Improved Iterative Methods for NAPL Transport Through Porous Media

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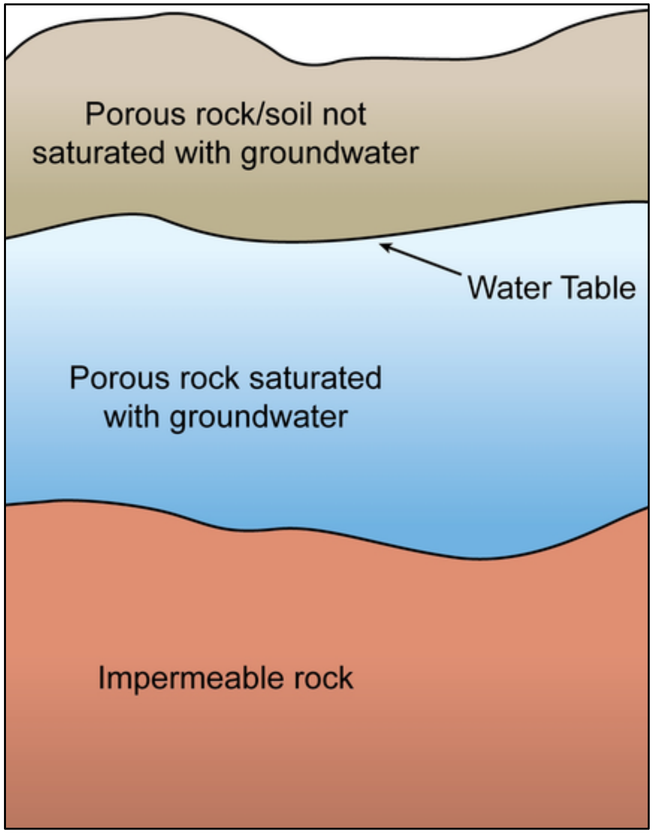
Background

- Non-aqueous phase liquid (NAPL)
  - Gasoline
  - Pesticides
  - Mercury

Background (cont.)

- Aquifer
  - Water
  - Pores



The Problem

- Spills
- Leakage
- Agricultural run–off

Can we model and simulate the flow of these contaminants?

Past Work

- Abriola et al.
  - VALOR
    - Version 1.0: 2D model, 3–phase flow
    - Now: 3D model, 2–phase flow
- Well–established theory

L. Abriola, K. Rathfelder, M. Maiza, and S. Yadav, VALOR Code Version 1.0: A PC Code for Simulating Immiscible Contaminant Transport in Subsurface Systems, Tech. Rep. EPRI TR-101018, The University of Michigan, Ann Arbor, Michigan, September 1992.

This Work

- Explore changes to VALOR solution algorithm

Goal: Improve runtime without sacrificing accuracy

Outline

- Model
- Discretization
- IMPES
- Solution Scheme
- Simulation Results
- Conclusion

Model

- Conservation of mass

$$\frac{\partial}{\partial t}[\underbrace{\phi S_\alpha \rho_\alpha}_{\text{Effective mass density}}] = -\nabla \cdot [\rho_\alpha \underbrace{\phi S_\alpha \mathbf{v}_\alpha}_{\text{Volumetric flux}}] + q_\alpha$$

- Effective Mass Density

$$\frac{V_{pore}}{V}\frac{V_{fluid}}{V_{pore}}\frac{m}{V_{fluid}}$$

Model (cont.)

- Modified Darcy's Law

$$\underbrace{\phi S_\alpha \mathbf{v}_\alpha}_{\text{Volumetric flux}} = -\frac{\boldsymbol{\kappa} k_{r\alpha}}{\mu_\alpha}[\nabla P_\alpha - \underbrace{\rho_\alpha g}_{\gamma_\alpha} \nabla z]$$

- Transmissibility

$$\boldsymbol{\lambda}_\alpha \equiv \frac{\rho_\alpha \boldsymbol{\kappa} k_{r\alpha}}{\mu_\alpha}$$

J. Bear, Dynamics of fluids in porous media, Dover, 1988.

Model (cont.)

- Final Equation

$$\frac{\partial}{\partial t}[\phi S_\alpha \rho_\alpha] = \nabla \cdot [\boldsymbol{\lambda}_\alpha(\nabla P_\alpha - \gamma_\alpha \nabla z)] + q_\alpha$$

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Discretization

- Sample space and time on discrete grid
- Round values to nearest floating-point number

Finite problem

Discretization (cont.)

- Finite Differences
  - Approximate derivatives

$$u'(x) \approx \begin{cases} \frac{u(x+h)-u(x)}{h} & \equiv \Delta^{+}u(x) \\ \frac{u(x)-u(x-h)}{h} & \equiv \Delta^{-}u(x) \\ \frac{u(x+h/2)-u(x-h/2)}{h} & \equiv \Delta^{0}u(x) \end{cases}$$

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IMPES

- Explicit schemes
  - $u(\mathbf{x}, t + \Delta t) = f[u(\mathbf{x}, 0 : t), \mathbf{x}, 0 : t]$
  - CFL conditions
- Implicit schemes
  - $g[u(\mathbf{x}, t + \Delta t), u(\mathbf{x}, 0 : t), \mathbf{x}, 0 : t] = 0$
  - Expensive

R. LeVeque, Finite Difference Methods for Ordinary and Partial Differential Equations: Steady-State and Time-Dependent Problems, Classics in Applied Mathematics, Society for Industrial and Applied Mathematics, 2007.

IMPES (cont.)

- Implicit-Pressure, Explicit-Saturation (IMPES)
- Expand time-derivative with product-rule
- Express NAPL pressure in terms of water pressure and capillary pressure

IMPES (cont.)

- Saturation Equations

$$\phi\rho_w\frac{\partial S_w}{\partial t} =$$

$$\nabla\cdot[\boldsymbol{\lambda}_w(\nabla P_w-\gamma_w\nabla z)]-(\phi S_w\frac{\partial\rho_w}{\partial P_w}+\rho_w S_w\frac{\partial\phi}{\partial P_w})\frac{\partial P_w}{\partial t}+q_w$$

$$\phi\rho_o\frac{\partial S_o}{\partial t} =$$

$$\nabla\cdot[\boldsymbol{\lambda}_o(\nabla P_w+\nabla P_{cow}-\gamma_o\nabla z)]-(\phi S_o\frac{\partial\rho_o}{\partial P_o}+\rho_o S_o\frac{\partial\phi}{\partial P_o})\frac{\partial P_w}{\partial t}+q_o$$

IMPES (cont.)

- Pressure Equation

$$
\begin{aligned}
&(d_{w2}d_{o1} + d_{o2}d_{w1})\frac{\partial P_w}{\partial t} = \\
&\quad d_{w2}\nabla \cdot [\boldsymbol{\lambda}_o(\nabla P_w + \nabla P_{cow} - \gamma_o \nabla z)] + d_{w2}q_o \\
&+d_{o2}\nabla \cdot [\boldsymbol{\lambda}_w(\nabla P_w - \gamma_w \nabla z)] + d_{o2}q_w
\end{aligned}
$$

$$
d_{\alpha 1} \equiv \phi S_\alpha \frac{\partial \rho_\alpha}{\partial P_\alpha} + \rho_\alpha S_\alpha \frac{\partial \phi}{\partial P_\alpha} \qquad d_{\alpha 2} \equiv \phi \rho_\alpha
$$

IMPES (cont.)

- Problems
  - Density is pressure-dependent
  - Capillary pressures and relative permeabilities have saturation-dependent functional form

Nonlinear system

J. C. Parker, R. J. Lenhard, and T. Kuppusamy, A parametric model for constitutive properties governing multiphase flow in porous media, Water Resour. Res., 23 (1987), pp. 618–624.

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Solution Scheme

- Picard Linearization
  - Solve a fixed point equation

$$x = F(x)$$

  - Iteration

$$x^{(0)} = x_0$$
$$x^{(k)} = F(x^{(k-1)})$$

Solution Scheme (cont.)

- Parallel Picard

$$
\begin{aligned}
\delta\mathbf{P}_t^{(0)} &= 0 \\
\mathbf{S}_t^{(0)} &= \mathbf{S}_{t-1} \\
\delta\mathbf{P}_t^{(k)} &= A^{-1}(\delta\mathbf{P}_t^{(k-1)}, \mathbf{S}_t^{(k-1)})\mathbf{b}(\delta\mathbf{P}_t^{(k-1)}, \mathbf{S}_t^{(k-1)}) \\
\mathbf{S}_t^{(k)} &= \mathbf{S}_{t-1} + G(\delta\mathbf{P}_t^{(k)}, \mathbf{S}_t^{(k-1)})
\end{aligned}
$$

Solution Scheme (cont.)

- Predictor–Corrector Picard

$$\mathbf{S}_t^{(0)} = \mathbf{S}_{t-1}$$

$$\delta\mathbf{P}_t^{(0,p)} = 0$$

$$\delta\mathbf{P}_t^{(k,p)} = A^{-1}(\delta\mathbf{P}_t^{(k-1,p)}, \mathbf{S}_t^{(p-1)})\mathbf{b}(\delta\mathbf{P}_t^{(k-1,p)}, \mathbf{S}_t^{(p-1)})$$

$$\mathbf{S}_t^{(p)} = \mathbf{S}_{t-1} + G(\delta\mathbf{P}_t^{(p)}, \mathbf{S}_t^{(p-1)})$$

Solution Scheme (cont.)

- Generalized minimal residual method (GMRES)
  - Solve $Ax = b$
  - Each step:

$$x_k = \underset{x \in K_k}{\operatorname{argmin}} \, ||Ax - b||$$

Y. Saad and M. H. Schultz, GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems, SIAM Journal on Scientific and Statistical Computing, 7 (1986), pp. 856–869

Solution Scheme (cont.)

- GMRES(k)
  - Restart GMRES
  - Minimize over only *k* vectors
  - Choice of *k* important

Y. Saad, Iterative Methods for Sparse Linear Systems, Society for Industrial and Applied Mathematics, 2003.

Solution Scheme (cont.)

- Preconditioning
  - New matrix, new spectrum
  - Right preconditioning:

$$AM^{-1}y = b$$

$$x = M^{-1}y$$

Solution Scheme (cont.)

- Jacobi

$$M = \mathrm{diag}(A)$$

- Algebraic Multigrid (AMG)

$$M = \text{Multigrid V-cycle}$$

U. Trottenberg, C. Oosterlee, and A. Schüller, Multigrid, Academic Press, 2001.

Solution Scheme (cont.)

- Terminating GMRES
  - Iterations
  - Absolute residual norm
  - Relative residual norm
  - Stagnation

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Simulation Results

- Test Problem Parameters
  - 2.8GHz Intel® Xeon, 16GB RAM
  - $N_x, N_y, N_z = 65, 21, 141$
  - $h_x, h_y, h_z = 0.25m, 0.5m, 0.05m$
  - Medium properties generated in T-PROGS
  - 5 days of simulation

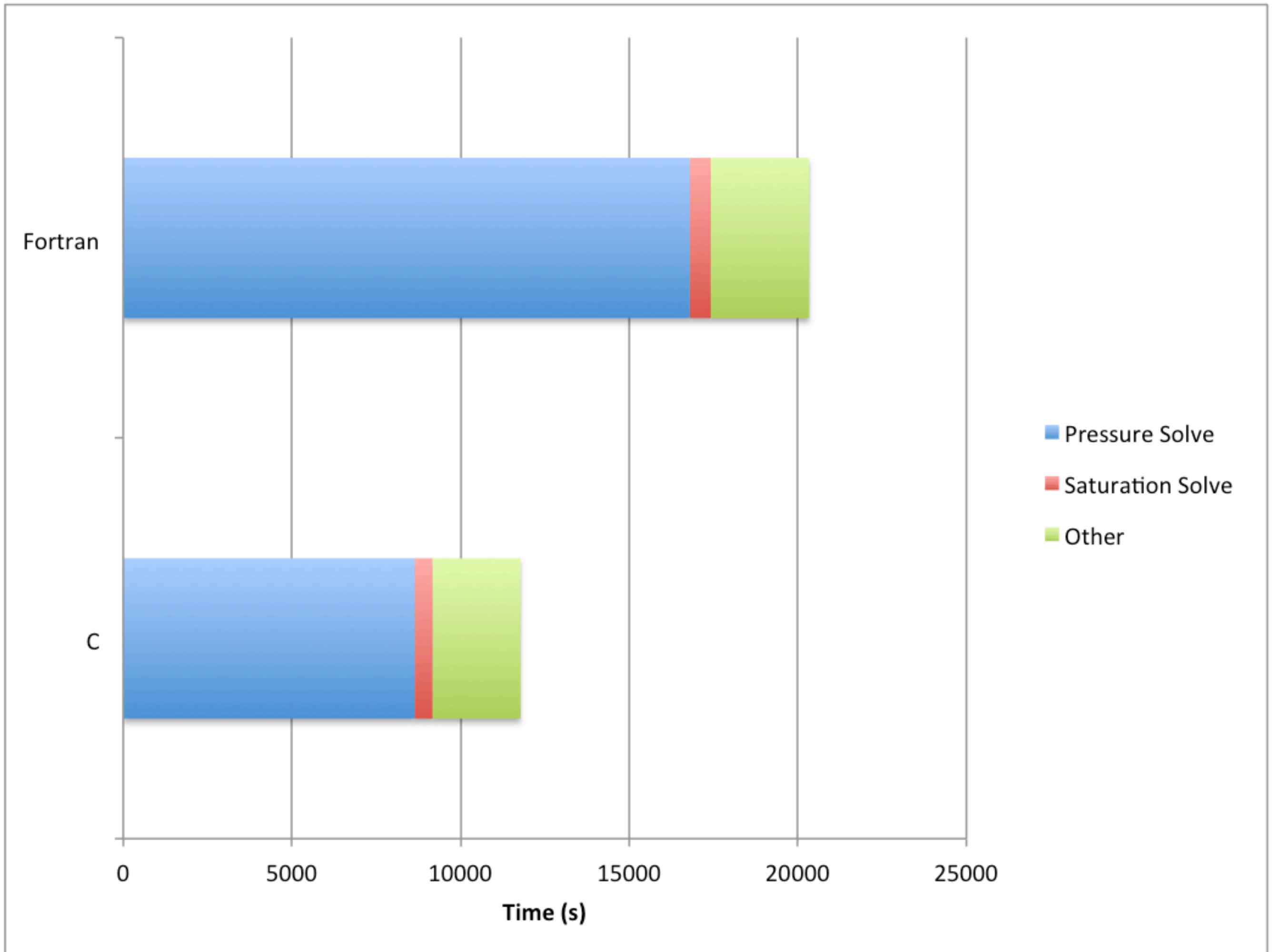
S. F. Carle, T-PROGS: Transition Probability Geostatistical Software and User's Guide, University of California, 1999.

Simulation Results (cont.)

- Original (Fortran) vs PETSc (C)
  - Left Jacobi
  - 30 GMRES iterations

S. Balay, J. Brown, , K. Buschelman, V. Eijkhout, W. D. Gropp, D. Kaushik, M. G. Knepley, L. C. McInnes, B. F. Smith, and H. Zhang, PETSc users manual, Tech. Rep. ANL- 95/11 - Revision 3.2, Argonne National Laboratory, 2011.

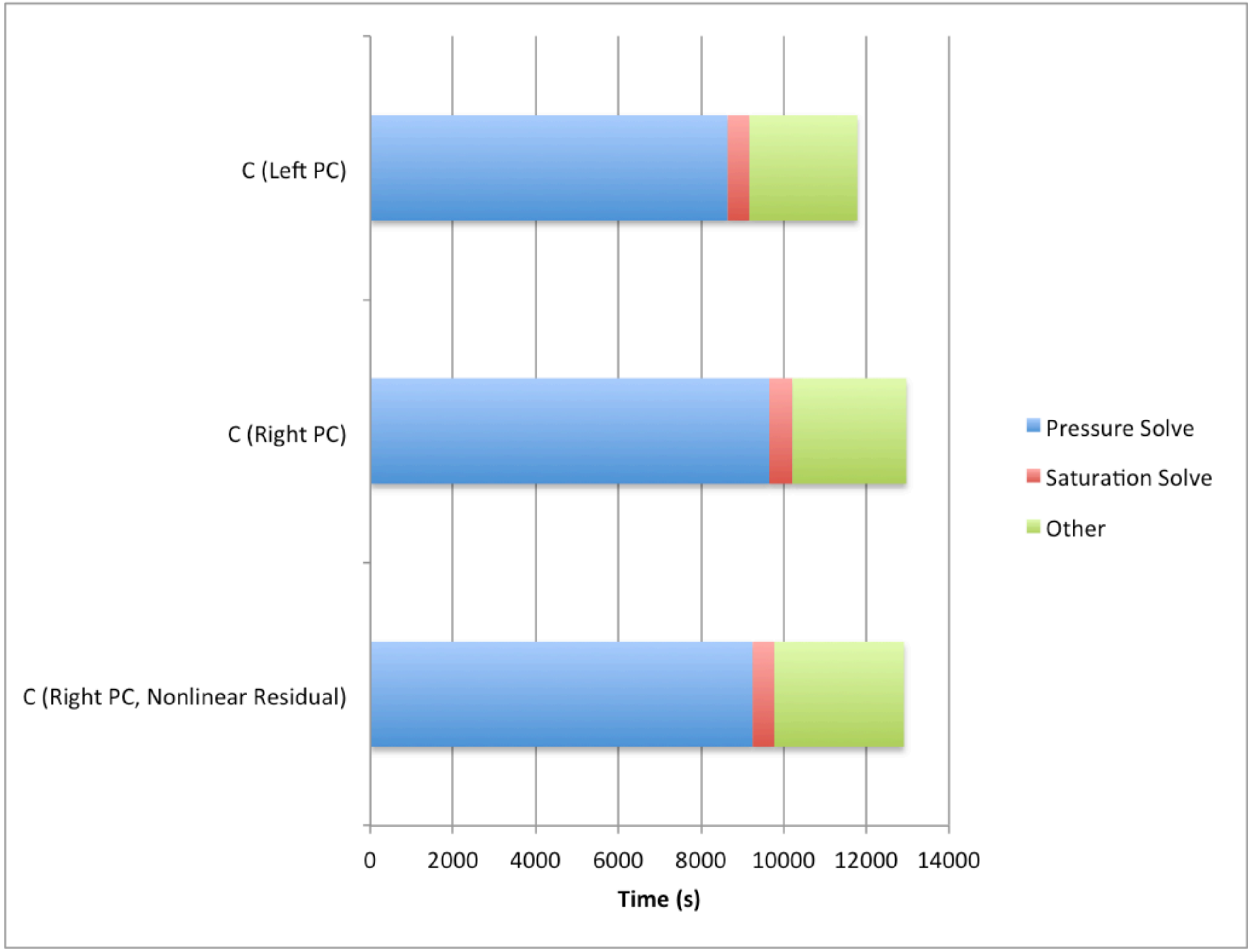
Simulation Results (cont.)



Simulation Results (cont.)

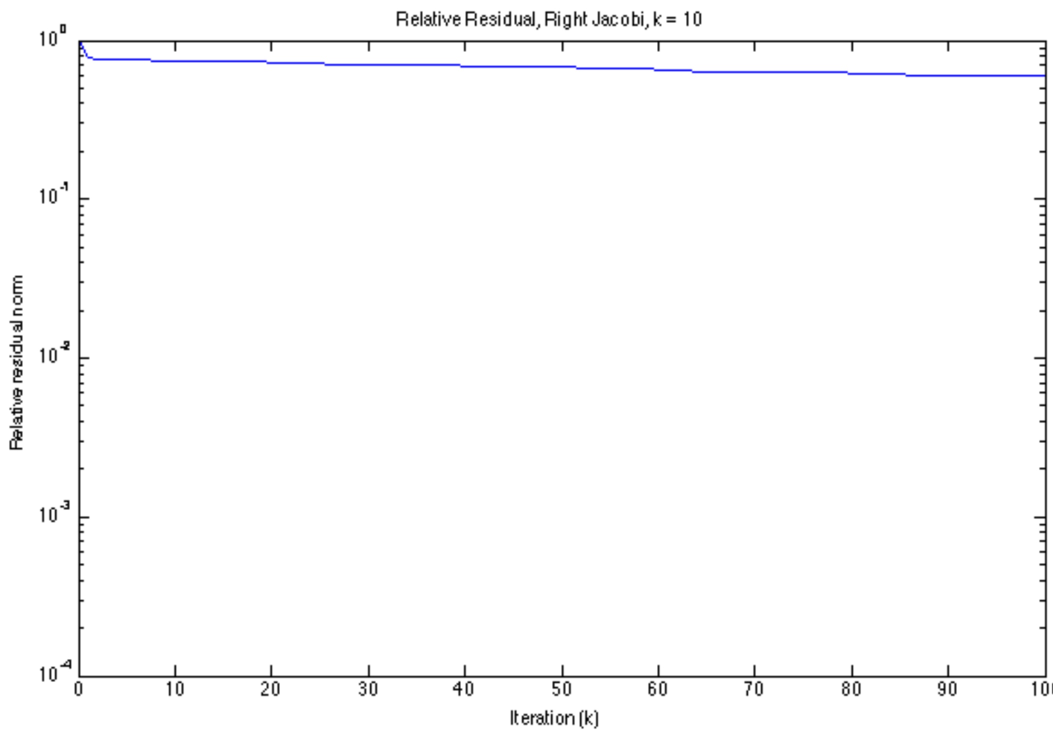
- Preliminary changes
  - Switch to right Jacobi
  - Enforce check of nonlinear residual

Simulation Results (cont.)

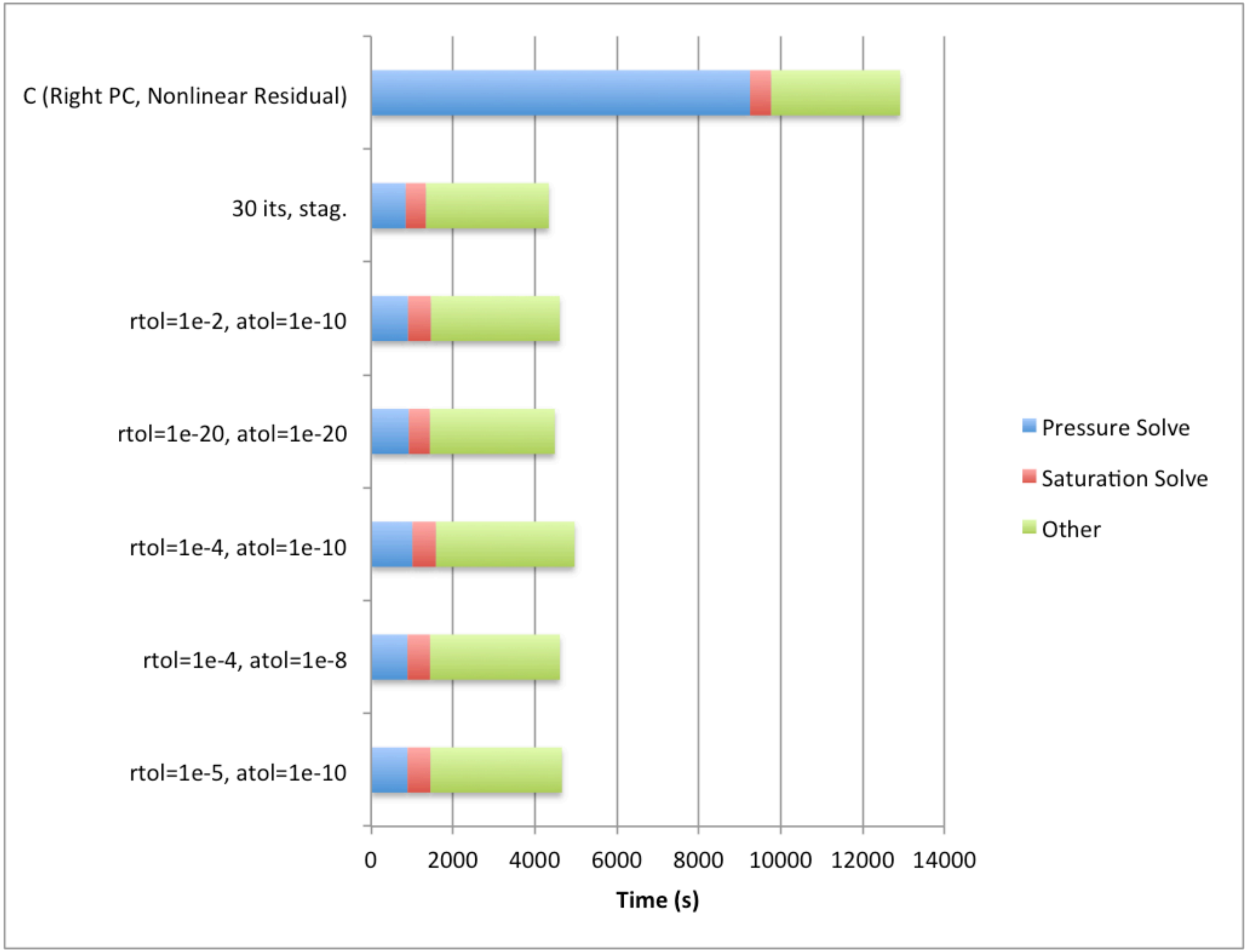


Simulation Results (cont.)

- Varying GMRES Tolerances

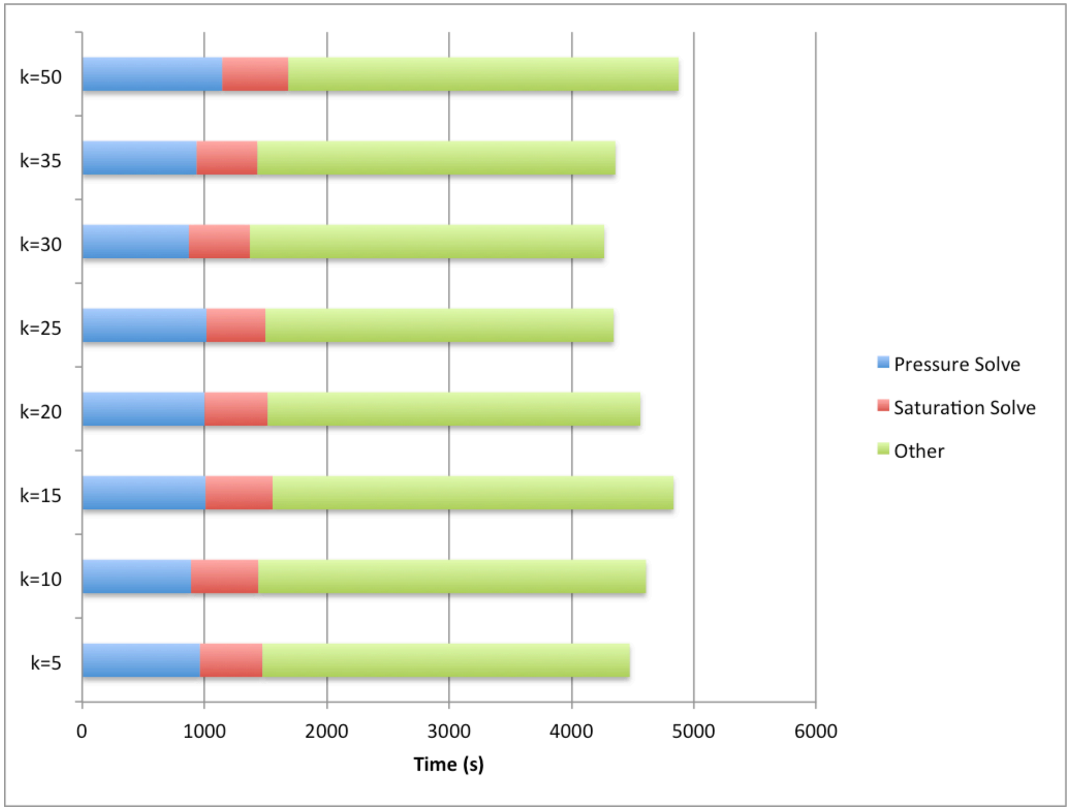


Simulation Results (cont.)



Simulation Results (cont.)

- Varying Restart Parameter

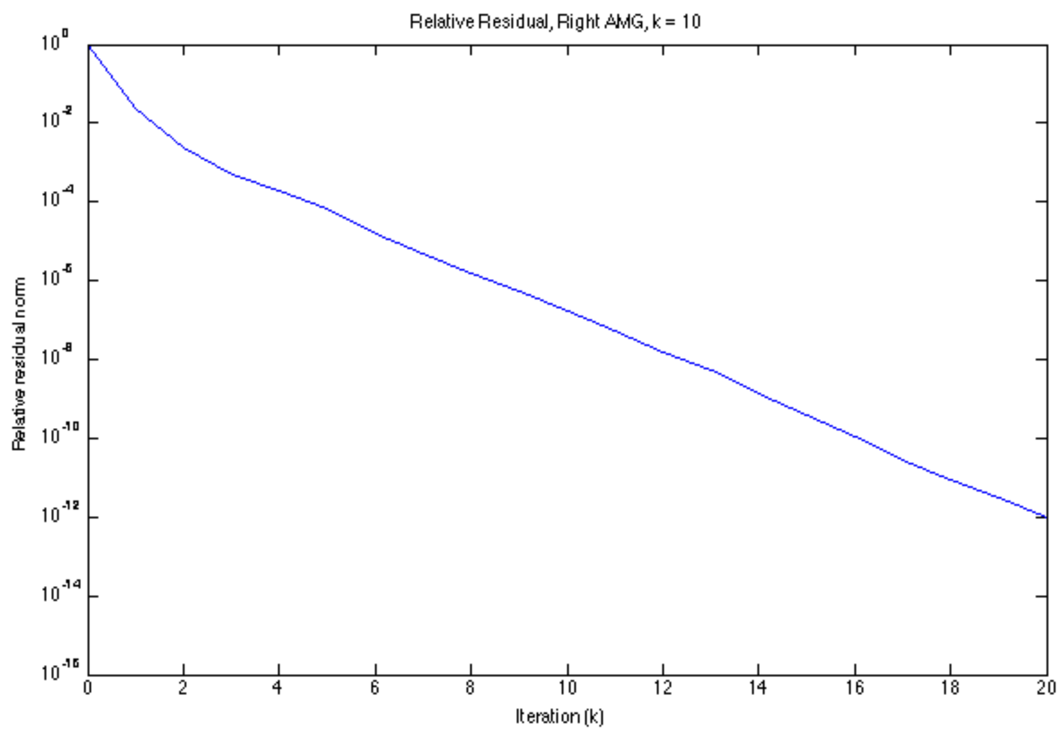


Simulation Results (cont.)

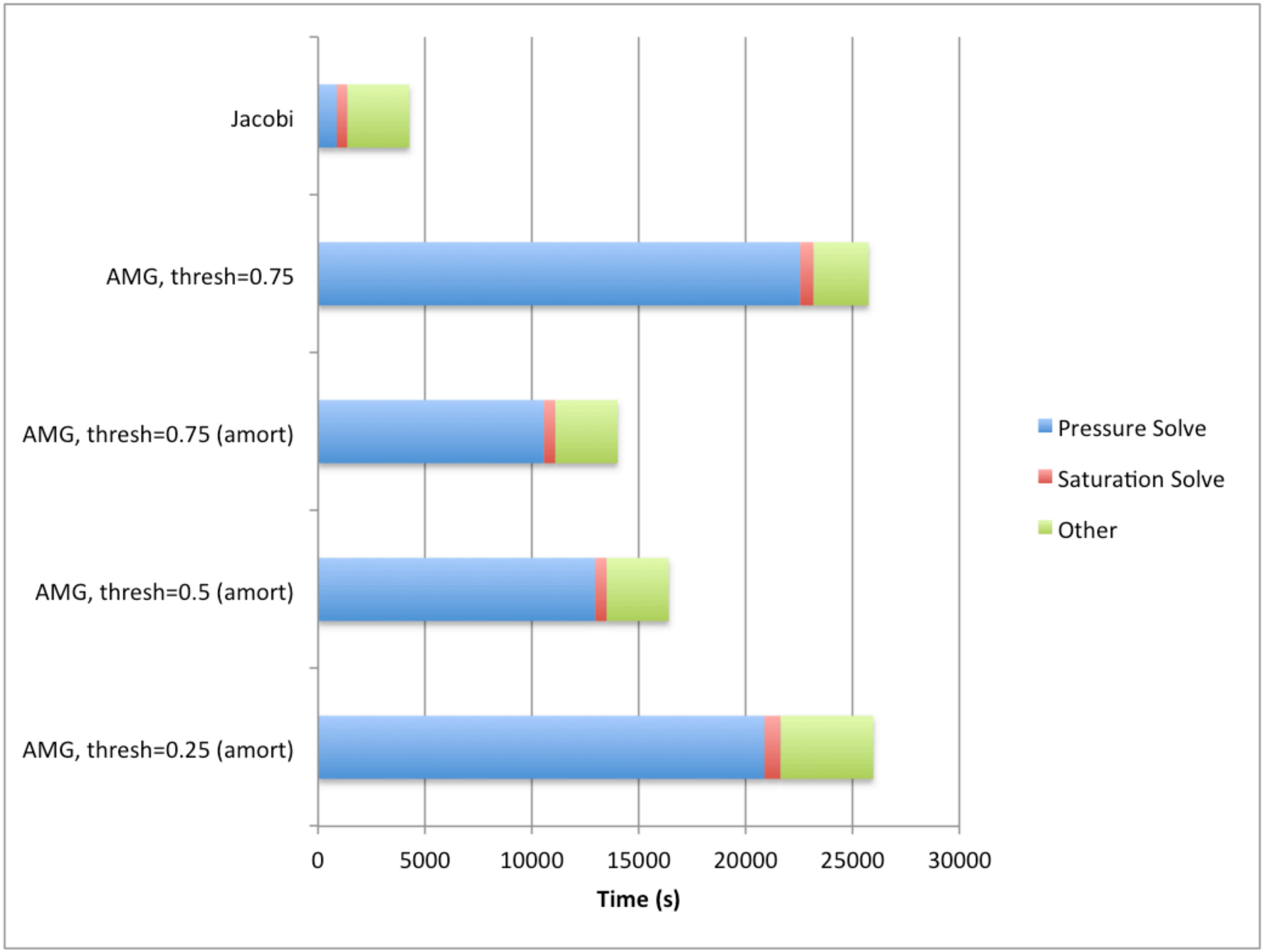
- Jacobi vs AMG
  - “Amortize” construction
  - Experiment with strength threshold

Simulation Results (cont.)

- AMG convergence



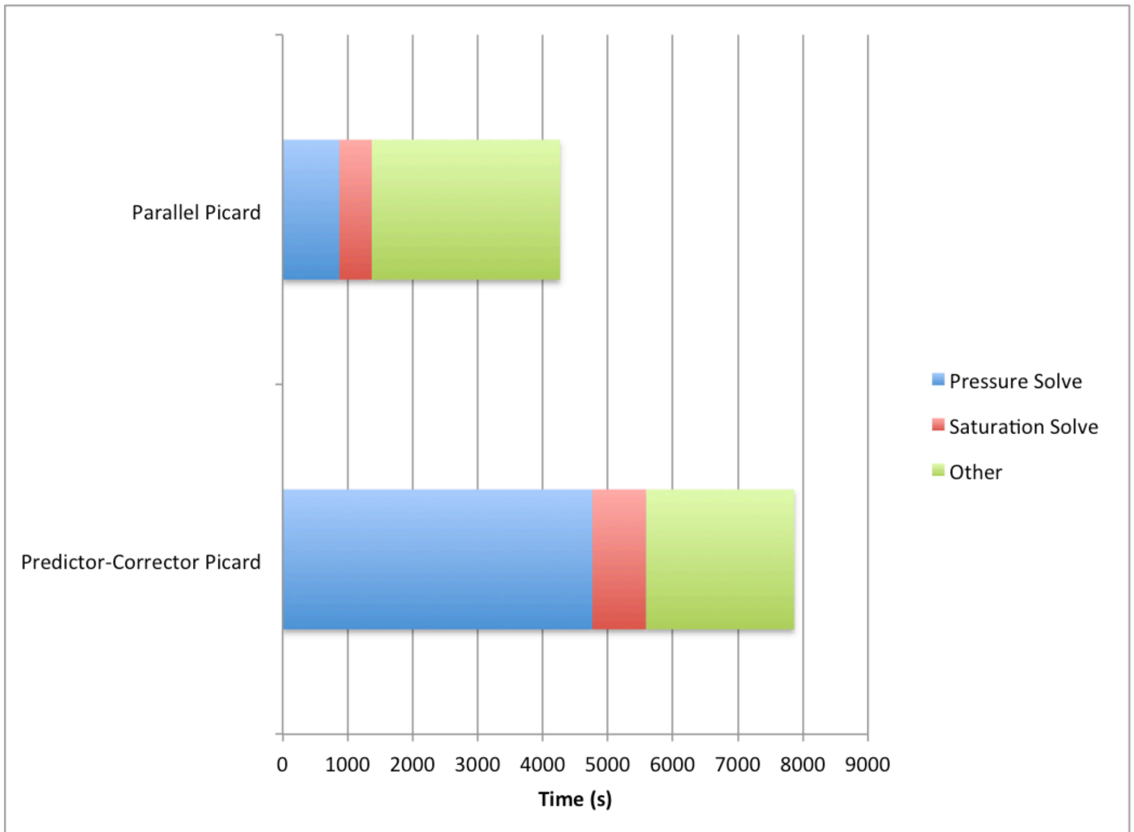
Simulation Results (cont.)

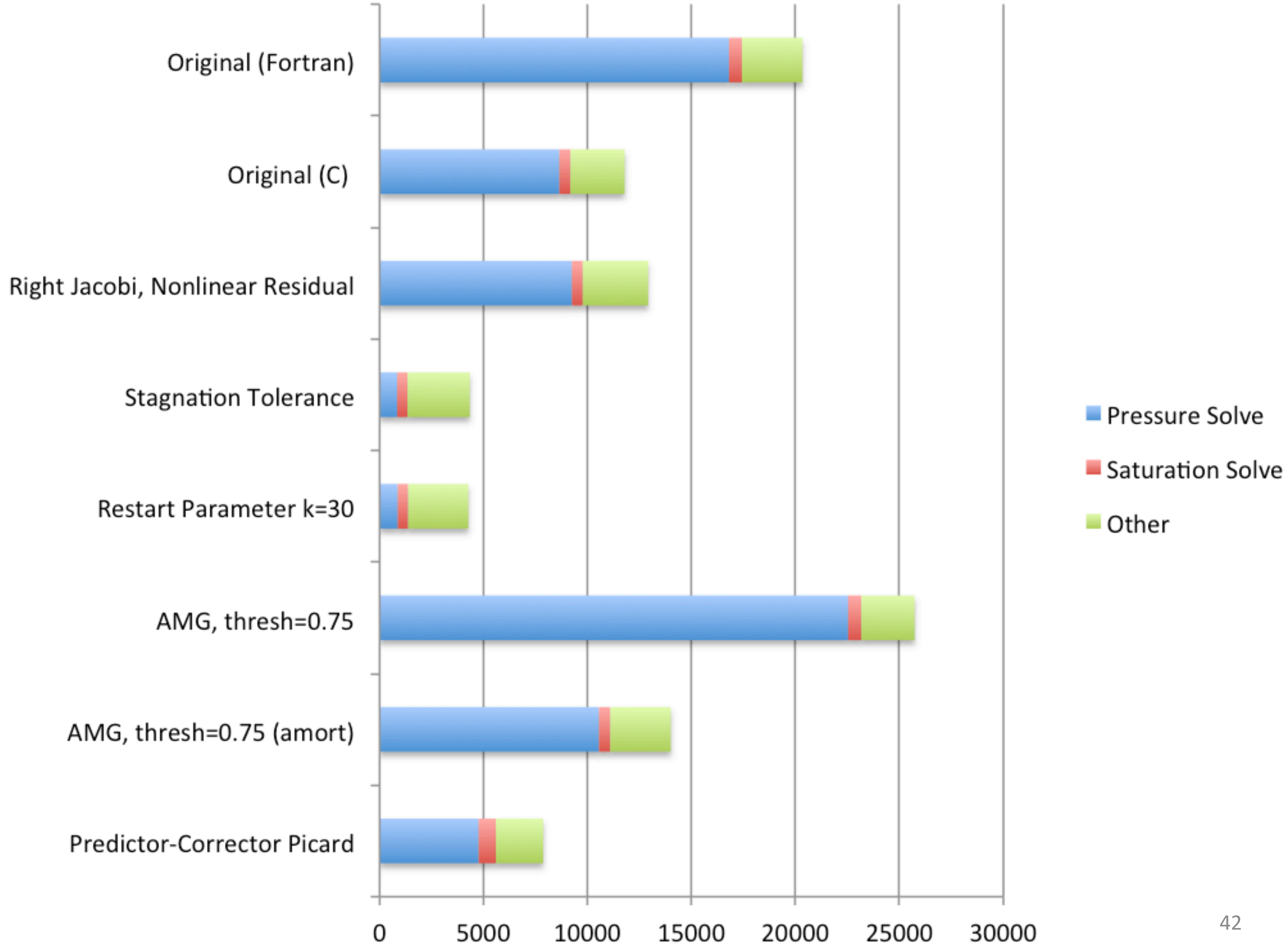


[20] V. E. Henson and U. M. Yang, Boomeramg: a parallel algebraic multigrid solver and preconditioner, Applied Numerical Mathematics, 41 (2000), pp. 155–177.

Simulation Results (cont.)

- Alternative Linearization




Original (Fortran)
Original (C)
Right Jacobi, Nonlinear Residual
Stagnation Tolerance
Restart Parameter k=30
AMG, thresh=0.75
AMG, thresh=0.75 (amort)
Predictor-Corrector Picard
0
5000
10000
15000
20000
25000
30000
Pressure Solve
Saturation Solve
Other

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Conclusion

- Summary of Results
  - C, right Jacobi, stagnation, restart
    - 4.75x speed-up on one test problem, 6.25x on another
    - Stagnation tolerance single biggest improvement
  - AMG, restructure
    - Increased runtime
    - Restructure: difference norm O(1e-2)

Conclusion (cont.)

- Future work
  - Validation
  - Jacobi vs AMG
    - Streamline saturation update?

U. Trottenberg, C. Oosterlee, and A. Schüller, Multigrid, Academic Press, 2001.

Thank You!

- Acknowledgements
- Questions?

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Extra Slides

- Assumptions
- Variables

Assumptions

- Isothermal system
- Viscosity independent of pressure
- Pore space does not change with time
- Fluid saturations account totally for pore volume
- Liquid compressibility constant

Variables

- Pressure – P_α
- Saturation – S_α
- Porosity – ϕ
- Density – ρ_α
- Velocity – $\mathbf{v}_\alpha$
- Source/Sink – q_α
- Intrinsic soil permeability – $\boldsymbol{\kappa}$
- Relative permeability – $k_{r\alpha}$
- Viscosity – μ_α