

Algebraic Multigrid

Copper Mountain 2019 Tutorial

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<https://github.com/copper-multigrid-conference/2019-tutorials>

A helpful reminder ... projection methods

- **The Problem**

$$Ax = b$$

- Residual

$$r = b - Ax$$

- Subspace

$$V$$

- Finds the “best” approximation

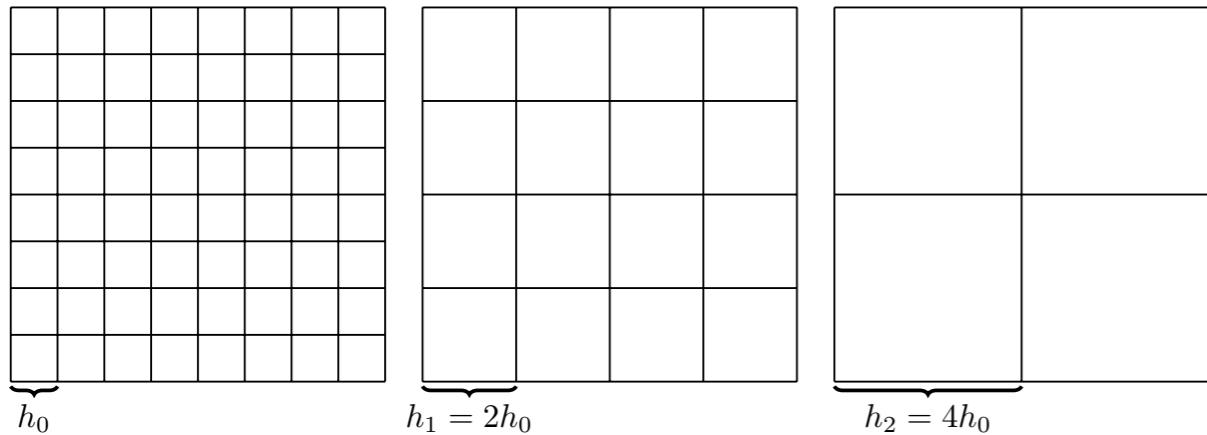
$$x \leftarrow x + V(V^T A V)^{-1} V^T r$$

FEM, CG, Jacobi, Multigrid...

Multigrid Basics

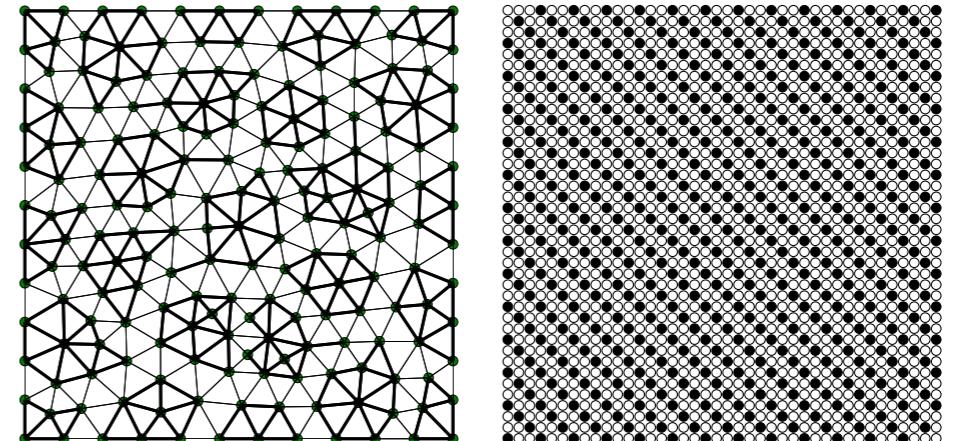
Geometric

- Grids are fixed
- Construct interpolation
- Find the best smoother



Algebraic

- Relaxation method is fixed
- Find coarse grids
- construct interpolation



Two Grid Algorithm

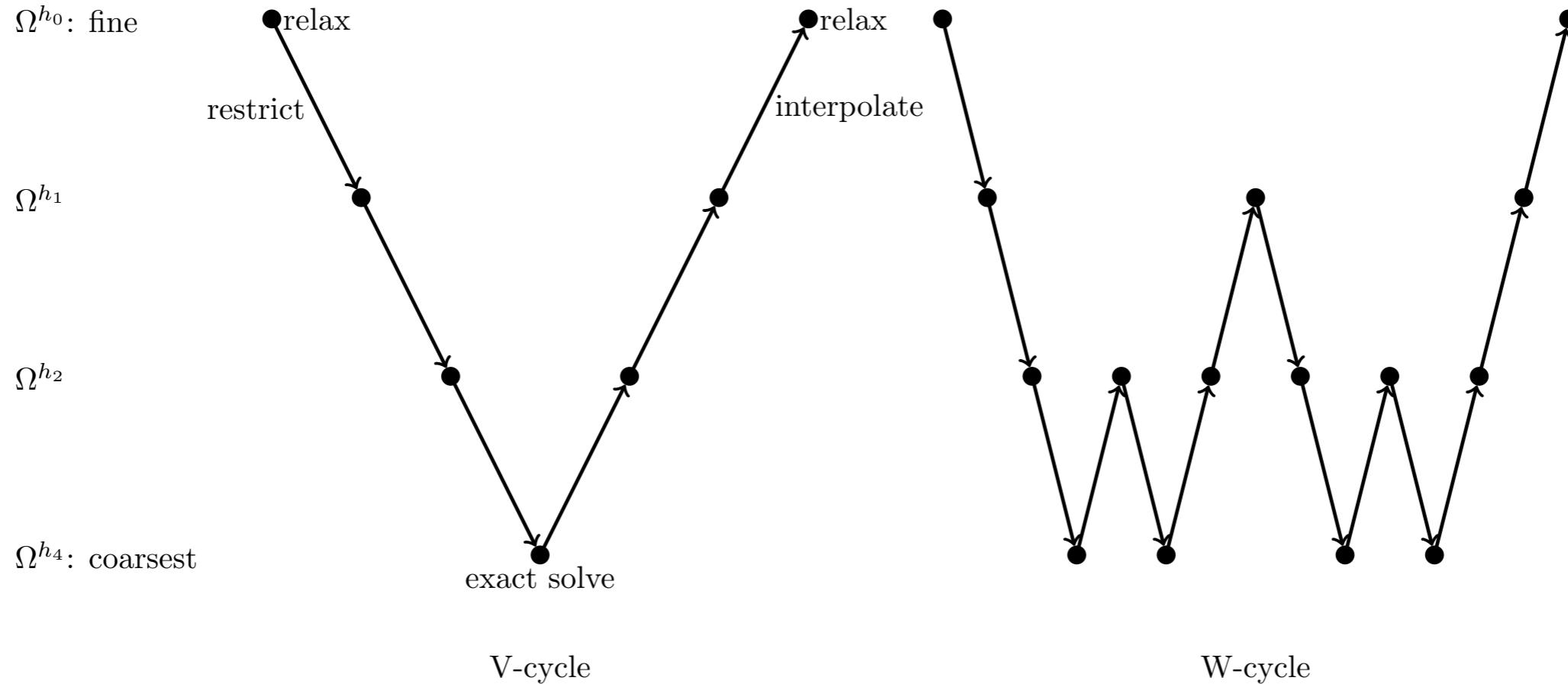
Algorithm 1: CGC

```
1 Input:  $u^h, f^h, \alpha_1$ , and  $\alpha_2$ 
2 Return:  $u^h$ 
3
4  $\omega\text{Jacobi}(A^h, u^h, f^h, \alpha_1)$                                 {pre-relaxation}
5  $r^h = f^h - A^h u^h$                                          {fine-grid residual}
6  $r^{2h} = I_h^{2h} r^h$                                          {restriction}
7 solve  $A^{2h} e^{2h} = r^{2h}$                                      {coarse problem}
8  $u^h \leftarrow u^h + I_{2h}^h e^{2h}$                                {interpolation and correction}
9  $\omega\text{Jacobi}(A^h, u^h, f^h, \alpha_2)$                                 {post-relaxation}
```

- Coarse grid operators
 - Rediscretized
 - Galerkin

$$A_{2h} = RAP = I_h^{2h} A_h I_{2h}^h$$

The Multigrid V-Cycle and W-Cycle



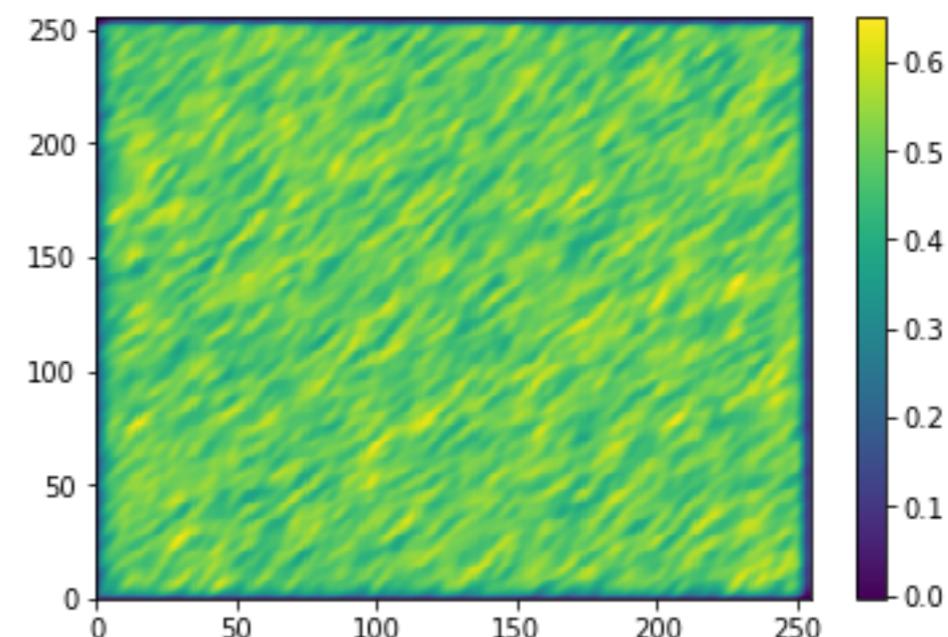
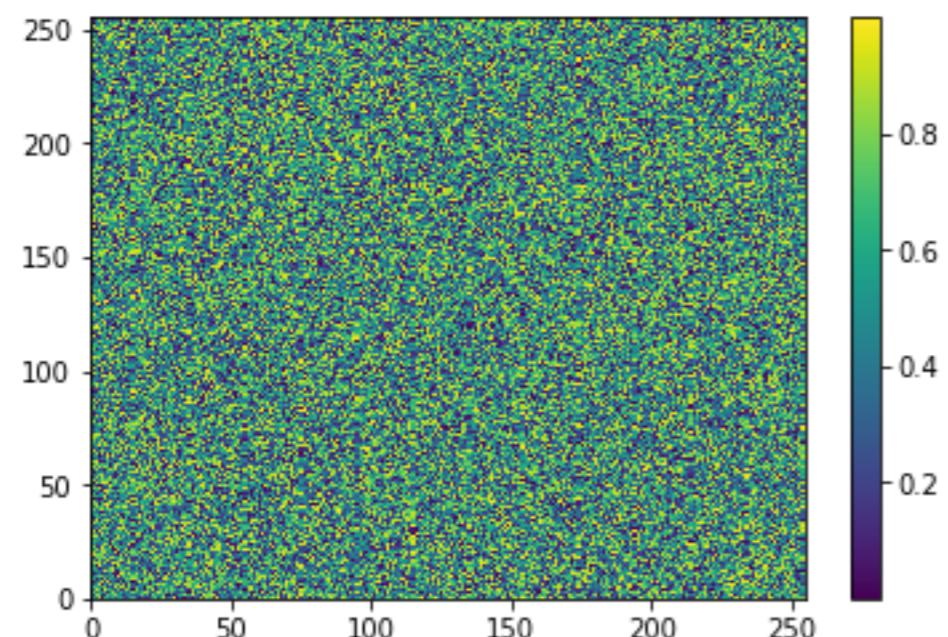
- Two-grid cycle can expose issues with coarser interpolation
- W-Cycle can account for inadequate coarser level solves
- **Exact solve?** Usually a pseudo-inverse

What can go wrong?!

- Demo: [0-multigrid-in-2d.ipynb](#) Consider an *anisotropic problem*

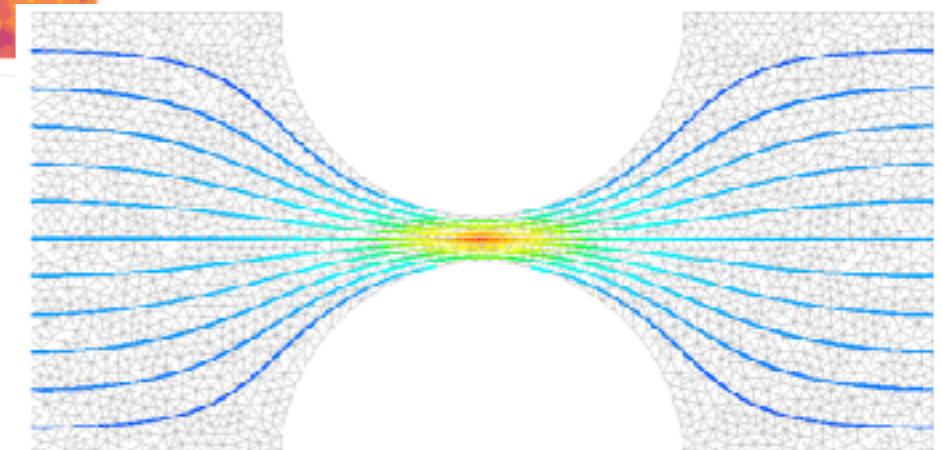
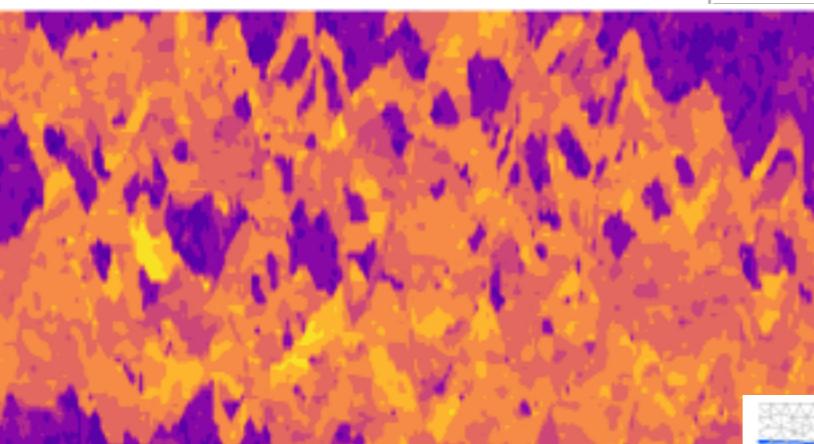
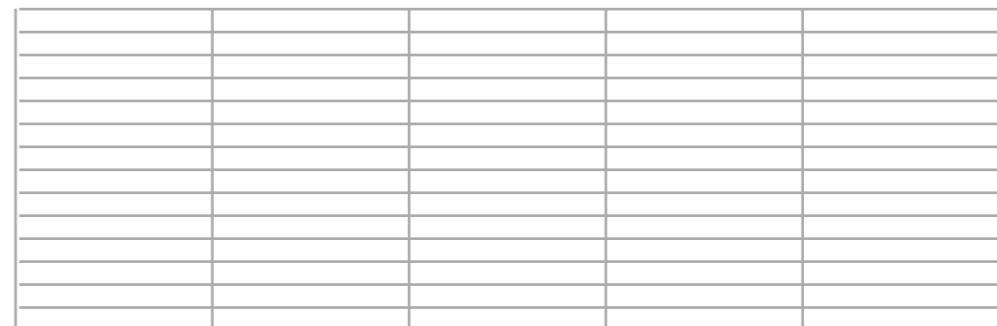
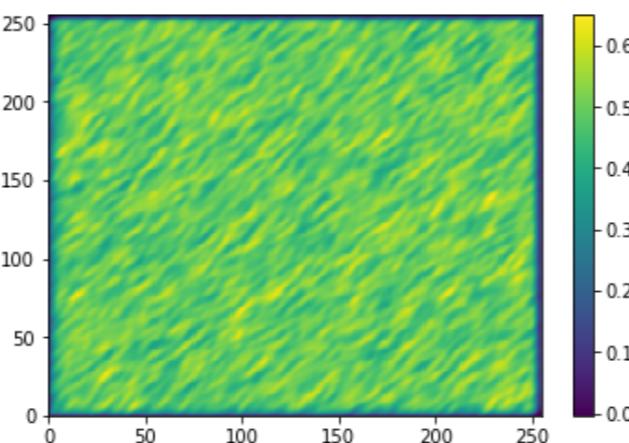
$$-u_{xx} - \epsilon u_{yy} = f$$

$$-\nabla \cdot \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \epsilon \end{bmatrix} \begin{bmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{bmatrix} \nabla u = f$$



What can go wrong?!

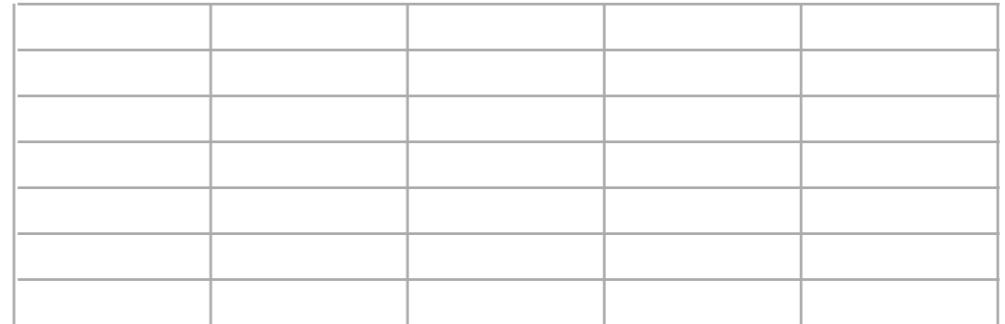
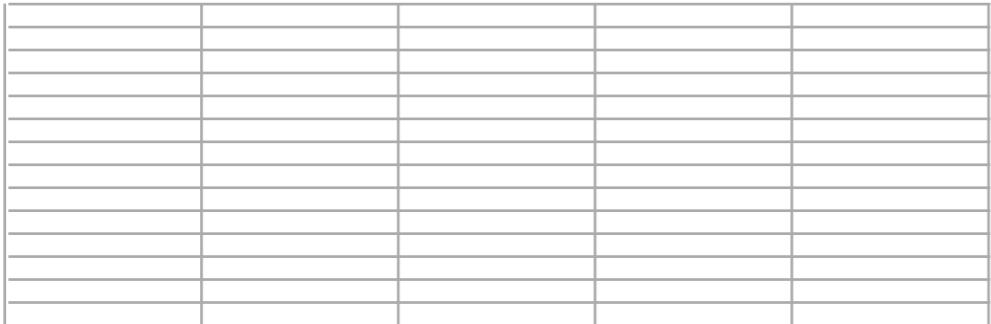
- Anisotropy
- Mesh stretching
- Jumping coefficients
- Non-elliptic



Options for more robust Multigrid

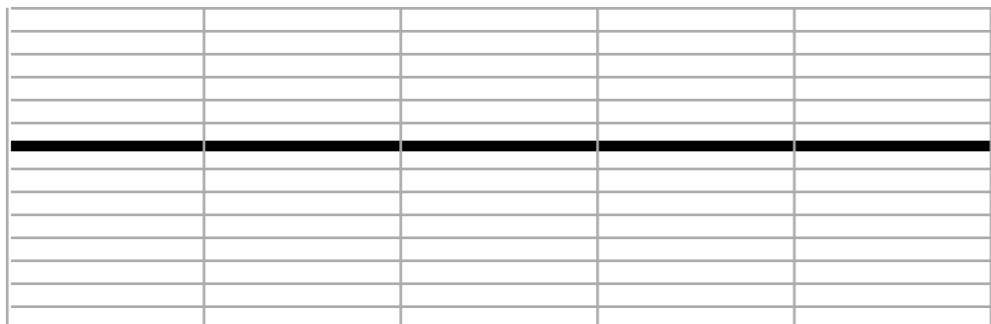
- **Semicoarsening**

Coarsen in the direction of smoothness



- **Line/plane relaxation**

Perform relaxation in groups (in a line)



- **Operator based Interpolation** (e.g. BoxMG)

$$Ae = 0$$

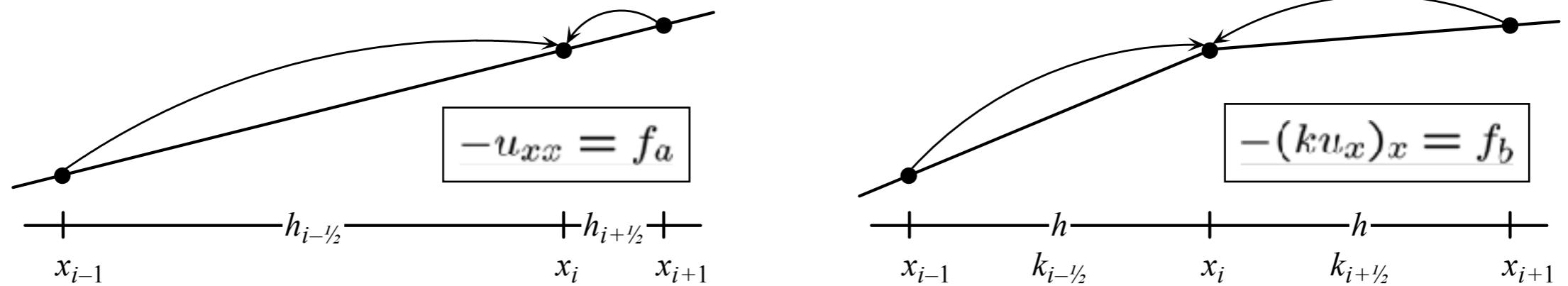
J. E. Dendy, Black box multigrid, J. Comput. Phys., 1982

J. E. Dendy and J. D. Moulton, Black box multigrid with coarsening by a factor of three, J. Numer. Lin. Alg. App., 2010

Algebraic Multigrid (AMG) uses matrix coefficients

- Geometric information alone is not sufficient

Linear Interpolation Operator-Dependent Interpolation

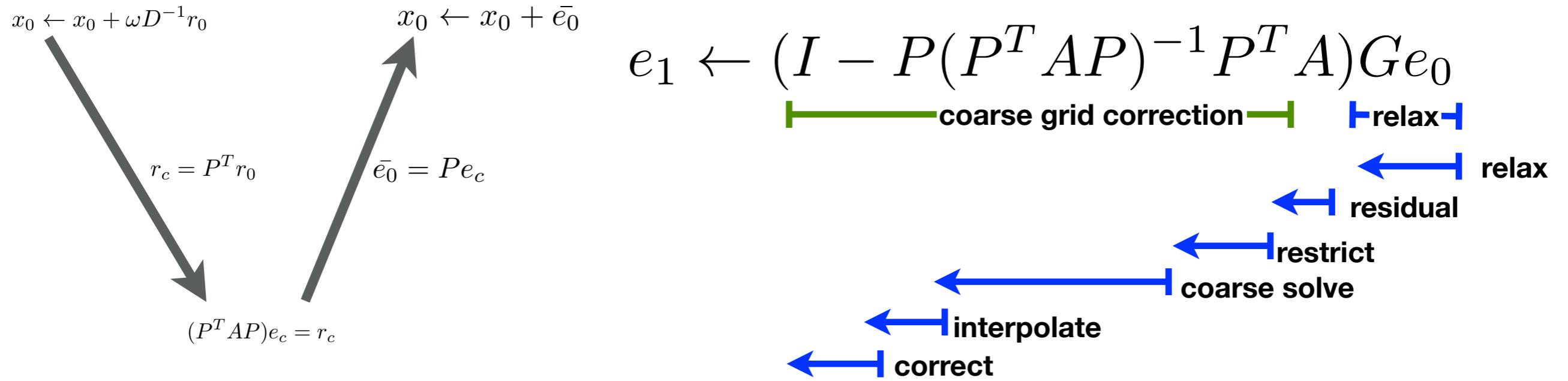


- AMG does not use geometric information, but captures both linear & operator-dep interpolation

$$(A\mathbf{u})_i = a_{i,i-1}u_{i-1} + a_{i,i}u_i + a_{i,i+1}u_{i+1}$$

$$u_i = \left(-\frac{a_{i,i-1}}{a_{i,i}} \right) u_{i-1} + \left(-\frac{a_{i,i+1}}{a_{i,i}} \right) u_{i+1}$$

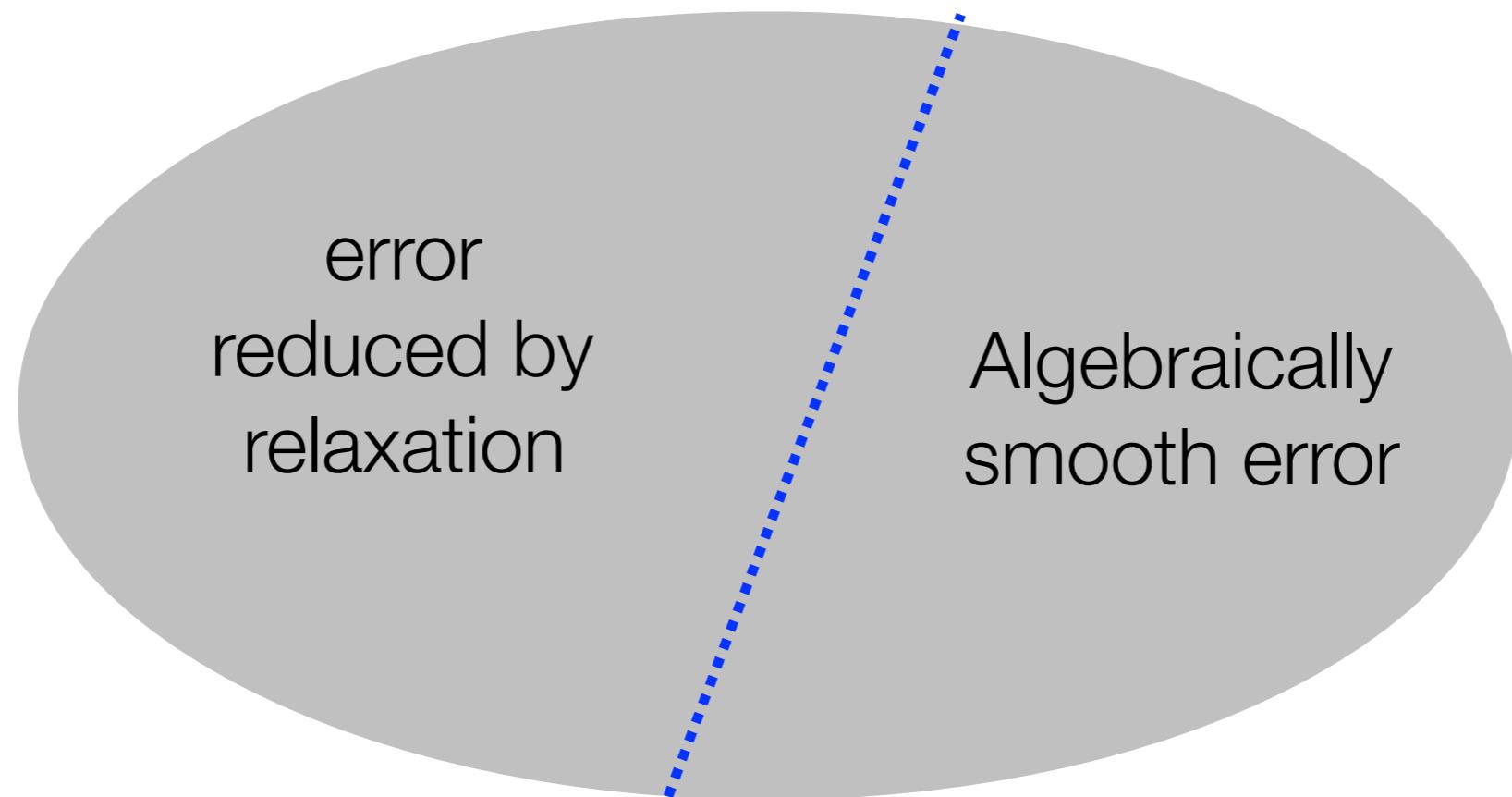
Algebraic Observation



$$Ge_0 \in \mathcal{R}(P) \quad \Rightarrow \quad e_1 = 0$$

interpolation should capture what relaxation misses

Algebraically Smooth Error

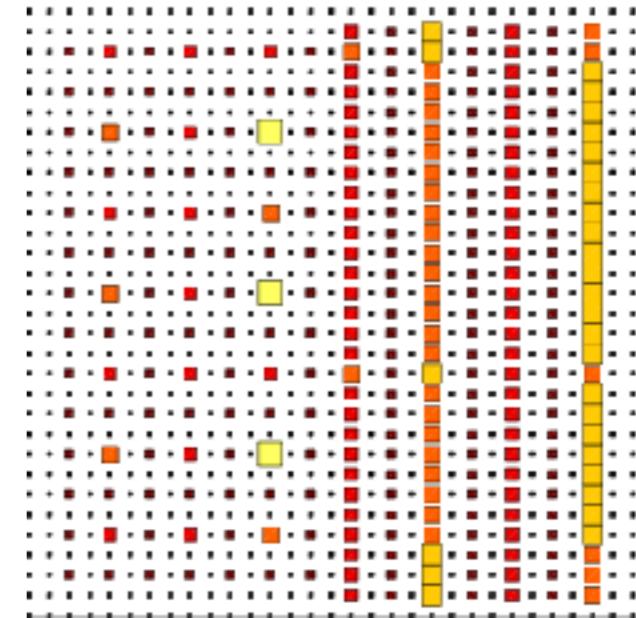
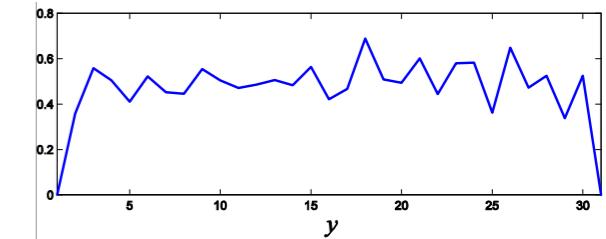
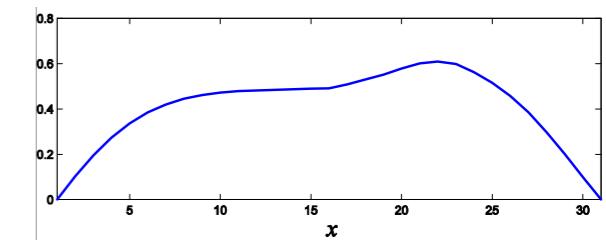
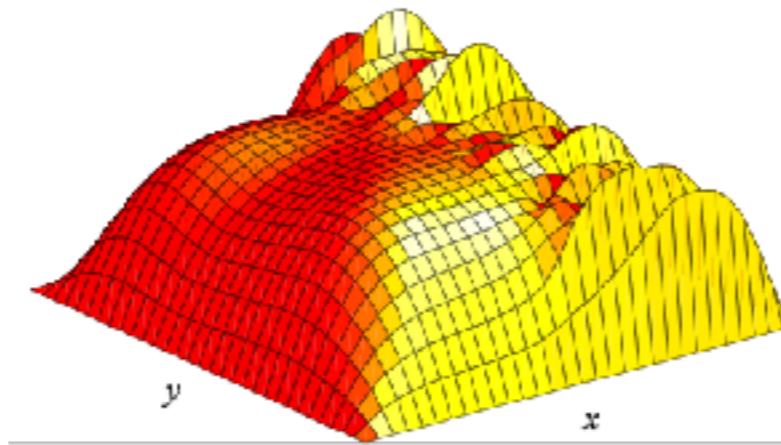


- “**Algebraically smooth**” error may not be geometrically smooth

Error left by relaxation can be geometrically oscillatory

- 7 GS sweeps on
 $-au_{xx} - bu_{yy} = f$

$$\begin{array}{|c|c|} \hline a & b \\ \hline \end{array} \quad \begin{array}{|c|c|} \hline a \gg b \\ \hline \end{array}$$



- Caution: this example
 - targets geometric smoothness
 - uses pointwise smoothers

AMG coarsens grids in the direction of geometric smoothness

Main idea: Algebraically smooth error

- Take a relaxation scheme such as w-Jacobi

$$e \leftarrow (I - M^{-1}A)e$$

- If relaxation stagnates, then the remaining error exhibits poor convergence, so

$$(I - M^{-1}A)e \approx e \Rightarrow M^{-1}Ae \approx 0 \Rightarrow r \approx 0$$

- Formally (characterized by small eigenvalues)

$$\langle Ae, e \rangle \ll 1$$

Main idea: Algebraically smooth error

- We then have $\langle Ae, e \rangle = \sum_i e_i (A_{ii}e_i + \sum_{j \neq i} A_{ij}e_j)$ assume zero row sum
$$\begin{aligned} &= \sum_i e_i \left(\sum_{j \neq i} -A_{ij}(e_i - e_j) \right) \\ &= \sum_{i < j} -A_{ij} \cdot e_i \cdot (e_i - e_j) + \sum_{i > j} -A_{ij} \cdot e_i \cdot (e_i - e_j) \quad \text{swap } i, j \\ &= \sum_{i < j} -A_{ij} \cdot e_i \cdot (e_i - e_j) - \sum_{i < j} -A_{ij} \cdot e_i \cdot (e_i - e_j) \\ &= \sum_{i < j} -A_{ij} \cdot (e_i - e_j)^2 \end{aligned}$$
- Ok, so smooth error varies **slowly** in the direction of large matrix coefficients

Main idea: Algebraically smooth error

- We have assumed **geometric** smoothness to show

$$\mathbf{e}^T A \mathbf{e} = \sum_{i < j} (-a_{ij})(e_i - e_j)^2 \ll 1$$

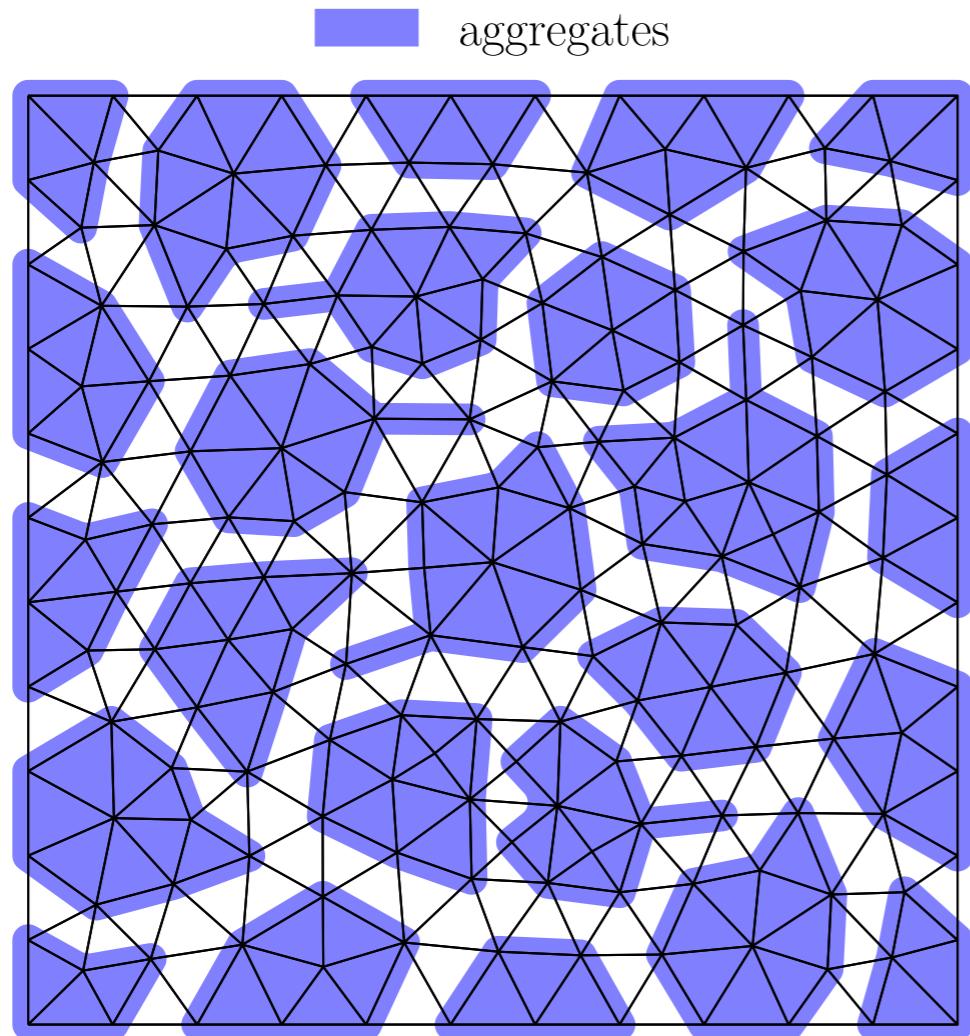
- **CF AMG:** Smooth error varies slowly in the direction of “large” matrix coefficients
- **Strength of connection:** Given a threshold $0 < \theta \leq 1$, we say that variable u_i strongly depends on variable u_j if

$$-a_{ij} \geq \theta \max_{k \neq i} \{-a_{ik}\}$$

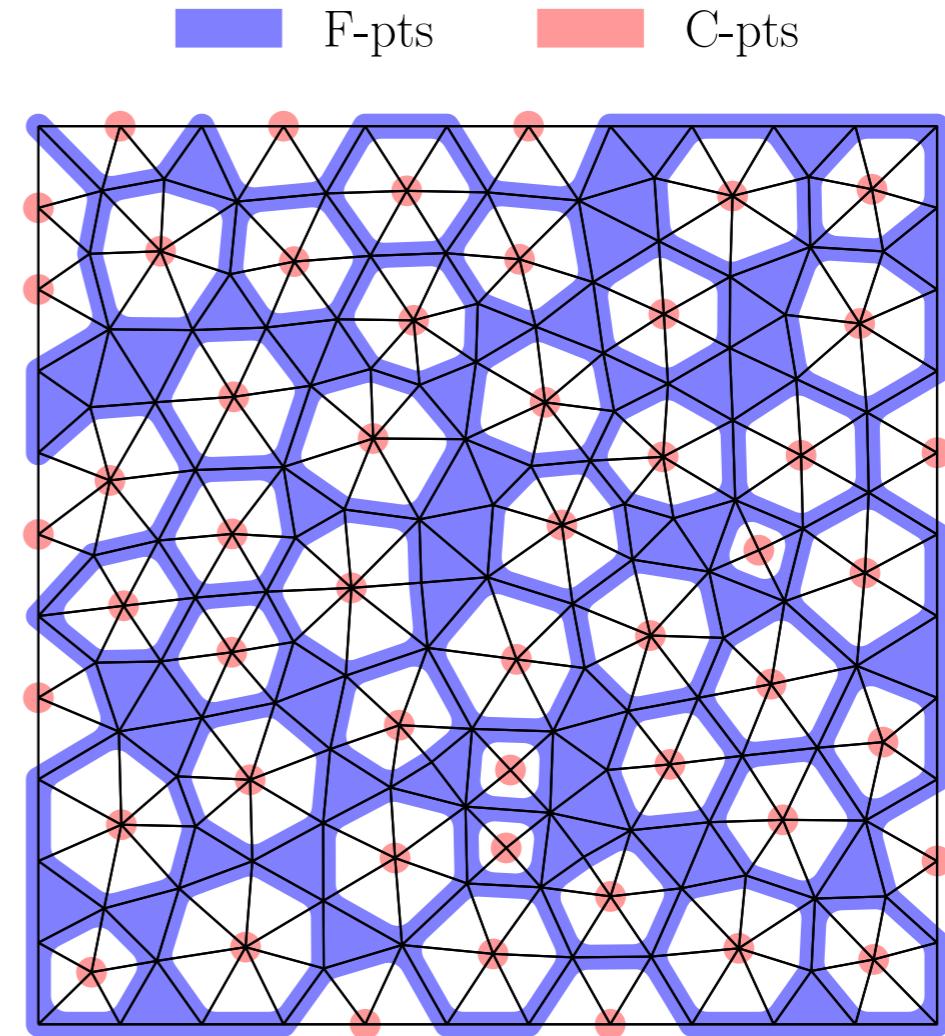
- Often positive off-diagonals are treated as **weak**
- This definition of strength of connection is not symmetric

Demo: [1-AMG-coarse-mesh-example.ipynb](#)

Two (general) forms of AMG



- Smoothed Aggregation AMG (SA-AMG)
- Interpolation constructed from candidate vectors
- Clear approach to *optimize* interpolation



- Coarse-Fine AMG (CF-AMG) or Ruge-Stüben
- Coarse grid points are a subset of the fine grid points
- Edge-wise construction of interpolation, allowing straightforward control of sparsity
- Incorporating near-nullspace is not straightforward

CF AMG

- **Goal:** select grid points to form the coarse grid where smooth error is well represented
- **Idea:** the variable at j would be a good **C-point** if it strongly influences the variable at i
- Strongly depend on...

$$S_i = \{j : -A_{ij} \geq \theta \max_{k \neq i} -A_{ik}\}$$

- Strongly influence...

$$S_i^T = \{j : i \in S_j\}$$

J. W. Ruge K. Stüben, Algebraic Multigrid,
1987

CF AMG

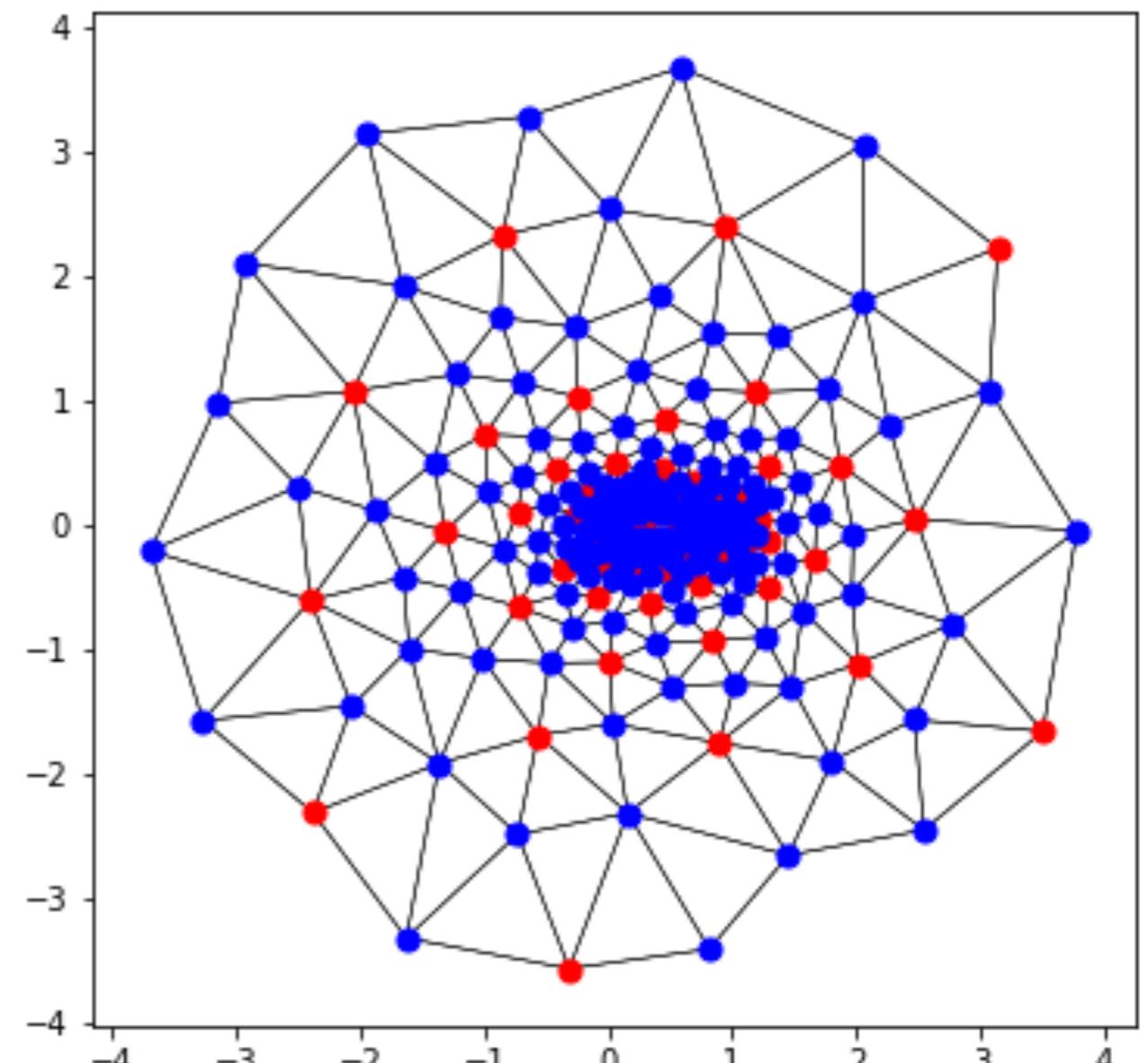
- **C-points:** coarse grid points
- **F-points:** fine grid points
- Either a C-pt or an F-pt

$$\Omega = C \cup F \quad C \cap F = \emptyset$$

- Coarse interpolatory set

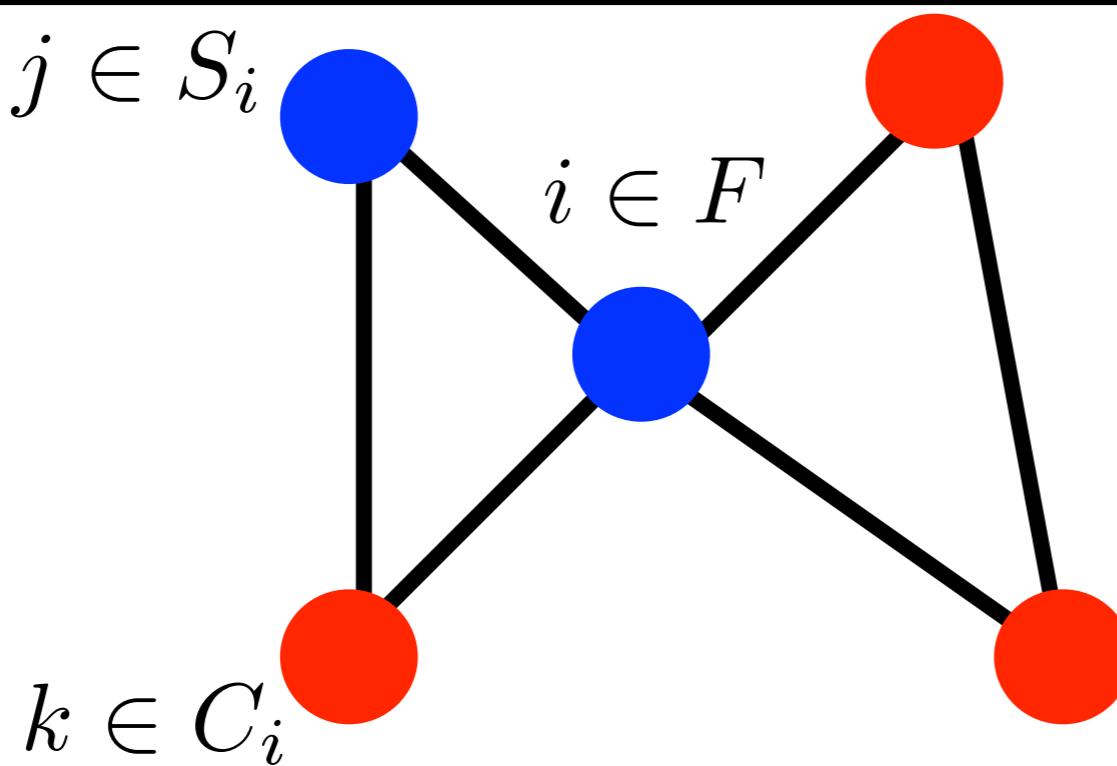
C_i

C-pts that are used to
interpolated F-pt i.



CF AMG

- (C1) Each $i \in F$ should strongly depend on either
 - A point in C
 - A point that strongly depends on a point in C_i



CF AMG

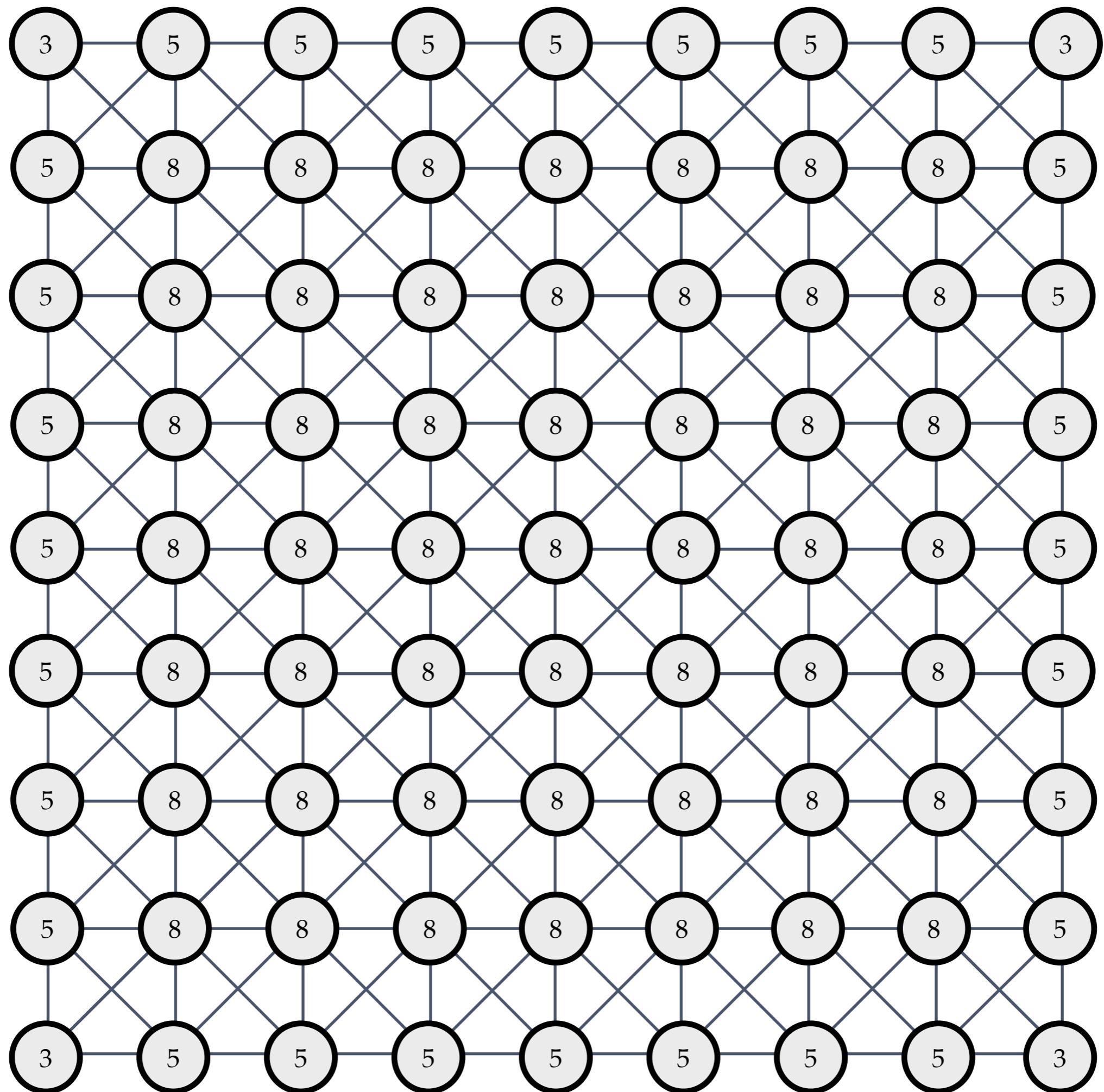
- (C2) The C-points should be *maximal* with no C-point depending on another C-point
- (C1) increases the size of the coarse grid (C-points)
- (C2) puts constraints on the size of the coarse grid
- Must satisfy (C1) in order to construct interpolation. Use (C2) to help limit computational complexity

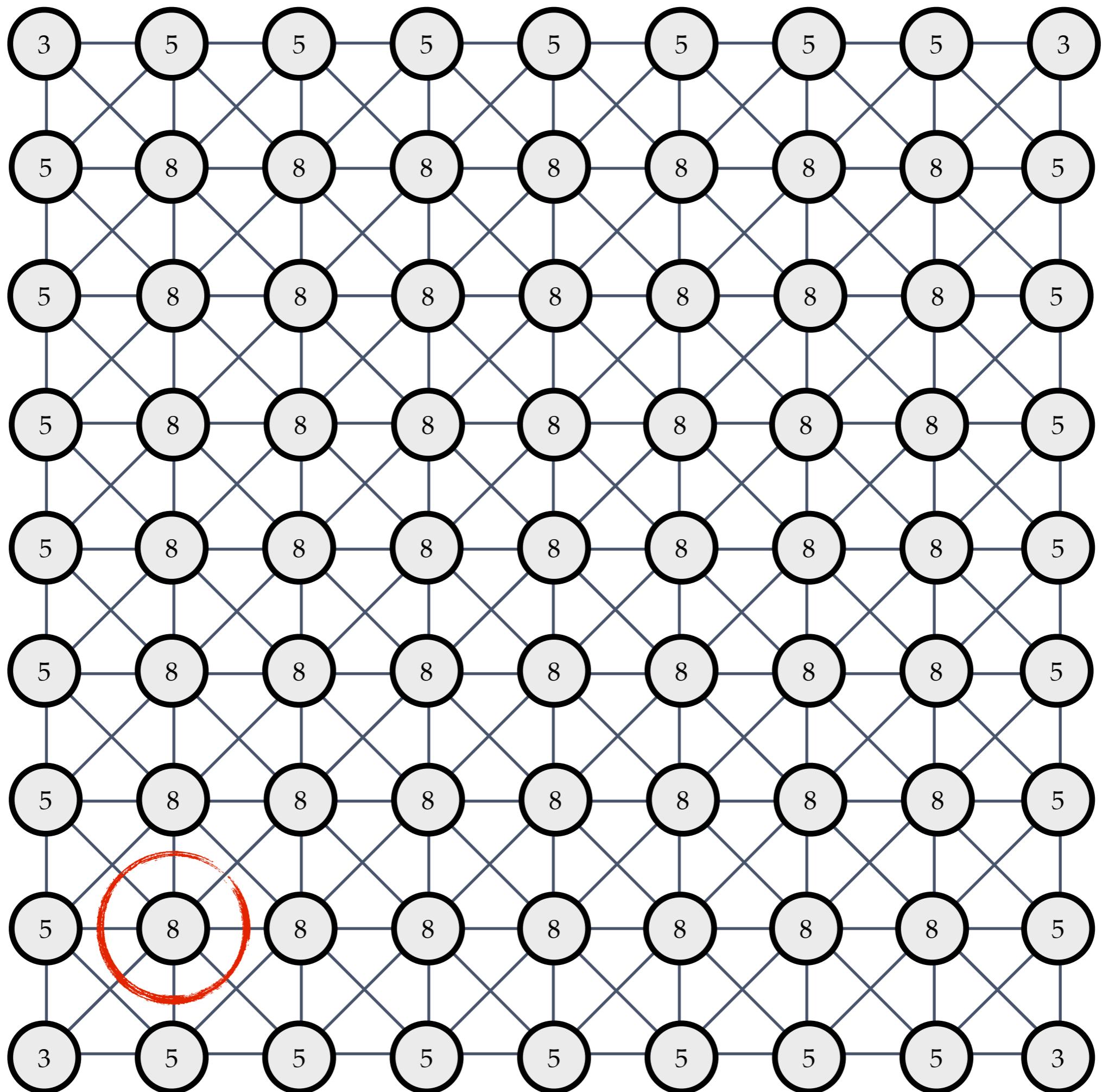
Ruge-Stüben

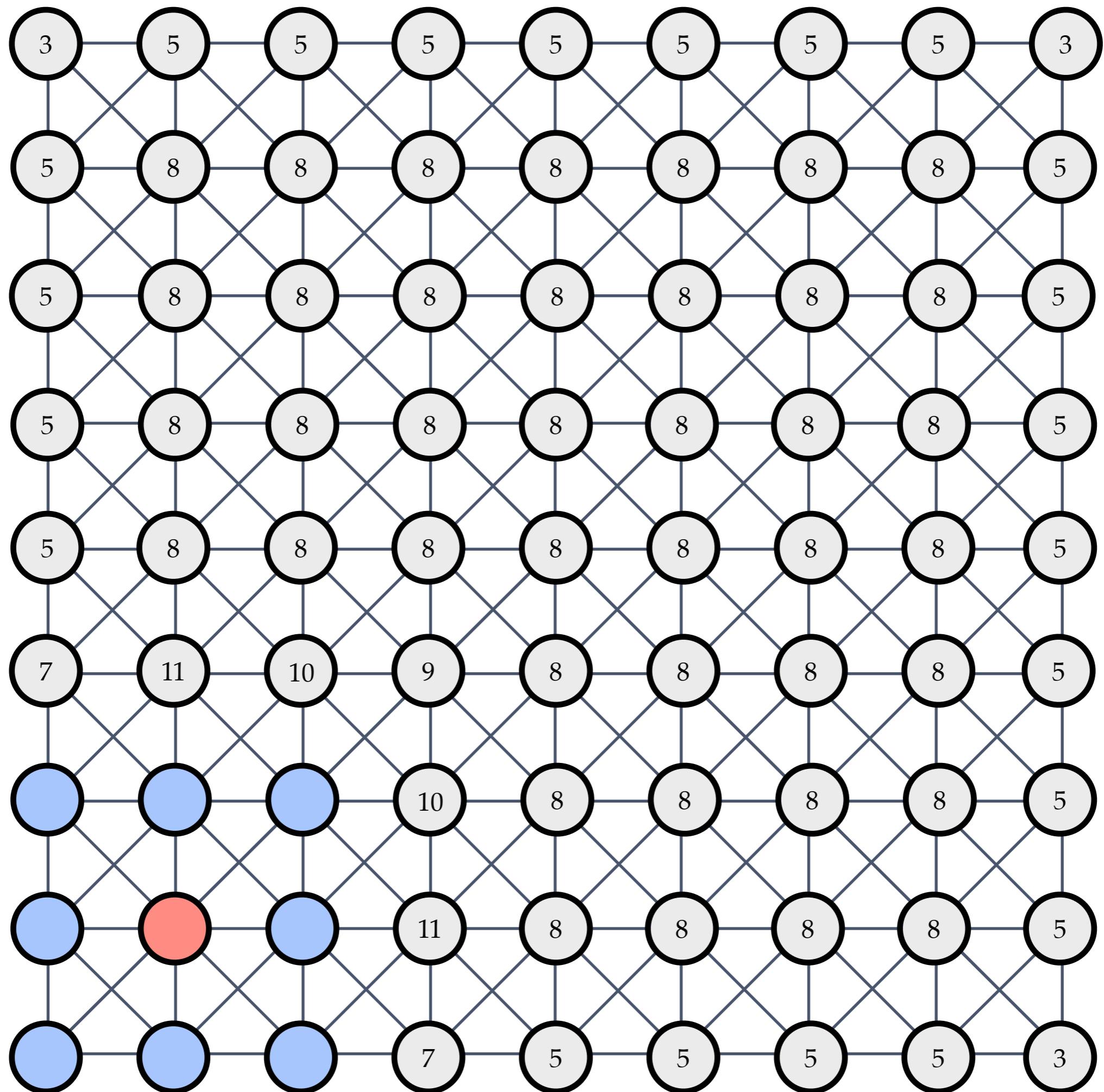
Algorithm 3. RUGE-STÜBEN.

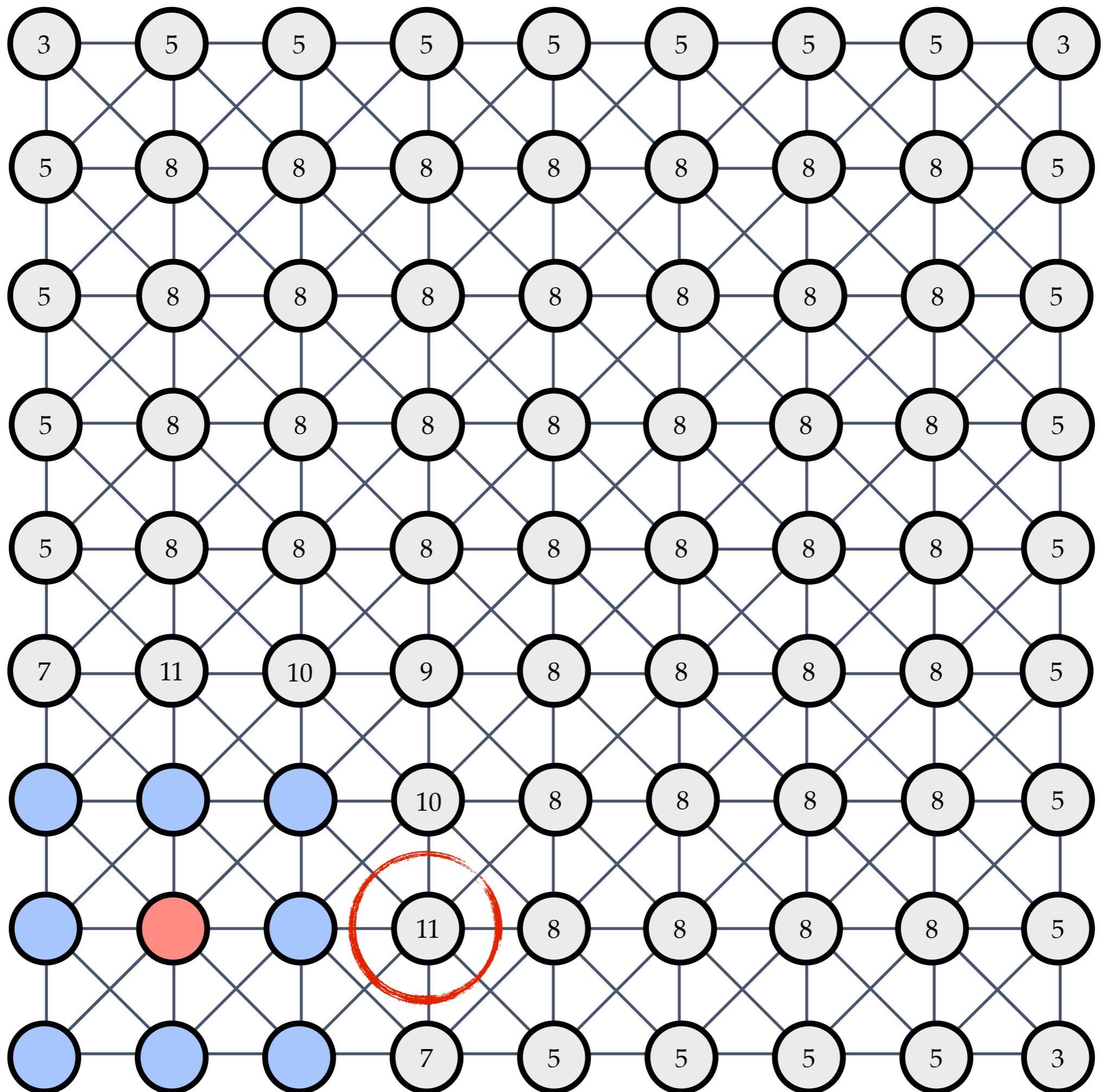
Initialize:

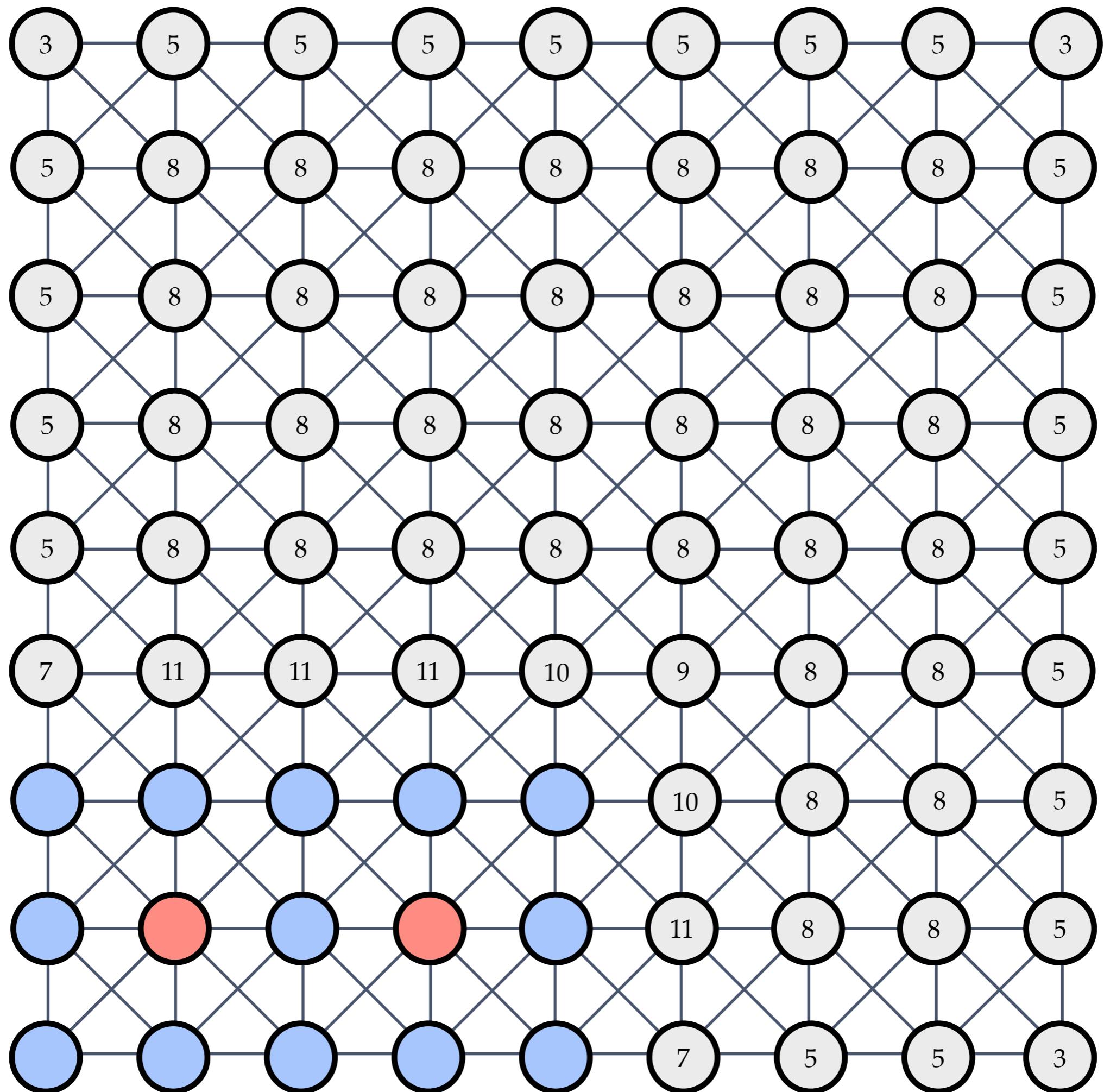
```
 $U = \Omega, C = \emptyset, F = \emptyset$ 
1. for all  $i \in \Omega$  do
2.    $w_i \leftarrow |S_i^T|$ 
3. end for
4. while  $|U| > 0$  do {First pass}
5.   select  $i: w_i \geq w_j, \forall j \in U$ 
6.    $U \leftarrow U \setminus \{i\}$ 
7.    $C \leftarrow C \cup \{i\}$ 
8.   for all  $j \in S_i^T \cap U$  do
9.      $U \leftarrow U \setminus \{j\}$ 
10.     $F = F \cup \{j\}$ 
11.    for all  $k \in S_j \cap U$  do
12.       $w_k \leftarrow w_k + 1$ 
13.    end for
14.  end for
15. end while
16. for all  $i \in F$  do {Second pass}
17.   for all  $j \in S_i \cap S_i^T \cap F$  do
18.     if  $S_i \cap S_j \cap C = \emptyset$  then
19.       make  $i$  or  $j$  into  $C$ -point
20.     end if
21.   end for
22. end for
```

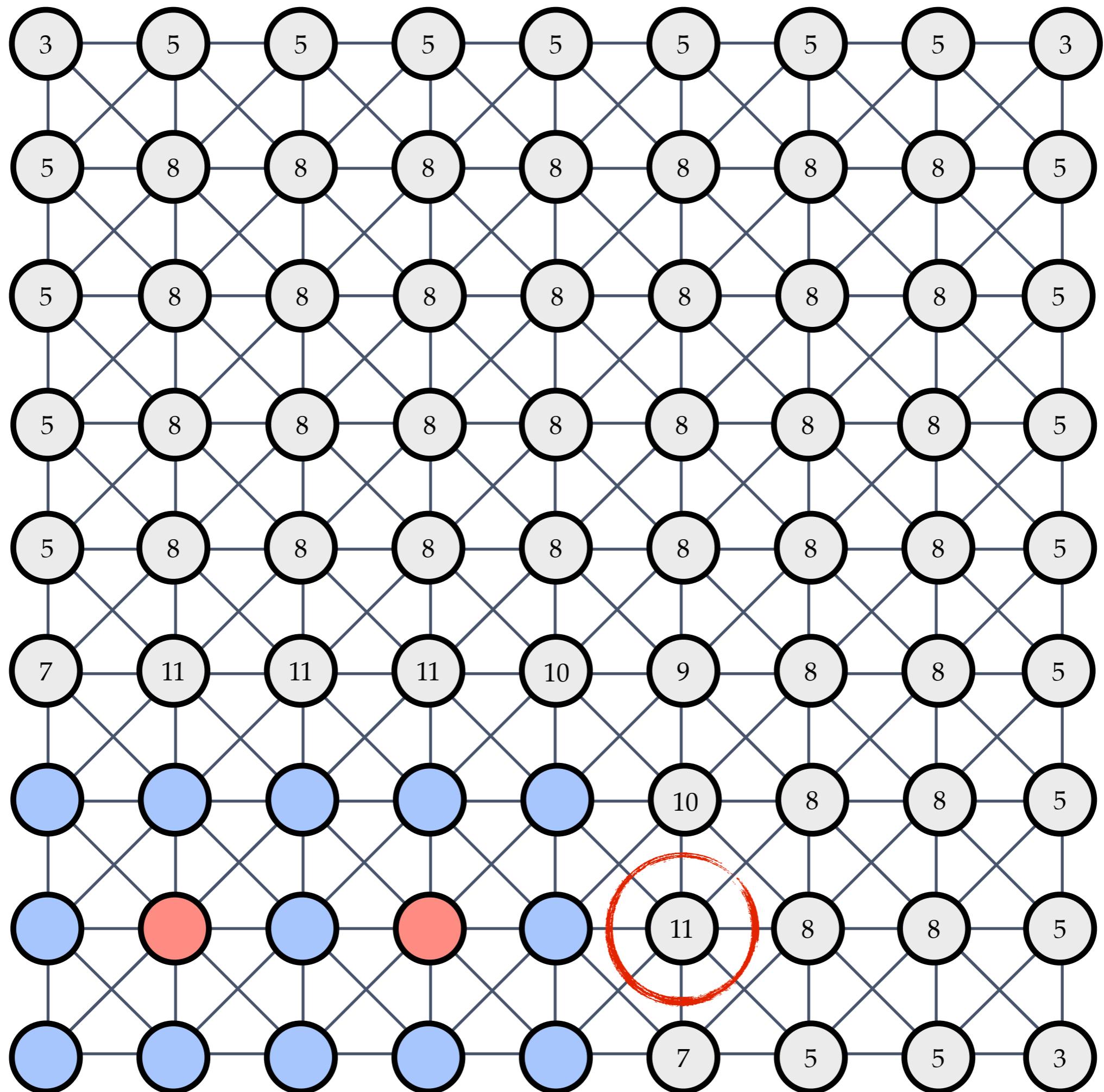


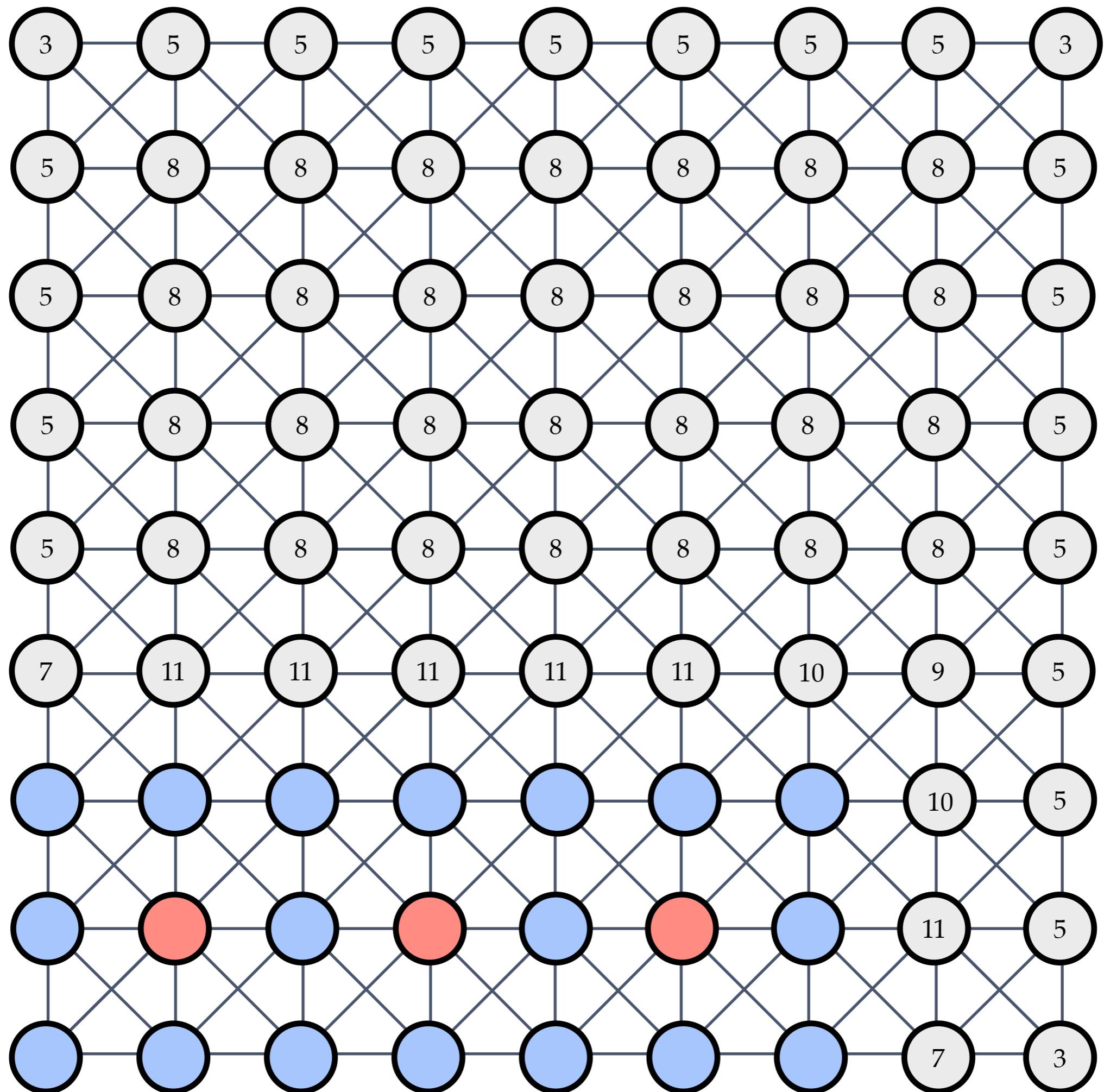


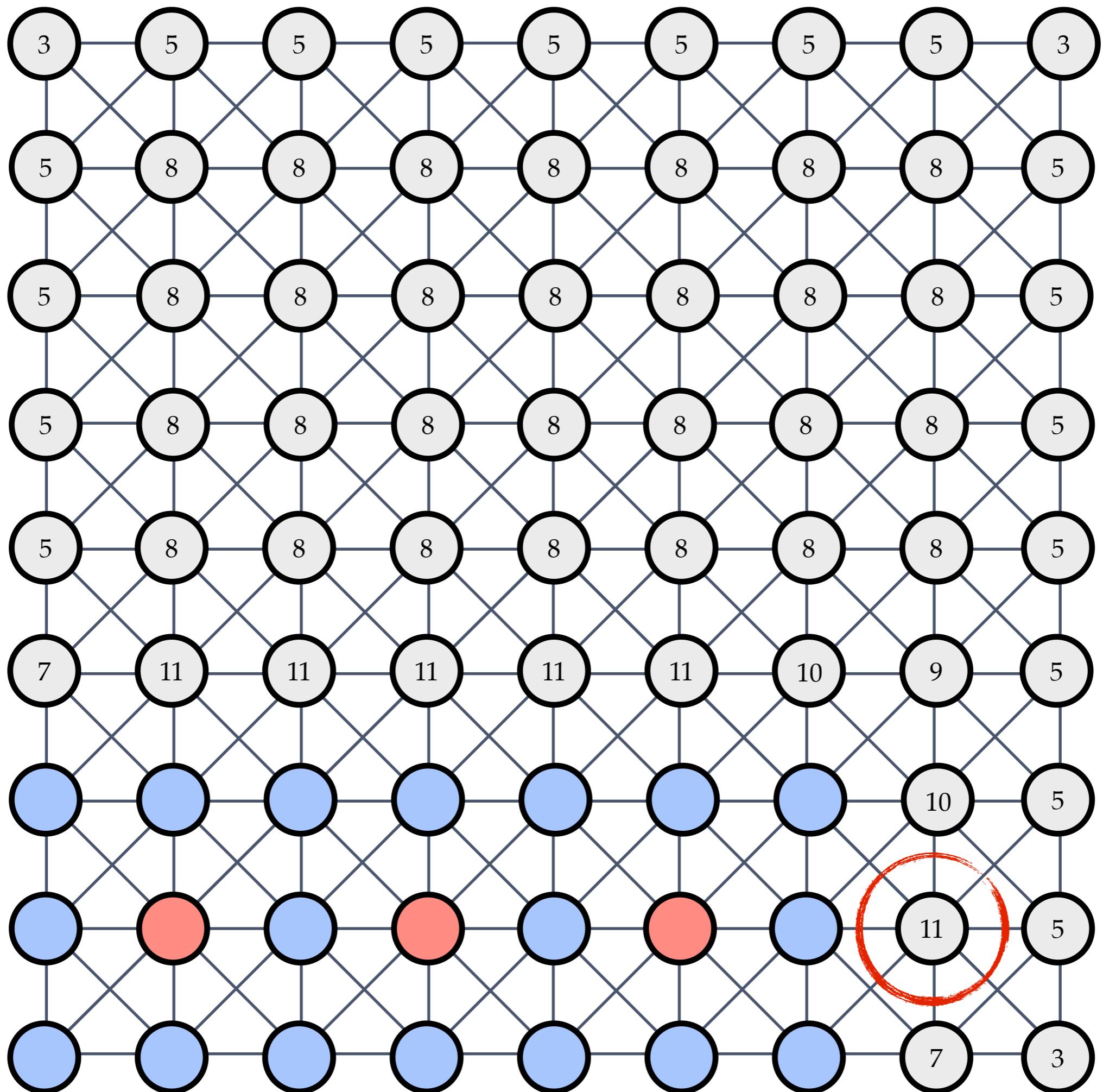


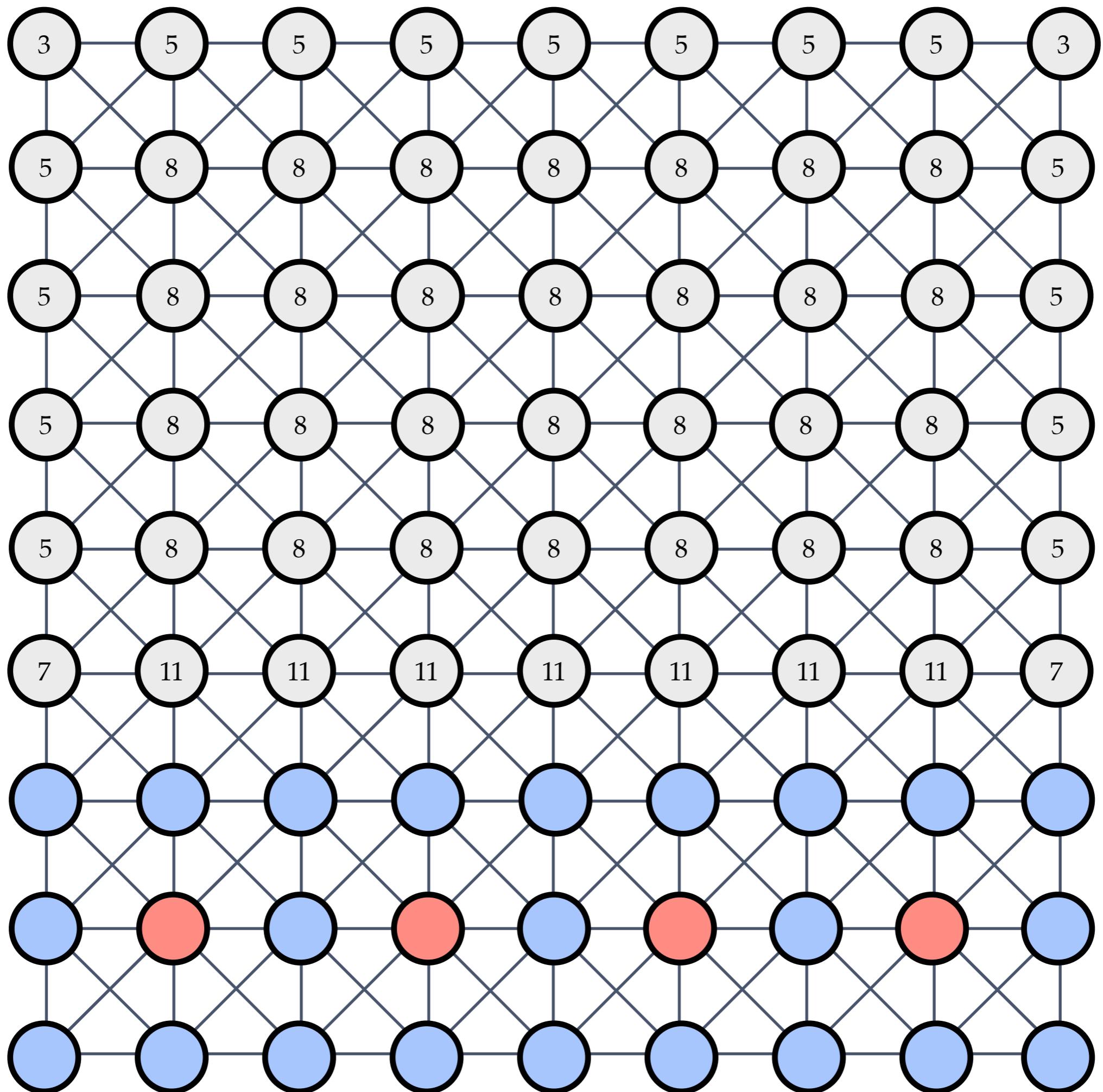


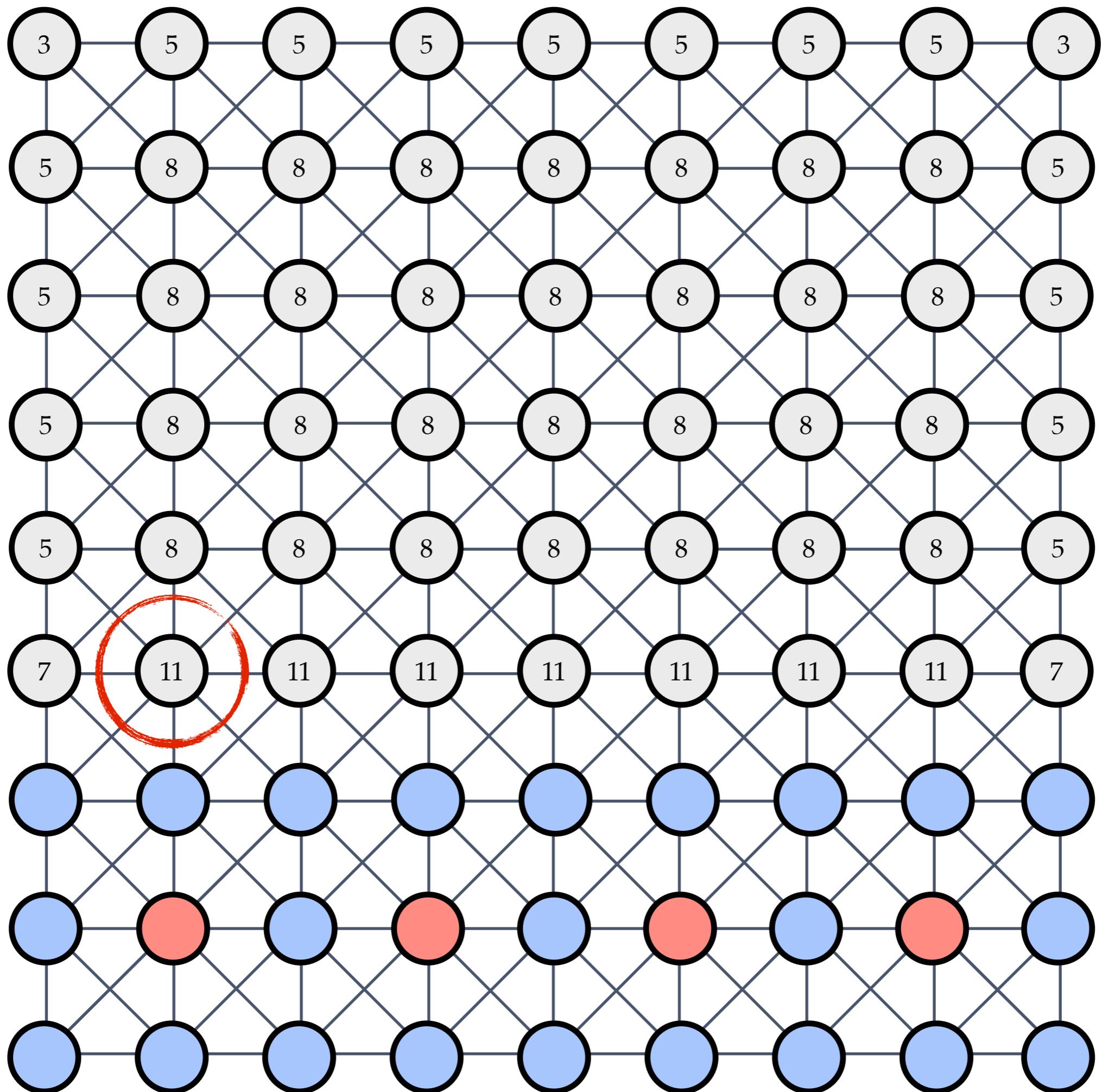


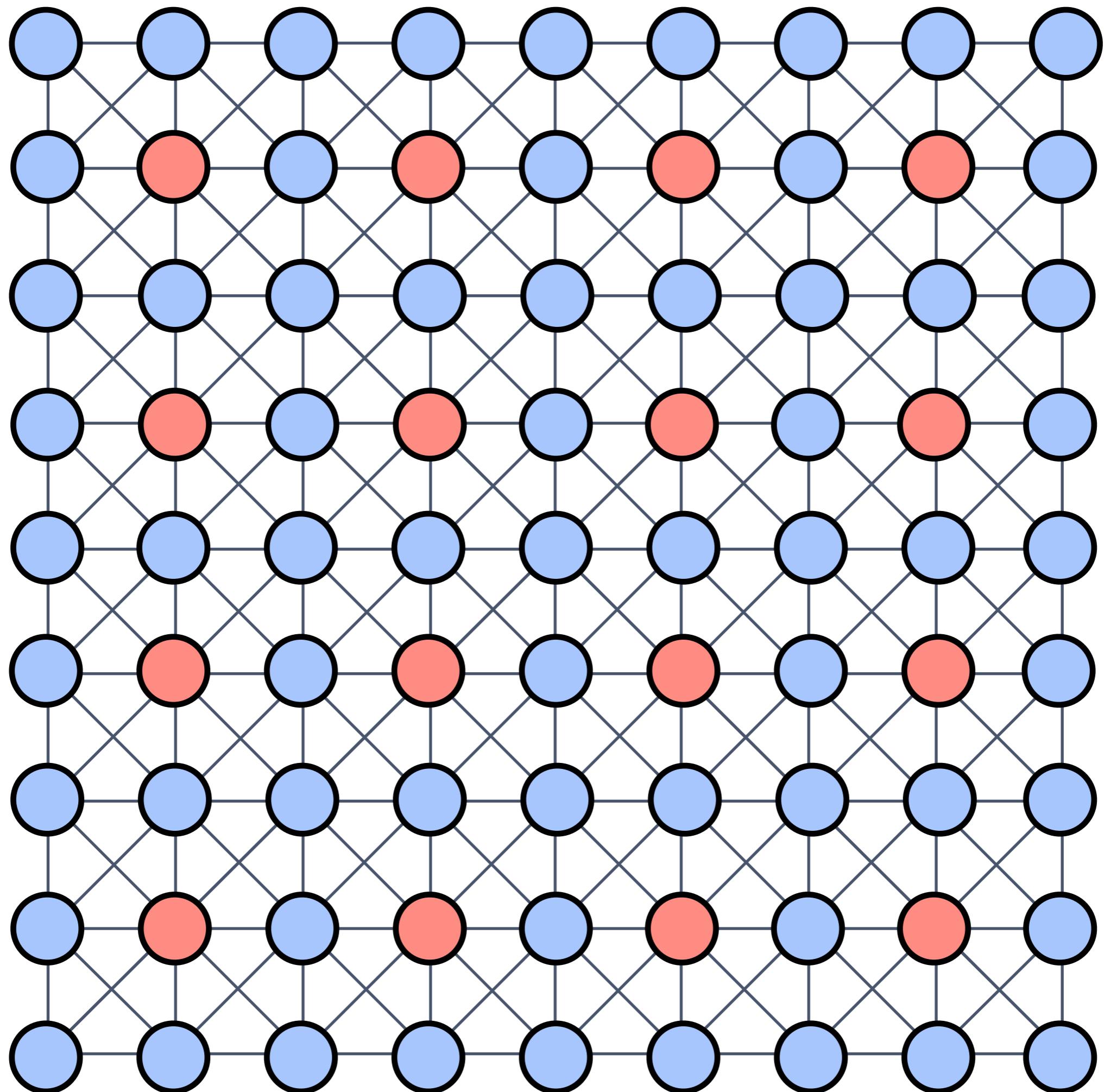












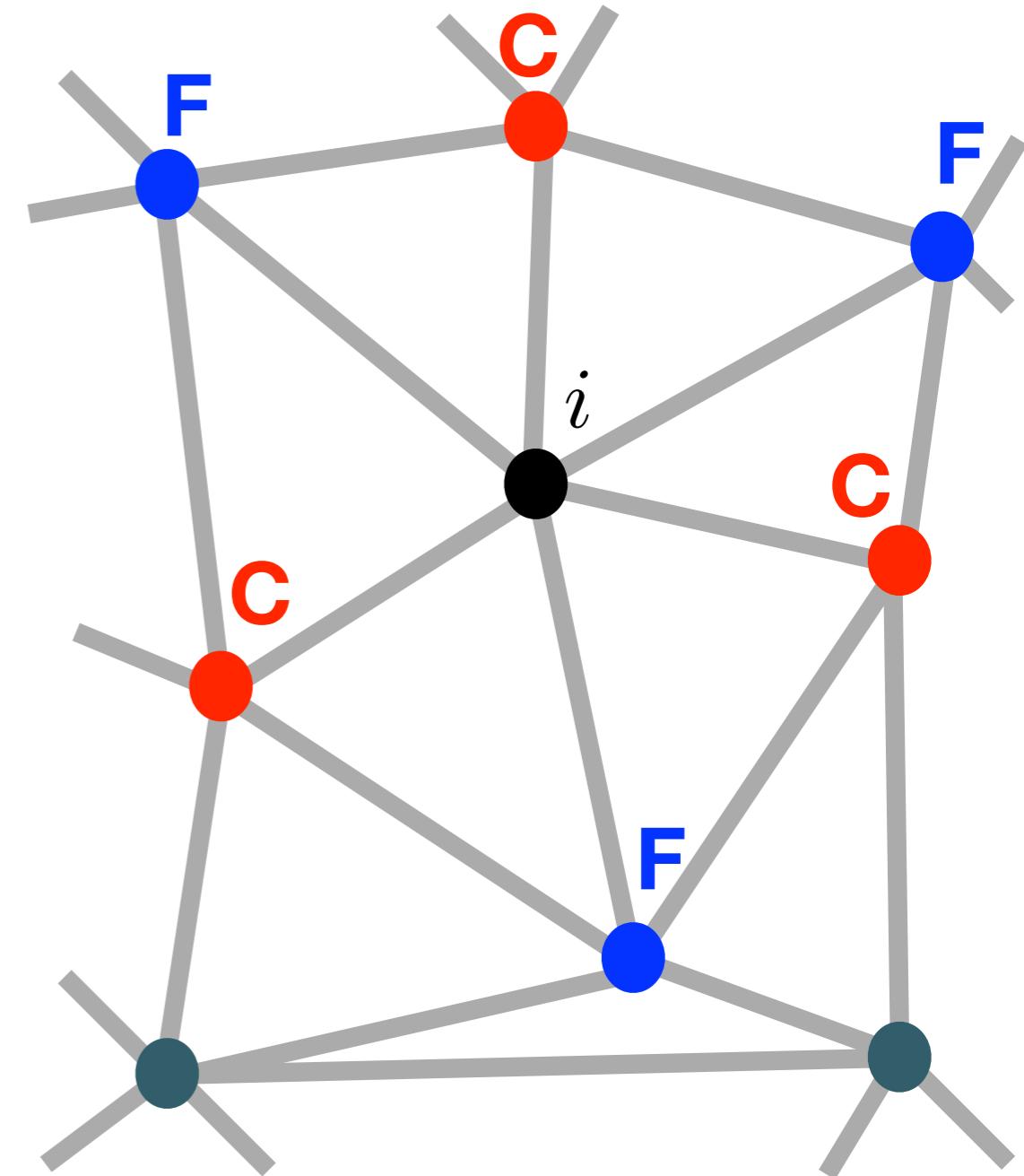
CF AMG

- With a coarse grid (C-points) defined, we can turn to interpolation.
- Write interpolation as a weighted sum of points in the coarse interpolatory set

$$(\vec{Pe})_i = \begin{cases} e_i & i \in C \\ \sum_{j \in C_i} \omega_{ij} e_j & i \in F \end{cases}$$

- Or

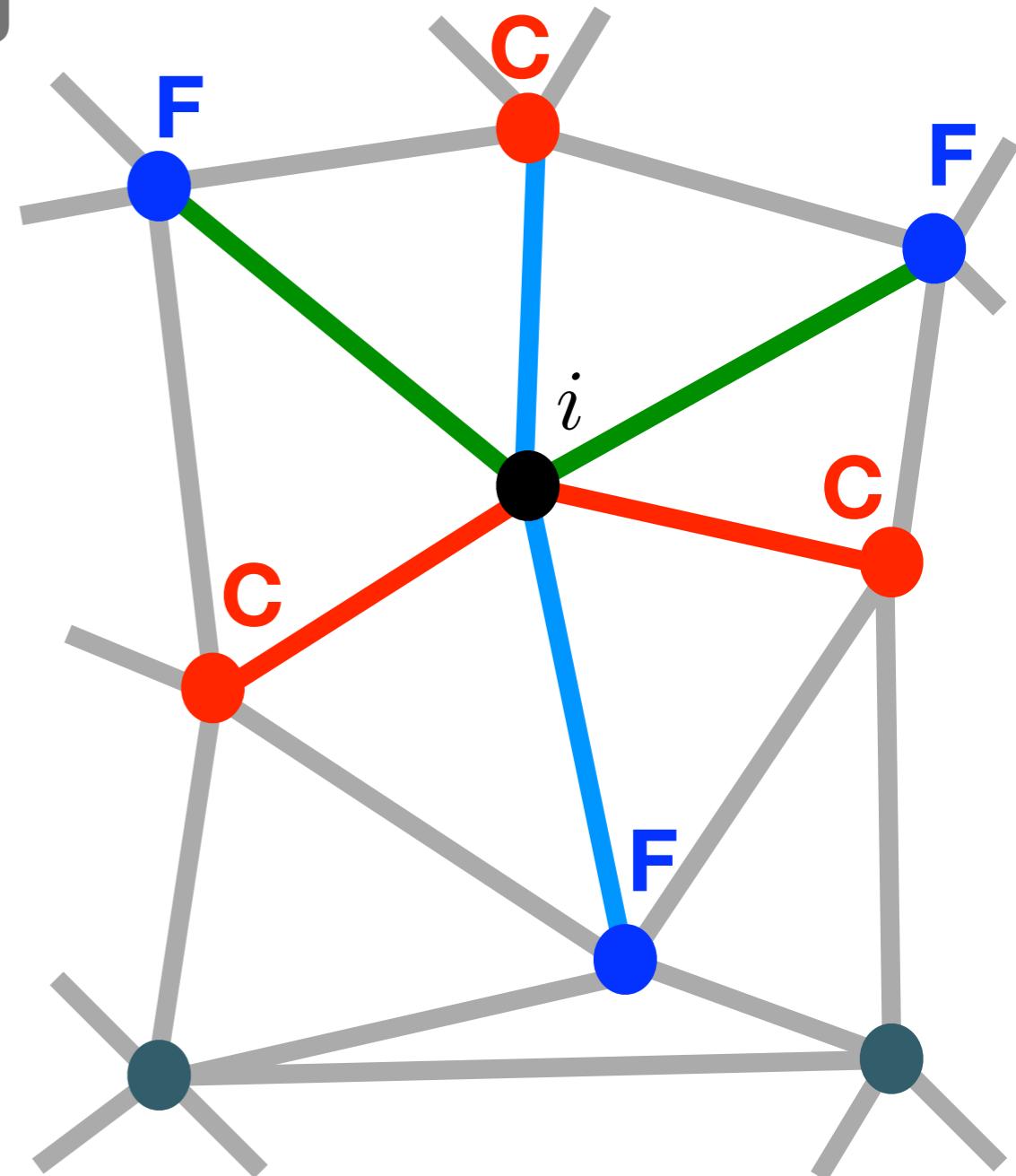
$$\vec{Pe} = P \begin{bmatrix} \vec{e}_C \\ \vec{e}_F \end{bmatrix} = \begin{bmatrix} I \\ W \end{bmatrix} \begin{bmatrix} \vec{e}_C \\ \vec{e}_F \end{bmatrix}$$



Example from MG Tutorial

CF AMG

- To interpolate, distinguish **strong** and **weak** connections to interpolate from
- C_i are **strong C-points**
- D_i^s are **strong F-points**
- D_i^w are **weak C/F-points**



CF AMG

- Start with smooth error

$$Ae \approx 0$$

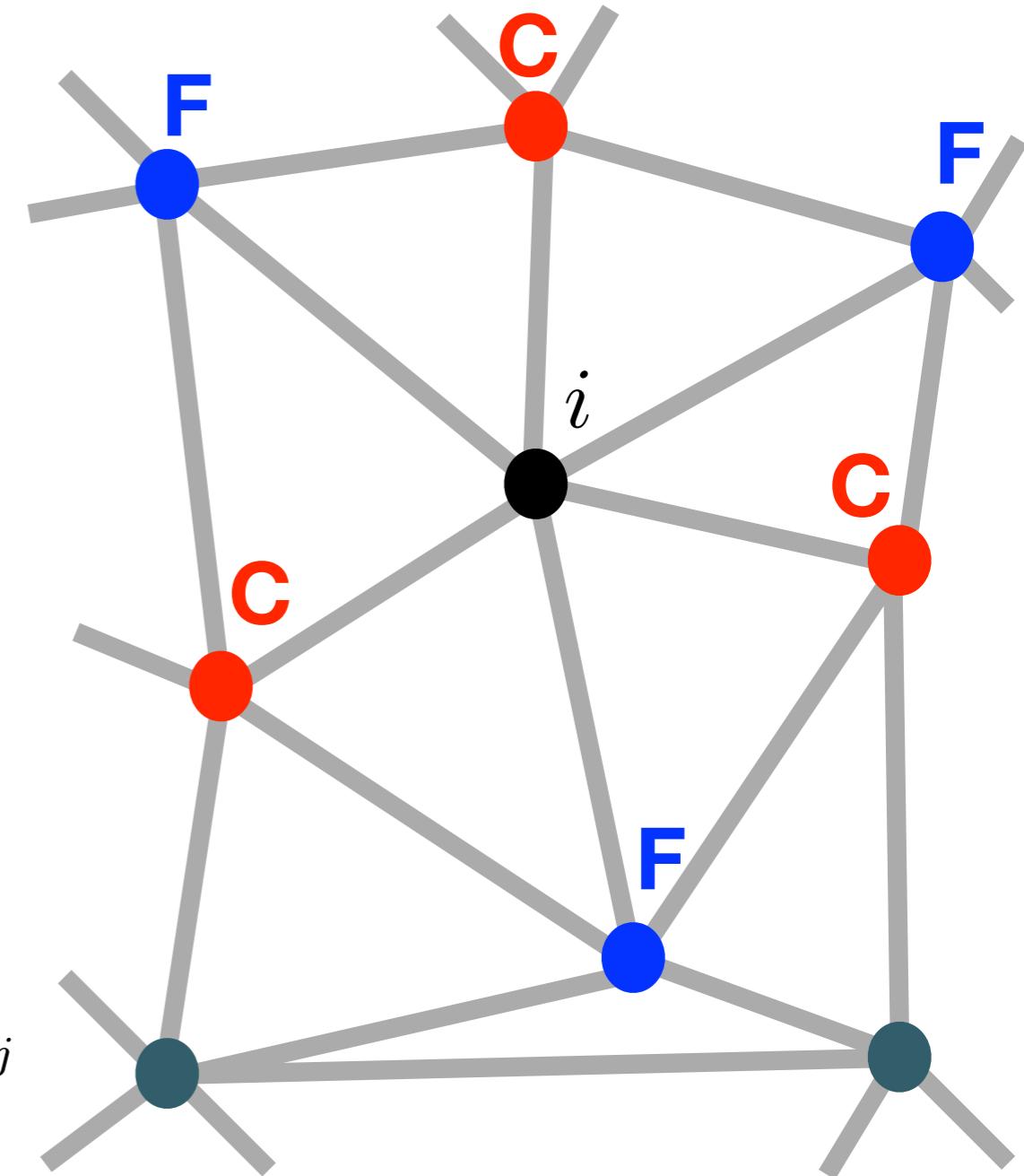
- Then “solve” for i

$$A_{ii}e_i = \sum_{j \neq i} A_{ij}e_j$$

- Then split into types

$$A_{ii}e_i = \sum_{j \in C_i} A_{ij}e_j + \sum_{j \in D_i^s} A_{ij}e_j + \sum_{j \in D_i^w} A_{ij}e_j$$

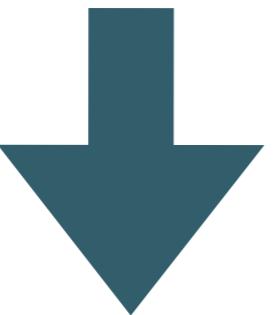
strong C **strong F** **weak**



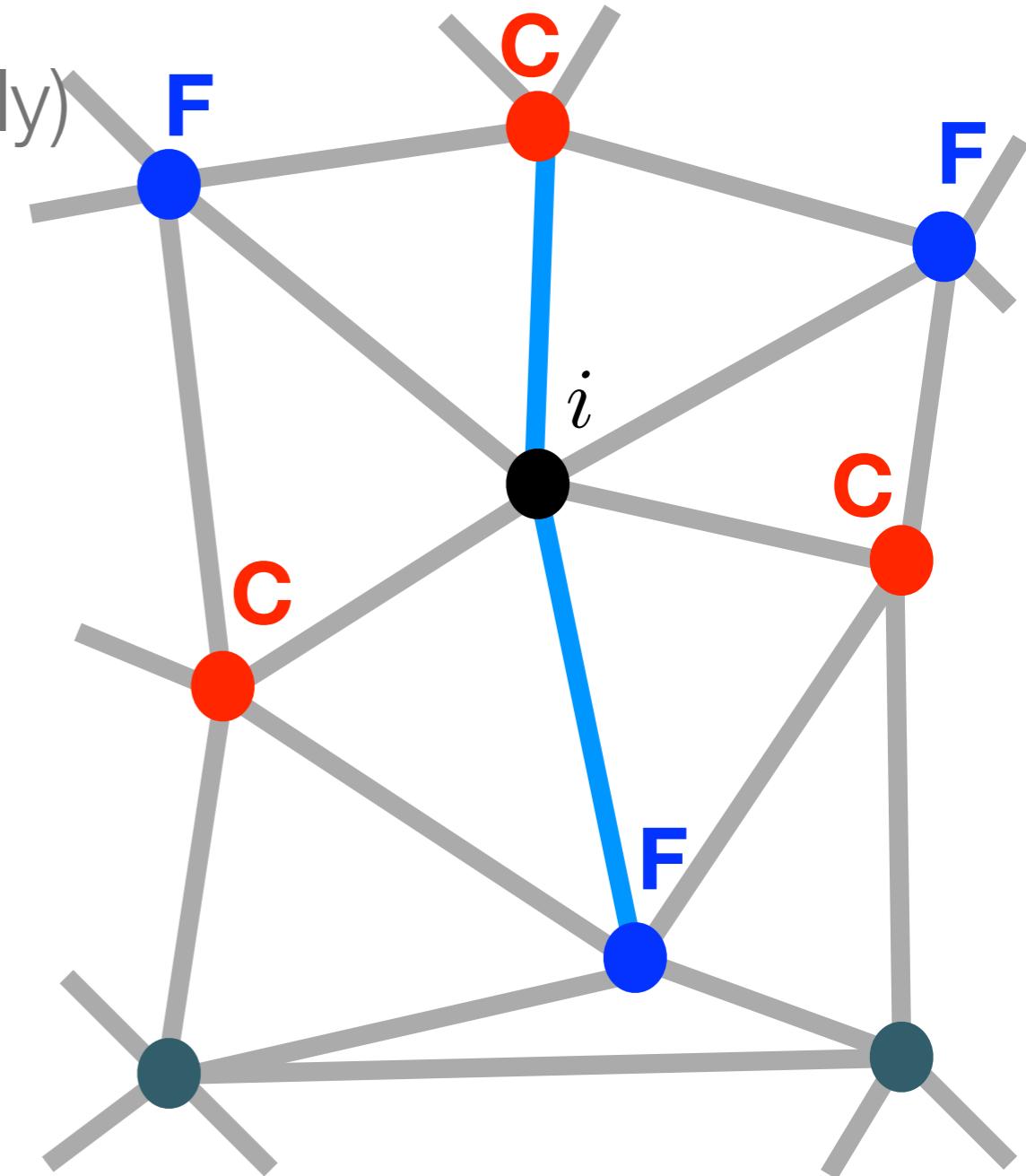
CF AMG

- **Weak:** assume $e_j \approx e_i$ in case there is dependence (=vary slowly)

$$A_{ii}e_i = \sum_{j \in C_i} A_{ij}e_j + \sum_{j \in D_i^s} A_{ij}e_j + \sum_{j \in D_i^w} A_{ij}e_j$$



$$\left(A_{ii} + \sum_{j \in D_i^w} A_{ij} \right) e_i = \sum_{j \in C_i} A_{ij}e_j + \sum_{j \in D_i^s} A_{ij}e_j$$



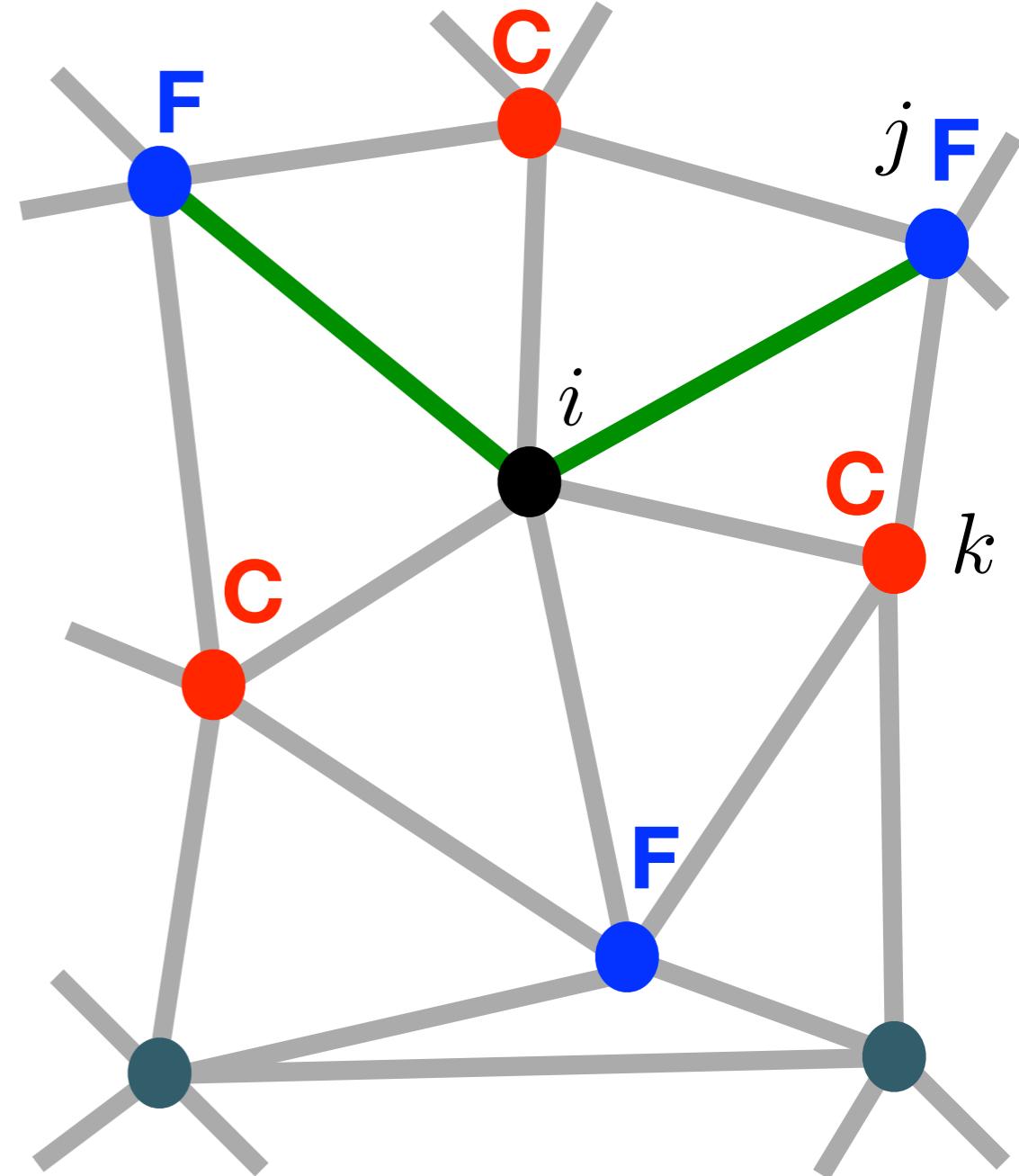
CF AMG

- **Strong F:** approximate e_j by points in $C_i \cap C_j$

$$e_j \approx \frac{\sum_{k \in C_i} A_{jk} e_k}{\sum_{k \in C_i} A_{jk}}$$

- This gives weights

$$\omega_{ij} = -\frac{A_{ij} + \sum_{j \in D_i^s} \frac{A_{ik} A_{kj}}{\sum_{m \in C_i} A_{km}}}{A_{ii} + \sum_{n \in D_i^w} A_{in}}$$



CF AMG Setup Algorithm

Algorithm 2: CF_setup()

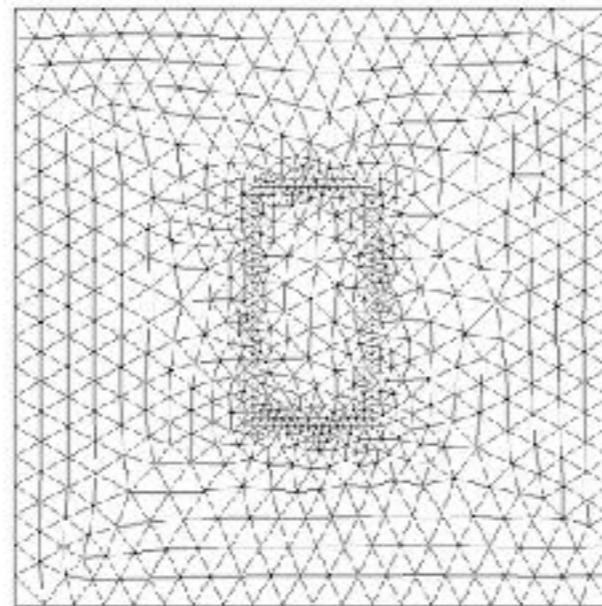
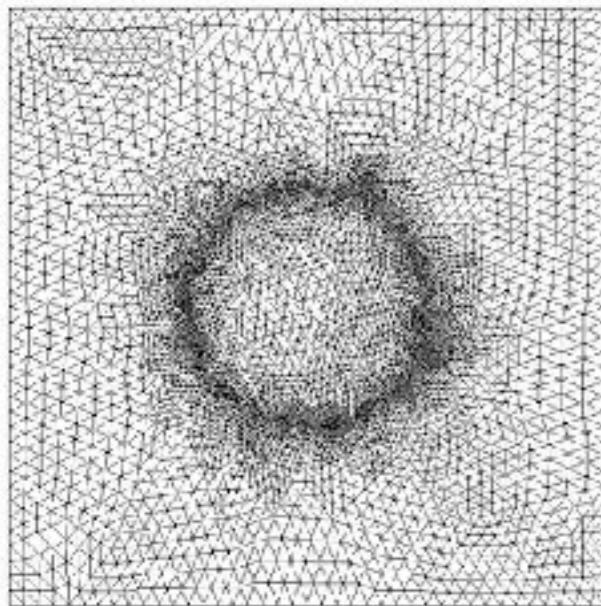
Input: A_0 : fine-grid operator
max_size: threshold for max size of coarsest problem

Output: A_1, \dots, A_L ,
 P_0, \dots, P_{L-1}

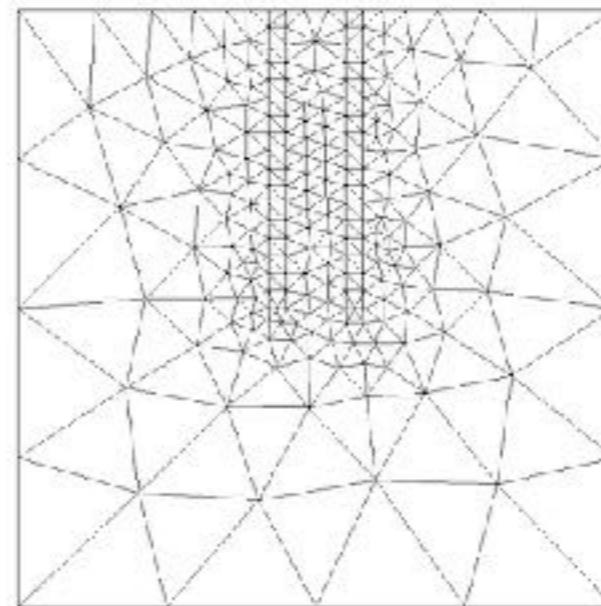
```
1  $\ell = 0$ 
2 while size( $A_\ell$ ) > max_size
3    $S_\ell = \text{strength}(A_\ell)$                                 {Strength-of-connection}
4    $\mathcal{C}_\ell, \mathcal{F}_\ell = \text{splitting}(S_\ell)$           {C/F-splitting}
5    $W = \text{weights}(S_\ell, A_\ell, \mathcal{C}_\ell, \mathcal{F}_\ell)$     {Interpolation weights}
6    $P_\ell = \begin{bmatrix} W \\ I \end{bmatrix}$                       {Form interpolation}
7    $A_{\ell+1} = P_\ell^T A_\ell P_\ell$                          {Coarse-grid operator}
8    $\ell = \ell + 1$ 
```

AMG grid hierarchies for several 2D problems

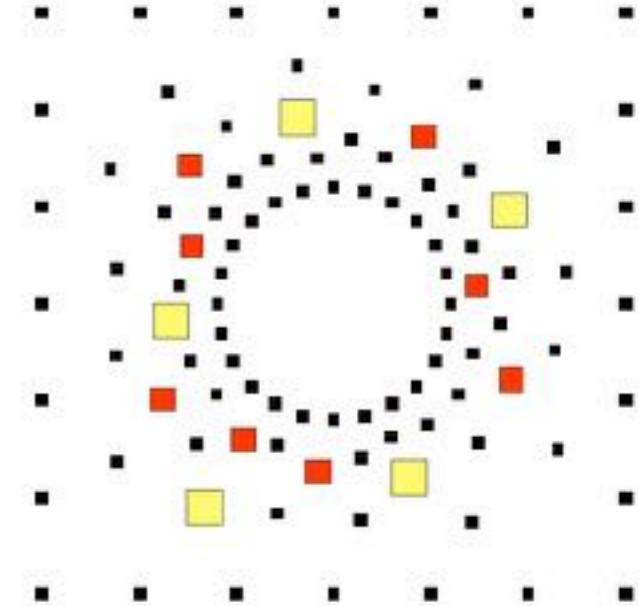
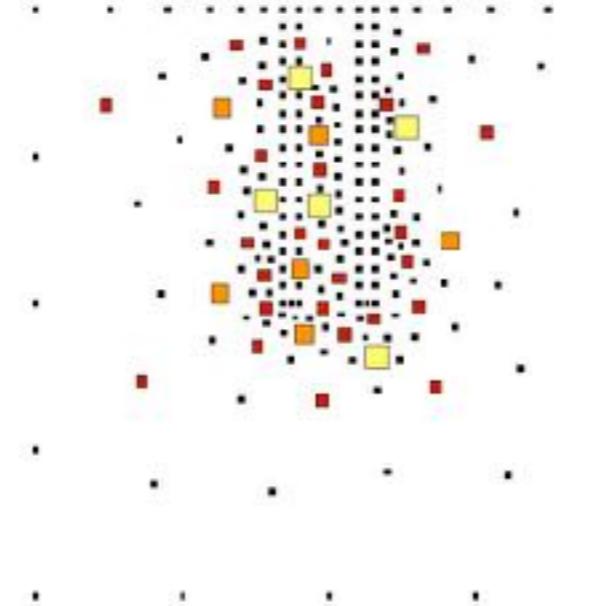
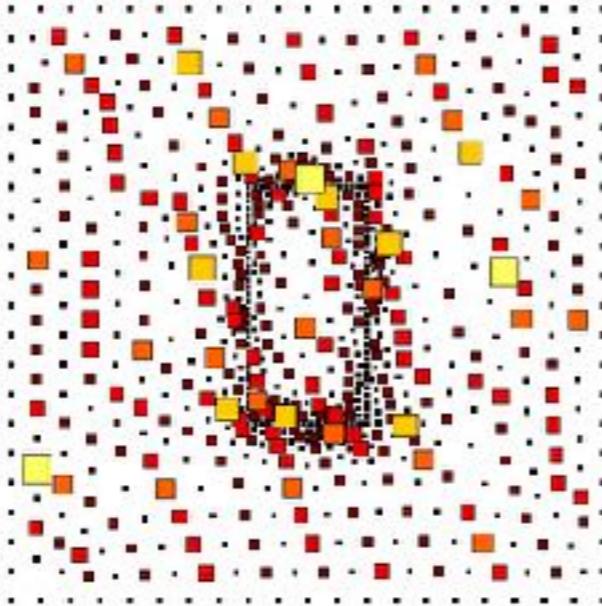
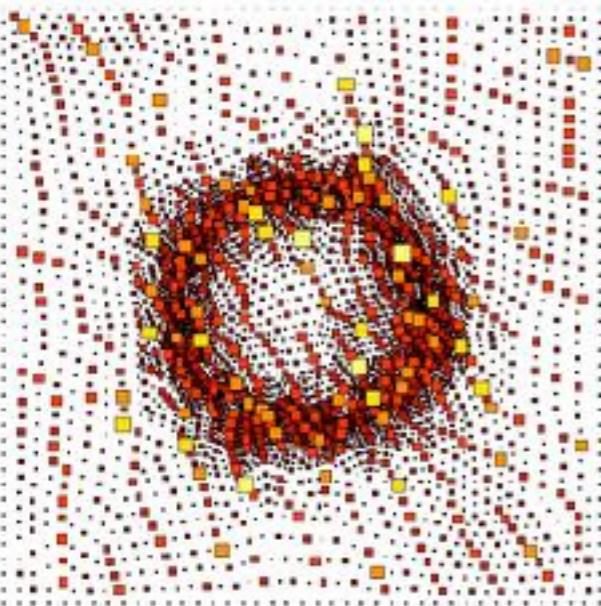
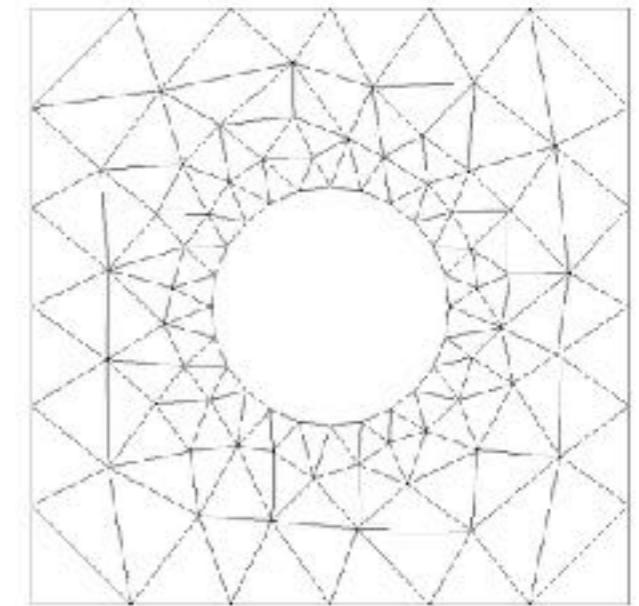
domain1 - 30° domain2 - 30°



pile



square-hole

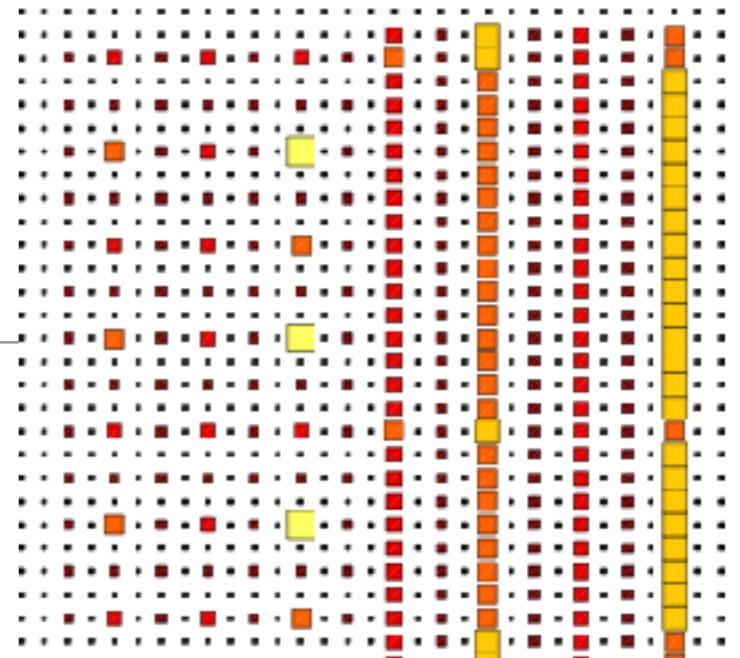


Demo: [2-AMG-complexity.ipynb](#)

Example CF-AMG results

$$-au_{xx} - bu_{yy} = f$$

$$\begin{array}{c|c} a = b & \\ \hline & a \gg b \end{array}$$



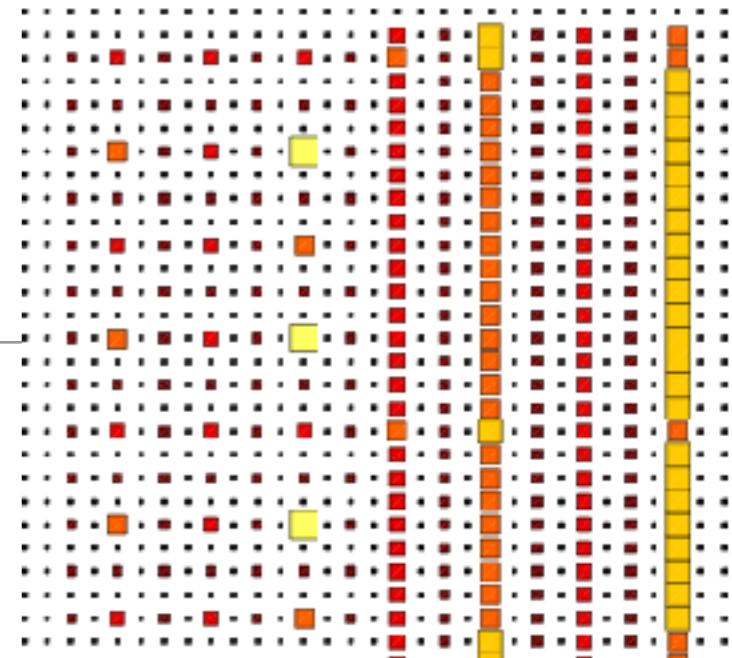
CF-AMG coarse grids

N	Iters	Conv factor	Coarse grids	Grid comp	Oper comp	Setup time	Solve time
61×61	10	0.23	6	1.6	1.6	0.01	0.02
121×121	9	0.23	8	1.6	1.7	0.05	0.07
241×241	9	0.23	9	1.6	1.7	0.25	0.32
481×481	9	0.23	12	1.7	1.7	1.02	1.27
961×961	11	0.29	13	1.7	1.7	4.42	6.28

Example CF-AMG results

$$-au_{xx} - bu_{yy} = f$$

$$\begin{array}{c|c} a = b & \\ \hline & a \gg b \end{array}$$



CF-AMG coarse grids

N	Iters	Conv factor	Coarse grids	Grid comp	Oper comp	Setup time	Solve time
61×61	10	0.23	6	1.6	1.6	0.01	0.02
121×121	9	0.23	8	1.6	1.7	0.05	0.07
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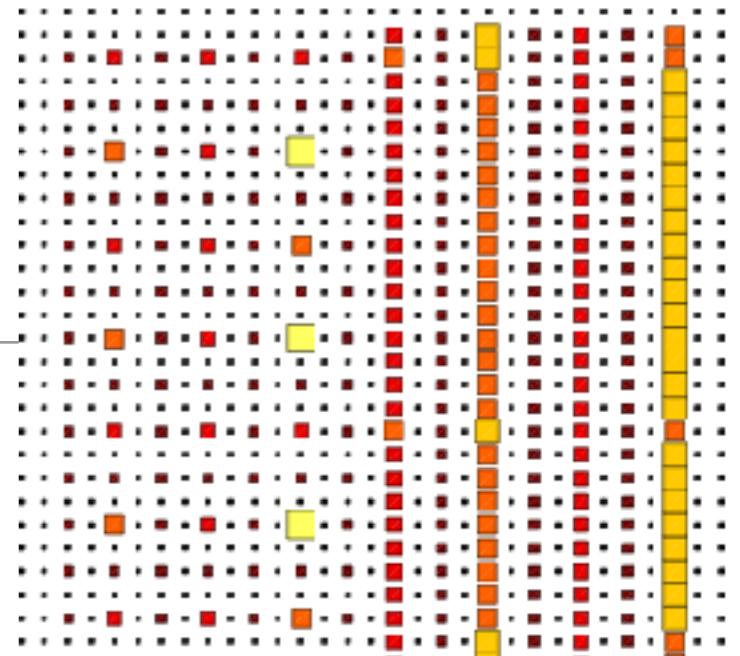


Iterations to a certain tolerance

Example CF-AMG results

$$-au_{xx} - bu_{yy} = f$$

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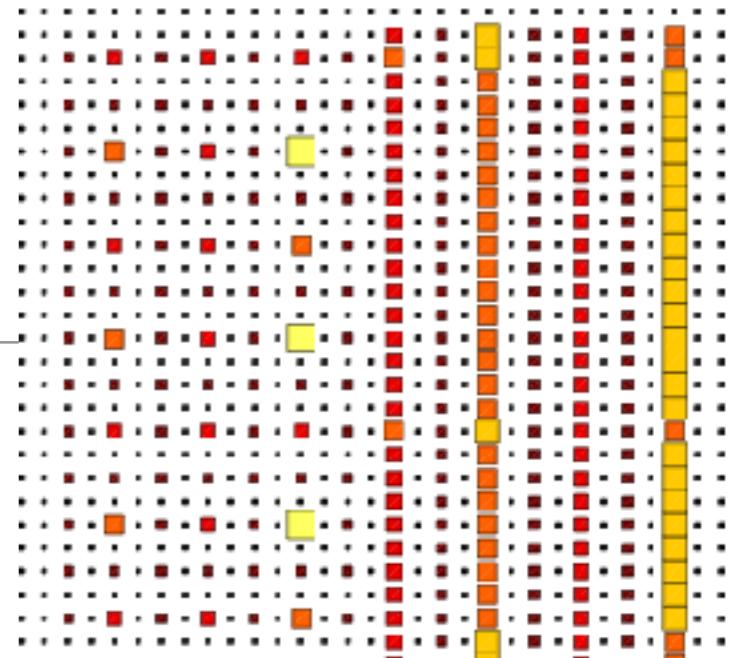


Convergence factor: factor by which the norm of the residual is reduced in each iteration

Example CF-AMG results

$$-au_{xx} - bu_{yy} = f$$

$$\begin{array}{c|c} a = b & \\ \hline & a \gg b \end{array}$$



CF-AMG coarse grids

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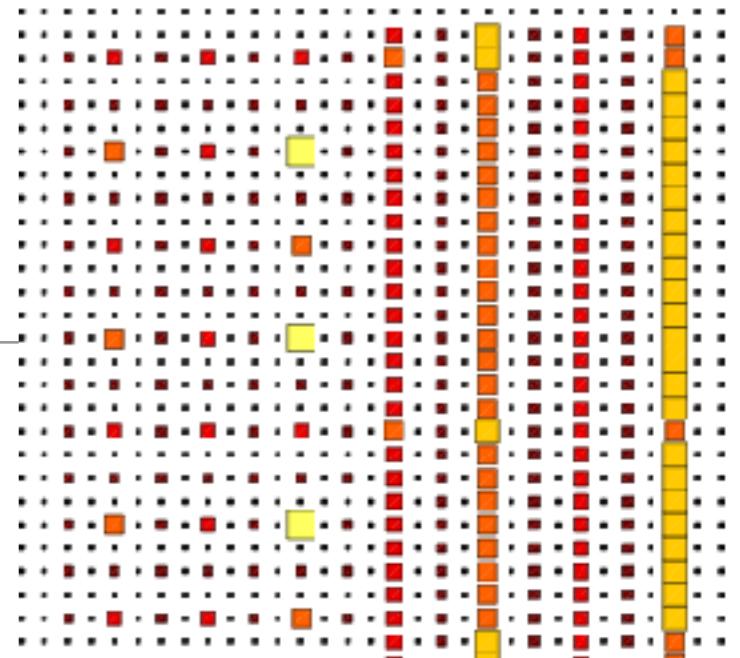


Coarse grids: number of coarse “grids”

Example CF-AMG results

$$-au_{xx} - bu_{yy} = f$$

$$\begin{array}{c|c} a = b & \\ \hline & a \gg b \end{array}$$



CF-AMG coarse grids

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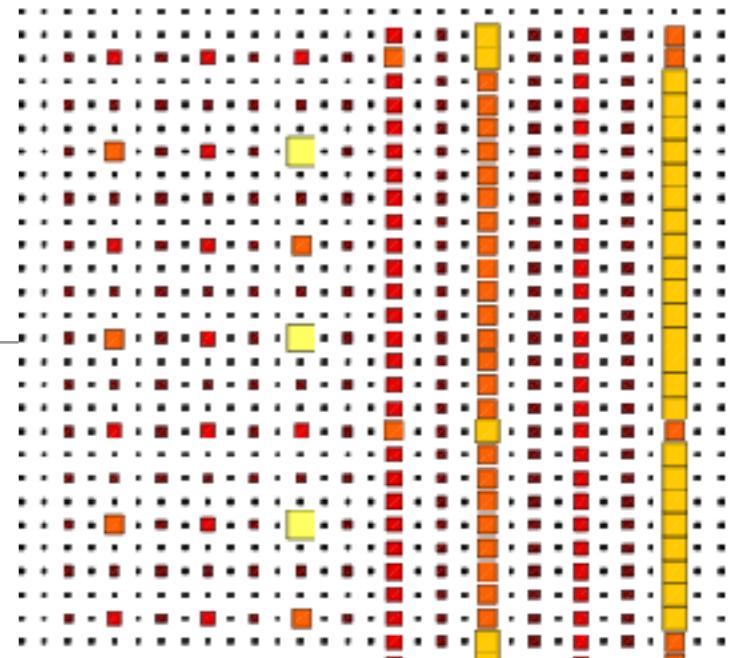


Grid complexity: total number of grid points (system size) on all levels / number of grids points on the fine level

Example CF-AMG results

$$-au_{xx} - bu_{yy} = f$$

$$\begin{array}{c|c} a = b & \\ \hline & a \gg b \end{array}$$



CF-AMG coarse grids

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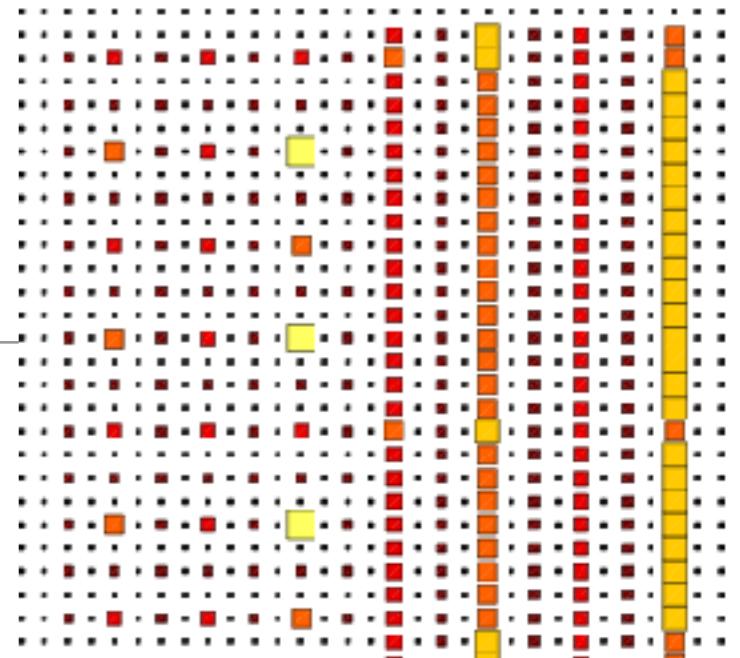


Operator complexity: total number non-zeros on all levels / number of non-zeros on the fine level

Example CF-AMG results

$$-au_{xx} - bu_{yy} = f$$

$$\begin{array}{c|c} a = b & \\ \hline & a \gg b \end{array}$$



CF-AMG coarse grids

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Setup/solve times: can vary *a lot* depending on the problem, but the setup is significant!

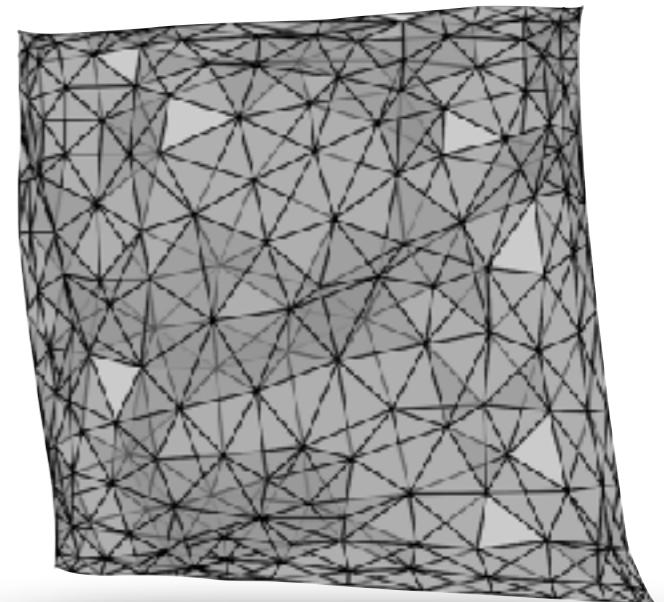
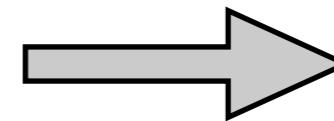
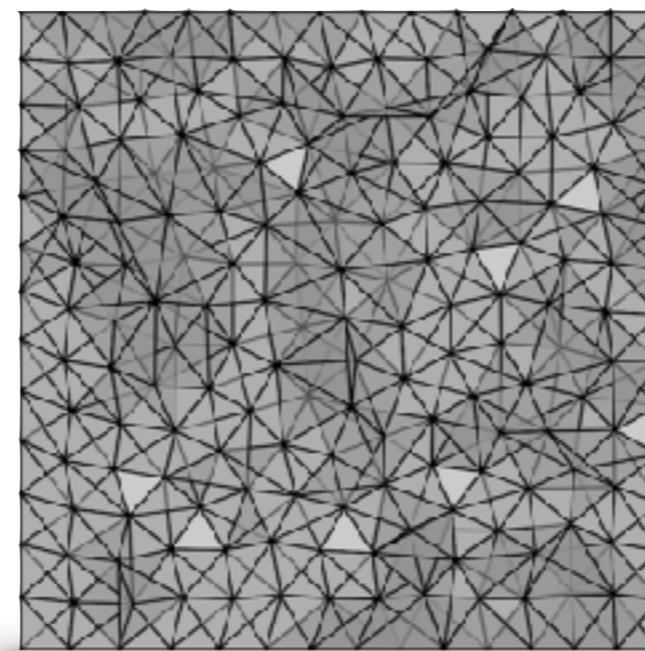
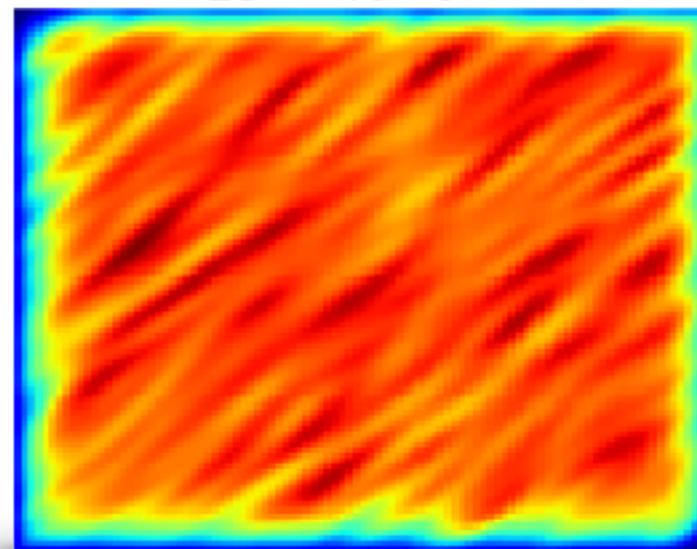
SA AMG

- Smoothed Aggregation based AMG takes a *different* approach
- Still, the same steps:
 1. strength between points
 2. find a coarse grid (this time **aggregates** of points)
 3. define interpolation
 4. compute the coarse grid operator

P. Vaněk, J. Mandel, M. Brezina, Algebraic multigrid by smoothed aggregation for second and fourth order elliptic problems, Computing, 1996

SA AMG

- SA AMG relies on “candidate” vectors or the near null space or smooth error
- vector of ones
- pre-smooth guesses
- adapting a cycle
- *a priori* knowledge
- topological inference



Symmetric Strength

- i strongly depends on j if

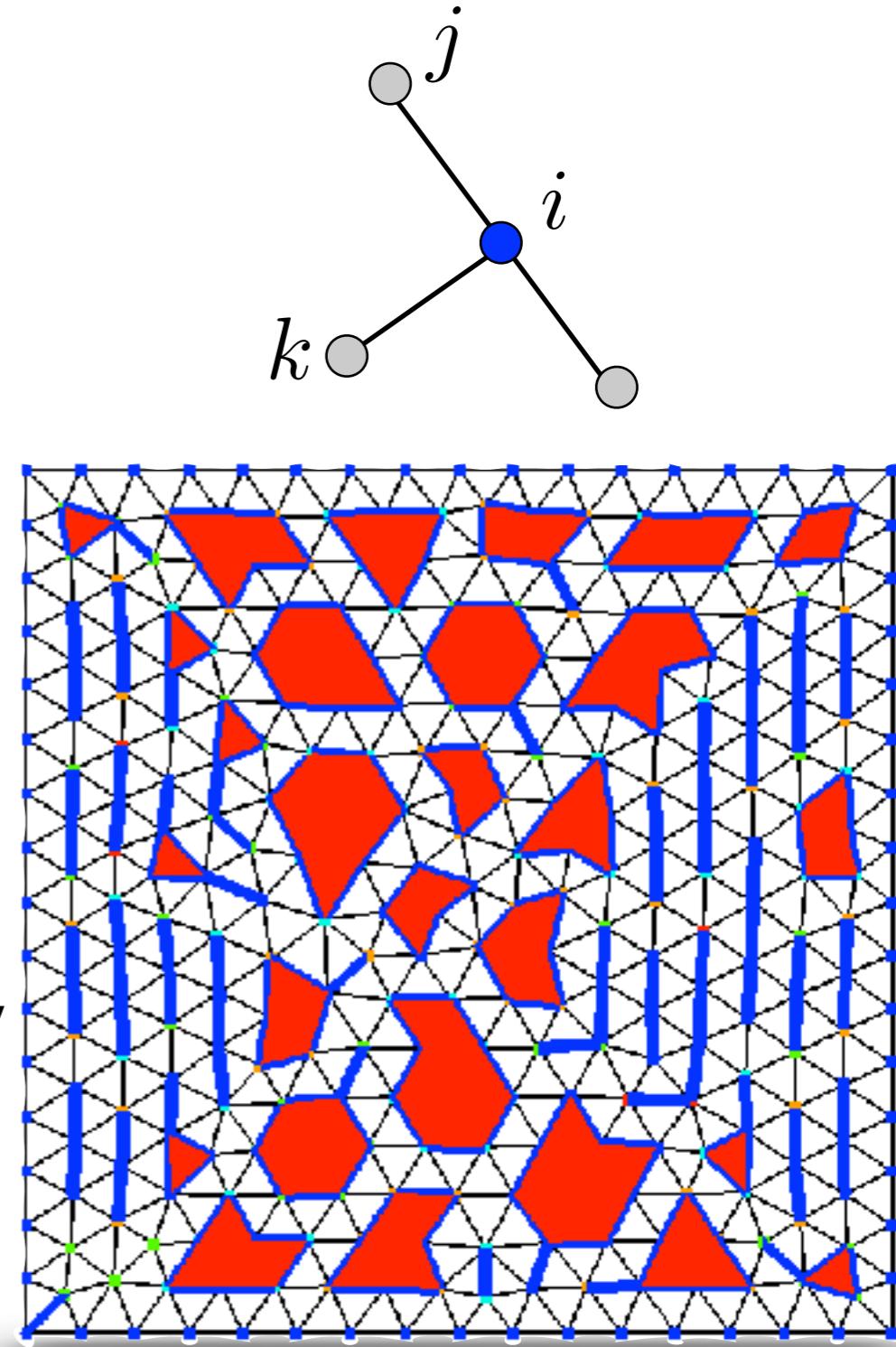
$$-A_{ij} \geq tol * \max_{k \neq i} -A_{ik}$$

- i strongly depends on j if

$$\frac{|A_{ij}|}{\sqrt{A_{ii}A_{jj}}} \geq tol$$

both “think” elliptic

↑
anisotropy
|

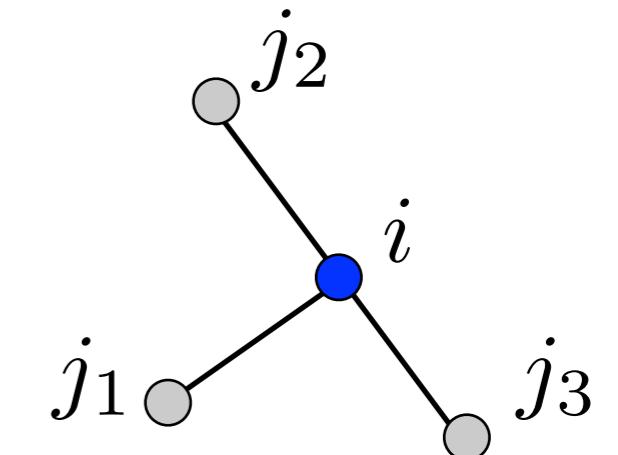
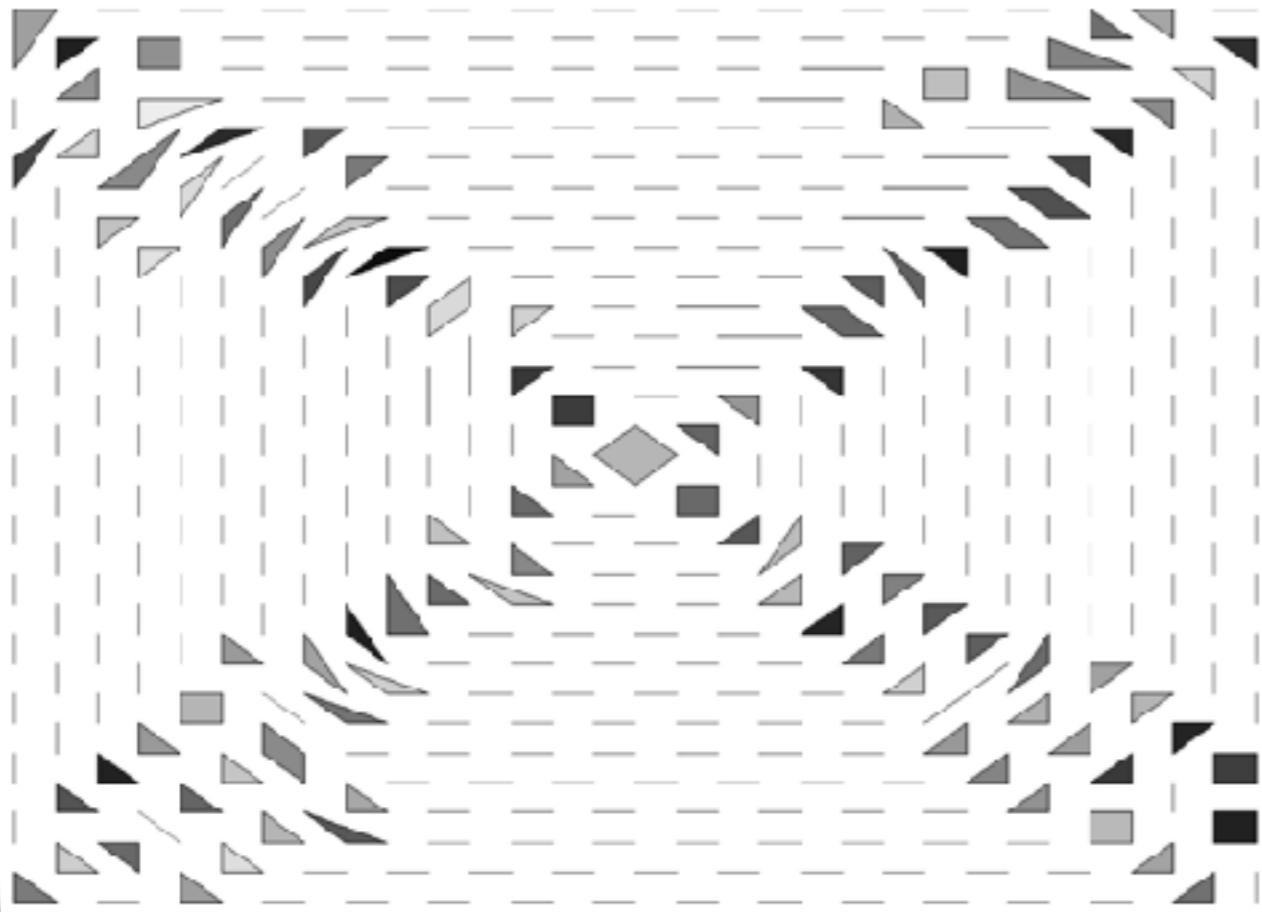


Advanced feature: evolution measure

1. drop point source at a node

2. evolve point source with A

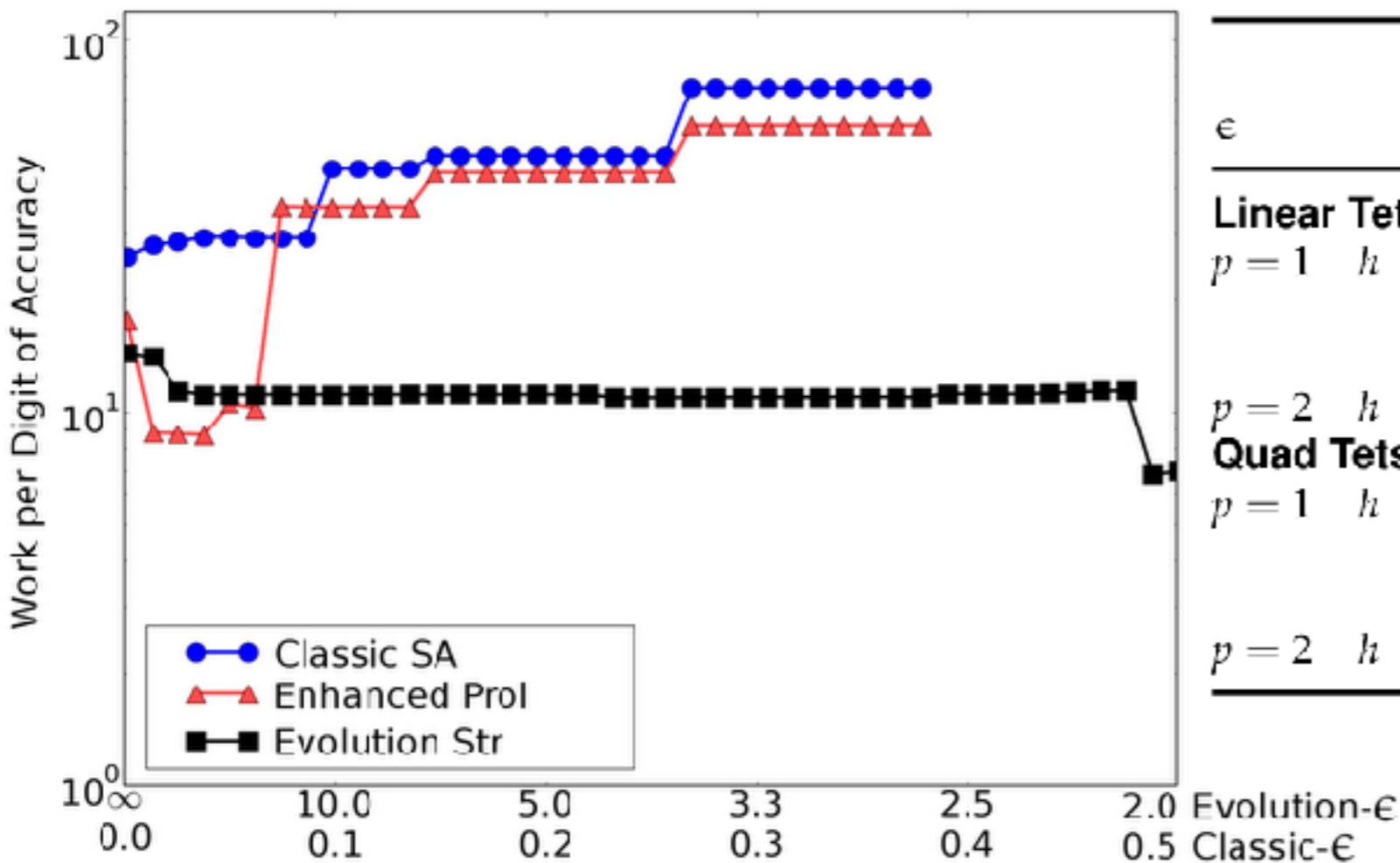
3. evaluate diffusivity at neighbors in comparison to known low energy



- efficient
- parameter insensitive
- Euler flow
- wave problems
- high-order
- discontinuous elements

Impact of the Evolution Measure

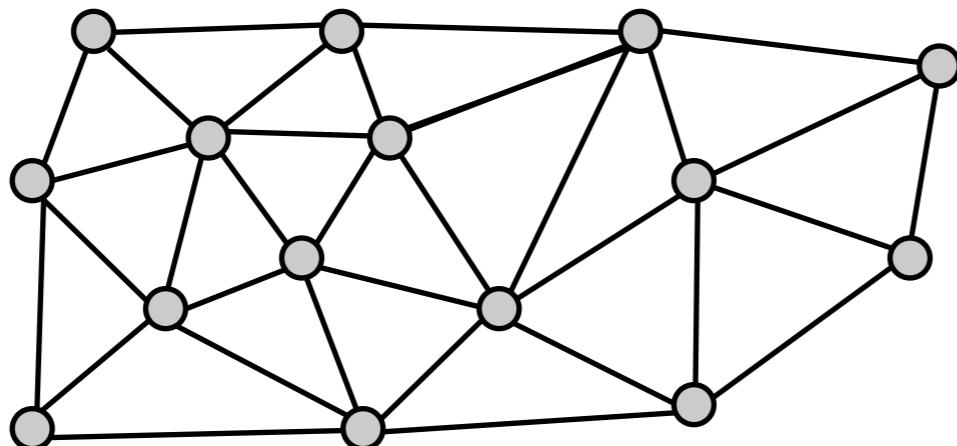
- less sensitive to drop tolerances
- single largest improvement we see in practice
- necessary for any complicated physics or discretization



ϵ	Classic SA		with P_{opt}		Evol
	0	$\frac{1}{4}$	0	$\frac{1}{4}$	4.00
Linear Tets					
$p = 1$	h	18	48	15	27
	$h/2$	17	74	14	62
	$h/4$	26	130	20	92
$p = 2$	h	41	85	24	46
	$h/2$	21	44	26	33
	$h/4$	45	88	67	67
Quad Tets					
$p = 1$	h	63	148	129	129
	$h/2$	49	86	61	61
	$h/4$	49	86	61	61

Algebraic Framework

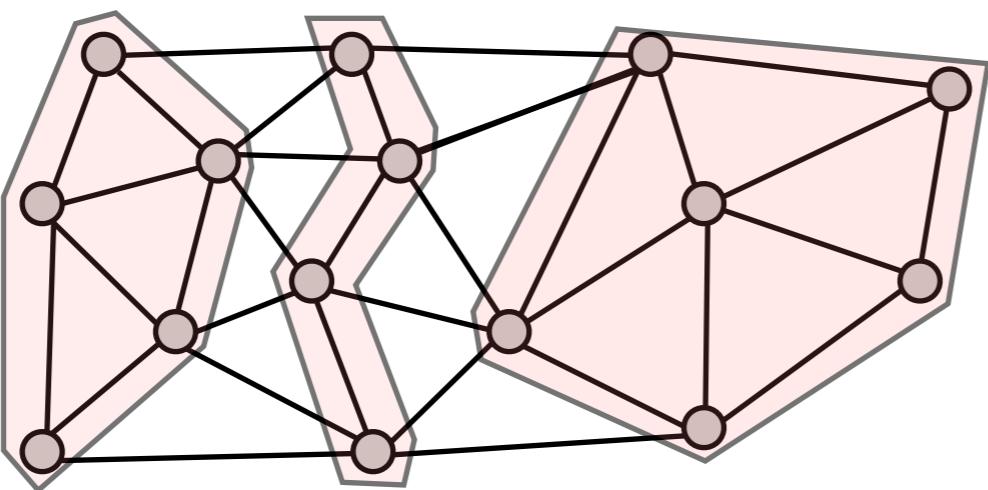
- aggregation: groups of fine nodes form coarse nodes



- an initial interpolation pattern
- find an optimal interpolation operator P that contains low energy

Algebraic Framework

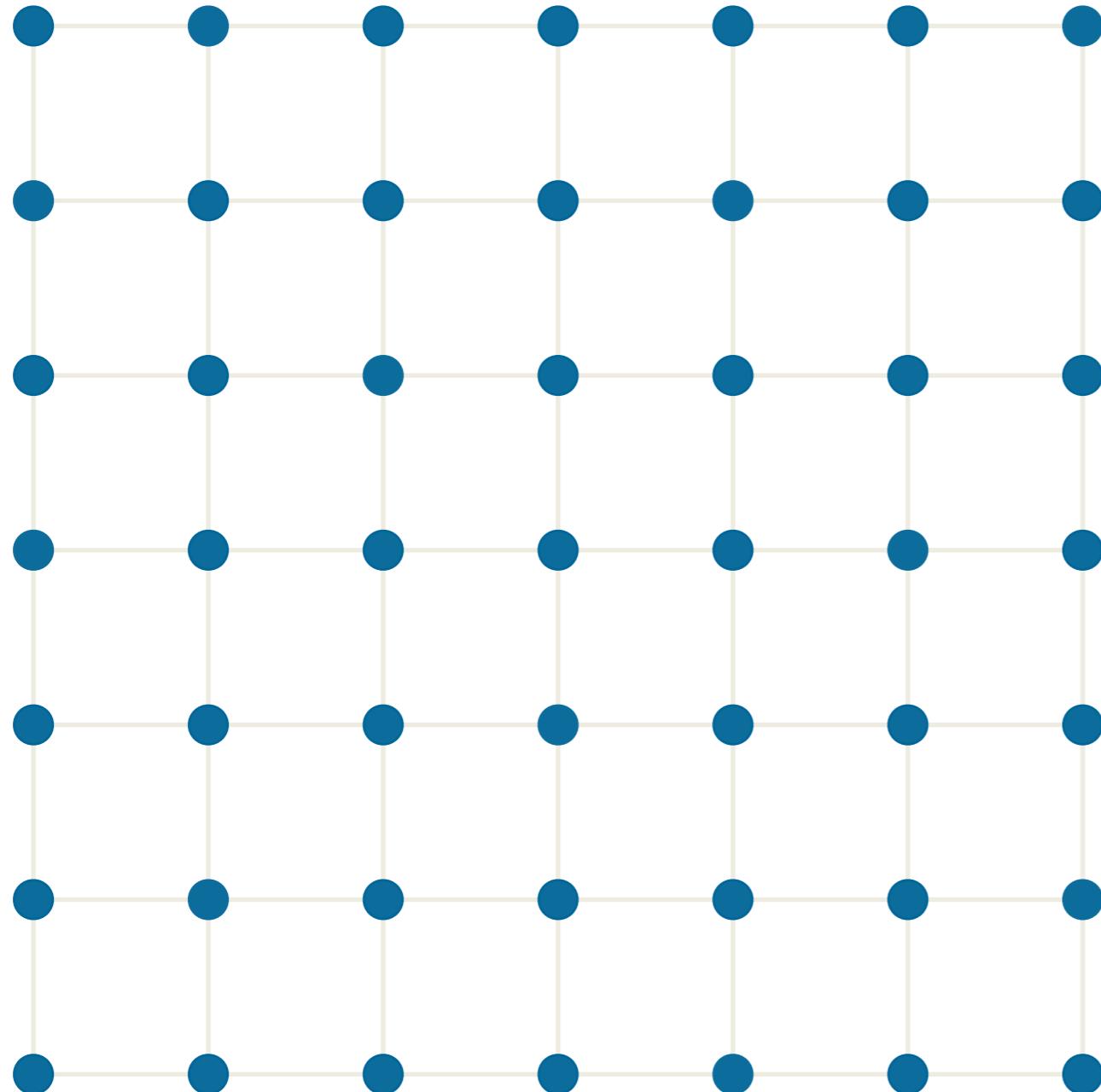
- aggregation: groups of fine nodes form coarse nodes



fine: 15
coarse: 3

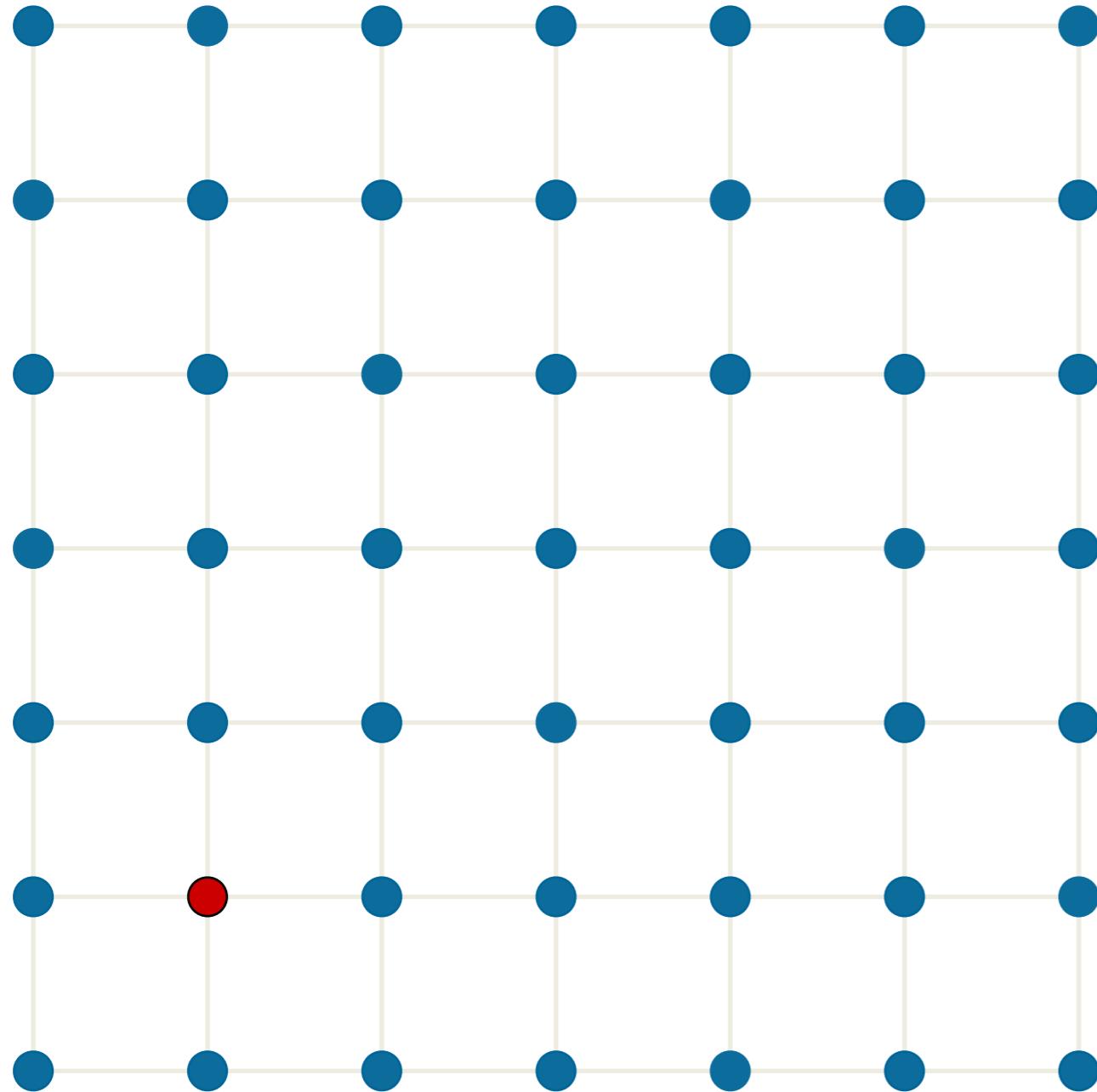
- an initial interpolation pattern
- find an optimal interpolation operator P that contains low energy

SA coarsening (5-pt Laplacian)



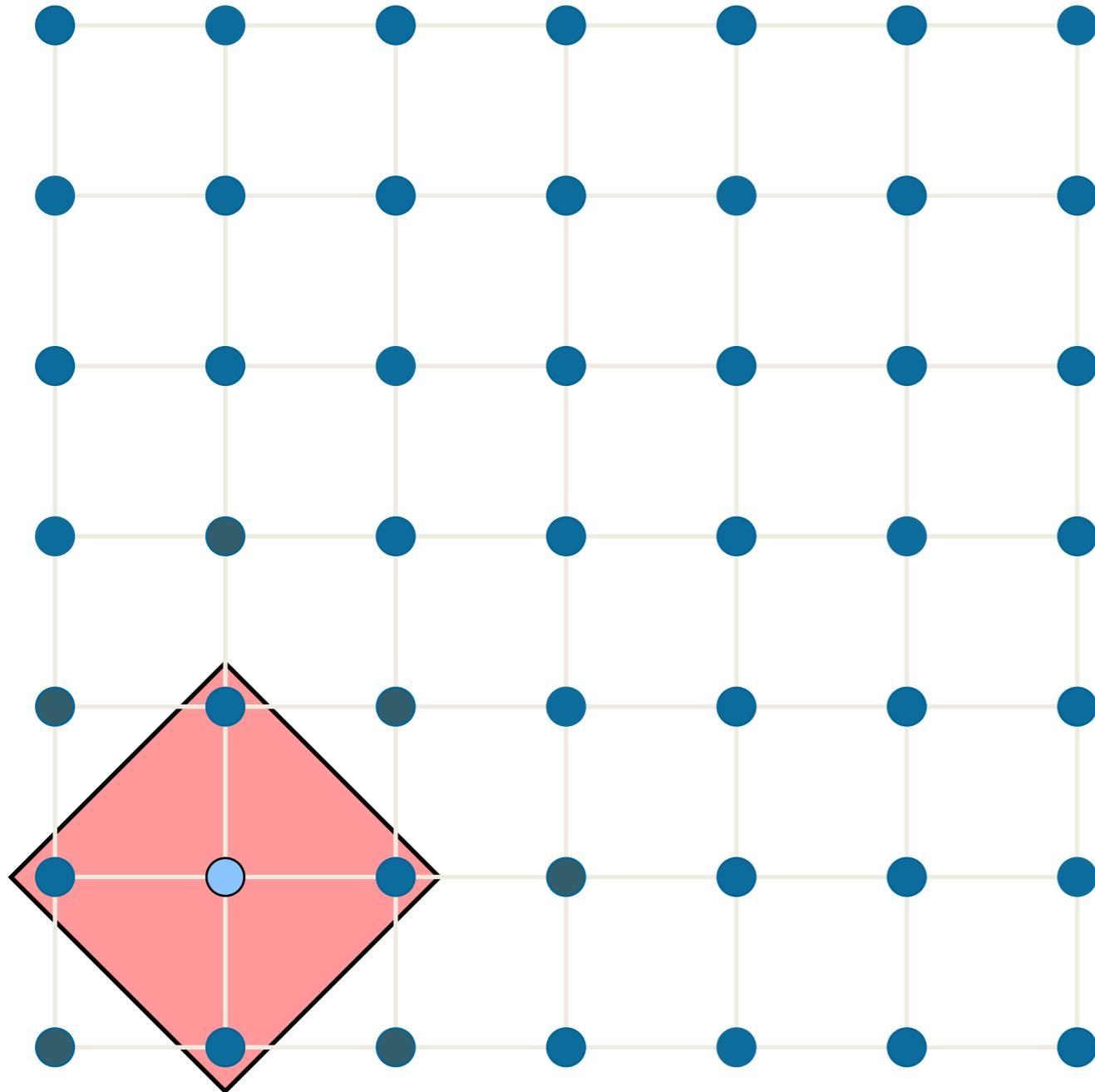
- Phase 1:**
- a) *Pick root pt not adjacent to agg*
 - b) *Aggregate root and neighbors*
- Phase 2:**
- Move pts into nearby aggs or new aggs*

SA coarsening (5-pt Laplacian)



- Phase 1:**
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SA coarsening (5-pt Laplacian)



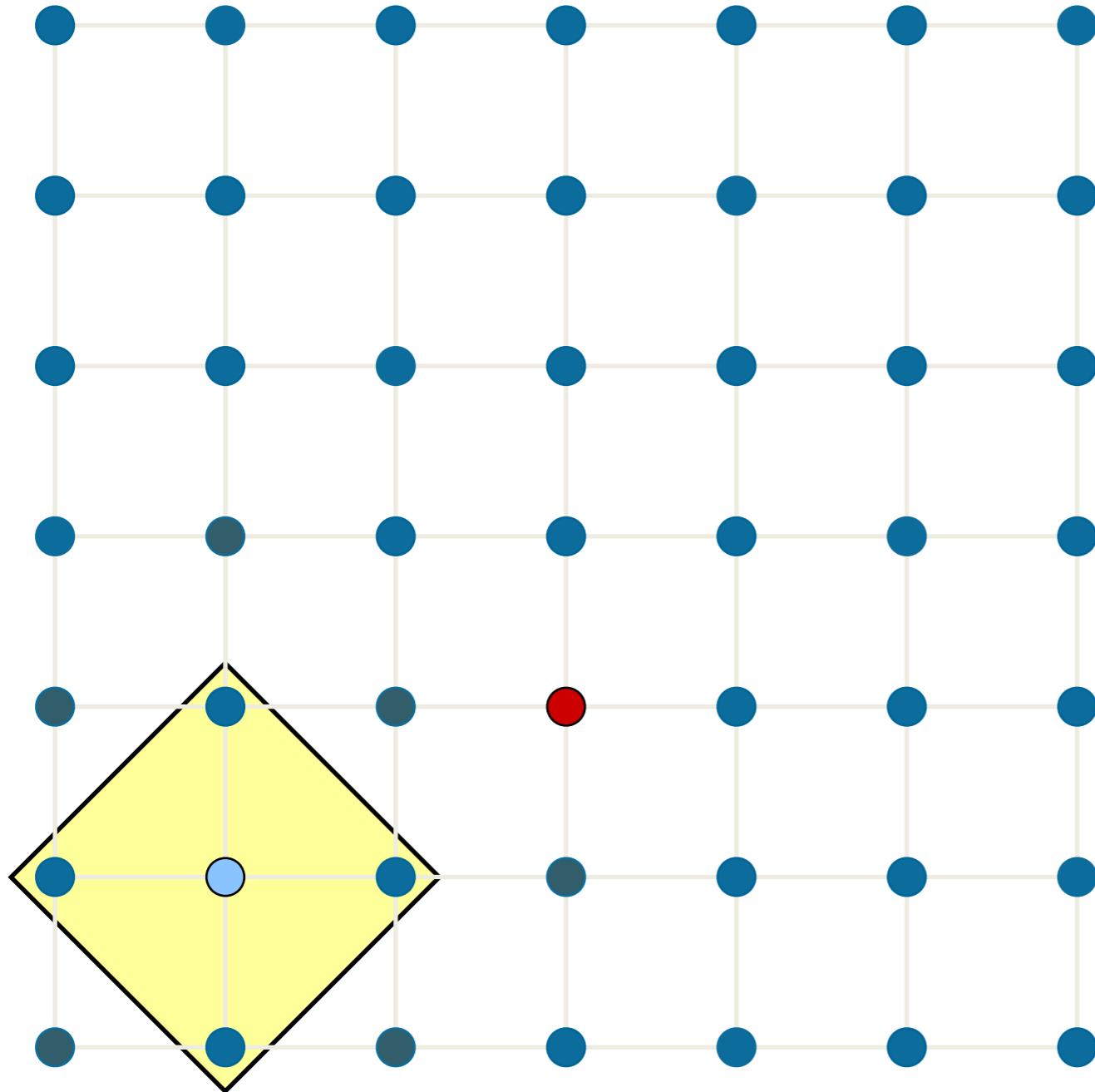
Phase 1:

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Phase 2:

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SA coarsening (5-pt Laplacian)



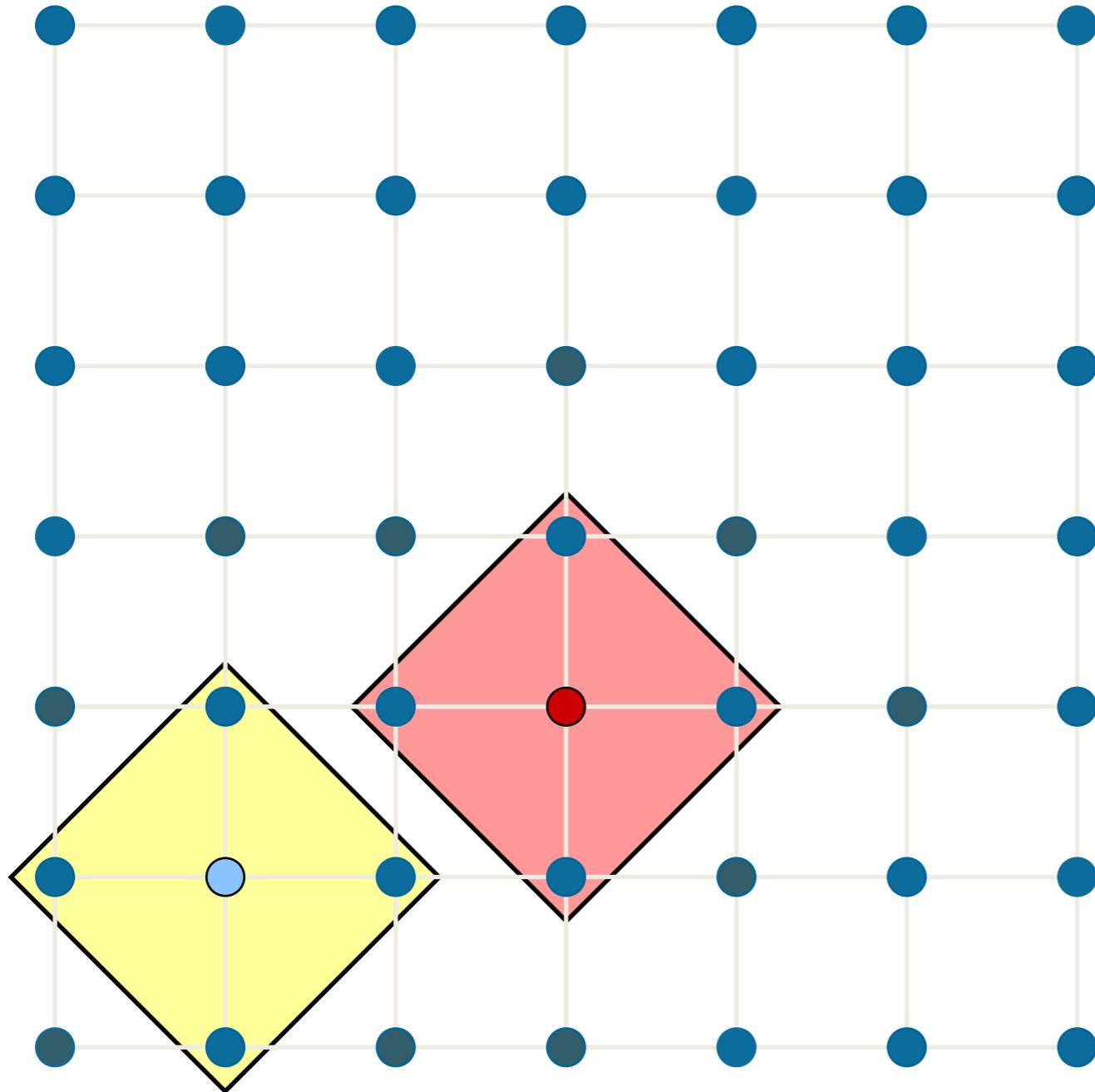
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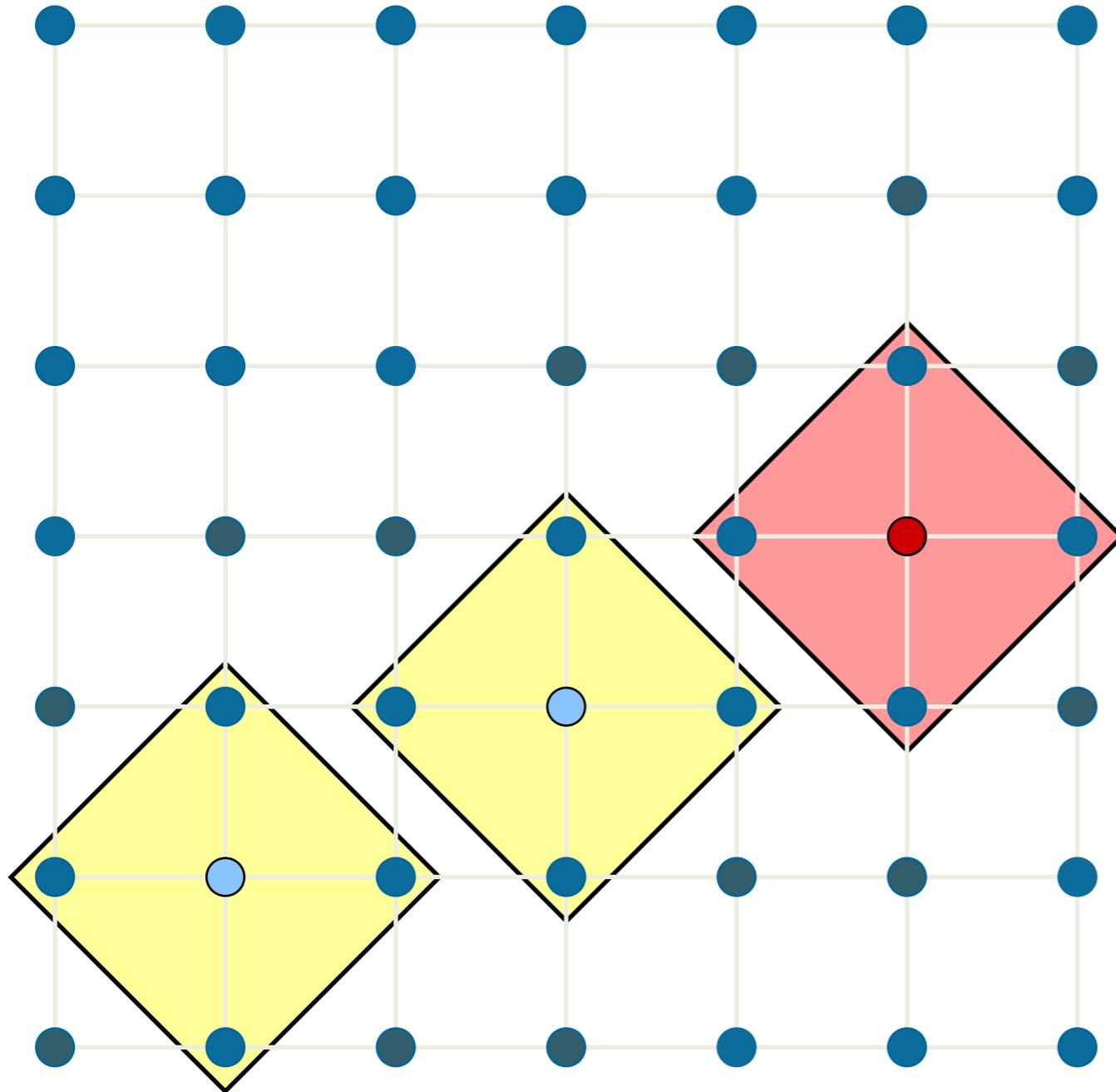
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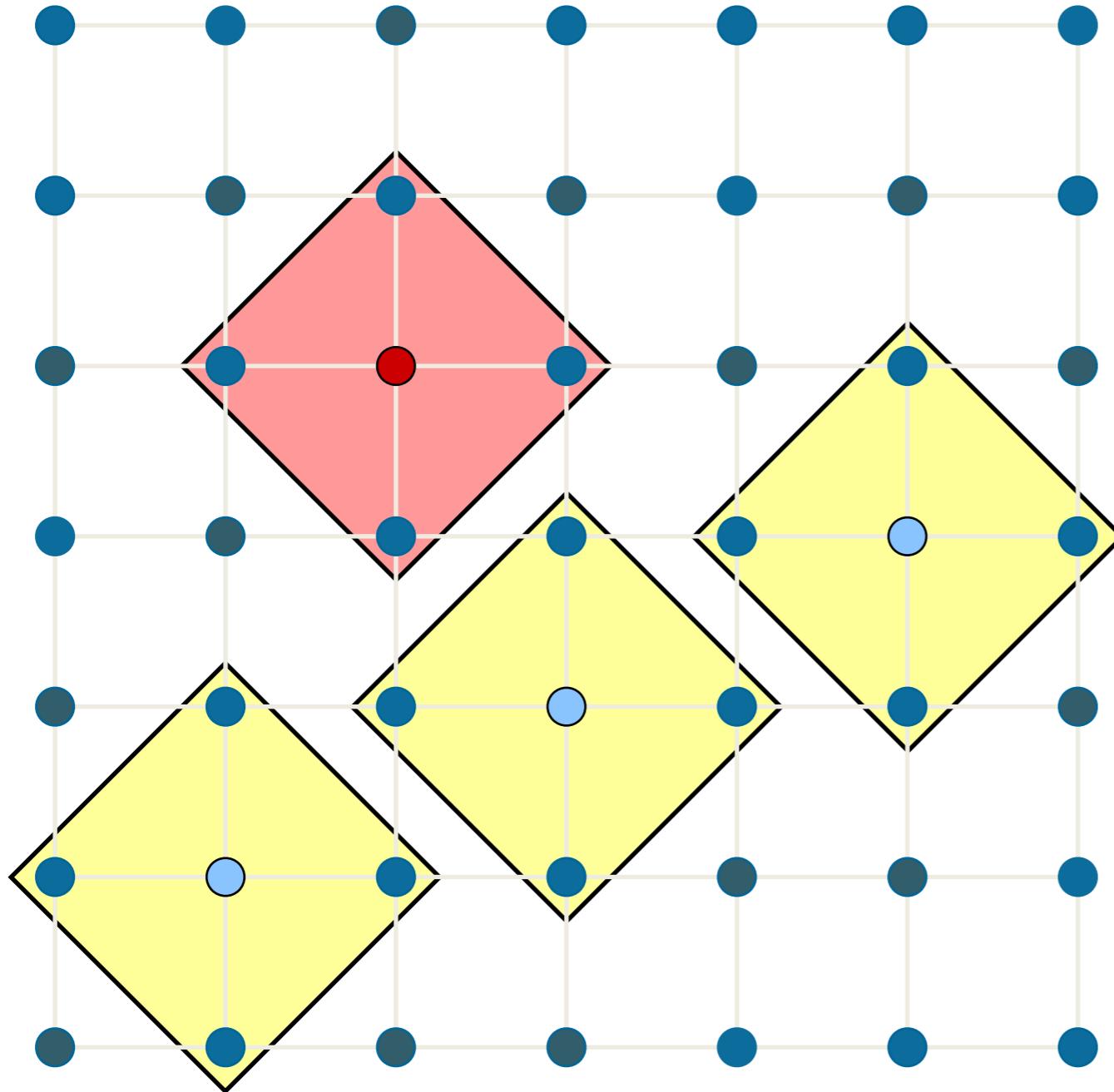
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SA coarsening (5-pt Laplacian)



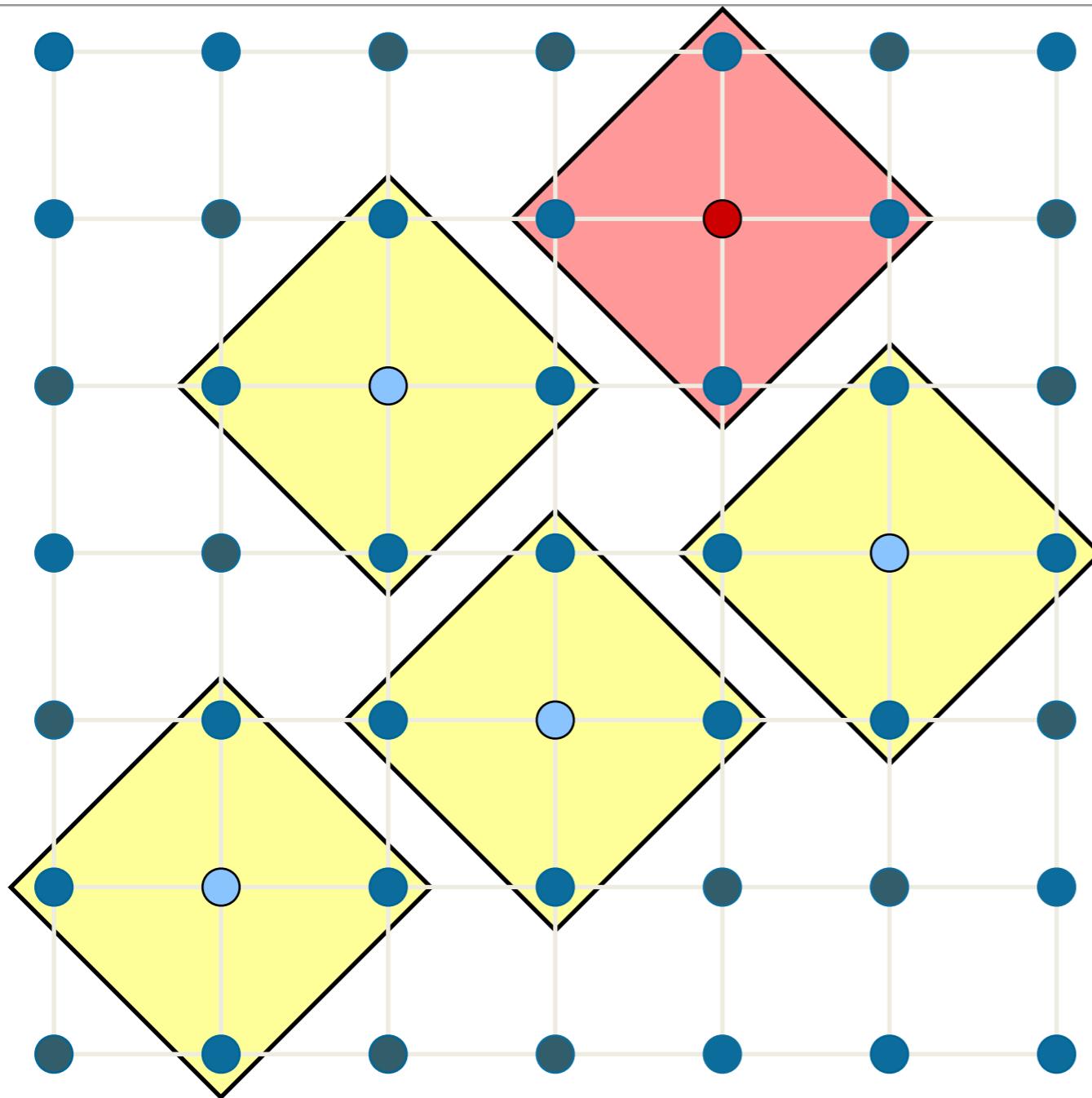
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SA coarsening (5-pt Laplacian)



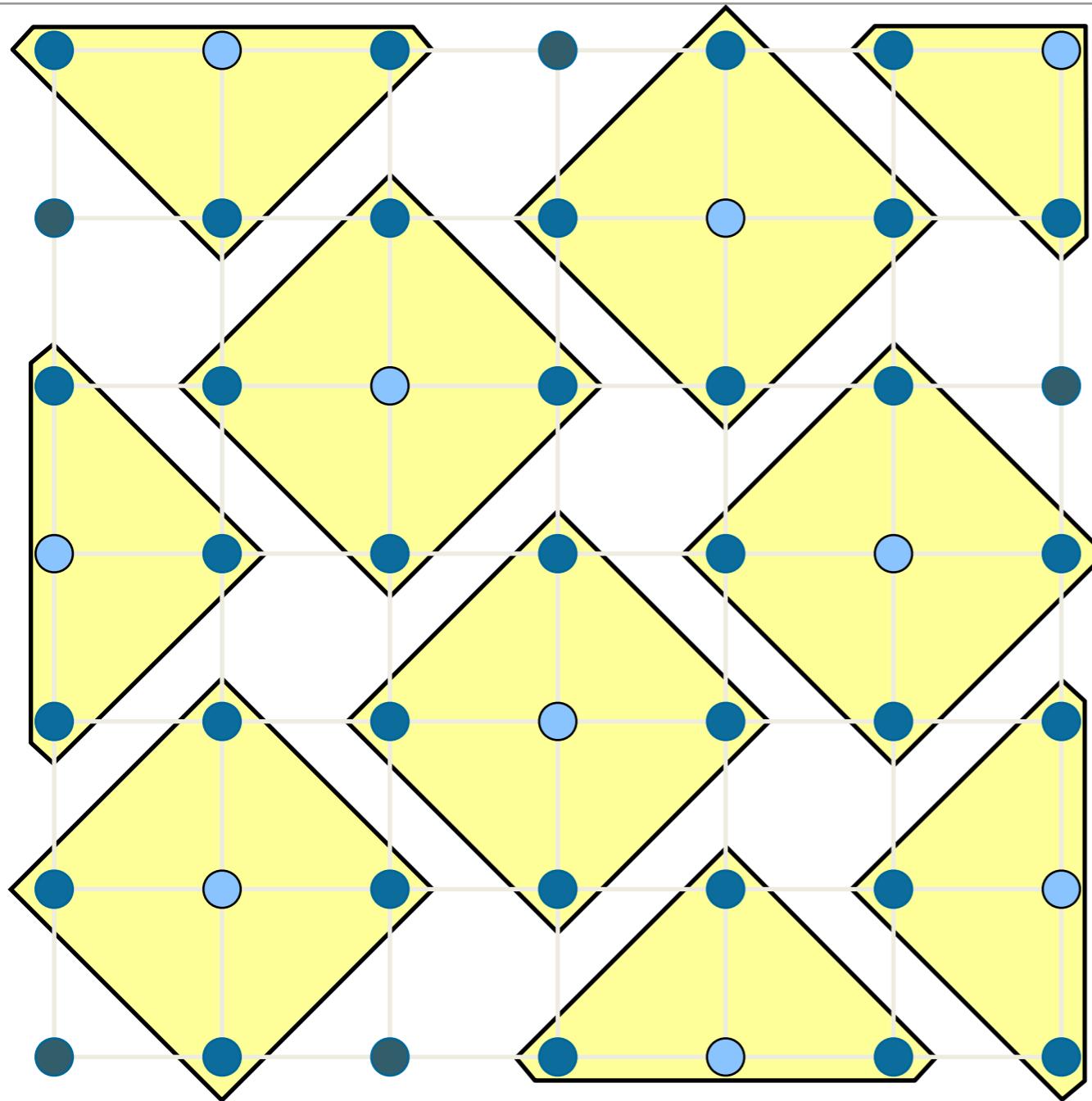
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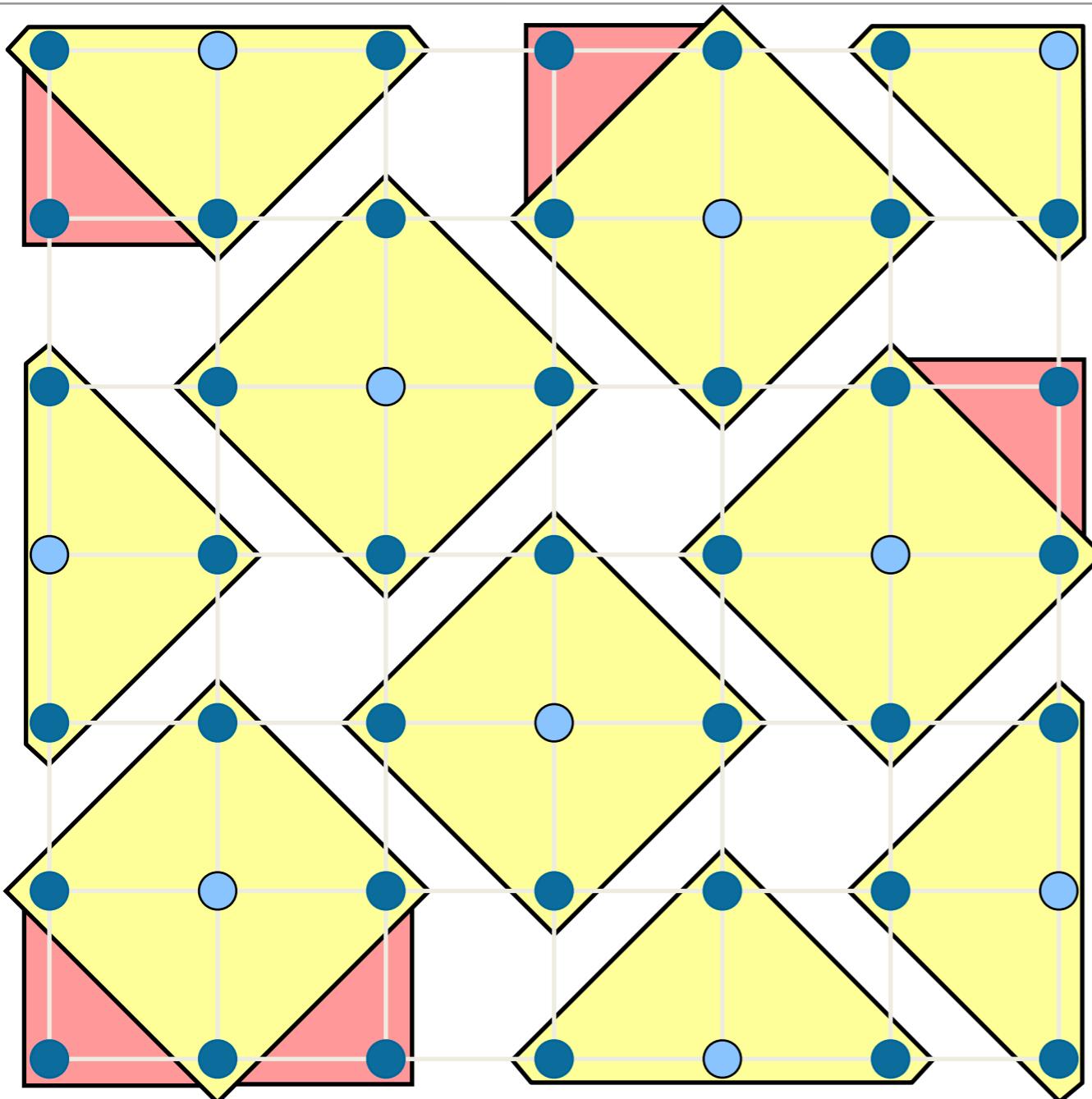
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SA coarsening (5-pt Laplacian)



Phase 1:

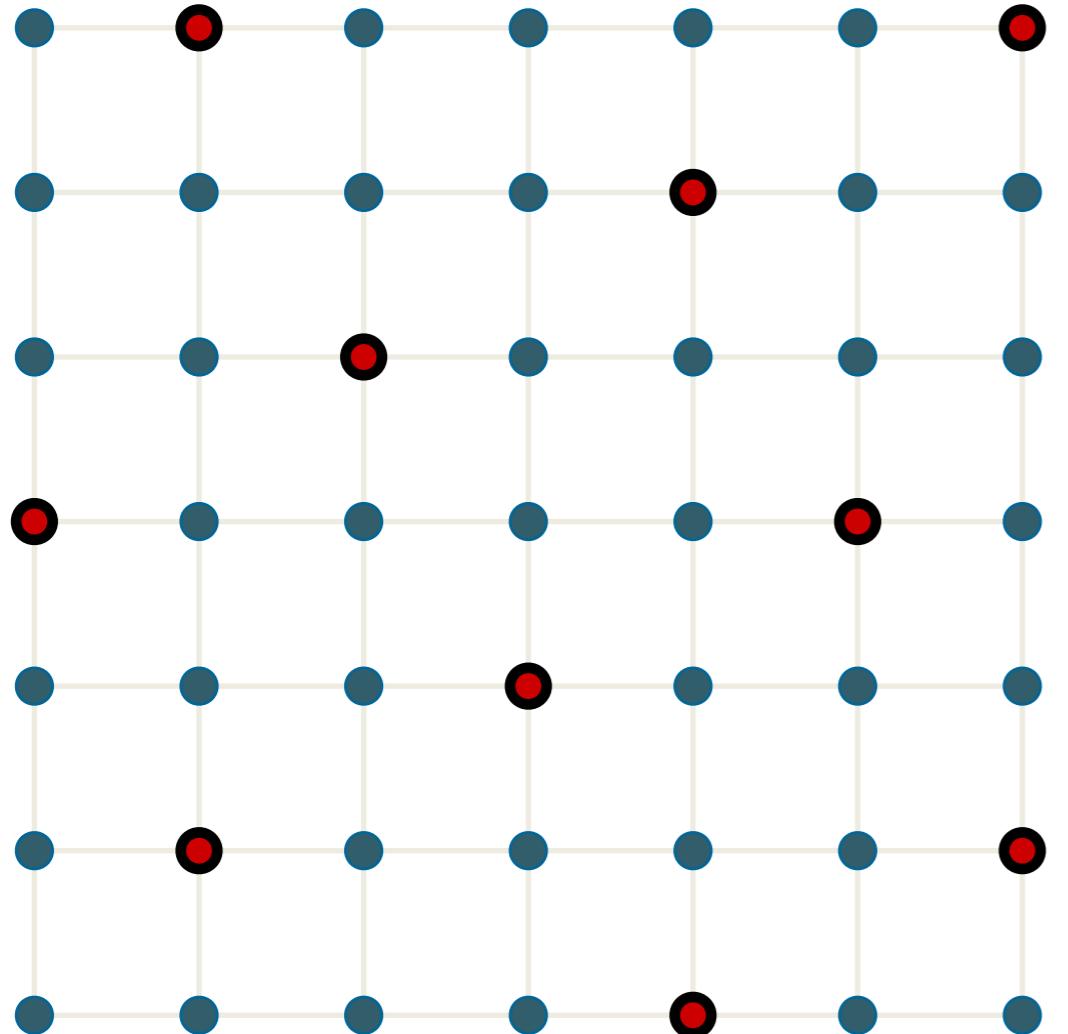
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Phase 2:

Move pts into nearby aggs or new aggs

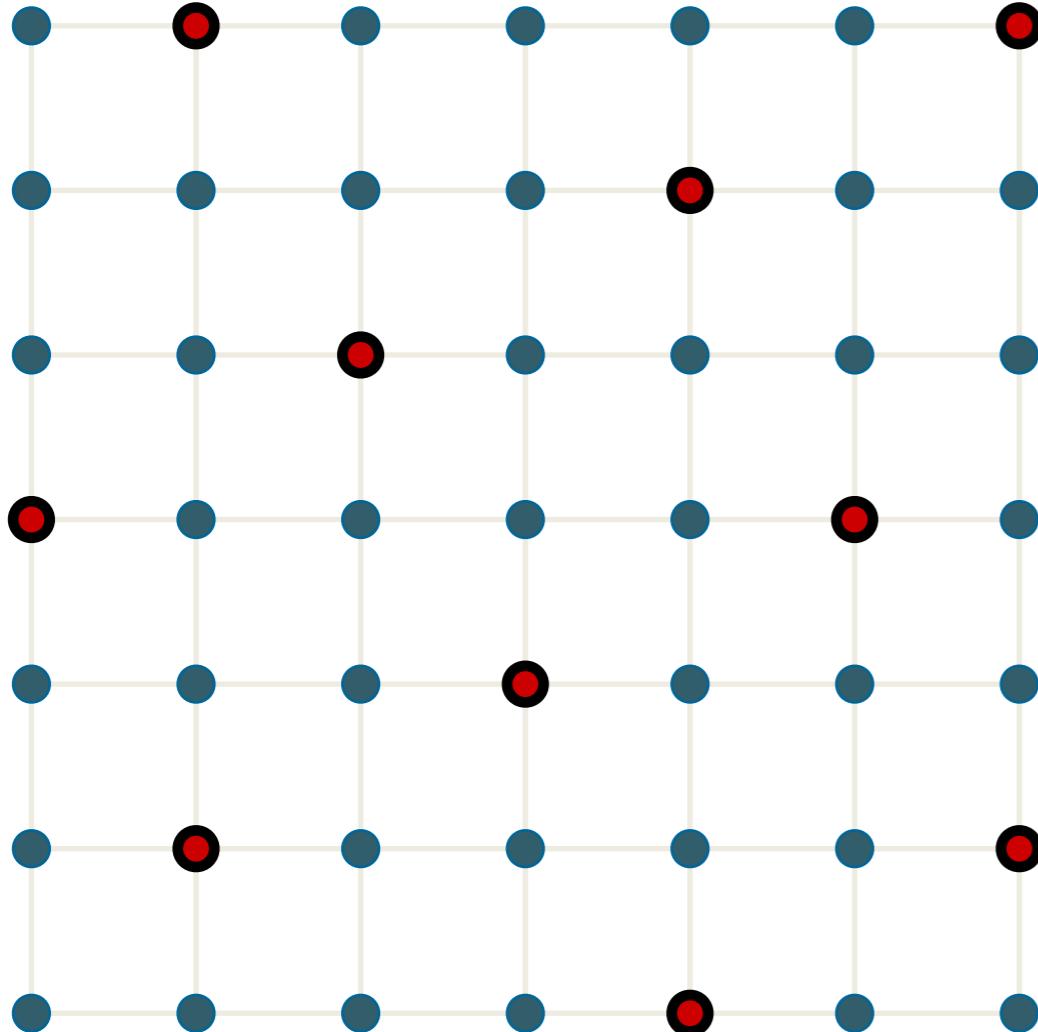
SA coarsening is traditionally more aggressive than
C-AMG coarsening (5-pt Laplacian example)

SA Seed Points (10)

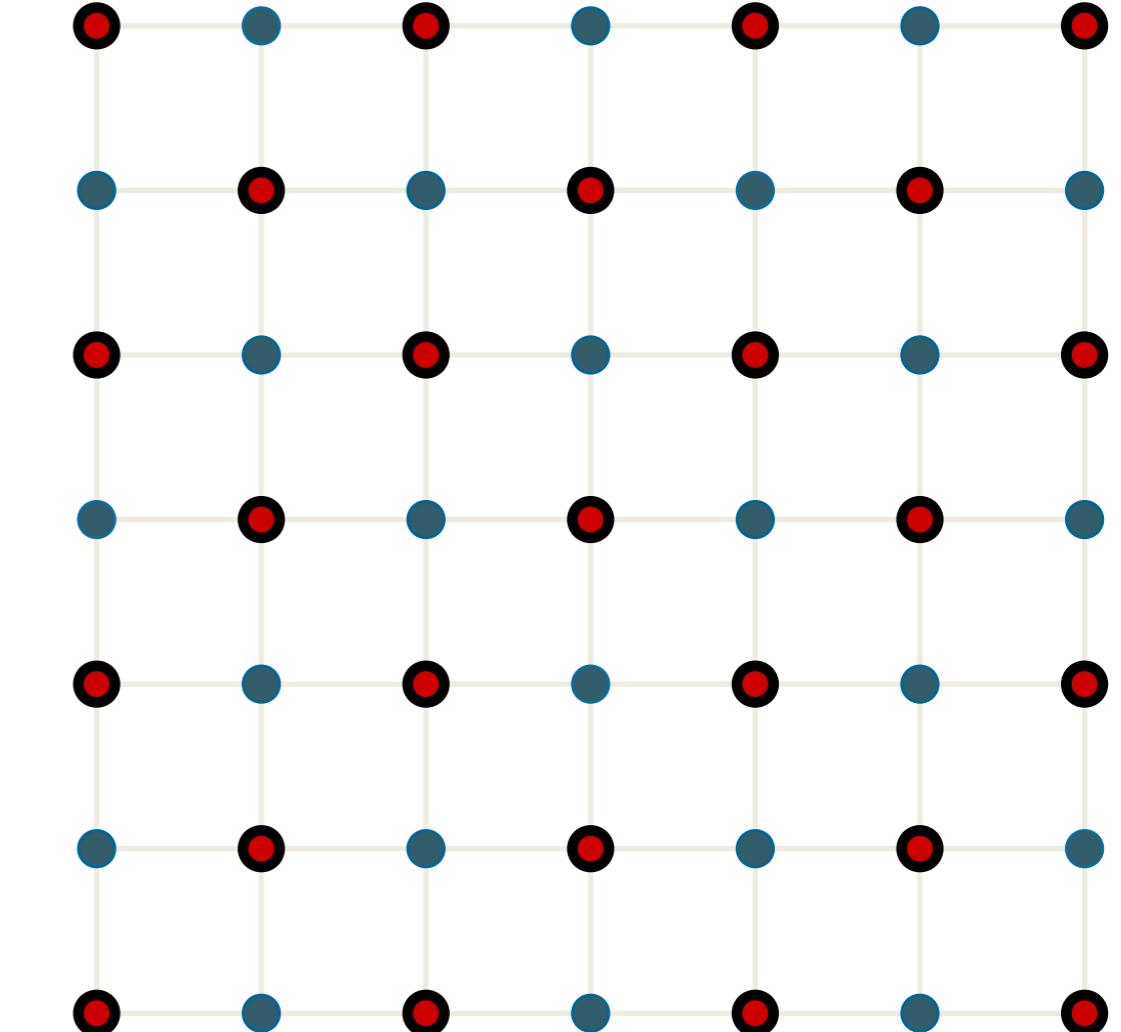


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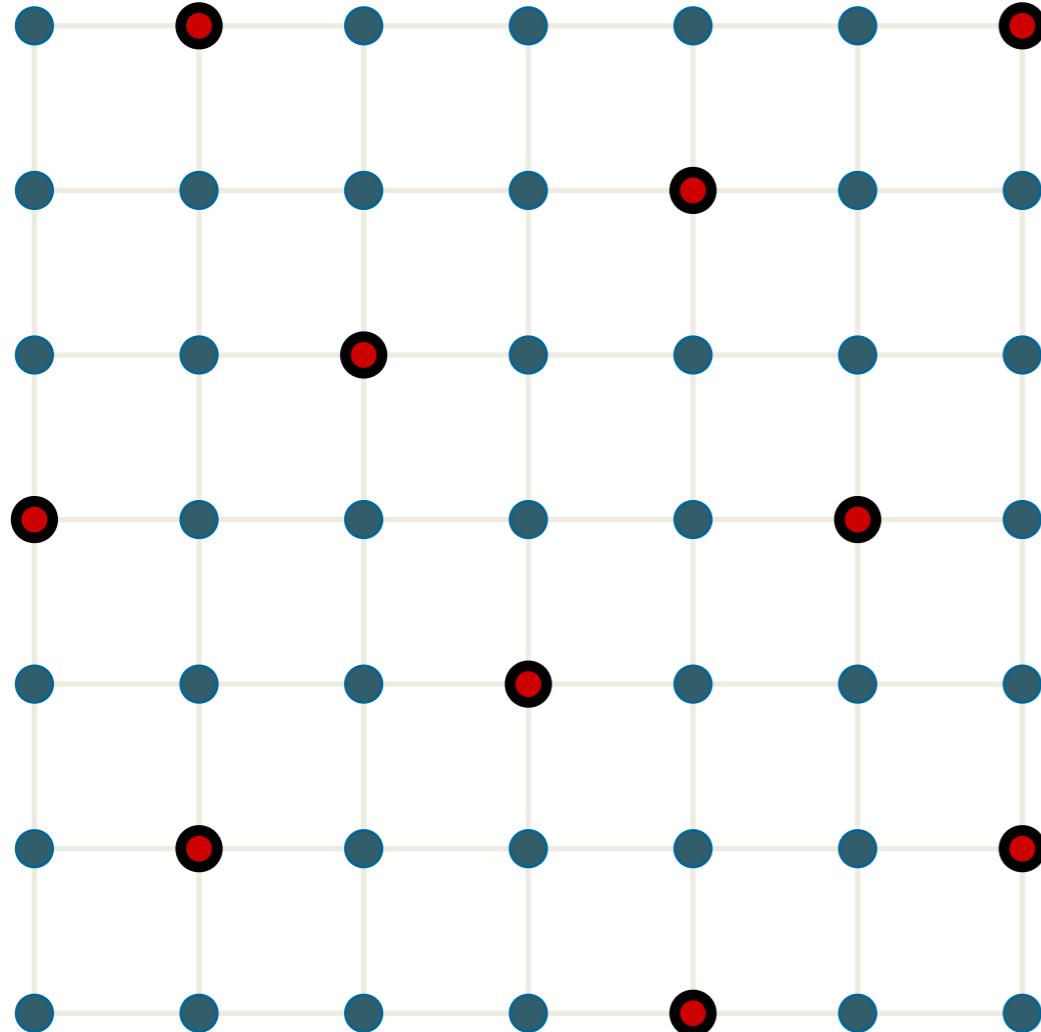


C-AMG Grid (25)

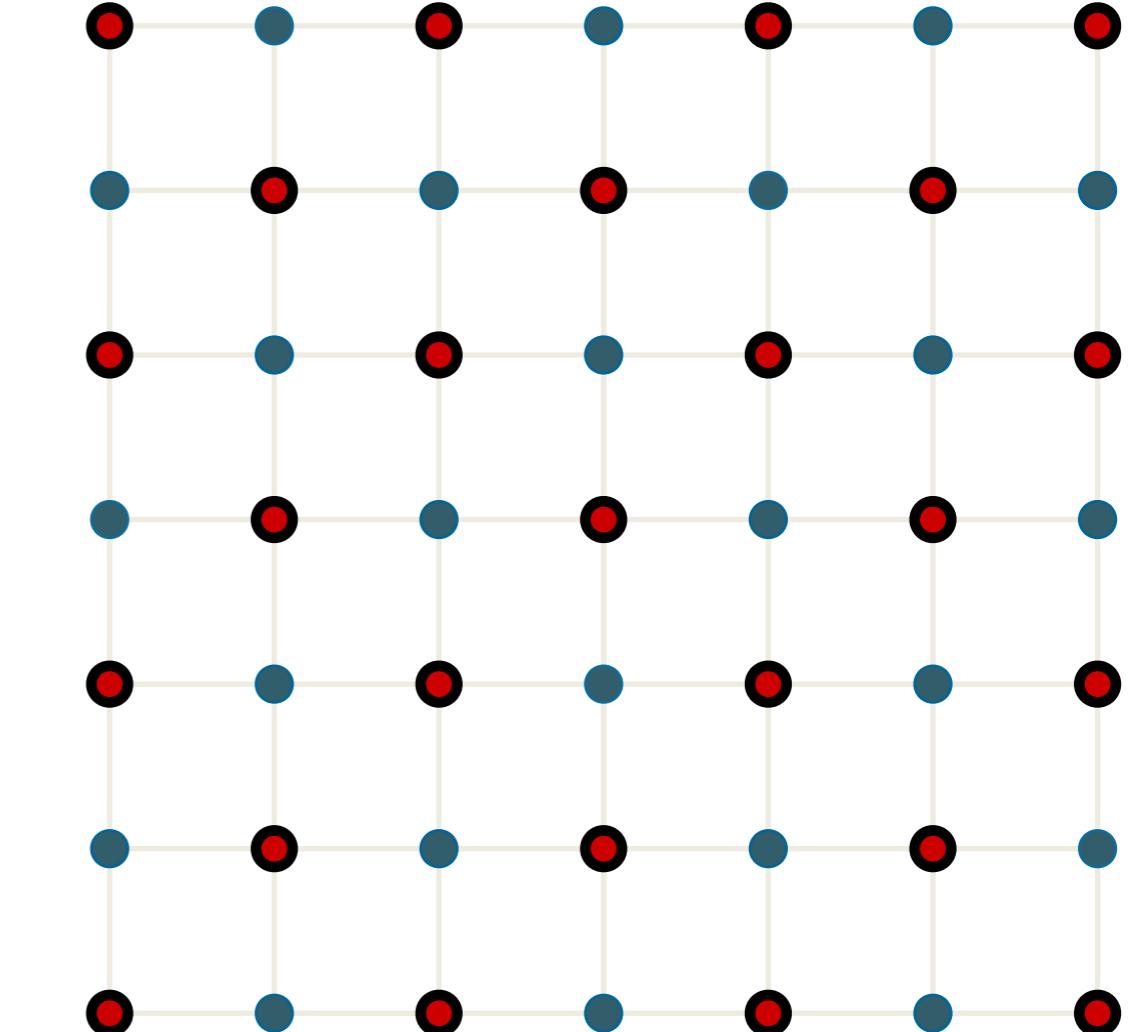


SA coarsening is traditionally more aggressive than C-AMG coarsening (5-pt Laplacian example)

SA Seed Points (10)



C-AMG Grid (25)



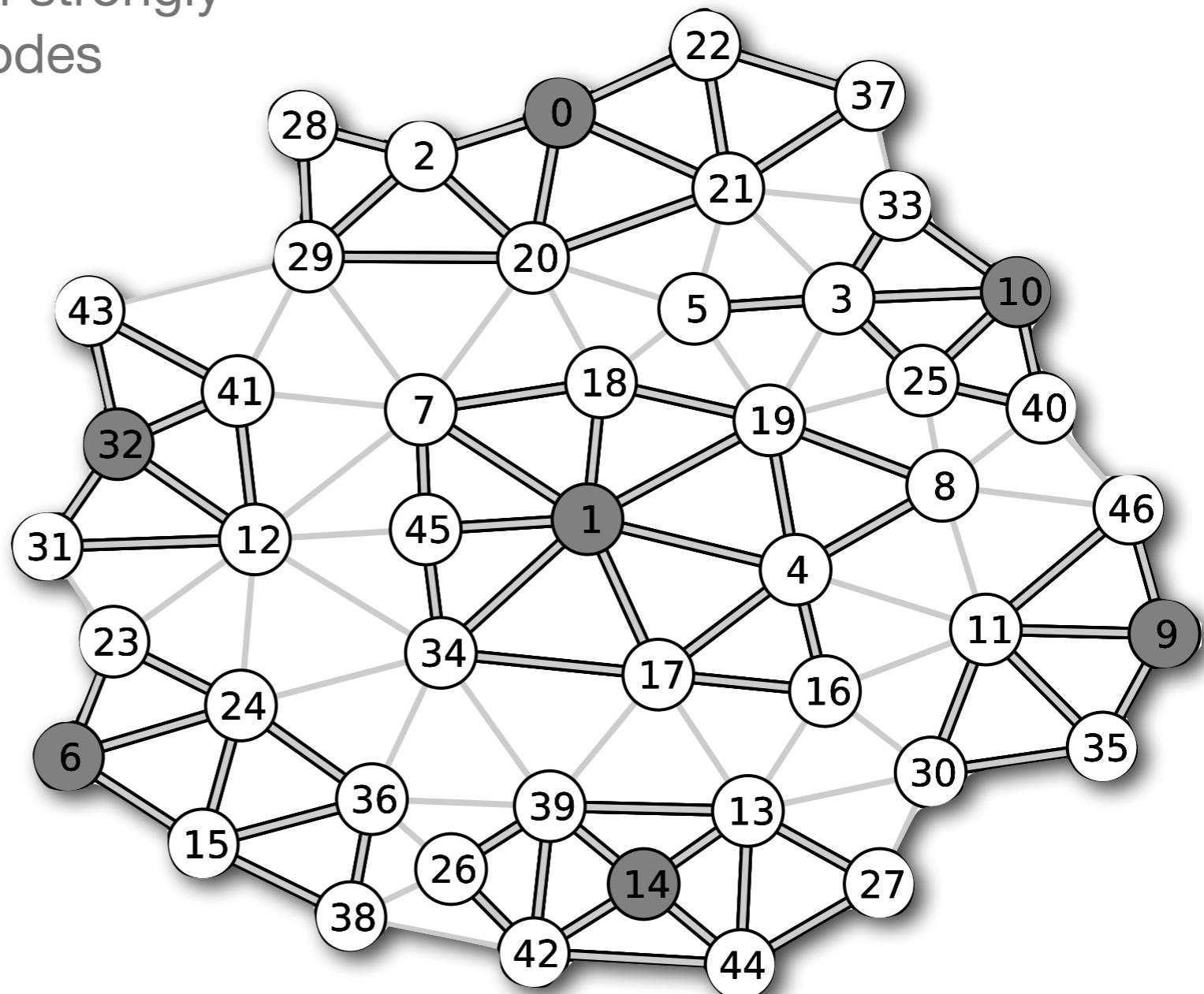
Operator complexities are usually smaller, too

MIS-based Graph Aggregation

- Greedy: group collections of strongly connected unaggregated nodes

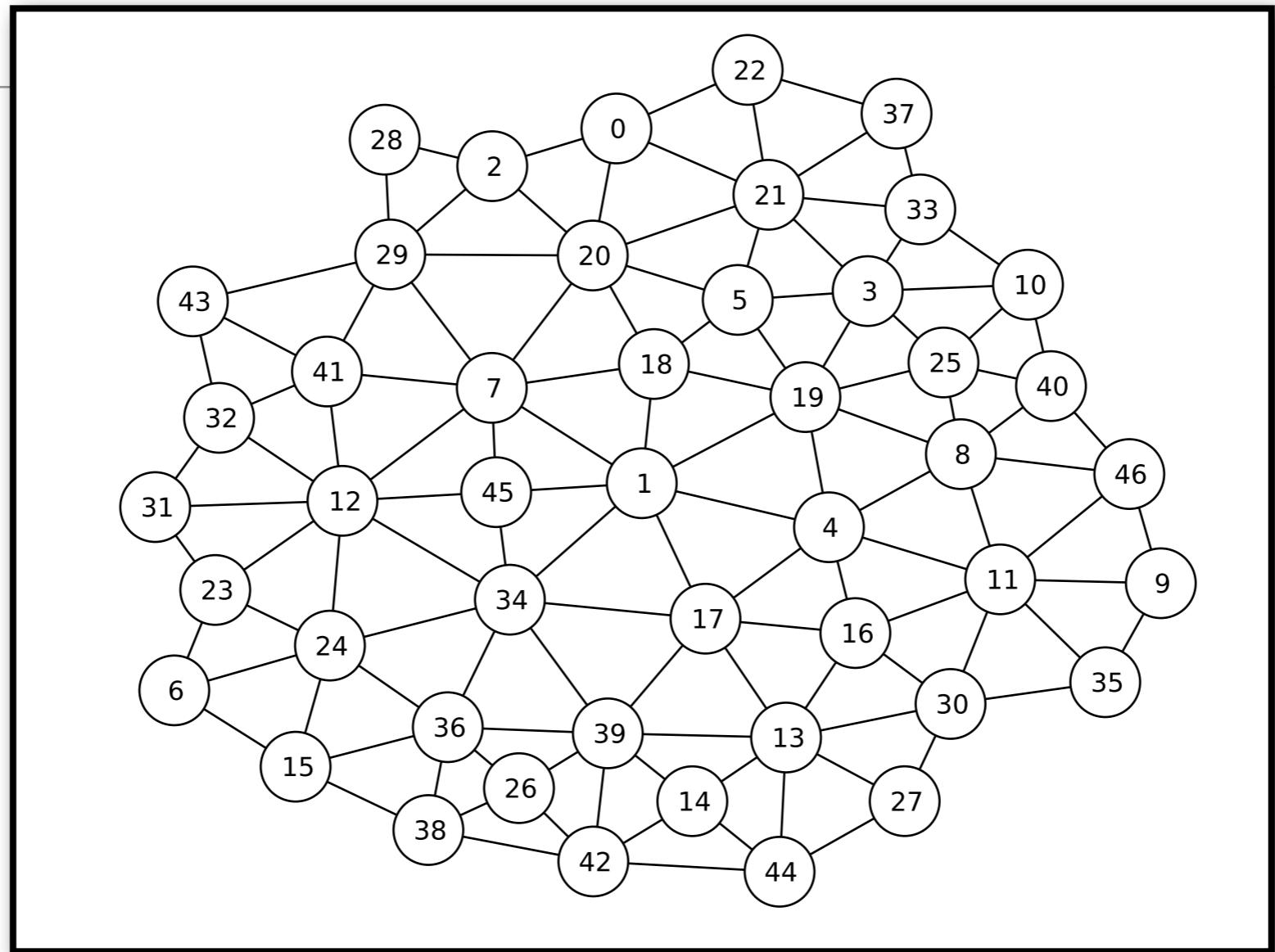
- Problems:

1. size fixed
2. sequential (greedy)



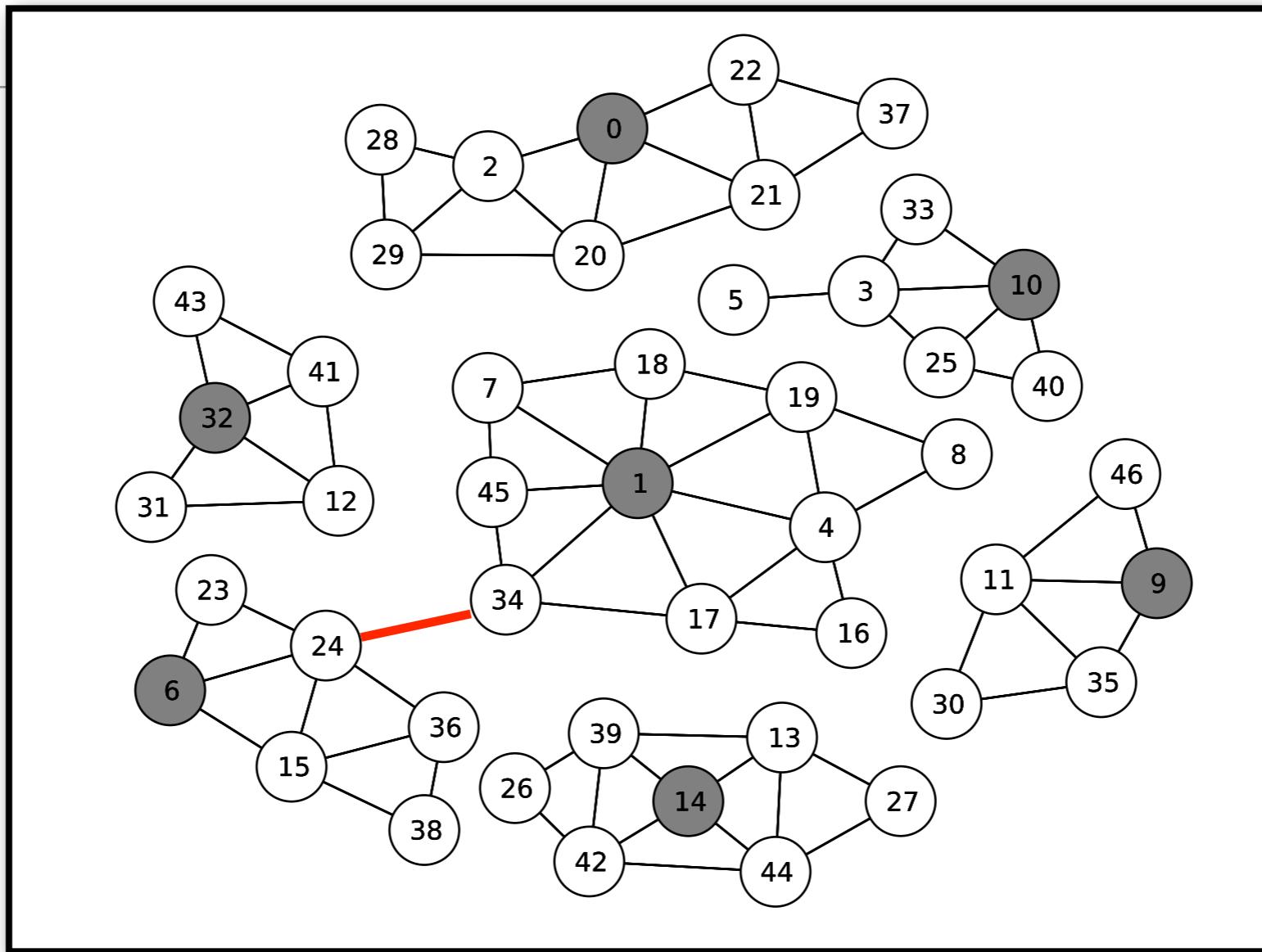
MIS(2)

3



MIS(2)

3



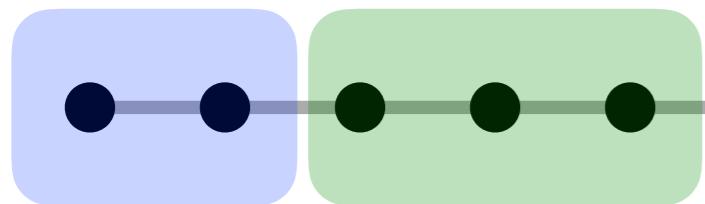
- root nodes more than 2 edges apart ($>$ distance-2)
 - an unaggregated node more than 2 edges from a root can become a root

MIS(2)

maximal

SA AMG Interpolation

- Here we use 1) the aggregation pattern
and 2) the candidate vectors



$$AggOpp = \begin{bmatrix} * & 0 & 0 \\ * & 0 & 0 \\ 0 & * & 0 \\ 0 & * & 0 \\ 0 & * & 0 \\ 0 & 0 & * \\ 0 & 0 & * \\ 0 & 0 & * \\ 0 & 0 & * \end{bmatrix}$$

$$Q_1 R_1 \quad Q_2 R_2 \quad Q_3 R_3$$

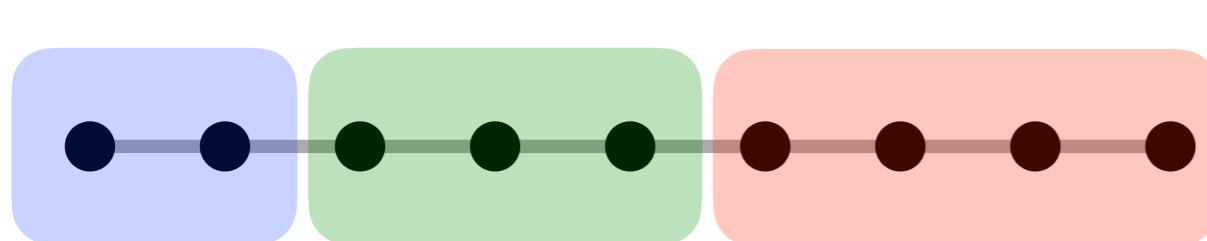
$$B = \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \\ B_{31} & B_{32} \\ B_{41} & B_{42} \\ B_{51} & B_{52} \\ B_{61} & B_{62} \\ B_{71} & B_{72} \\ B_{81} & B_{82} \\ B_{91} & B_{92} \end{bmatrix} \quad \hat{T} = \begin{bmatrix} B_{11} & B_{12} & & & \\ B_{21} & B_{22} & B_{31} & B_{32} & \\ & & B_{41} & B_{42} & \\ & & B_{51} & B_{52} & B_{61} & B_{62} \\ & & & & B_{71} & B_{72} \\ & & & & B_{81} & B_{82} \\ & & & & B_{91} & B_{92} \end{bmatrix} \quad T = \begin{bmatrix} Q_1 & & \\ & Q_2 & \\ & & Q_3 \end{bmatrix}$$

$$B_C = \begin{bmatrix} R_1 \\ R_2 \\ R_3 \end{bmatrix}$$

$T B_C = B$

SA AMG Interpolation

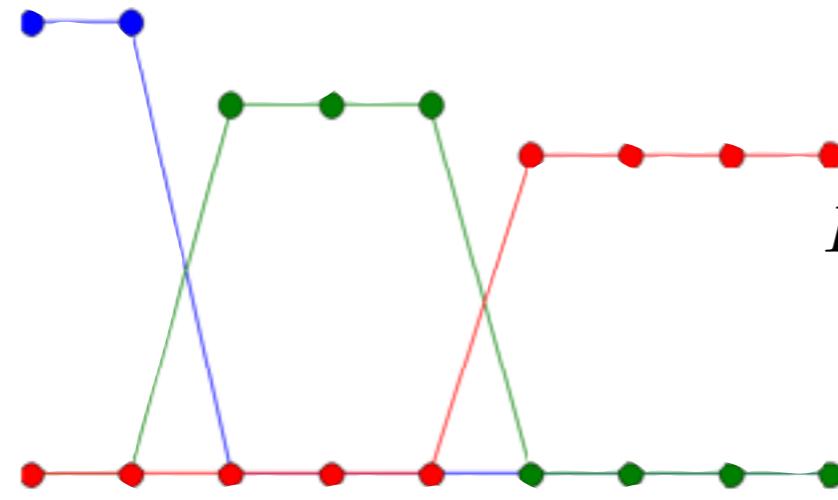
- Example



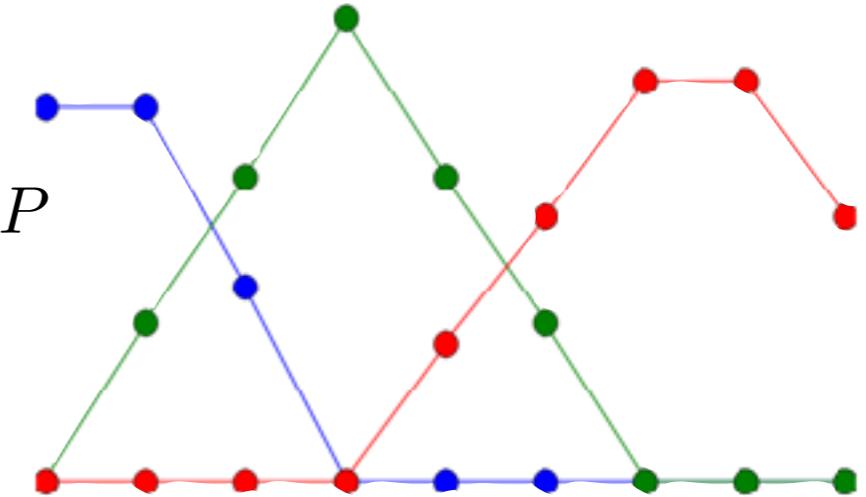
$$\hat{T} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

$$T = \begin{bmatrix} \frac{\sqrt{2}}{2} & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & \frac{\sqrt{3}}{3} & 0 \\ 0 & 0 & \frac{\sqrt{4}}{4} \end{bmatrix}$$

- Now make interpolation **better**



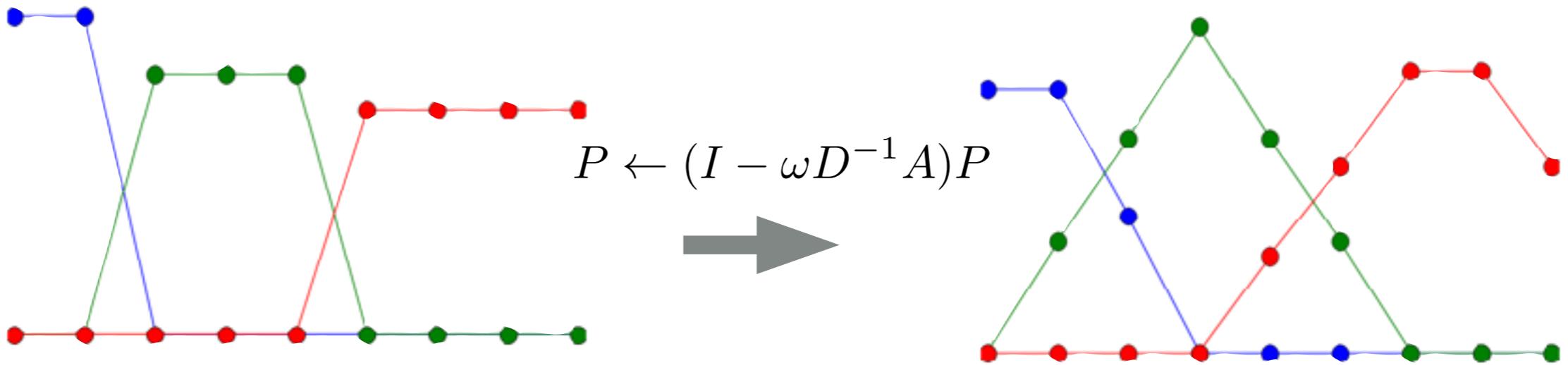
$$P \leftarrow (I - \omega D^{-1} A)P$$



SA AMG Interpolation

- reduce energy
- improve accuracy
- increase complexity

- Improving interpolation



- Makes the columns of P **smoother**
- Makes the sparsity of P **denser**

Demo: [3-SA-AMG-in-1D.ipynb](#)

SA AMG Interpolation

$$e_1 \leftarrow (I - P(P^T A P)^{-1} P^T A) G e_0$$

$$G e_0 \in \mathcal{R}(P) \quad \Rightarrow \quad e_1 = 0$$

interpolation should capture what relaxation misses

- P should have low energy (low A -norm or $A^* A$ -norm)
 1. determine sparsity pattern
 2. minimize energy column-wise (parallel)

SA AMG Interpolation

- Want P so that $u_{low} \in \mathcal{R}(P)$

1. Grow and fix sparsity pattern as $S^k P_{tent}$

2. Minimize residual of

$$AP_j = 0 \quad \text{for each column } j$$

3. Constraint the minimization with

$$PB_c = B$$

SA AMG General Interpolation

- Hermitian (and positive definite): use CG

$$AP_j = 0 \Leftrightarrow \min \|P_j\|_A$$

$$R = P^*$$

- Non-Hermitian: use GMRES

$$AP_j = 0 \Leftrightarrow \min \|P_j\|_{A^* A}$$

$$A^* R_j^* = 0 \Leftrightarrow \min \|R_j^*\|_{AA^*}$$

- Range of interpolation targets “right” low-energy

W. L. Wan, T. F. Chan, and B. Smith, An energy-minimizing interpolation for robust multi-grid methods, SIAM J. Sci. Comput., 2000

- Range of restriction* targets “left” low-energy

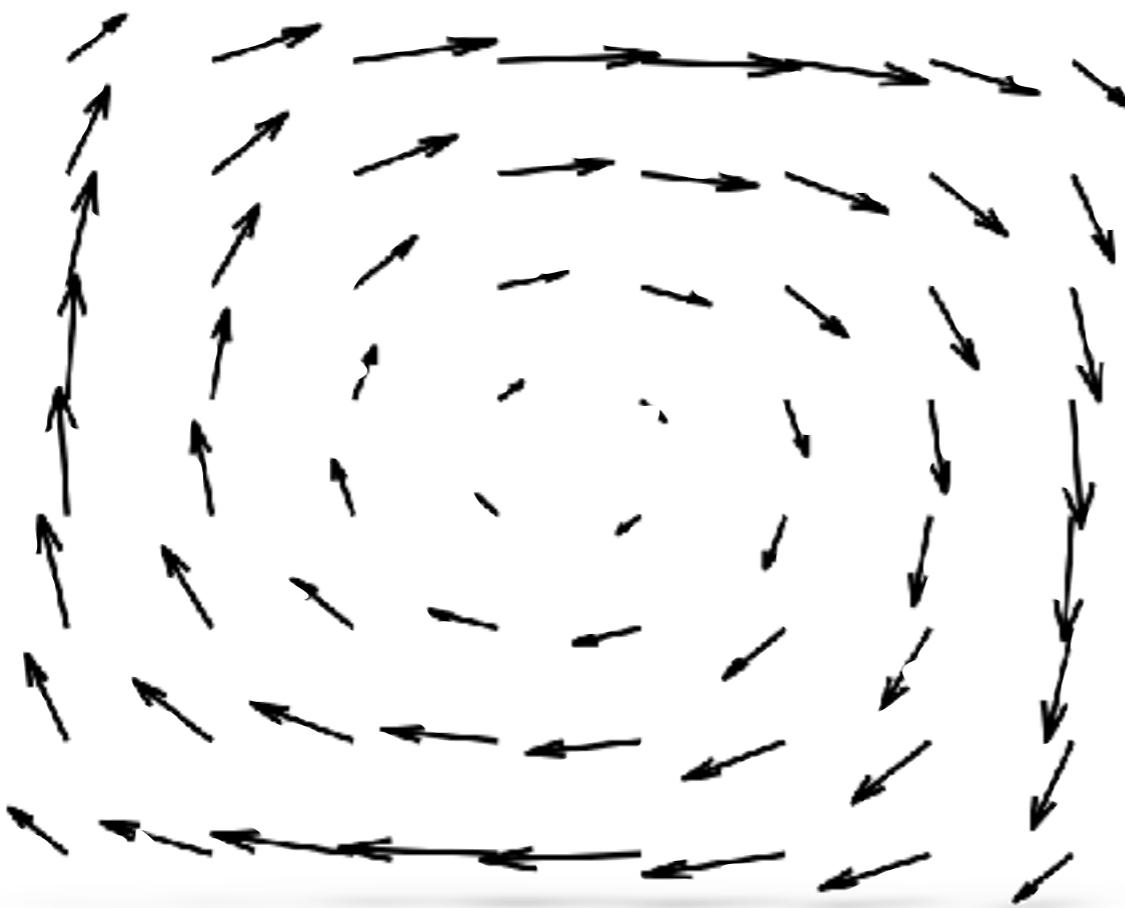
J. Xu and L. Zikatanov, On an energy minimizing basis for algebraic multigrid methods, Comput. Vis. Sci., 2004

- Cost is comparable to that of standard smoothing

Luke N. Olson , Jacob Schroder , Raymond S. Tuminaro, A General Interpolation Strategy for Algebraic Multigrid Using Energy Minimization, SISC, 2011

SA AMG General Interpolation

- P should have low energy
(low A -norm or A^*A -norm)
 1. determine sparsity pattern
 2. minimize energy column-wise (parallel)



h	std.	opt.
1/64	>150	24
1/128	>150	28
1/256	>150	33
1/512	>150	33

Aggregation Based Setup

B

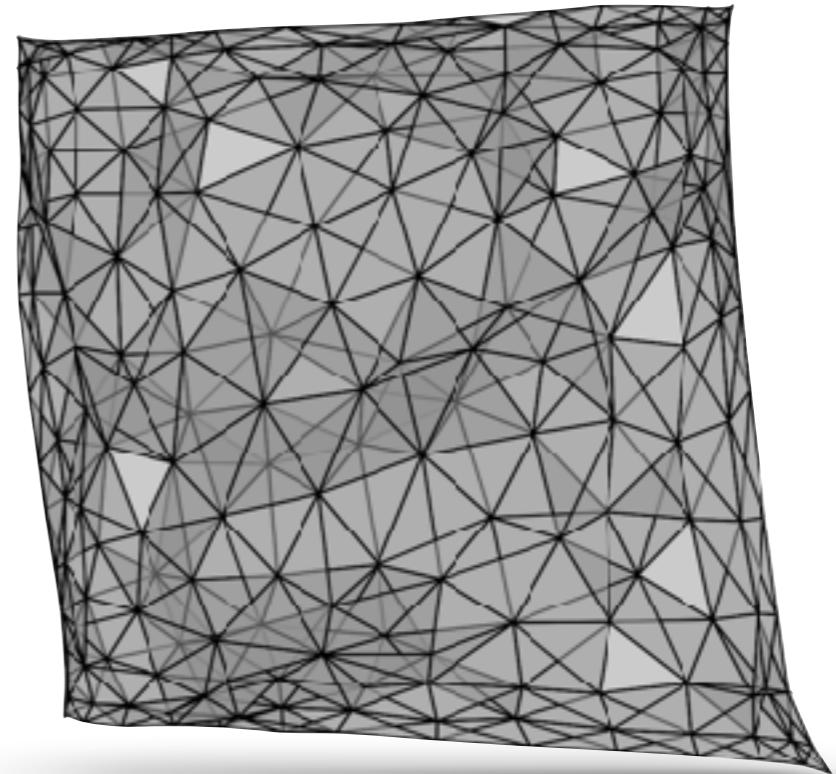
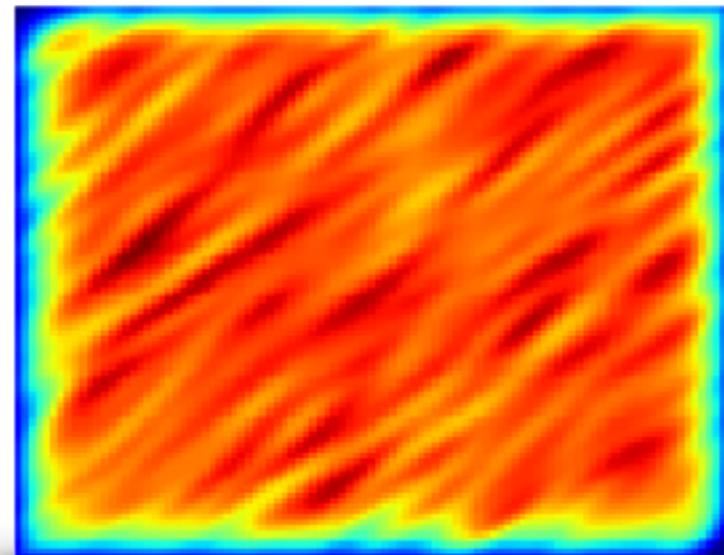
$S \leftarrow \text{strength}(A, B)$

$C \leftarrow \text{aggregate}(S)$

$P^{(0)}, B^C \leftarrow \text{inject}(C, B)$

$P \leftarrow \text{improve}(A, P^{(0)})$

$R = P^* \quad A^C = RAP$



Aggregation Based Setup

B

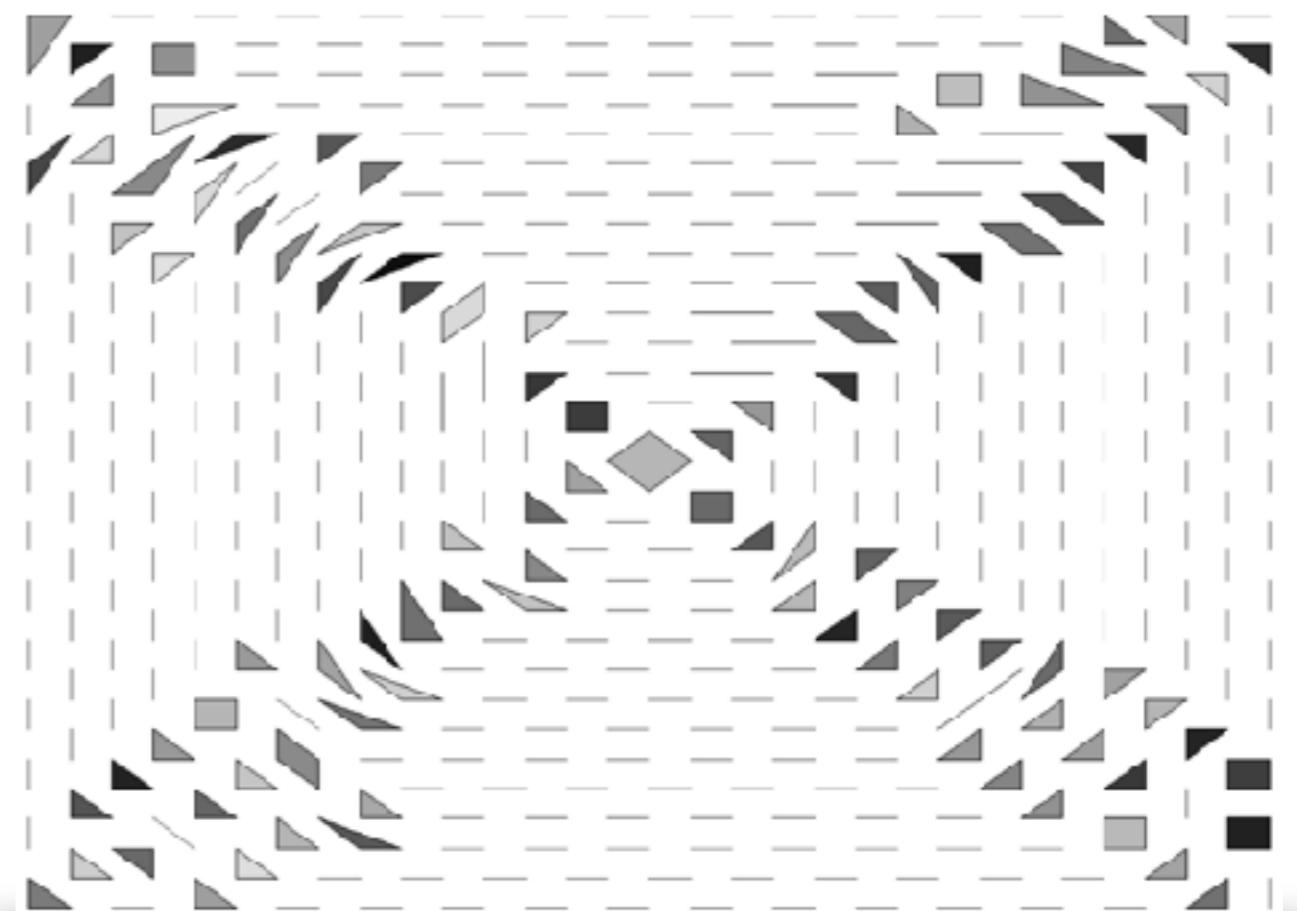
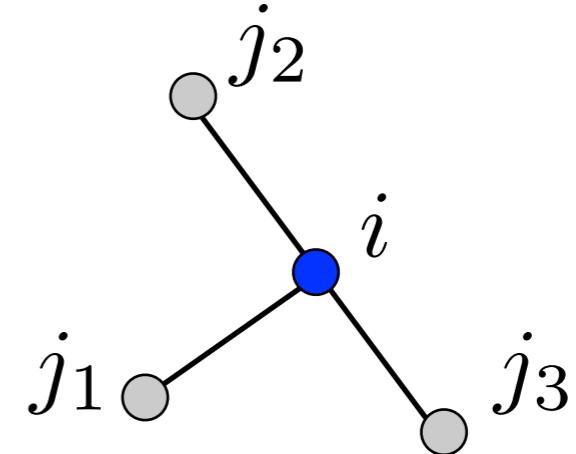
$S \leftarrow \text{strength}(A, B)$

$C \leftarrow \text{aggregate}(S)$

$P^{(0)}, B^C \leftarrow \text{inject}(C, B)$

$P \leftarrow \text{improve}(A, P^{(0)})$

$R = P^* \quad A^C = RAP$



Aggregation Based Setup

B

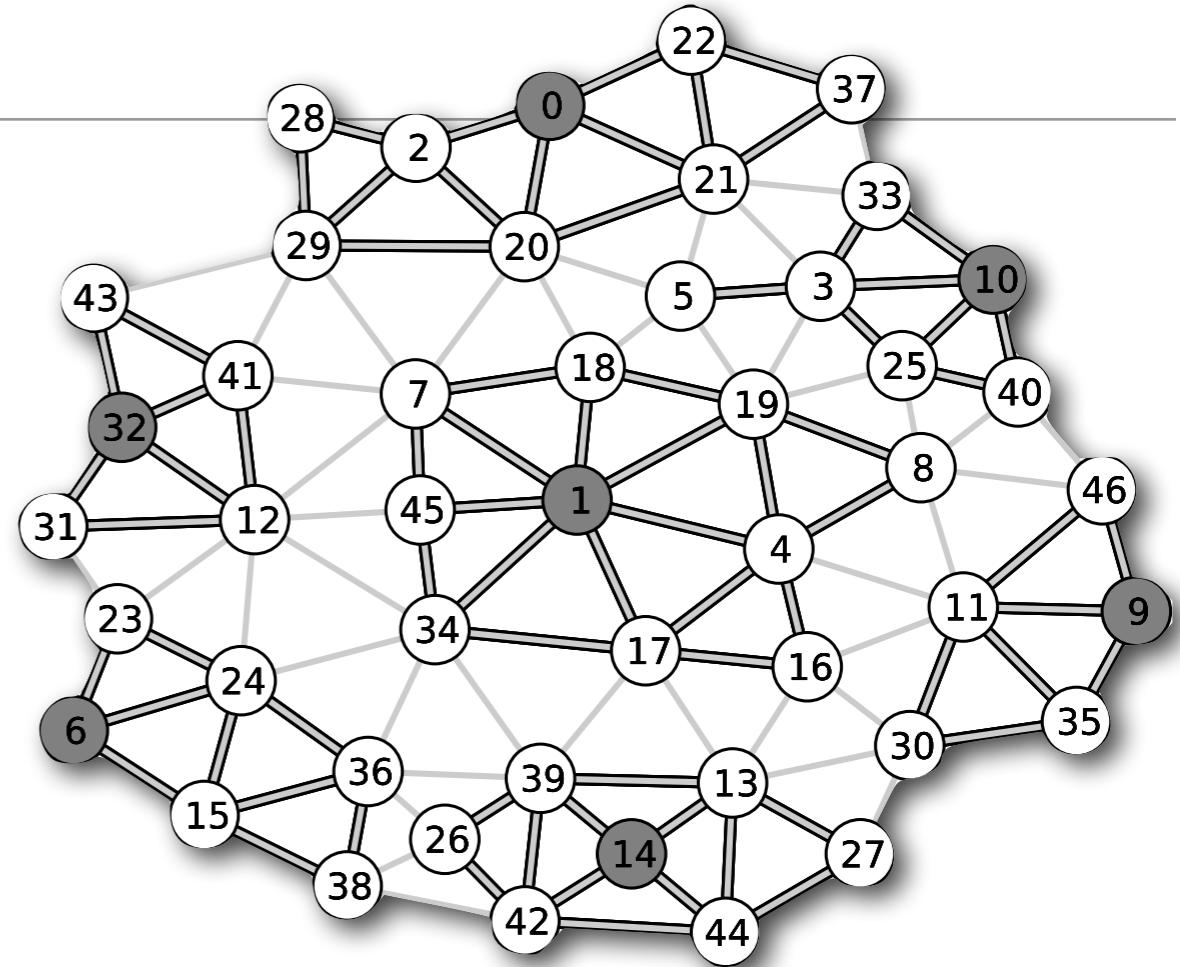
$S \leftarrow \text{strength}(A, B)$

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$P \leftarrow \text{improve}(A, P^{(0)})$

$R = P^* \quad A^C = RAP$



- Group nodes
- based on strong connections
- variable size

Aggregation Based Setup

B

$S \leftarrow \text{strength}(A, B)$

$C \leftarrow \text{aggregate}(S)$

$P^{(0)}, B^C \leftarrow \text{inject}(C, B)$

$P \leftarrow \text{improve}(A, P^{(0)})$

$R = P^* \quad A^C = RAP$

$$B = \begin{bmatrix} b_{00} & b_{01} \\ b_{10} & b_{11} \\ b_{20} & b_{21} \\ b_{30} & b_{31} \\ b_{40} & b_{41} \\ b_{50} & b_{51} \\ b_{60} & b_{61} \\ b_{70} & b_{71} \\ b_{80} & b_{81} \\ b_{90} & b_{91} \end{bmatrix}$$

$$P_{\text{tent}} = \begin{bmatrix} b_{00} & b_{01} & & & \\ b_{10} & b_{11} & & & \\ & & b_{20} & b_{21} & \\ & & b_{30} & b_{31} & \\ & & b_{40} & b_{41} & \\ & & & & b_{50} & b_{51} \\ & & & & b_{60} & b_{61} \\ & & & & b_{70} & b_{71} \\ & & & & & b_{80} & b_{81} \\ & & & & & b_{90} & b_{91} \end{bmatrix}$$

Aggregation Based Setup

B

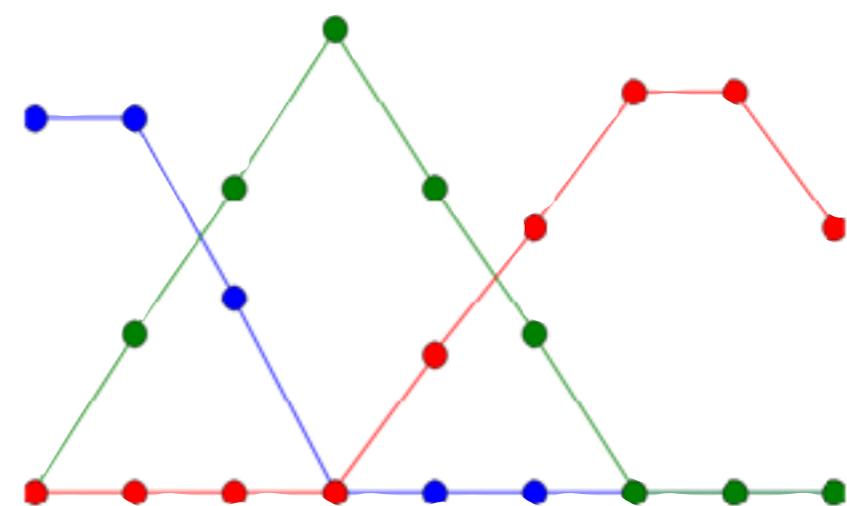
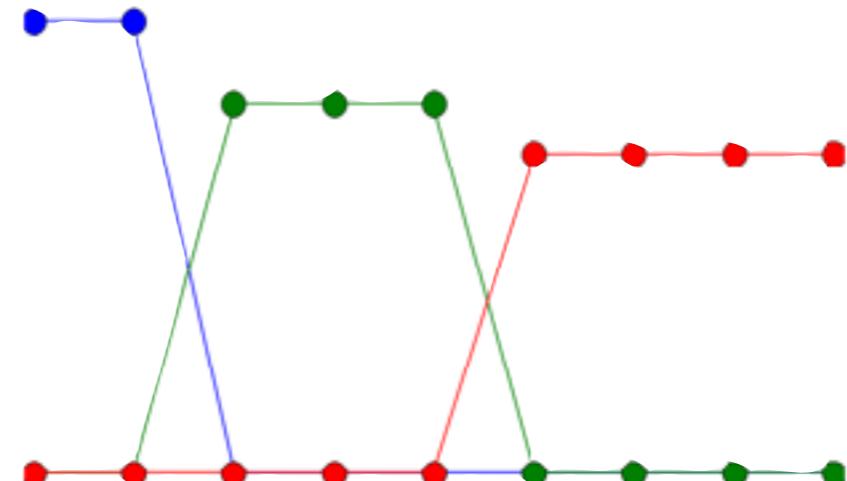
$S \leftarrow \text{strength}(A, B)$

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$P^{(0)}, B^C \leftarrow \text{inject}(C, B)$

$$P \leftarrow \text{improve}(A, P^{(0)})$$

$$R = P^* \quad A^C = RAP$$



SA AMG Setup Algorithm

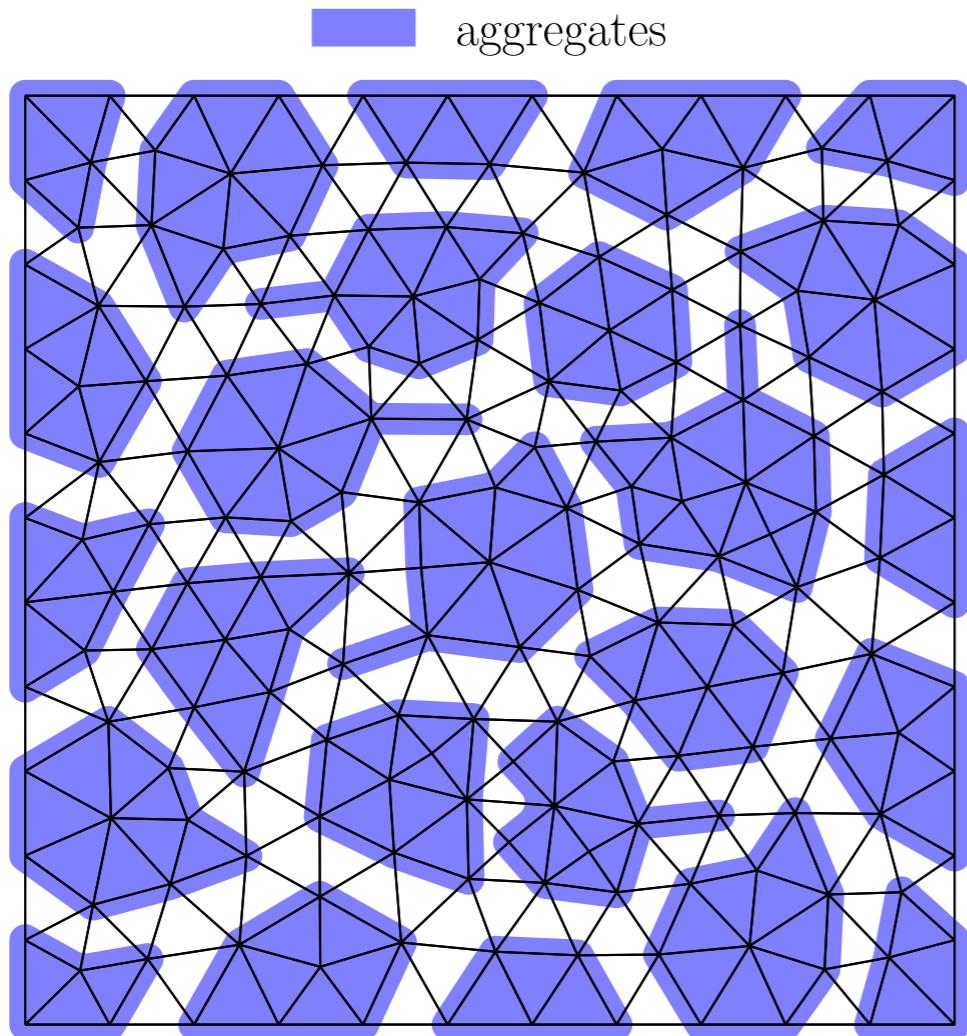
Algorithm 1: SA_setup()

Input: A_0 : fine-grid operator
 B_0 : fine-grid candidate vectors
max_size: threshold for max size of coarsest problem

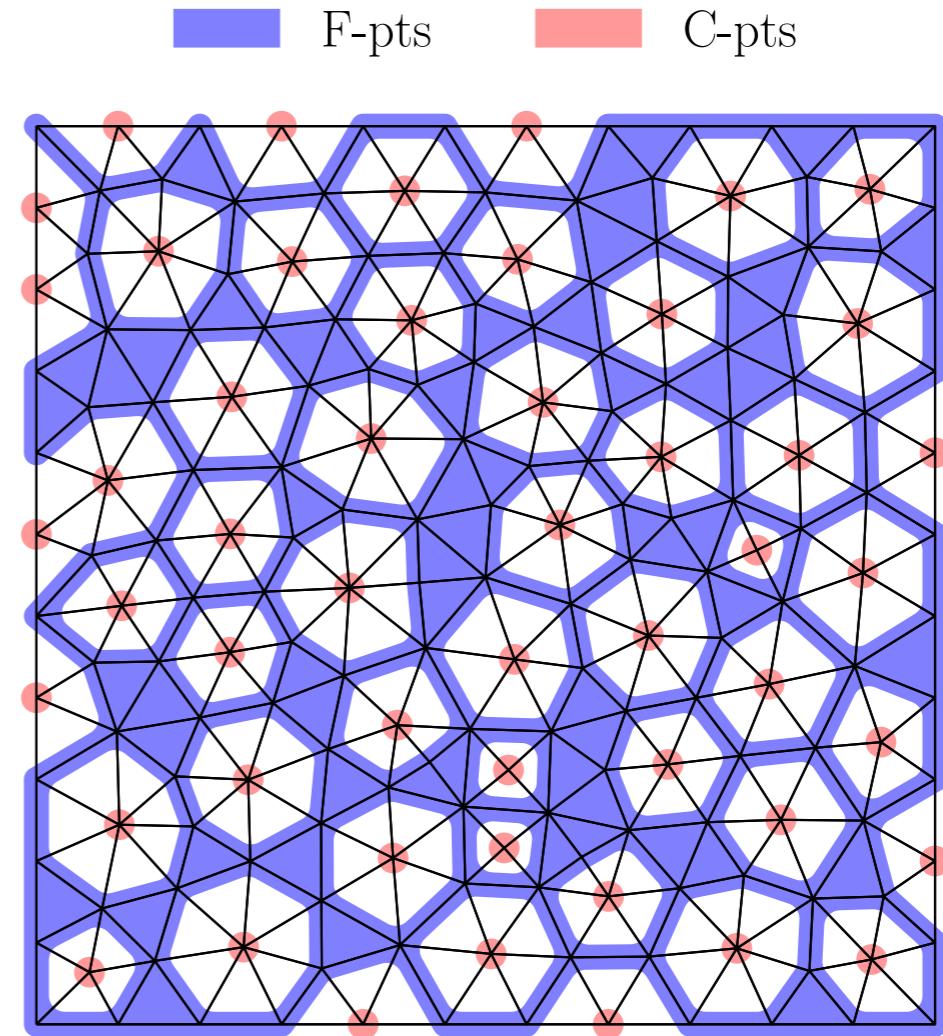
Output: A_1, \dots, A_L ,
 P_0, \dots, P_{L-1}

```
1  $\ell = 0$ 
2 while size( $A_\ell$ ) > max_size
3    $S_\ell = \text{strength}(A_\ell)$                                 {Strength-of-connection}
4    $\mathcal{A}_\ell = \text{aggregate}(S_\ell)$                       {Aggregation}
5    $T_\ell, B_{\ell+1} = \text{inject}(\mathcal{A}_\ell, B_\ell)$     {Form tentative interpolation and coarse candidates}
6    $P_\ell = \text{smooth}(A_\ell, T_\ell)$                         {Smooth  $T_\ell$ }
7    $A_{\ell+1} = P_\ell^T A_\ell P_\ell$                          {Coarse-grid operator}
8    $\ell = \ell + 1$ 
```

AMG



- Smoothed Aggregation AMG (SA-AMG)
- Interpolation constructed from candidate vectors
- Clear approach to *optimize* interpolation



- Coarse-Fine AMG (CF-AMG) or Ruge-Stüben
- Edge-wise construction of interpolation, allowing straightforward control of sparsity
- Incorporating near-nullspace is not straightforward

Theory

Bounds on convergence guide the design of methods.

- strength of connection
- coarse grids
- interpolation
- etc

Look at the Operators

- Smoothing

$$\mathbf{u} \leftarrow G\mathbf{u} + (I - G)A^{-1}\mathbf{f} \quad \text{or} \quad \mathbf{e} \leftarrow G\mathbf{e}.$$

$$G = I - \omega D^{-1} A$$

- Coarse-grid Correction

$$\mathbf{e} \leftarrow \left(I - P \left(P^T A P \right)^{-1} P^T A \right) \mathbf{e}$$

$$T$$

Consider V(0,1) convergence...

Assumption 1

Assume A is symmetric and positive-definite, P is full rank, G is a norm-convergent relaxation operator ($\|G\|_A < 1$), and $T = I - P(P^T A P)^{-1} P^T A$.

- Goal: Bound the reduction in error after G and T

$$\|GT\mathbf{e}\|_A^2 \leq (1 - \delta^*) \|\mathbf{e}\|_A^2$$

- Target a Sharp Bound:

$$\|GT\|_A^2 := \sup_{\mathbf{e} \neq \mathbf{0}} \frac{\|GT\mathbf{e}\|_A^2}{\|\mathbf{e}\|_A^2} = 1 - \delta^*$$

Assume Relaxation is Convergent on *SOMETHING*

- Assume relaxation is effective on the Range of T

$$\|GTe\|_A^2 \leq (1 - \delta) \|Te\|_A^2 \quad \text{for all } \mathbf{e}$$

- Then, since T is an A -orthogonal projector

$$\|GTe\|_A^2 \leq (1 - \delta) \|\mathbf{e}\|_A^2 \quad \text{for all } \mathbf{e}$$

- Can show this also holds

$$\|Gv\|_A^2 \leq \|v\|_A^2 \quad \text{for all } v \perp \mathcal{R}(T)$$

Smoothing Property

Theorem 2

Under Assumption 1, if there is a $\delta > 0$ such that

$$\|G\mathbf{e}\|_A^2 \leq \|\mathbf{e}\|_A^2 - \delta \|T\mathbf{e}\|_A^2 \quad \text{for all } \mathbf{e},$$

then

$$\|GT\|_A^2 \leq 1 - \delta.$$

- If relaxation reduces error after coarse-grid correction
- Then the V(0,1)-cycle is convergent
- Is it **sharp**?

Yes, it is sharp

Theorem 3

Under Assumption 1, if

$$\hat{\delta} = \inf_{\mathbf{e}: T\mathbf{e} \neq \mathbf{0}} \frac{\|\mathbf{e}\|_A^2 - \|G\mathbf{e}\|_A^2}{\|T\mathbf{e}\|_A^2},$$

then $\hat{\delta}$ defines a sharp bound on the two-grid V(0,1)-cycle convergence factor; that is,

$$\|GT\|_A^2 = 1 - \hat{\delta}.$$

- Great!
- What's the problem?

Yes, it is sharp

Theorem 3

Under Assumption 1, if

$$\hat{\delta} = \inf_{\mathbf{e}: T\mathbf{e} \neq \mathbf{0}} \frac{\|\mathbf{e}\|_A^2 - \|G\mathbf{e}\|_A^2}{\|T\mathbf{e}\|_A^2},$$

then $\hat{\delta}$ defines a sharp bound on the two-grid V(0,1)-cycle convergence factor; that is,

$$\|GT\|_A^2 = 1 - \hat{\delta}.$$

- Great!
- What's the problem?

COMPUTABILITY

Break up the Relaxation Assumption

$$\delta(e) = \frac{\|e\|_A^2 - \|Ge\|_A^2}{\|Te\|_A^2}$$

$$\delta(e) = \frac{\|e\|_A^2 - \|Ge\|_A^2}{\|e\|_{AD^{-1}A}^2} \frac{\|e\|_{AD^{-1}A}^2}{\|Te\|_A^2}$$

Break up the Relaxation Assumption

$$\delta(e) = \frac{\|e\|_A^2 - \|Ge\|_A^2}{\|Te\|_A^2}$$

$$\delta(e) = \frac{\|e\|_A^2 - \|Ge\|_A^2}{\|e\|_{AD^{-1}A}^2} \frac{\|e\|_{AD^{-1}A}^2}{\|Te\|_A^2}$$

$\hat{\alpha}$

Break up the Relaxation Assumption

$$\delta(e) = \frac{\|e\|_A^2 - \|Ge\|_A^2}{\|Te\|_A^2}$$

$$\delta(e) = \frac{\|e\|_A^2 - \|Ge\|_A^2}{\|e\|_{AD^{-1}A}^2} \frac{\|e\|_{AD^{-1}A}^2}{\|Te\|_A^2}$$

$\hat{\alpha}$ $\frac{1}{\hat{\beta}}$

Break up the Relaxation Assumption

$$\delta(e) = \frac{\|e\|_A^2 - \|Ge\|_A^2}{\|e\|_{AD^{-1}A}^2} \frac{\|e\|_{AD^{-1}A}^2}{\|Te\|_A^2}$$
$$\hat{\alpha} \quad \frac{1}{\hat{\beta}}$$

$$\|GTe\|_A^2 \leq \|Te\|_A^2 - \hat{\alpha} \|Te\|_{AD^{-1}A}^2$$

$$\leq \|Te\|_A^2 - \frac{\hat{\alpha}}{\hat{\beta}} \|Te\|_A^2$$

$$= \left(1 - \frac{\hat{\alpha}}{\hat{\beta}}\right) \|Te\|_A^2$$

$$\leq \left(1 - \frac{\hat{\alpha}}{\hat{\beta}}\right) \|\mathbf{e}\|_A^2$$

Split Theory

Theorem 4

Under Assumption 1, if there exists $\bar{\alpha}_g > 0$ such that

$$\|G\mathbf{e}\|_A^2 \leq \|\mathbf{e}\|_A^2 - \bar{\alpha}_g g(\mathbf{e}) \quad \text{for all } \mathbf{e} \quad (\text{smoothing}),$$

and there exists $\bar{\beta}_g > 0$ such that

$$\|T\mathbf{e}\|_A^2 \leq \bar{\beta}_g g(T\mathbf{e}) \quad \text{for all } \mathbf{e} \quad (\text{approximation}),$$

then $\|GT\|_A \leq \sqrt{1 - \bar{\alpha}_g / \bar{\beta}_g}$.

$$g(\mathbf{e}) = \|\mathbf{e}\|_{AD^{-1}A}^2$$

- Making an assumption on smoothing and the interpolation results in a convergent method.

Example

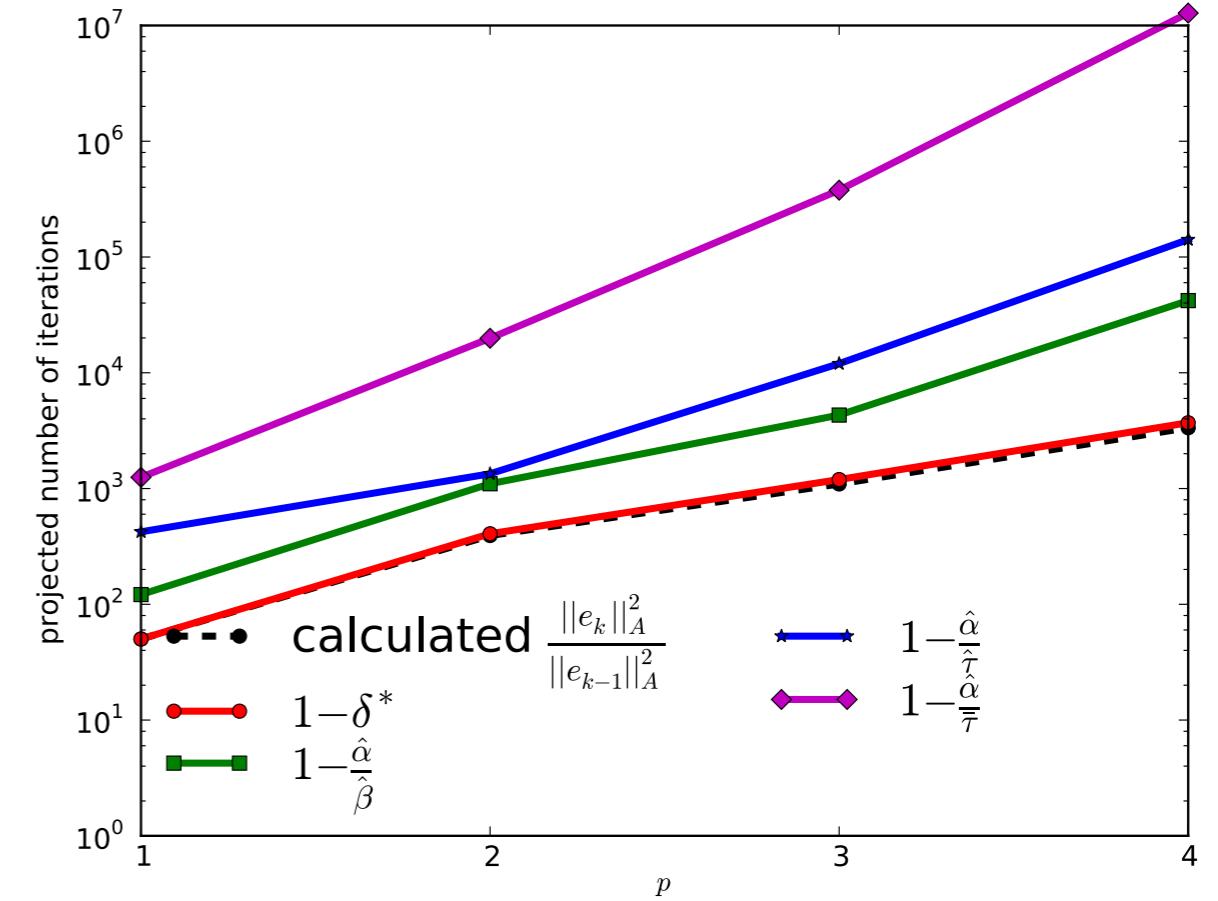
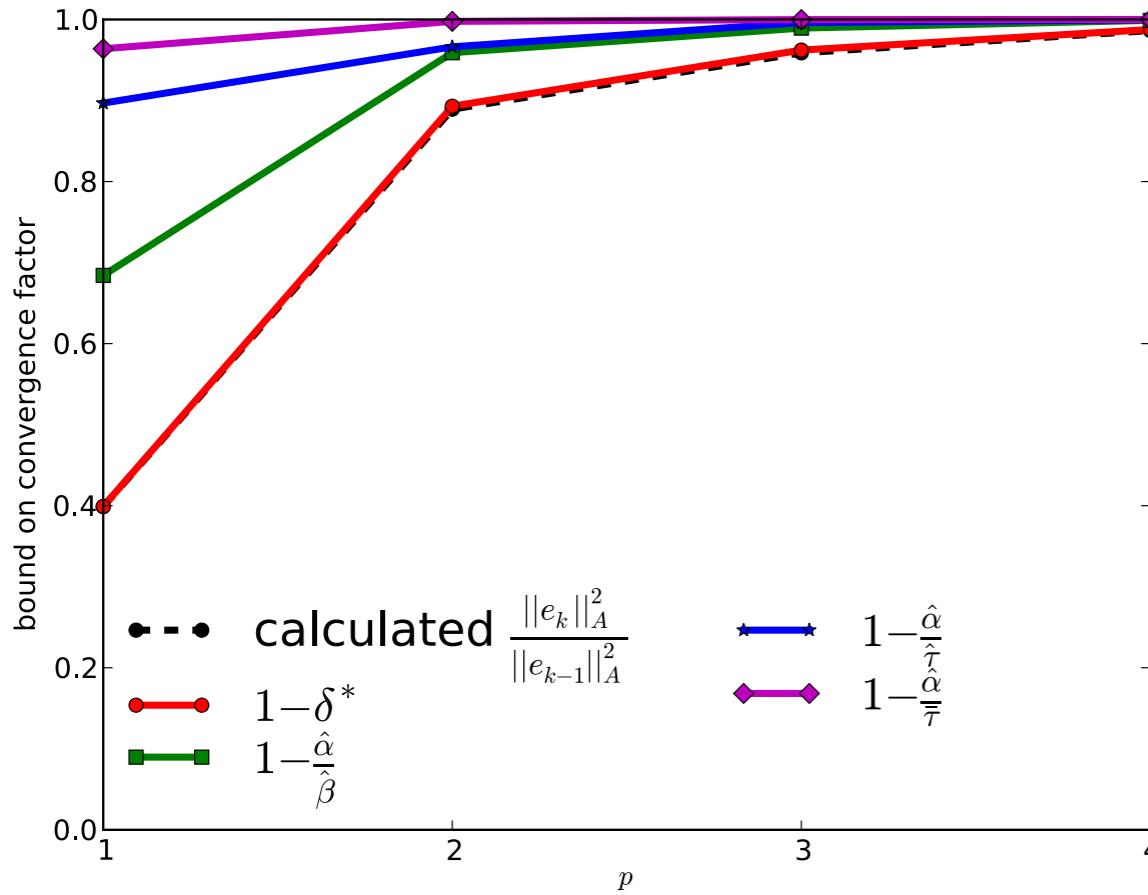
$$\rho^2 = \lim_{k \rightarrow \infty} \frac{\|\mathbf{e}_{k+1}\|_A^2}{\|\mathbf{e}_k\|_A^2}$$

$$\text{iterations} \approx \frac{10}{\log_{10} \rho_{\text{bound}}}$$

Varying p : an unstructured triangulation with $\varepsilon = 1$ (isotropic) is constructed. The finite element order is varied from $p = 1, \dots, 4$.

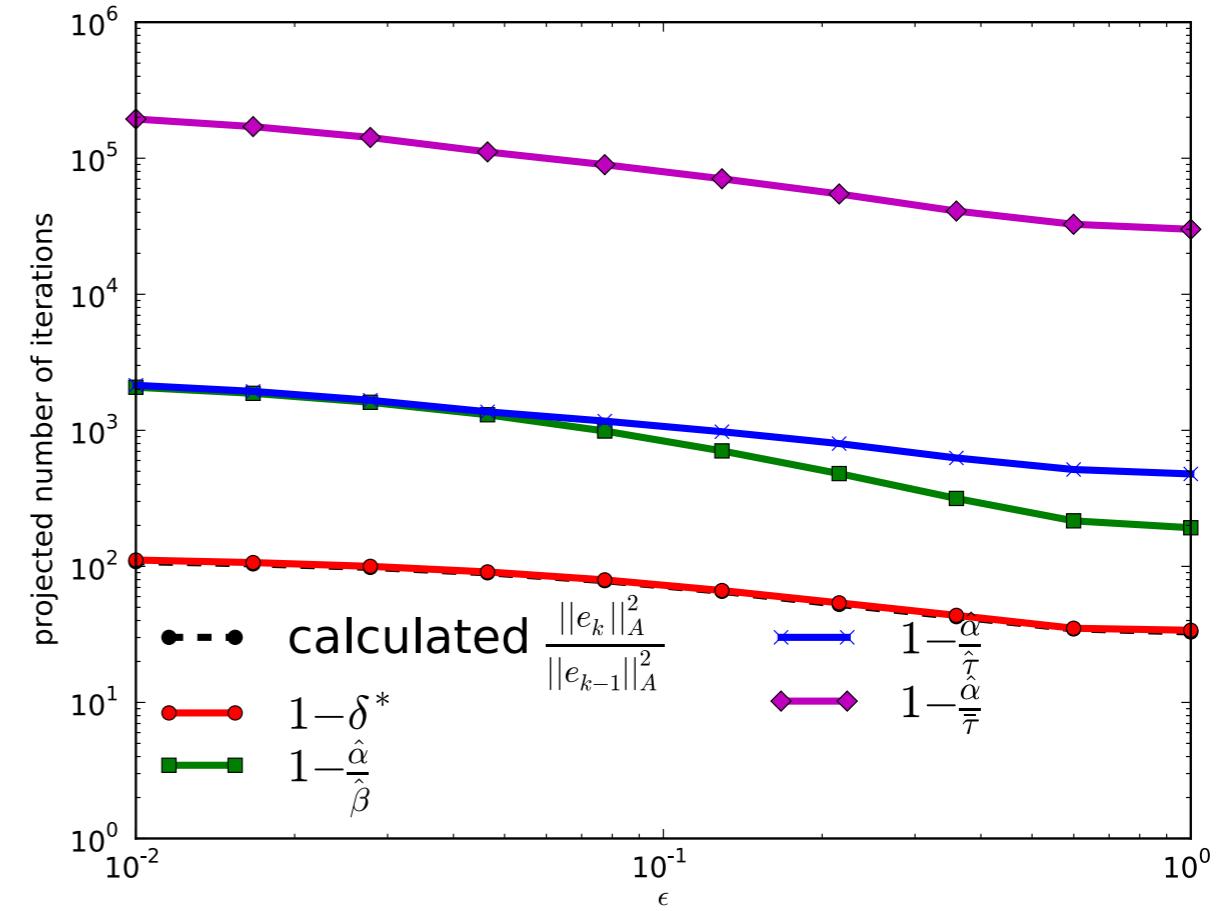
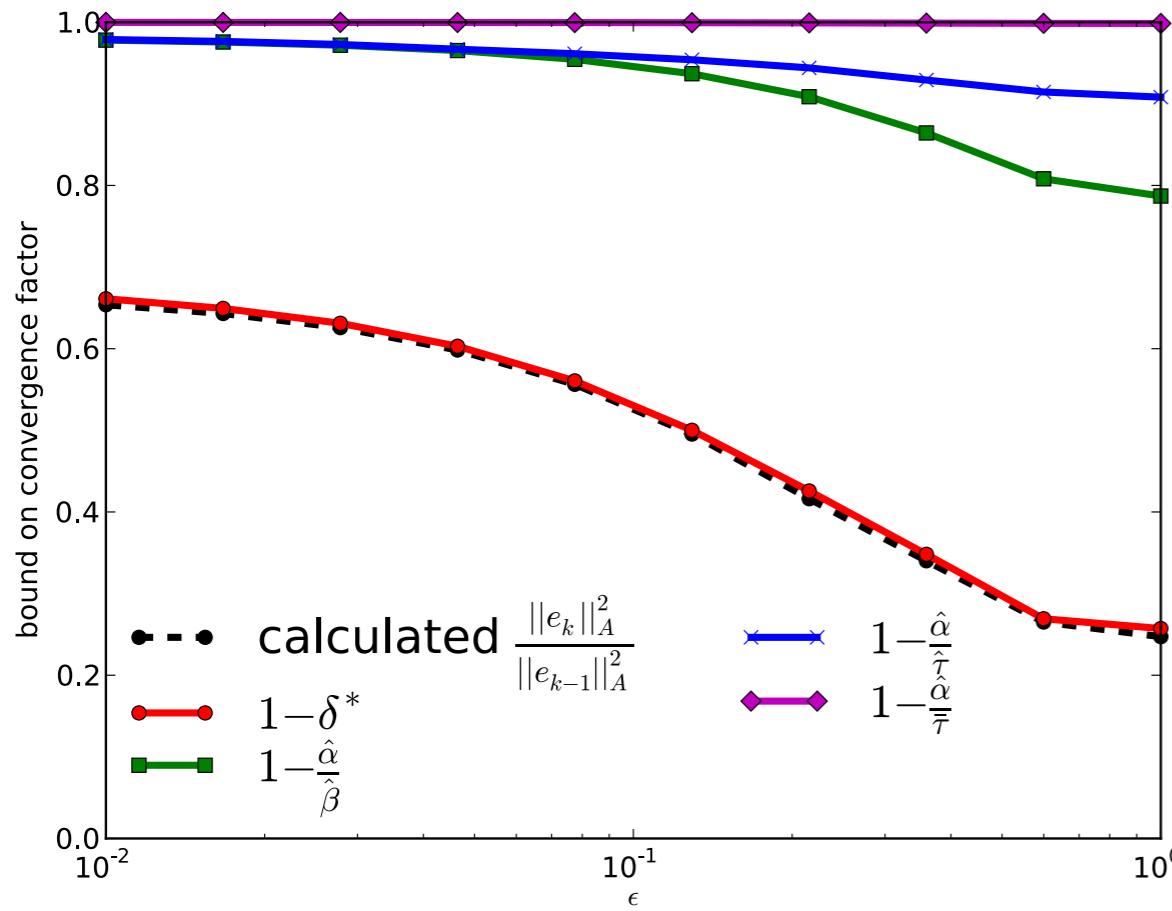
Varying ε : a structured triangulation with $p = 1$ (linear elements) is constructed. The anisotropy is rotated by $\theta = \pi/4$, and the strength is varied from $\varepsilon = 1.0, \dots, 0.01$.

Vary polynomial Order



- Bounds how *badly* the method can be
- Does not bound how *good* the method might be

Vary Anisotropy



- Bounds how *badly* the method can be
- Does not bound how *good* the method might be

Generalized AMG Theory

- Smoother (symmetric or non-symmetric)

$$e \leftarrow (I - M^{-1}A)$$

- Assume s.p.d. A and $M + M^T - A$

- The *symmetrized* smoother is given as

$$\tilde{M} = M(M^T + M - A)^{-1}M^T$$

- or

$$(I - \tilde{M}^{-1}A) = (I - M^{-T}A)(I - M^{-1}A)$$

Robert D. Falgout and Panayot S. Vassilevski,
On Generalizing the Algebraic Multigrid
Framework, 2004

Generalized AMG Theory

- **Interpolation:** $P : \mathbb{R}^{n_c} \rightarrow \mathbb{R}^n$

- Some **restriction** (not MG restriction):

$$R : \mathbb{R}^n \rightarrow \mathbb{R}^{n_c}$$

- Define such that

$$PR = I$$

Here, RP is a **projection** onto the range of P

- For any SPD matrix X and any full-rank matrix B , denote the **X -orthogonal projection** onto $\text{range}(B)$ by

$$\pi_X(B) = B(B^T X B)^{-1} B^T X$$

- Define the **two-grid multigrid** error propagator by

$$E_{TG} = (I - M^{-1}A)(I - \pi_A(P))$$

Generalized two-grid theory splits construction of coarse-grid correction into two parts

- Theorem: For any projection PR

$$\|E_{TG}\|_A^2 \leq 1 - \frac{1}{K}; \quad K = \sup_e \frac{\|(I - PR)e\|_{\tilde{M}}^2}{\|e\|_A^2}$$

- Fix R so that it does not depend on P
 - Defines the **coarse-grid variables**, $u_c = Ru$
 - Example: $R = [0, I]$ ($P^T = [W^T, I]^T$), i.e., subset of the fine grid
- Theorem: Pick a coarse grid and interpolation P

$$K \leq \eta K_*; \quad \eta = \|PR\|_A; \quad K_* = \inf_P \sup_e \frac{\|(I - PR)e\|_{\tilde{M}}^2}{\|e\|_A^2}$$

- Small K_* insures coarse grid quality – use compatible relaxation (CR)**
- Small η insures interpolation quality – necessary condition that does not depend on relaxation!**

Compatible relaxation (CR)

A. Brandt, General highly accurate algebraic coarsening, Electron. Trans. Numer. Anal. 2000

- CR (Brandt, 2000) is a modified relaxation scheme that keeps the coarse-level variables, Ru , invariant
- “a general measure for the quality of the set of coarse variables is the convergence rate of compatible relaxation”
- **Theorem:** (fast convergence) good coarse grid

$$K_{\star} \leq \left(\frac{\Delta^2}{2 - \omega} \right) \frac{1}{1 - \rho_{cr}}$$

$\Delta \geq 1$ measures the deviation of M from its symmetric part M_{σ} and $0 < \omega < 2$ is a kind of smoothing parameter

$$\Delta^2 = \left\| M_{\sigma}^{-1/2} M M_{\sigma}^{-1/2} \right\|^2; \quad \omega = \lambda_{\max}(M_{\sigma}^{-1} A)$$

Several general *CR* methods

- Define S : $\mathbb{R}^n = \text{range}(S) \oplus \text{range}(R^T)$
 $RS = 0$
- Example:
 $R = \begin{bmatrix} 0 & I \end{bmatrix}$
 $S = \begin{bmatrix} I \\ 0 \end{bmatrix}$
 $P = \begin{bmatrix} W \\ I \end{bmatrix}$
- Main *CR* method – where M is explicitly available
$$e \leftarrow (I - (S^T M S)^{-1} (S^T A S)) e$$
- Habituated *CR* – not as sharp, but always computable
$$e \leftarrow (S^T (I - M^{-1} A) S) e \quad \text{with } S^T S = I$$

CR provides an alternative approach for coarsening

- All AMG algorithms need to select coarse grids
- But, most **coarsening algorithms** are based on a (particular) notion of “strength of connection”
 - assumes an *M*-matrix
 - assumes a pointwise smoother

Stretched quad example ($\Delta x \rightarrow \infty$):

$$A = \begin{bmatrix} -1 & -4 & -1 \\ 2 & 8 & 2 \\ -1 & -4 & -1 \end{bmatrix}$$

Direction of smoothest error is not readily apparent

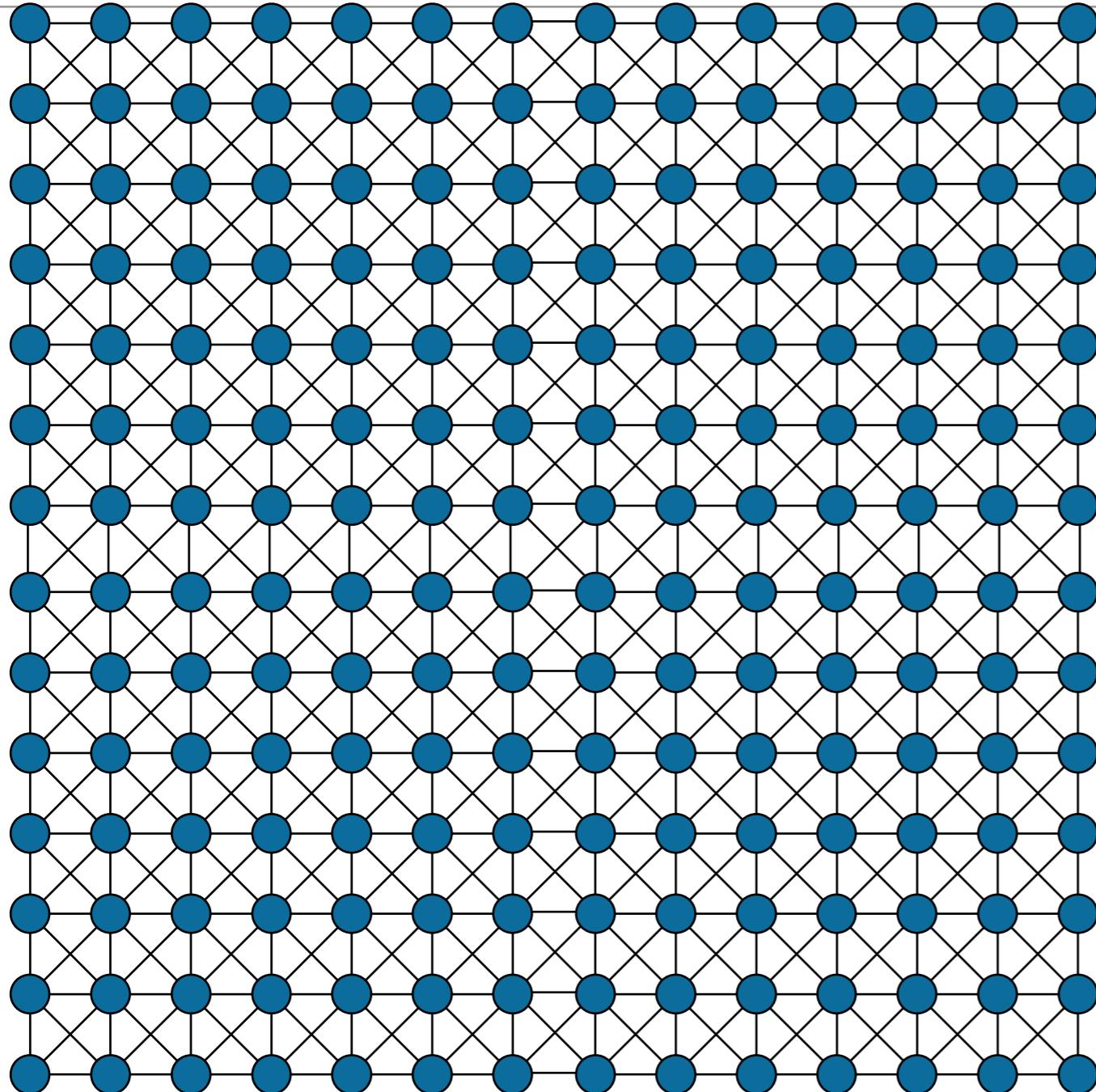
- ***CR* coarsening does not use strength of connection**

Using CR to choose the coarse grid

- **Simplest case:** the coarse grid is a subset of the fine grid $\rightarrow CR$ is just F -relaxation
- Relax on the homogeneous equations $A_{ff}x = 0$
- Basic CR coarsening algorithm (θ_{cr} , θ_{cs}):
$$\gamma_i = |x_i|/\|x\|_\infty$$

```
Initialize C = ∅
Run CR → ρcr, e
While ρcr > θcr
{
    Compute candidate set measures {γi : i ∈ C}
    U = {i ∈ C : γi > θcs}
    C = C ∪ {independent set of U}
    Run CR → ρcr, e
}
```

Using CR to choose the coarse grid



Initialize U-pts

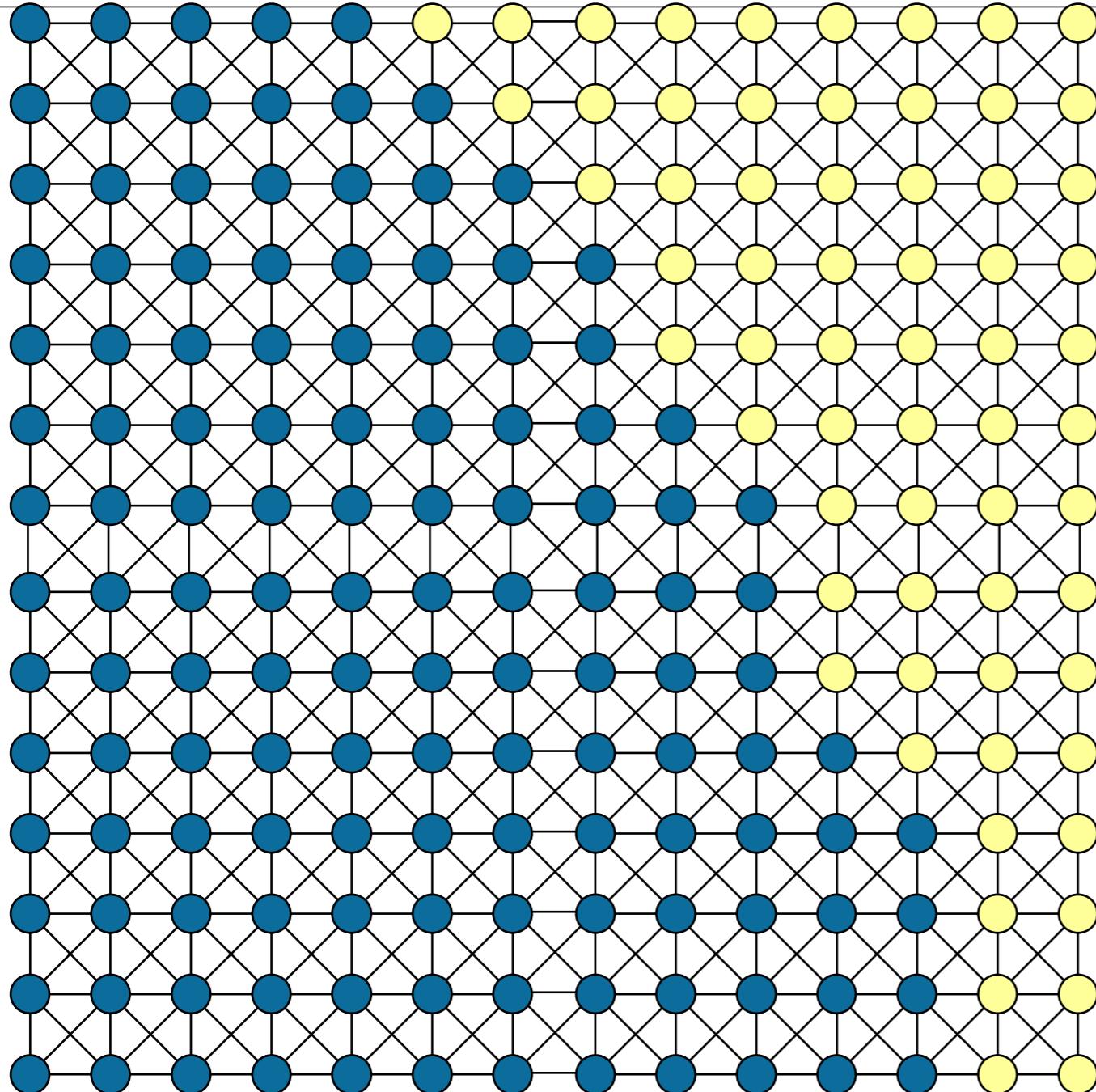


Do CR and redefine
U-pts as points slow
to converge



Select new C-pts as
indep. set over U

Using CR to choose the coarse grid



Initialize U-pts

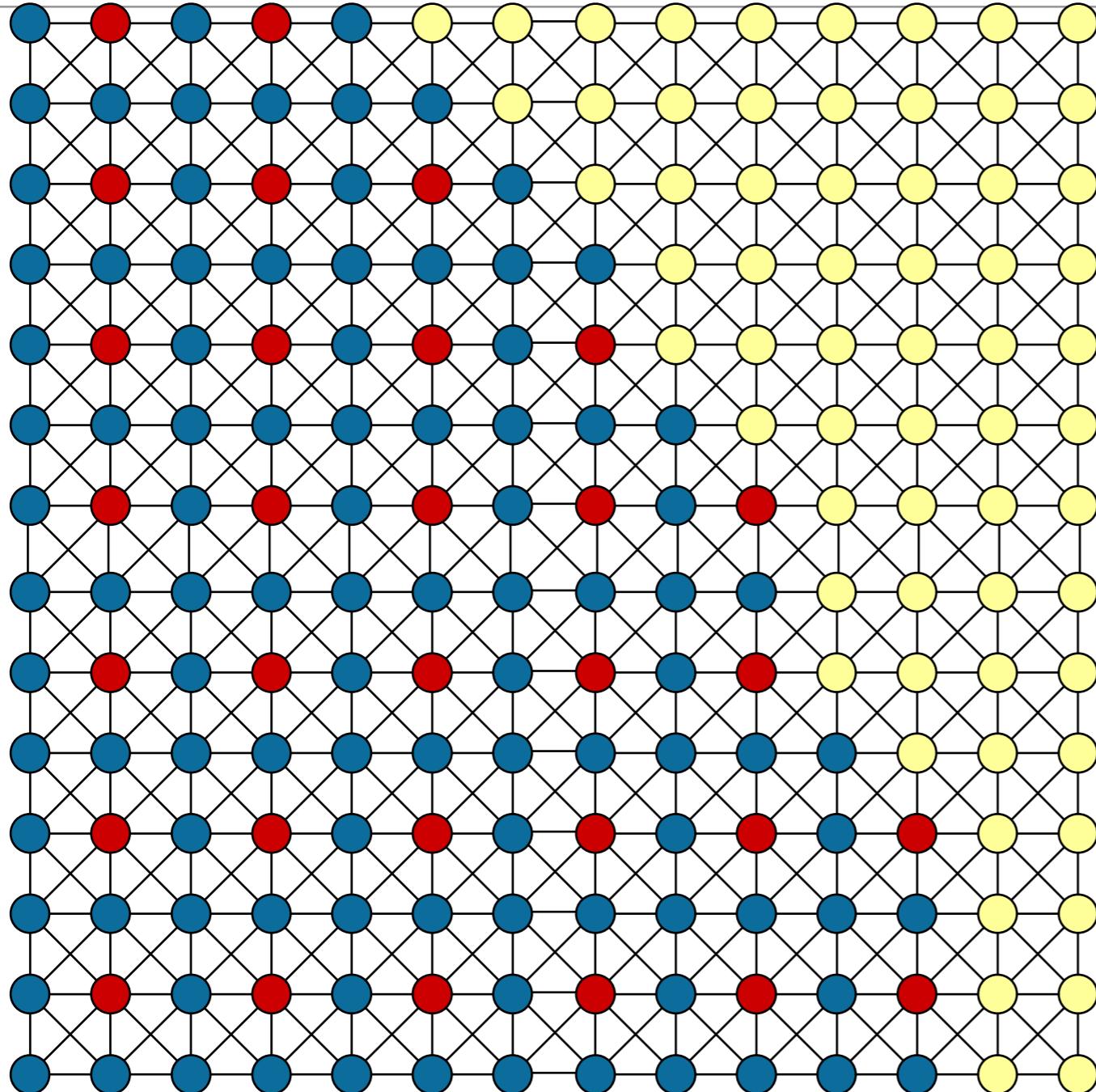


**Do CR and redefine
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Select new C-pts as
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Using CR to choose the coarse grid



Initialize U-pts

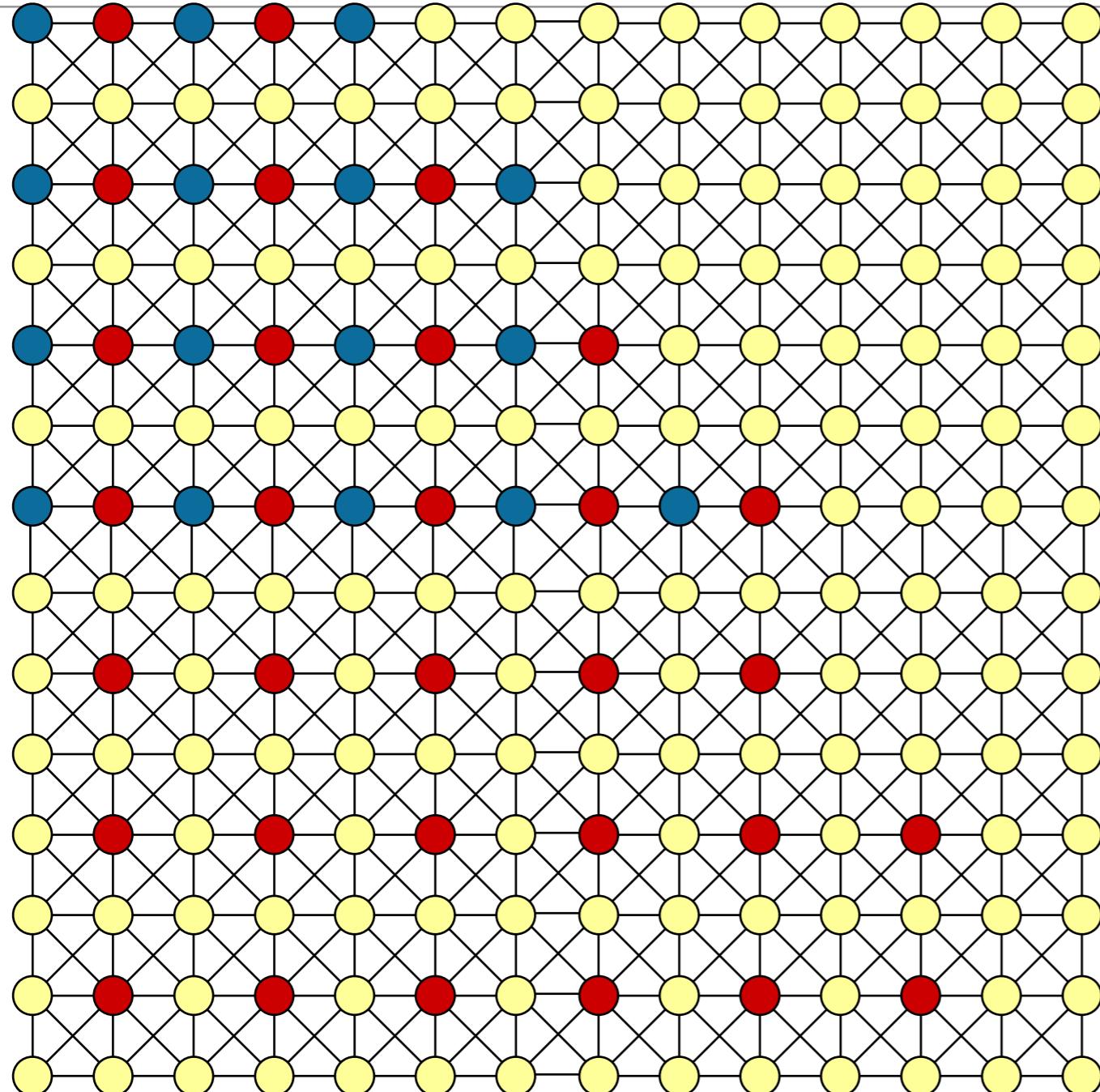


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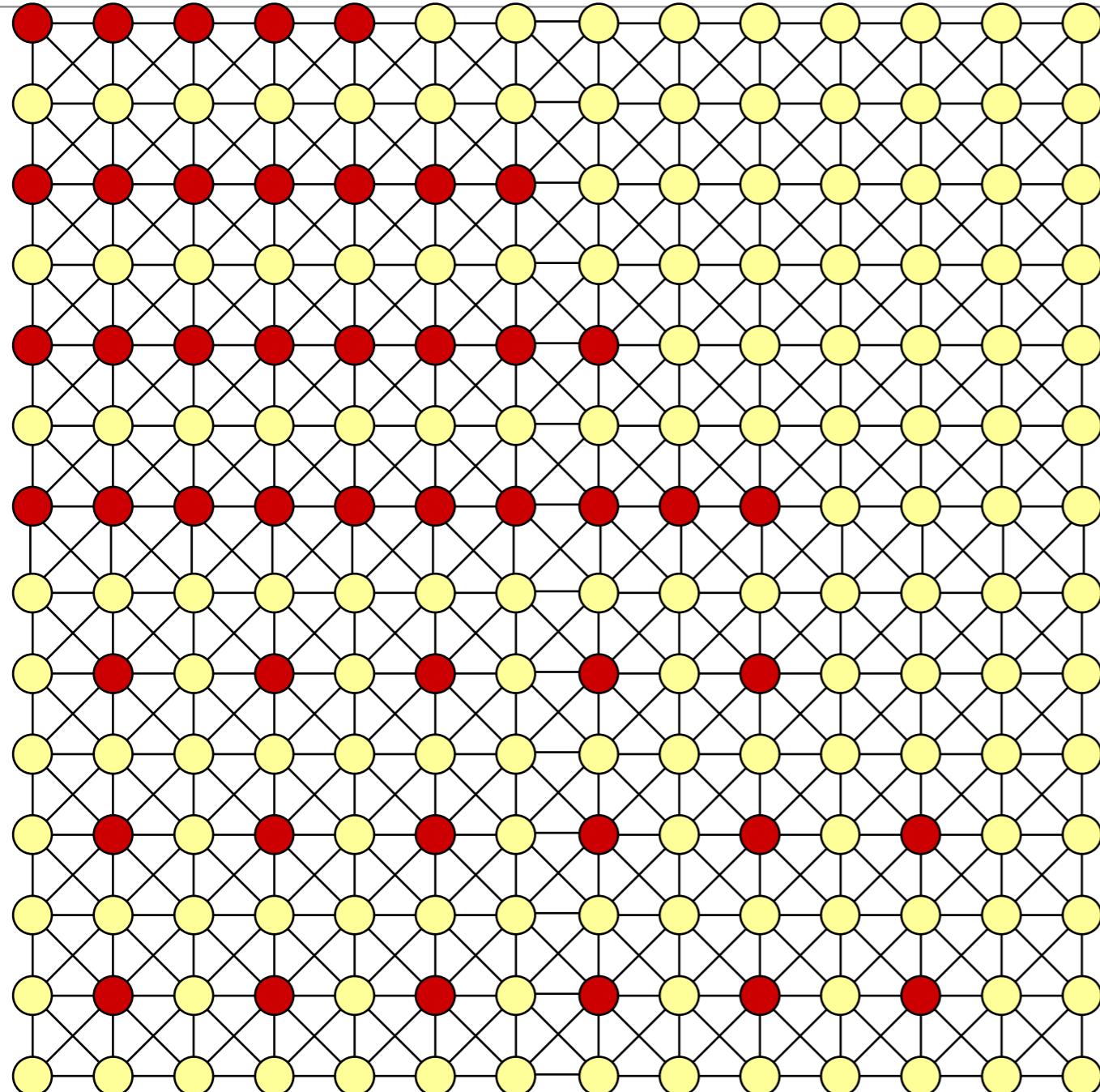
?

**Do CR and redefine
U-pts as points slow
to converge**



Select new C-pts as
indep. set over U

Using CR to choose the coarse grid



Initialize U-pts



Do CR and redefine
U-pts as points slow
to converge



Select new C-pts as
indep. set over U

The candidate set measure and parameters are currently somewhat heuristic in nature

- CR algorithm relaxes on $Ax=0$ with
$$\mathbf{x}_0 = \mathbf{1} + \text{rand}(0, 0.1)$$

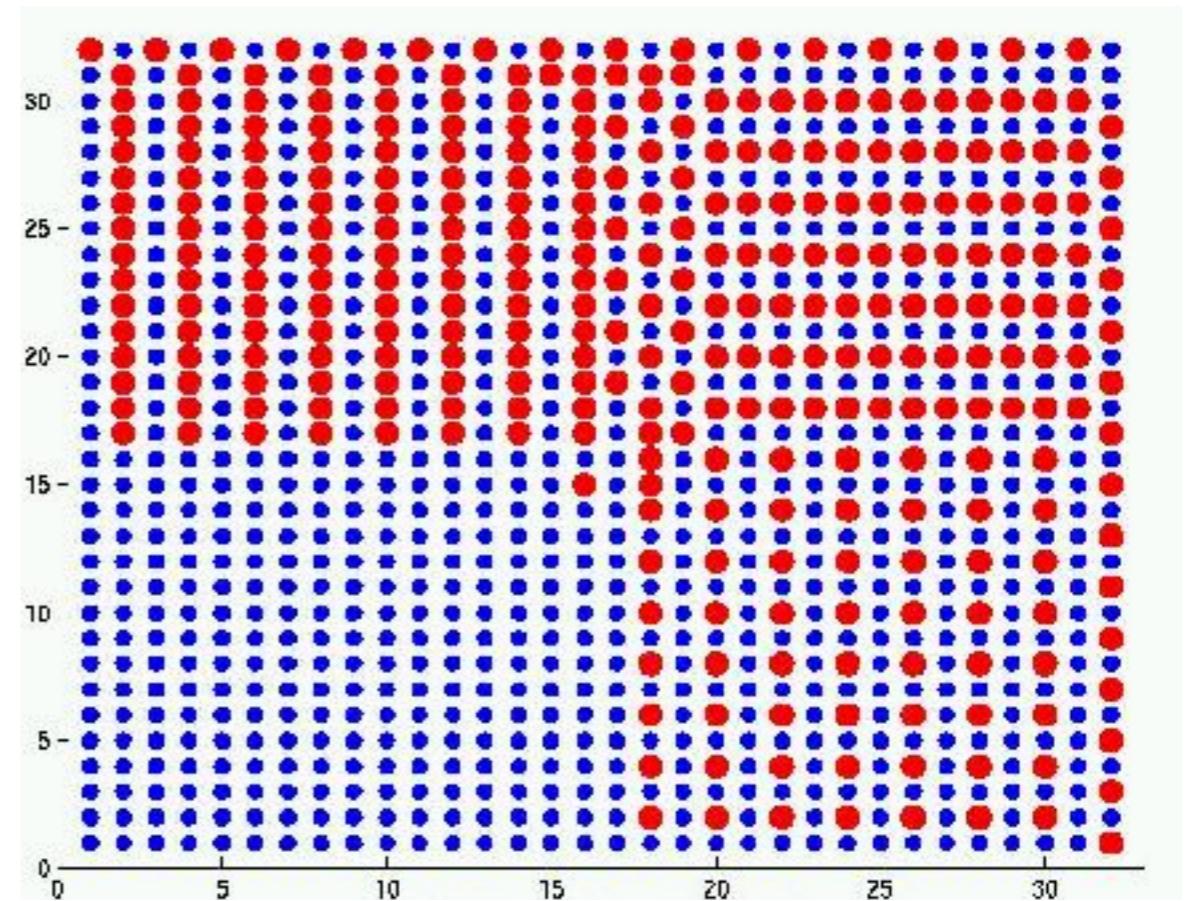
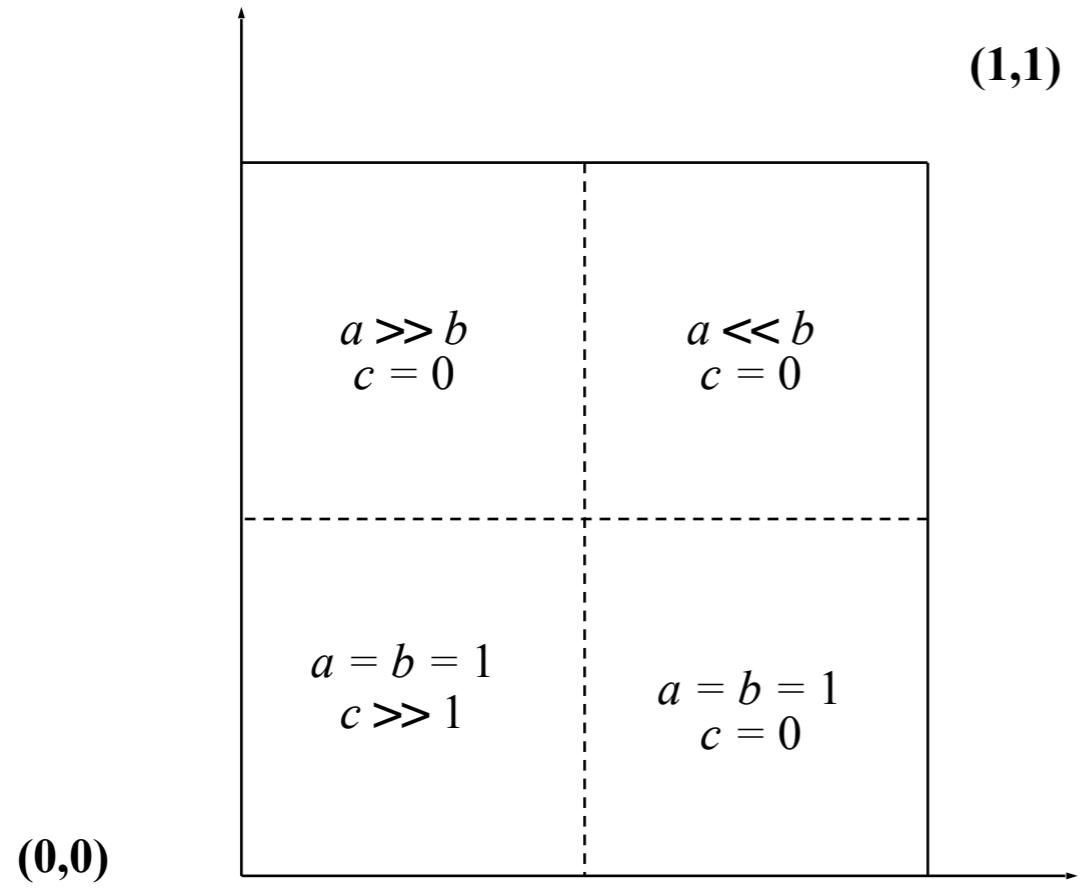
and candidate set measure

$$\gamma_i = |x_i|/\|x\|_\infty$$

- Candidate set threshold θ_{cs} is set to 0.1 on the first phase and 0.5 on subsequent phases
 - Helps to stay close to boundaries
- CR convergence threshold θ_{cr} is between 0.5 and 0.7

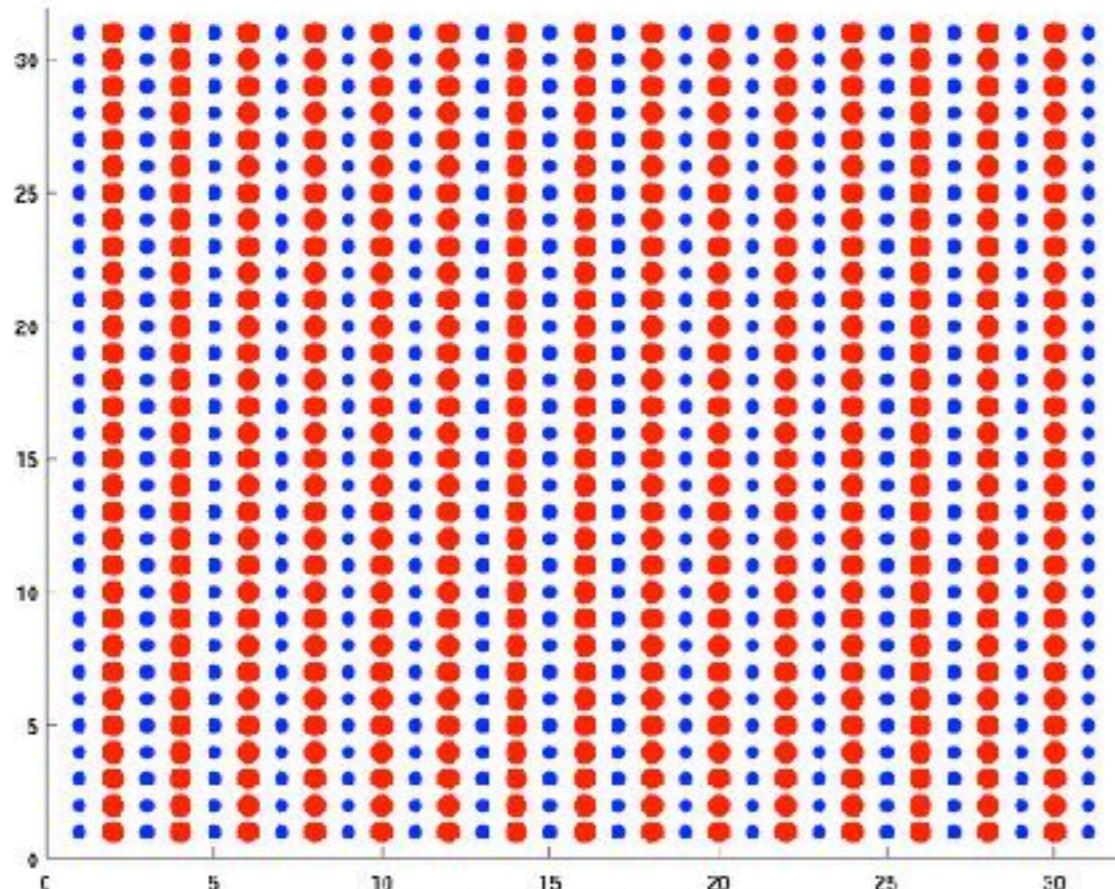
Tests: 4 region diffusion, 9-pt FE... coarse grids reflect the anisotropies

$$-au_{xx} - bu_{yy} + cu = f$$

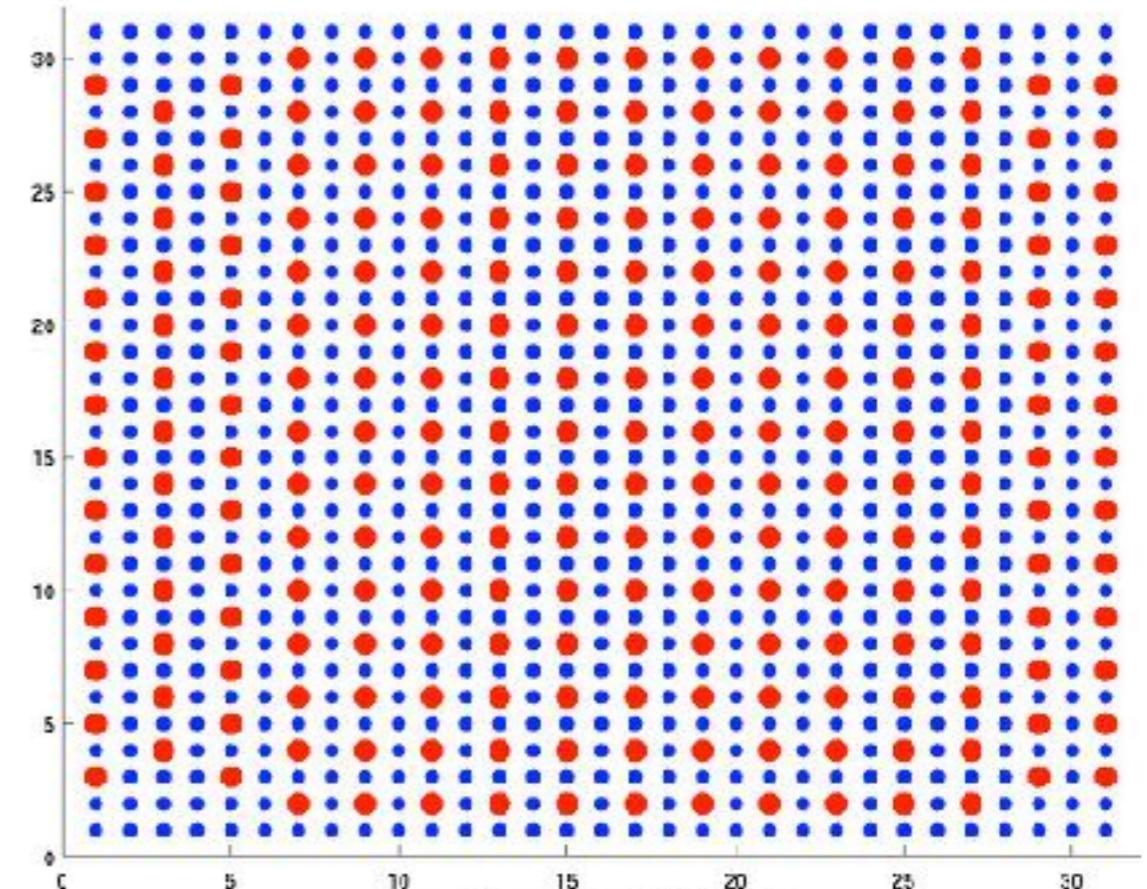


Tests: anisotropic 9-pt FE... coarse grids reflect smoother used for *CR*

- Pointwise Gauss-Seidel *CR*



$$\rho_{cr} = 0.19$$

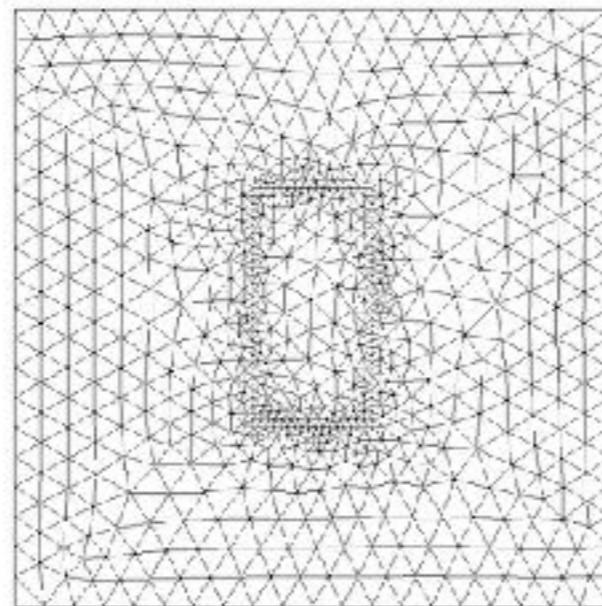
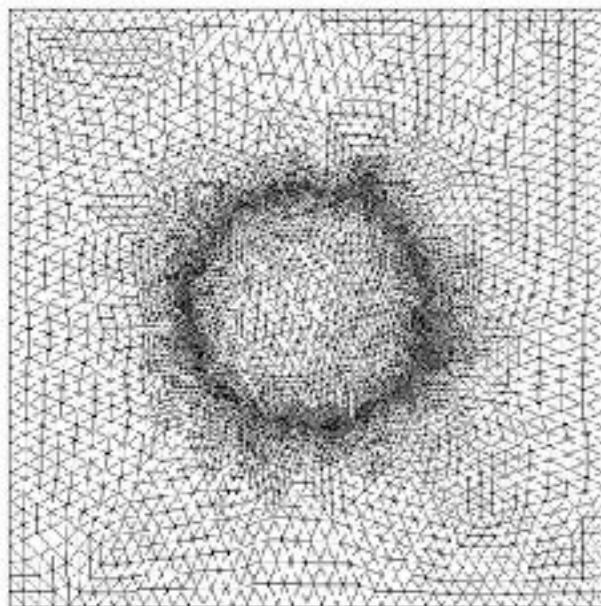


$$\rho_{cr} = 0.45$$

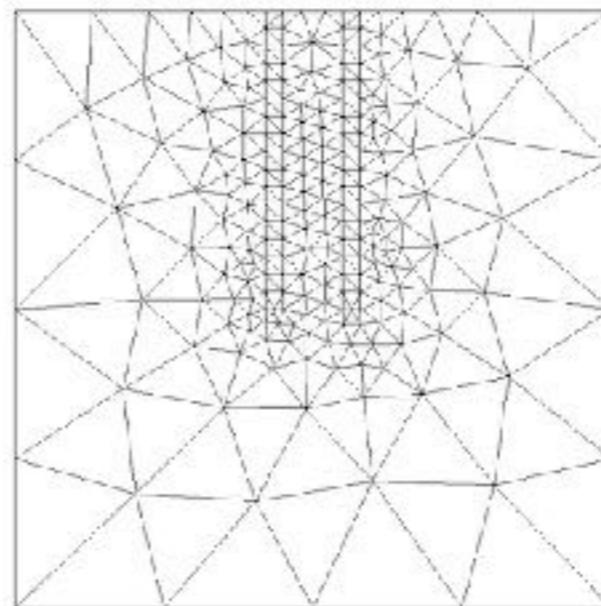
Not possible with standard definitions of strength

CR-AMG grid hierarchies for several 2D problems

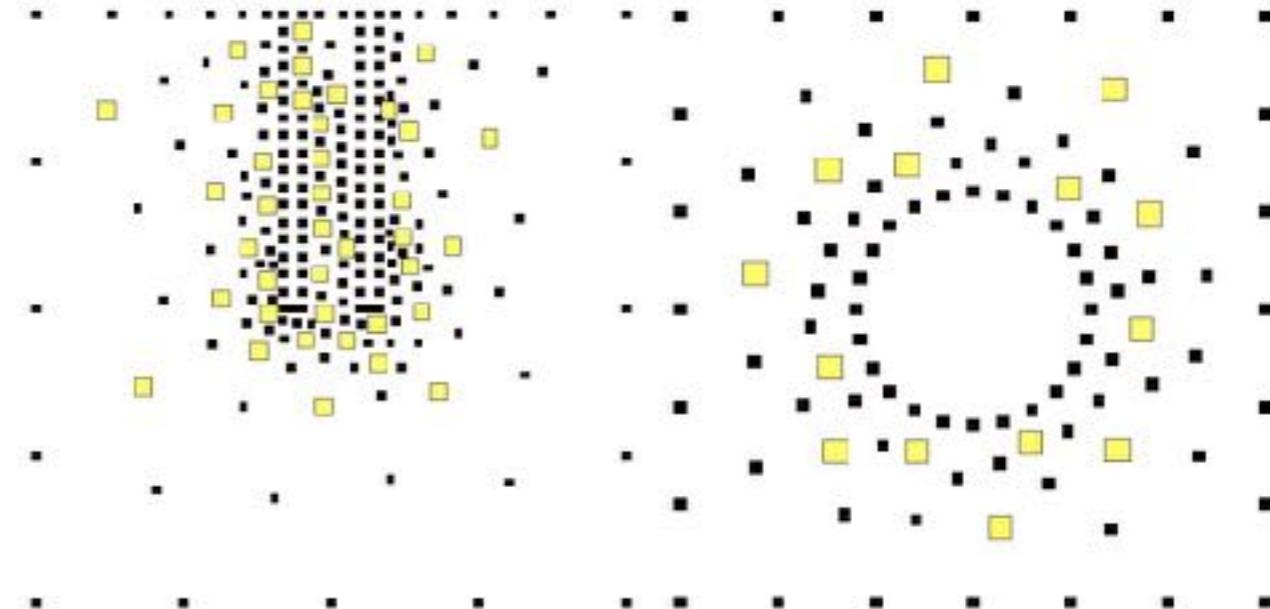
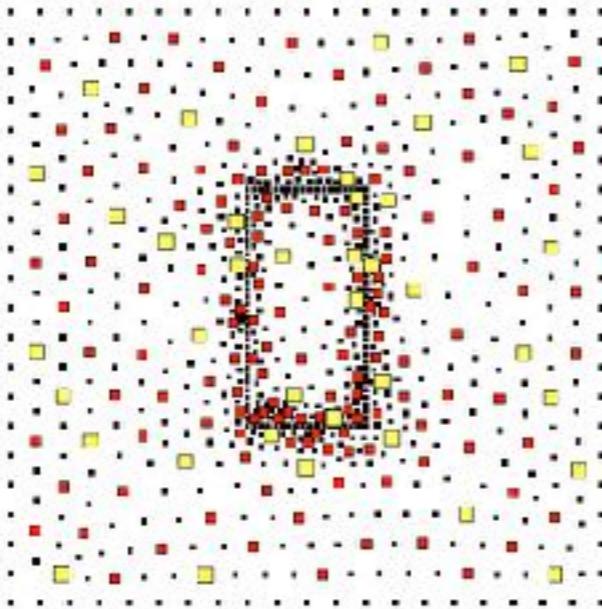
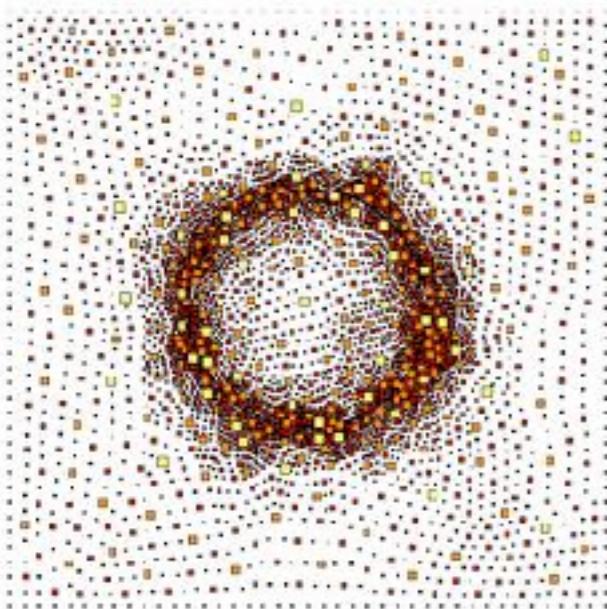
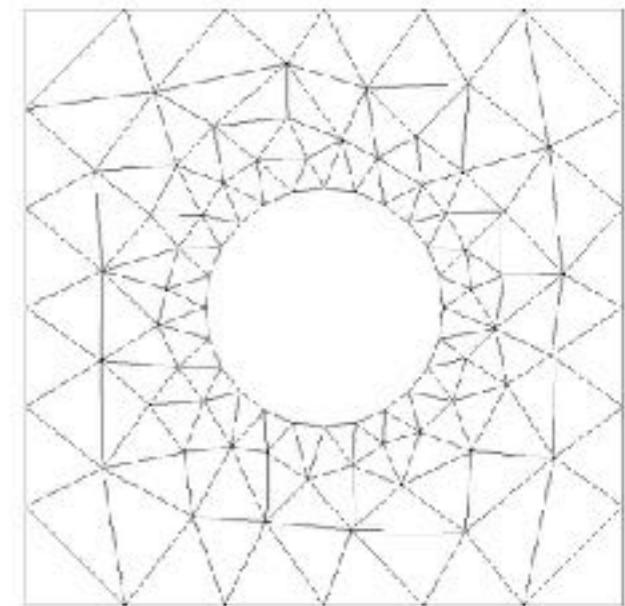
domain1 - 30° domain2 - 30°



pile



square-hole



Adaptive AMG: use the method to improve the method

- Requires no *a-priori* knowledge of the near null space
- Idea: uncover *representatives* of slowly-converging error by applying the “current method” to $Ax = 0$, then use these to adapt (improve) the method
- Achi Brandt’s *Bootstrap AMG* is an adaptive method
- PCG can be viewed as an adaptive method
 - Not optimal because it uses a global view
 - The key is to view representatives locally

α SA automatically builds the global basis for SA

- Generate the basis one vector at a time
 - Start with relaxation on $Au=0 \rightarrow u_1 \rightarrow \alpha\text{SA}(u_1)$
 - Use $\alpha\text{SA}(u_1)$ on $Au=0 \rightarrow u_2 \rightarrow \alpha\text{SA}(u_1, u_2)$
 - Etc., until we have a good method
- Setup is expensive, but is amortized over many RHS's
- Helpful analysis tool

Brannick, Brezina, Keyes, Livne, Livshits, MacLachlan, Manteuffel, McCormick, Ruge, and Zikatanov, "Adaptive smoothed aggregation in lattice QCD," Springer (2006)

Brezina, Falgout, MacLachlan, Manteuffel, McCormick, and Ruge, "Adaptive smoothed aggregation (α SA)," SIAM J. Sci. Comput. (2004)

Other AMG methods

- AMGe
 - Use local stiffness matrices to define smooth error

M. Brezina, A. J. Cleary, R. D. Falgout, V. E. Henson, J. E. Jones, T. A. Manteuffel, S. F. McCormick, and J. W. Ruge, Algebraic multigrid based on element interpolation (AMGe), SIAM J. Sci. Comput., 2000

- Element-Free AMGe
 - Builds “local element matrices” directly from global matrix
 - Requires the definition of an **extension map**

V. E. Henson and P. S. Vassilevski, Element-free AMGe: General algorithms for computing interpolation weights in AMG, SIAM J. Sci. Comput., 2001

- Spectral AMGe
 - Based on a variant of the AMGe measure
 - Coarse dofs are no longer simple subsets of fine-grid dofs
 - Requires solution of local eigenvalue problems

T. Chartier, R. D. Falgout, V. E. Henson, J. Jones, T. Manteuffel, S. McCormick, J. Ruge, and P. S. Vassilevski, Spectral AMGe (pAMGe), SIAM J. Sci. Comput., 2003

Advanced Demos

Demo: [5-AMG-advanced-options-anisotropy.ipynb](#)

Demo: [6-AMG-advanced-options-nonsymmetric-flow.ipynb](#)

Demo: [7-AMG-advanced-options-systems-elasticity.ipynb](#)