AMG Preconditioner for Multiphase Flow in Engineered Simulation Domains

Heeho D Park, Glenn E Hammond, and Albert J Valocchi

Sandia National Laboratories, Albuquerque, NM and University of Illinois at Urbana–Champaign, Urbana, IL

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Applications of Multiphase Porous Media Flow

Nuclear waste repositories

Enhanced recovery of petroleum reservoirs

Contaminant remediation

Geothermal engineering

Carbon sequestration

Coupled overland/groundwater flow

U.S. Department of Energy - PFLOTRAN development for deep geologic disposal

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PFLOTRAN

Flow and reactive transport in porous media

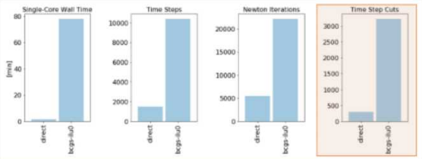
- Developed by DOE
- Modern Fortran ('08)
- Open-source and community-driven
- PETSc parallel framework
- Runs in massively parallel computing architectures, workstations, and down to a laptop

OPEN

Analysis of Iterative Linear Solver Failure

Linear Solver Failure

Direct solver vs BiCGSTAB-ILU(0) (1 core)



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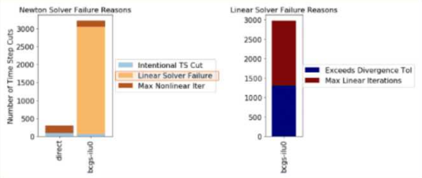

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Direct solver, block-Jacobi-ILU(0), and block-Jacobi-ILU(5) (4 cores) (3D, 274k unknowns)

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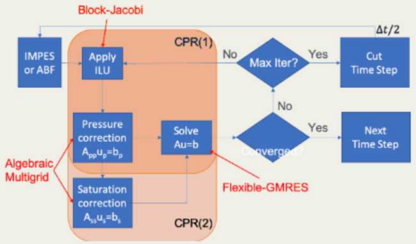
CPR-AMG Preconditioner

Constrained Pressure Residual (CPR) - Algebraic Multigrid (AMG) Preconditioner

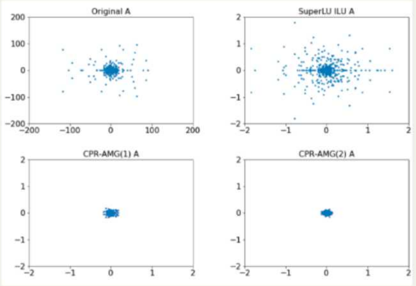


Decoupling Techniques

OPEN

Results/Conclusions

Eigenvalue Spectrum



Preconditioners reduce the eigenvalue

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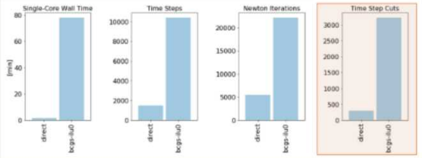

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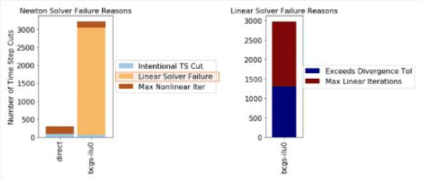

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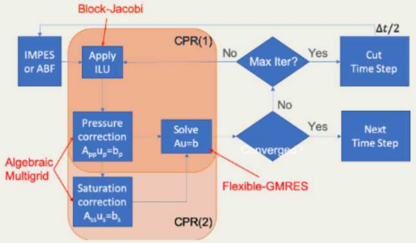

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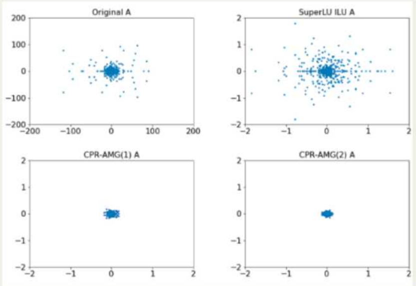

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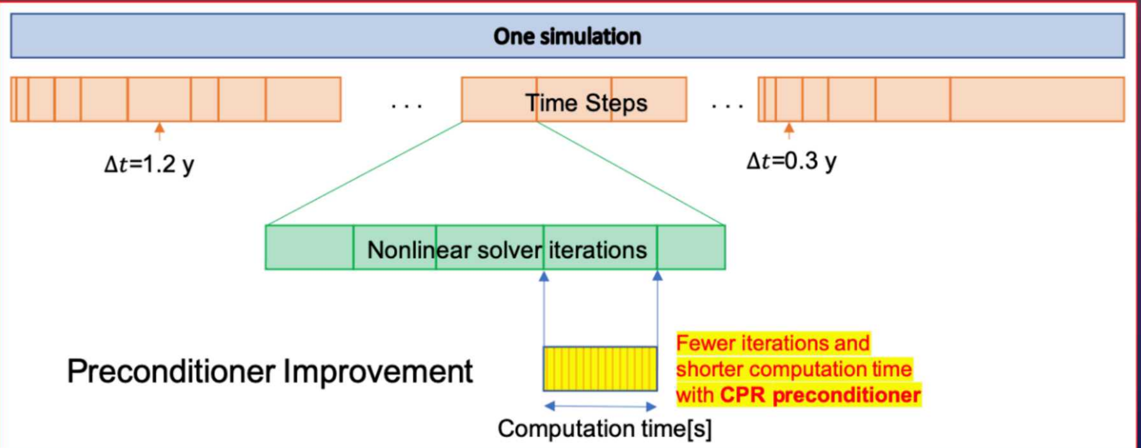
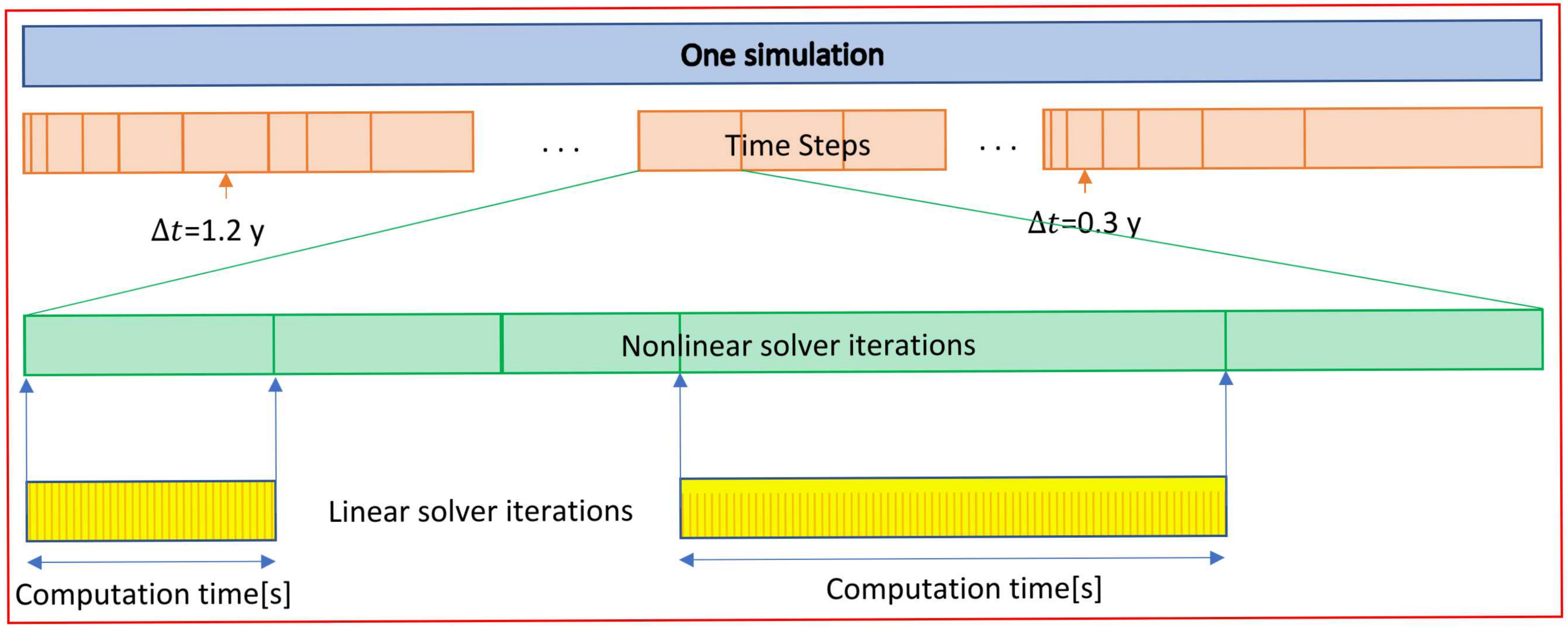


Bottom Right Slide 1



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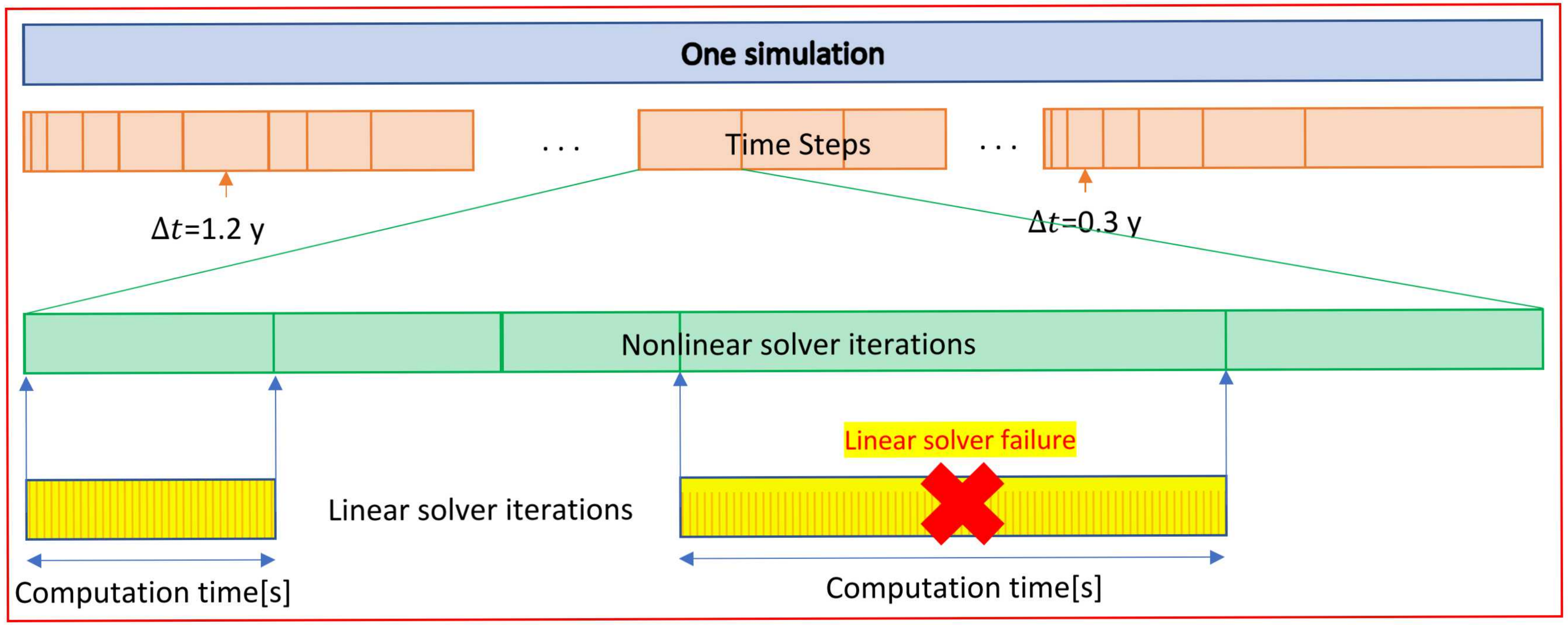

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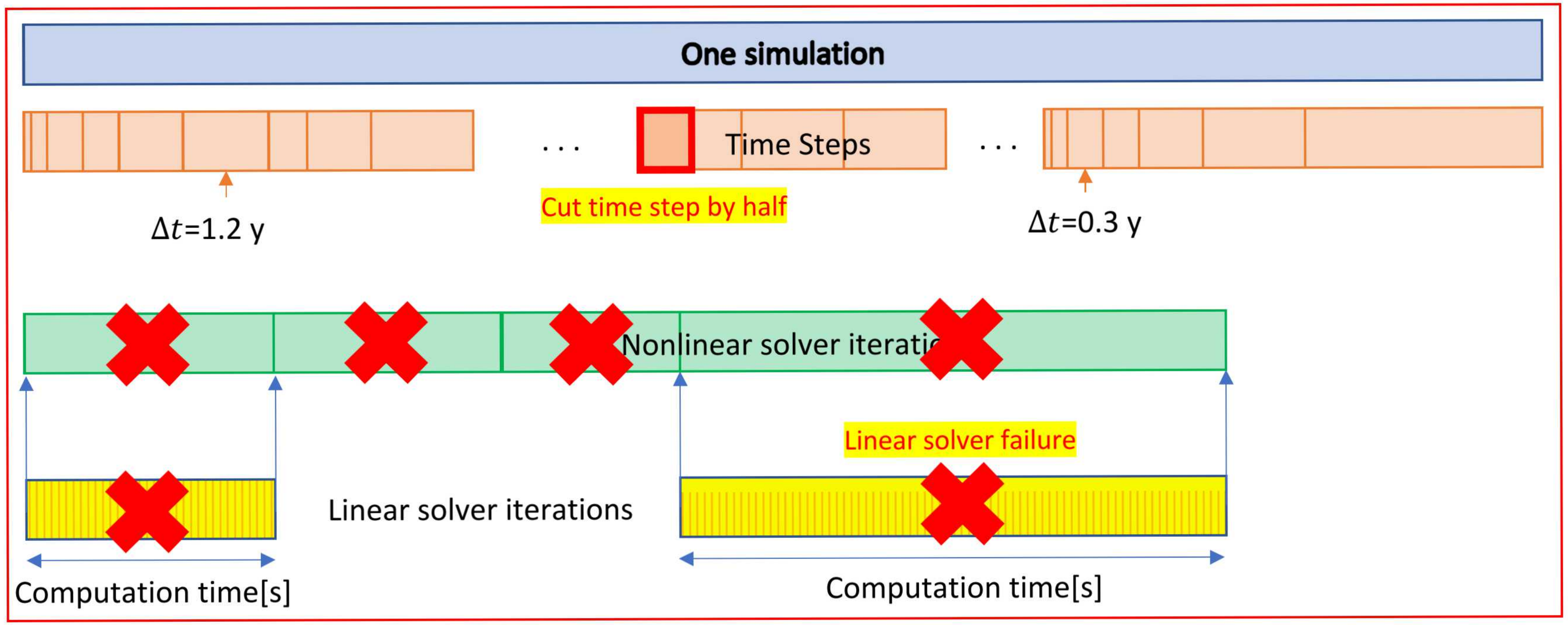

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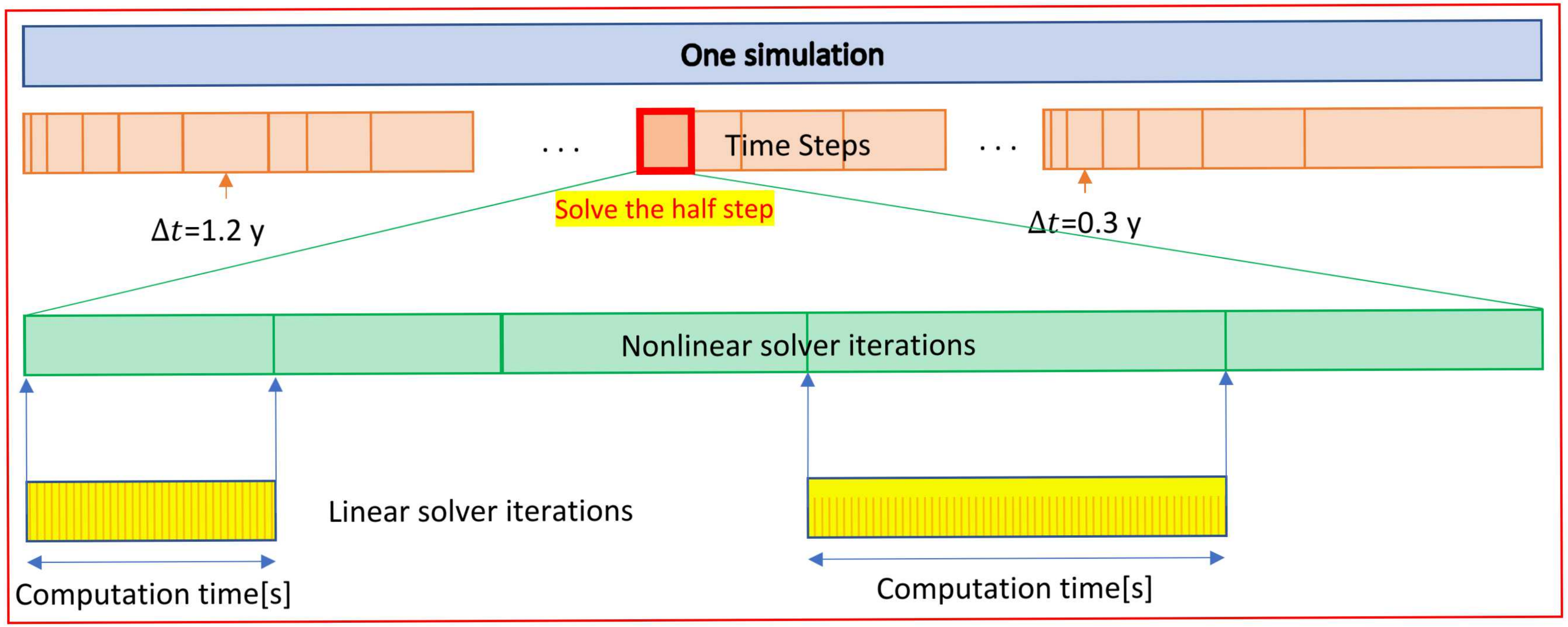

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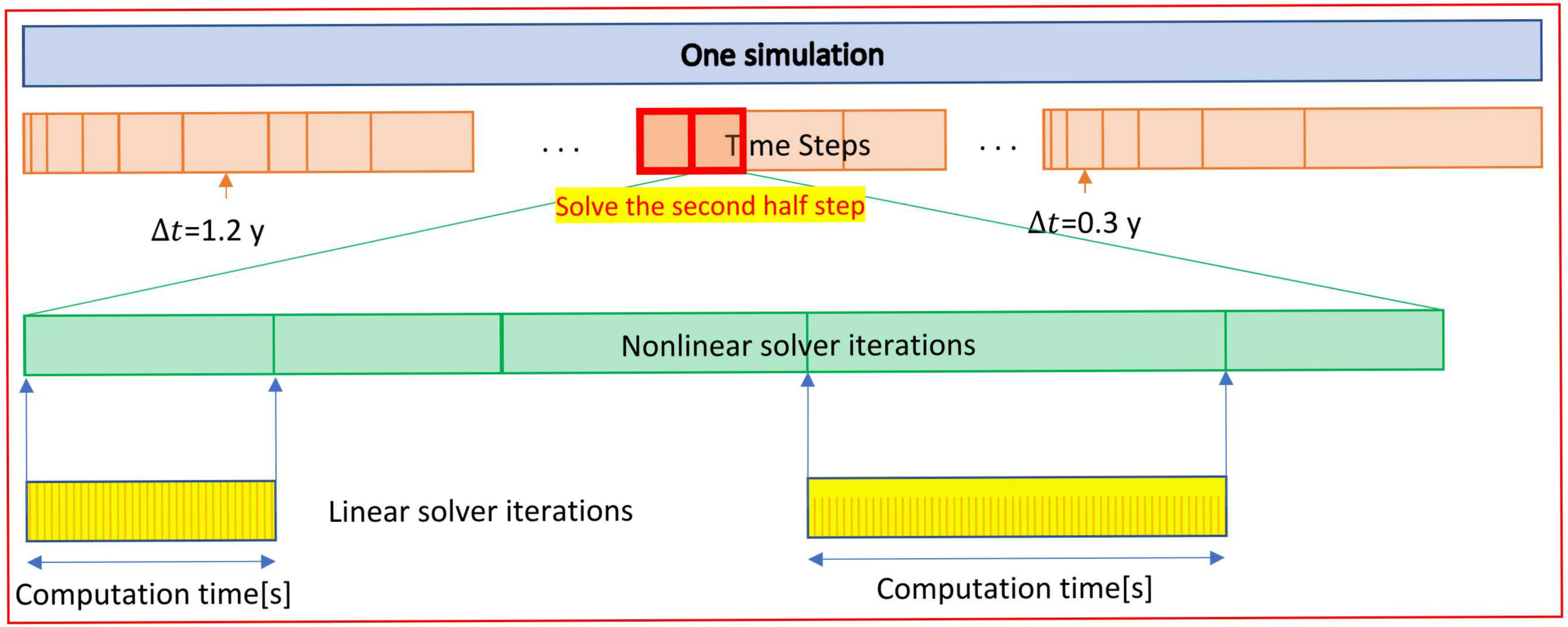

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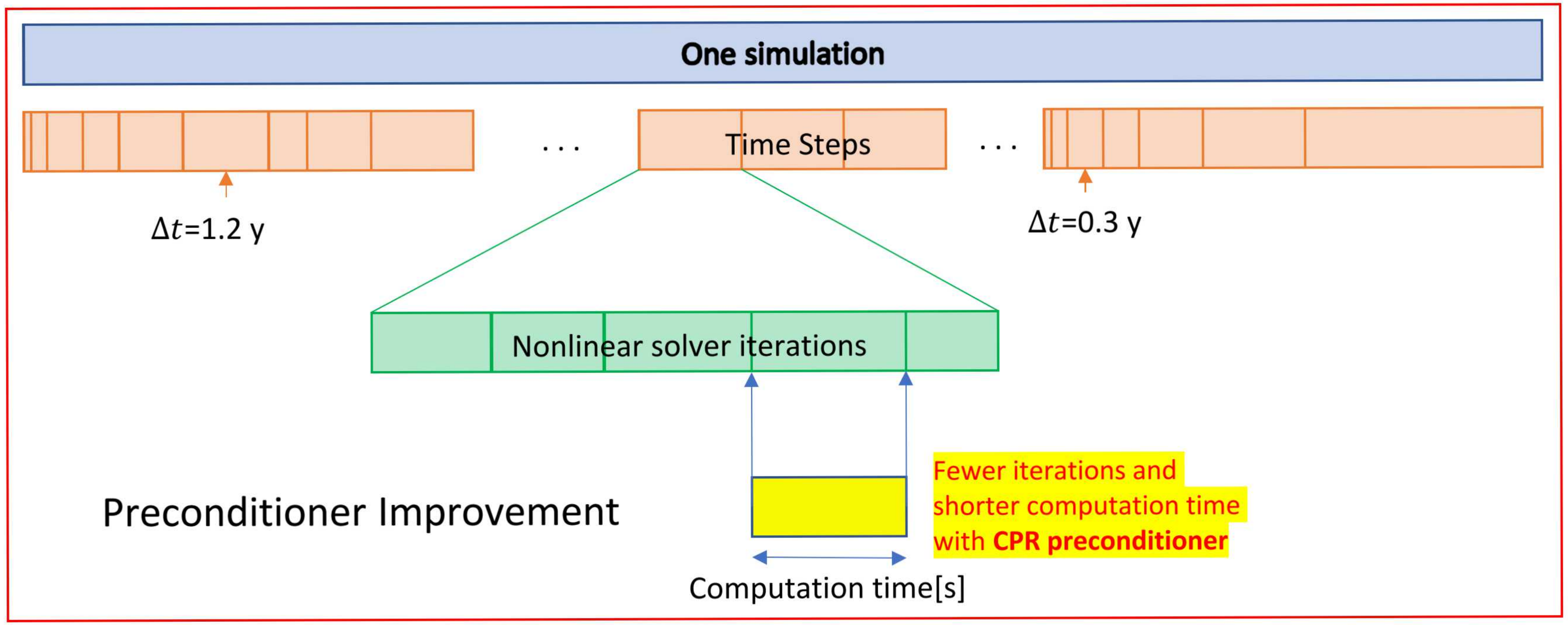

Top Left

Nuclear waste repositories

Enhanced recovery of petroleum reservoirs

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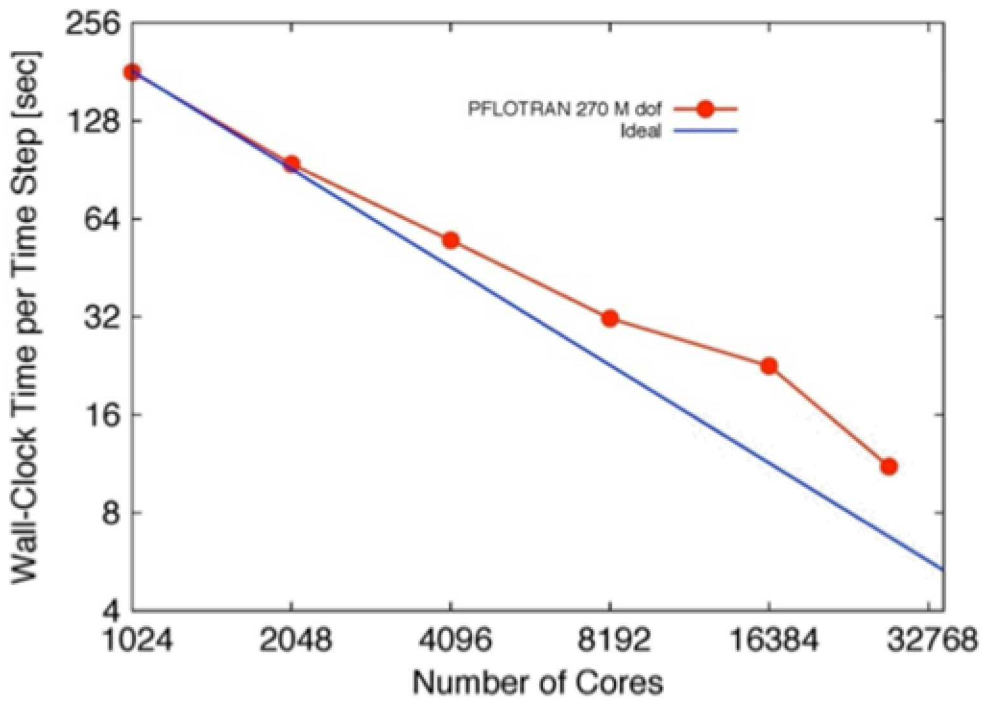
U.S. Department of Energy - PFLOTRAN development for deep geologic disposal of nuclear waste

- Geologic Disposal Safety Assessment (GDSA) Framework: an open-source software toolkit for performance assessment (PA) of deep geologic repositories for nuclear waste applied to generic repository concepts in salt, argillite, and crystalline host rocks. Generic PAs assume a regulatory period of 1 million years for high-level wastes. (DOE - Office of Nuclear Energy)
- Future use in PA for Waste Isolation Pilot Plant (WIPP): The probability and consequence of potential transuranic radionuclide release from the repository to the accessible environment for 10,000 years. WIPP started its operation since 1999. (DOE - Environmental Management)

Bottom Left

Flow and reactive transport in porous media

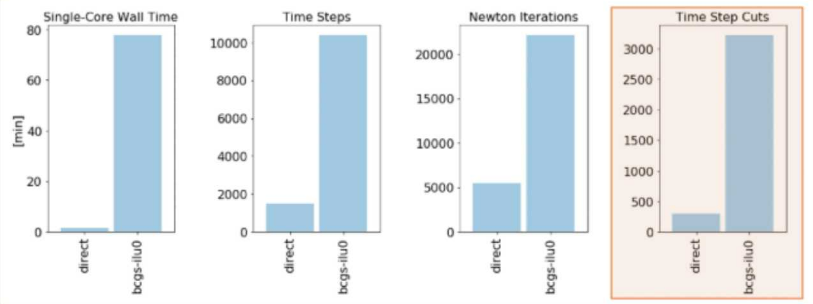
- Developed by DOE
- Modern Fortran ('08)
- Open-source and community-driven
- PETSc parallel framework
- Runs in massively parallel computing architectures, workstations, and down to a laptop
- Has been run on up to 262k processor cores with 2 billion degrees of freedom using the domain decomposition
- Applies the finite volume method with backward Euler temporal 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



Middle Left

Linear Solver Failure

Direct solver vs BiCGSTAB-ILU(0) (1 core)



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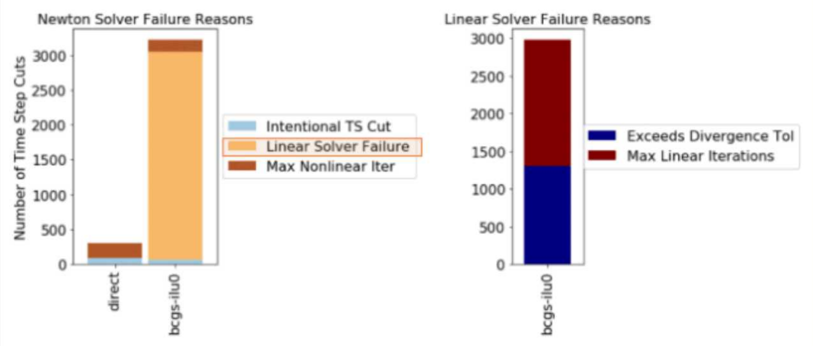
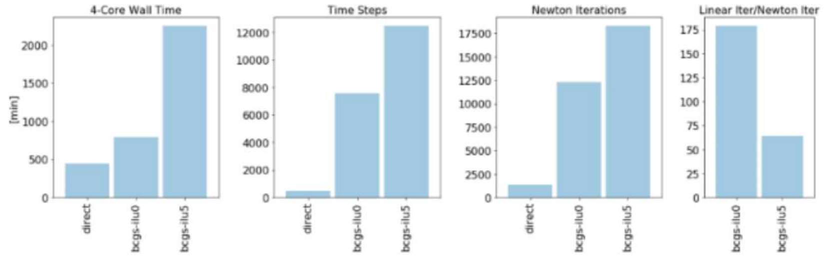


BiCGSTAB-ILU(0) shows Newton iteration failure due to linear solver divergence and reaching maximum iterations.

Direct solver, block-Jacobi-ILU(0), and block-Jacobi-ILU(5) (4 cores) (3D, 274k unknowns)



Convergence criteria	Wall time [hr]	Time steps	Nonlinear iterations	Linear iterations	Wasted linear iterations
3D WIPP (274k unknowns) – 10,000-year simulation BICGSTAB					
Direct – 4 cores	7.40	511	1379	-	-
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

Block Jacobi preconditioner loses information without any communication among 4 cores and is unable to provide an accurate approximate inverse of the matrix.

Middle Left

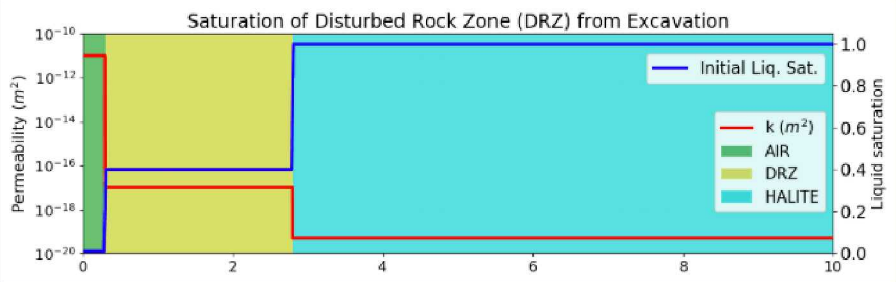
Potential Causes

1. Highly contrasting intrinsic permeability at discrete boundaries.

Excavation (AIR): $10^{-11} \mathrm{m}^2$

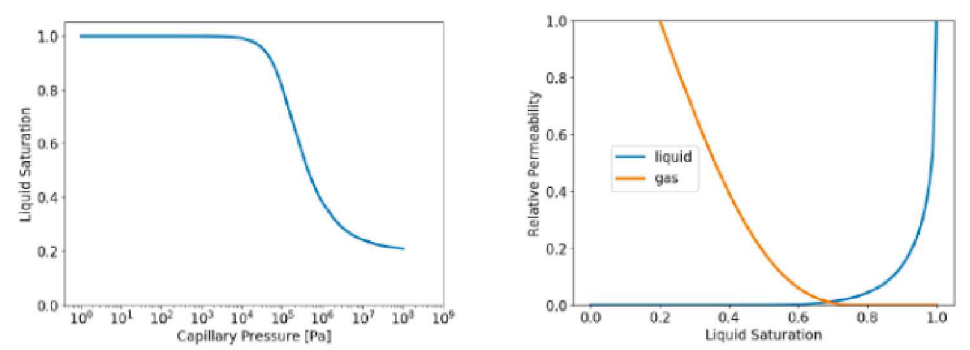
Disturbed Rock Zone (DRZ): $10^{-17} \mathrm{m}^2$

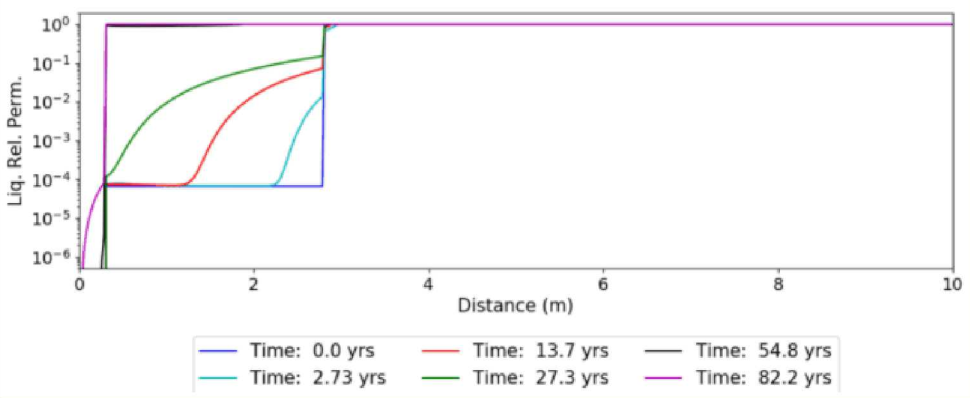
Salt Rock (HALITE): $5 \times 10^{-20} \mathrm{m}^2$



2. Rapidly changing water retention function

Multiplying the low liquid relative permeability to the low intrinsic permeability can generate some extremely small coefficients for the linear system of equations.





Changes in liquid relative permeability over time as brine seeps in from the intact salt (HALITE) to the excavation (AIR).

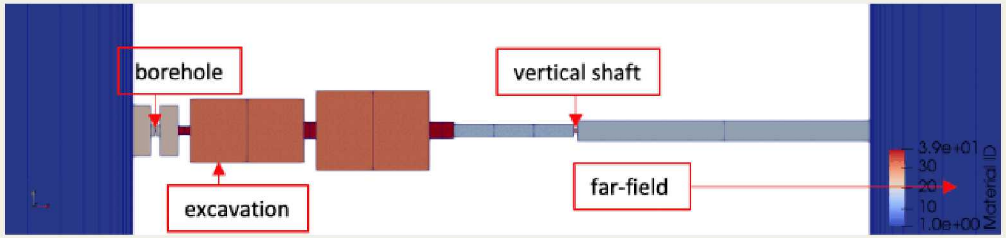
Middle Left

3. Large contrasts of grid cell volumes in a simulation domain

A borehole grid cell volume: $0.014\mathrm{m}^3$

An excavation grid cell volume: $1621\mathrm{m}^3$

A far-field grid cell volume: $10^9\mathrm{m}^3$



4. Simulation time steps

When the simulation must run out to 10,000 years to 1,000,000 years, large time steps are needed to complete the simulation in reasonable computation time.

Minimum time step: 1 minute

Maximum time step: 1000 years

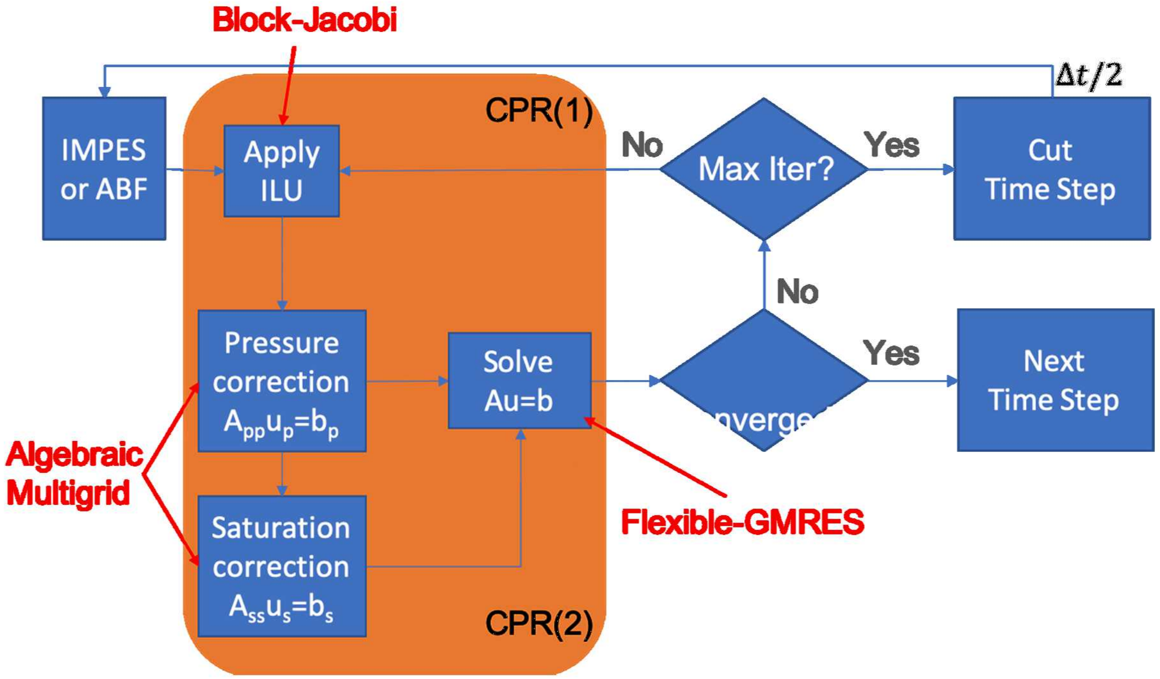
Extreme condition Number

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) = 10k. Information can be lost if the matrix is scaled improperly.

Some of the matrices that could not be solved with BiCGSTAB-ILU(0) for the 3D case had a condition number of $10^{17} - 10^{19}$

Middle Right

Constrained Pressure Residual (CPR) - Algebraic Multigrid (AMG) Preconditioner



Decoupling Techniques

Stacked Jacobian format

$$A = \begin{bmatrix} A_{pp} & A_{ps} \\ A_{sp} & A_{ss} \end{bmatrix}, r = \begin{bmatrix} r_p \\ r_s \end{bmatrix}$$

Schur Complement

$$A_{pp}x + A_{ps}y = r_p$$
$$A_{sp}x + A_{ss}y = r_s$$
$$\left(A_{pp} - A_{ps}A_{ss}^{-1}A_{sp}\right)x = r_p - A_{ps}A_{ss}^{-1}r_s$$

There are three methods that approximate the inverse matrix and reduce matrix-matrix multiplications to vector-matrix multiplications.

Middle Right

True-implicit pressure explicit saturation (IMPES)

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

Quasi-IMPES

$$A_{pp} - D_{ps}D_{ss}^{-1}A_{sp}, \text{where } D = \mathrm{diag}(A)$$

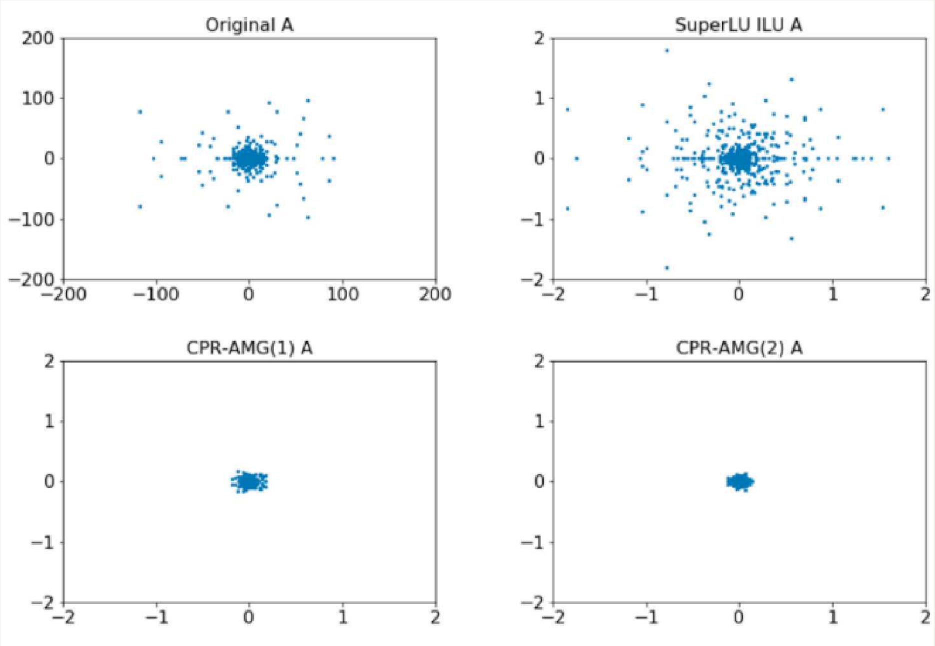
Alternate Block Factorization (ABF)

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

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

Top Right

Eigenvalue spectrum



Preconditioners reduce the eigenvalue spectrum.

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

Condition number

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

Preconditioners lowered condition numbers significantly.

CPR solve result

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)

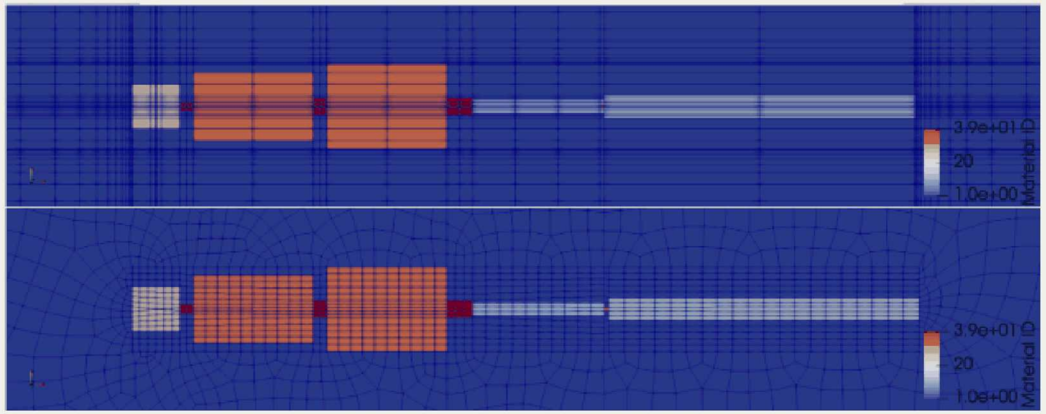
*Failed to converge in 1 of 9 matrices

This 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

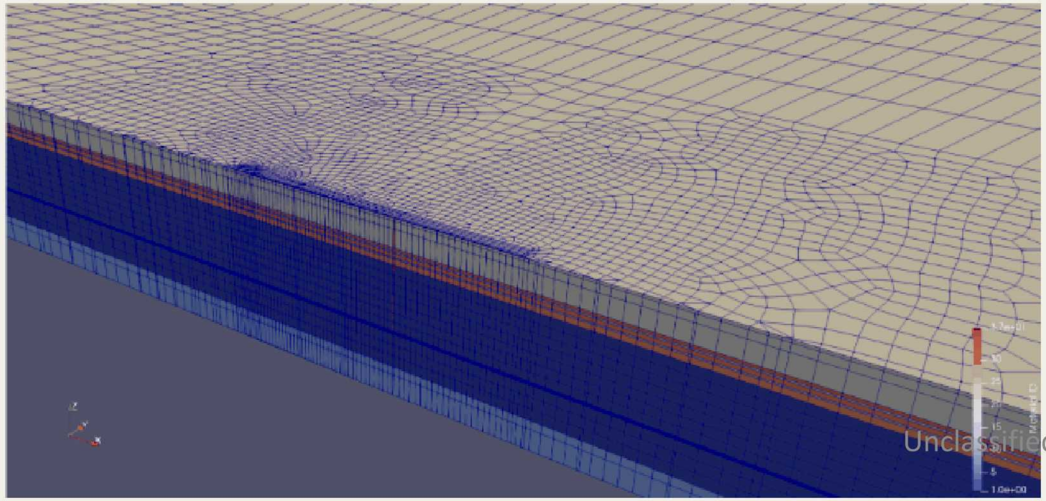
Top Right

CPR in PFLOTRAN

Structured grid vs Paved grid



3D view of the grid



CPR results

Methods	# of Cores	Wall Time [hr]	Time Steps	Nonlinear iterations	Linear iterations
3D Structured Grid (137k cells, 274k unknowns) – 10,000-year simulation					
BiCGSTAB-ILU(0)	4	13.25	7544	12,331	2,202,112
Direct solver	4	7.39	511	1379	-
FGMRES-CPR	4	3.09 (4.28x)	1578	3150	849,666
3D Paved Grid (237k cells, 474k unknowns) – 10,000-year simulation					
BiCGSTAB-ILU(0)	8	83.7	15,265	26,120	24,810,791
Direct solver	8	15.3	1,242	4,171	-
FGMRES-CPR	8	1.02 (83x)	1,338	4,252	126,796
3D Hexahedral Grid (1.6M cells, 3.2M unknowns) – 5-year finding initial condition simulation					
BiCGSTAB-ILU(0)	24 (1.5x)	25.8	3,254	15,889	1,293,210
Direct solver	16	>168 (incomplete)	-	-	-
FGMRES-CPR	16	10.8 (3.5x)	3,218	15,922	234,109

Even with the same convergence criteria, flexible generalized minimal residual (FGMRES) with IMPES-CPR may have provided more accurate solutions. Therefore, it showed a speed-up of 3 to 80 times.

CONCLUSION

Generally, FGMRES-IMPES-CPR is more robust and efficient in parallel for large-scale engineered subsurface systems compared to BiCGSTAB-block-Jacobi-ILU or Direct Solver.

CV

Heeho D Park

Experience

Sandia National Laboratories (5yrs 11mos)

- Senior Member of Technical Staff (Jan 2017 - present)

- Member of Technical Staff (Jan 2014 - Jan 2017)

The University of Michigan - Ann Arbor (4 years)

- Research Computer Specialist (May 2012 - Aug 2013)

- Student Research Assistant (Sep 2009 - May 2012)

Education

The University of Illinois at Urbana-Champaign (Aug 2016 - present)

- Ph.D., Multi/Interdisciplinary Studies with Civil & Environmental Engineering and Computational Science & Engineering

The University of Michigan - Rackham Graduate School (Sep 2011 - Apr 2012)

- M.S.E, Nuclear Engineering & Radiological Sciences

The University of Michigan - College of Engineering (Sep 2007 - Apr 2011)

- B.S.E, Nuclear Engineering & Radiological Sciences

DISCLOSURES

✖

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ABSTRACT

✖

An engineered system such as a geologic nuclear waste repository can be difficult to simulate due to extreme contrasts in permeability and extreme grid cell aspect ratios caused by a small area of interest in a large domain. As an example, a typical nuclear waste repository simulation has a domain of a few kilometers with nuclear waste canisters at the meter scale. Excavated volumes that are not backfilled may be simulated with very high permeability in the porous media flow simulation, while the host rock and engineered barriers tend to have comparatively low permeability. The regulatory horizon of 10,000 to 1 million years requires large time steps to complete performance assessment in reasonable amount of computation time. These characteristics can result in ill-conditioned matrices that are difficult to solve with iterative solvers in parallel using conventional preconditioners such as parallel block Jacobi incomplete lower-upper matrix decomposition (ILU). In order to improve parallel performance, iterative solvers require proper scaling of matrix coefficients, and preconditioners that are well-suited for the characteristics of the multi-phase problem. Algebraic multigrid (AMG) is well-known for efficiently and robustly solving the elliptic pressure equation. To test the performance of the AMG preconditioner, the matrices from Newton solves that failed to converge due to iterative linear solver failure using the block Jacobi ILU preconditioner are extracted from PFLOTRAN simulations and solved by applying preconditioners (available in the Python library PyAMG) that are more optimized to the classification of the matrices. This presentation compares performance of the block Jacobi ILU preconditioner coupled with stabilized biconjugate gradient (BiCGSTAB) solver, a parallel direct solver (MUMPS), and the flexible generalized minimal residual (FGMRES)-AMG solver applied to two-stage additive or combinative constrained pressure residual (CPR) preconditioner with different matrix decoupling techniques, including true implicit pressure and explicit saturation (true-IMPES), quasi-IMPES, and alternate block factorization (ABF).

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