# Multigrid

#### optimal solvers for linear and nonlinear elliptic PDEs

Ed Bueler

UAF Math 692 Scalable Seminar

Spring 2023

### Outline



- 2 simple iterations?
- 2-grid method, and the coarse-grid correction
  - V-cycle multigrid
- 5 nonlinear multigrid

### a linear PDE problem



• 
$$\nabla^2$$
 is a negative-definite operator

#### 1. Poisson problem

for a given source function f(x, y), find u(x, y) so that

$$-
abla^2 u = f ext{ on } \Omega, \qquad u \big|_{\partial \Omega} = 0$$



#### a nonlinear PDE problem

- the second problem is nonlinear, but still elliptic
- claim 1. the area of surface z = v(x, y) over  $\Omega$  is

$$I[v] = \int_{\Omega} \sqrt{1 + |\nabla v|^2} \, dx \, dy$$

• claim 2. for given g, continuous along  $\partial \Omega$ ,

$$u = \min_{\{v : v \mid \partial \Omega = g\}} I[v]$$

solves the boundary value problem below

### 2. minimal surface problem

for given boundary function (wire frame) g(x, y), find u(x, y) so that

$$-\nabla \cdot \left( rac{
abla u}{\sqrt{1+|
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ight) = 0 \ ext{on } \Omega, \qquad u\big|_{\partial\Omega} = g$$



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#### finite difference discretization

- PDEs are infinite-dimensional problems, but discretization yields finite systems of equations
- for example, finite differences (FD):

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2)$$



- grid spacings:  $h_x = \frac{1}{m_x 1}$ ,  $h_y = \frac{1}{m_y 1}$
- grid points:  $(x_i, y_j) = (ih_x, jh_y)$  for  $i = 0, ..., m_x - 1$  and  $j = 0, ..., m_y - 1$
- 5-point stencil for the Laplacian:

$$\nabla^2 u(x_i, y_j) \approx \frac{u_{i-1,j} - 2u_{ij} + u_{i+1,j}}{h_x^2} + \frac{u_{i,j-1} - 2u_{ij} + u_{i,j+1}}{h_y^2}$$





### $\mathsf{PDE} \implies \mathsf{linear system } A \mathbf{u} = \mathbf{b}$

• FD discretize  $-\nabla^2 u = f$ :

- o note we keep the boundary values in the system
- $N = m_x m_y$  total unknowns on the grid
  - $m_x = 4, m_y = 3$  shown at right
- unknowns  $\{u_{ij}\}$  are globally ordered:  $u_{\ell} = u_{ij}$
- get a linear system for  $\mathbf{u} \in \mathbb{R}^N$ :



•  $A \in \mathbb{R}^{N \times N}$  is sparse

- A has positive diagonal
- A is symmetric positive definite
- A has O(1) nonzeros per row  $\leftarrow$  at most 5, actually

•  $\mathbf{b} \in \mathbb{R}^N$  has entries  $b_\ell = f(x_i, y_j)$ 

- for  $m_x = m_y = 5$ : 9 non-trivial eqns (middle right)
- for  $m_x = m_y = 8$ : 36 non-trivial eqns (lower right)





• the linear system  $A\mathbf{u} = \mathbf{b}$  can be set-up using 6N memory locations

- A has 5 nonzero entries per row, plus one entry of b
- can we solve  $A \mathbf{u} = \mathbf{b}$  in O(N) work and time as  $N \to \infty$ ?
  - o if so, the solver is optimal

• *A* is banded, with bandwidth  $\approx \min\{m_x, m_y\} \approx \sqrt{N}$ • so banded Gaussian elimination will solve in  $O(N^2)$ 

• let's back up and ask:

what operations using our A are obviously O(N)?

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### cheap O(N) operations: mat-vec and residual

for A from PDE discretization, we can compute Av in O(N) flops
 this is because A has O(1) nonzero entries per row

• also the residual is O(N)

#### Definition

given  $\mathbf{v} \in \mathbb{R}^N$ , the *residual* for the linear system  $A\mathbf{u} = \mathbf{b}$  is

$$\mathbf{r}(\mathbf{v}) = \mathbf{b} - A\mathbf{v}$$

observe that:

$$A\mathbf{u} = \mathbf{b} \iff \mathbf{r}(\mathbf{u}) = \mathbf{0}$$

## are simple iterations cheap O(N) operations?

#### Definition

for the linear system  $A\mathbf{u} = \mathbf{b}$  and an invertible matrix  $M \in \mathbb{R}^{N \times N}$ , simple iteration is

$$\mathbf{v}_{k+1} = \mathbf{v}_k + \alpha M^{-1} \underbrace{(\mathbf{b} - A\mathbf{v}_k)}_{=\mathbf{r}(\mathbf{v}_k)}$$

•  $\alpha \in \mathbb{R}$  is a tuning parameter, with default  $\alpha = 1$ 

• if M = A and  $\alpha = 1$  then  $\mathbf{v}_{k+1} = \mathbf{u}$ , so one iteration solves it!

• ... not practical, and usually not O(N)

- *Richardson iteration*  $\mathbf{v}_{k+1} = \mathbf{v}_k + \alpha \mathbf{r}(\mathbf{v}_k)$  is the M = I case
  - observation: Richardson iteration for the Poisson equation is *gradient* descent for the quadratic functional  $I[v] = \alpha \int_{\Omega} \frac{1}{2} |\nabla v|^2 fv$
  - each Richardson iteration is clearly O(N) work
- a simple iteration is  $O(N) \dots$  if M is the right kind of matrix!

#### Definition

if a matrix or linear map  $M \in \mathbb{R}^{N \times N}$  is invertible, we say

$$M^{-1}Au = M^{-1}b$$

is a *(left-) preconditioned* system for  $A \mathbf{u} = \mathbf{b}$ 

- the preconditioned system has the same solutions as before
- the new residual is  $\tilde{\mathbf{r}}(\mathbf{v}) = M^{-1}\mathbf{b} M^{-1}A\mathbf{v}$
- observation: Richardson iteration on the new system is equivalent to simple iteration

$$\mathbf{v}_{k+1} = \mathbf{v}_k + \alpha \, \tilde{\mathbf{r}}(\mathbf{v}) \quad \iff \quad \mathbf{v}_{k+1} = \mathbf{v}_k + \alpha \, M^{-1} \, (\mathbf{b} - A \mathbf{v}_k)$$

### Definition

a matrix or linear map *M* is a *fast preconditioner* if solving  $M\mathbf{z} = \mathbf{c}$  requires O(N) work

- example: if A has nonzero diagonal entries, the diagonal M = D is a fast preconditioner
- do *not* actually form the matrix  $M^{-1}$  when solving  $M\mathbf{z} = \mathbf{c}$
- warning: a preconditioner *M* can be fast without being a useful tool!
- preconditioning is an apparently simple idea, but in the 21st century it is used all over the space of solvers

### O(N) simple iterations: Jacobi and Gauss-Seidel

• suppose we split A into diagonal and triangular parts:

$$A = D + L + U$$

• the linear system can be rearranged using the splitting:

$$A \mathbf{u} = \mathbf{b} \iff D\mathbf{u} = \mathbf{b} - (L+U)\mathbf{u}$$
  
 $\iff \mathbf{u} = \mathbf{u} + D^{-1}(\mathbf{b} - A\mathbf{u})$ 

• solving 
$$D\mathbf{z} = \mathbf{c}$$
 is  $O(N)$ 

#### Definition

a Jacobi iteration applies a fast preconditioner:

$$\mathbf{v}_{k+1} = \mathbf{v}_k + D^{-1}(\mathbf{b} - A\mathbf{v}_k)$$

### O(N) simple iterations: Jacobi and Gauss-Seidel

• suppose we split A into diagonal and triangular parts:

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$$A \mathbf{u} = \mathbf{b} \iff (D+L)\mathbf{u} = \mathbf{b} - U\mathbf{u}$$
  
 $\iff \mathbf{u} = \mathbf{u} + (D+L)^{-1}(\mathbf{b} - A\mathbf{u})$ 

• solving  $(D + L)\mathbf{z} = \mathbf{c}$  is O(N) (for our A)

#### Definition

a Gauss-Seidel (GS) iteration applies a fast preconditioner:

$$\mathbf{v}_{k+1} = \mathbf{v}_k + (D+L)^{-1}(\mathbf{b} - A\mathbf{v}_k)$$

#### example of Gauss-Seidel iteration

the matrix-splitting view obscures the simplicity of Gauss-Seidel? *example*: consider the linear system Au = b with

$$A = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_N \end{bmatrix}$$

o in this case, Gauss-Seidel iteration computes

$$v_{j}^{[k+1]} = \frac{b_{j}}{2} + \frac{1}{2} \left( v_{j-1}^{[k+1]} + v_{j+1}^{[k]} \right)$$

- this is a *relaxation* method ... update *v<sub>j</sub>* using average of neighbors
- one can prove this method converges
- $\circ~$  this example is relevant because A  $\sim -\nabla^2$  in 1D

#### Jacobi and Gauss-Seidel iterations as solvers

- for the Poisson problem linear system Au = b, one can prove that Gauss-Seidel and Jacobi converge
- but, after initial progress, residual norm decrease is *agonizingly slowly* on fine grids
- these simple iterations stagnate
- an iteration v<sub>k+1</sub> = φ(v<sub>k</sub>) stagnates or stalls if the ratio of successive residual norms {||r(v<sub>k+1</sub>)||/|r(v<sub>k</sub>)||} goes to one



• Achi Brandt, an inventor of multigrid:

Stalling numerical processes must be wrong. Whenever the computer grinds very hard for small or slow effect, there must be a better way to achieve the same goal.

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#### Jacobi and Gauss-Seidel iterations as smoothers

- observation: functions become much smoother after a few iterations
- the first multigrid paper (Federenko, 1961) observed this?



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### grid transfers

 multiple grid resolutions will allow us to exploit smoothers to generate fast solutions, but we need grid transfer operators between the different grids



- for a function v defined on a finer grid, define its restriction Rv to a coarser grid to be its value on the coarse grid points (*injection*), or restrict by averaging onto the coarser grid (*full weighting*)
- for a function **w** defined on the coarser grid, define its *prolongation Pw* to a finer grid by (linear) *interpolation*
- *R*, *P* are linear operators
  - R, P are rectangular (non-square) matrices
  - RP = I, or approximately so

### 2-arid method

put these ideas together!

• the 2-grid method approximately solves the PDE on the finer grid:

```
def twogrid(v,pre=2,post=2):
    for k in range(pre):
         v = smooth(A, b, v)
    rc = restrict(b - A * v)
    ec = solve(Ac, rc)
                              # solve error equation
    v = v + prolong(ec)
    for k in range(post):
         v = smooth(A, b, v)
    return v
```

#### where

A,b = discretize(m,m) # fine grid Ac, \_ = discretize(m/2,m/2) # coarse grid

- smooth() does one Jacobi or GS iteration
- solve () might be Gaussian elimination, etc., for  $A^c e^c = r^c$

- what do I mean by the error equation?
- for the linear system  $A\mathbf{u} = \mathbf{b}$ , consider some  $\mathbf{v}$  which is *not* a solution

### Definition

for any vector  $\mathbf{v}$ , the *error equation* corresponding to the linear system  $A\mathbf{u} = \mathbf{b}$  is the equation

$$Ae = r(v)$$

• here's the logic:

$\mathbf{e} = \mathbf{u} - \mathbf{v}$	definition of the error		
$A \mathbf{e} = A \mathbf{u} - A \mathbf{v}$	multiply by A		
$A \mathbf{e} = \mathbf{b} - A \mathbf{v} = \mathbf{r}(\mathbf{v})$	error equation		

#### the coarse grid correction

- the essential 3 lines in twogrid() form a coarse-grid correction:
  - ec = solve(Ac, rc)v = v + prolong(ec)
- rc = restrict(b A\*v) # restrict the residual
  - # coarse-grid solve
    - # add back as correction
- this is a kind of simple iteration:  $\mathbf{v} \leftarrow \mathbf{v} + P(A^c)^{-1}R(\mathbf{b} A\mathbf{v})$
- define the coarse-grid correction matrix:

$$B^c = P(A^c)^{-1}R$$

so twogrid() mixes two flavors of simple iteration:

 $\mathbf{v} \leftarrow \mathbf{v} + M^{-1}(\mathbf{b} - A\mathbf{v})$ the smoother  $\mathbf{v} \leftarrow \mathbf{v} + B^c (\mathbf{b} - A\mathbf{v})$ the coarse-grid correction

• Q is  $B^c \approx A^{-1}$ ?

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 $\begin{aligned} \mathbf{v} \leftarrow \mathbf{v} + M^{-1}(\mathbf{b} - A\mathbf{v}) & the \, smoother \\ \mathbf{v} \leftarrow \mathbf{v} + B^c(\mathbf{b} - A\mathbf{v}) & the \, coarse-grid \, correction \end{aligned}$ 

• Q: is  $B^c \approx A^{-1}$ ?

#### A: yes, but only for smooth inputs

#### 2-grid method: the effect on error

• look at twogrid() again:

```
def twogrid(v,pre=2,post=2):
    for k in range(pre):
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    return v
```

• a fairly-quick calculation shows that twogrid() applies a linear operator, which is close to the zero operator, to e = u - v:

$$\mathbf{e} \leftarrow (I - M^{-1}A)^{\text{post}}(I - B^{c}A)(I - M^{-1}A)^{\text{pre}}\mathbf{e}$$

• Q: how should we solve the coarse-grid problem  $A^c e^c = r^c$ ?

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Q: how should we solve the coarse-grid problem A<sup>c</sup>e<sup>c</sup> = r<sup>c</sup>?

- A: if we can have two levels of grids, we can have many!
- when faced with a coarse-grid solve, just do another 2-grid ... and keep going down to some really easy and cheap coarse grid



• restrictions *R* and prolongations *P* are needed in this grid hierarchy

E	b=	Bu	el	er

#### recursive V-cycle

```
def vcycle(b,v,lev,pre=2,post=2):
A,_ = discretize(lev)
if lev == 0:
    return solve(A,b)  # the buck stops here
for k in range(pre):
    v = smooth(A,b,v)
rc = restrict(b - A*v)
ec = vcycle(r,0,lev-1)  # descend a grid level
v = v + prolong(ec)
for k in range(post):
    v = smooth(A,b,v)
return v
```





Multigrid

#### how well does it work?

• so, how well does it work on our Poisson problem  $-\nabla^2 u = f$ ?

absurdly well!

• here is scaling out to m = 4097, when  $N = 1.6 \times 10^7$ 





#### how well does it work?

• so, how well does it work on our Poisson problem  $-\nabla^2 u = f$ ?

- absurdly well!
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#### on multigrid costs: single V-cycle

- let us analyze the work (flops) of applying a single V-cycle
  - note: multiple V-cycles are generally needed to solve the problem

#### Definitions

$$|\Omega^{(k)}| = ($$
number of grid points (unknowns) on grid  $\Omega^{(k)})$ 

 $W_k^{k-1} = \begin{pmatrix} \text{smoother work done on grid } \Omega^{(k)}, \text{ plus cost of} \\ \text{restriction/prolongation to/from next-coarser grid } \Omega^{(k-1)} \end{pmatrix}$ 

 $W_0 = ($ solver work done on the coarsest level)

• *K* = 3 case:



Multigrid

#### on multigrid costs: single V-cycle

total cost of a single V-cycle:

$$\overline{W} = W_{K}^{K-1} + W_{K-1}^{K-2} + \cdots + W_{1}^{0} + W_{0}$$

for 2D grids, each coarse grid is 4 times smaller:

$$|\Omega^{(k-1)}| \approx \frac{1}{4} |\Omega^{(k)}|$$

since smoothers and restriction/prolongation are O(1) per grid point:

$$W_k^{k-1} \leq C |\Omega^{(k)}|$$

• for some C independent of k

• since  $N = |\Omega^{(K)}|$  is the number of points in the finest grid,

$$\begin{split} \overline{W} &\leq C |\Omega^{(K)}| + C |\Omega^{(K-1)}| + \dots + C |\Omega^{(1)}| + W_0 \\ &\approx CN \left( 1 + \frac{1}{4} + \dots + \frac{1}{4^{K-1}} \right) + W_0 \\ &\approx CN \frac{1}{1 - (1/4)} = \frac{4}{3}CN \quad \text{optimal} \end{split}$$



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### multigrid variations

• there are many variations on linear multigrid:

- choose different smoothers (● is pre-smoother, is post-smoother)
- $\circ~$  choose different values for  ${\tt pre}~{\tt and}~{\tt post}~{\tt smoother}$  iterations
- choose different coarse-grid solvers (□)
- repeat the coarse-grid correction a couple of times (W cycles)



#### • multigrid combines three conceptual threads:

- a few classical iterations, such as Jacobi and GS, are cheap smoothers of the residual and the error
- a coarse-grid correction does a good job of updating the fine-grid solution when acting on a smooth residual
- the coarse-grid correction is cheap because restriction and prolongation are cheap
- but the Poisson problem is too easy!

#### minimal surfaces, a nonlinear problem



#### minimal surface problem

for given boundary function (wire frame) g(x, y), find u(x, y) so that

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ight) = 0 \, ext{ on } \Omega, \qquad u \big|_{\partial\Omega} = g$$

#### discretization gets you ... more general equations

• at each point  $(x_i, y_j)$  on the target (finest) grid  $\Omega^{(K)}$  we discretize to get an FD approximation of the PDE:

$$f_{ij}(u_{i-1,j}, u_{i+1,j}, u_{i,j-1}, u_{i,j+1}, u_{i,j}) = 0$$

- o roughly-speaking, anyway ... see details next slide
- unknowns must be globally-ordered into a vector  $\mathbf{u} \in \mathbb{R}^N$ :

$$U_{\ell} = U_{i,j}$$

where  $\ell = \ell(i, j)$  is a global-to-local indexing function

nonlinear discretization principle enforcing the PDE at grid point ( $x_i$ ,  $y_j$ ) gives one scalar equation  $f_{ij}(\mathbf{u}) = 0$ 

also globally-order the equations (functions), *f*<sub>ℓ</sub>(**u**) = *f*<sub>ij</sub>(**u**), to get a nonlinear system of *N* scalar equations in *N* scalar unknowns:

$$\mathbf{F}(\mathbf{u}) = \mathbf{0}$$

• **F** is a sparse function, as each  $f_{\ell}$  depends on only O(1) entries of **u** 

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#### details: 9-point stencil with staggered diffusivity

• how do you discretize 
$$\nabla \cdot \left( \frac{\nabla u}{\sqrt{1 + |\nabla u|^2}} \right)$$
?

- technique: generalize first!
- discretize  $\nabla \cdot (D(w)\nabla u)$  where

$$D(w) = (1 + w)^{-1/2}$$
$$w = |\nabla u|^2$$

• centered FD, using *staggered* values of D(w), gets  $O(h_x^2 + h_y^2)$  truncation error and symmetry:



$$\nabla \cdot (D(w)\nabla u) \approx \frac{D(w_e)(u_{i+1,j} - u_{i,j}) - D(w_w)(u_{i,j} - u_{i-1,j})}{h_x^2} + \frac{D(w_h)(u_{i,j+1} - u_{i,j}) - D(w_s)(u_{i,j} - u_{i,j-1})}{h_y^2}$$
$$w_e = \left[ |\nabla u|^2 \right]_{i+\frac{1}{2},j} \approx \left( \frac{u_{i+1,j} - u_{i,j}}{h_x} \right)^2 + \left( \frac{u_{i,j+1} + u_{i+1,j+1} - u_{i,j} - u_{i+1,j}}{4h_y} \right)^2$$

#### 9-point stencil Jacobian: sparsity

• on a 6 × 6 grid, the Jacobian  $J(\mathbf{v})$  has this sparsity pattern:



#### Newton's method

Q: how do we solve our nonlinear system F(u) = 0?
 A: Newton's method!:

$$egin{array}{ll} J(\mathbf{u}^{
ho})\,\mathbf{s} = -\mathbf{F}(\mathbf{u}^{
ho}) \ \mathbf{u}^{
ho+1} = \mathbf{u}^{
ho} + \mathbf{s} \end{array}$$

where  $J(\mathbf{v})$  is the Jacobian

$$J(\mathbf{v})_{r,s} = \left[\frac{\partial f_r(\mathbf{v})}{\partial v_s}\right]$$

Q: how do you calculate the Jacobian? (*cause it's a pain in the ...*)
 A: more finite differencing:

$$J(\mathbf{v})_{r,s} \approx \frac{f_r(\mathbf{v} + \epsilon \mathbf{1}_s) - f_r(\mathbf{v})}{\epsilon}$$

A': symbolically?

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#### Newton's method with finite-differenced Jacobian

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Q: how do you calculate the Jacobian? (*cause it's a pain in the ...*)
 A: more finite differencing:

$$J(\mathbf{v})_{r,s} \approx \frac{f_r(\mathbf{v} + \epsilon \mathbf{1}_s) - f_r(\mathbf{v})}{\epsilon}$$

A': symbolically?

• Q: how do you *efficiently* calculate the FD Jacobian? A: graph coloring

Ed Bueler

#### Newton-multigrid

• Q: how do you solve each linear system in the Newton iteration?

A: solve  $J(\mathbf{u}^{p}) \mathbf{s} = -\mathbf{F}(\mathbf{u}^{p})$  using multigrid:

```
def newtonmultigrid(v,lev,maxnewts=50,cycles=1):
    for p in range(maxnewts):
        b = -F(v)
        s = 0
        for _ in range(cycles):
            s = vcycle(b,s,lev)
        v = v + s
    return v
```

o details:

- inside vcycle(), the matrix  $A = A^{(k)}$  on each grid level  $\Omega^{(k)}$  is computed using the Jacobian on that grid level (*rediscretization*)
- the finest-level iterate  $\mathbf{u}^{p}$  must be restricted (injected) down to  $\Omega^{(k)}$ :

$$A^{(k)} = J^{(k)}(R^{K-k}\mathbf{u}^{p})$$

 $\circ~J^{(k)}$  is approximated using FD and graph coloring on  $\Omega^{(k)}$ 

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### nonlinear multigrid F-cycle solvers

- but wait, ... there's more!
- Q: how do you find a good initial iterate u<sup>0</sup> for the Newton iteration?
   A: by solving the problem on a coarser grid, and prolonging
- justification: the domain of Newton convergence is larger on the smaller (= coarser) version of the PDE
- this strategy is called *nested iteration* or *grid sequencing*
- if you also solve at each level with Newton-multigrid, then this is a *nonlinear multigrid F-cycle*...the most powerful solver you've seen!



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#### minimal surface PDE problem: results



#### run-time demo:

- \$ cd p4pdes/c/ch7/
- \$ make minimal
- \$ mpiexec -n 6 ./minimal -snes\_fd\_color -pc\_type mg \
   -{snes,ksp}\_converged\_reason -snes\_grid\_sequence 10

<sup>-</sup>snes\_monitor\_solution draw -mg\_levels\_{snes,ksp}\_converged\_reason

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#### summary

- a multigrid V-cycle combines three conceptual threads to build an optimal solver for linear elliptic PDEs:
  - classical iterations = cheap smoothers
  - coarse-grid correction effective, if starting from a smooth residual
  - restriction and prolongation are cheap

#### there is also algebraic multigrid, but that is a different talk ...

• for nonlinear elliptic PDEs:

wrap a Newton iteration around multigrid V-cycles: Newton-multigrid

- grid sequencing generates a high-quality finest-grid initial iterate
- thus: a nonlinear multigrid F-cycle solver
- Newton-multigrid is not the only nonlinear option ... there is also **full approximation scheme** multigrid, but that is a different talk ...

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Achi Brandt

