Opportunities for reducing communication and improving adaptivity in nonlinear multigrid methods

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This talk: http://59A2.org/files/20140915-UCDenver.pdf

Plan: ruthlessly eliminate communication

- Eliminate, not “aggregate and amortize”

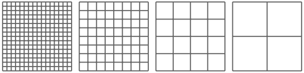
Why?

- Local recovery despite global coupling
- Tolerance for high-frequency load imbalance
  - From irregular computation or hardware error correction
- More scope for dynamic load balance

Requirements

- Must retain optimal convergence with good constants
- Flexible, robust, and debuggable

Multigrid Preliminaries



Multigrid is an $O(n)$ method for solving algebraic problems by defining a hierarchy of scale. A multigrid method is constructed from:

1. a series of discretizations
   - coarser approximations of the original problem
   - constructed algebraically or geometrically
2. intergrid transfer operators
   - residual restriction I_h^H (fine to coarse)
   - state restriction $\hat{I}_h^H$ (fine to coarse)
   - partial state interpolation I_H^h (coarse to fine, 'prolongation')
   - state reconstruction $\mathbb{I}_H^h$ (coarse to fine)
3. Smoothers (S)
   - correct the high frequency error components
   - Richardson, Jacobi, Gauss-Seidel, etc.
   - Gauss-Seidel-Newton or optimization methods

τ formulation of Full Approximation Scheme (FAS)

- classical formulation: “coarse grid *accelerates* fine grid $\searrow\nearrow$
- τ formulation: “fine grid feeds back into coarse grid” $\nearrow\searrow$
- To solve $Nu = f$, recursively apply

$$\begin{aligned}
\text{pre-smooth} \quad & \tilde{u}^h \leftarrow S^h_{\text{pre}}(u^h_0, f^h) \\
\text{solve coarse problem for } u^H \quad & N^H u^H = \underbrace{I^H_h f^h}_{f^H} + \underbrace{N^H \hat{I}^H_h \tilde{u}^h - I^H_h N^h \tilde{u}^h}_{\tau^H_h} \\
\text{correction and post-smooth} \quad & u^h \leftarrow S^h_{\text{post}}\left(\tilde{u}^h + I^h_H(u^H - \hat{I}^H_h \tilde{u}^h), f^h\right)
\end{aligned}$$

I^H_h	residual restriction	$\hat{I}^H_h$	solution restriction
I^h_H	solution interpolation	$f^H = I^H_h f^h$	restricted forcing
$\{S^h_{\text{pre}}, S^h_{\text{post}}\}$	smoothing operations on the fine grid		

- At convergence, $u^{H*} = \hat{I}^H_h u^{h*}$ solves the τ-corrected coarse grid equation $N^H u^H = f^H + \tau^H_h$, thus τ^H_h is the “fine grid feedback” that makes the coarse grid equation accurate.
- τ^H_h is *local* and need only be recomputed where it becomes stale.
- Interpretation by Achi Brandt in 1977, many tricks followed

Model problem: $\mathfrak{p}$-Laplacian with slip boundary conditions

- 2-dimensional model problem for power-law fluid cross-section

$$-\nabla\cdot\left(|\nabla u|^{\mathfrak{p}-2}\nabla u\right) - f = 0, \qquad 1 \le \mathfrak{p} \le \infty$$

  Singular or degenerate when $\nabla u = 0$

- Regularized variant

$$-\nabla\cdot(\eta\nabla u) - f = 0$$

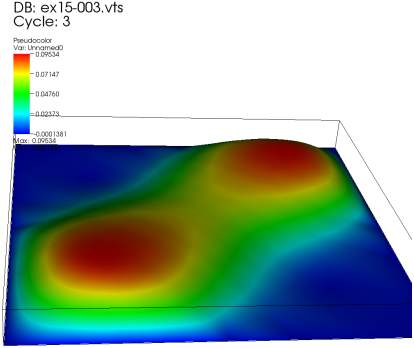
$$\eta(\gamma) = (\varepsilon^2 + \gamma)^{\frac{\mathfrak{p}-2}{2}} \qquad \gamma(u) = \frac{1}{2}|\nabla u|^2$$

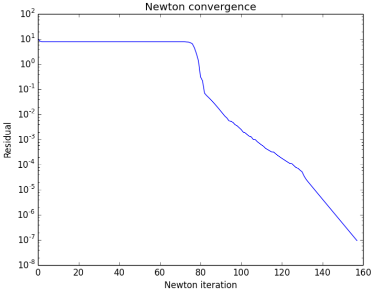
- Friction boundary condition on one side of domain

$$\nabla u \cdot n + A(x)\,|u|^{q-1}\,u = 0$$

Model problem: $\mathfrak{p}$-Laplacian with slip boundary conditions

- $\mathfrak{p} = 1.3$ and $q = 0.2$, checkerboard coefficients $\{10^{-2}, 1\}$
- Friction coefficient $A = 0$ in center, 1 at corners





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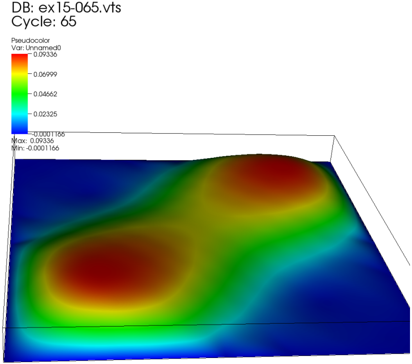

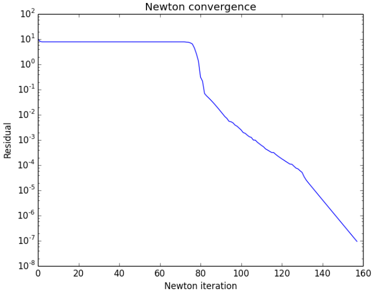

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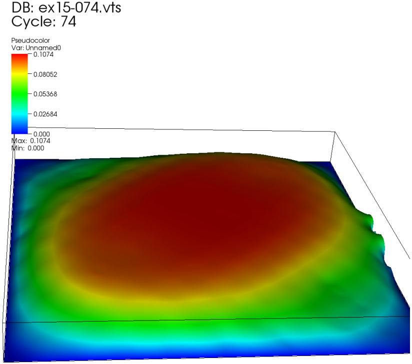

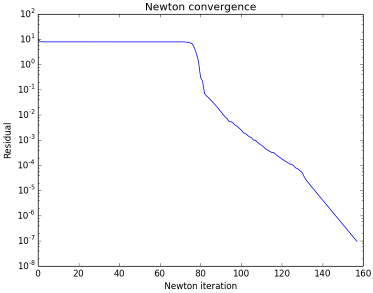

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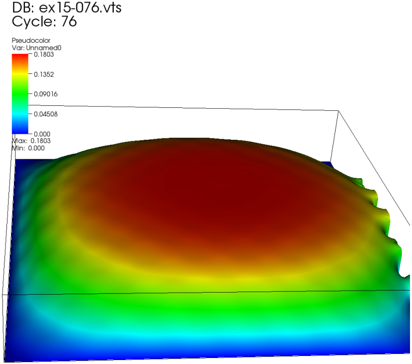

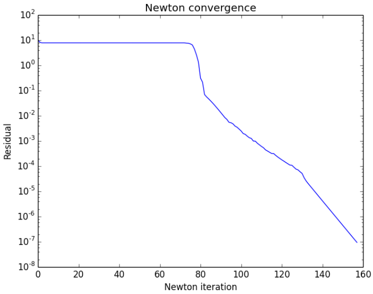

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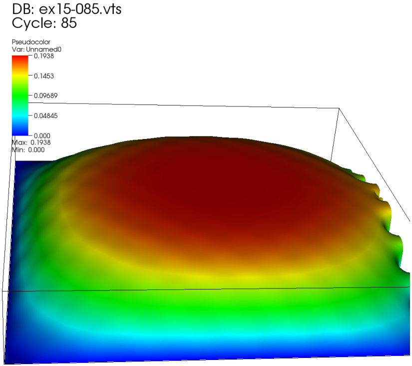

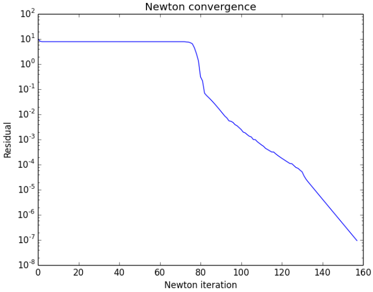

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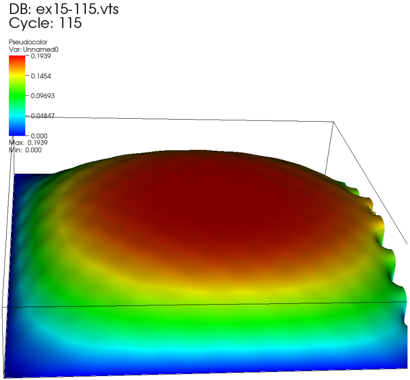
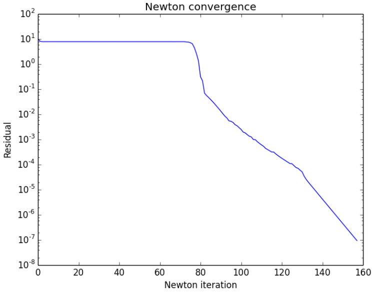
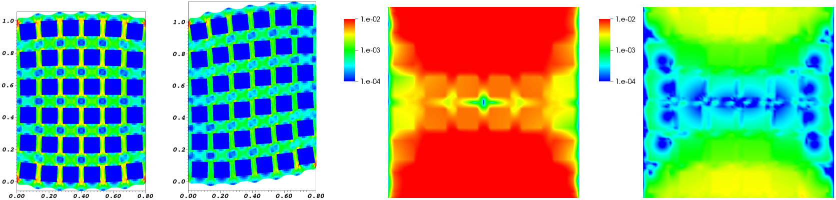




τ corrections



- Plane strain elasticity, $E = 1000, \nu = 0.4$ inclusions in $E = 1, \nu = 0.2$ material, coarsen by 3^2.
- Solve initial problem everywhere and compute $\tau_h^H = A^H \hat{I}_h^H u^h - I_h^H A^h u^h$
- Change boundary conditions and solve FAS coarse problem

$$N^H \acute{u}^H = \underbrace{I_h^H \acute{f}^h}_{\acute{f}^H} + \underbrace{N^H \hat{I}_h^H \tilde{u}^h - I_h^H N^h \tilde{u}^h}_{\tau_h^H}$$

- Prolong, post-smooth, compute error $e^h = \acute{u}^h - (N^h)^{-1} \acute{f}^h$
- Coarse grid *with* τ is nearly $10\times$ better accuracy

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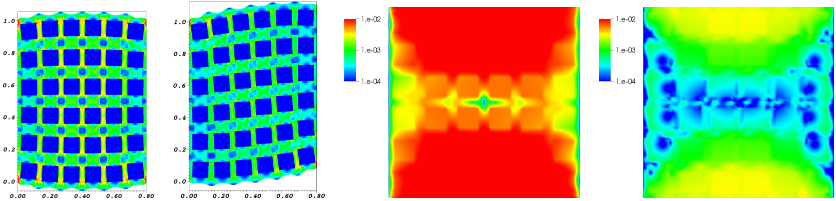

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τ adaptivity: an idea for heterogeneous media

- Applications with localized nonlinearities
  - Subduction, rifting, rupture/fault dynamics
  - Carbon fiber, biological tissues, fracture
- Adaptive methods fail for heterogeneous media
  - Rocks are rough, solutions are not “smooth”
  - Cannot build accurate coarse space without scale separation
- τ adaptivity
  - Fine-grid work needed everywhere at first
  - Then τ becomes accurate in nearly-linear regions
  - Only visit fine grids in “interesting” places: active nonlinearity, drastic change of solution

Comparison to nonlinear domain decomposition

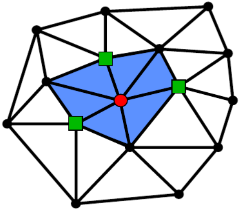
- ASPIN (Additive Schwarz preconditioned inexact Newton)
  - Cai and Keyes (2003)
  - More local iterations in strongly nonlinear regions
  - Each nonlinear iteration only propagates information locally
  - Many real nonlinearities are activated by long-range forces
    - locking in granular media (gravel, granola)
    - binding in steel fittings, crack propagation
  - Two-stage algorithm has different load balancing
    - Nonlinear subdomain solves
    - Global linear solve
- τ adaptivity
  - Minimum effort to communicate long-range information
  - Nonlinearity sees effects as accurate as with global fine-grid feedback
  - Fine-grid work always proportional to “interesting” changes

Nonlinear and matrix-free smoothing

- matrix-based smoothers require global linearization
- nonlinearity often more efficiently resolved locally
- nonlinear additive or multiplicative Schwarz
- nonlinear/matrix-free is good if

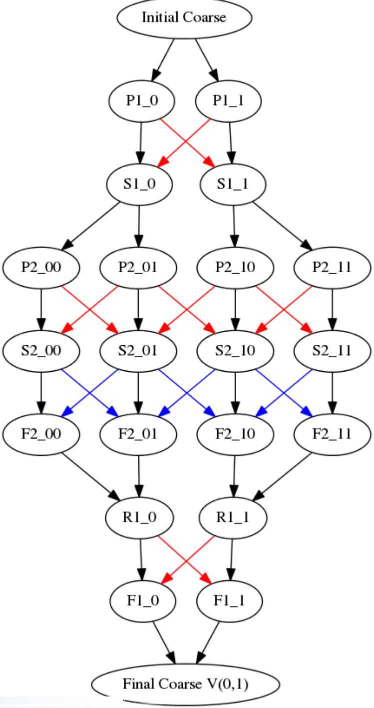
$$C = \frac{(\text{cost to evaluate residual at one “point”}) \cdot N}{(\text{cost of global residual})} \sim 1$$

  - finite difference: $C < 2$
  - finite volume: $C \sim 2$, depends on reconstruction
  - finite element: $C \sim$ number of vertices per cell
- larger block smoothers help reduce C
- additive correction (Jacobi/Chebyshev/multi-stage)
  - global evaluation, as good as $C = 1$
  - but, need to assemble corrector/scaling
  - need spectral estimates or wave speeds



Low communication MG

- red arrows can be removed by τ-FAS with overlap
- blue arrows can also be removed, but then algebraic convergence stalls when discretization error is reached
- no simple way to check that discretization error is obtained
- if fine grid state is not stored, use compatible relaxation to complete prolongation P
- “Segmental refinement” by Achi Brandt (1977)
- 2-process case by Brandt and Diskin (1994)

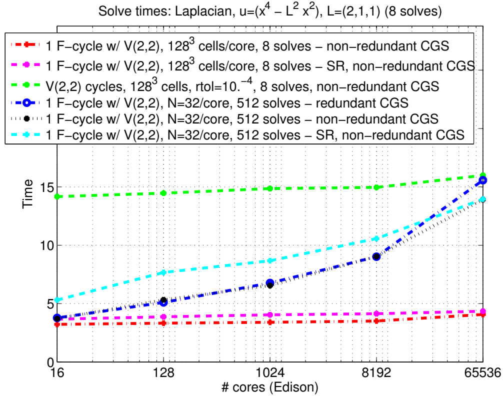


Segmental refinement: no horizontal communication

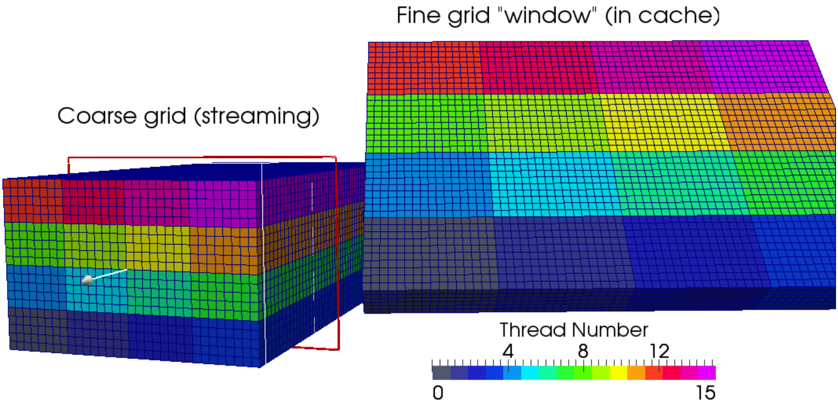
- 27-point second-order stencil, manufactured analytic solution
- 5 SR levels: 16^3 cells/process local coarse grid
- Overlap $=$ Base $+ (L - \ell)$Increment
  - Implementation requires even number of cells—round down.
- FMG with $V(2,2)$ cycles

Table: $\|e_{SR}\|_\infty / \|e_{FMG}\|_\infty$

	Base		
Increment	1	2	3
1	1.59	2.34	1.00
2	1.00	1.00	1.00
3	1.00	1.00	1.00



Reducing memory bandwidth



- Sweep through “coarse” grid with moving window
- Zoom in on new slab, construct fine grid “window” in-cache
- Interpolate to new fine grid, apply pipelined smoother (*s*-step)
- Compute residual, accumulate restriction of state and residual into coarse grid, expire slab from window

Arithmetic intensity of sweeping visit

- Assume 3D cell-centered, 7-point stencil
- 14 flops/cell for second order interpolation
- $\geq$ 15 flops/cell for fine-grid residual or point smoother
- 2 flops/cell to enforce coarse-grid compatibility
- 2 flops/cell for plane restriction
- assume coarse grid points are reused in cache
- Fused visit reads u^H and writes $\hat{I}_h^H u^h$ and $I_h^H r^h$
- Arithmetic Intensity

$$\frac{\overbrace{15}^{\text{interp}} + \overbrace{2\cdot(15+2)}^{\text{compatible relaxation}} + \overbrace{2\cdot 15}^{\text{smooth}} + \overbrace{15}^{\text{residual}} + \overbrace{2}^{\text{restrict}}}{3\cdot \texttt{sizeof(scalar)} / \underbrace{2^3}_{\text{coarsening}}} \gtrsim 30 \qquad (1)$$

- Still $\gtrsim$ 10 with non-compressible fine-grid forcing

Regularity

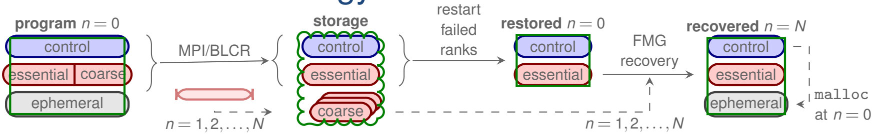
Accuracy of recovery depends on operator regularity

- Even with regularity, we can only converge up to discretization error, unless we add a *consistent* fine-grid residual evaluation
- Visit fine grid with some overlap, but patches do not agree exactly in overlap
- Need decay length for high-frequency error components (those that restrict to zero) that is bounded with respect to grid size
- Required overlap J is proportional to the number of cells to cover decay length
- Can enrich coarse space along boundary, but causes loss of coarse-grid sparsity
- Brandt and Diskin (1994) has two-grid LFA showing $J \lesssim 2$ is sufficient for Laplacian
- With L levels, overlap $J(k)$ on level k,

$$2J(k) \geq s(L-k+1)$$

where s is the smoothness order of the solution or the discretization order (whichever is smaller)

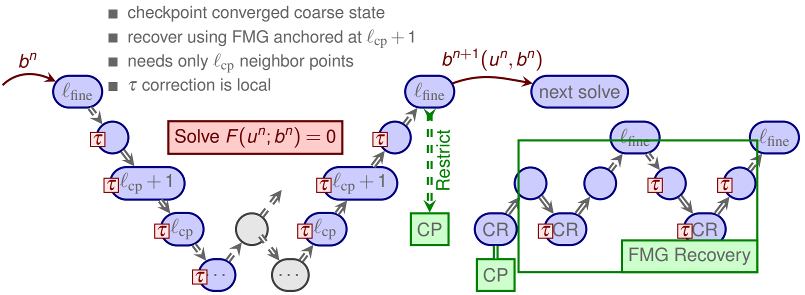
Basic resilience strategy



control	contains program stack, solver configuration, etc.
essential	program state that cannot be easily reconstructed: time-dependent solution, current optimization/bifurcation iterate
ephemeral	easily recovered structures: assembled matrices, preconditioners, residuals, Runge-Kutta stage solutions

- Essential state at time/optimization step n is inherently globally coupled to step $n-1$ (otherwise we could use an explicit method)
- *Coarse* level checkpoints are orders of magnitude smaller, but allow rapid recovery of essential state
- FMG recovery needs only nearest neighbors

Multiscale compression and recovery using τ form



- Normal multigrid cycles visit all levels moving from $n \rightarrow n+1$
- FMG recovery only accesses levels finer than ℓ_{CP}
- Lightweight checkpointing for transient adjoint computation
- Postprocessing applications, e.g., in-situ visualization at high temporal resolution in part of the domain

First-order cost model for FAS resilience

Extend first-order locality-unaware model of Young (1974):

- t_{W} time to write a heavy fine-grid checkpointed state
- t_{R} time to read back lost state
- R fraction of forward simulation needed for recomputation from a saved state
- P the heavy checkpoint interval
- M mean time to failure

Neglect cost of I/O for lightweight coarse-grid checkpoints

$$\text{Overhead} = 1 - \text{AppUtilization} = \underbrace{\frac{t_{\mathrm{W}}}{P}}_{\text{writing}} + \underbrace{\frac{t_{\mathrm{R}}}{M}}_{\text{reading after failure}} + \underbrace{\frac{RP}{2M}}_{\text{recomputation}}$$

Minimized for a heavy checkpointing interval $P = \sqrt{2Mt_{\mathrm{W}}/R}$

$$\text{Overhead}^* = \sqrt{2t_{\mathrm{W}}R/M} + t_{\mathrm{R}}/M$$

where the first term is always larger than the second. Conventional checkpointing schemes store only fine-grid state, thus $R = 1$ (recovery costs the same as initial computation).

Other uses

- Transient adjoints
  - Adjoint model runs backward-in-time, needs state from solution of forward model
  - Status quo: hierarchical checkpointing
  - Memory-constrained and requires computing forward model multiple times
  - If forward model is stiff, each step has global dependence
  - Compression via τ-FAS accelerates recomputation, can be local
- Visualization and analysis
  - Targeted visualization in small part of domain
  - Interesting features emergent so can't predict where to look

Outlook on τ-FAS adaptivity and compression

- Benefits of AMR without fine-scale smoothness
- Coarse-centric restructuring is a major interface change
- Nonlinear smoothers (and discretizations)
  - Smooth in neighborhood of “interesting” fine-scale features
  - Which discretizations can provide efficient matrix-free smoothers?
  - Does there exist an efficient smoother based on element Neumann problems?
- Dynamic load balancing
- Reliability of error estimates for refreshing τ
  - We want a coarse indicator for whether τ needs to change
- Worthwhile for resilience and to better use hardware