Parallel System Solvers for the Navier-Stokes Equations

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Outline

1. **Present preconditioned schemes for solving the resulting "segregated" and "reordered" linear systems.**

2. **Use for the stabilized and unstabilized finite element formulations.**

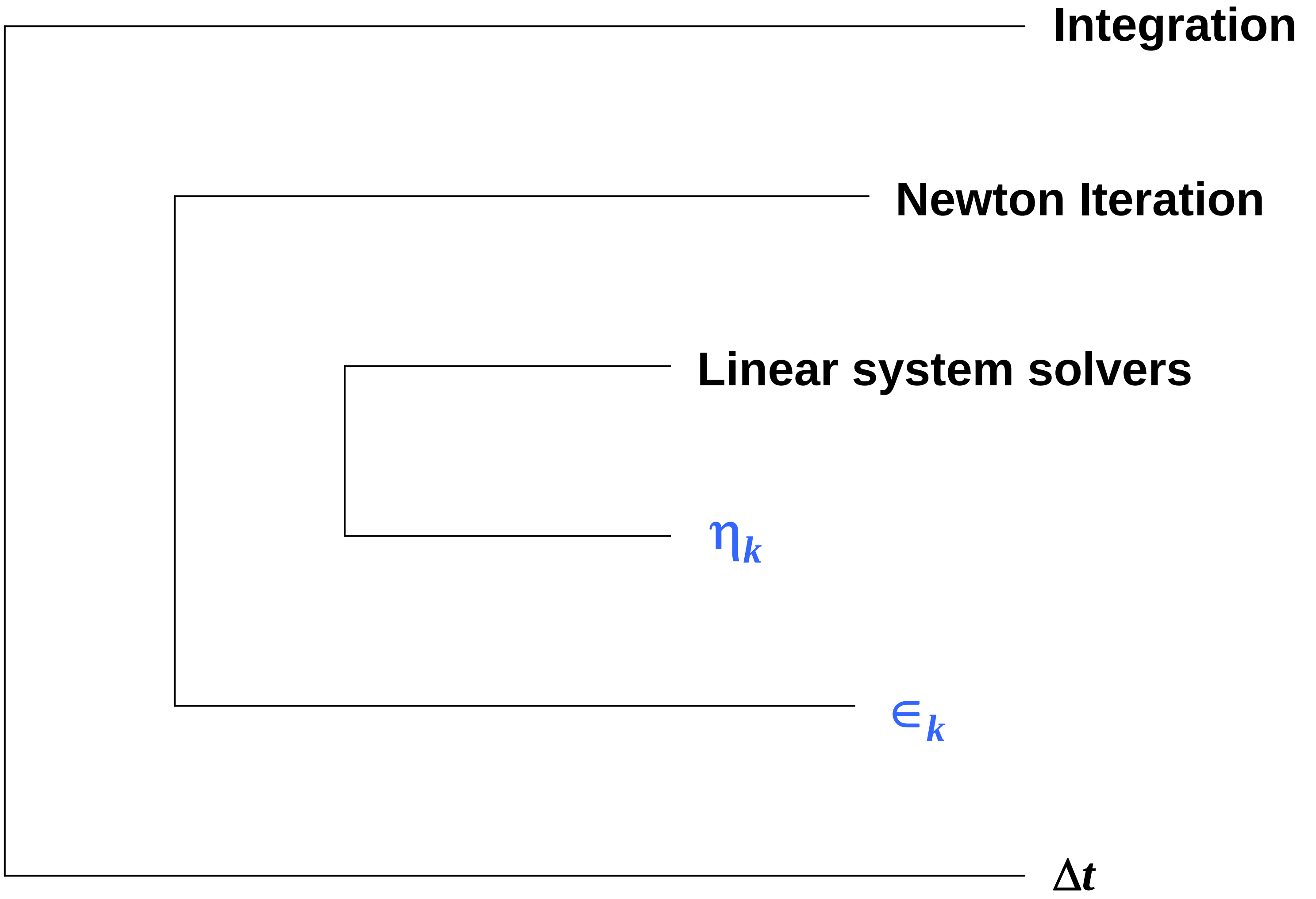
3. **Effectiveness of solvers demonstrated on model problems in –**
   - ***time-accurate solutions in fluid-structure/solid interaction***
   - ***steady-state case***

4. **Concluding remarks.**

Applications

- Space-time flow computation:
  - a simplified parachute model
  - flow past a hemisphere.
- Particulate flow
- Incompressible fluid flow within a "leaky" lid-driven cavity problem steady-state case.

Adaptive Tolerances



Linear Systems

$$\begin{bmatrix} A & B \\ C^T & G \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{bmatrix}$$

- $A \neq A^T$:= $(n \times n)$, rank = n
- B, C := $(n \times m)$, maximal col. rank <= m
- G := symmetric +*ve* semi-definite
- $m < n$

Preconditioned Scheme

Solve $\begin{pmatrix} A & B \\ C^T & G \end{pmatrix}\begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{pmatrix}$

via a Krylov subspace method

Preconditioner

$$M = \begin{pmatrix} E & B \\ C^T & G \end{pmatrix}$$

Solve $M\boldsymbol{z} = \boldsymbol{r}$ via Richardson scheme

$$\boldsymbol{z}_{k+1} = \boldsymbol{z}_k + \hat{M}^{-1}(\boldsymbol{r} - M\boldsymbol{z}_k)$$

where,

$$\hat{M} = \begin{pmatrix} \hat{A} & B \\ C^T & G \end{pmatrix}$$

Solving $\hat{M}\mathbf{u} = \mathbf{c}$

Solve $\begin{pmatrix} \hat{A} & B \\ C^T & G \end{pmatrix} \begin{pmatrix} \mathbf{v} \\ \mathbf{w} \end{pmatrix} = \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix}$

Since

$$\begin{pmatrix} \hat{A} & B \\ C^T & G \end{pmatrix} = \begin{pmatrix} \hat{A} & 0 \\ C^T & I \end{pmatrix} \begin{pmatrix} \hat{A}^{-1} & 0 \\ 0 & G - C^T \hat{A}^{-1} B \end{pmatrix} \begin{pmatrix} \hat{A} & B \\ 0 & I \end{pmatrix}$$

Then solution scheme is given by,

- solve $\hat{A}\mathbf{v} = \mathbf{a}$
- solve $(G - C^T \hat{A}^{-1} B)\mathbf{w} = \mathbf{b} - C^T \mathbf{v}$
- solve $\hat{A}\mathbf{v} = \mathbf{a} - B\mathbf{w}$

- ***Solve*** $\hat{A}v = h$
  - $\hat{A}$ = approximate LU factorization of E, or
  - $\hat{A}^{-1}$ ***: approximate sparse inverse of*** E

    e.g., $\min \left\| I - E\hat{A}^{-1} \right\|_F$ for a given sparsity structure of $\hat{A}^{-1}$.
  - ***Action of*** $\hat{A}^{-1}$ ***is realized via iterative solvers involving E.***
- ***Solve*** $(G-C^T\hat{A}^{-1}B)y = h$

  using a Krylov subspace method with a relaxed stopping criterion

$$\left\|\boldsymbol{r}_k\right\|_2 / \left\|\boldsymbol{r}_0\right\|_2 < \text{tol.}$$

Convergence

Need to have $\rho(I - \hat{M}^{-1}M) < 1$

- $\lambda(I - \hat{M}^{-1}M) := 0, \mu$
- $\mu = \lambda[(I + K)(I - \hat{A}^{-1}E)]$
- $K = \hat{A}^{-1}B(G - C^T\hat{A}^{-1}B)^{-1}C^T$

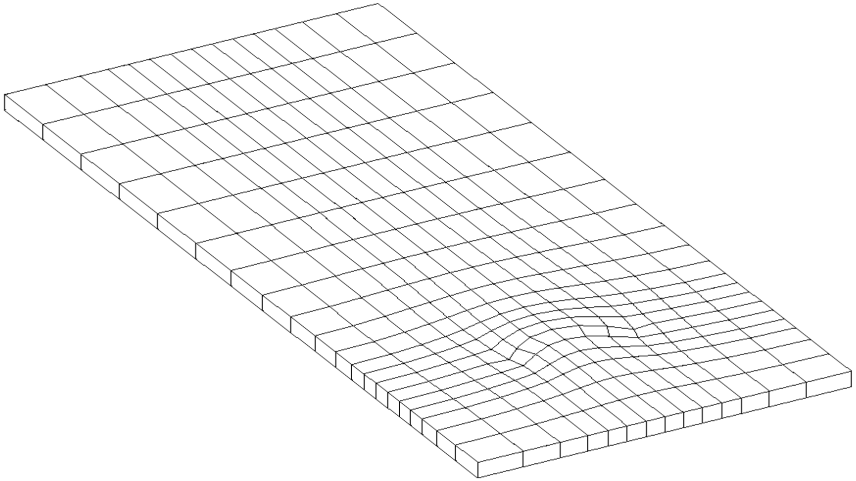
$$\lambda(K) = \lambda[(C^T\hat{A}^{-1}B)(G - C^T\hat{A}^{-1}B)^{-1}]$$

- $\rho(I - \hat{A}^{-1}E) \leq \alpha < 1$

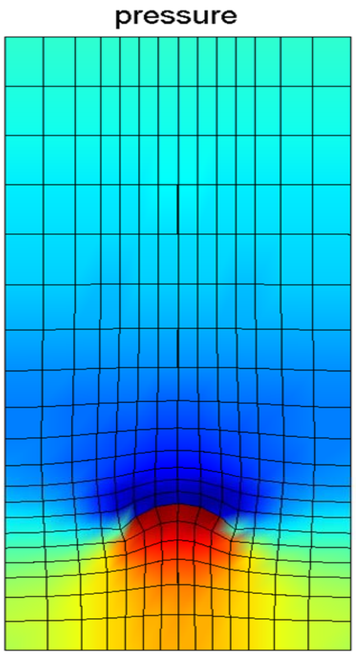
Case 1

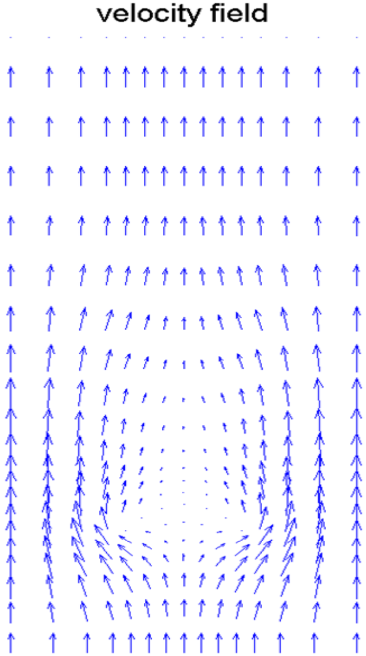
Space-Time Computation

1. Simplified Parachute Model

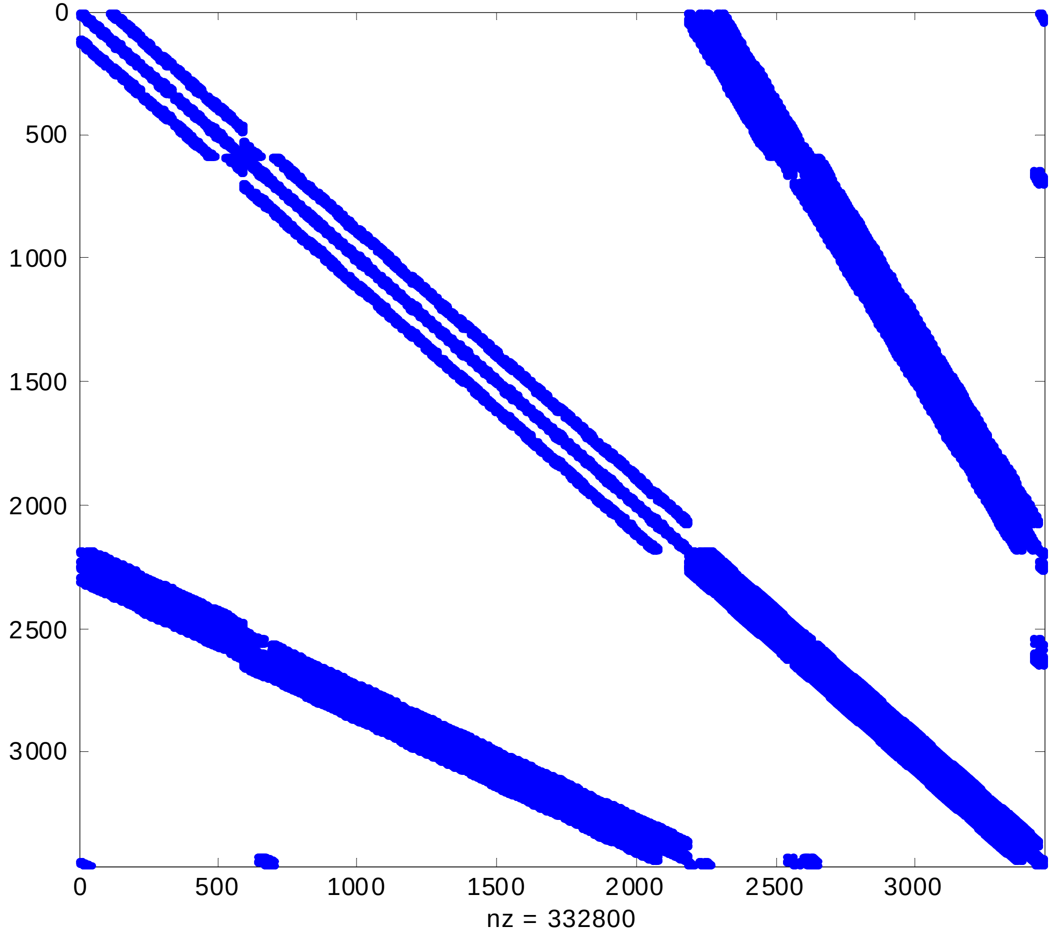


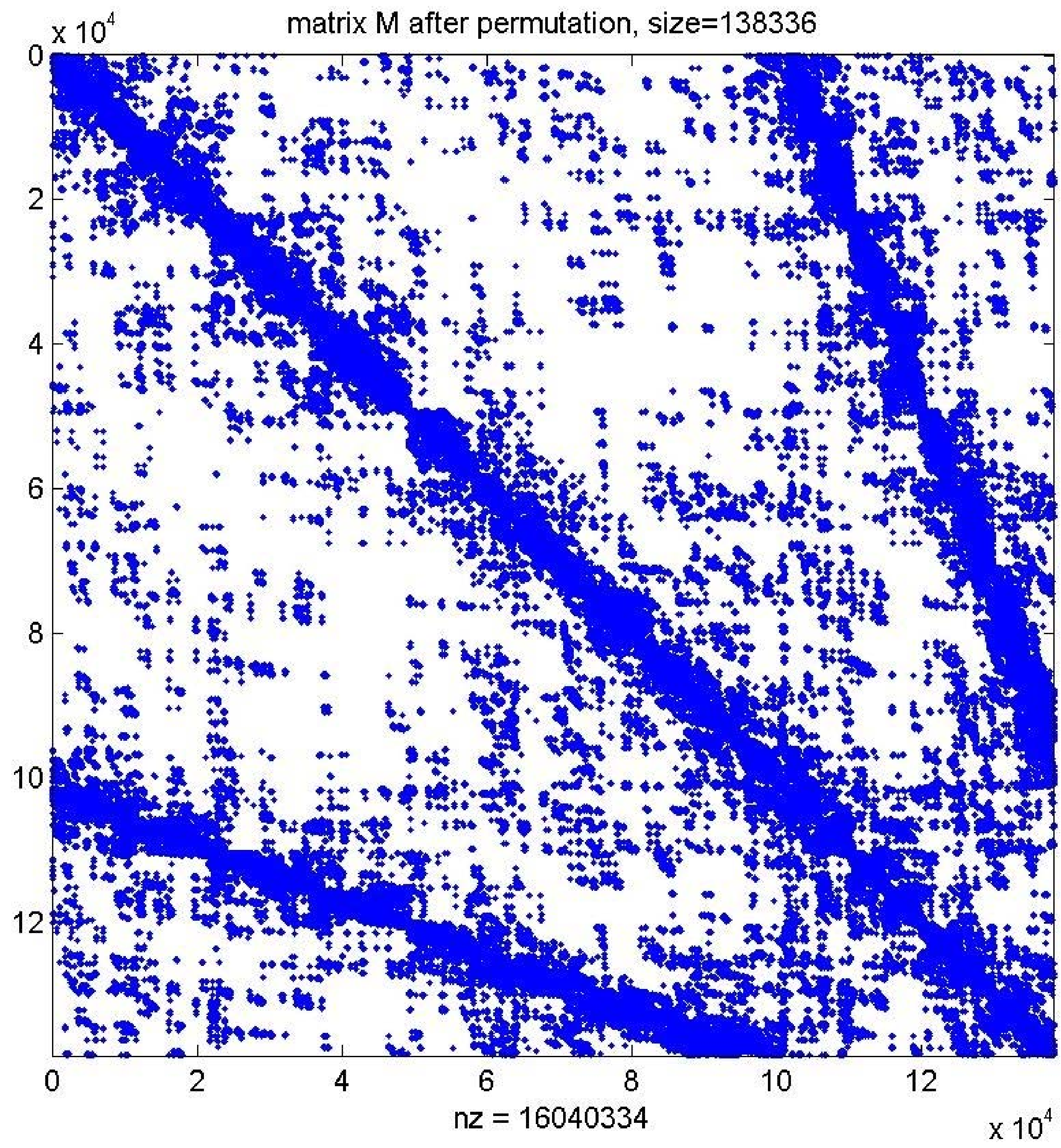
Flow Results:





The Linear System Matrix $\tilde{A}$





matrix M after permutation, size=138336
x 10^4
0
2
4
6
8
10
12
0
2
4
6
8
10
12
nz = 16040334
x 10^4

Parachute model…

- Re = 1000
- Choose $E = A$ and remove outer layer.
- $\hat{A} = LU$
  incomplete LU-factorization of A with no fill-in, or any of its parallel counterparts.

Solve $\begin{bmatrix} A & B \\ C^T & G \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{bmatrix}$

via Richardson scheme: $\left\| r_{Richardson} \right\|_2 \leq 10^{-5}.$

- $\hat{M} = \begin{bmatrix} LU & B \\ C^T & G \end{bmatrix}$

$$\begin{bmatrix} \boldsymbol{u}_{k+1} \\ \boldsymbol{p}_{k+1} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_k \\ \boldsymbol{p}_k \end{bmatrix} + \hat{M}^{-1} \left[\begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{pmatrix} - \begin{pmatrix} A & B \\ C^T & G \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_k \\ \boldsymbol{p}_k \end{pmatrix} \right]$$

Note:

Solve $(G - C^T \hat{A}^{-1} B)\boldsymbol{w} = \boldsymbol{s}$ via bicgstab with relative residual $< 10^{-1}$.

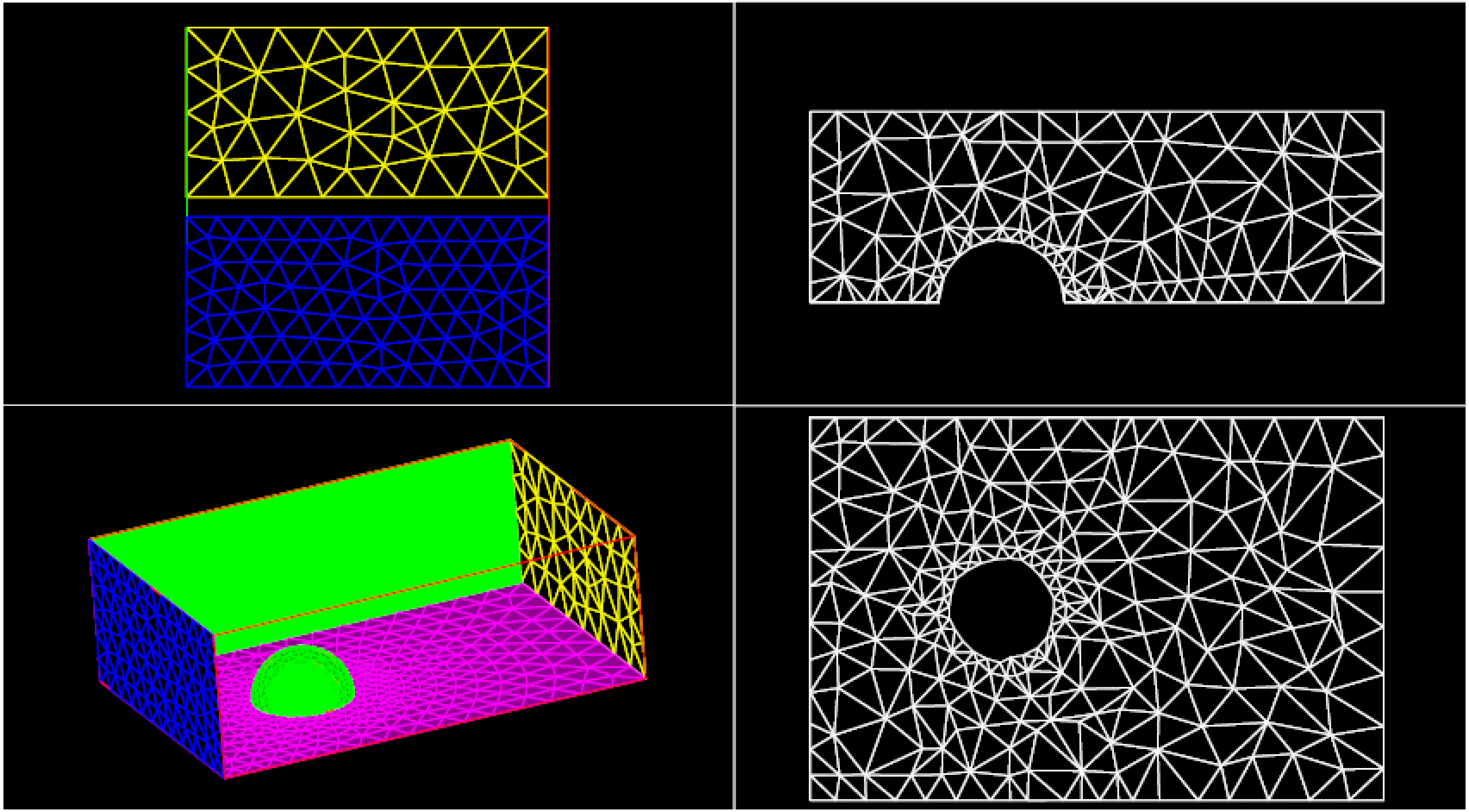
G1 := preconditioner

Richardson: Incomplete LU - Bicgstab (10^{-1})

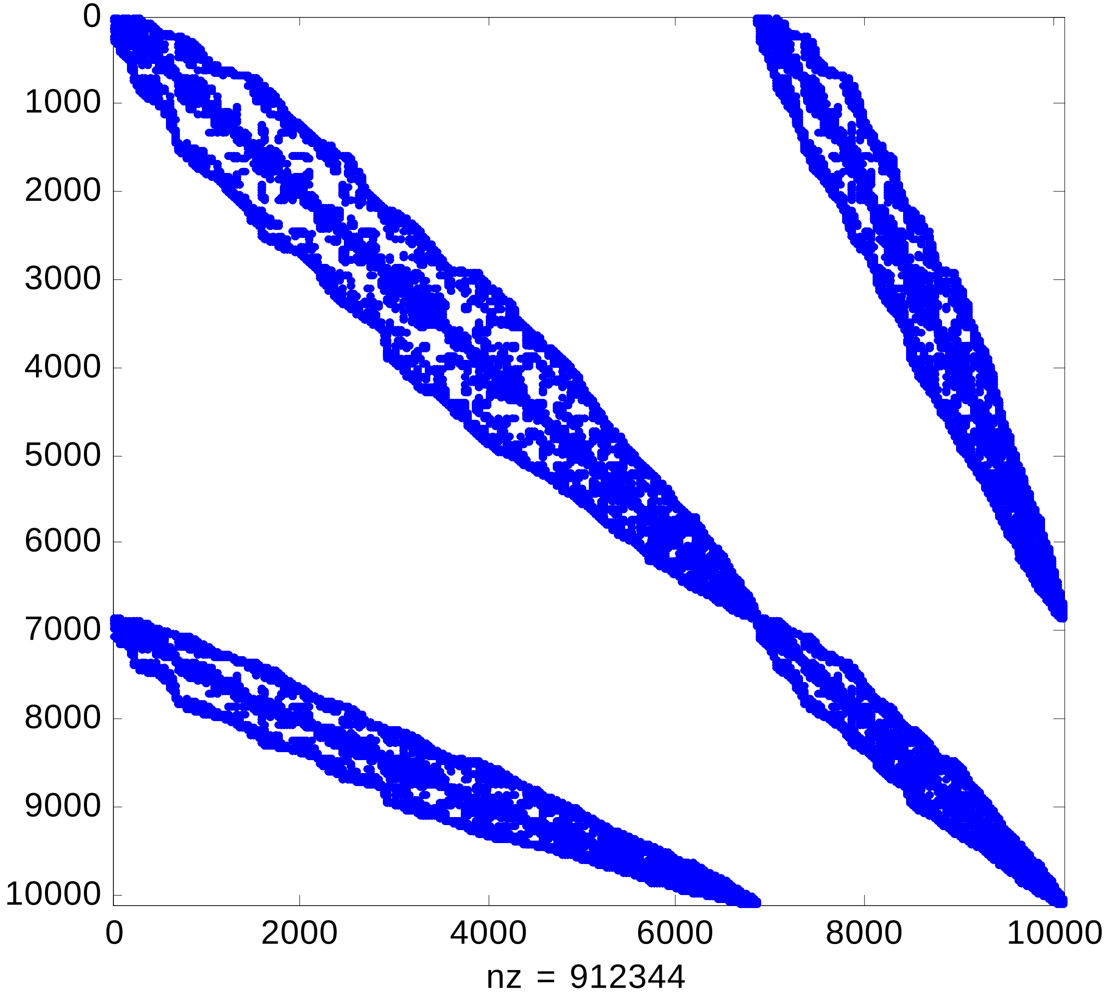
2. Flow past an inflatable hemisphere

- *Fluctuating inflow.*
- *Reynold's number = 100*
- *System under consideration is extracted at a given time step.*
- ***Cond(A) ~ 1.5 e+3***
- ***Cond [A, B; C^T, G] ~ 0.8 e+5***

Flow past a hemisphere



Linear System



Flow past a hemisphere…

- Re = 100.
- Choose $E = A$ and remove outer layer.
- *Action of $\hat{A}^{-1}$ is realized via solving systems of the form $A\, x = b$ using Bicgstab with a diagonal approximate inverse of A as a preconditioner.*

Preconditioned Scheme

Solve $\begin{pmatrix} A & B \\ C^T & G \end{pmatrix} \begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{pmatrix}$

via a Krylov subspace method

Preconditioner

$$M = \begin{pmatrix} E & B \\ C^T & G \end{pmatrix}$$

Solve $Mz = r$ via Richardson scheme

$$\boldsymbol{z}_{k+1} = \boldsymbol{z}_k + \hat{M}^{-1}(\boldsymbol{r} - M\boldsymbol{z}_k)$$

where,

$$\hat{M} = \begin{pmatrix} \hat{A} & B \\ C^T & G \end{pmatrix}$$

Flow past a hemisphere…

- ***Action of $\hat{A}^{-1}$ is realized via solving systems of the form $A\,x = b$ using Bicgstab with a diagonal approximate inverse of A as a preconditioner.***
  - *# of bicgstab iterations < 20 for relative residuals of $O(10^{-9})$.*
- **Solve $S\,y = h$, where $S = (G - C^T \hat{A}^{-1} B)$, via bicgstab with a diag. approximate inverse of S to achieve a relative residual < 10^{-2}.**

Solve $\begin{bmatrix} A & B \\ C^T & G \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{bmatrix}$

via Richardson scheme with relative residual < 10^{-6}

- $\hat{M} = \begin{pmatrix} \hat{A} & B \\ C^T & G \end{pmatrix}$

$$\begin{bmatrix} \boldsymbol{u}_{k+1} \\ \boldsymbol{p}_{k+1} \end{bmatrix} = \begin{bmatrix} \boldsymbol{u}_k \\ \boldsymbol{p}_k \end{bmatrix} + \hat{M}^{-1} \left[\begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{pmatrix} - \begin{pmatrix} A & B \\ C^T & G \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_k \\ \boldsymbol{p}_k \end{pmatrix} \right]$$

Note:

Solve $(G - C^T \hat{A}^{-1} B)y = h$ via bicgstab with relative residual $< 10^{-2}$.
Preconditioner: diagonal approximate inverse

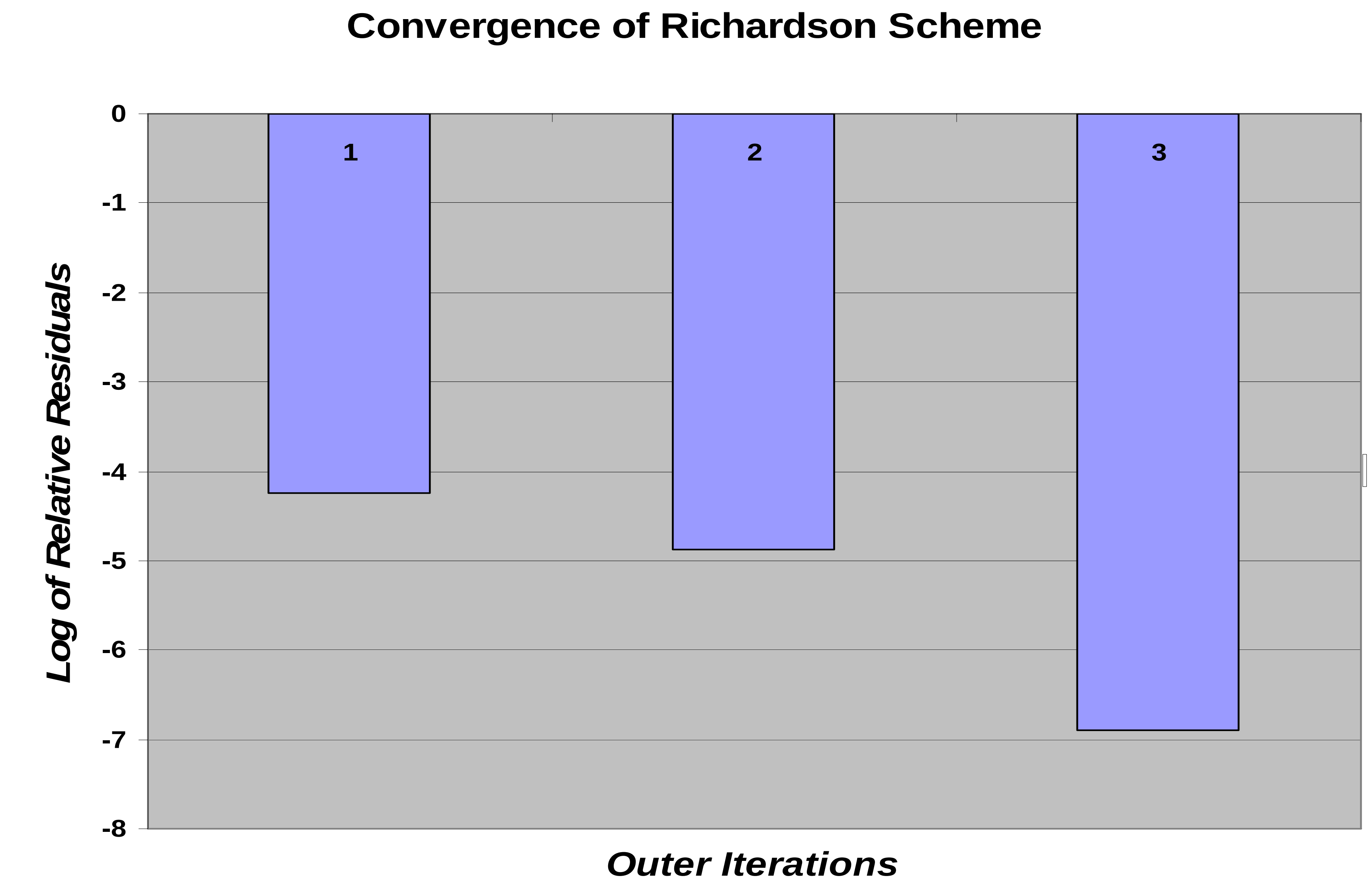
Convergence

Need to have $\rho(I - \hat{M}^{-1}M) < 1$

- $\lambda(I - \hat{M}^{-1}M) := 0, \mu$
- $\mu = \lambda[(I + K)(I - \hat{A}^{-1}E)]$
- $K = \hat{A}^{-1}B(G - C^T\hat{A}^{-1}B)^{-1}C^T$

$$\lambda(K) = \lambda[(C^T\hat{A}^{-1}B)(G - C^T\hat{A}^{-1}B)^{-1}]$$

- $\rho(I - \hat{A}^{-1}E) \leq \alpha < 1$

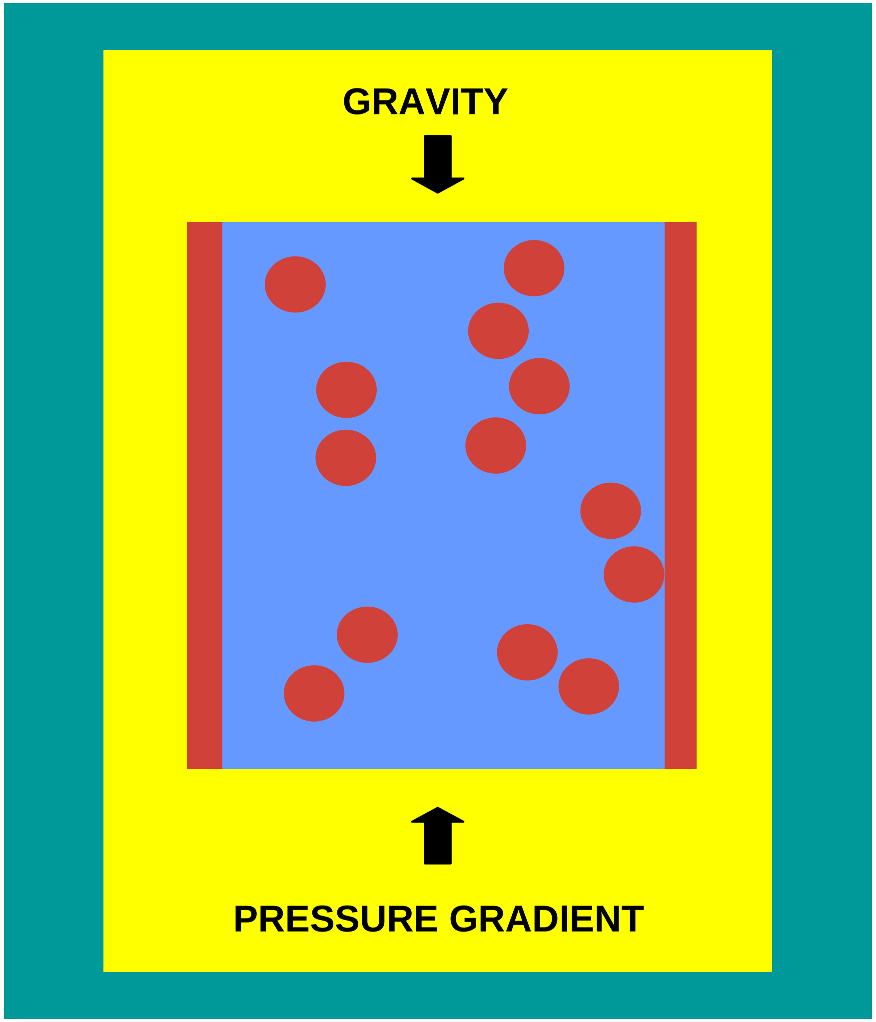


37 inner Bicgstab(10^{-2}) iterations for solving S y = h / outer iteration

Case 2

Particulate Flow

Motivating Application: Particulate Flows



Modeling Particulate Flows

- Navier-Stokes equations coupled with Newton's equations for particles

$$\rho \frac{\partial u}{\partial t} + \rho(u \bullet \nabla u) = \rho g - \nabla p + \nabla \bullet \tau$$

$$\nabla \bullet u = 0$$

$$M \frac{dU}{dt} = F$$

$$\frac{dX}{dt} = U$$

$$\tau = \mu(\nabla u + \nabla u^T)$$

- No-slip on particle surface.
- Unstructured mesh, generated after every few steps.
- Mixed finite elements approximation: *P*2/*P*1 pair of elements.

Case 2…

Particulate Flow:

- viscosity = 1/100
- G = zero matrix
- $E = A_s = (A + A^T)/2$
- $\hat{A}^{-1}$:= **diagonal approximate inverse of A_s,** i.e.

$$\min \left\| I - \hat{A}^{-1} A_s \right\|_F$$

- $\rho (I - \hat{A}^{-1} A_s) = \alpha < 1$

Preconditioned Scheme: Case 2

Solve $\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix}\begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{pmatrix}$

via Gmres $\left[\|\boldsymbol{r}_k\| / \|\boldsymbol{r}_0\| \leq 10^{-6} \right]$

Preconditioner

$$M = \begin{pmatrix} A_s & B \\ B^T & 0 \end{pmatrix}$$

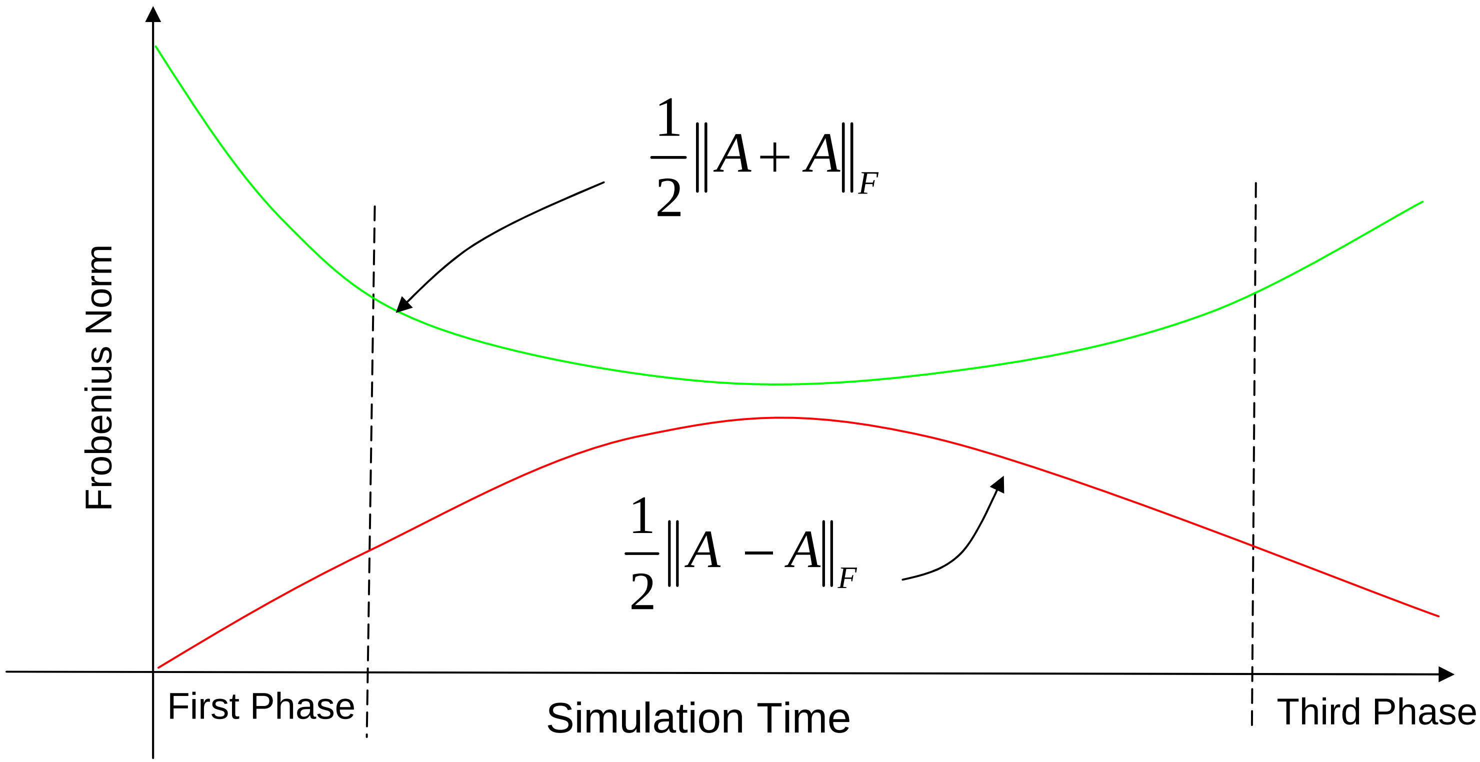
Solve $Mz = r$ via Richardson scheme $\left[\|\boldsymbol{r}_k\| / \|\boldsymbol{r}_0\| \leq 10^{-6} \right]$

$$\boldsymbol{z}_{k+1} = \boldsymbol{z}_k + \hat{M}^{-1}(\boldsymbol{r} - M\boldsymbol{z}_k)$$

where,

$$\hat{M} = \begin{pmatrix} \hat{A} & B \\ B^T & 0 \end{pmatrix}$$

Frobenius Norm of the Skew-Symmetric Part of A



- To quantify the skew-symmetry, we introduce the “degree of skewness” measured by $\dfrac{\|A-A^T\|_F}{\|A+A^T\|_F} = \|A_{ss}\|_F / \|A_s\|_F$.

Solving $\hat{M}\boldsymbol{u} = \boldsymbol{c}$; Case 2

Solve $\begin{pmatrix} \hat{A} & B \\ B^T & 0 \end{pmatrix}\begin{pmatrix} \boldsymbol{v} \\ \boldsymbol{w} \end{pmatrix} = \begin{pmatrix} \boldsymbol{a} \\ \boldsymbol{b} \end{pmatrix}$

Since

$$\begin{pmatrix} \hat{A} & B \\ B^T & 0 \end{pmatrix} = \begin{pmatrix} \hat{A} & 0 \\ B^T & I \end{pmatrix}\begin{pmatrix} \hat{A}^{-1} & 0 \\ 0 & -\hat{G} \end{pmatrix}\begin{pmatrix} \hat{A} & B \\ 0 & I \end{pmatrix}$$, with $\hat{G} = B^T \hat{A}^{-1} B,$

the solution scheme is given by,

- $\boldsymbol{v} = \hat{A}^{-1}\boldsymbol{a}$
- $\hat{G}\boldsymbol{w} = B^T\boldsymbol{v} - \boldsymbol{b}$ via CG with $\|\boldsymbol{r}_k\|_2 / \|\boldsymbol{r}_0\| \leq 10^{-2}.$
- $\boldsymbol{v} = \hat{A}^{-1}(\boldsymbol{a} - B\boldsymbol{w})$

Convergence….

- $\lambda(I - \hat{M}^{-1} M) := 0, \mu$
- $\mu = \lambda[(I - K)(I - \hat{A}^{-1} A_s)]$
- $\lambda(K) = \lambda[\hat{A}^{-1/2} B(B^T \hat{A}^{-1} B)^{-1} B^T \hat{A}^{-1/2}]$; [a projector]
- Thus $\rho(I - \hat{M}^{-1} M) < 1$

$$\hat{A}^{-1} := SPAI(A_s) \quad \text{[diagonal]}$$

$$\alpha = \rho(I - \hat{A}^{-1} A_s) < 1$$

t	# particles	system size	Gmres(k)		
			k	outer	inner
20 Δt	20	8,777	20	1	13
100 Δt	240	95,749	50	3	14
200 Δt	240	111,326	50	4	15

Robustness of solver $\left(\|r_k\|_2 / \|r_0\|_2 < 10^{-6} \right)$

- **Gmres with approx. LU factorizations of $\tilde{A}$ (as preconditioners) has failed.**

Case 3

Driven Cavity: steady-state case

Case 3…

- Square domain: $-1 \le x, y \le 1$

  B.C$^{S.}$: $\boldsymbol{u}_x = \boldsymbol{u}_y = 0$ on $x, y = -1\ ;\ x = 1$

  $\boldsymbol{u}_x = 1, \boldsymbol{u}_y = 0$ on $y = 1$
- Picard's iterations; **Q2/Q1 elements**: Linearized equations (**Oseen problem**)
- $G \equiv 0$
- $E = A_s = (A + A^T)/2$
- viscosity: 0.1, 0.02, 0.01,0.002

Preconditioned Scheme

Solve $\begin{pmatrix} A & B \\ B^T & 0 \end{pmatrix}\begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{pmatrix}$

via a Krylov subspace method

Preconditioner

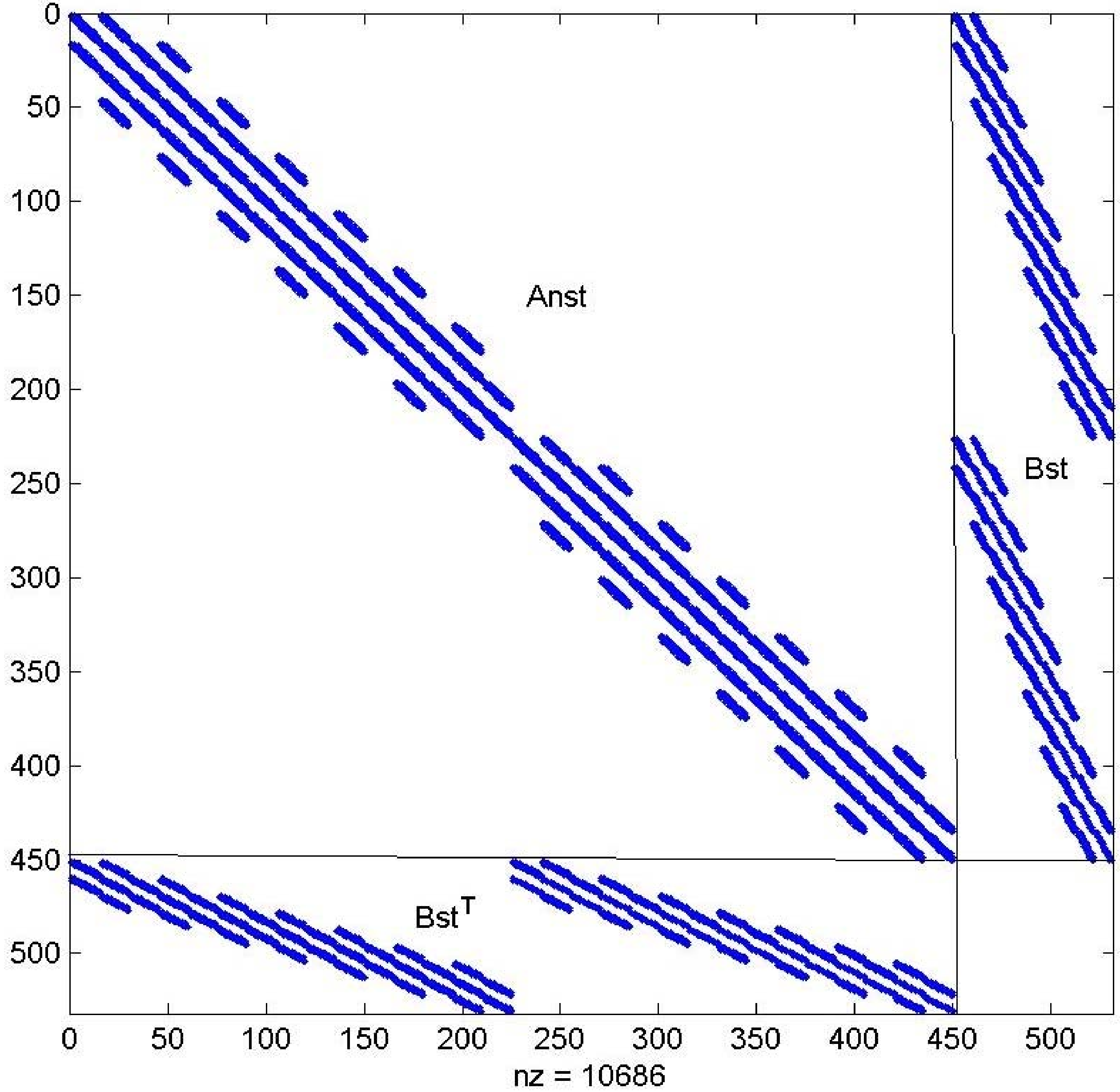
$$M = \begin{pmatrix} A_s & B \\ B^T & 0 \end{pmatrix} \; ; \; A_s = (A + A^T)/2$$

Solve $M\boldsymbol{z} = \boldsymbol{r}$ via Richardson scheme

$$\boldsymbol{z}_{k+1} = \boldsymbol{z}_k + \hat{M}^{-1}(\boldsymbol{r} - M\boldsymbol{z}_k)$$

where,

$$\hat{M} = \begin{pmatrix} \hat{A} & B \\ B^T & 0 \end{pmatrix}$$



Anst
Bst
Bst^T
nz = 10686

Case 3…

- $A_s = P + N;$ [Axelsson & Kolotolina]

  $P(i,i) = 0\ ;\ P(i,j) \geq 0$

  $N(i,i) > 0\ ;\ N(i,j) \leq 0$

- $D\,\boldsymbol{e} = P\,\boldsymbol{e}$

  $D :=$ diagonal ; $\boldsymbol{e}^T = (1,1,\ldots,1)$

- $\hat{A} = D + N$

  $\hat{A}$ is a Stieltjes matrix

  $\hat{A}(i,i) > 0\ ;\ \hat{A}(i,j) \leq 0;\ \hat{A}^{-1} > 0$

Case 3: Scheme I

Solving $\hat{M}\boldsymbol{u} = \boldsymbol{c}$; Case 3

Solve $\begin{pmatrix} \hat{A} & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{v} \\ \boldsymbol{w} \end{pmatrix} = \begin{pmatrix} \boldsymbol{a} \\ \boldsymbol{b} \end{pmatrix}$

Since

$$\begin{pmatrix} \hat{A} & B \\ B^T & 0 \end{pmatrix} = \begin{pmatrix} \hat{A} & 0 \\ B^T & I \end{pmatrix} \begin{pmatrix} \hat{A}^{-1} & 0 \\ 0 & -\hat{G} \end{pmatrix} \begin{pmatrix} \hat{A} & B \\ 0 & I \end{pmatrix}, \text{ with } \hat{G} = B^T \hat{A}^{-1} B$$

we solve the following systems using pcg with $\|\boldsymbol{r}_k\|_2 / \|\boldsymbol{r}_0\| \leq 10^{-1}$.

- $\hat{A}\boldsymbol{v} = \boldsymbol{a}$
- $\hat{G}w = B^T \boldsymbol{v} - \boldsymbol{b}$
- $\hat{A}\boldsymbol{v} = \boldsymbol{a} - B\boldsymbol{w}$

Each requires no more than 2 pcg iterations.

Convergence of Richardson Scheme

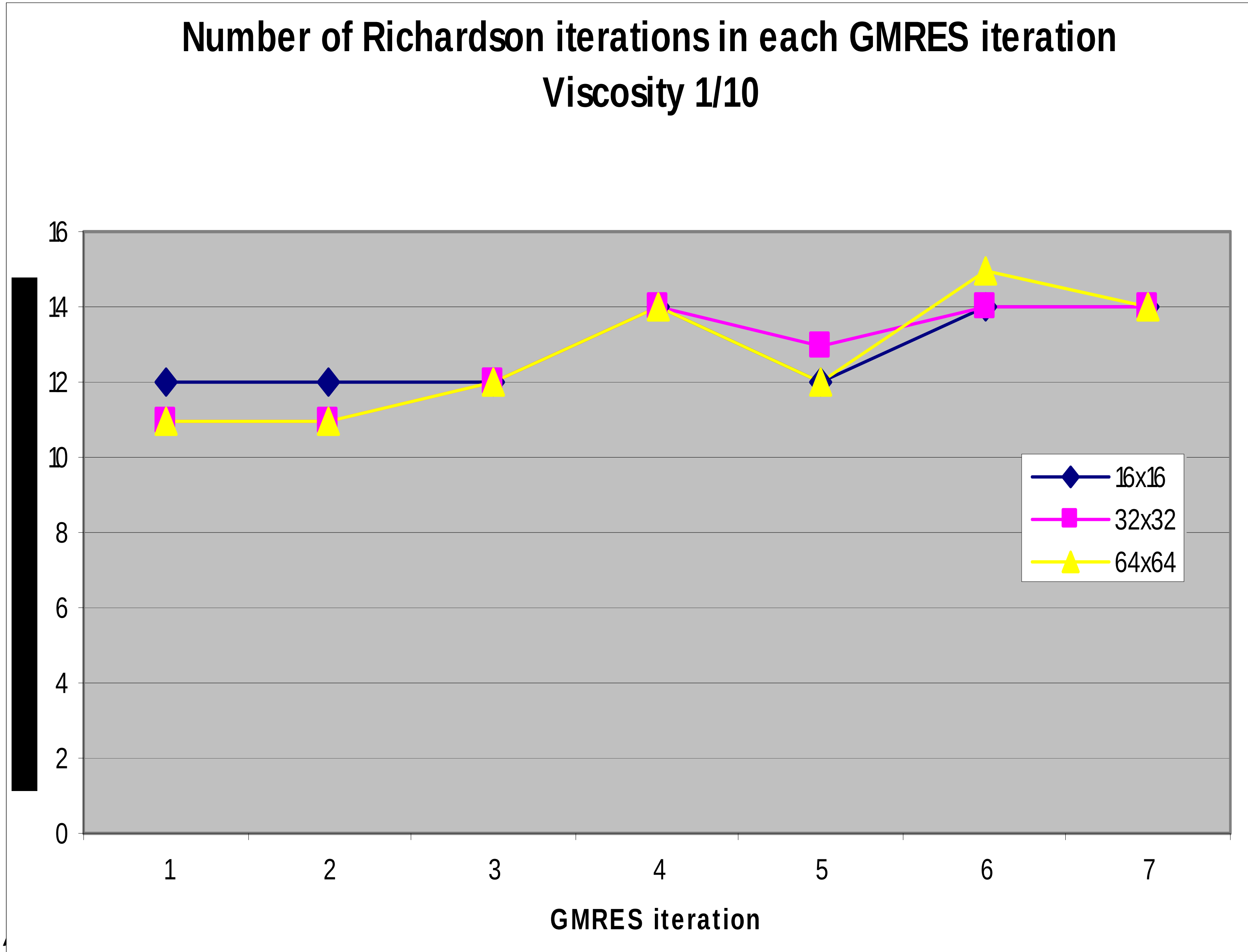
$$\rho(I - \hat{A}^{-1}A_s) = \sim 0.37$$

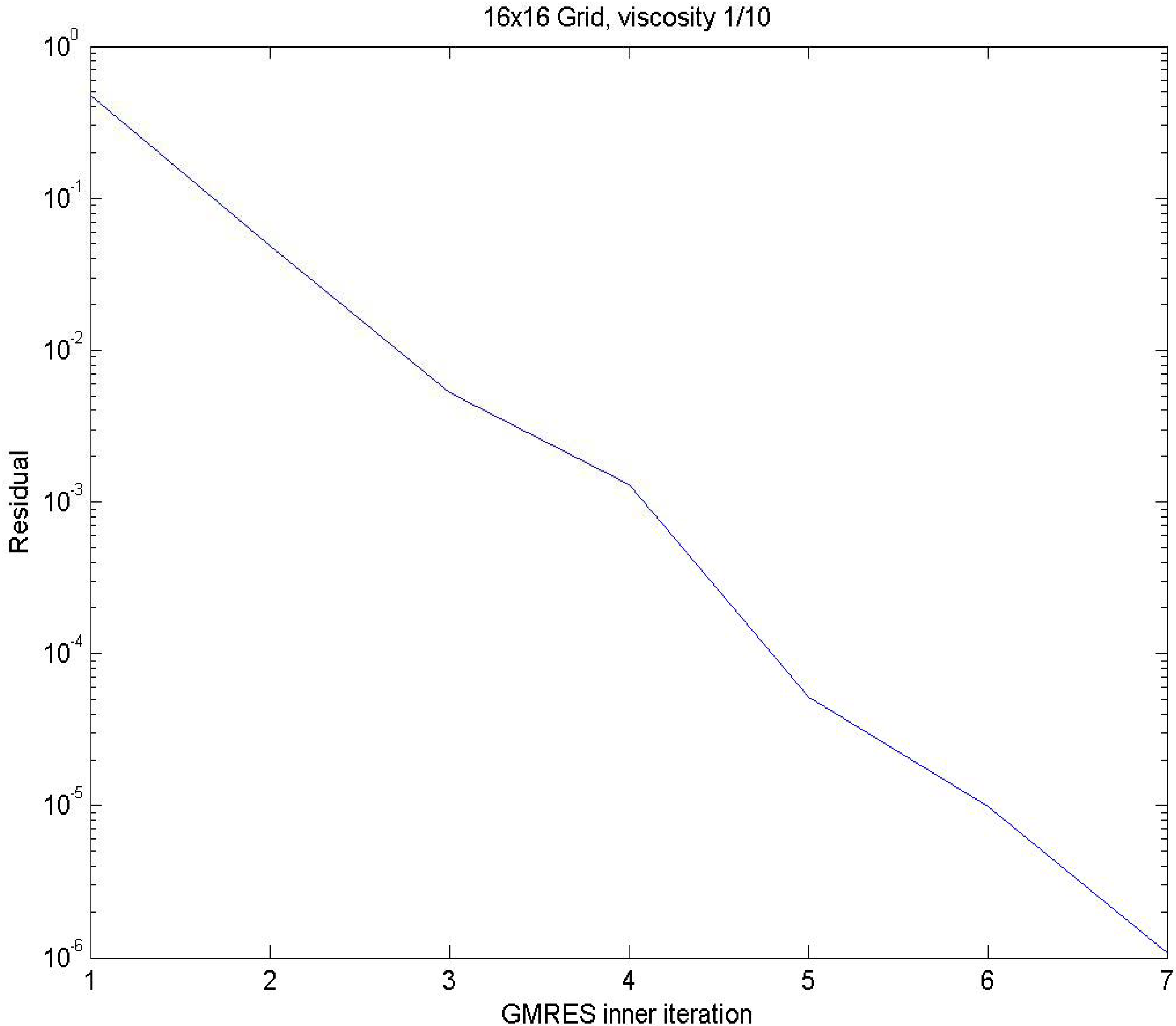
- for all mesh sizes: $2^k \times 2^k$

  k = 4, 5, 6, 7, 8,…

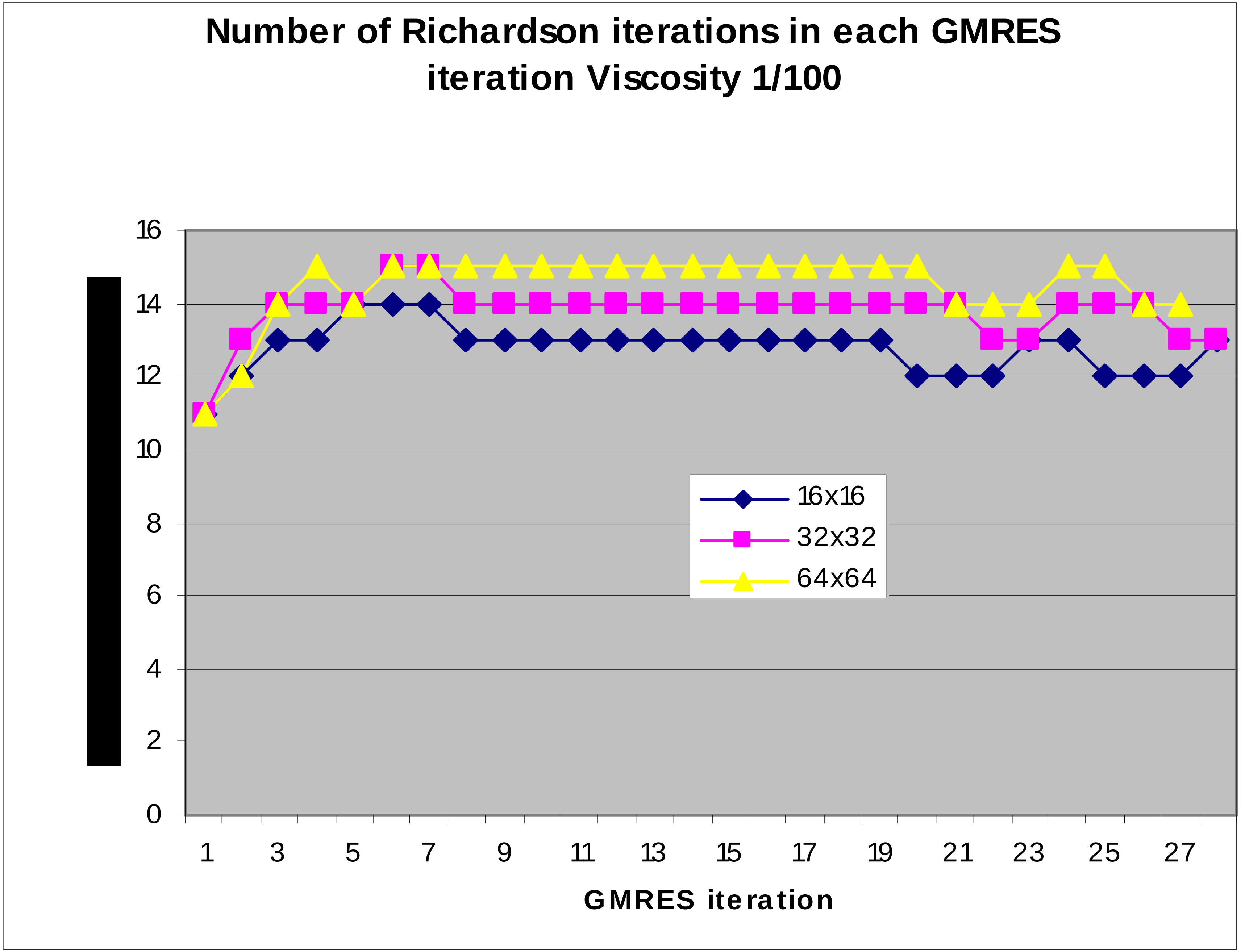
- for viscosity:

  0.1; 0.02; 0.01; 0.002

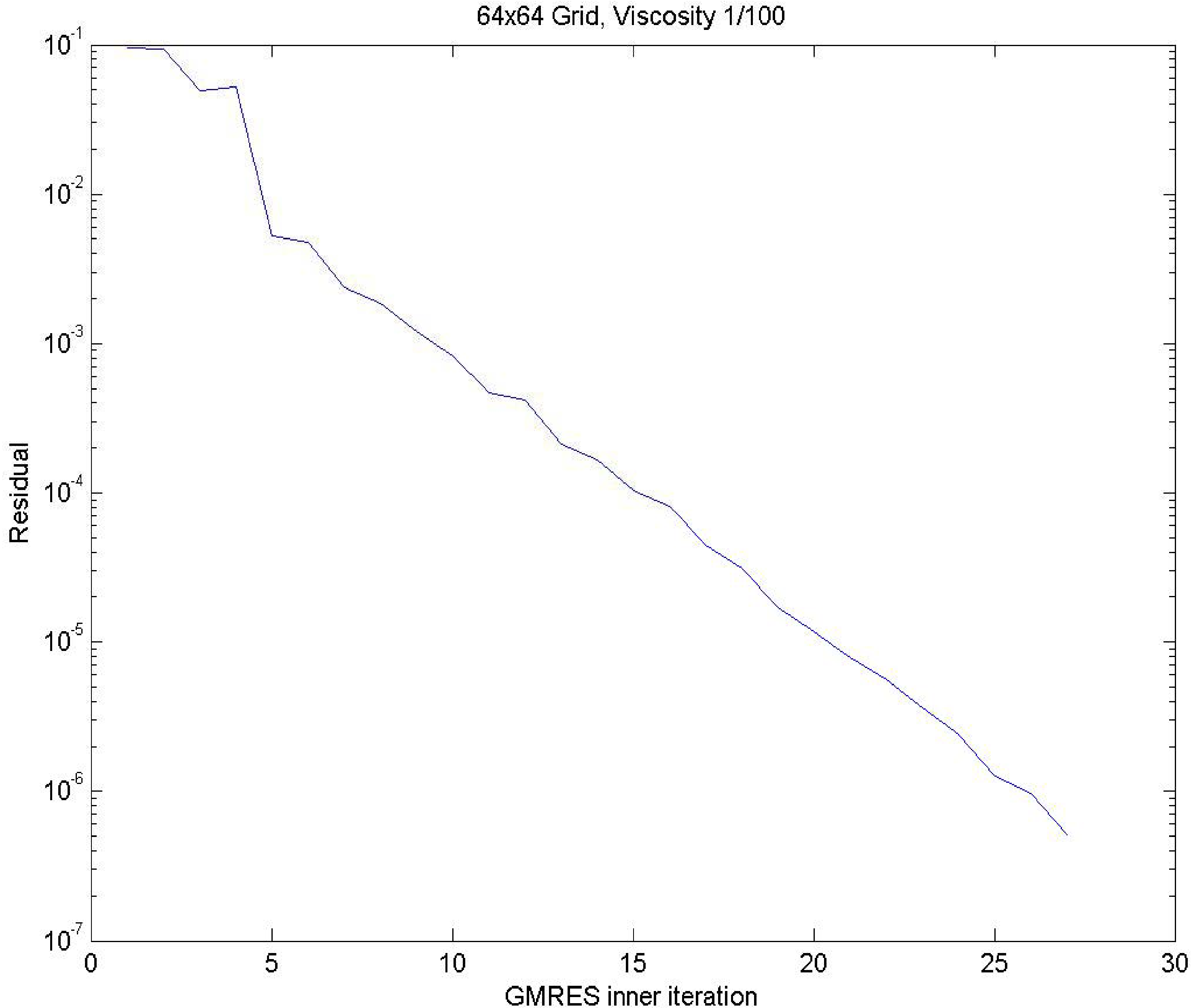

Number of Richardson iterations in each GMRES iteration
Viscosity 1/10
[redacted]
16
14
12
10
8
6
4
2
0
1
2
3
4
5
6
7
GMRES iteration
16x16
32x32
64x64



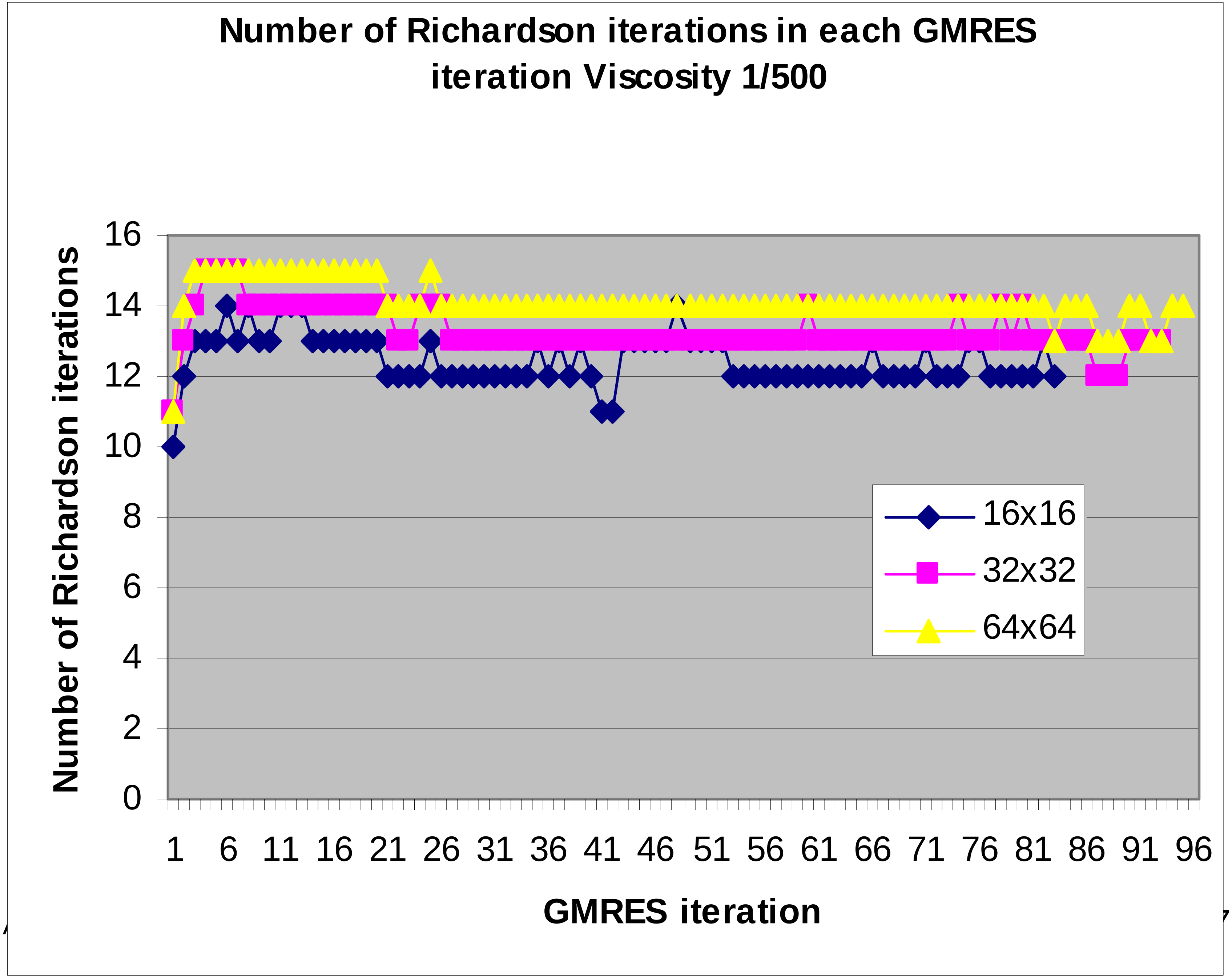
16x16 Grid, viscosity 1/10
Residual
GMRES inner iteration
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
1
2
3
4
5
6
7

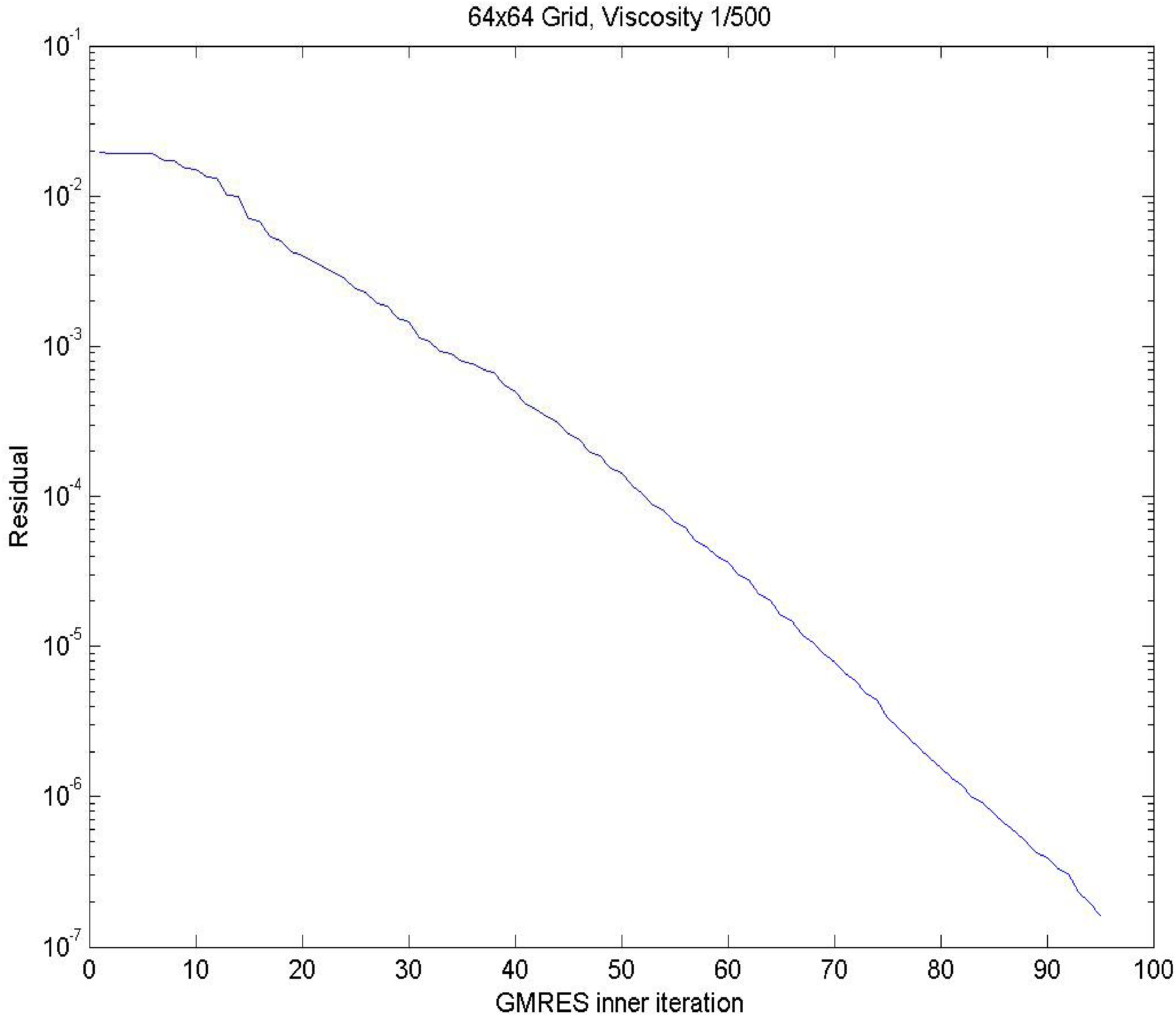


Number of Richardson iterations in each GMRES iteration Viscosity 1/100
16
14
12
10
8
6
4
2
0
1
3
5
7
9
11
13
15
17
19
21
23
25
27
GMRES iteration
16x16
32x32
64x64



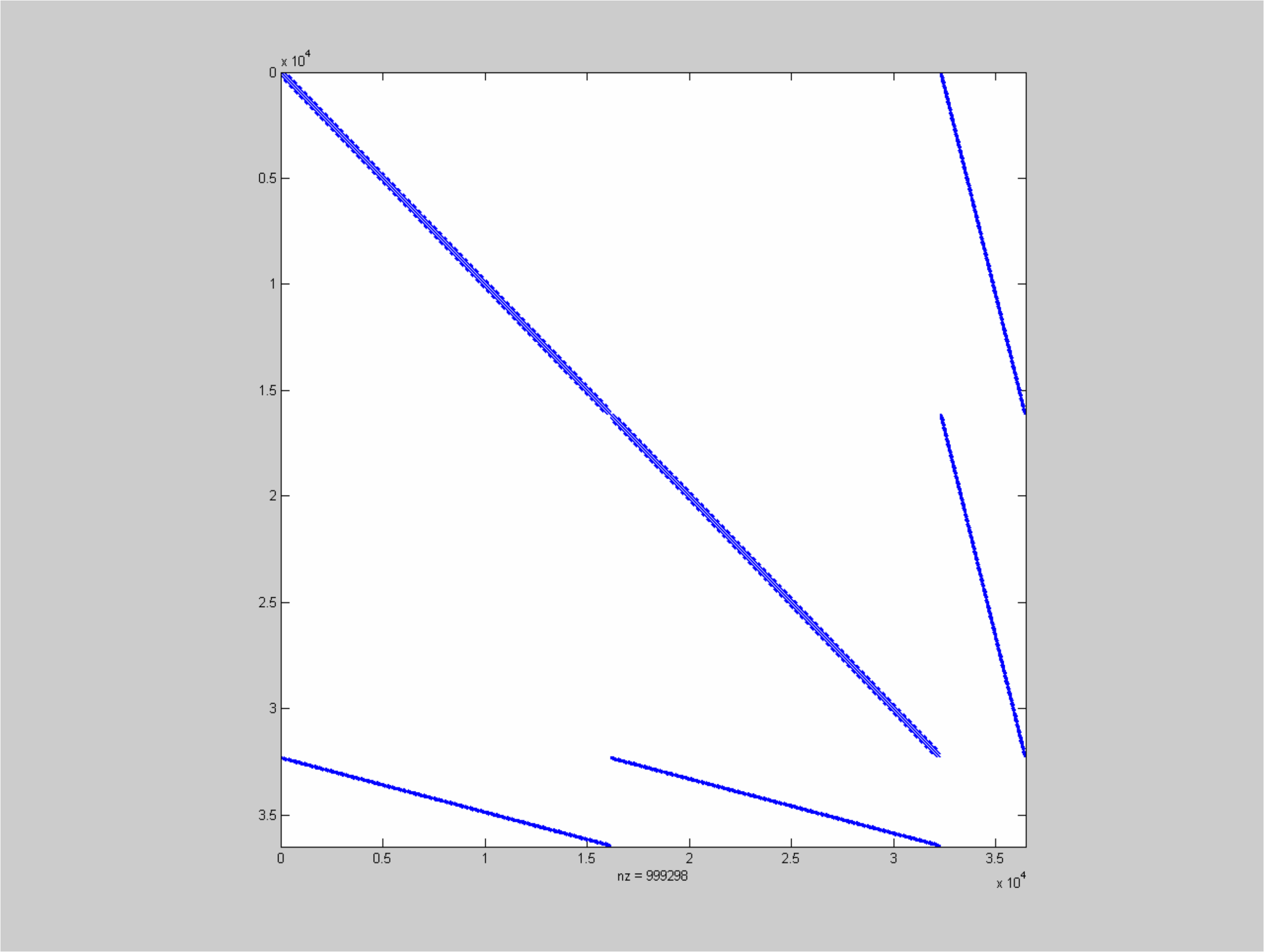
64x64 Grid, Viscosity 1/100
Residual
GMRES inner iteration
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
0
5
10
15
20
25
30


Number of Richardson iterations in each GMRES iteration Viscosity 1/500
Number of Richardson iterations
GMRES iteration
16
14
12
10
8
6
4
2
0
1
6
11
16
21
26
31
36
41
46
51
56
61
66
71
76
81
86
91
96
16x16
32x32
64x64

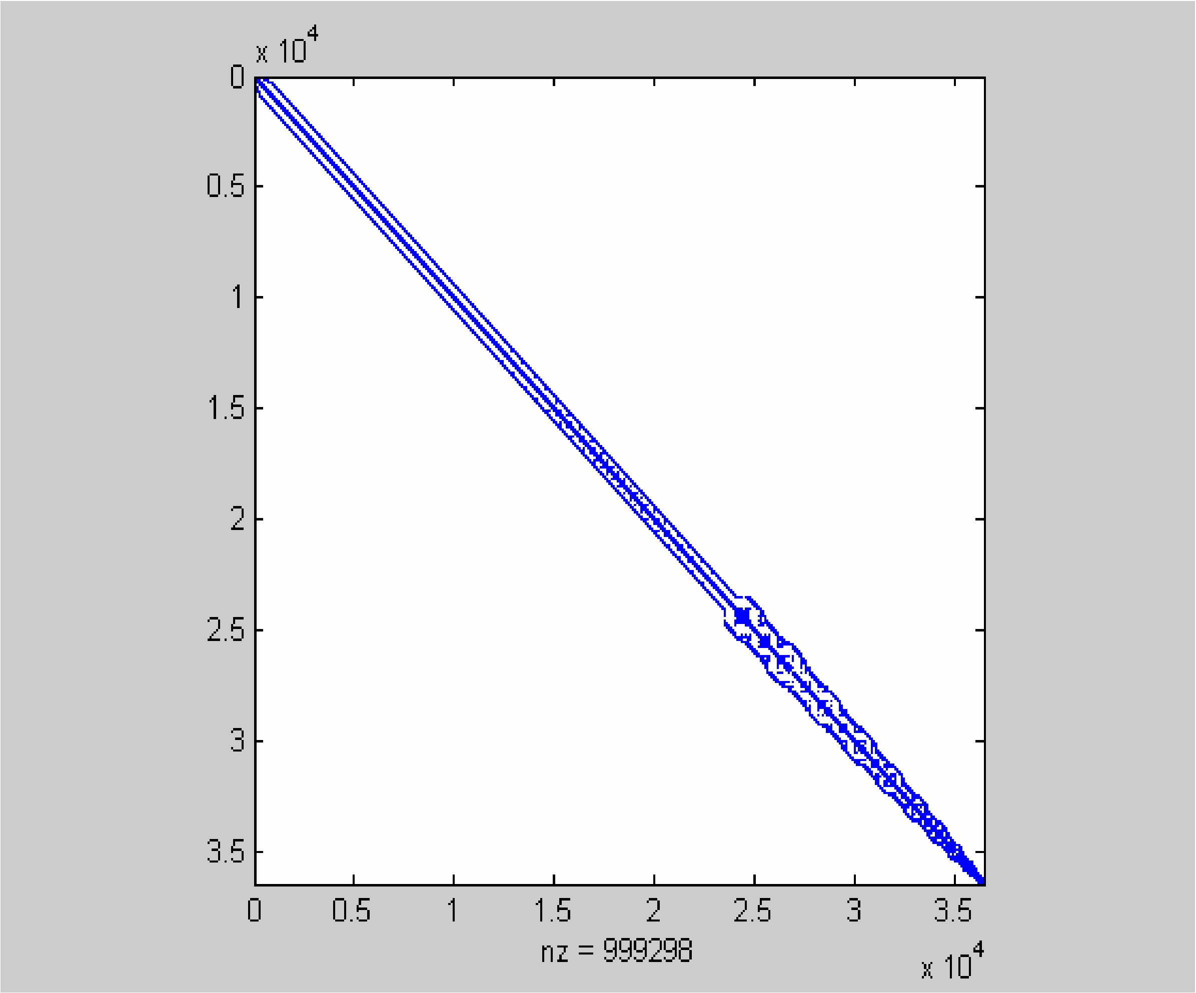

64x64 Grid, Viscosity 1/500
Residual
GMRES inner iteration
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
0
10
20
30
40
50
60
70
80
90
100

Case 3: Scheme II

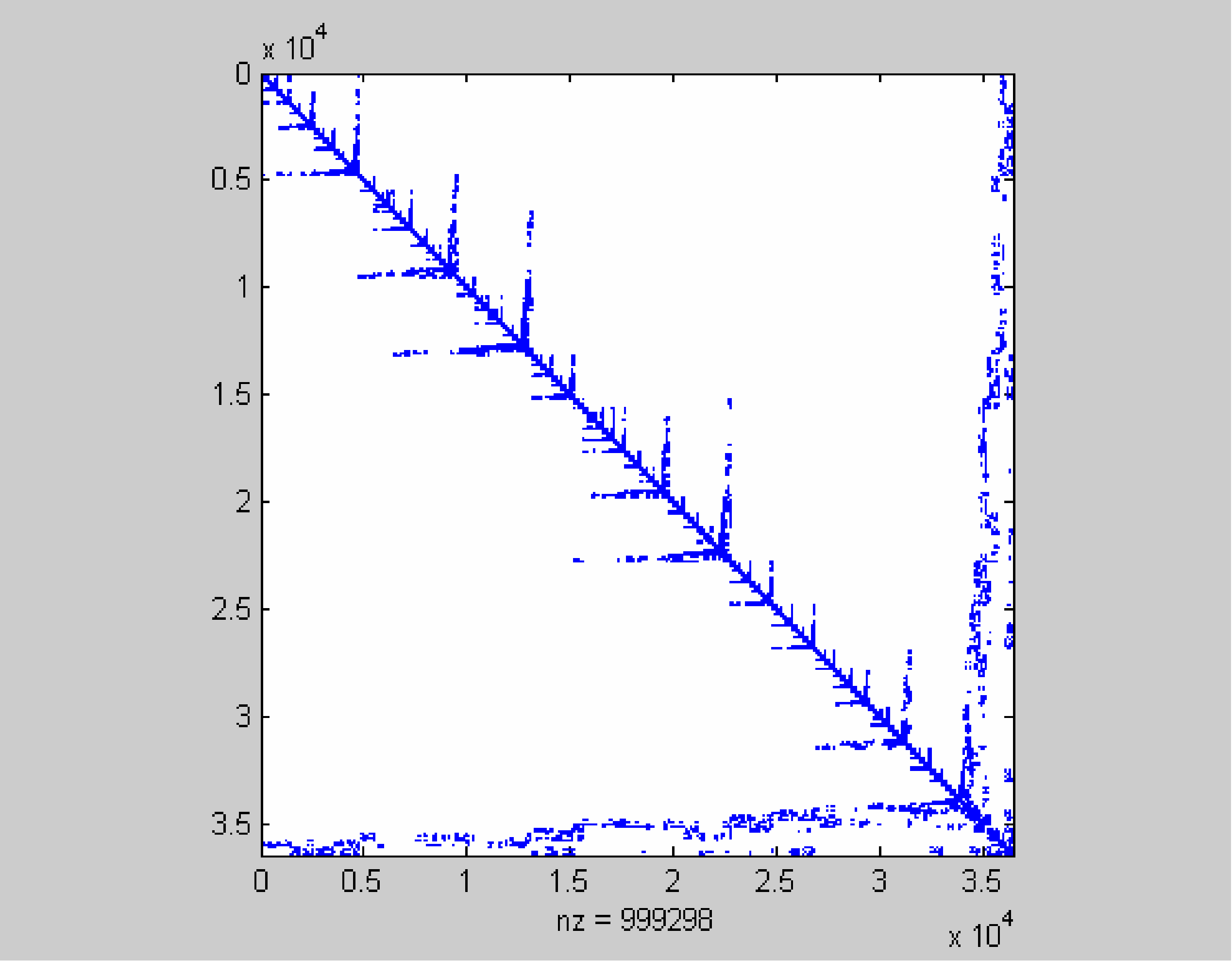
Linear system for 128 x 128 grid



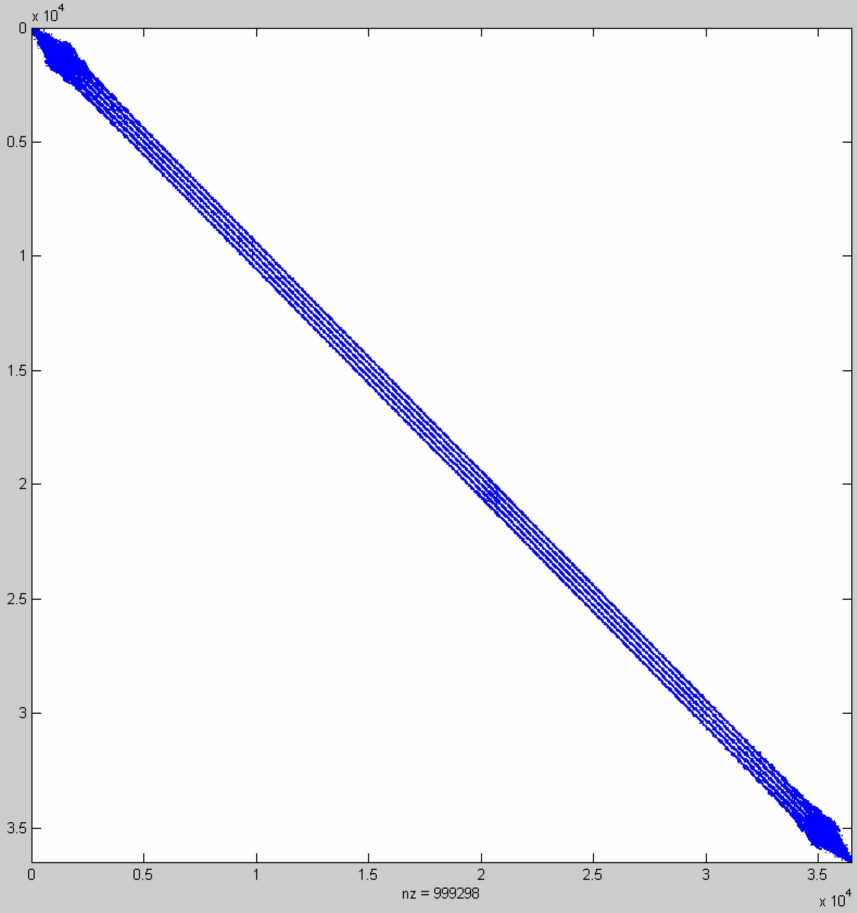
after RCM reordering



after approx. min. degree reordering



after spectral reordering



Spectral Reordering

- *Obtain second smallest eigenpairs of the Laplacian.*
- *Sort the elements of the eigenvector (Fielder vector).*
- *Permute the rows and columns of the matrix using the sorted order.*
- *W : [sum of magnitudes of the elements within the selected band] / [sum of the magnitudes of all the matrix elements]*
  - ***W = 99.9 %, for bandwidth = 1401, and viscosity=1/50.***

MA48 as a preconditioner for GMRES on a uniprocessor

Droptol	# of iter.	T(factor.)	T(GMRES iters.)	nnz(L+U)	final residual	v
0	2	142.7	0.3	7,195,157	2.07E-13	1/50
1.00E-04	24	115.5	1.4	2,177,181	2.83E-09	1/50
1.00E-03	248	109.6	17.3	1,611,030	5.11E-08	1/50

** for drop tolerance = .0001, total time ~ 117 sec.

** No convergence for a drop tolerance of 10^{-2}

Spike – Pardiso *for solving systems involving the banded preconditioner*

- ***On 4 nodes (8 CPU's) of a Xeon-Intel cluster:***
  - ***bandwidth of extracted preconditioner = 1401***
  - ***total time = 16 sec.***
  - ***# of Gmres iters. = 131***
  - ***2-norm of residual = 10^{-7}***
- ***Speed improvement over sequential procedure with drop tolerance = .0001:***
  - ***117/16 ~ 7.3***

Conclusion & Future Work

1. **Proposed nested scheme is:**
   - **versatile with appropriate choice of preconditioners at the three nesting levels,**
   - **suitable for implementation on parallel computing platforms.**

2. **Reordering the resulting "segregated" system yields often a prominent band that can be used as an effective parallel preconditioner.**
3. **Plan to build an environment for construction of these solvers with fewer input parameters from the application user.**

Thank you!