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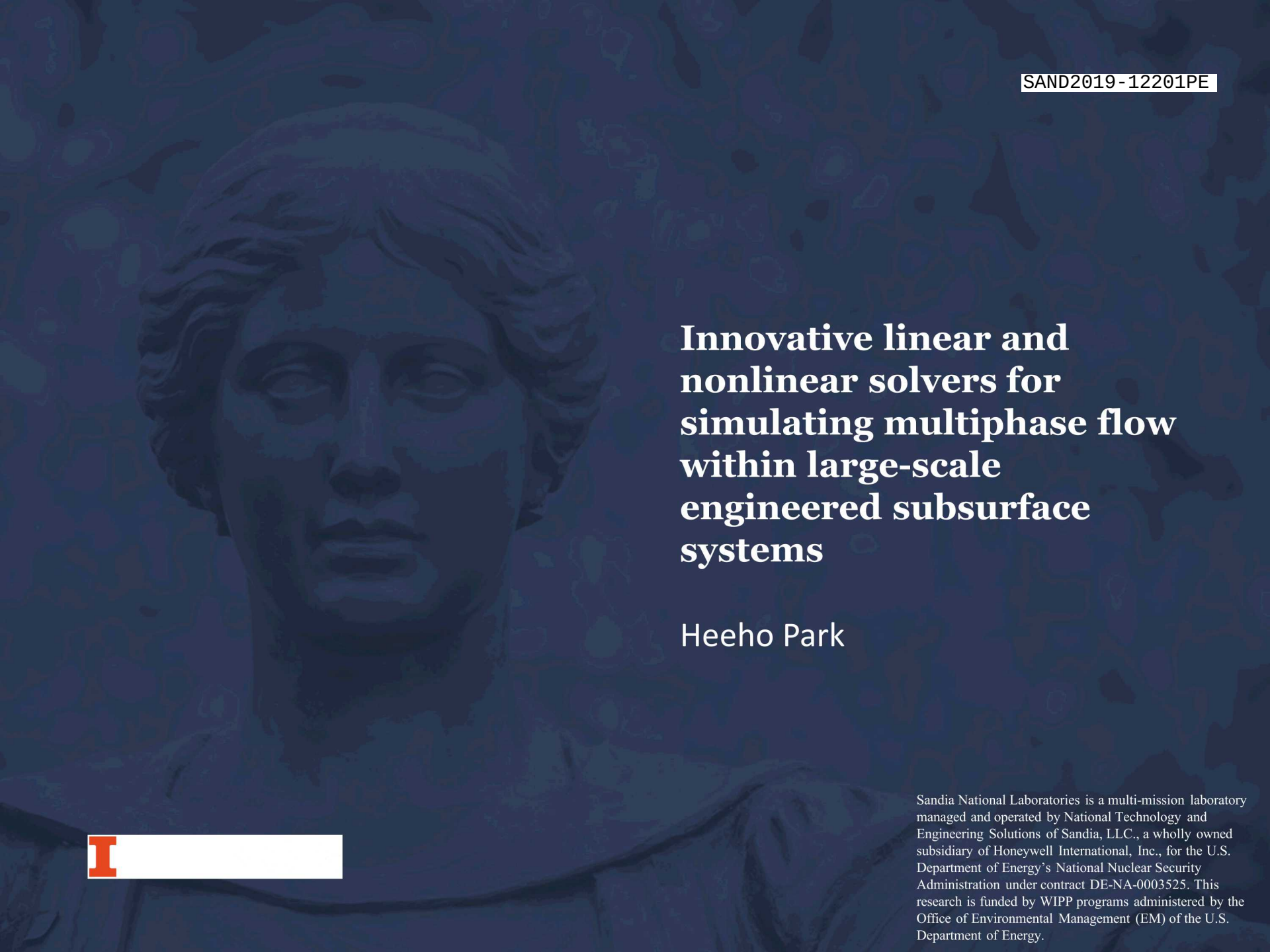

Innovative linear and nonlinear solvers for simulating multiphase flow within large-scale engineered subsurface systems

Heeho Park

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Thank you

- The committee
  - Al Valocchi
  - Glenn Hammond
  - Luke Olson
  - Praveen Kumar

Overview

- Introduction
- WIPP model engineered challenges
  - WIPP simulation domain and governing equations
  - Analysis of iterative linear solver failure
  - Preliminary results for advanced preconditioner
  - Proposed research
- GDSA model unsaturated zone challenges
  - GDSA simulation description and governing equations
  - Nonlinear solver oscillations
  - Preliminary results for advanced nonlinear solvers (trust region)
  - Proposed research

Introduction

Applications of multiphase porous media flow

- Applications
  - Nuclear waste repositories
  - Enhanced recovery of petroleum reservoirs
  - Contaminant remediation
  - Geothermal engineering
  - Carbon sequestration
- U.S. Department of Energy projects
  - Geologic Disposal Safety Assessment (GDSA) Framework
    - High-level waste impact analysis to the environment within 1 million years
  - Performance Assessment (PA) for Waste Isolation Pilot Plant (WIPP)
    - The probability and consequence of potential radionuclide releases from the repository to the accessible environment for 10,000 years

National Research Council et al. The Waste Isolation Pilot Plant: A Potential Solution for the Disposal of Transuranic Waste. National Academies Press, 1996

Introduction
PFLOTRAN

- Flow and reactive transport in porous media code
  - Developed by DOE
  - Modern Fortran (’08)
    - Open-source and community driven
  - PETSc Framework
    - Runs in massively parallel computing architectures, workstations, and laptops
    - Has been run on up to 2^{18} processor cores with 2 billion degrees of freedom
  - Backward Euler temporal discretization and finite volume spatial discretization
  - Non-isothermal/isothermal and immiscible/miscible multiphase
  - Multicomponent aqueous complexation, sorption, precipitation/dissolution
  - METIS/PARMETIS libraries for unstructured grids
  - HDF5 and ASCII files for input/output
- Suited for WIPP and GDSA projects

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WIPP Model
Background

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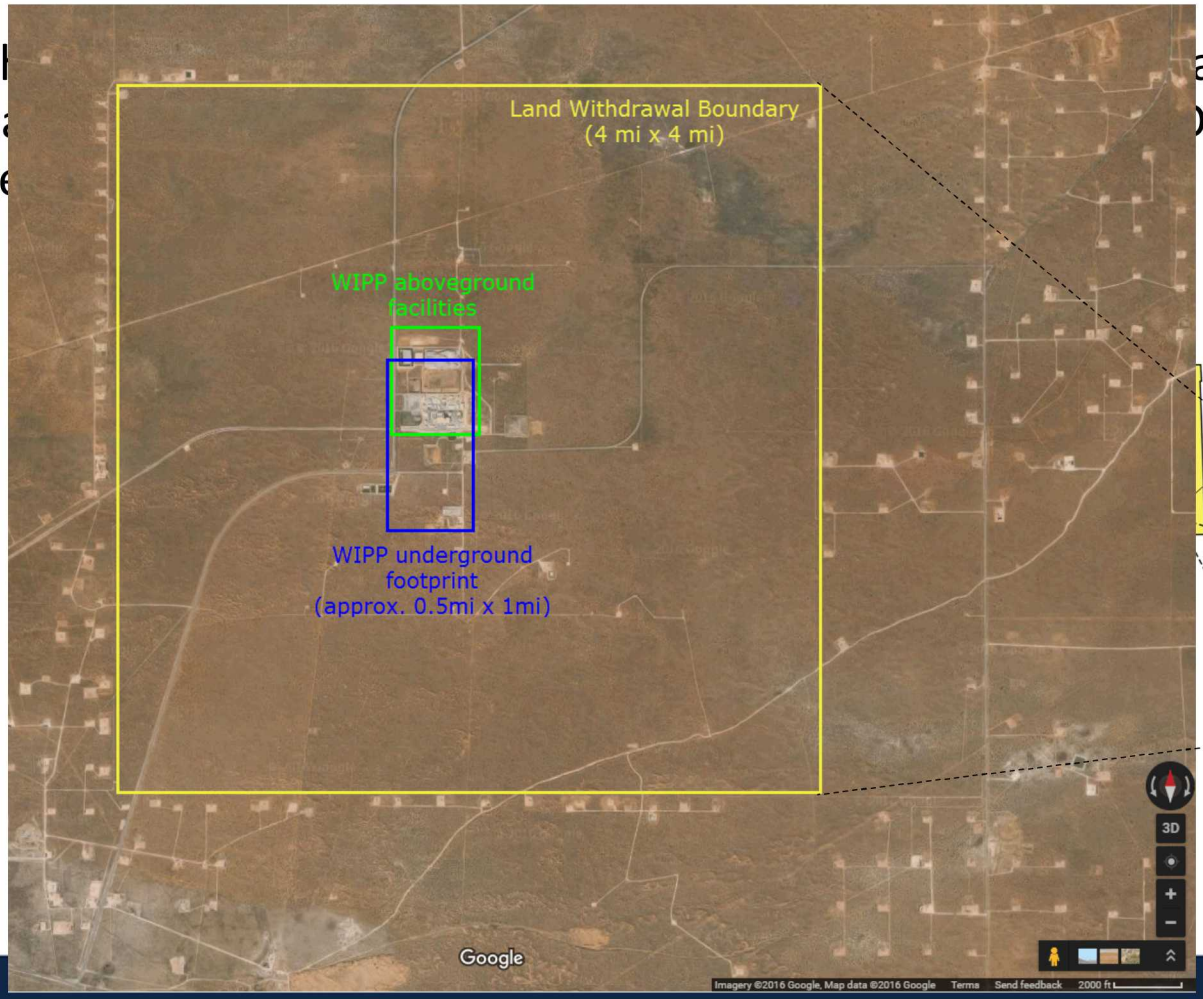
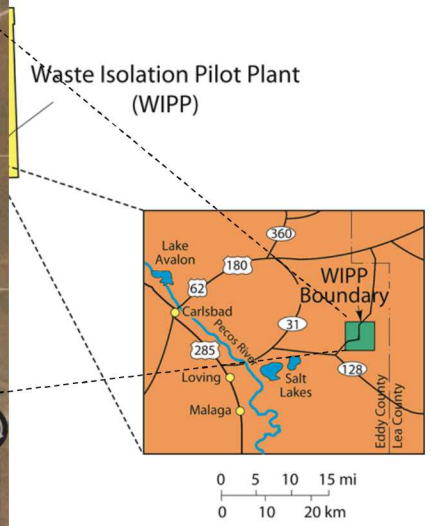
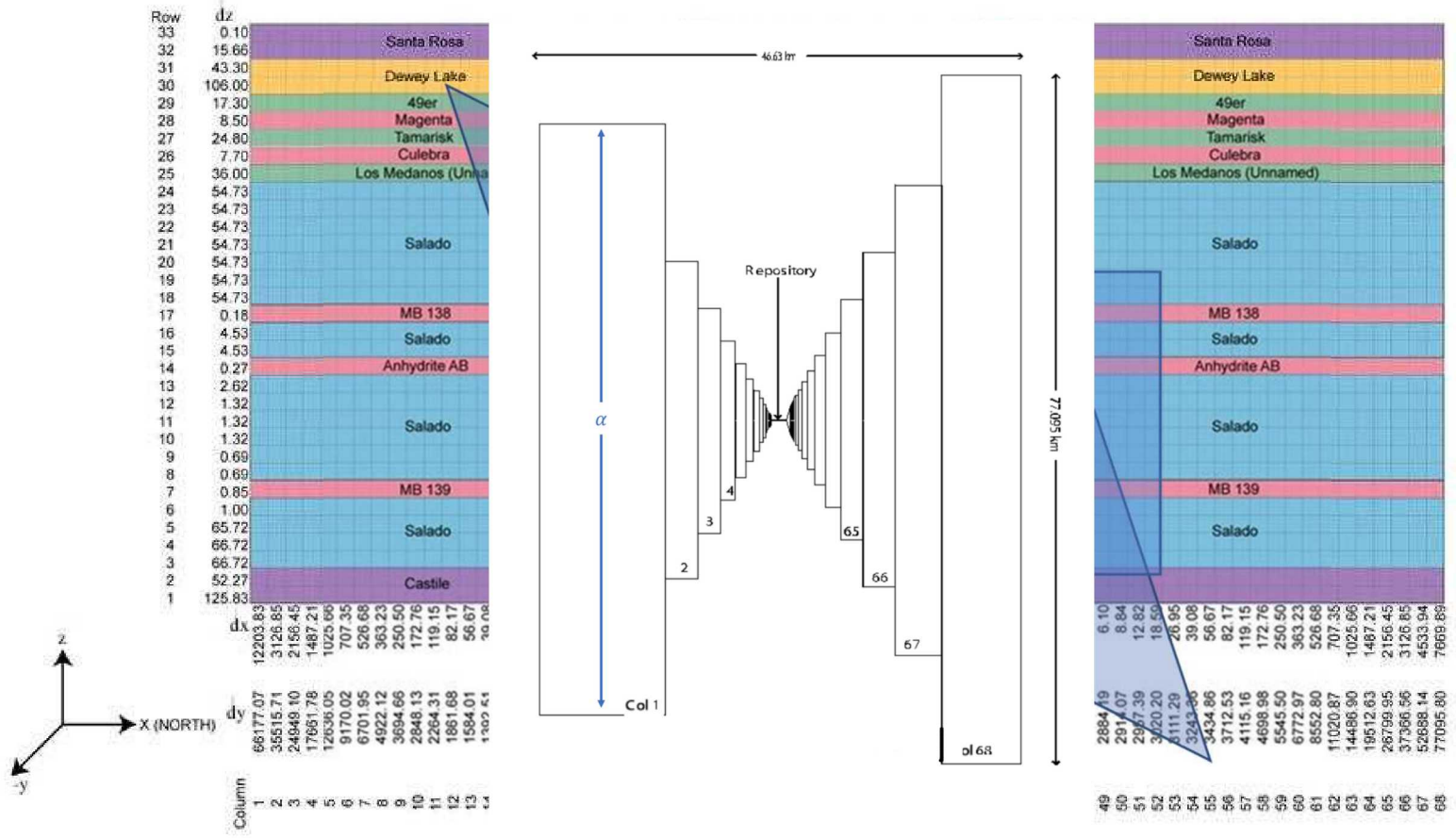




Kenneth S. Johnson (1978). Salt Deposits in the United States and Regional Geologic Characteristcs importan for Storage of Radioactive Waste.

WIPP Model
Background (2)



National Research Council et al. The Waste Isolation Pilot Plant: A Potential Solution for the Disposal of Transuranic Waste. National Academies Press, 1996

Emily R. Stein et al. Update to the pflotran-bragflo benchmark: Comparison of test cases and simulations on the 2-d flared grid. Technical report, Sandia National Labs.(SNL), Albuquerque, NM (United States), 2017.

WIPP Model

Isothermal immiscible two-phase porous flow

- Governing equations and constraints
  - All phases exist in all simulation grid cells
    - Liquid phase

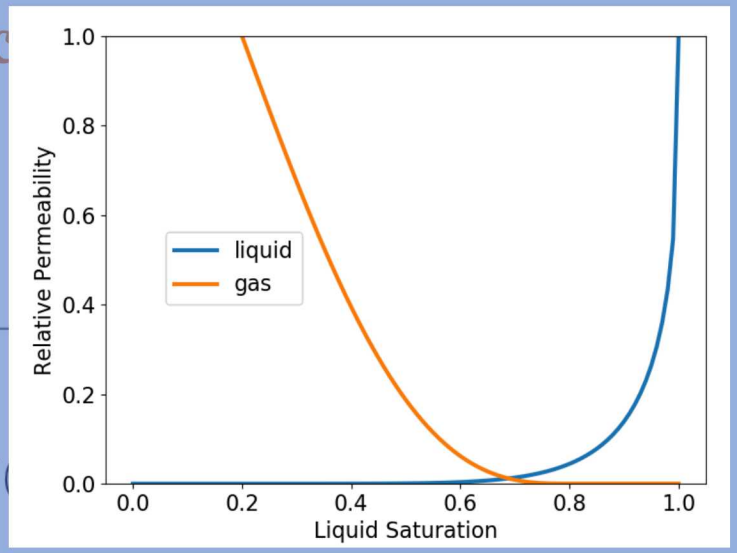
$$\frac{\partial}{\partial t}(\phi \rho_w s_w) = \nabla \cdot \left[\frac{\rho_w k k_{rw}}{\mu_w} (\nabla p_w - \rho_w g \hat{z}) \right] + Q_w,$$

    - Gas phase

$$\frac{\partial}{\partial t}(\phi \rho_g s_g) = \nabla \cdot \left[\frac{\rho_g k k_{rg}}{\mu_g} (\nabla p_g - \rho_g g \hat{z}) \right] + Q_g.$$

  - Constraints
    - Saturation $s_g + s_w = 1$
    - Capillary pressure $p_c = p_g - p_w$

WIPP Model



- van Genuchten water retention function
  - Capillary pressure

$$p_c(s_l) = \frac{1}{\alpha}\left(s_e^{-1/m} - 1\right)^{1/n}$$

$$s_e = \frac{s_l - s_{rl}}{1 - s_{rl}}$$

Relative permeability

$$k_{rl} = \sqrt{s_{el}}\left(1 - \left(1 - s_{el}^{1/m}\right)^m\right)^2 \qquad s_{el} = \frac{s_l - s_{rl}}{1 - s_{rl}}$$

$$k_{rg} = \sqrt{1 - s_{eg}}\left(1 - s_{eg}^{1/m}\right)^{2m} \qquad s_{eg} = \frac{s_l - s_{rl}}{1 - s_{rl} - s_{rg}}$$

WIPP Model

Newton-Raphson linearized system

- Newton-Raphson Iteration
  - Jacobian

$$J_F(u_n)(\delta u) = -F(u_n) \text{ and } u_{n+1} = u_n + \delta u$$

$$\rightarrow A\vec{x} = b \leftarrow$$

  - Convergence tolerance

$$||F(u_n)|| < \text{Tol}_{\text{absolute}}, \quad \frac{||F(u_n)||}{||F(u_0)||} < \text{Tol}_{\text{relative}}, \quad \text{and/or} \quad \frac{||u_n - u_{n-1}||}{||u_{n-1} - u_{n-2}||} < \text{Tol}_{\text{rel\_update}}$$

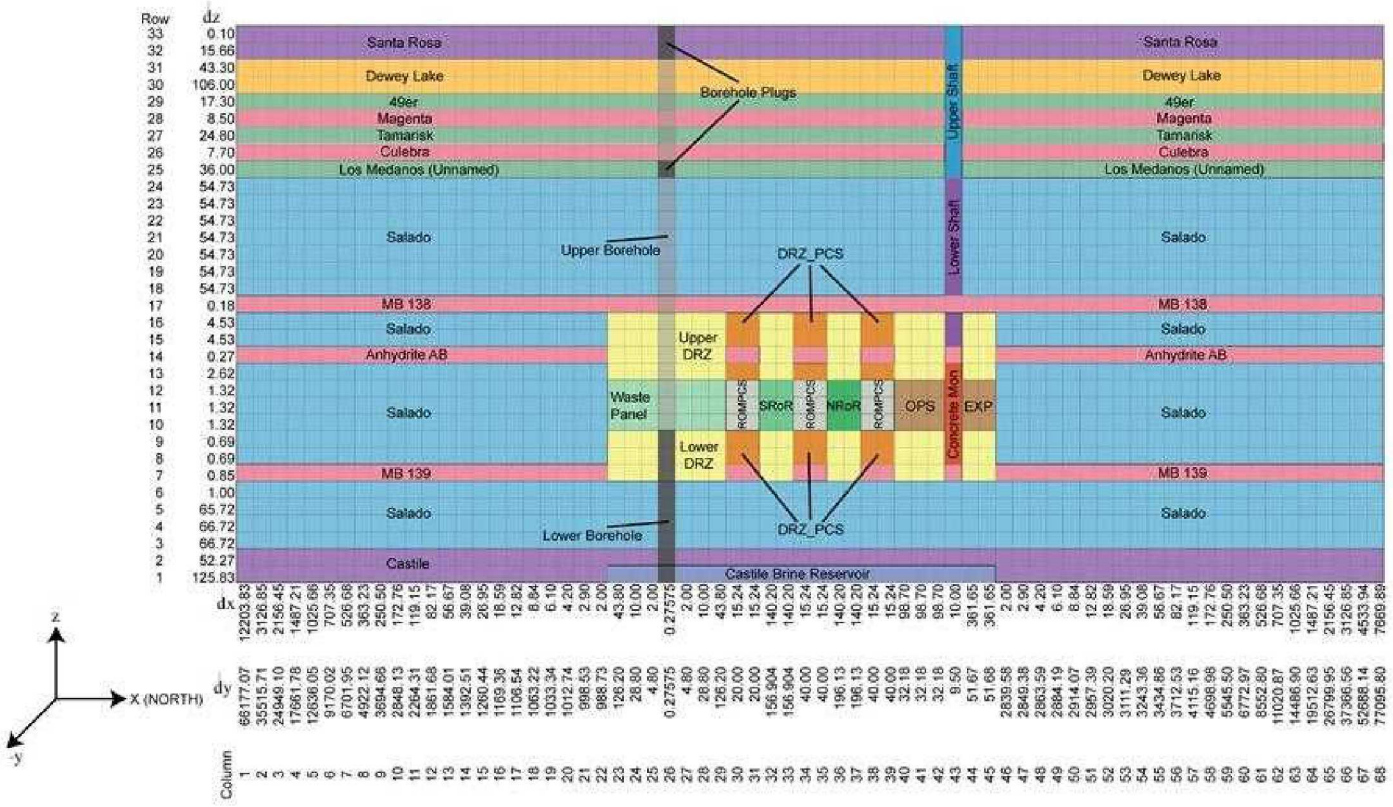
  - Linearized system of equations

$$\begin{bmatrix} \frac{\partial F_w}{\partial p_w} & \frac{\partial F_w}{\partial s_g} \\ \frac{\partial F_g}{\partial p_w} & \frac{\partial F_g}{\partial s_g} \end{bmatrix}_n \begin{bmatrix} \delta p_w \\ \delta s_g \end{bmatrix} = - \begin{bmatrix} F_w \\ F_g \end{bmatrix}_n$$

WIPP Model

2D WIPP simulation domain

- The 10,000-year simulations containing 2,244 elements were run



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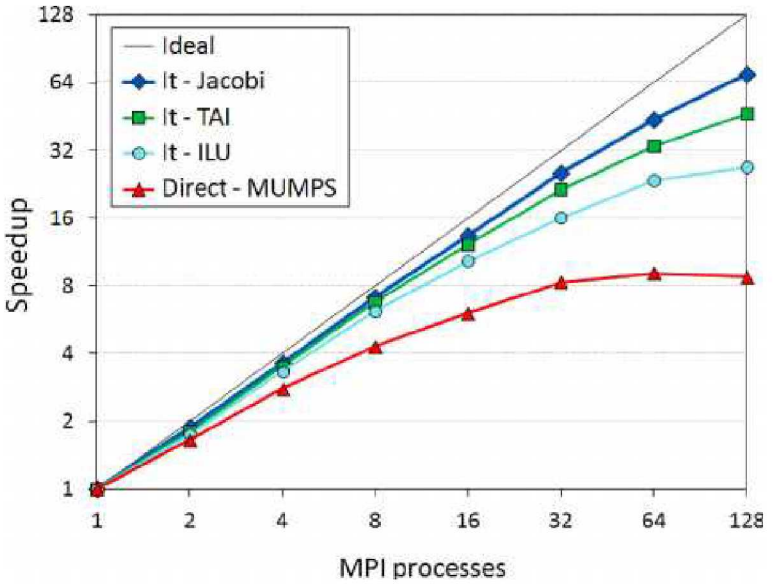
WIPP Model

Importance of scalability of iterative methods

- Direct solvers have limited scalability
  - 32 cores to have 8x speed up
  - 16 cores to have 5x speed up
- Conventional iterative solvers
  - Block Jacobi with ILU(0) breaks down
- Proposed research
  - Use tailored preconditioner
    - Algebraic multigrid (AMG)
    - Decoupling techniques
    - Constrained pressure residuals (CPR)

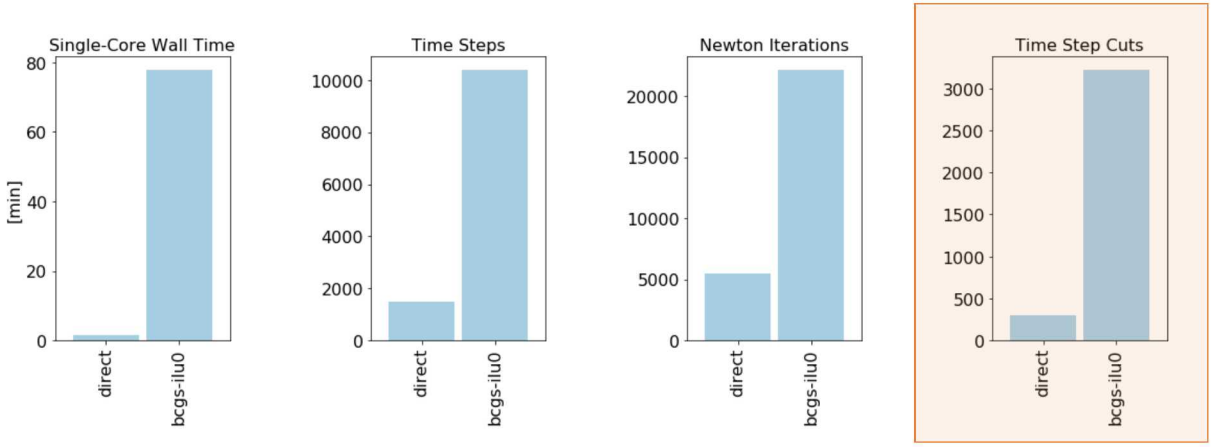


Vladimir Puzyrev and José María Cela. A review of block krylov subspace methods for multisource electromagnetic modelling. Geophysical Journal International, 202(2): 1241–1252, 2015

WIPP Model

Analysis of iterative linear solver failure (1 core)

- Direct solver vs. BiCGSTAB-ILU(0) comparison

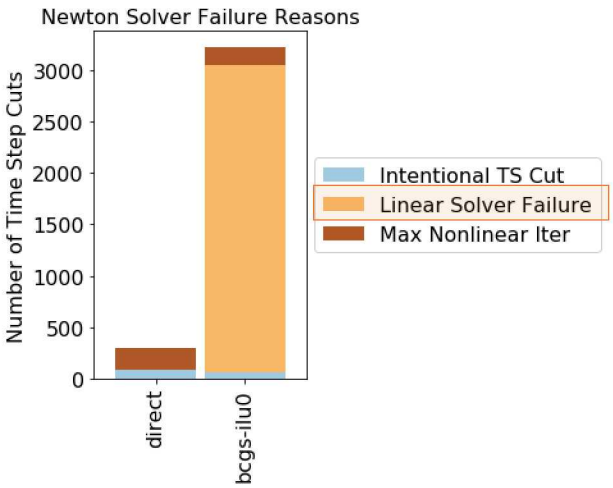


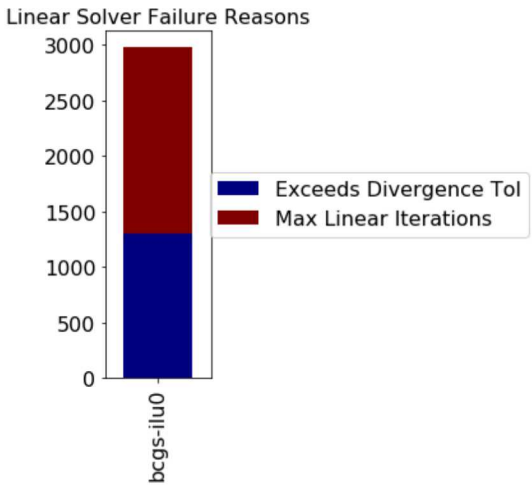
- There are many more wasted number of Newton iterations and linear iterations due to exceedingly high number of time step cuts.

WIPP Model

Analysis of iterative linear solver failure (1 core)

- Direct solver vs. BiCGSTAB-ILU(0) comparison
- Newton iteration failure due to **linear solver divergence**
- Newton iteration failure due to **linear solver reaching maximum iterations**

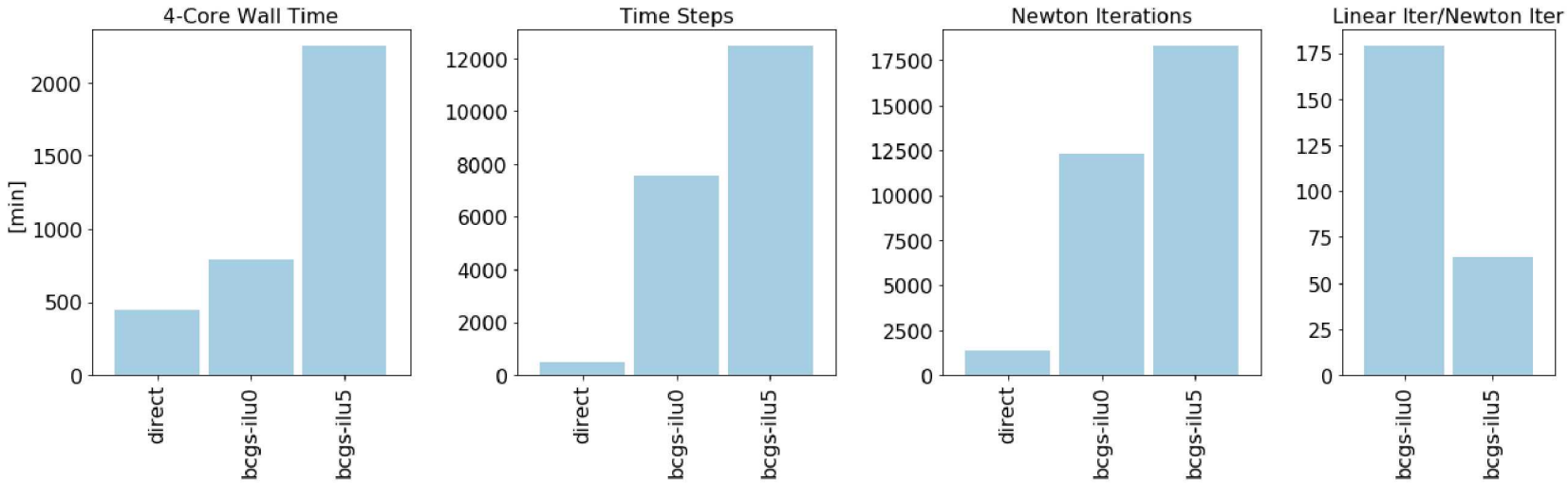




WIPP Model

Analysis of iterative linear solver failure (4 core)

- Direct, BiCGSTAB-ILU(0), BiCGSTAB-ILU(5)



ILU(5) experienced nearly 4000 linear solver break downs whereas ILU(0) has 1900 break downs. The break downs cause time step cuts and there is clearly a price looking at 4-Core Wall Time bar graph where ILU(0) simulation took approximately 800 minutes and ILU(5) simulation took about 2200 minutes.

WIPP Model

Analysis of iterative linear solver failure (4 core)

- Why? Block Jacobi ILU loses information.

Convergence criteria	Wall time [hr]	Time steps	Nonlinear iterations	Linear iterations	Waste linear iterations
3D WIPP Flared Grid (274k unknowns) – 10,000-year simulation BICGSTAB					
Direct – 4 cores	7.40	511	1379	-	-
ILU(5) – 1 core	3.50	514	1675	40732	1,223
ILU(5) – 4 cores	37.5	12,453	18,282	1,169,217	64,065
ILU(0) – 4 cores	13.3	7,544	12,331	2,202,112	137,301

WIPP Model

Iterative linear solver accuracy

Convergence criteria [4 cores]	Wall time [hr]	Time steps	Nonlinear iterations	Linear iterations	Waste linear iterations
3D WIPP Flared Grid (274k unknowns) – 10,000-year simulation BICGSTAB-ILU(0)					
Rel. Tol < 1.E-5	13.3	7544	12,331	2,202,112	137,301
Rel. Tol < 1.E-8	44.3	10,846	15,089	15,167,887	7,538,017
Rel. Tol < 1.E-12	73.5	20,000	21,484	26,635,131	8,014,421
Direct Solve	7.40	511	1379	-	-

- The accurate solver requires more linear iterations to reach the lower convergence criteria.
- The conventional preconditioner block Jacobi ILU(0) fails before it reaches the lower convergence criteria.

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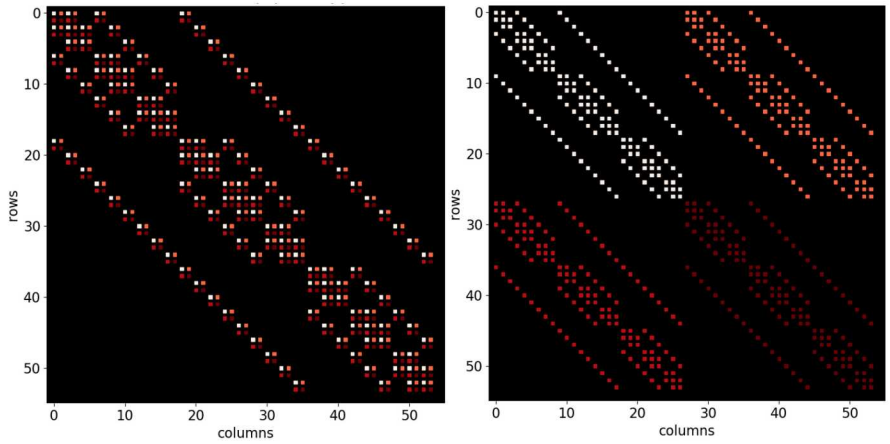
WIPP Model
Decoupling Techniques

- Stacked Jacobian format

$$A = \begin{bmatrix} A_{pp} & A_{ps} \\ A_{sp} & A_{ss} \end{bmatrix}$$

- Decoupling matrix

$$MAu = Mr.$$



- True-implicit pressure explicit saturation (IMPES)

$$M = \begin{bmatrix} I & -\mathrm{colsum}(A_{ps})\mathrm{colsum}(A_{ss})^{-1} \\ 0 & I \end{bmatrix}$$

- Quasi-IMPES

$$M = \begin{bmatrix} I & -\mathrm{diag}(A_{ps})\mathrm{diag}(A_{ss})^{-1} \\ 0 & I \end{bmatrix}$$

- Alternate-block-factorization (ABF)

$$M = \begin{bmatrix} \Lambda^{-1} & 0 \\ 0 & \Lambda^{-1} \end{bmatrix} \begin{bmatrix} D_{ss} & -D_{ps} \\ -D_{sp} & D_{pp} \end{bmatrix}$$

$$\Lambda = D_{pp}D_{ss} - D_{ps}D_{sp}.$$

WIPP Model
Decoupling Techniques

- Stacked Jacobian format

$$A = \begin{bmatrix} A_{pp} & A_{ps} \\ A_{sp} & A_{ss} \end{bmatrix}$$

- Decoupling matrix

$$MAu = Mr.$$

- Schur Complement

$$Ax + By = a$$
$$Cx + Ey = b$$

$$(A - BE^{-1}C)x = a - BE^{-1}b$$

- True-implicit pressure explicit saturation (IMPES) A_{pp}

$$A_{pp} - \text{colsum}(A_{ps})\text{colsum}(A_{ss})^{-1}(A_{sp})$$

- Quasi-IMPES A_{pp}

$$A_{pp} - \text{diag}(A_{ps})\text{diag}(A_{ss})^{-1}(A_{sp})$$

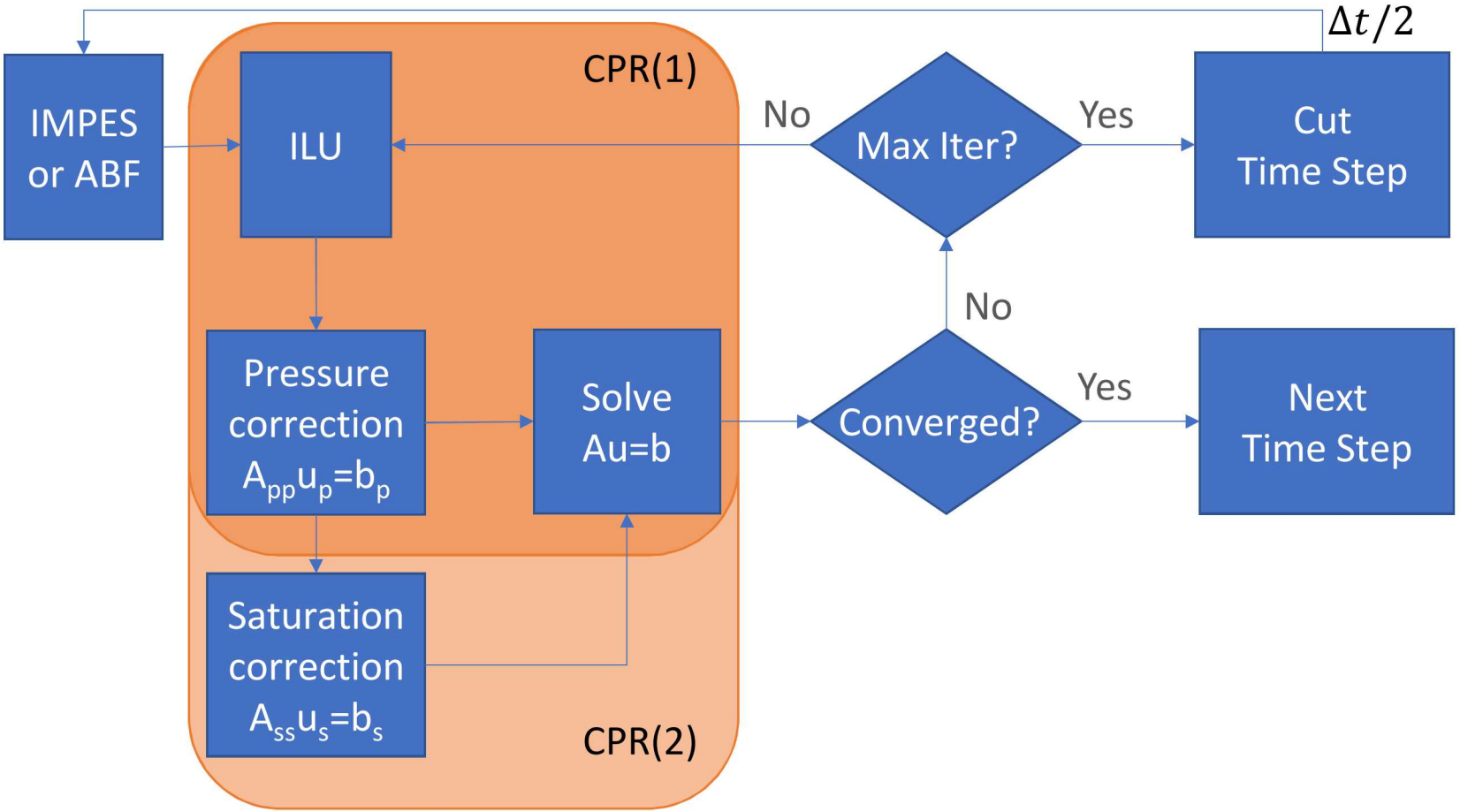
- ABF A_{pp}

$$(D^{-1}A)(Dx) = b$$

$$\Lambda^{-1}D_{ss}A_{pp} - \Lambda^{-1}D_{ps}A_{sp}$$

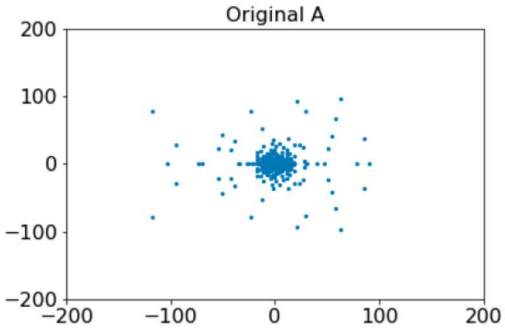
WIPP Model

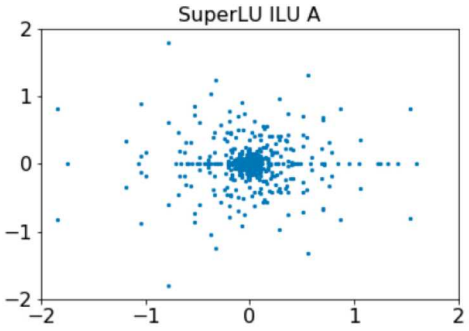
Constrained pressure residual algorithm

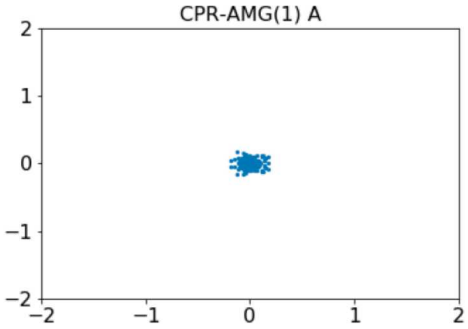


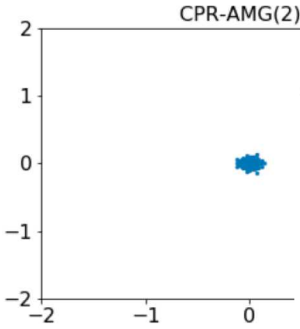
WIPP Model

Eigenvalue spectrum and condition number









- Preconditioners reduced the eigenvalue spectrum
- Preconditioners lowered condition numbers significantly

Preconditioner	Condition Number
Not preconditioned	3.39E+19
SuperLU ILU	4.59E+09
CPR-ABF-AMG(1)	2.74E+12
Two-iteration CPR-ABF-AMG(1)	2.96E+08
CPR-ABF-AMG(2)	1.93E+09
Two-iteration CPR-ABF-AMG(2)	4.11E+06

You may lose up to k digits of accuracy on top of what would be lost to the numerical method for Condition number $k(A) = 10^k$. Information can be lost if the matrix is scaled improperly.

WIPP Model

Preliminary results (PyAMG)

Solver	Preconditioner	Linear Iter (Max)	Wall Clock (Max) [s]
BiCGSTAB	ILU(0)	-	-
BiCGSTAB	SuperLU ILU	-	-
FGMRES	CPR-quasi-IMPES-AMG(1)	3.2 (4)	19.6 (23.9)
FGMRES*	CPR-true-IMPES-AMG(1)*	5.0 (9)	26.8 (53.0)
FGMRES	CPR-ABF-AMG(1)	3.2 (4)	12.8 (15.7)
FGMRES	CPR-ABF-AMG(2)	2.9 (3)	12.1 (14.4)

*Failed to converge in 1 of 9 matrices

This preliminary result shows that these matrices that could not be solved with ILU(0) preconditioners can be solved with just a few iterations with more optimized preconditioners.

The advantage of AMG in parallel compared to the block Jacobi ILU is that it **inherently requires communications** among all the nodes to restrict and interpolate which minimizes loss of information.

WIPP Model

Preliminary results (PFLOTRAN-BoomerAMG)

Methods	# of Cores	Wall Time [hr]	Time Steps	Nonlinear iterations	Linear iterations
3D WIPP Flared Grid (137k cells, 274k unknowns) – 10,005-year simulation					
BiCGSTAB-ILU(0)	4	43.7	13,545	22,689	12,223,601
FGMRES-CPR	4	3.2 (13.6x)	1,514	3,517	777,874
3D WIPP Paved Grid (261k cells, 522k unknowns) – 10,000-year simulation					
BiCGSTAB-ILU(0)	12	53.1	9,748	58,584	8,972,495
FGMRES-CPR	8	11.5 (6.6x)	2,441	2,844	1,795,677
3D WIPP Hexahedral Grid (1.6M cells, 3.2M unknowns) – 5-year simulation					
BiCGSTAB-ILU(0)	24	25.8	3,254	15,889	1,293,210
FGMRES-CPR	16	10.8 (3.5x)	3,218	15,922	234,109

Even with same convergence criteria FGMRES-CPR may provide more accurate solution. Generally, FGMRES-CPR is more robust, but I've observed in many other cases where it doesn't increase time step size and takes too long to complete the simulation.

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Proposed Research (WIPP)

Tasks and new questions

- New findings in peer-reviewed journals
  - Does the scaling of the coefficients in the linear system of equations impact linear solver convergence? And how significant is the impact?
  - What is the performance of different decoupling matrix techniques in parallel?
  - Does applying AMG to the saturation block further simplify the ill-conditioned matrix to outperform CPR with AMG only applied to the pressure block?
  - Is it possible to use a hybrid solver approach where the solver uses the conventional approach like BiCGSTAB-ILU(0) but if it fails, it switches to CPR-AMG preconditioner with FGMRES?
- Tasks
  - Restructure PFLOTRAN block structured matrix to a stacked matrix
  - Implement parallel CPR algorithms and matrix decoupling techniques
  - Develop several test problems for studying matrix scaling and hybrid conventional/CPR-AMG preconditioner

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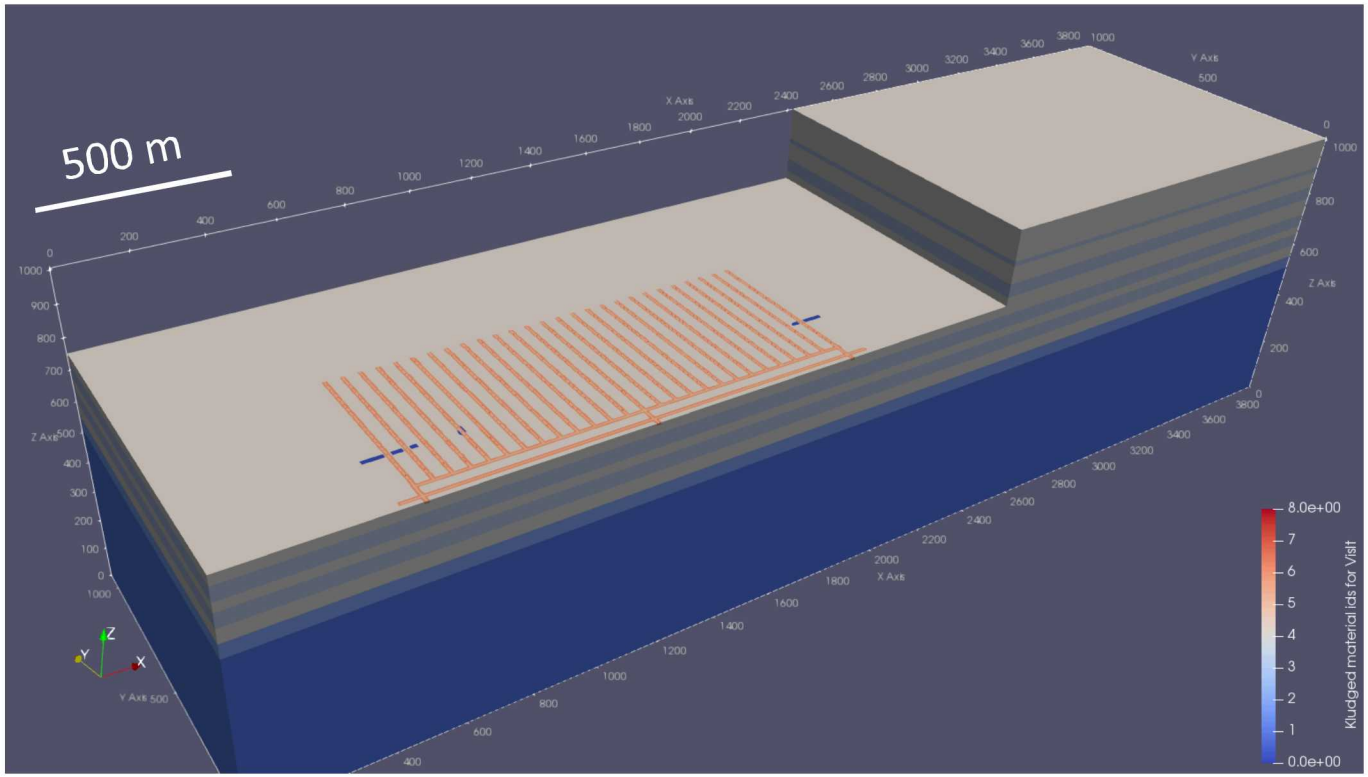
GDSA Model

Preliminary results (PFLOTRAN-BoomerAMG)

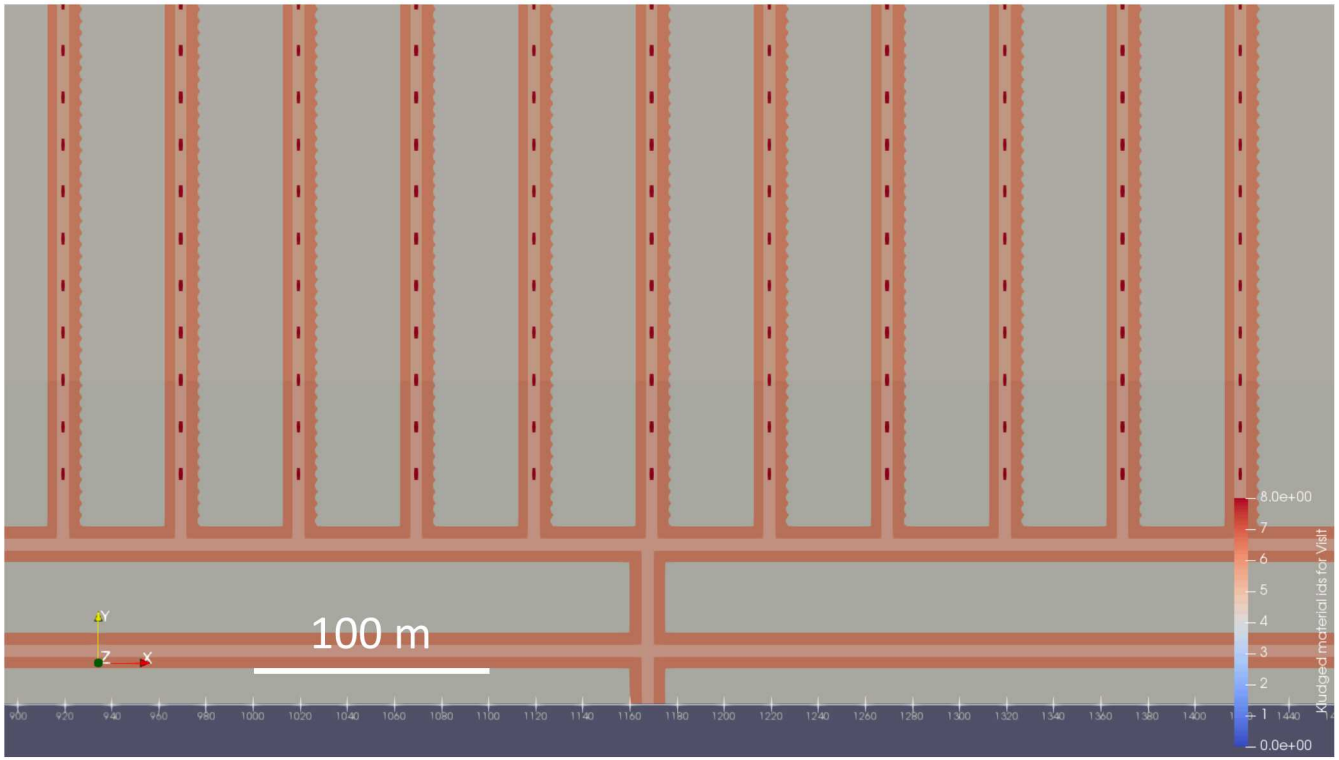
- GDSA UZ reference case (repository depth of 250m)



GDSA Model

Preliminary results (PFLOTRAN-BoomerAMG)

- Zoomed view of the waste drifts (dark reds represent waste packages)



GDSA Model

Non-isothermal miscible two-phase porous flow

- Governing equations and constraints
  - Each grid cell can have a different state depending on the phase presence
    - Water component (water and vapor)

$$\frac{\partial}{\partial t}\phi(s_l\rho_l x_w^l + s_g\rho_g x_w^g) + \nabla\cdot(\vec{q_l}\rho_l x_w^l + \vec{q_g}\rho_g x_w^g - \phi s_l D_l\rho_l\nabla x_w^l - \phi s_g D_g\rho_g\nabla x_w^g) = Q_w$$

    - Air component (air and dissolved air)

$$\frac{\partial}{\partial t}\phi(s_l\rho_l x_a^l + s_g\rho_g x_a^g) + \nabla\cdot(\vec{q_l}\rho_l x_a^l + \vec{q_g}\rho_g x_a^g - \phi s_l D_l\rho_l\nabla x_a^l - \phi s_g D_g\rho_g\nabla x_a^g) = Q_a$$

    - Energy

$$\sum_{\alpha=l,g}\left[\frac{\partial}{\partial t}(\phi s_\alpha\rho_\alpha U_\alpha) + \nabla\cdot(\vec{q_\alpha}\rho_\alpha H_\alpha)\right] + \frac{\partial}{\partial t}\left(((1-\phi)\rho_{rock}C_pT) - \nabla\cdot(\kappa\nabla T)\right) = Q$$

    - Constraints

$$\sum_\alpha s_\alpha = 1 \qquad \sum_i x_i^\alpha = 1 \qquad p_c = p_g - p_l \qquad U_\alpha = H_\alpha - \frac{p_\alpha}{\rho_\alpha}$$

GDSA Model

Linearized system of the three states

- Single-phase liquid state

$$\begin{bmatrix} \frac{\partial F_{p_l}}{\partial p_l} & \frac{\partial F_{p_l}}{\partial x_a^l} & \frac{\partial F_{p_l}}{\partial T} \\ \frac{\partial F_{x_a^l}}{\partial p_l} & \frac{\partial F_{x_a^l}}{\partial x_a^l} & \frac{\partial F_{x_a^l}}{\partial T} \\ \frac{\partial F_T}{\partial p_l} & \frac{\partial F_T}{\partial x_a^l} & \frac{\partial F_T}{\partial T} \end{bmatrix}_n \begin{bmatrix} \delta p_l \\ \delta x_a^l \\ \delta T \end{bmatrix} = - \begin{bmatrix} F_{p_l} \\ F_{x_a^l} \\ F_T \end{bmatrix}_n$$

- Two-phase state

$$\begin{bmatrix} \frac{\partial F_{p_g}}{\partial p_g} & \frac{\partial F_{p_g}}{\partial s_g} & \frac{\partial F_{p_g}}{\partial T} \\ \frac{\partial F_{s_g}}{\partial p_g} & \frac{\partial F_{s_g}}{\partial s_g} & \frac{\partial F_{s_g}}{\partial T} \\ \frac{\partial F_T}{\partial p_g} & \frac{\partial F_T}{\partial s_g} & \frac{\partial F_T}{\partial T} \end{bmatrix}_n \begin{bmatrix} \delta p_g \\ \delta s_g \\ \delta T \end{bmatrix} = - \begin{bmatrix} F_{p_g} \\ F_{s_g} \\ F_T \end{bmatrix}_n$$

- Single-phase gas state

$$\begin{bmatrix} \frac{\partial F_{p_g}}{\partial p_g} & \frac{\partial F_{p_g}}{\partial x_w^g} & \frac{\partial F_{p_g}}{\partial T} \\ \frac{\partial F_{x_w^g}}{\partial p_g} & \frac{\partial F_{x_w^g}}{\partial x_w^g} & \frac{\partial F_{x_w^g}}{\partial T} \\ \frac{\partial F_T}{\partial p_g} & \frac{\partial F_T}{\partial x_w^g} & \frac{\partial F_T}{\partial T} \end{bmatrix}_n \begin{bmatrix} \delta p_g \\ \delta x_w^g \\ \delta T \end{bmatrix} = - \begin{bmatrix} F_{p_g} \\ F_{x_w^g} \\ F_T \end{bmatrix}_n$$

- A single solution vector can have all the different states presented here
- Each Newton iteration linear solve can have a different set of primary variables compared to the previous iterations.

$$J_F(u_n)(\delta u) = -F(u_n) \text{ and } u_{n+1} = u_n + \delta u$$

$$Ax = b$$

Overview

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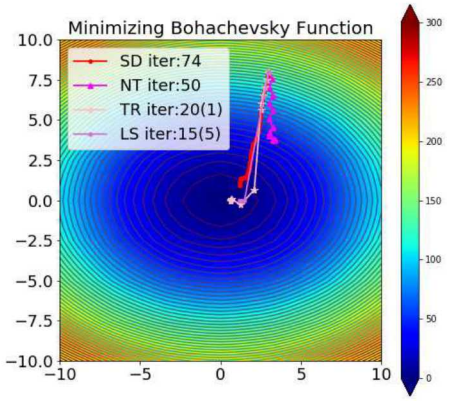
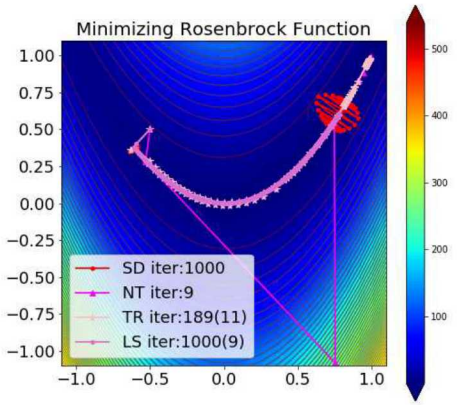
GDSA Model

Iterative nonlinear solver oscillations

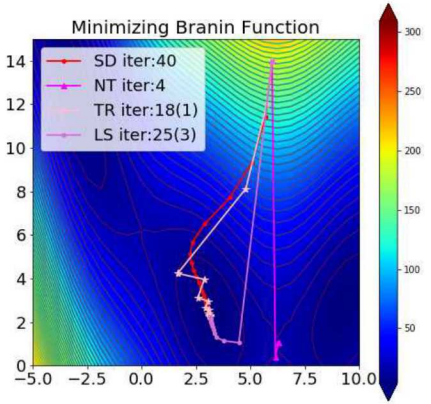
- Basic Newton iteration failures
  - **Infinity norm oscillations**
  - **L2-norm oscillations**
  - **State transition oscillations**
- Reasons
  - Discontinuities from the phase state changes
  - Inflection points in nonlinear equations
- Behaviors on test functions
  - Bohachevsky f(x,y)
  - Rosenbrock f(x,y)
  - Branin f(x,y)



Oscillations



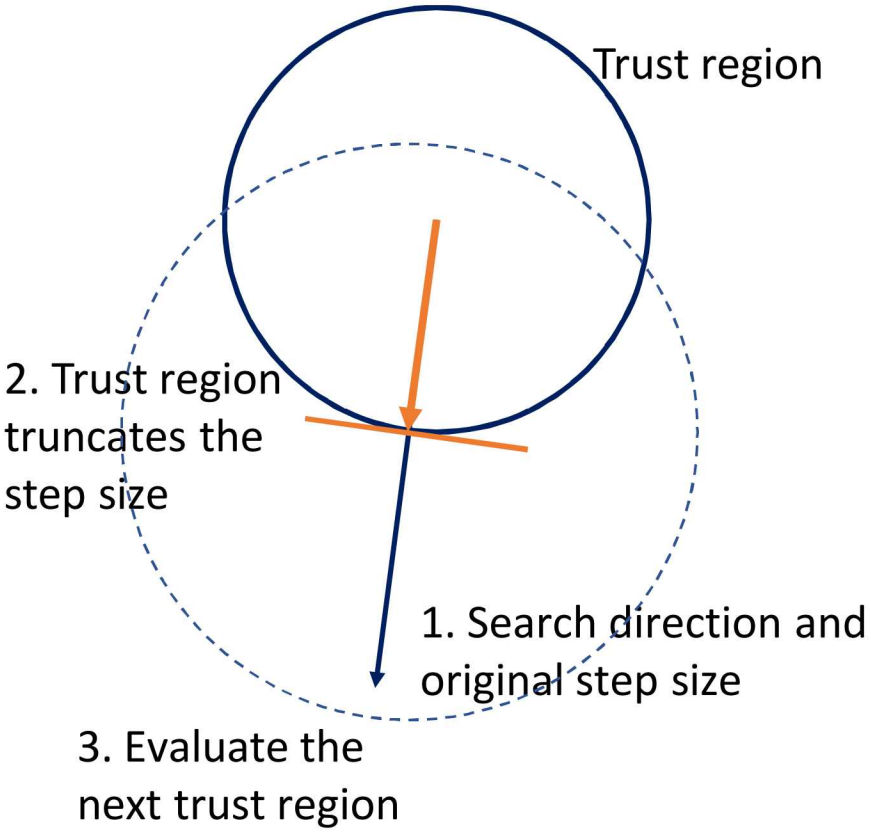
Overshoot

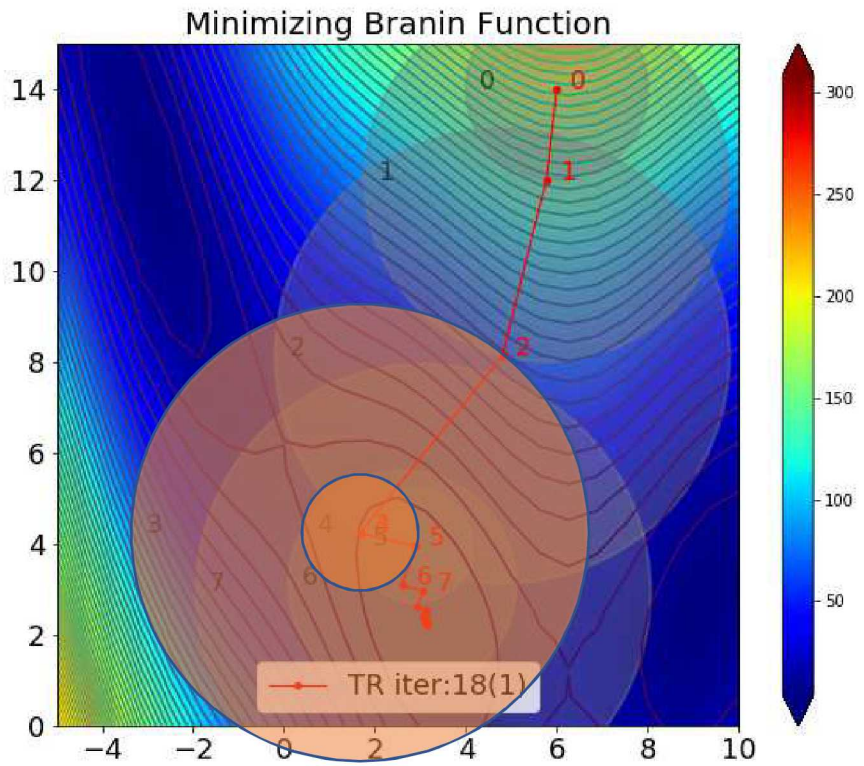


Saddle point

GDSA Model

Newton Trust Region





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GDSA Model

Newton Trust Region Preliminary Results

Nonlinear Solver	Time Steps	Nonlinear Iter	Linear Iter	Wall Clock
1D Capillary Barrier (Figure 17, 400 unknowns, 1 core)				
Newton's method(NT)	1100	4000	4000	14 sec
Trust Region(TR)	2800	3400	3600	17 sec
3D Coarse Unsaturated Zone 24-PWR Repository (190k unknowns, 8 cores)				
NT	1300	1500	420000	48 min
TR	430	710	180000	29 min
3D Coarse UZ 37-PWR Repository (190k unknowns, 8 cores)				
NT	2300	19000	1200000	180 min
TR	830	3400	310000	52 min
3D Fine 4-by-4 Array 37-PWR Waste Packages (120k unknowns, 16 cores)				
NT	8500	9400	220000	34 min
TR	2600	2600	68000	11 min

[+]All results are rounded to 2 digits; Pressurized water reactor (PWR)

- In all cases, Newton trust region performed 2 to 3 times better than basic Newton except 1D, because TR is algorithmically more complicated.

GDSA Model

Newton Trust Region Preliminary Results

Nonlinear Solver	Simulation Time	Wall Clock	ST/WC
3D Fine UZ 12-PWR Repository (313k unknowns, 8 core)			
Newton's method(NT)*	300 y	24 h	13 y/hr
Trust Region(TR)	1000000 y	4.7h	210000 y/hr
3D Fine UZ 24-PWR Repository (313k unknowns, 8 core)			
Newton's method(NT)*	444 y	7.2 h	62.0 y/hr
Trust Region(TR)	1000000 y	20.3h	49000 y/hr
3D Fine UZ 37-PWR Repository (313k unknowns, 8 core)			
Newton's method(NT)*	90 y	1.0 h	90 y/hr
Trust Region(TR)	1000000 y	27.9	36000 y/hr

+All results are rounded to 2 digits

*Failed to complete the simulation due to divergence and oscillation

- In all cases, TR was able to complete the 1 million year simulations where the best basic Newton's method could reach was 300 years near the peak temperature of the nuclear waste repository

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Proposed Research (GDSA)

Tasks and new questions

- New findings in peer-reviewed journals
  - Is solving the TR subproblem more robust and efficient than the current implementation of TR in PETSc?
  - Is applying AMG to either the gas or liquid pressure block robust enough to outperform the conventional preconditioner for non-isothermal miscible flow?
  - AMG has many tuning parameters. What are the best setting for the pressure, saturation, and pressure blocks?
  - How do we best determine what preconditioners, linear solvers, and nonlinear solvers to use for a given simulation?
- Tasks
  - Develop the full algorithm and work flow to use CPR-AMG preconditioner for the linear solver and TR as the nonlinear solver in parallel for primary variable switching non-isothermal miscible flow.
  - Modify higher order nonlinear solvers that properly handles state changes for non-isothermal miscible flows in parallel.

Thank you

- The committee
  - Al Valocchi
  - Glenn Hammond
  - Praveen Kumar
  - Luke Olson

Backup slides

- Linear solver failures output
- Nonlinear solver oscillations output
- TR algorithm
- TR equations

WIPP Model

Iterative linear solver failure

- Newton iteration failure due to **linear solver divergence**

```
== WIPP IMMISCIBLE MULTIPHASE FLOW ============================================
    Rsn: ---L---|--  789 -1.13E+00    0 -3.01E-03    0  0.00E+00    0  0.00E+00
  0 2r: 1.95E+00 2x: 0.00E+00 2u: 0.00E+00 ir: 1.13E+00 iu: 0.00E+00 rsn:   0
    Rsn: ---LGPS|-- 1930  1.07E+02 1114  2.03E+01 2001 -3.24E-02  843  7.04E-03
  1 2r: 1.11E+02 2x: 3.85E+08 2u: 2.76E+05 ir: 1.07E+02 iu: 5.51E+04 rsn:   0
 -> Cut time step: snes= -3 icut=  1[282] t=  1.01258E+03 dt=  1.55405E+00
Newton solver reason: The linear solver failed.
Linear solver reason: The linear solver diverged due to dtol based on the
equation: norm(r) >= dtol*norm(b) where r = b-Ax for the linear system Ax=b
within the Krylov solver. norm(r) = 7.2976E+00).
    Rsn: ---L---|--  789 -5.64E-01    0 -1.51E-03    0  0.00E+00    0  0.00E+00
  0 2r: 9.77E-01 2x: 0.00E+00 2u: 0.00E+00 ir: 5.64E-01 iu: 0.00E+00 rsn:   0
    Rsn: ---LGPS|-- 1930  1.47E+01 1114  4.14E+00 2001 -1.64E-02  843  4.03E-03
  1 2r: 1.58E+01 2x: 3.85E+08 2u: 1.41E+05 ir: 1.47E+01 iu: 2.80E+04 rsn:   0
    Rsn: ----G--|--    0  3.13E-02  910 -1.28E-01    0 -1.00E-04    0 -5.67E-05
  2 2r: 1.34E-01 2x: 3.85E+08 2u: 2.53E+03 ir: 1.28E-01 iu: 3.30E+02 rsn:   0
    Rsn: -------|--    0 -1.45E-05    0 -3.07E-05    0  2.76E-07    0 -5.92E-08
  3 2r: 4.19E-05 2x: 3.85E+08 2u: 3.95E+00 ir: 3.07E-05 iu: 4.55E-01 rsn: 999

Step   1190 Time=  1.01413E+03 Dt=  1.55405E+00 [y] snes_conv_reason:  999
 newton =   4 [    4038] linear =   676 [    490584] cuts =  1 [ 282]
 --> SNES Linear/Non-Linear Iterations =          578  /           3
 --> SNES Residual:   4.190453E-05  1.867403E-08  3.073555E-05
 --> max chng: dpl=   2.8014E+04 dpg=   2.8014E+04 dsg=   4.0624E-03
```

WIPP Model

Iterative linear solver failure

- Newton iteration failure due to **linear solver reaching maximum iterations**

```
== WIPP IMMISCIBLE MULTIPHASE FLOW ============================================
    Rsn: ---LG--|--  789 -2.03E+00 1114 -1.88E-02    0  0.00E+00    0  0.00E+00
  0 2r: 2.61E+00 2x: 0.00E+00 2u: 0.00E+00 ir: 2.03E+00 iu: 0.00E+00 rsn:   0
    Rsn: ---LGPS|--  706 -8.97E+01 1114 -3.67E+02 2001 -2.84E-02  777 -1.01E-02
  1 2r: 4.20E+02 2x: 3.85E+08 2u: 2.74E+05 ir: 3.67E+02 iu: 4.65E+04 rsn:   0
    Rsn: ---LG-S|--  706  1.11E+01  910  2.13E+01    0  2.12E-03  777  6.36E-03
  2 2r: 3.20E+01 2x: 3.85E+08 2u: 1.19E+05 ir: 2.13E+01 iu: 1.12E+04 rsn:   0
 -> Cut time step: snes= -3 icut=  1[289] t=  1.06902E+03 dt=  2.57096E+00
Newton solver reason: The linear solver failed.
Linear solver reason: The linear solver took too many iterations, beyond the
allowable number set by maxits (10000).
    Rsn: ---L---|--  789 -1.01E+00    0 -9.39E-03    0  0.00E+00    0  0.00E+00
  0 2r: 1.30E+00 2x: 0.00E+00 2u: 0.00E+00 ir: 1.01E+00 iu: 0.00E+00 rsn:   0
    Rsn: ---LGPS|-- 1930  5.60E+00 1114  8.21E+00 2001 -1.47E-02  789 -4.62E-03
  1 2r: 1.23E+01 2x: 3.85E+08 2u: 1.56E+05 ir: 8.21E+00 iu: 2.39E+04 rsn:   0
    Rsn: ----G--|--    0  7.37E-03  910 -2.48E-02    0  7.23E-06    0 -7.56E-06
  2 2r: 3.00E-02 2x: 3.85E+08 2u: 2.58E+02 ir: 2.48E-02 iu: 3.23E+01 rsn:   0
    Rsn: -------|--    0 -1.99E-05    0  7.22E-05    0 -2.83E-08    0 -1.24E-08
  3 2r: 8.23E-05 2x: 3.85E+08 2u: 9.01E-01 ir: 7.22E-05 iu: 1.11E-01 rsn: 999

Step   1214 Time=  1.07160E+03 Dt=  2.57096E+00 [y] snes_conv_reason:  999
 newton =   5 [    4123] linear =  6088 [    543639] cuts =  1 [ 289]
 --> SNES Linear/Non-Linear Iterations =          788  /            3
 --> SNES Residual:   8.230478E-05  3.667771E-08  7.217836E-05
 --> max chng: dpl=   2.3864E+04 dpg=   2.3864E+04 dsg=   4.6149E-03
```

GDSA Model

Iterative nonlinear solver oscillations

- Newton iteration failure due to **infinity norm oscillation**

```
 0 2r: 5.35E-03 2x: 0.00E+00 2u: 0.00E+00 ir: 8.83E-05 iu: 0.00E+00 rsn:   0
 1 2r: 1.38E-04 2x: 3.90E+08 2u: 6.55E+00 ir: 1.12E-04 iu: 2.33E+00 rsn:   0
 2 2r: 1.42E-04 2x: 3.90E+08 2u: 4.60E+00 ir: 1.09E-04 iu: 3.28E+00 rsn:   0
 3 2r: 1.44E-04 2x: 3.90E+08 2u: 4.69E+00 ir: 1.12E-04 iu: 3.28E+00 rsn:   0
 4 2r: 1.42E-04 2x: 3.90E+08 2u: 4.69E+00 ir: 1.09E-04 iu: 3.28E+00 rsn:   0
 5 2r: 1.44E-04 2x: 3.90E+08 2u: 4.69E+00 ir: 1.12E-04 iu: 3.28E+00 rsn:   0
 6 2r: 1.42E-04 2x: 3.90E+08 2u: 4.69E+00 ir: 1.09E-04 iu: 3.28E+00 rsn:   0
 7 2r: 1.44E-04 2x: 3.90E+08 2u: 4.69E+00 ir: 1.12E-04 iu: 3.28E+00 rsn:   0
 8 2r: 1.42E-04 2x: 3.90E+08 2u: 4.69E+00 ir: 1.09E-04 iu: 3.28E+00 rsn: -88
-> Cut time step: snes=-88 icut=  2[***] t=  4.20361E+02 dt=  1.60181E-03
Newton solver reason: Unknown(-88).
 0 2r: 5.35E-03 2x: 0.00E+00 2u: 0.00E+00 ir: 8.83E-05 iu: 0.00E+00 rsn:   0
 1 2r: 1.38E-04 2x: 3.90E+08 2u: 3.31E+00 ir: 1.11E-04 iu: 1.17E+00 rsn:   0
 2 2r: 1.34E-04 2x: 3.90E+08 2u: 2.30E+00 ir: 1.02E-04 iu: 1.55E+00 rsn:   0
 3 2r: 1.42E-04 2x: 3.90E+08 2u: 2.34E+00 ir: 1.11E-04 iu: 1.56E+00 rsn:   0
 4 2r: 1.34E-04 2x: 3.90E+08 2u: 2.34E+00 ir: 1.02E-04 iu: 1.56E+00 rsn:   0
 5 2r: 1.42E-04 2x: 3.90E+08 2u: 2.34E+00 ir: 1.11E-04 iu: 1.56E+00 rsn:   0
 6 2r: 1.34E-04 2x: 3.90E+08 2u: 2.34E+00 ir: 1.02E-04 iu: 1.56E+00 rsn:   0
 7 2r: 1.42E-04 2x: 3.90E+08 2u: 2.34E+00 ir: 1.11E-04 iu: 1.56E+00 rsn:   0
 8 2r: 1.34E-04 2x: 3.90E+08 2u: 2.34E+00 ir: 1.02E-04 iu: 1.56E+00 rsn: -88
-> Cut time step: snes=-88 icut=  3[***] t=  4.20361E+02 dt=  8.00903E-04
Newton solver reason: Unknown(-88).
 0 2r: 5.35E-03 2x: 0.00E+00 2u: 0.00E+00 ir: 8.83E-05 iu: 0.00E+00 rsn:   0
 1 2r: 1.36E-04 2x: 3.90E+08 2u: 1.71E+00 ir: 1.08E-04 iu: 5.85E-01 rsn:   0
 2 2r: 1.14E-04 2x: 3.90E+08 2u: 1.23E+00 ir: 8.36E-05 iu: 9.44E-01 rsn: 999

Step   7207 Time=  4.20362E+02 Dt=  8.00903E-04 [y] snes_conv_reason:  999
 newton =  26 [   33567] linear =   519 [    895508] cuts =  3 [2989]
 --> SNES Linear/Non-Linear Iterations =          42  /           2
 --> SNES Residual:   1.138415E-04  1.088934E-09  8.364154E-05
 --> max chng: dpl=   1.6873E-03 dpg=   8.2578E-01 dpa=   1.1490E+00
               dxa=   9.7392E-11  dt=   1.0563E-03 dsg=   5.9443E-05
```

GDSA Model

Iterative nonlinear solver oscillations

- Newton iteration failure due to **state transition oscillation**

```
== GENERAL MULTIPHASE FLOW ================================================
  0 2r: 6.16E-03 2x: 0.00E+00 2u: 0.00E+00 ir: 1.07E-04 iu: 0.00E+00 rsn:   0
 (1): State Transition: Gas -> 2 Phase at Cell    18055
 (4): State Transition: 2 Phase -> Gas at Cell    99640
  1 2r: 1.93E-04 2x: 3.90E+08 2u: 1.88E+03 ir: 1.20E-04 iu: 2.10E+02 rsn:   0
 (0): State Transition: 2 Phase -> Gas at Cell    19405
  2 2r: 4.77E-03 2x: 3.90E+08 2u: 3.65E+04 ir: 3.08E-03 iu: 2.33E+04 rsn:   0
 (0): State Transition: Gas -> 2 Phase at Cell    19405
 (0): State Transition: Gas -> 2 Phase at Cell    19406
 (0): State Transition: Gas -> 2 Phase at Cell    19407
  3 2r: 2.47E-03 2x: 3.90E+08 2u: 1.30E+05 ir: 1.70E-03 iu: 9.27E+04 rsn:   0
 (0): State Transition: 2 Phase -> Gas at Cell    19406
  4 2r: 1.81E-01 2x: 3.90E+08 2u: 3.16E+04 ir: 1.27E-01 iu: 2.56E+04 rsn:   0
 (0): State Transition: 2 Phase -> Gas at Cell    19407
  5 2r: 5.75E-02 2x: 3.90E+08 2u: 1.40E+04 ir: 4.04E-02 iu: 1.20E+04 rsn:   0
  6 2r: 1.80E-02 2x: 3.90E+08 2u: 3.42E+04 ir: 1.29E-02 iu: 3.19E+04 rsn:   0
 (0): State Transition: 2 Phase -> Gas at Cell    18919
  7 2r: 3.91E-01 2x: 3.90E+08 2u: 1.16E+06 ir: 3.18E-01 iu: 1.07E+06 rsn:   0
 (0): State Transition: Gas -> 2 Phase at Cell    18919
 (0): State Transition: Gas -> 2 Phase at Cell    18920
 (0): State Transition: Gas -> 2 Phase at Cell    18921
 (0): State Transition: Gas -> 2 Phase at Cell    19407
  8 2r: 1.20E-02 2x: 3.90E+08 2u: 8.27E+05 ir: 8.59E-03 iu: 5.79E+05 rsn: -88
-> Cut time step: snes=-88 icut=  1[***] t=  3.46773E+02 dt=  6.25000E-01
Newton solver reason: Unknown(-88).
```

Newton TR algorithm

Algorithm TR Newton Trust Region(Δ)[35][36] - Cauchy Point

1. Set $x = x_0$, initial guess, $\Delta_0 = 2.0$ and iteration counter, $k = 0$.
2. Iteration starts:
   (a) Solve for $\vec{p}$ using Cauchy point which minimizes Eq. 46
   (b) Evaluate $m(\vec{p})$ in Eq. 46
   (c) Evaluate ρ in Eq. 47
   (d) If Δ is suited, $x_{k+1} = x_k - (-\vec{p})$ and may increase Δ; else, $x_{k+1} = x_k$ and re-evaluate with smaller Δ (inner iteration, no update on x_{k+1}).
   (e) Continue iteration if not converged or not reached max iteration number.

Newton TR algorithm

- Quadratic model

$$m_k(\vec{p}) = f_k + g_k^T \vec{p} + \frac{1}{2}\vec{p}^T B_k \vec{p} \ s.t. \ ||\vec{p}|| <= \Delta_k$$

- Ratio of actual improvement and the predicted improvement

$$\rho_k = \frac{f(x_k) - f(x_k + p_k)}{m_k(0) - m_k(p_k)}$$

Line Search Backtracking

Algorithm LS Line Search Backtracking[33]

1. Set $x = x_0$, initial guess, $\alpha_0 = 1.0$ and iteration counter, $k = 0$.
2. Iteration starts:
   (a) Set inner iteration counter $j = 0$.
   (b) Inner iteration starts:
      i. Compute $-\nabla f$ as a steepest descent direction, $\vec{p_k}$.
      ii. Set $t = -c\vec{p}^T \nabla f(\vec{x})$ where c is a control parameter.
      iii. If $f(\vec{x}) - f(\vec{x} + \alpha_j \vec{p}) \leq \alpha_j t$, select α_j else, $\alpha_{j+1} = \tau \alpha_j$, where τ is a control parameter.
   (c) $\vec{x}_{k+1} = \vec{x}_k - \alpha \nabla f(\vec{x})$
   (d) Continue iteration if not converged or not reached max iteration number.

Newton's Method

Algorithm NT Newton's Method[33]

1. Set $x = x_0$, initial guess, and iteration counter, $k = 0$.
2. Iteration starts:
   (a) Find gradient, $\nabla f = \begin{bmatrix} \frac{\partial f(x,y)}{\partial x} \\ \frac{\partial f}{\partial y} \end{bmatrix}$ and Hessian, $H = \begin{bmatrix} \frac{\partial f(x,y)}{\partial x^2} & \frac{\partial f}{\partial x \partial y} \\ \frac{\partial f}{\partial y \partial x} & \frac{\partial f}{\partial y^2} \end{bmatrix}$.
   (b) Solve the linear system, $H\vec{x} = -\nabla f$
   (c) $x_{k+1} = x_k + \vec{x}$
   (d) Continue iteration if not converged or not reached max iteration number.

Newton TR verification