Multilevel preconditioners for solving systems of partial differential equations

RAL-Bath NA Day

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Goal

Solve linear systems arising from (systems of) Partial Differential Equations

Example: nonlinear diffusion equation

$$\frac{\partial E(T)}{\partial t} = \mathsf{div}(K(T)\nabla T) + f,$$

with appropriate boundary conditions

This has applications in many problems arising in physics

Other example: 3 temperature radiative transfer model

$$\rho \frac{\partial E_i(T_i)}{\partial t} = \mathrm{div}(K_i \nabla T_i) + \alpha(T_e - T_i),$$

$$\rho \frac{\partial E_e(T_e)}{\partial t} = \mathrm{div}(K_e \nabla T_e) - \alpha(T_e - T_i) - c(a\sigma_E T_e^4 - \sigma_A T_r^4),$$

$$\rho \frac{\partial a T_r^4}{\partial t} = \mathrm{div}(K_r \nabla a T_r^4) + c(a\sigma_E T_e^4 - \sigma_A T_r^4).$$

Unknowns are T_e, T_i, T_r (ρ is known)

This is a system of nonlinear PDEs whose behavior depends on the relative values of diffusion and relaxation terms

Using finite volumes or finite elements in space and backward Euler in time, one obtains at each time step a nonlinear system with $3 \times N$ unknowns which is linearized with the Newton's method

At every nonlinear iteration a (large) linear system has to be solved

We would like to solve large sparse linear systems on parallel computer in a scalable way

$$Ax = b$$

with A a nonsingular sparse matrix of order n, n may be several tens or hundreds millions

To reach this goal one can use Domain Decomposition or Multigrid

Here we use Krylov iterative methods

Today, we will concentrate on symmetric systems using CG

When solving problems arising from PDEs one can use (geometric) multigrid

However, it is not always easy to define the coarse grids when using unstructured meshes

A possibility is to use algebraic preconditioners relying only on the matrix

$$Ax = b$$

A symmetric positive definite $\Rightarrow$ PCG

For PCG to be scalable the preconditioner must be s.t.:

- the number of iterations is (almost) constant when the size of the problem increases
- the complexity of applying the preconditioner is proportional to n

Algebraic multigrid was introduced by J. Ruge and K. Stuben (1985)

It mimics geometric multigrid

A "grid" $\equiv$ (sub)space of unknowns (vertices) of the matrix graph

- The main difficulty is to have a method both efficient and parallel

Multilevel preconditioners (V-cycle)

Starting from the null vector :

0– on the coarsest level, solve exactly using Gauss, otherwise

1– Do ν smoothing iterations

2– Restrict the residual r to $r_c = Rr$ (next coarse level)

3– Recursively solve $A_c e_c = r_c$, $A_c = RAP$, $R = P^T$

4– Interpolate e_c to $e = Pe_c$ (next fine level)

5– Add the correction e to the current iterate

6– Do ν smoothing iterations

Smoothers

- symmetric Gauss–Seidel (not //)
- incomplete Cholesky (not //) LDL^T
  - IC(0)
  - IC with fill–in (values)
  - IC with fill–in (levels)

$$LD^{-1}L^T(x^{k+1} - x^k) = b - Ax^k$$

◦ Approximate inverse AINV from M. Benzi (Emory Univ.) and al.

$$M \approx A^{-1}, \quad M = ZD^{-1}Z^T$$

where Z is upper triangular with 1 on the diagonal and D is diagonal

The parameter τ defines which elements are kept in Z as the factorization (by columns) proceeds

It works for H–matrices, for SPD matrices one uses SAINV (Stabilized AINV)

Smoother: Richardson iteration defined as

$$x^{k+1} = x^k + M(b - Ax^k)$$

Influence matrix

How to define the coarse levels?

$$\mathcal{N} = \{1, \ldots, n\}, \quad \mathcal{N} = F \cup C$$

Set of indices: standard AMG choice (Ruge-Stuben) for M–matrices

i is a row index

$$S_i = \{j | -a_{i,j} > \theta \max_{k \neq i}(-a_{i,k}), \quad \theta < 1\}$$

From S_i we construct S (matrix with 1 and 0 elements)

General case

$$S_i^A = \{j \neq i \mid |a_{i,j}| > \tau \max_k |a_{i,k}|, \quad \tau < 1\}$$

We keep at least one 1 for the largest modulus element ('b')

τ parameter to be chosen

It is usually better to symmetrically normalize the matrix

Coarsening algorithm

The "standard" algorithm is:

Weights w_i = nb of points which depend on i (using S)

1- Choose a point i of maximal weight as a C point

2- Flag the points that i influences (with S) as F points

3- Add 1 to the weights of points influencing these new F points (to give them a better chance to be chosen as C points in the next steps)

4- Decrease by 1 the weights of points that depend on i

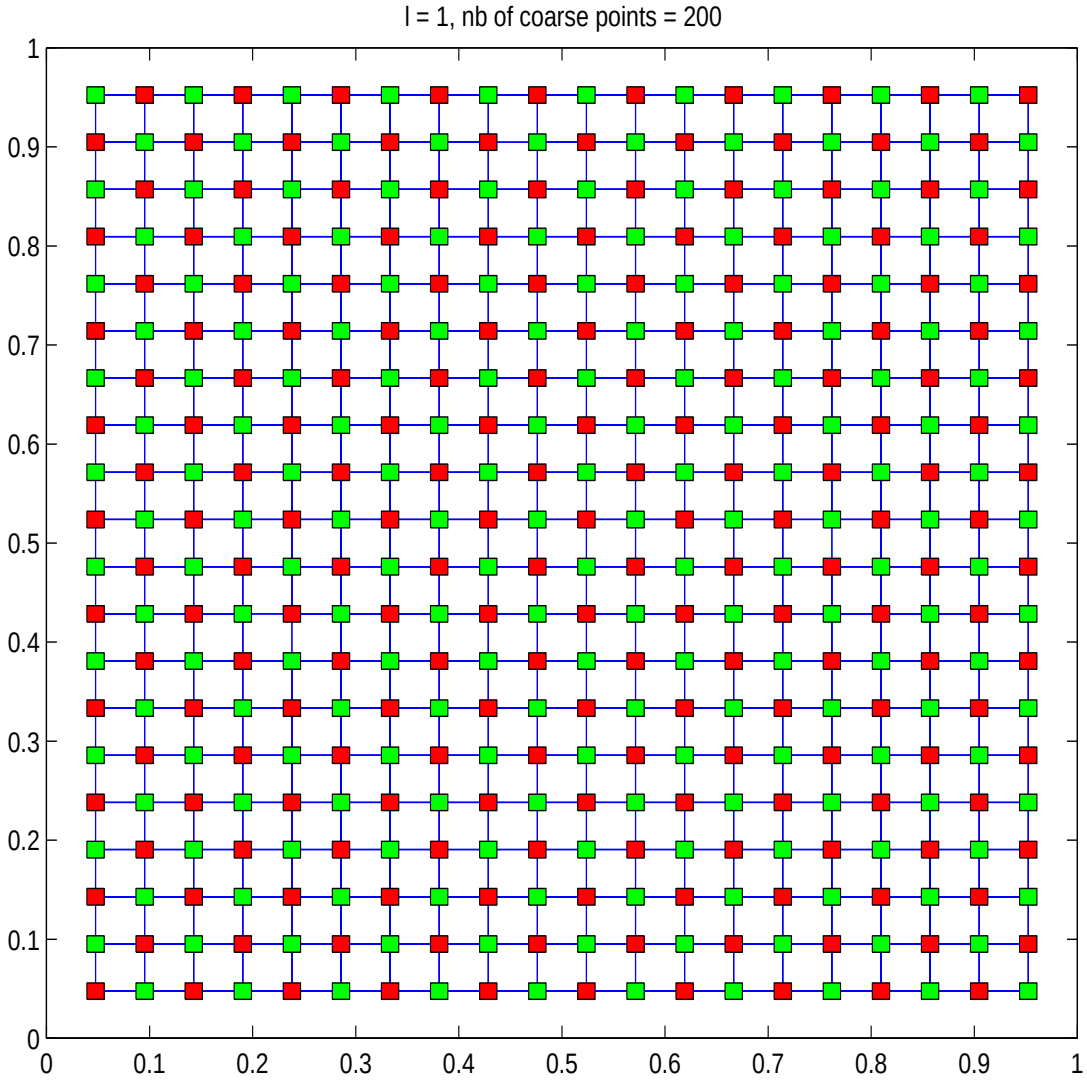
Repeat steps 1-4 until all the points are labelled

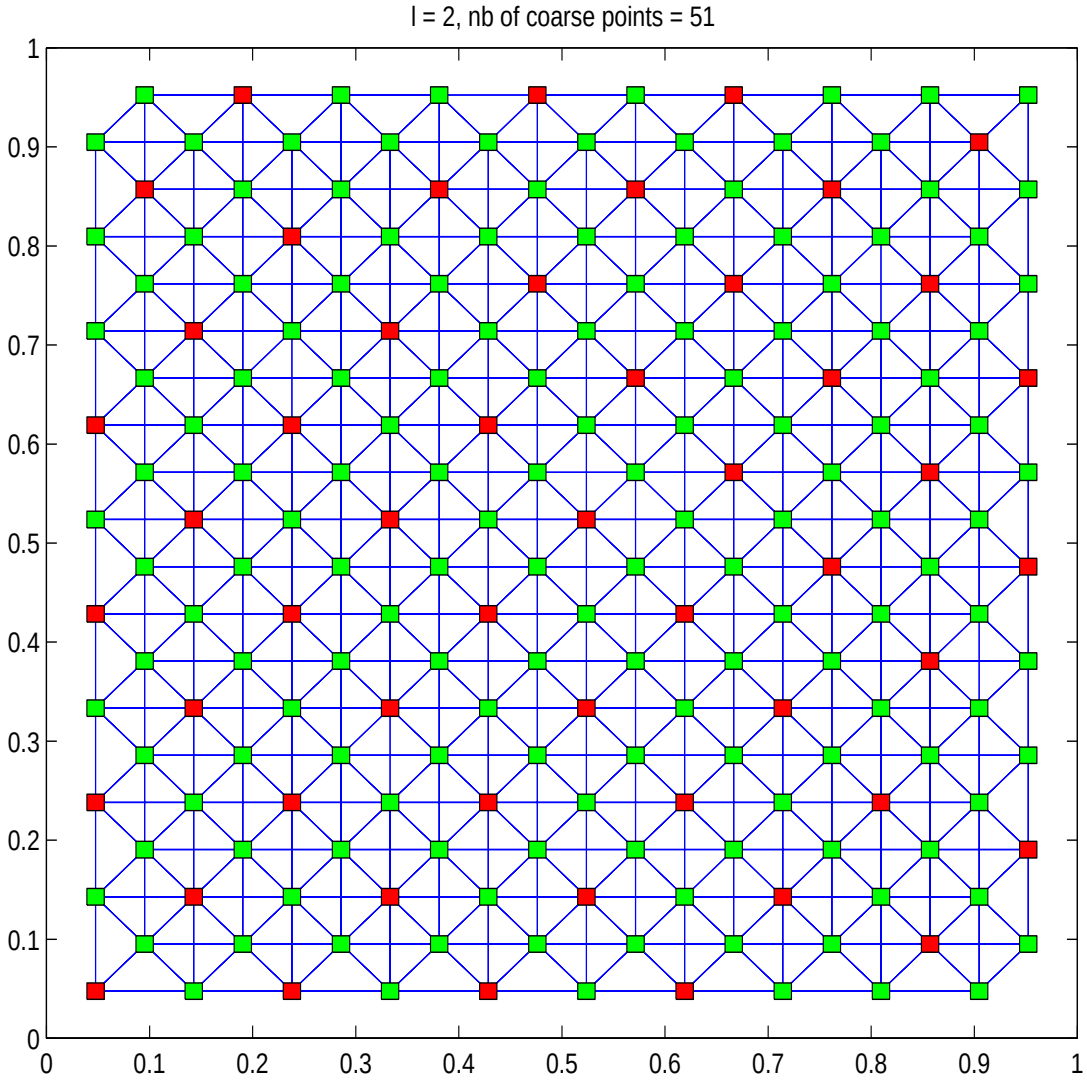
Example: Poisson equation in a square, 5-point finite differences, $n = 400$

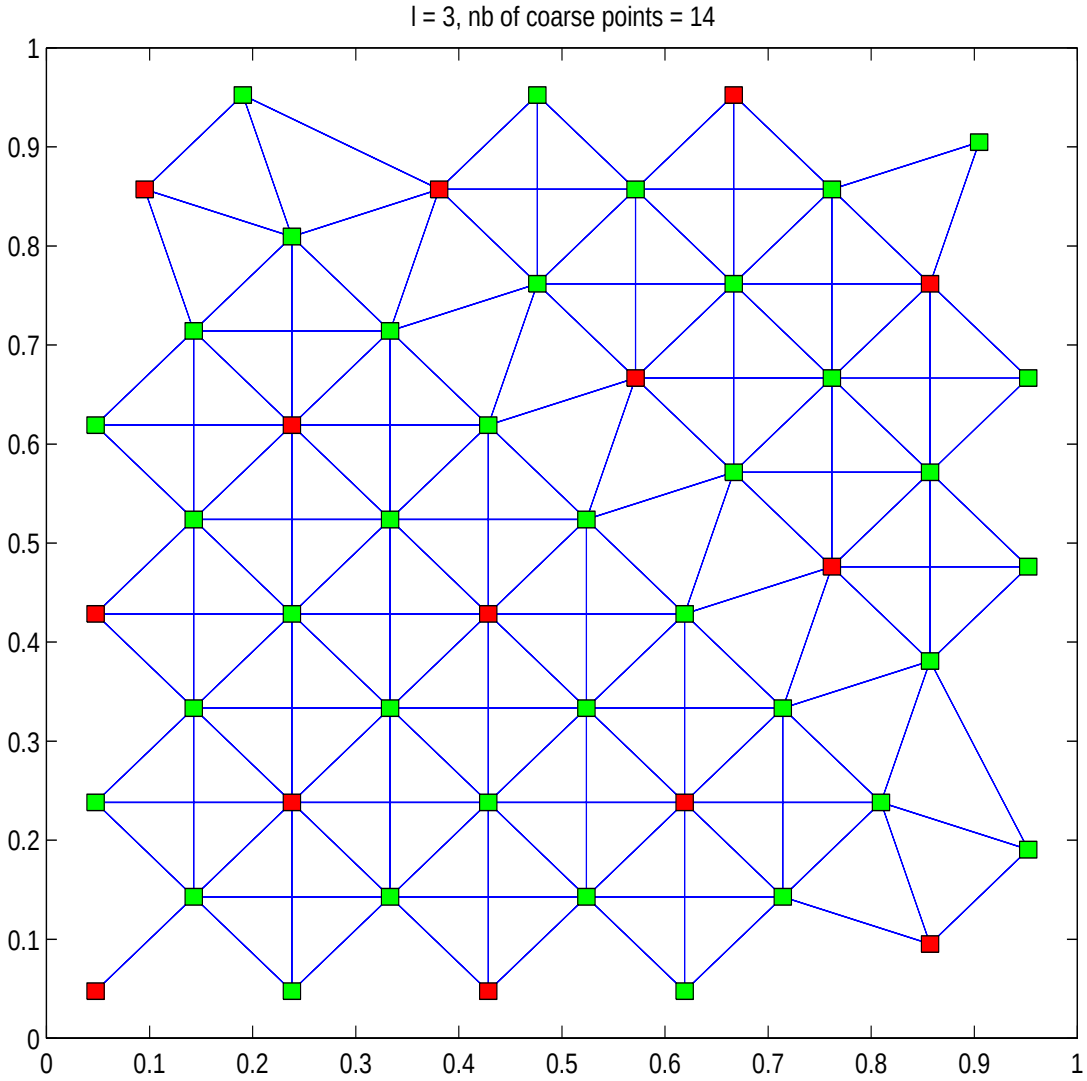
The graph of A is the same as the mesh

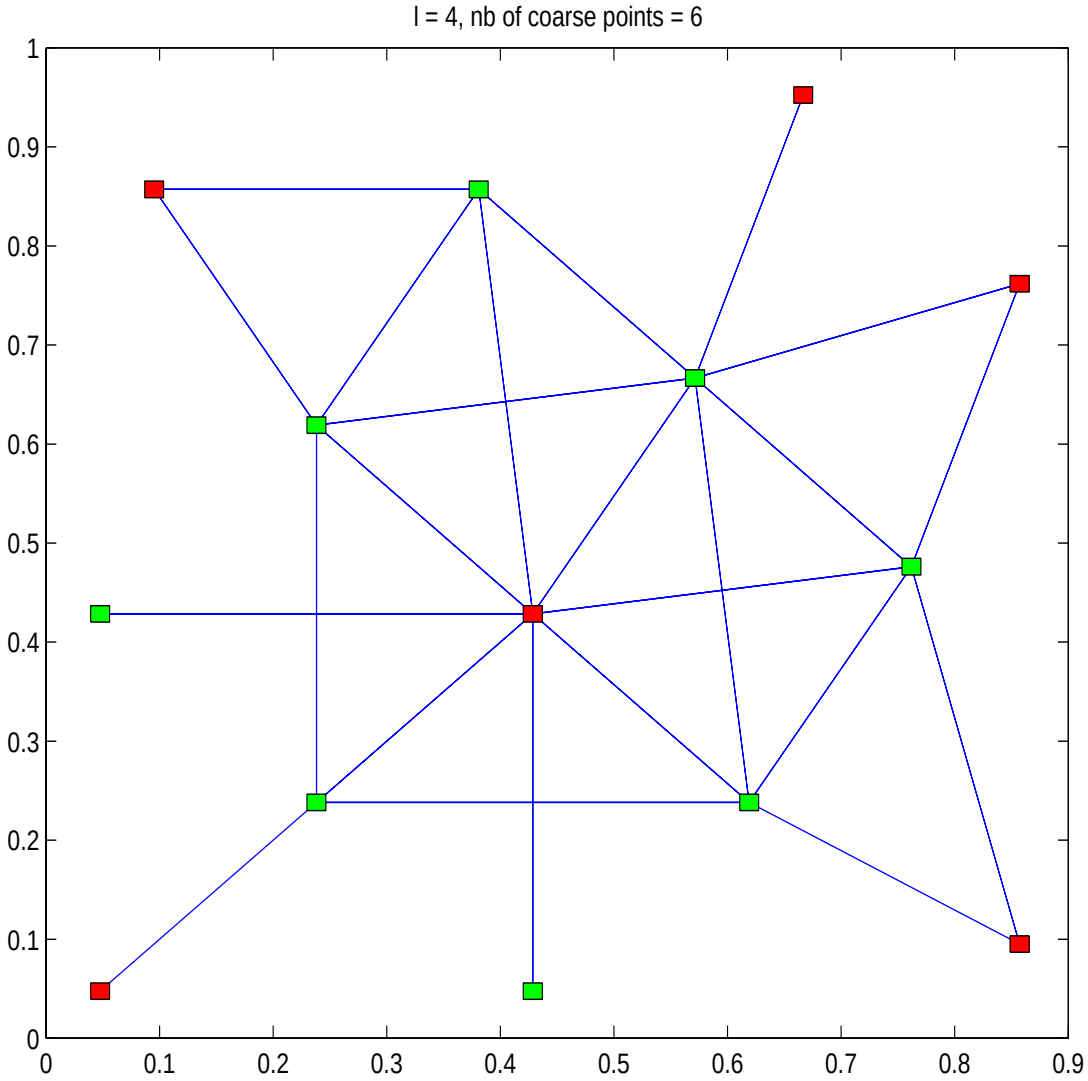
The matrix is normalized with ones on the diagonal

graphs and C and F points for all levels


l = 1, nb of coarse points = 200
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


l = 2, nb of coarse points = 51
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


l = 3, nb of coarse points = 14
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1


l = 4, nb of coarse points = 6
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9

Interpolation algorithm

- $i \in F, j \in C$

$$\omega_{i,j} = -\frac{a_{i,j} + \sum_{k \in D_i^S} \frac{a_{i,k} a_{k,j}}{\sum_{m \epsilon C_i} a_{k,m}}}{a_{i,i} + \sum_{k \in D_i^W} a_{i,k}}$$

D_i^S and D_i^W are strong and weak couplings

This comes from writing $Ae = 0$ and using $e_j \approx e_i$ for weak connections and a weighted average for connections with F points

Coarse matrices

The interpolation algorithm defines P and $R = P^T$

$$A_C = RAP$$

How to parallelize the smoothers?

Domain decomposition

◦ Partition the graph of A (or sometimes S) with or without overlapping (ghost nodes)

◦ symmetric Gauss–Seidel

parallelized by using Jacobi for interface nodes (SGSJ)

◦ incomplete Cholesky or AINV

parallelized by ignoring dependencies between subdomains (ICp, SAINVp)

Only the finest level is partitioned, this may cause load balancing problems on coarse levels

Parallel coarsening

◦ LLNL algorithms (Cleary, Falgout, Henson and Jones)

• They start on several "independent" nodes at the same time

◦ Other method :

• Start by coarsening the overlapping or the interface

• Flag the (subdomain) neighbors of these C points as F points (without introducing $F - F$ connections)

• Coarsen the subdomains using the preceding step as "boundary conditions"

Numerical results

5 point finite differences, unit square, $m \times m$ cartesian mesh

b random, $x^0 = 0$

stopping criterion: $\|r^k\| \leq 10^{-10}\|r^0\|$

Small sequential problems

PCG, Poisson, $\tau = 0.06$, ('ic', 'a', 'st', 'st'), $\gamma = 1$

m	$\nu = 1$	$\nu = 2$
40	5 op=1598145, /n=998.8 str=35667, /n=22.3 $\kappa = 1.03$	5 op=2631408, /n=1644 $\kappa = 1.01$
50	5 op=2528438, /n=1011 str=56497, /n=22.6 $\kappa = 1.02$	5 op=4165773, /n=1666 $\kappa = 1.01$
60	6 op=4265230, /n=1185 str=81388, /n=22.6 $\kappa = 1.03$	5 op=6008813, /n=1669 $\kappa = 1.01$

Numerical results on the CEA TERA 1

(HP-Compaq, Alpha EV6 processors 1Ghz)

5 (7) point finite differences, unit square (cube), $m \times m$ mesh, b random

$x^0 = 0$

stopping criterion $\|r^k\| \leq 10^{-10}\|r^0\|$

Domain decomposition with squares (cubes), $m_p^{2(3)}$ unknowns per processor

- A is distributed by rows

- Poisson equation
- Diffusion problem with discontinuous and anisotropic coeff

Partition of $[0,1]^2$ in 4 squares

diffusion coeff $(1,1),(10,100),(100,10),(1000,1000)$

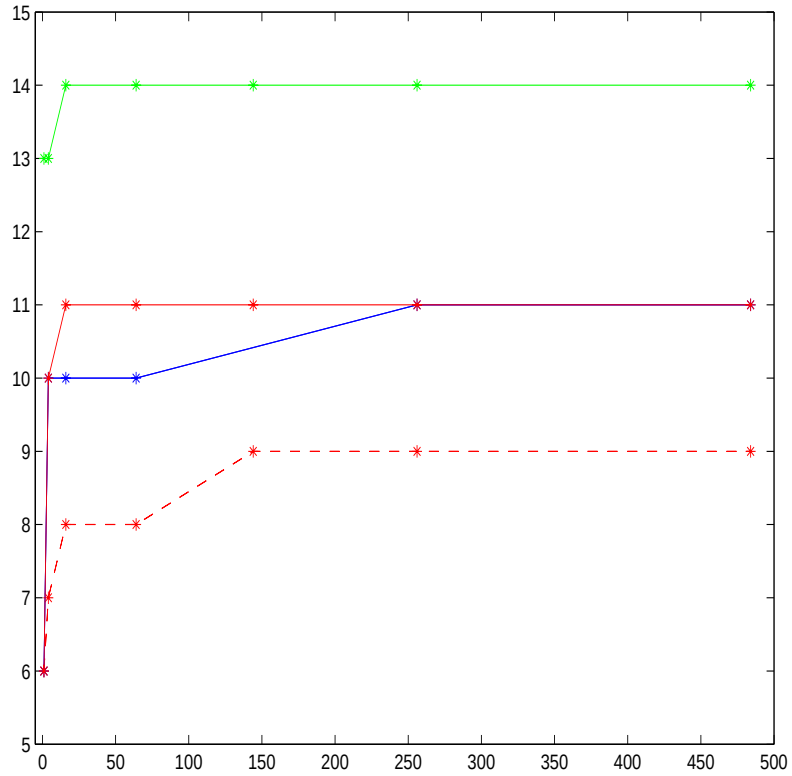
First experiment

- Poisson

$m_p = 250 \rightarrow 62500$ unknowns per processor,

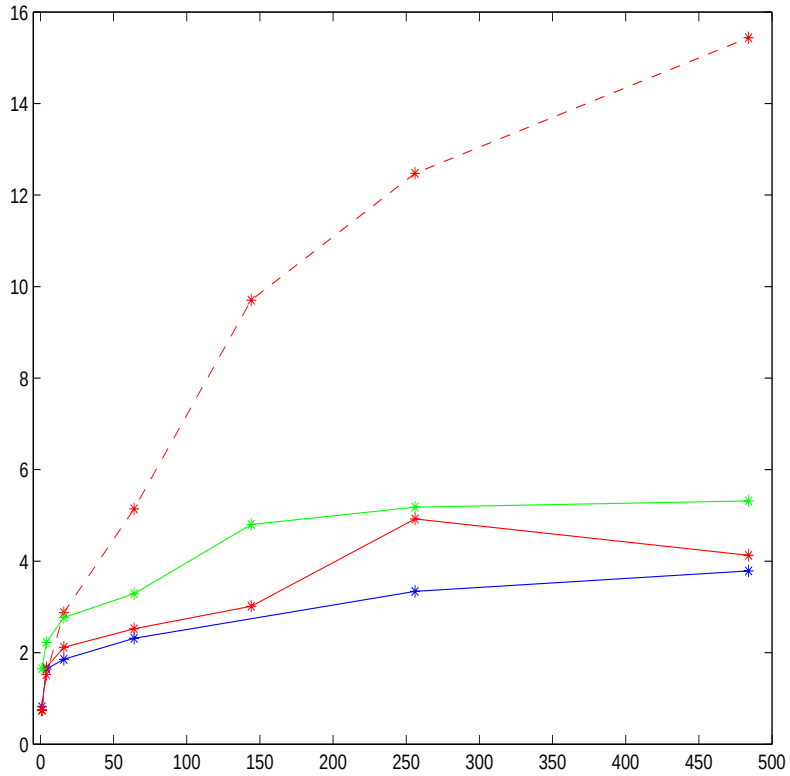
$p = 1, 4, 16, 64, 144, 256, 484$

- largest problem has $\simeq 30\ 10^6$ unknowns



Nb of iterations for Poisson as a function of p

coarsening : LLNL, blue: SGSJ, red dashed: IC, red: ICp, green: SAINVp



"elapsed" time (s) for Poisson as a function of p

coarsening : LLNL, blue: SGSJ, red dashed: IC, red: ICp, green: SAINVp

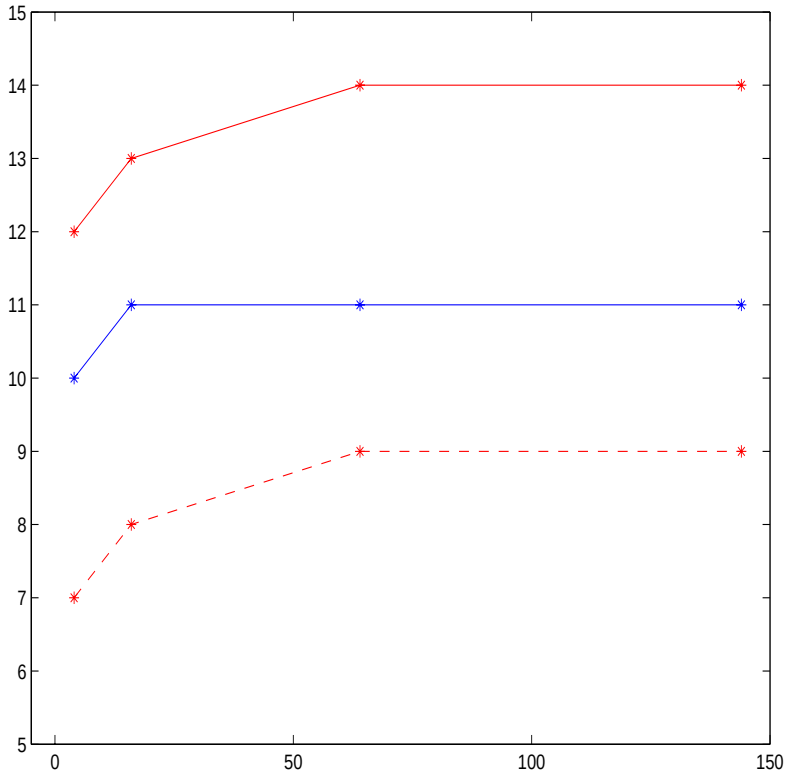
Second experiment

- Discontinuous and anisotropic problem

$m_p = 250 \rightarrow 62500$ unknowns per processor

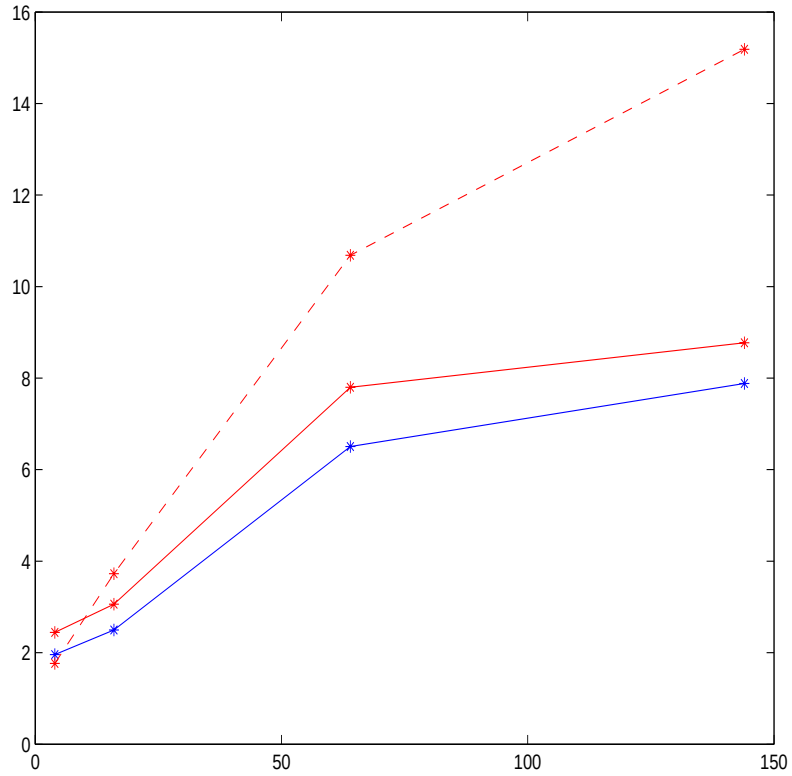
$p = 4, 16, 64, 144$

- Largest problem has $4\ 10^6$ unknowns



Nb of iterations for the discontinuous and anisotropic pb as a function of p

coarsening : LLNL, blue: SGSJ, red dashed: IC, red: ICp

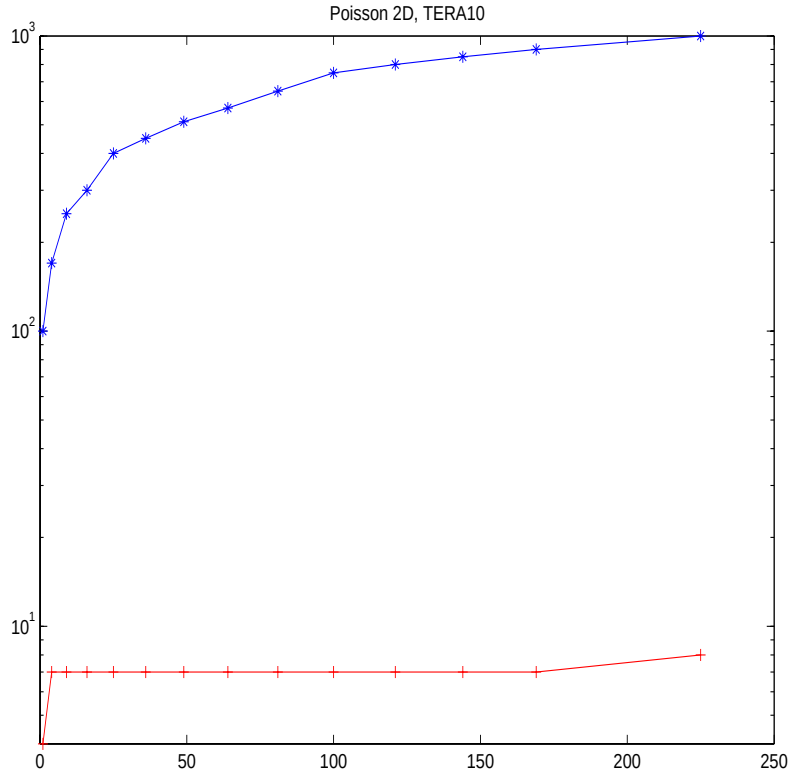


"elapsed" time (s) for the discontinuous and anisotropic pb as a function of p

coarsening : LLNL, blue: SGSJ, red dashed: IC, red: ICp

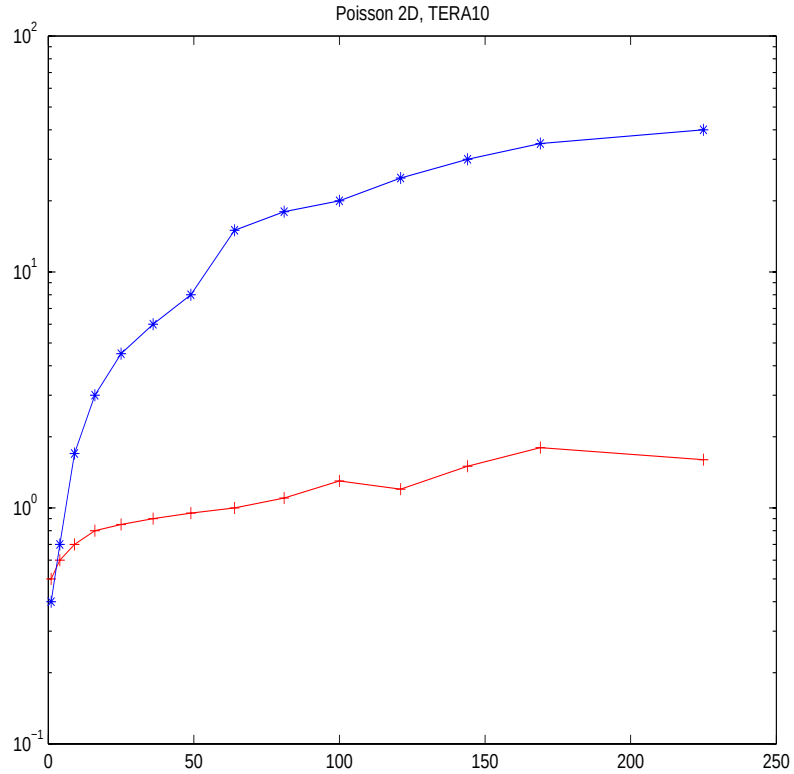
The CEA TERA 10 parallel computer

	TERA-1	TERA-10
Processor	Alpha EV6 - 1 Ghz	Intel Montecito - 1.6 Ghz
Node	4 processors	16 cores (8 Montecito)
Memory per node	4 GB - 16 GB - 32 GB	48 GB - 128 GB
Peak performance	8 Gflops	> 100 Gflops
Interconnexion Network	2 "rails" ELAN - 3 Latency 5 us - Links 400 MB/s	3 "rails" ELAN - 4 Latency 4 us - Links 900 MB/s
Number of nodes	608	544
Peak performance	5 Tflops	> 60 Tflops
Sustained performance	1.35 Tflops	12.5 Tflops
Memory size	3 TB	30 TB
Disk space	50 TB	1 PB
Disk bandwidth	7.5 GB/s	100 GB/s
Storage network	32 HiPPI links (800 Mbits/s)	20 IB 4x links (1 GB/s)
User access	20 1 Gbits links	10 10 Gbits links



Nb of iterations for 2D Poisson as a function of p

TERA10, red: AMG, blue: IC, $10\ 000$ unkn/p



Elapsed time (s) for 2D Poisson as a function of p

TERA10, red: AMG, blue: IC, $10\ 000$ unkn/p

Extension to block matrices

Goal: solve linear systems arising from PDE systems (several unknowns per element or node)

These systems can be solved with a (point) multilevel preconditioner

However, results are not always so good

This motivated the development of a block extension of the AMG preconditioner

In our example, blocks are 3×3

Smoothers

- iterations of (symmetric) block Gauss–Seidel/Jacobi

Small $p \times p$ systems are solved by Gaussian elimination

- block IC/ILU

Influence matrix

Define influences between blocks:

block I depends on block J (J influences I) if

$$\|A_{I,J}\|_F \geq \tau \max_{K \neq I} \|A_{I,K}\|_F$$

This gives S of order n/size of blocks

Coarsening

The (block) graph of A is coarsened using S with the same algorithms as in the point case

Interpolation P

Interpolation is done component by component:

$$e_I = \sum_{J \in C_I} W_{I,J} e_J,$$

C_I: coarse nodes influencing I, $W_{I,J}$ diagonal $p \times p$ matrix, no coupling between different types of unknowns

Use the same formula as in the point case

$$R = P^T$$

$$A_{\text{grossier}} = RAP$$

This couples the unknowns

Model problem

Block 5-diagonal symmetric matrix with 3×3 blocks

Constant diffusion and relaxation coefficients

Diagonal blocks:

$$\begin{pmatrix} 4\alpha + \mu h^2 & -\mu h^2 & 0 \\ -\mu h^2 & 4\alpha + (\mu + \sigma) h^2 & -\sigma h^2 \\ 0 & -\sigma h^2 & 4\alpha + \sigma h^2 \end{pmatrix}$$

Nonzero nondiagonal blocks are $-\alpha I_3$, $h = 1/(m+1)$

$$\alpha = 1, \mu = 10, \sigma = 200$$

m	n	nb it block GS	nb it block IC
10	300	6	5
20	1200	7	6
30	2700	7	6
40	4800	7	6
50	7500	7	6

Conclusions

- These multilvel preconditioners are (almost) scalable
- Drawback: setup phase is "expensive"
- They are useful only for difficult and/or very large problems