Optimal Model Complexity in Geological Carbon Sequestration: A Design of Experiment (DoE) & Response Surface (RS) Uncertainty Analysis

Project Number: DE-FE-0009238

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U.S. Department of Energy

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Carbon Storage R&D Project Review Meeting
Developing the Technologies and
Infrastructure for CCS

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Presentation Outline

- Project major goals and benefits;
- Detailed project objectives & success criteria;
- Accomplishments to date;
- Summary of results;
- Appendix (organization chart; Gantt chart; additional results).

Benefit to the Program

Major goals:

Support industry's ability to predict CO_2 storage capacity in geologic formations to within ±30% accuracy; Develop and validate technologies to ensure 99% storage permanence.

Project benefits:

We will facilitate the development and implementation of efficient workflows for modeling field-scale geological carbon sequestration (GCS) in a variety of geochemically reactive environments, where subsurface formations exhibit multiple scales of permeability (k) heterogeneity.

Project Overview:

Specific Goals and Objectives

- Develop, test, and verify the DoE and RS uncertainty analysis for a fully heterogeneous reference model (FHM) & increasingly lower resolution "geologic models" created from upscaling the FHM. For all models:

  (1) within the uncertainty framework over multiple time scales, identify influential parameters (and processes) on making various predictions and to quantify their prediction uncertainties: *pressure evolution, CO_2 footprint, CO_2 storage ratio, CO_2/brine leakage, distributions of geochemical species, and ϕ/k changes in the storage system (reservoir + caprock) and their feedback with flow modeling*.

  (2) At increasing time scales, evaluate optimal heterogeneity resolution(s) by comparing the uncertainty analysis outcomes of all models.

- Investigate the effect of increasing reservoir permeability (k) variance and depth on the uncertainty outcomes including optimal heterogeneity resolution(s). At deep depth, investigate gravity-stable injection.

Project Overview:

Success Criteria

- At increasing depth, for both weakly and strongly heterogeneous systems, the geologic models can capture the FHM CO_2 behaviors *within the full parameter space*; → **Reduced characterization cost;**

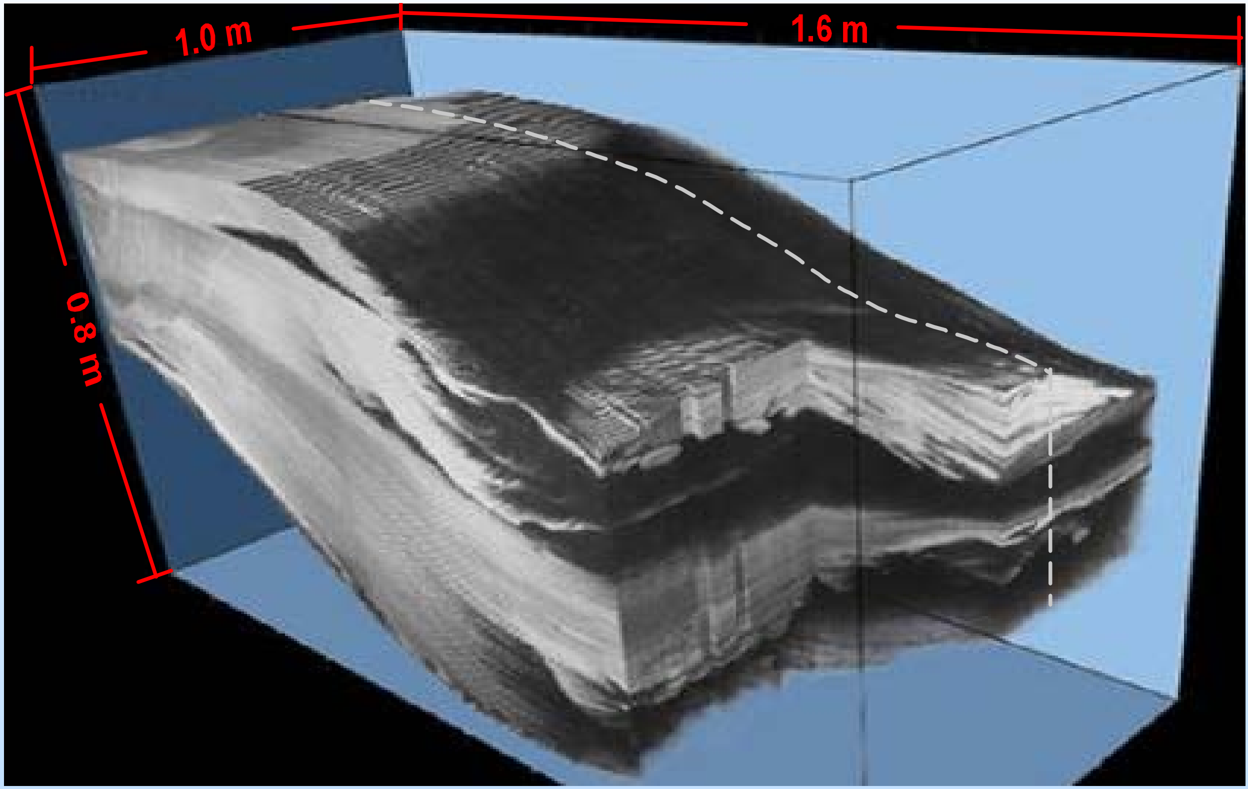
- RS analytical models are successfully verified against full-physics reservoir simulations via HPC, thus prediction uncertainty of any outcome at any time can be assessed *using the low-resolution model(s)* running the efficient RS models. → **Enhanced computation efficiency;**

- Deep injection: within the uncertainty analysis framework, identify the combination(s) of favorable parameters & reservoir condition that give rise to *gravity stable* flow → **Enhanced storage security**.

Accomplishments to Date

- High-resolution 3D reservoir k heterogeneity (3.2 M) & geologic models of decreasing k resolutions;
- Permeability upscaling & single-phase flow verification;
- (poster tomorrow) Multiscale dispersivity upscaling & verification via a new parallel RWPT with div(D);
- CO_2 modeling with PFLOTRAN & performance scaling on the petascale Yellowstone supercomputer at NWSC;
- Preliminary model comparison & DoE/RS analysis.

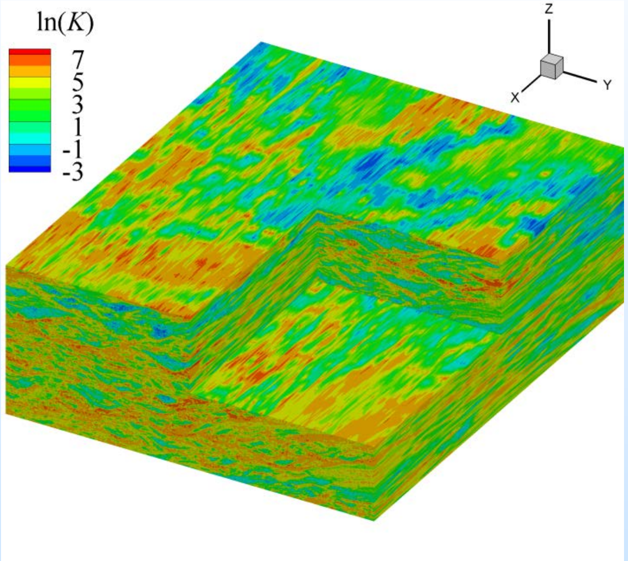
Sediment Experiment at SAFL



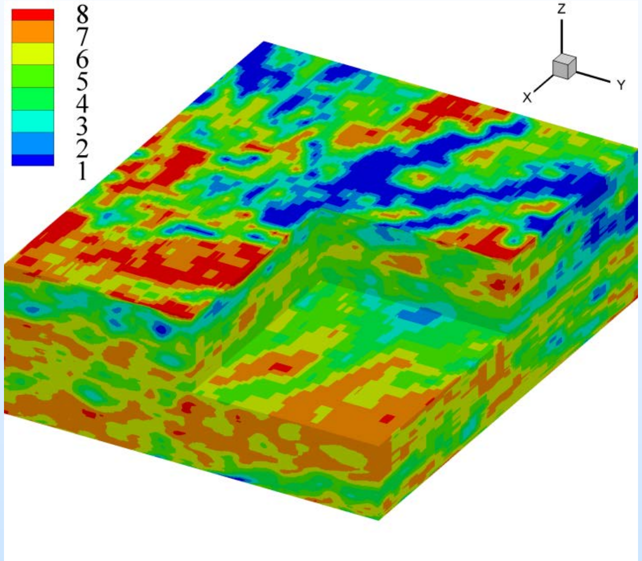
http://www.safl.umn.edu/
Project lead: Prof. Chris Paola
Funding: NSF & oil industry consortium

Reservoir Heterogeneity v. Geologic Models

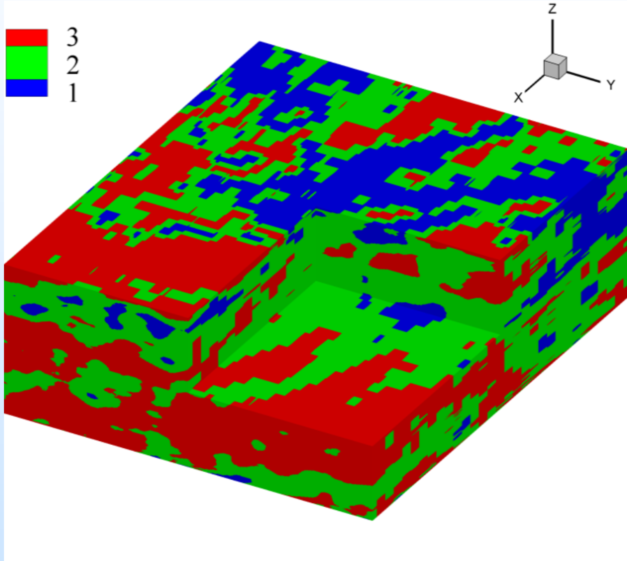
Nx=251, Ny=251, Nz=50 (total grid cells = 3.2M)



FHM



8-unit facies model



3-unit facies model

- A 1-unit homogeneous “formation” model is also created (not shown);
- A homogeneous shale caprock unit is added to all models (not shown);

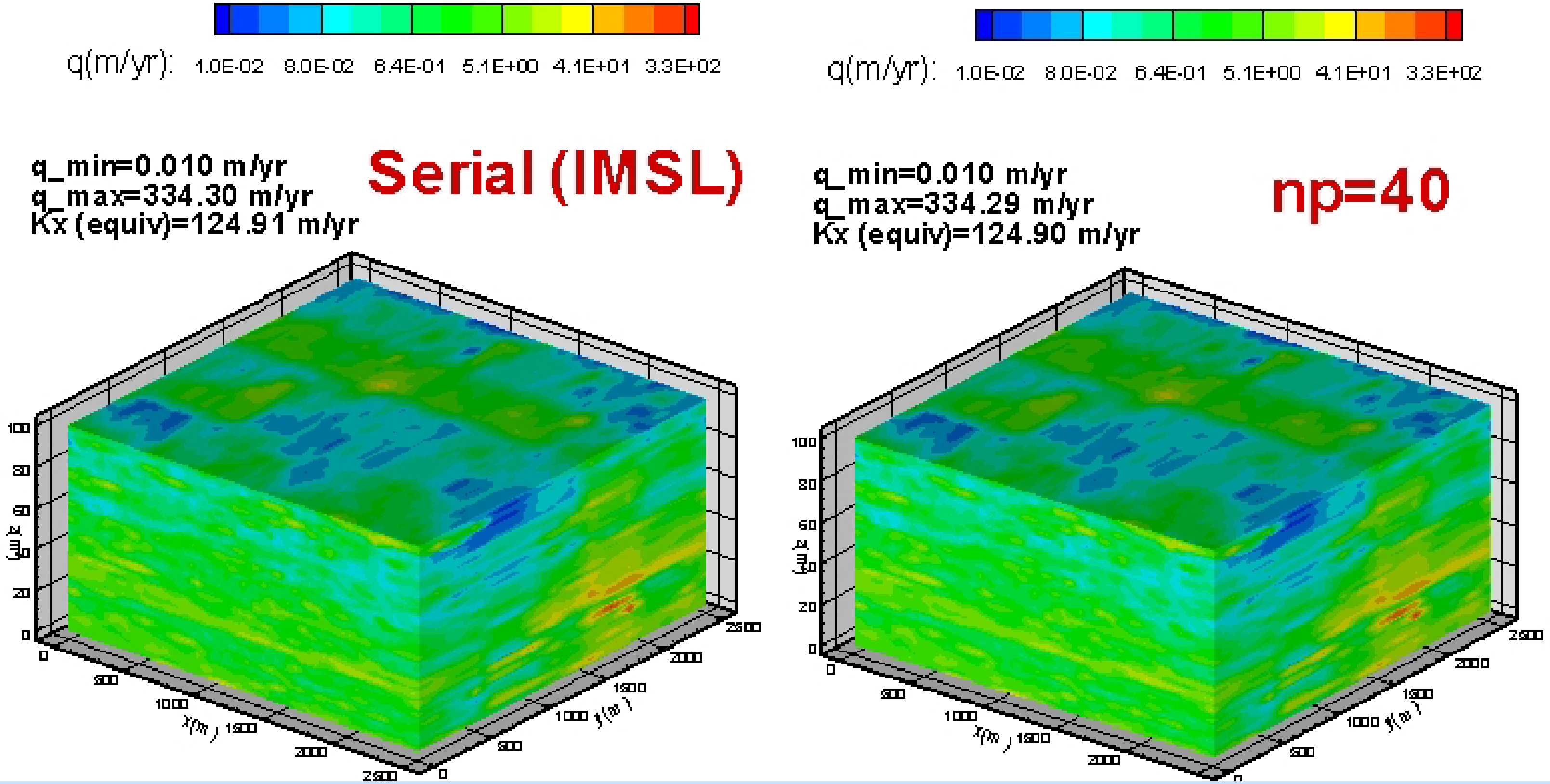
Intrinsic Permeability Upscaling

$$
\begin{array}{l|ccccccccc|}
 & \left\langle \frac{\partial\Phi}{\partial x}\right\rangle_1 & \left\langle \frac{\partial\Phi}{\partial y}\right\rangle_1 & \left\langle \frac{\partial\Phi}{\partial z}\right\rangle_1 & 0 & 0 & 0 & 0 & 0 & 0 \\
\mathrm{BC}_1 & 0 & 0 & 0 & \left\langle \frac{\partial\Phi}{\partial x}\right\rangle_1 & \left\langle \frac{\partial\Phi}{\partial y}\right\rangle_1 & \left\langle \frac{\partial\Phi}{\partial z}\right\rangle_1 & 0 & 0 & 0 \\
 & 0 & 0 & 0 & 0 & 0 & 0 & \left\langle \frac{\partial\Phi}{\partial x}\right\rangle_1 & \left\langle \frac{\partial\Phi}{\partial y}\right\rangle_1 & \left\langle \frac{\partial\Phi}{\partial z}\right\rangle_1 \\
\hline
 & \left\langle \frac{\partial\Phi}{\partial x}\right\rangle_2 & \left\langle \frac{\partial\Phi}{\partial y}\right\rangle_2 & \left\langle \frac{\partial\Phi}{\partial z}\right\rangle_2 & 0 & 0 & 0 & 0 & 0 & 0 \\
\mathrm{BC}_2 & 0 & 0 & 0 & \left\langle \frac{\partial\Phi}{\partial x}\right\rangle_2 & \left\langle \frac{\partial\Phi}{\partial y}\right\rangle_2 & \left\langle \frac{\partial\Phi}{\partial z}\right\rangle_2 & 0 & 0 & 0 \\
 & 0 & 0 & 0 & 0 & 0 & 0 & \left\langle \frac{\partial\Phi}{\partial x}\right\rangle_2 & \left\langle \frac{\partial\Phi}{\partial y}\right\rangle_2 & \left\langle \frac{\partial\Phi}{\partial z}\right\rangle_2 \\
\hline
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
\hline
 & \left\langle \frac{\partial\Phi}{\partial x}\right\rangle_m & \left\langle \frac{\partial\Phi}{\partial y}\right\rangle_m & \left\langle \frac{\partial\Phi}{\partial z}\right\rangle_m & 0 & 0 & 0 & 0 & 0 & 0 \\
\mathrm{BC}_m & 0 & 0 & 0 & \left\langle \frac{\partial\Phi}{\partial x}\right\rangle_m & \left\langle \frac{\partial\Phi}{\partial y}\right\rangle_m & \left\langle \frac{\partial\Phi}{\partial z}\right\rangle_m & 0 & 0 & 0 \\
 & 0 & 0 & 0 & 0 & 0 & 0 & \left\langle \frac{\partial\Phi}{\partial x}\right\rangle_m & \left\langle \frac{\partial\Phi}{\partial y}\right\rangle_m & \left\langle \frac{\partial\Phi}{\partial z}\right\rangle_m \\
\hline
 & 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
\text{Symmetry} & 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\
 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & -1 & 0
\end{array}
\cdot
\left\{\begin{array}{c} k_{xx} \\ k_{xy} \\ k_{xz} \\ k_{yx} \\ k_{yy} \\ k_{yz} \\ k_{zx} \\ k_{zy} \\ k_{zz} \end{array}\right\}
= (-\mu)
\left\{\begin{array}{c} \langle q_x\rangle_1 \\ \langle q_y\rangle_1 \\ \langle q_z\rangle_1 \\ \langle q_x\rangle_2 \\ \langle q_y\rangle_2 \\ \langle q_z\rangle_2 \\ \ldots \\ \langle q_x\rangle_m \\ \langle q_y\rangle_m \\ \langle q_z\rangle_m \\ 0 \\ 0 \\ 0 \end{array}\right\}
$$

Zhang et al. (2006) WRR; Li et al. (2011) WRR

Parallel Flow Simulation for Upscaling

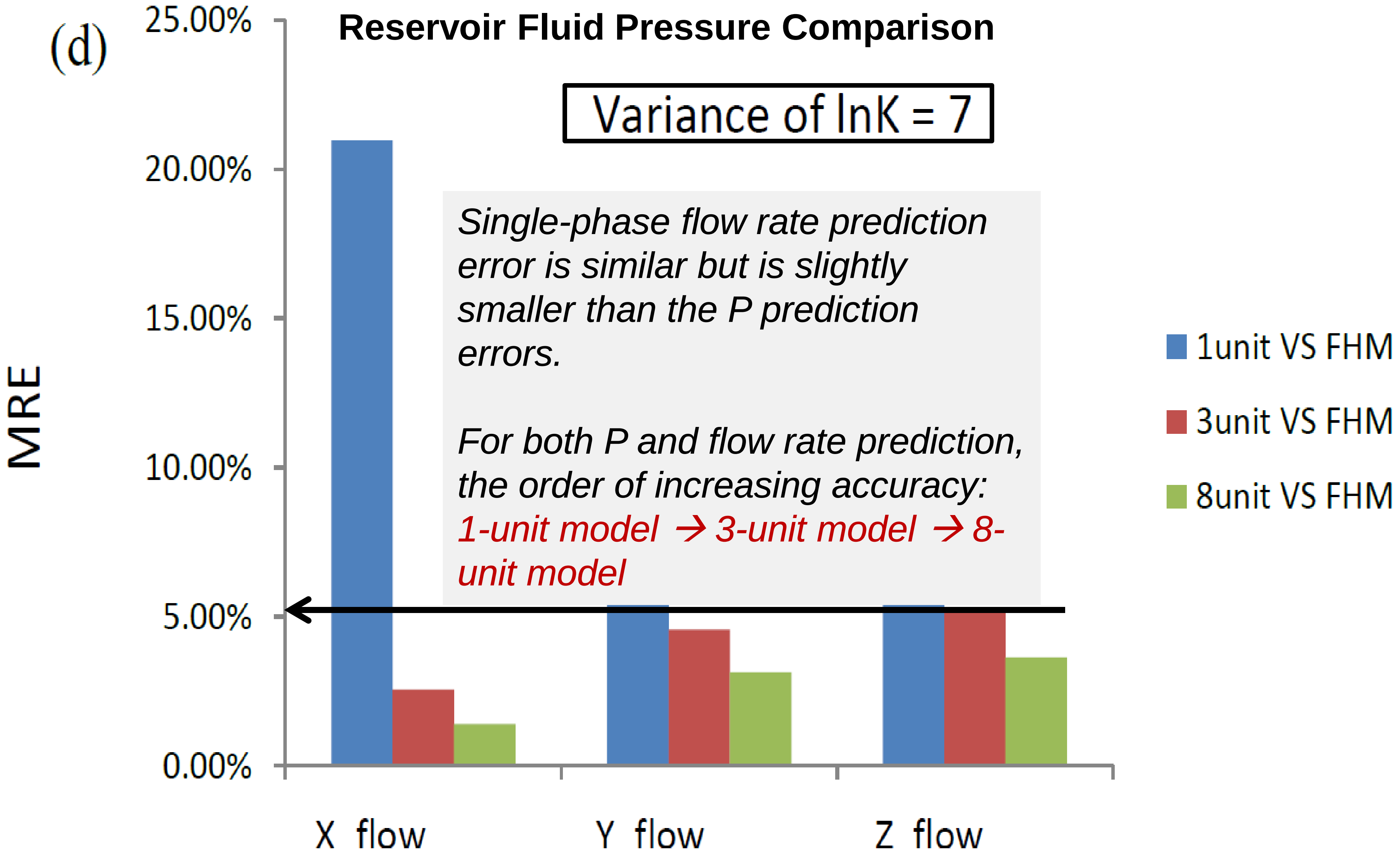
Test model (0.4M):



Serial time (calling an optimized IMSL on BigRed at IU): 1 hour

Parallel time (H2oc.gg.uwyo.edu): 37 sec (64 processors)

Upscaling Verification



Single-phase flow rate prediction error is similar but is slightly smaller than the P prediction errors.

For both P and flow rate prediction, the order of increasing accuracy: *1-unit model → 3-unit model → 8-unit model*

Upscaling Summary

- Global upscaling can homogenize irregularly shaped & hierarchical geologic models with reservoir-scale (long-range) k connectivity;
- Upscaling is successful even for high-variance systems (the highest successfully tested reservoir k varies ~10^6);
- Parallel HPC can overcome the computational hurdle associated with the global upscaling of large models;
- (poster tomorrow) A dispersivity upscaling analysis is conducted to estimate the effective longitudinal macrodispersivity for each unit of the geologic models, for both the low and high *lnk* variance systems.

CO_2 Modeling with PFLOTRAN

- Multicomponent-multiphase-multiphysics non-isothermal reactive flow and transport model;

- Massively parallel---based on the PETSc parallel framework;
  - Peta-scale performance
  - Highly scalable (run on over 265k cores)

- Supercritical CO_2-H_2O
  - Span-Wagner EOS for CO_2 density & fugacity coefficient
  - Mixture density for dissolved CO_2-brine (Duan et al., 2008)
  - Viscosity CO_2 (Fenghour et al., 1998)

- Finite Volume Discretization
  - Variable switching for changes in fluid phase
  - Structured/Unstructured grids

- Object Oriented Fortran 2003
  - Open Source (Multilab code: LANL, LBNL, ORNL, PNNL)

PFLOTRAN Scaling on Yellowstone

Yellowstone is a 1.5-petaflops supercomputer with 72,288 processor cores & 144.6 TB of memory.

http://www2.cisl.ucar.edu/resources/yellowstone

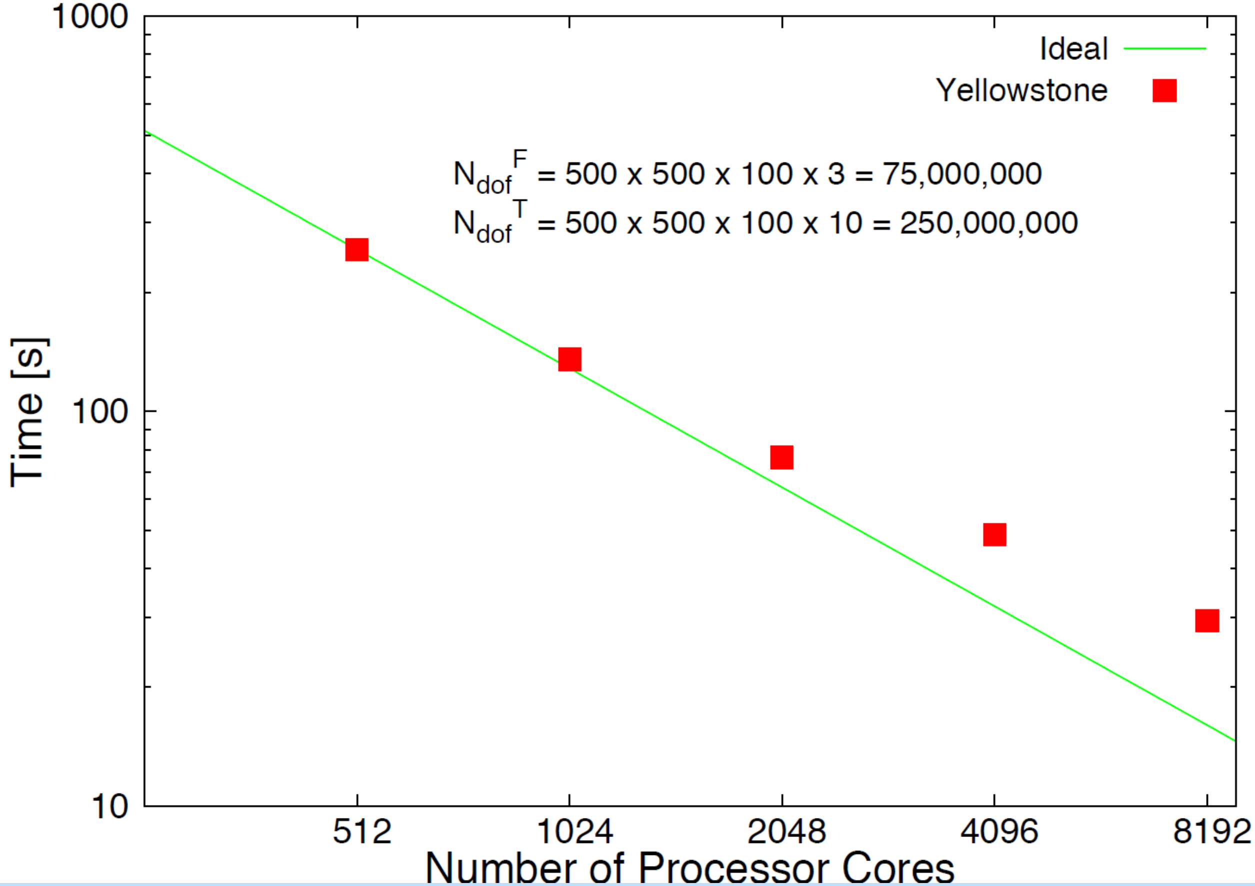
We can solve bigger problems, but we cannot access all these cores at all times!

1-unit model (3.2M):

** 20 yr CO_2 injection + 1000 yr monitoring*

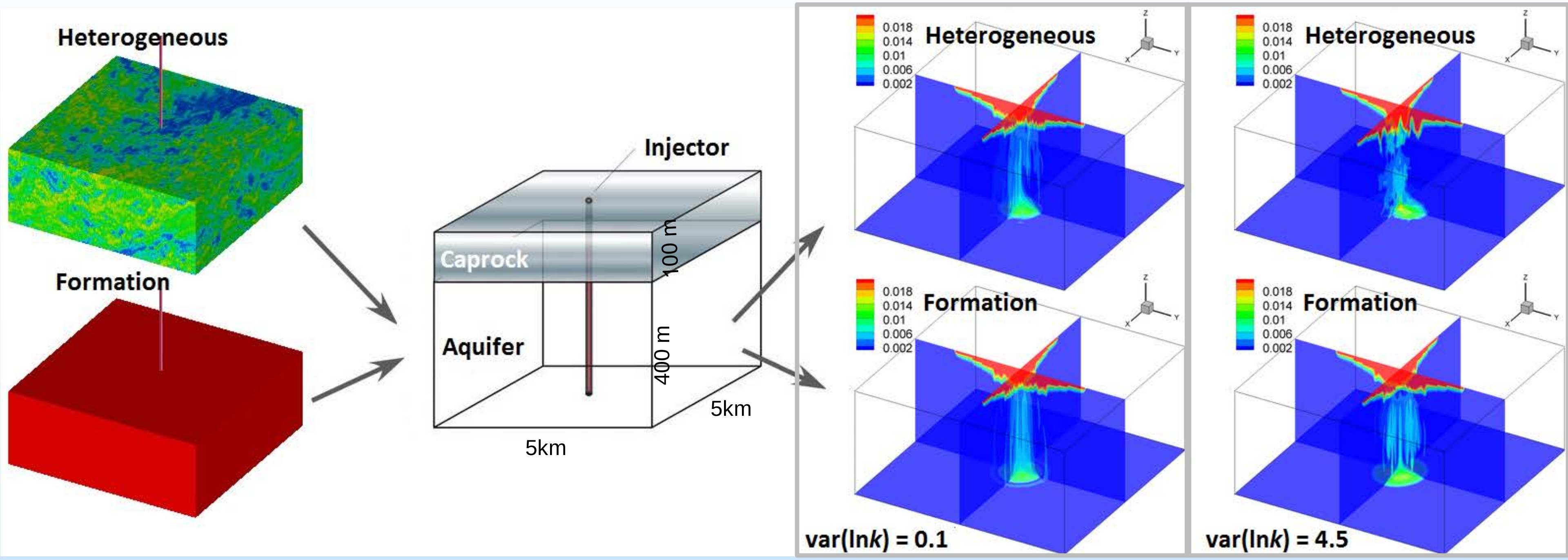
** **1024 cores**: 5 min = 2 min (injection) + 3 min (monitoring)*

1-unit model (25 M): CO_2 injection w/ reactive chemistry



CO_2 Simulation: FHM v. 1-Unit Model

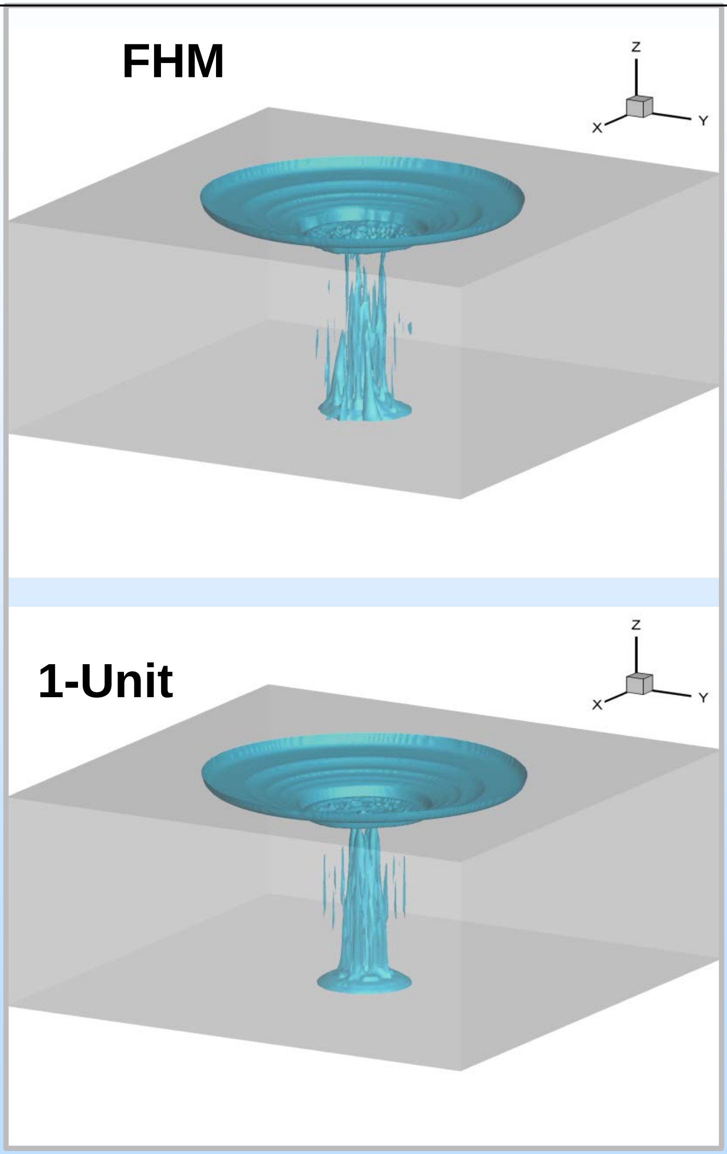
Dissolved CO_2 at the end of monitoring (inj rate= 0.05 Mt/yr):



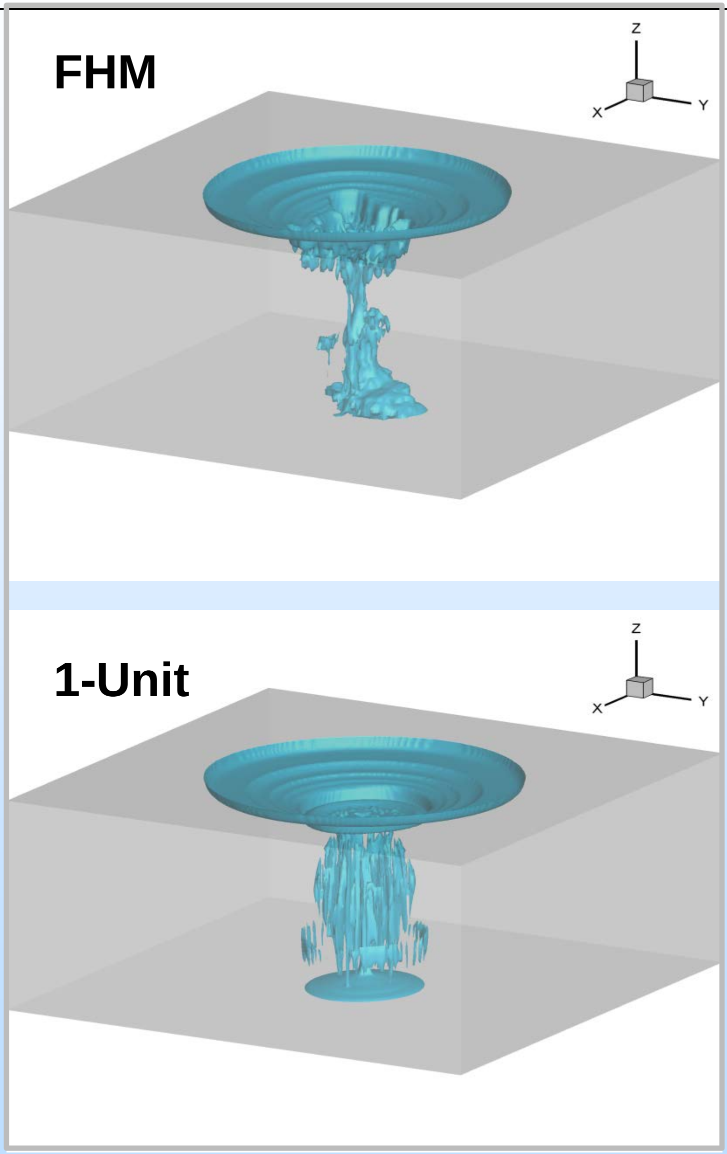
aquifer k varies over 5 orders of magnitude

- Under both low and high variance conditions, the 1-unit model can capture the plume footprint (see above) and fluid pressure (Appendix) of the FHM very well.
- Base on results of the upscaling study, the 8-unit and 3-unit models should yield more accurate CO_2 predictions than the 1-unit model → yet to be simulated.

End of Monitoring: Iso_conc = 0.004

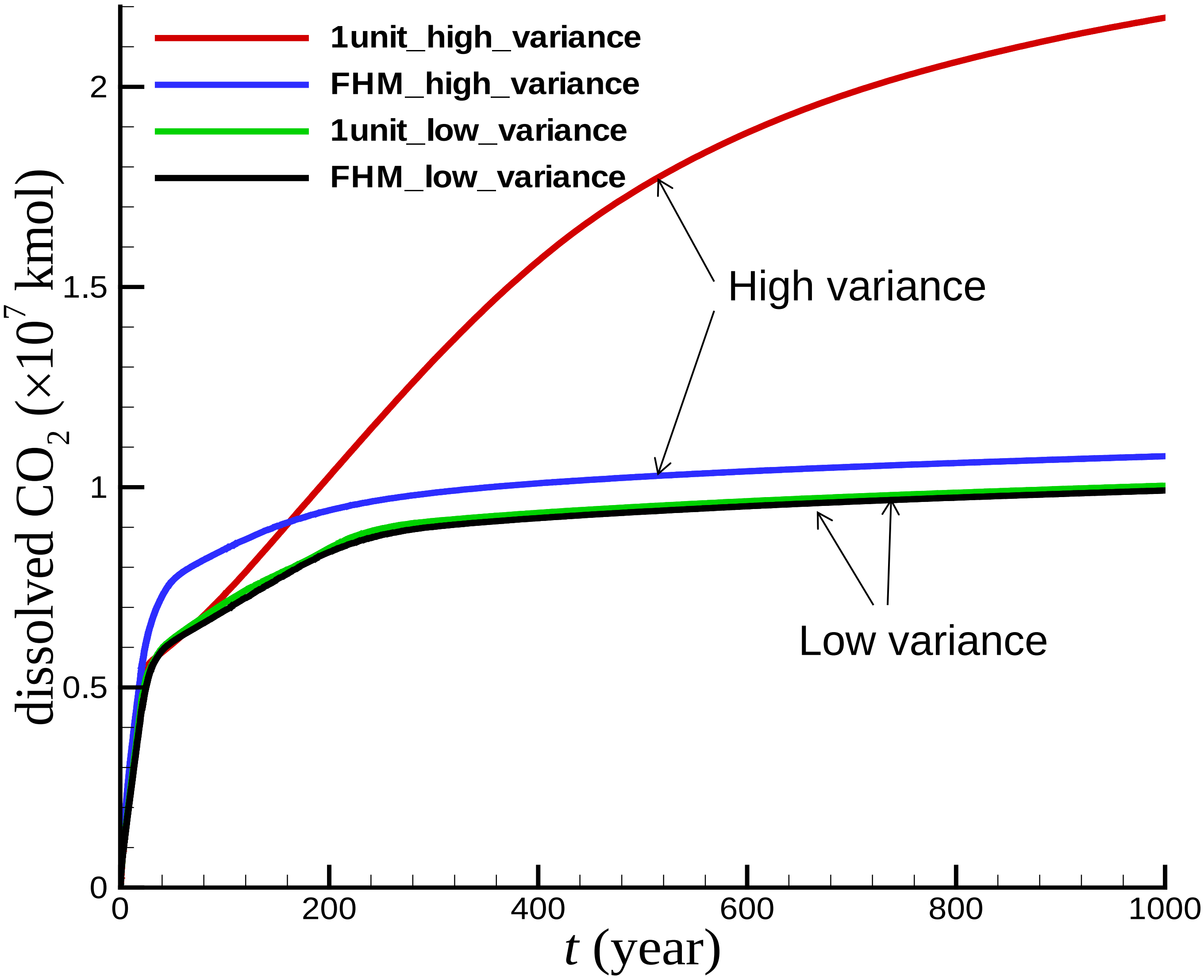


Var(lnk)=0.1



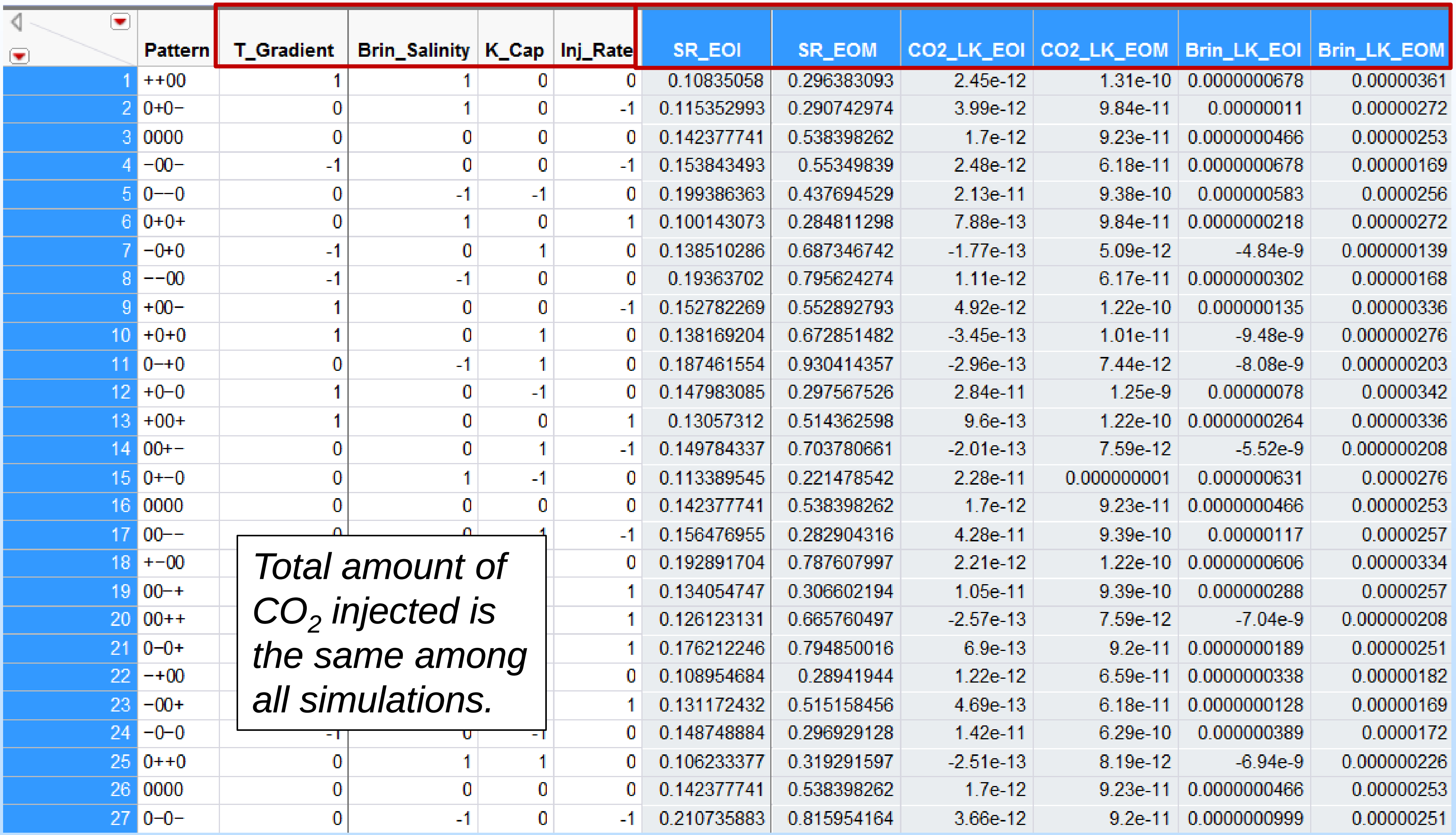
Var(lnk)=4.5

FHM v. 1-Unit Model: Dissolved CO_2



- Under low variance, the 1-unit model can capture the dissolved CO_2 well;
- Under high variance, the 1-unit model over-estimates the dissolved CO_2 because the equivalent kz is high → faster density-driven convection → more CO_2 dissolved per unit time;
- Under high variance, how accurate are the 8-unit and 3-unit models remain to be seen.

Design of Experiment: 1-Unit



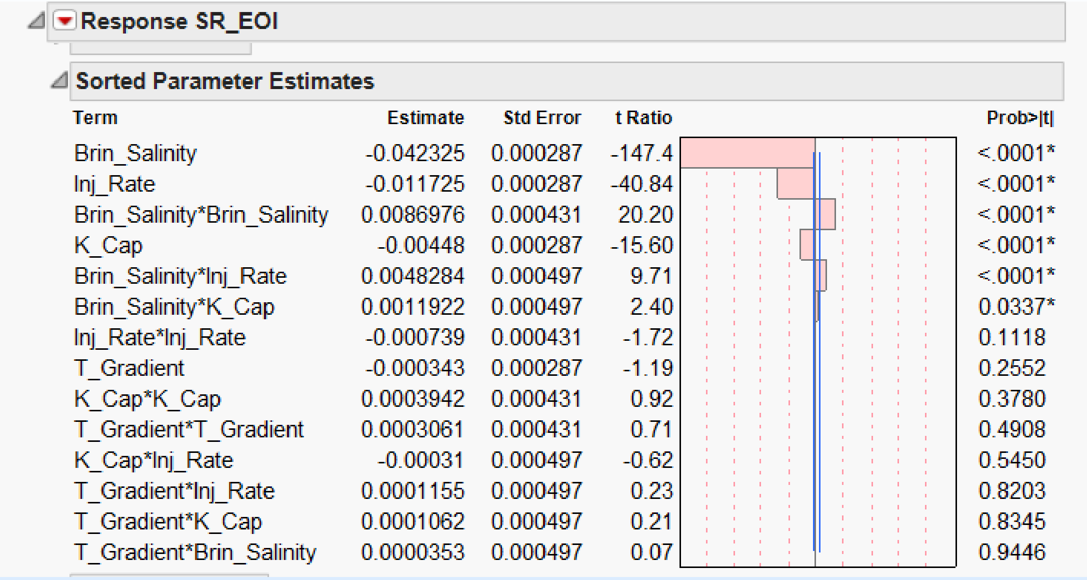
	Pattern	T_Gradient	Brin_Salinity	K_Cap	Inj_Rate	SR_EOI	SR_EOM	CO2_LK_EOI	CO2_LK_EOM	Brin_LK_EOI	Brin_LK_EOM
1	++00	1	1	0	0	0.10835058	0.296383093	2.45e-12	1.31e-10	0.0000000678	0.00000361
2	0+0−	0	1	0	-1	0.115352993	0.290742974	3.99e-12	9.84e-11	0.00000011	0.00000272
3	0000	0	0	0	0	0.142377741	0.538398262	1.7e-12	9.23e-11	0.0000000466	0.00000253
4	−00−	-1	0	0	-1	0.153843493	0.55349839	2.48e-12	6.18e-11	0.0000000678	0.00000169
5	0−−0	0	-1	-1	0	0.199386363	0.437694529	2.13e-11	9.38e-10	0.000000583	0.0000256
6	0+0+	0	1	0	1	0.100143073	0.284811298	7.88e-13	9.84e-11	0.0000000218	0.00000272
7	−0+0	-1	0	1	0	0.138510286	0.687346742	-1.77e-13	5.09e-12	-4.84e-9	0.000000139
8	−−00	-1	-1	0	0	0.19363702	0.795624274	1.11e-12	6.17e-11	0.0000000302	0.00000168
9	+00−	1	0	0	-1	0.152782269	0.552892793	4.92e-12	1.22e-10	0.000000135	0.00000336
10	+0+0	1	0	1	0	0.138169204	0.672851482	-3.45e-13	1.01e-11	-9.48e-9	0.000000276
11	0−+0	0	-1	1	0	0.187461554	0.930414357	-2.96e-13	7.44e-12	-8.08e-9	0.000000203
12	+0−0	1	0	-1	0	0.147983085	0.297567526	2.84e-11	1.25e-9	0.00000078	0.0000342
13	+00+	1	0	0	1	0.13057312	0.514362598	9.6e-13	1.22e-10	0.0000000264	0.00000336
14	00+−	0	0	1	-1	0.149784337	0.703780661	-2.01e-13	7.59e-12	-5.52e-9	0.000000208
15	0+−0	0	1	-1	0	0.113389545	0.221478542	2.28e-11	0.000000001	0.000000631	0.0000276
16	0000	0	0	0	0	0.142377741	0.538398262	1.7e-12	9.23e-11	0.0000000466	0.00000253
17	00−−	0	0	[illegible]	-1	0.156476955	0.282904316	4.28e-11	9.39e-10	0.00000117	0.0000257
18	+−00	[illegible]	[illegible]	[illegible]	0	0.192891704	0.787607997	2.21e-12	1.22e-10	0.0000000606	0.00000334
19	00−+	[illegible]	[illegible]	[illegible]	1	0.134054747	0.306602194	1.05e-11	9.39e-10	0.000000288	0.0000257
20	00++	[illegible]	[illegible]	[illegible]	1	0.126123131	0.665760497	-2.57e-13	7.59e-12	-7.04e-9	0.000000208
21	0−0+	[illegible]	[illegible]	[illegible]	1	0.176212246	0.794850016	6.9e-13	9.2e-11	0.0000000189	0.00000251
22	−+00	[illegible]	[illegible]	[illegible]	0	0.108954684	0.28941944	1.22e-12	6.59e-11	0.0000000338	0.00000182
23	−00+	[illegible]	[illegible]	[illegible]	1	0.131172432	0.515158456	4.69e-13	6.18e-11	0.0000000128	0.00000169
24	−0−0	-1	0	-1	0	0.148748884	0.296929128	1.42e-11	6.29e-10	0.000000389	0.0000172
25	0++0	0	1	1	0	0.106233377	0.319291597	-2.51e-13	8.19e-12	-6.94e-9	0.000000226
26	0000	0	0	0	0	0.142377741	0.538398262	1.7e-12	9.23e-11	0.0000000466	0.00000253
27	0−0−	0	-1	0	-1	0.210735883	0.815954164	3.66e-12	9.2e-11	0.0000000999	0.00000251

Total amount of CO_2 injected is the same among all simulations.

Parameter Ranking: 1-Unit

Outcome: dissolved CO_2

End of Injection

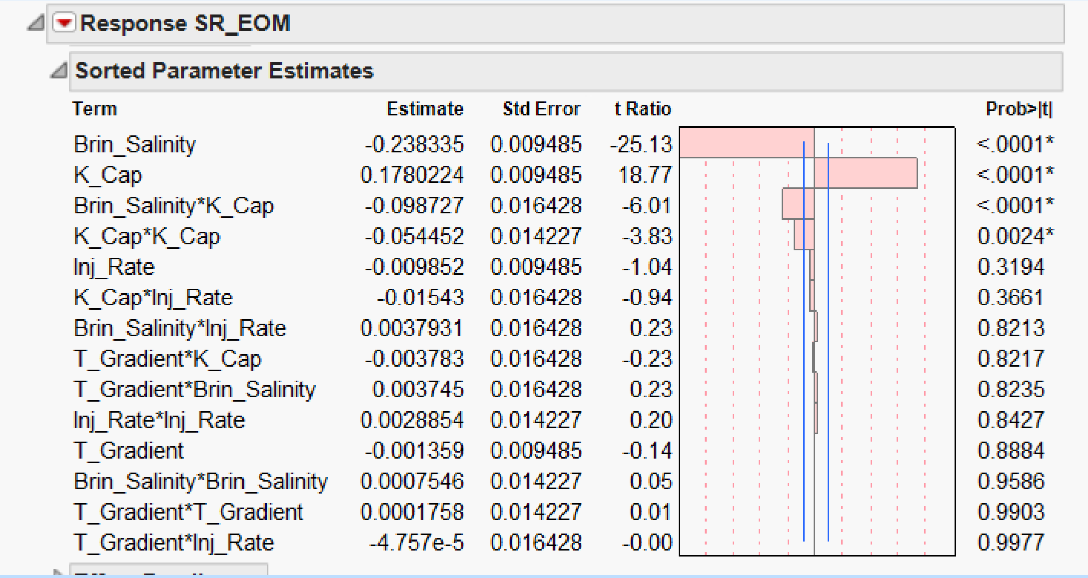


Response SR_EOI

Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Brin_Salinity	-0.042325	0.000287	-147.4	<.0001*
Inj_Rate	-0.011725	0.000287	-40.84	<.0001*
Brin_Salinity*Brin_Salinity	0.0086976	0.000431	20.20	<.0001*
K_Cap	-0.00448	0.000287	-15.60	<.0001*
Brin_Salinity*Inj_Rate	0.0048284	0.000497	9.71	<.0001*
Brin_Salinity*K_Cap	0.0011922	0.000497	2.40	0.0337*
Inj_Rate*Inj_Rate	-0.000739	0.000431	-1.72	0.1118
T_Gradient	-0.000343	0.000287	-1.19	0.2552
K_Cap*K_Cap	0.0003942	0.000431	0.92	0.3780
T_Gradient*T_Gradient	0.0003061	0.000431	0.71	0.4908
K_Cap*Inj_Rate	-0.00031	0.000497	-0.62	0.5450
T_Gradient*Inj_Rate	0.0001155	0.000497	0.23	0.8203
T_Gradient*K_Cap	0.0001062	0.000497	0.21	0.8345
T_Gradient*Brin_Salinity	0.0000353	0.000497	0.07	0.9446

End of Monitoring



Response SR_EOM

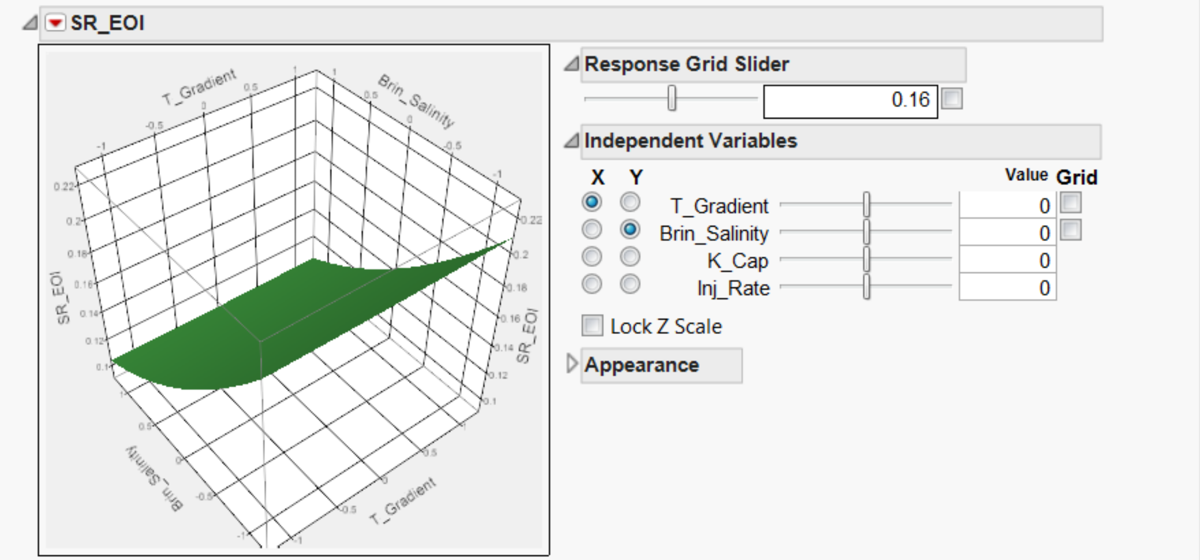
Sorted Parameter Estimates

Term	Estimate	Std Error	t Ratio	Prob>|t|
Brin_Salinity	-0.238335	0.009485	-25.13	<.0001*
K_Cap	0.1780224	0.009485	18.77	<.0001*
Brin_Salinity*K_Cap	-0.098727	0.016428	-6.01	<.0001*
K_Cap*K_Cap	-0.054452	0.014227	-3.83	0.0024*
Inj_Rate	-0.009852	0.009485	-1.04	0.3194
K_Cap*Inj_Rate	-0.01543	0.016428	-0.94	0.3661
Brin_Salinity*Inj_Rate	0.0037931	0.016428	0.23	0.8213
T_Gradient*K_Cap	-0.003783	0.016428	-0.23	0.8217
T_Gradient*Brin_Salinity	0.003745	0.016428	0.23	0.8235
Inj_Rate*Inj_Rate	0.0028854	0.014227	0.20	0.8427
T_Gradient	-0.001359	0.009485	-0.14	0.8884
Brin_Salinity*Brin_Salinity	0.0007546	0.014227	0.05	0.9586
T_Gradient*T_Gradient	0.0001758	0.014227	0.01	0.9903
T_Gradient*Inj_Rate	-4.757e-5	0.016428	-0.00	0.9977

Response Surfaces: 1-Unit

Outcome: dissolved CO_2

End of Injection



SR_EOI

Response Grid Slider 0.16 ☐

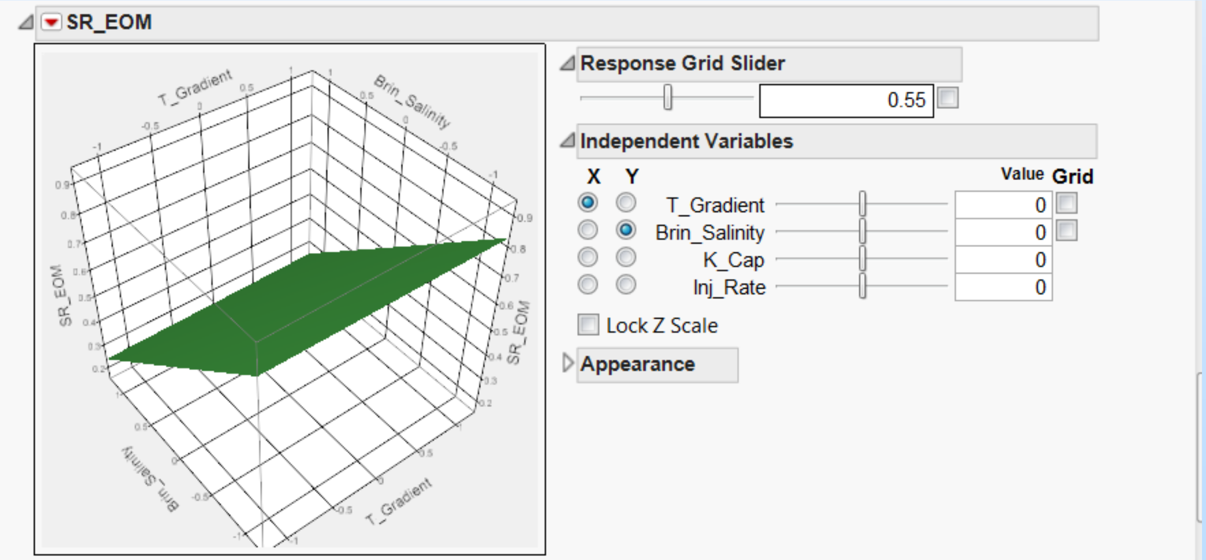
Independent Variables

X	Y		Value	Grid
●	○	T_Gradient	0	☐
○	●	Brin_Salinity	0	☐
○	○	K_Cap	0	
○	○	Inj_Rate	0	

☐ Lock Z Scale

Appearance

End of Monitoring



SR_EOM

Response Grid Slider 0.55 ☐

Independent Variables

X	Y		Value	Grid
●	○	T_Gradient	0	☐
○	●	Brin_Salinity	0	☐
○	○	K_Cap	0	
○	○	Inj_Rate	0	

☐ Lock Z Scale

Appearance

Summary

- Global upscaling computes equivalent *k*s for the geologic model with decreasing heterogeneity resolution; for increasing reservoir *lnk* variances (0.1, 1.0, 4.5), FHM pressure and flow rate are captured well by the geologic models, but errors increase with variance.

- (poster) Upscaled dispersivities for the 8-, 3-, and 1-unit models can capture plume moments (centroid, longitudinal plume covariance, BTC) when variance is low to modest.

- When the variance of ln(k) is low, the 1-unit model yields very similar reservoir fluid pressure, plume footprint, and dissolution fingering as the FHM. It thus accurately predicts the total dissolution storage at the end of the simulation time.

- When the variance of ln(k) is high, the 1-unit model yields similar reservoir fluid pressure (slight increase in error) and plume footprint as the FHM, but predicts more dissolution fingering per unit time (more optimistic storage estimate).

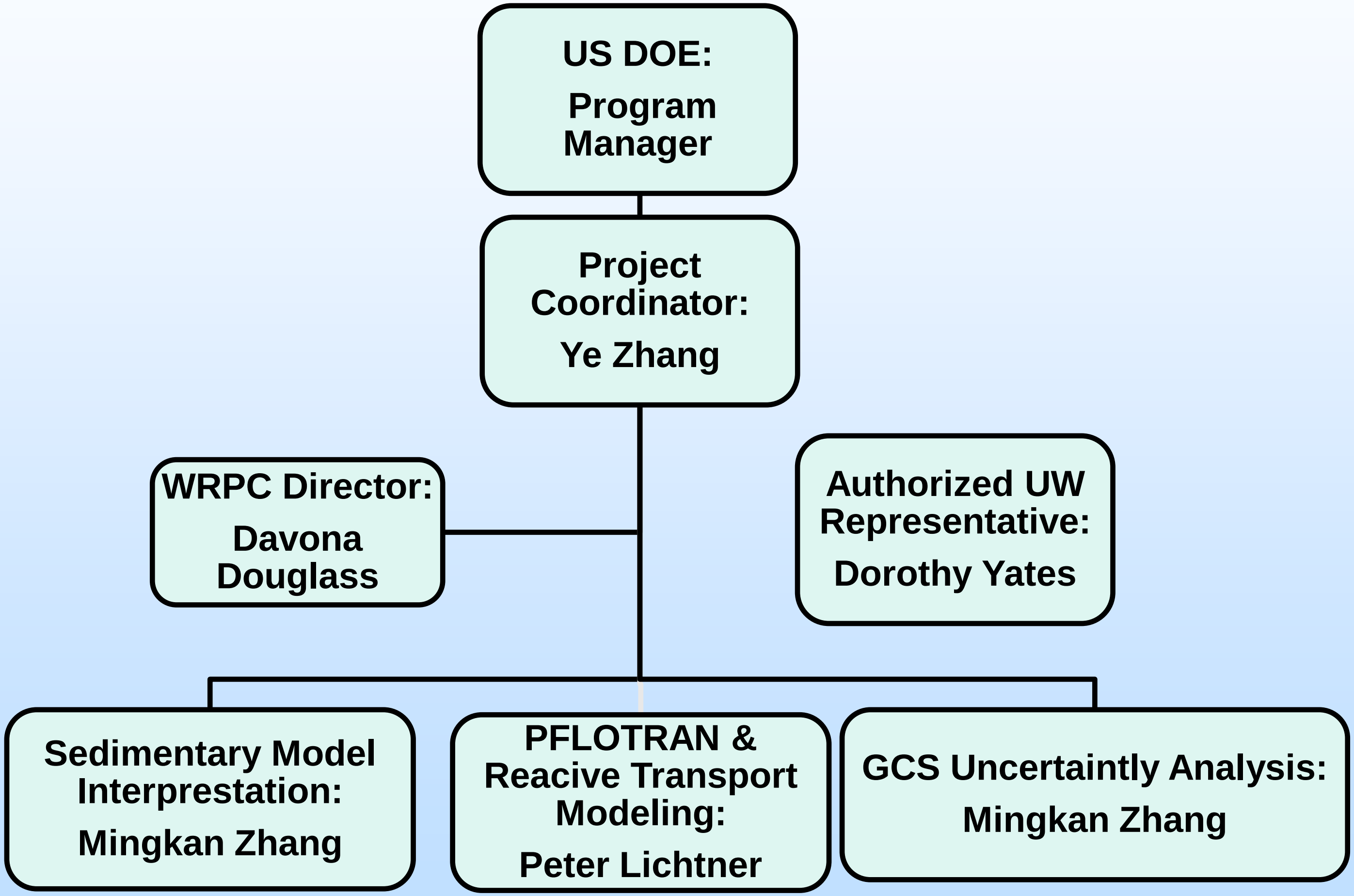
- Preliminary experimental design analysis suggests that brine salinity is the single most influential factor impacting CO_2 dissolution storage in the 1-unit model.

- Next step: For low and high variance systems, complete the DoE and RS analysis for all models to compare their parameter sensitivity & prediction uncertainty.

Appendix

- These slides will not be discussed during the presentation, but are mandatory

Organization Chart



US DOE:

Program Manager

Project Coordinator:

Ye Zhang

WRPC Director:

Davona Douglass

Authorized UW Representative:

Dorothy Yates

Sedimentary Model Interprestation:

Mingkan Zhang

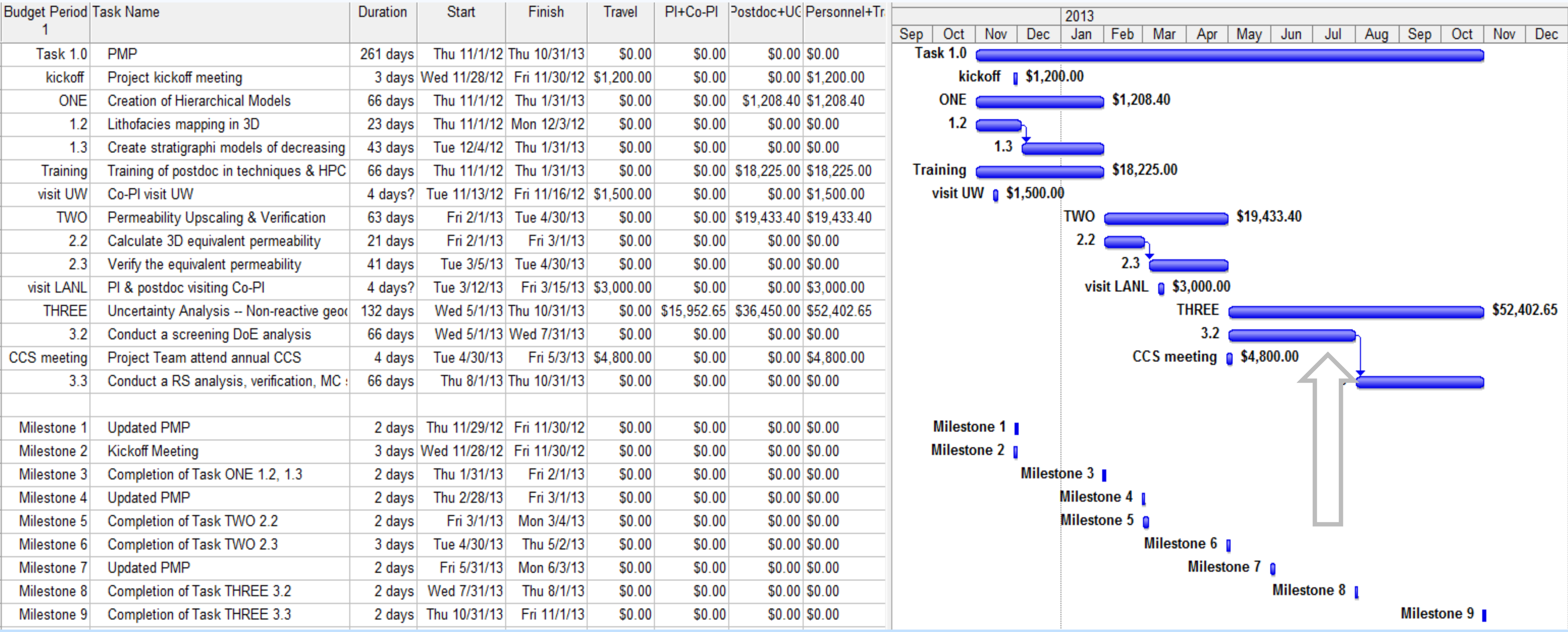
PFLOTRAN & Reacive Transport Modeling:

Peter Lichtner

GCS Uncertaintly Analysis:

Mingkan Zhang

Gantt Chart: Budget Period 1



Budget Period 1	Task Name	Duration	Start	Finish	Travel	PI+Co-PI	Postdoc+UC	Personnel+Tr
Task 1.0	PMP	261 days	Thu 11/1/12	Thu 10/31/13	$0.00	$0.00	$0.00	$0.00
kickoff	Project kickoff meeting	3 days	Wed 11/28/12	Fri 11/30/12	$1,200.00	$0.00	$0.00	$1,200.00
ONE	Creation of Hierarchical Models	66 days	Thu 11/1/12	Thu 1/31/13	$0.00	$0.00	$1,208.40	$1,208.40
1.2	Lithofacies mapping in 3D	23 days	Thu 11/1/12	Mon 12/3/12	$0.00	$0.00	$0.00	$0.00
1.3	Create stratigraphi models of decreasing	43 days	Tue 12/4/12	Thu 1/31/13	$0.00	$0.00	$0.00	$0.00
Training	Training of postdoc in techniques & HPC	66 days	Thu 11/1/12	Thu 1/31/13	$0.00	$0.00	$18,225.00	$18,225.00
visit UW	Co-PI visit UW	4 days?	Tue 11/13/12	Fri 11/16/12	$1,500.00	$0.00	$0.00	$1,500.00
TWO	Permeability Upscaling & Verification	63 days	Fri 2/1/13	Tue 4/30/13	$0.00	$0.00	$19,433.40	$19,433.40
2.2	Calculate 3D equivalent permeability	21 days	Fri 2/1/13	Fri 3/1/13	$0.00	$0.00	$0.00	$0.00
2.3	Verify the equivalent permeability	41 days	Tue 3/5/13	Tue 4/30/13	$0.00	$0.00	$0.00	$0.00
visit LANL	PI & postdoc visiting Co-PI	4 days?	Tue 3/12/13	Fri 3/15/13	$3,000.00	$0.00	$0.00	$3,000.00
THREE	Uncertainty Analysis -- Non-reactive geo	132 days	Wed 5/1/13	Thu 10/31/13	$0.00	$15,952.65	$36,450.00	$52,402.65
3.2	Conduct a screening DoE analysis	66 days	Wed 5/1/13	Wed 7/31/13	$0.00	$0.00	$0.00	$0.00
CCS meeting	Project Team attend annual CCS	4 days	Tue 4/30/13	Fri 5/3/13	$4,800.00	$0.00	$0.00	$4,800.00
3.3	Conduct a RS analysis, verification, MC	66 days	Thu 8/1/13	Thu 10/31/13	$0.00	$0.00	$0.00	$0.00
Milestone 1	Updated PMP	2 days	Thu 11/29/12	Fri 11/30/12	$0.00	$0.00	$0.00	$0.00
Milestone 2	Kickoff Meeting	3 days	Wed 11/28/12	Fri 11/30/12	$0.00	$0.00	$0.00	$0.00
Milestone 3	Completion of Task ONE 1.2, 1.3	2 days	Thu 1/31/13	Fri 2/1/13	$0.00	$0.00	$0.00	$0.00
Milestone 4	Updated PMP	2 days	Thu 2/28/13	Fri 3/1/13	$0.00	$0.00	$0.00	$0.00
Milestone 5	Completion of Task TWO 2.2	2 days	Fri 3/1/13	Mon 3/4/13	$0.00	$0.00	$0.00	$0.00
Milestone 6	Completion of Task TWO 2.3	3 days	Tue 4/30/13	Thu 5/2/13	$0.00	$0.00	$0.00	$0.00
Milestone 7	Updated PMP	2 days	Fri 5/31/13	Mon 6/3/13	$0.00	$0.00	$0.00	$0.00
Milestone 8	Completion of Task THREE 3.2	2 days	Wed 7/31/13	Thu 8/1/13	$0.00	$0.00	$0.00	$0.00
Milestone 9	Completion of Task THREE 3.3	2 days	Thu 10/31/13	Fri 11/1/13	$0.00	$0.00	$0.00	$0.00

PFLOTRAN formulations

To model GCS, the following mass and energy conservation equations are solved:

$$\frac{\partial}{\partial t}\left[\varphi \sum_{\alpha} (\rho_\alpha s_\alpha X_i^\alpha)\right] + \nabla \cdot \sum_{\alpha} (\rho_\alpha X_i^\alpha \vec{q}_\alpha - \varphi \rho_\alpha s_\alpha \tau_\alpha D_\alpha \nabla X_i^\alpha) = S_i \qquad (1)$$

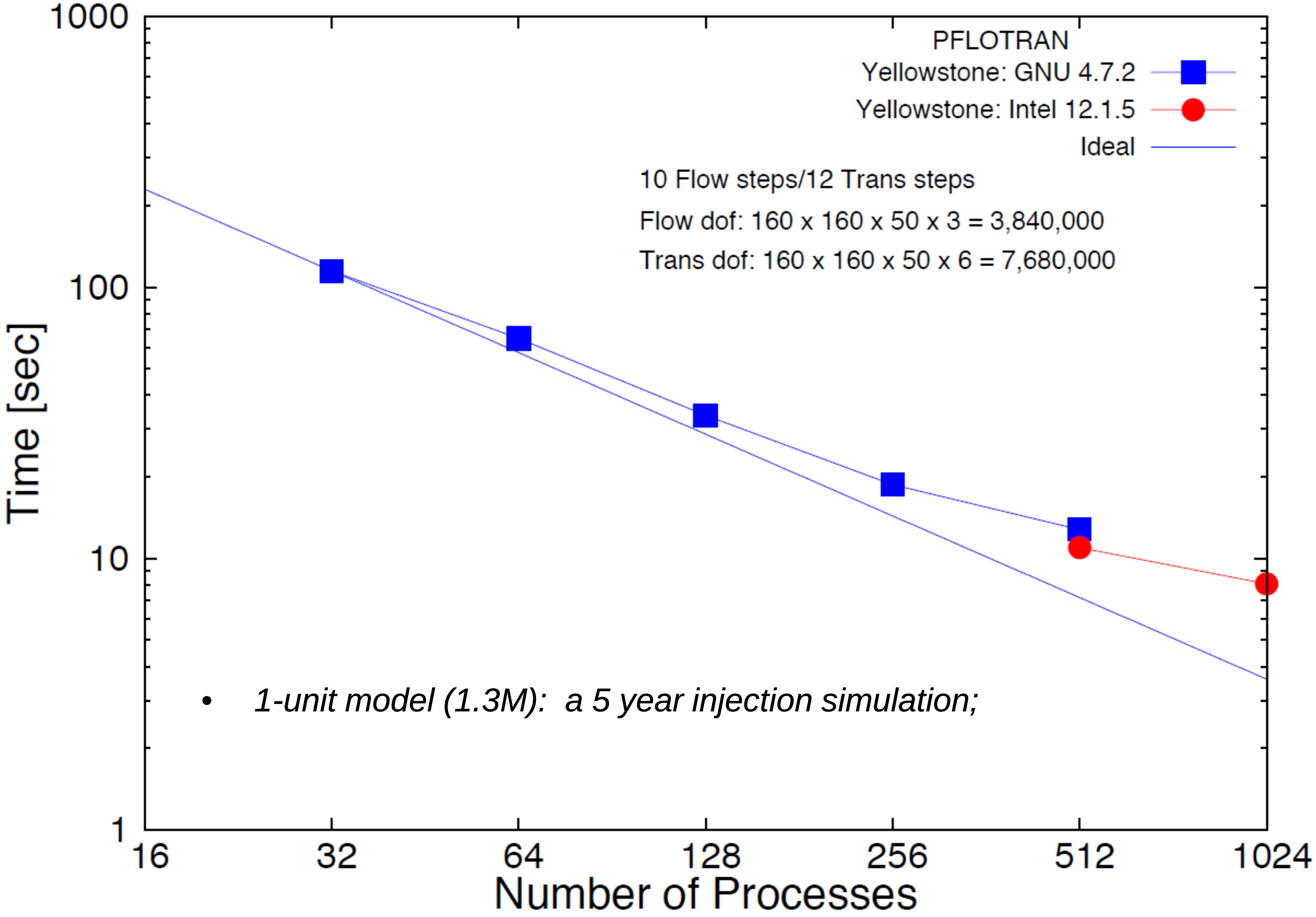
$$\frac{\partial}{\partial t}\left[\varphi \sum_{\alpha} (\rho_\alpha s_\alpha U_\alpha) + (1-\varphi)\rho_r C_{p,r} T\right] + \nabla \cdot \left[\sum_{\alpha} (\vec{q}_\alpha \rho_\alpha H_\alpha) - \lambda \nabla T\right] = Q \qquad (2)$$

φ denotes porosity, and $\rho_\alpha, s_\alpha, \tau_\alpha, D_\alpha, U_{\alpha,} H_\alpha$ refer to the density, saturation, tortuosity, diffusion coefficient, internal energy, and enthalpy of fluid phase α, respectively. Two fluid phases (CO_2, brine) will be modeled. The quantities X_i^α denote the mole fraction of component *i* in phase α. The quantities $C_{p,r}$ and λ denote the rock heat capacity and conductivity, respectively. The summation is carried out over all fluid phases present in the system. The system is assumed locally to be in thermodynamic equilibrium with temperature *T*($\vec{x}$*; t)* at position $\vec{x}$ and time *t*. The quantity *Q* denotes an energy source/sink term.

The quantity *Si* denotes a source/sink term for the *i*th primary species describing reaction with minerals given by $S_i = -\sum_m \nu_{im} I_m$, with stoichiometric reaction coefficients ν_{im} and kinetic rate I_m for the *m*th mineral, taken as positive for precipitation and negative for dissolution.

The flow rate $\vec{q}_\alpha$ of fluid phase α is given by the extended Darcy's law: $\vec{q}_\alpha = -\frac{\bar{\bar{k}} k_\alpha}{\mu_\alpha}(\nabla p_\alpha - \rho_\alpha g z)$, with intrinsic permeability $\bar{\bar{k}}$, relative permeability k_α, fluid viscosity μ_α, and pressure p_α of phase α.

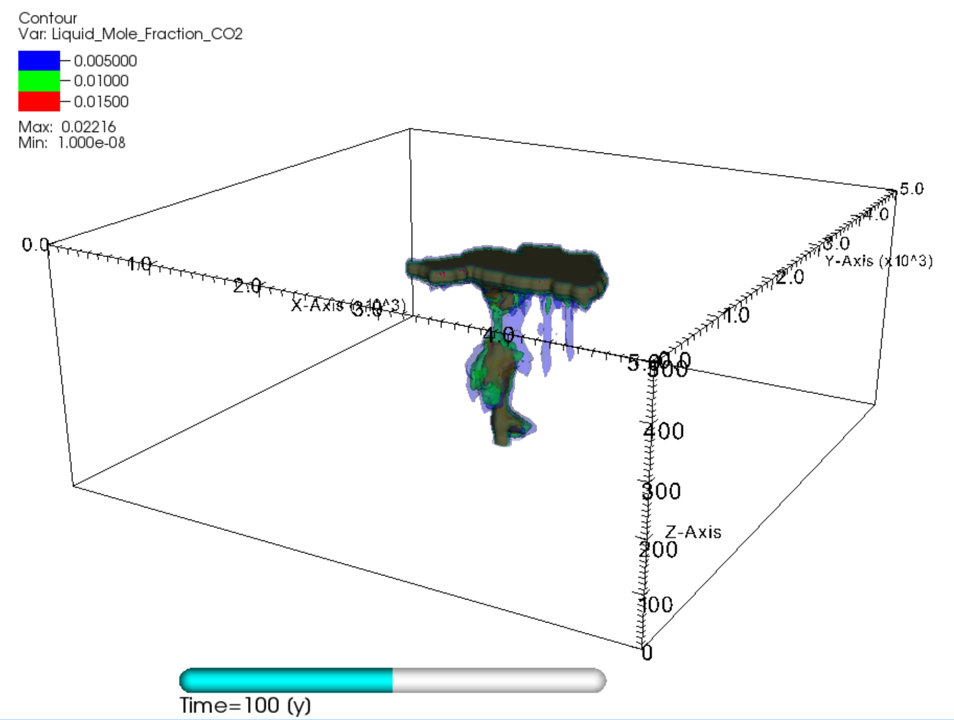
PFLOTRAN Scaling on Yellowstone



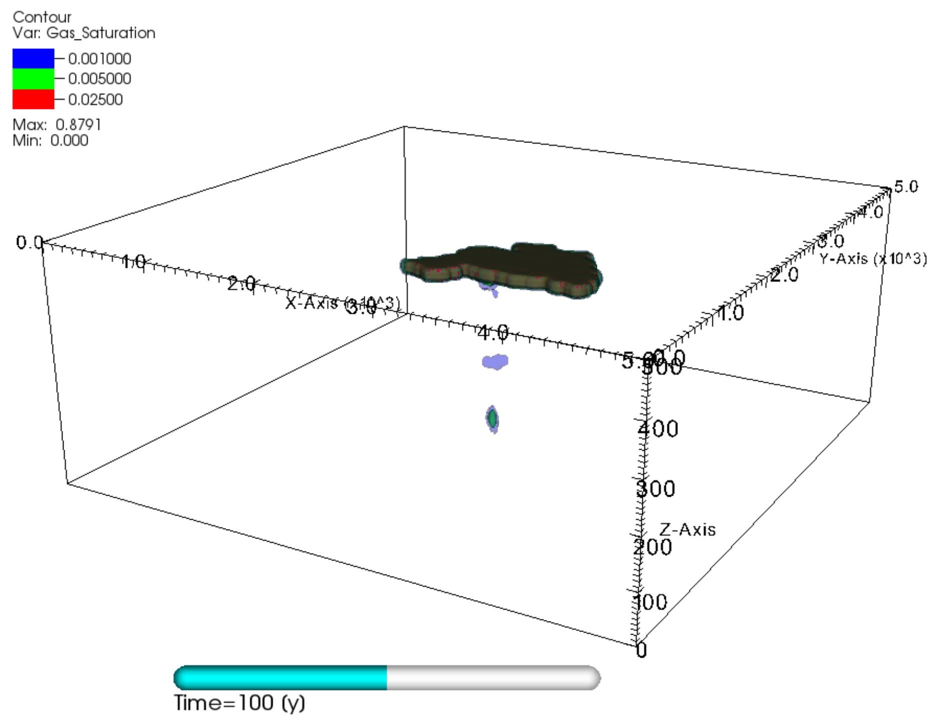
- *1-unit model (1.3M): a 5 year injection simulation;*

CO_2 Simulation: FHM (Var[lnk]=4.5)

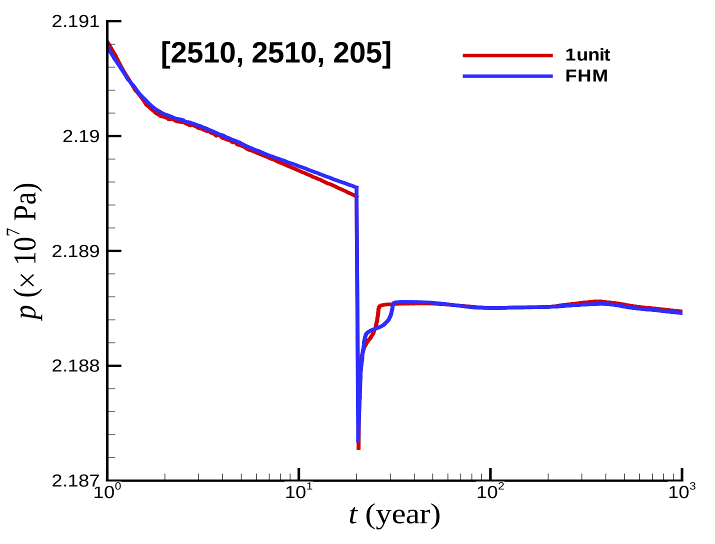
Dissolved CO_2

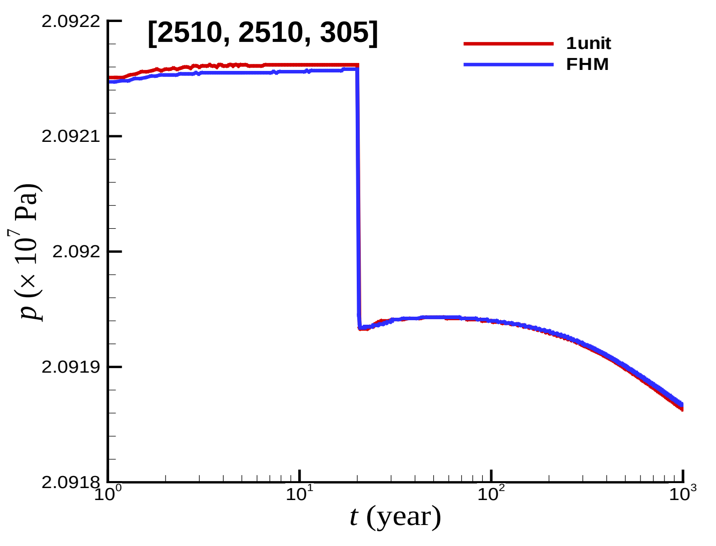


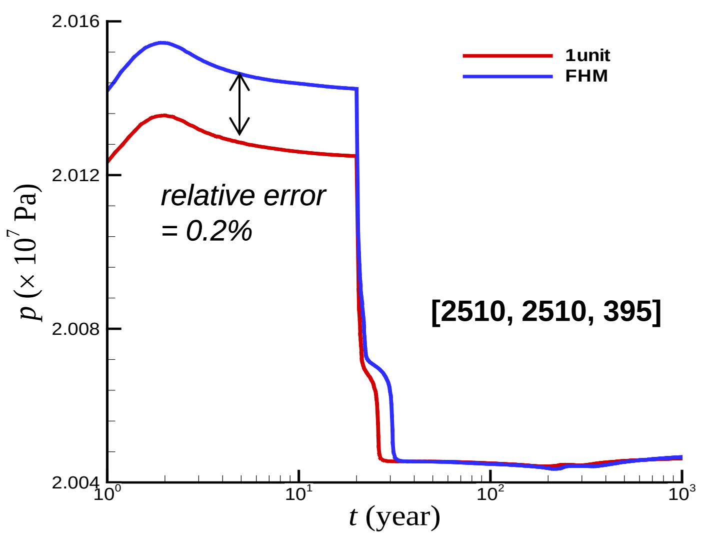
$scCO_2$

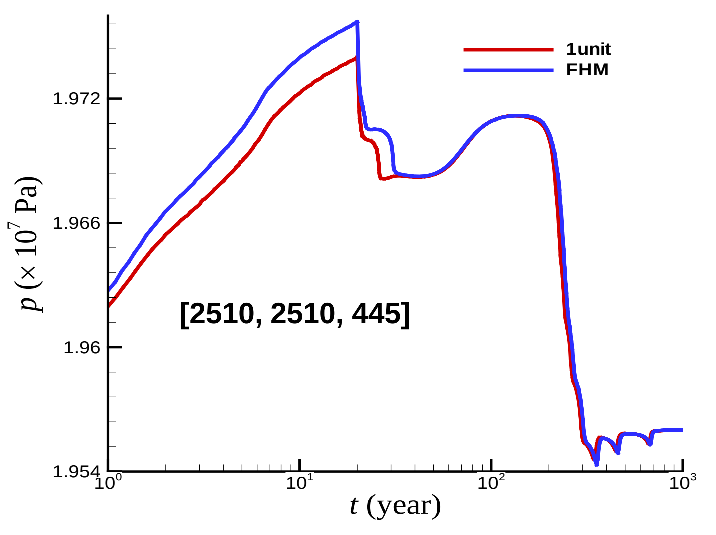


FHM v. 1-Unit Model: $\sigma^2_{\ln k}$=0.1

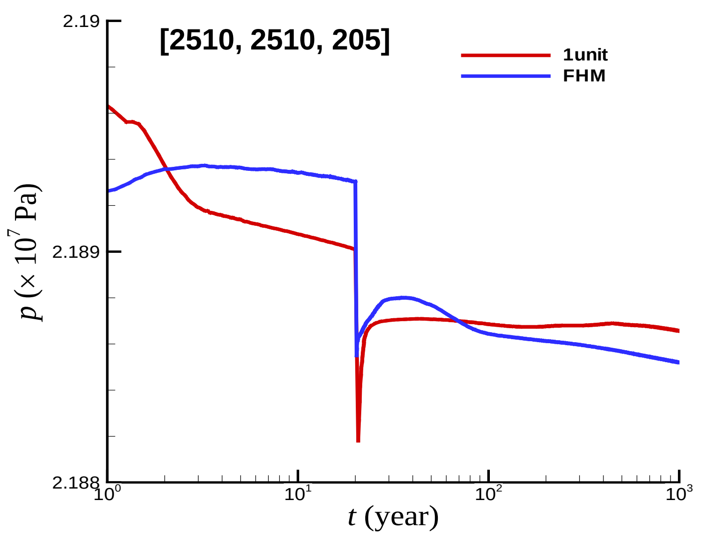


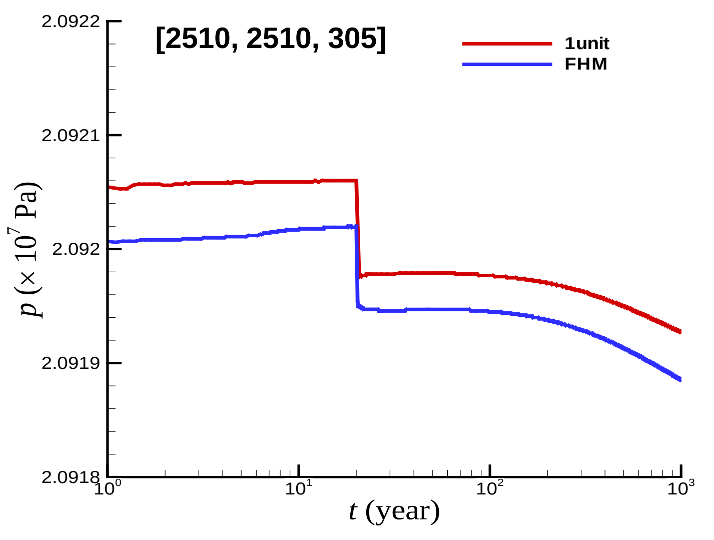


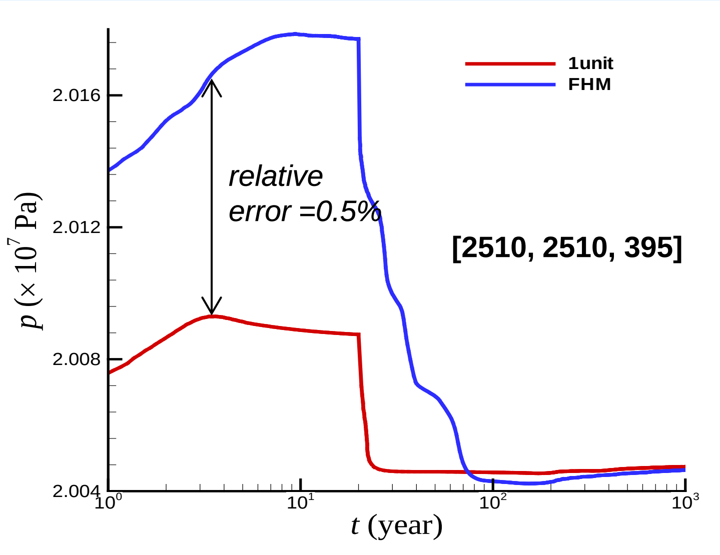

relative error = 0.2%

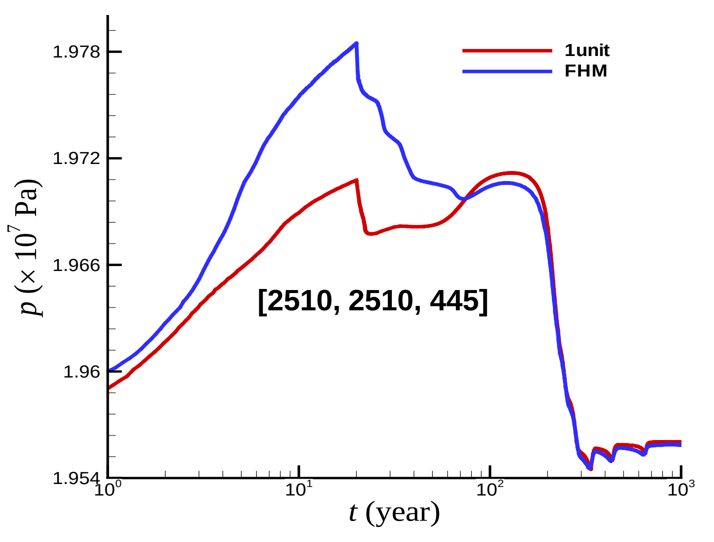


FHM v. 1-Unit Model: $\sigma^2_{\ln k}=4.5$









Potential Causes for Delay

CISL Daily Bulletin - August 19, 2013:

Yellowstone InfiniBand recabling set to start Monday, September 30

CISL, IBM, and Mellanox have set Monday, September 30, as the start date for the process of replacing the Yellowstone InfiniBand cables, previously announced in July. Users should plan for Yellowstone being out of service for up to three weeks from that date.