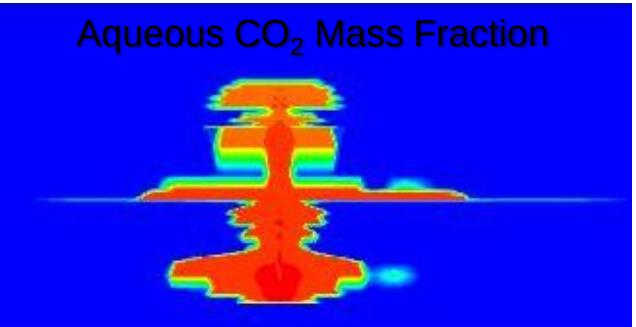
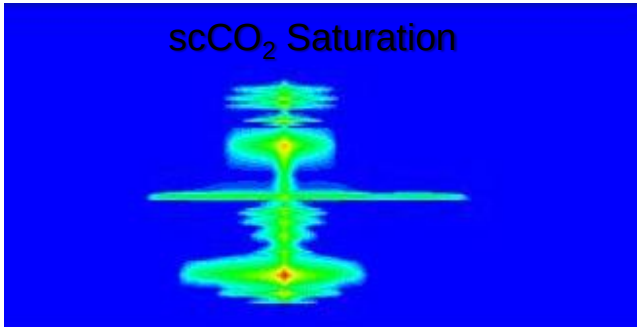
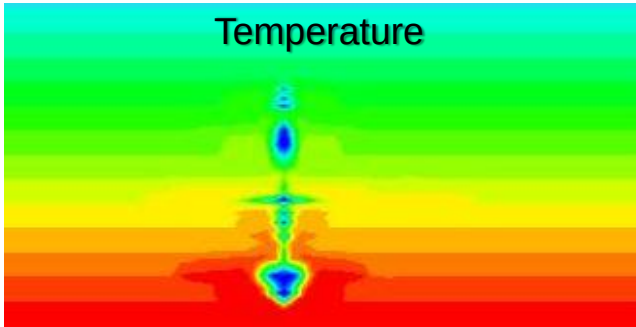
eSTOMP-CO_2

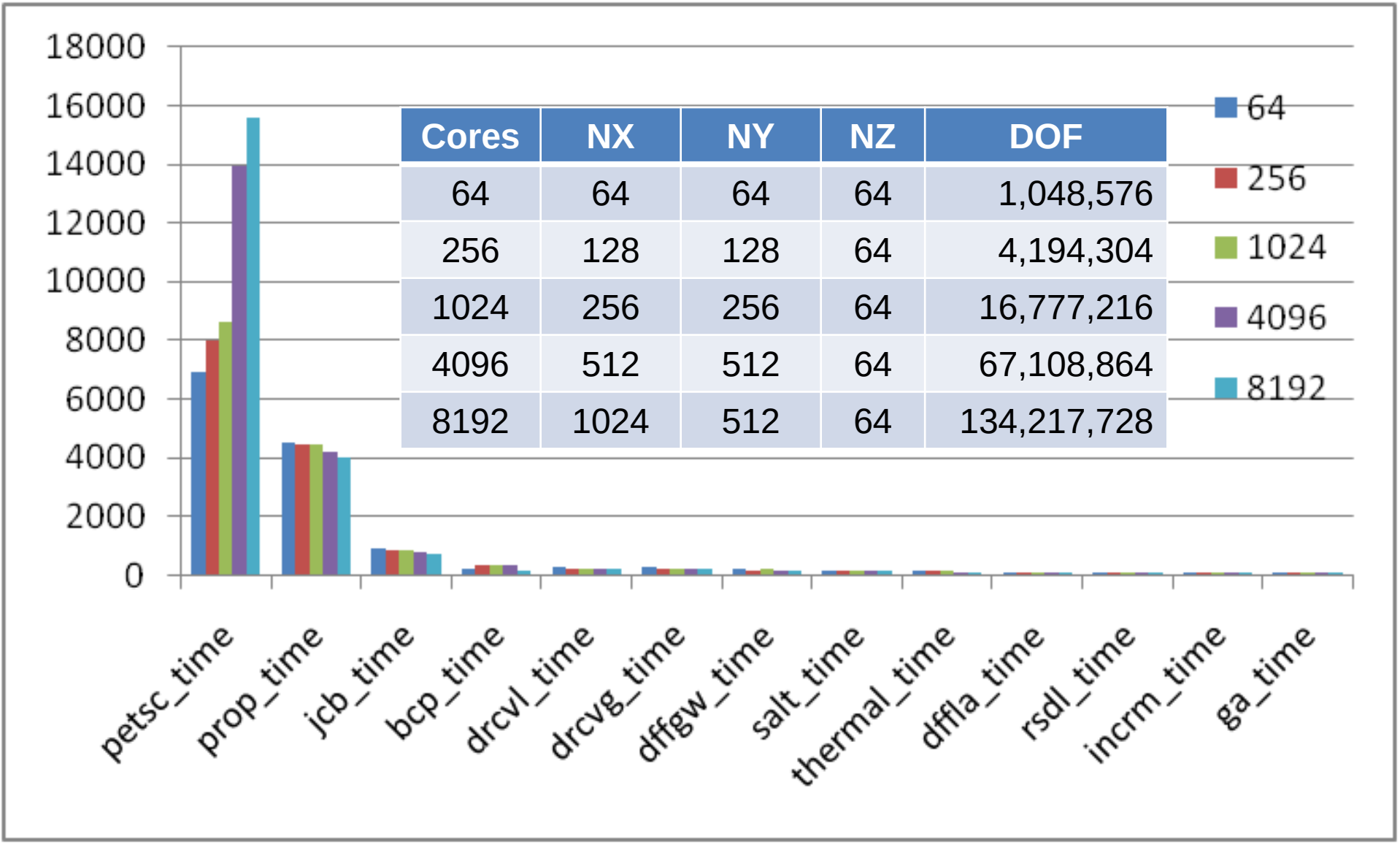
- General parallelization approach: GA + grid component
- Nonisothermal multiphase algorithms conversion complete
- Application to Illinois Basin
  - 4 unknowns per grid cell: aqueous pressure, $scCO_2$ saturation, temperature, brine concentration
  - 2 wells each injecting 1 MMt/yr of $scCO_2$ into heterogeneous Mt. Simon Sandstone
  - Vertical heterogeneity in permeability, porosity, saturation fcns







eSTOMP-CO_2 Weak Scaling

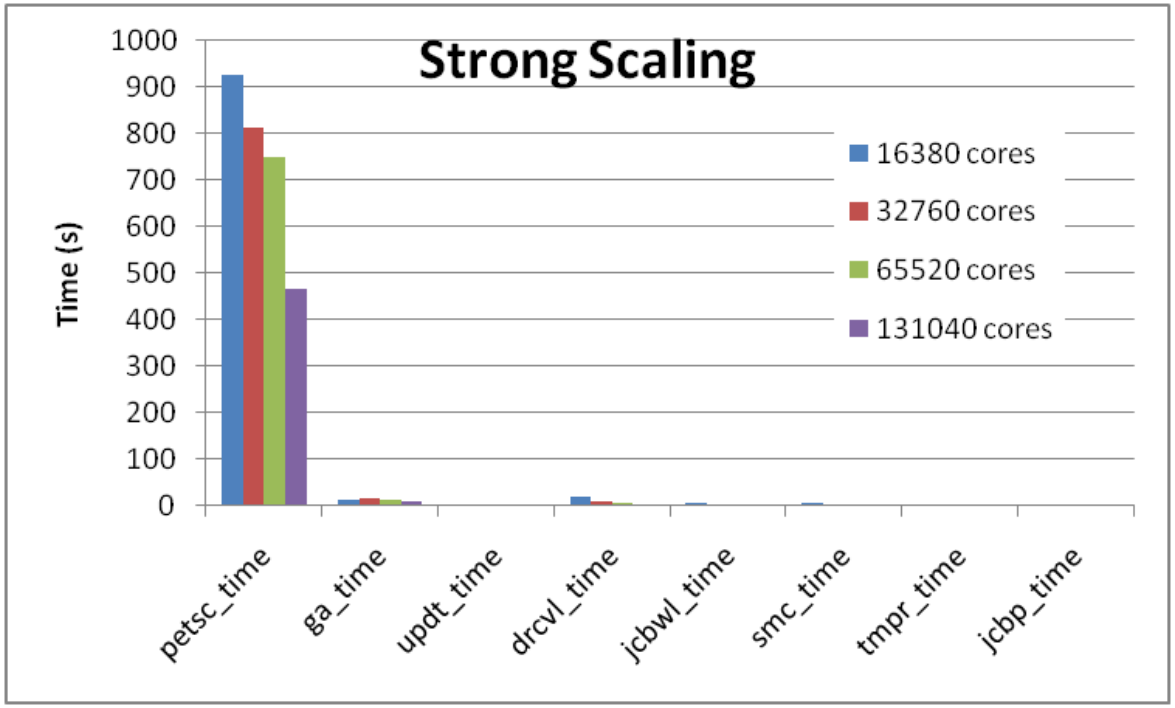


Cores	NX	NY	NZ	DOF
64	64	64	64	1,048,576
256	128	128	64	4,194,304
1024	256	256	64	16,777,216
4096	512	512	64	67,108,864
8192	1024	512	64	134,217,728

Petascale

- Successful proposal to use 2.3 PFLOPS OLCF Jaguar
- Bottlenecks identified and removed: strong scaling up to 131,040 cores

6400x6400x15 = 0.61 x 10^9 nodes
(12 tasks/node)



ASCR Software Metric for Computational Effectiveness

- Jaguar (18,688 nodes; 224,256 processing cores)
  - FY11 metric: capability usage > 40%; > 2X improvement
  - 25 M core-hour grant
- Uranium Bioremediation Problem
  - 0.1 m resolution = 2,268,000 grid cells, maximum 0.1 h timestep
  - 52,800 processor cores
  - 1 simulated day = 400 GB of output
- Objectives
  - Reduce the wall clock time to simulation completion
  - Improve the scalability/efficiency of this eSTOMP application.

In Silico *Geobacter sulfurreducens* Model

- Replaces Fe(III) TEAP reactions and rate law

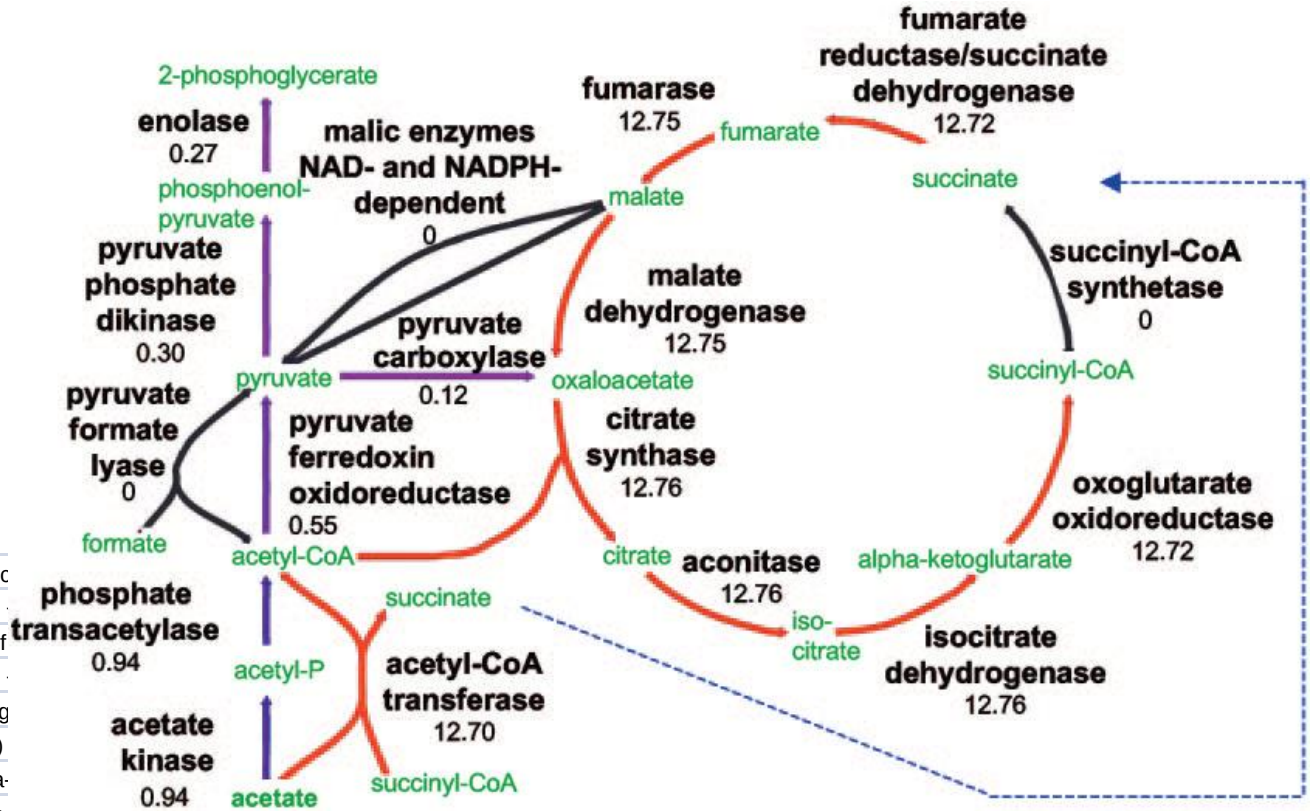
$$0.125CH_3COO^- + FeOOH(s) + 1.875H^+ = Fe^{++} + 1.5H_2O + 0.25HCO_3^-$$

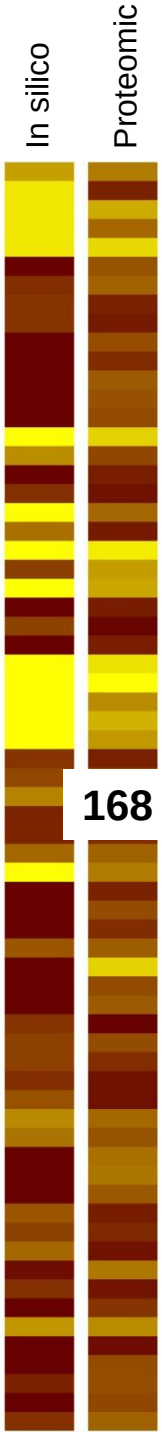
$$R_C^{bio} = -\sum_{eA}^{N_{eA}} \mu_{m,eA} B_m \left(\frac{C_C}{K_{s,C} + C_C} \right) \left(\frac{C_{eA}}{K_{s,eA} + C_{eA}} \right) f(\Delta G_r)$$

- Constraint-based metabolic model of intra-cellular and environmental exchange reactions (588 genes associated with 467 metabolic reactions, 541 metabolites)
- Inputs
  - Initial biomass (planktonic, attached not differentiated)
  - Biomass growth rate
  - Acetate, Fe(III), ammonium uptake rate
- Outputs
  - Acetate, phosphate, ammonium consumption
  - Biomass, Fe(II) production, bicarbonate

List of intracellular reactions		Metabolic Pathway Classification			
Abbreviation	Equation	Subsystem	Gene	Protein	Flux(mmol/gdw h
AACPAT	[c] : accoa + acp --> acacp + coa	Fatty Acid Synthesis	GSU1601, GSU0290	FabHAB	0.015075082
ACBIPGT	[c] : adcobap + gtp + h --> adgcoba + ppi	Vitamins & Cofactor Biosynthesis	GSU3010	CobU	0
ACCOAC	[c] : accoa + atp + hco3 --> adp + h + malcoa + pi	Lipid & Cell Wall Metabolism	GSU1402, GSU2370, GSU2020, GSU201	AccAD, Ac	0.25581673
ACGK	[c] : acglu + atp --> acg5p + adp	Amino Acid Metabolism	GSU0150	ArgB	0.012094597
ACGS	[c] : accoa + glu-L --> acglu + coa + h	Amino Acid Metabolism	GSU2061	ArgA	0
ACHBS	[c] : 2obut + h + pyr --> 2ahbut + co2	Amino Acid Metabolism	GSU1911, GSU1736, GSU1910	IlvB, IlvN1	0.01204339
ACKr	[c] : ac + atp <==> actp + adp	Central Metabolism	GSU3448, GSU2707	AckA2, Ac	0.93881496
ACLS	[c] : h + (2) pyr --> alac-S + co2	Amino Acid Metabolism	GSU1911, GSU1736, GSU1910	IlvB, IlvN1	0.040216412
ACMA					075082
ACNPL					0
ACONT					518787
ACOTA					094597
ACt2					917248
ADCL					0
ADCOE					0
ADCOE					0
ADCOE					0
ADCS					0
ADK1					679421
ADK2					0
ADNK1					0
ADOCE					0
ADPT					0
ADSK					028616
ADSL1					269554
ADSL2					517873
ADSS					269554
AGPAT					0
AGPR					094597
AHC					0
AHCYSNS	[c] : ahc			fs2, Pfs1	0
AHMMPS	[c] : air			hiC1, ThiC	0
AICART	[c] : 10f			urH	0.013391588
AIRC	[c] : air			urE	0.009517873
AKGD	[c] : akg			pd, SucA	0
ALAALA	[c] : (2)			dl	0
ALAD_L	[c] : ala-			ld	0
ALAR	[c] : ala-L <==> ala-D	Lipid & Cell Wall Metabolism	GSU0606	Alr	0.001337047
ALATA_L	[c] : akg + ala-L <==> glu-L + pyr	Amino Acid Metabolism	GSU1242	AlaT	-0.023678235

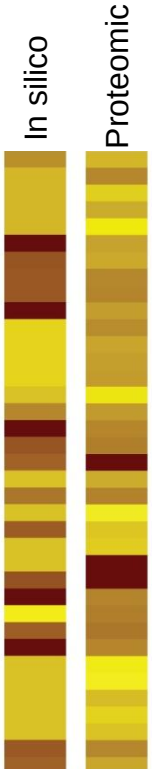
Metabolic functions were assigned to the genes in the *G. sulfurreducens genome* based on available biochemical and genetic evidence and sequence similarity.





Ammonium growth

GSU0097 Pyruvate ferredoxin/flavodoxin oxioreductase
GSU0110 ATP synthase F1, delta subunit
GSU0111 ATP synthase F1, alpha subunit
GSU0112 ATP synthase F1, gamma subunit
GSU0113 ATP synthase F1, beta subunit
GSU0135 Delta-aminolevulinic acid dehydratase
GSU0153 Arginosuccinate synthase
GSU0160 Dihydrodipicolinate reductase
GSU0162 Aromatic aminotransferase, putative
GSU0337 Glutamate-1-semialdehyde-2,1-aminomutase
GSU0339 NADH dehydrogenase I, B subunit
GSU0340 NADH dehydrogenase I, C subunit
GSU0341 NADH dehydrogenase I, D subunit
GSU0343 NADH dehydrogenase I, F subunit
GSU0490 Succinyl:acetate CoA transferase
GSU0580 Pyruvate phosphate dikinase
GSU0604 Thiamine biosynthesis protein ThiC
GSU0609 Phosphoribosylaminoimidazolecarboxamide formyltransferase/IMP cyclohydrolase
GSU0994 Fumarate hydratase, class I
GSU1061 Aspartate aminotransferase
GSU1106 Citrate synthase
GSU1110 Nucleoside diphosphate kinase
GSU1177 Fumarate reductase
GSU1219 Glutamyl-tRNA synthetase
GSU1276 Carbamoyl-phosphate synthase, large subunit
GSU1305 Glu/Leu/Phe/Val dehydrogenase family protein
GSU1465 Isocitrate dehydrogenase
GSU1466 Malate dehydrogenase
GSU1468 Keto/oxoacid ferredoxin oxioreductase, alpha subunit
GSU1469 Keto/oxoacid ferredoxin oxioreductase, beta subunit
GSU1470 Keto/oxoacid ferredoxin oxioreductase, gamma subunit
GSU1605 3-oxoacyl-(acyl-carrier-protein) synthase II



N_2 fixing growth

GSU0097 Pyruvate ferredoxin/flavodoxin oxioreductase
GSU0110 ATP synthase F1, delta subunit
GSU0111 ATP synthase F1, alpha subunit
GSU0112 ATP synthase F1, gamma subunit
GSU0113 ATP synthase F1, beta subunit
GSU0135 Delta-aminolevulinic acid dehydratase
GSU0153 Arginosuccinate synthase
GSU0160 Dihydrodipicolinate reductase
GSU0162 Aromatic aminotransferase, putative
GSU0337 Glutamate-1-semialdehyde-2,1-aminomutase
GSU0339 NADH dehydrogenase I, B subunit
GSU0340 NADH dehydrogenase I, C subunit
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GSU0490 Succinyl:acetate CoA transferase
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GSU0661 Ribose-phosphate pyrophosphokinase
GSU0994 Fumarate hydratase, class I
GSU1061 Aspartate aminotransferase
GSU1106 Citrate synthase
GSU1110 Nucleoside diphosphate kinase
GSU1177 Succinate dehydrogenase flavoprotein subunit
GSU1178 Succinate dehydrogenase/fumarate reductase iron-sulfur subunit
GSU1183 O-acetyl-L-homoserine sulfhydrylase
GSU1219 Glutamyl-tRNA synthetase
GSU1239 Glutamate synthetase-related protein
GSU1276 Carbamoyl-phosphate synthase, large subunit
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GSU1465 Isocitrate dehydrogenase
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GSU1469 Keto/oxoacid ferredoxin oxioreductase, beta subunit
GSU1470 Keto/oxoacid ferredoxin oxioreductase, gamma subunit
GSU1605 3-oxoacyl-(acyl-carrier-protein) synthase II

168 detected *Geobacter sulfurreducens* genes, 77 associated with in silico reactions

GSU1651 Fructose-1,6-bisphosphatase
GSU1660 Aconitate hydratase 2
GSU1691 Riboflavin synthase, beta subunit
GSU1700 NADP-dependent malic enzyme
GSU1735 Branched-chain amino acid ABC transporter, periplasmic amino acid-binding protein, putative
GSU1799 Aspartate kinase, monofunctional class
GSU1835 Glutamine synthetase, type I
GSU1875 Adenosylhomocysteinase
GSU1880 S-adenosylmethionine synthetase
GSU1895 CTP synthase
GSU1902 3-isopropylmalate dehydratase, small subunit, putative
GSU1906 2-isopropylmalate synthase
GSU1911 Acetolactate synthase, large subunit, biosynthetic type
GSU1912 Dihydroxy-acid dehydratase
GSU2286 Enolase
GSU2428 Pyruvate carboxylase
GSU2819 Nitrogenase molybdenum-iron protein, beta subunit
GSU2820 Nitrogenase molybdenum-iron protein, alpha chain
GSU2821 Nitrogenase iron protein
GSU2878 Aspartate-semialdehyde dehydrogenase, putative
GSU2879 3-isopropylmalate dehydrogenase
GSU2919 Transketolase, N-terminal subunit
GSU2977 Transaldolase, putative
GSU3142 3-deoxy-D-arabino-heptulosonate 7-phosphate (DAHP) synthase
GSU3285 Porphobilinogen deaminase
GSU3291 V-type H(+)-translocating pyrophosphatase
GSU3299 Carboxyl transferase domain protein
GSU3302 Methylmalonyl-CoA mutase, putative
GSU3308 Adenylosuccinate synthetase
GSU3385 Phosphoenolpyruvate carboxykinase
GSU3401 Branched-chain amino acid ABC transporter, periplasmic amino acid-binding protein, putative

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GSU1660 Aconitate hydratase 2
GSU1691 Riboflavin synthase, beta subunit
GSU1700 NADP-dependent malic enzyme
GSU1734 Branched-chain amino acid ABC transporter, periplasmic amino acid-binding protein, putative
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GSU1799 Aspartate kinase, monofunctional class
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GSU1875 Adenosylhomocysteinase
GSU1880 S-adenosylmethionine synthetase
GSU1895 CTP synthase
GSU1902 3-isopropylmalate dehydratase, small subunit, putative
GSU1906 2-isopropylmalate synthase
GSU1911 Acetolactate synthase, large subunit, biosynthetic type
GSU1912 Dihydroxy-acid dehydratase
GSU2013 Phosphoglucomutase/phosphomannomutase family protein
GSU2286 Enolase
GSU2428 Pyruvate carboxylase
GSU2819 Nitrogenase molybdenum-iron protein, beta subunit
GSU2820 Nitrogenase molybdenum-iron protein, alpha chain
GSU2821 Nitrogenase iron protein
GSU2878 Aspartate-semialdehyde dehydrogenase, putative
GSU2879 3-isopropylmalate dehydrogenase
GSU2919 Transketolase, N-terminal subunit
GSU2977 Transaldolase, putative
GSU2999 Precorrin-8X methylmutase
GSU3142 3-deoxy-D-arabino-heptulosonate 7-phosphate (DAHP) synthase
GSU3285 Porphobilinogen deaminase
GSU3291 V-type H(+)-translocating pyrophosphatase
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GSU3308 Adenylosuccinate synthetase
GSU3385 Phosphoenolpyruvate carboxykinase
GSU3401 Branched-chain amino acid ABC transporter, periplasmic amino acid-binding protein, putative
GSU3453 Uroporphyrinogen decarboxylase

Comparison with Rifle Geobacter Sulfurreducens Proteomic Data

- Greatest protein abundances (acetyl-CoA transferase and citrate synthase) match the highest in silico fluxes.
- Pyruvate ferredoxin oxioreductase activity agrees with prediction that this enzyme converts acetate to pyruvate.
- Proteomics detects some activity through the “other” acetyl CoA transferase (GSU174), whereas model has all the flux going through GSU490.
- No phosphotransacetylase in the proteomics data although this protein was data searched with other Geobacter genomes: G. sulfurreducens genomic data may not match the environmental proteomics data.
- Evidence for phosphoenolpyruvate carboxykinase (GSU3385) activity; this enzyme converts phosphoenolpyruvate (formed from pyruvate) to oxaloacetate which then goes into the TCA cycle.

FY-2011

- Ongoing
  - CO_2 application to heterogeneous material properties
  - UQ application to Rifle IFRC
  - Joint hydrologic and geophysics inverse modeling
  - Incorporate nonisothermal, 2-phase flow into eSTOMP-H2O
  - Implement and demonstrate load balancing and fault tolerance in collaboration with XSCI projects
- Dr. Nitin Gawande starts post-doc position at the end of this month
- Interactions
  - eSTOMP-CO2 being used in NRAP
  - Automated 414.1c testing developed under ASCEM
  - CSI proposal for incorporating geomechanics into eSTOMP
  - eSTOMP application in 300 Area and Rifle IFRCs
  - GS^3 UQ/viz application using eSTOMP

eSTOMP Needs

- Capabilities
  - Unstructured grid
  - Geomechanics
  - N-phase multifluid formulation
  - Well models
- Infrastructure
  - Parallel I/O
  - Data management
  - Fault tolerance
- Software engineering
  - Consolidation of multiple STOMP modes
  - Componentization
- Challenges
  - Architecture-specific algorithms (e.g., GPU reaction solver)
  - More robust and efficient solution techniques

eSTOMP Presentations and Publications

- Invited presentations
  - 2010. DOE SBR PI Meeting: Modeling and Simulation of Subsurface Systems, Washington, D.C.
  - 2010. Gordon Conference on Flow and Transport in Porous Media, Lewiston, ME
  - 2010. AGU Meeting of the Americas, Foz do Iguassu, Brazil
  - 2010. Soil Science Society of America Annual Meeting, Long Beach, CA
- Journal articles submitted
  - Parallel Implementation of a Subsurface Flow and Reactive Transport Simulator using a Component-Based Approach" by Fang, Palmer, Yabusaki submitted to Computational Geosciences
  - Variably Saturated Flow and Multicomponent Biogeochemical Reactive Transport Modeling ..." Yabusaki, Fang, … submitted to the Journal of Contaminant Hydrology.