Notes – October 14, 2025

Topic: Discussion on Experimental Results of RBGS_GMRES, BGS_GMRES and built-in GMRES

1. Overview of Experiment Setup

Parameter	Description
Solver	RBGS-GMRES, BGS-GMRES, GMRES(built-in)
Runs	1
Matrices Tested	SiH4, Si10H16, e20r5000
Krylov basis	monomial basis, Newton basis (SiH4, e20r5000)
Sketch Sizes	s = 5, 8, 10, 20
Metric	Relative residual, $ \left\lVert A*x - b \right\rVert / \left\lVert b \right\rVert$

2. Experimental Results by Matrix

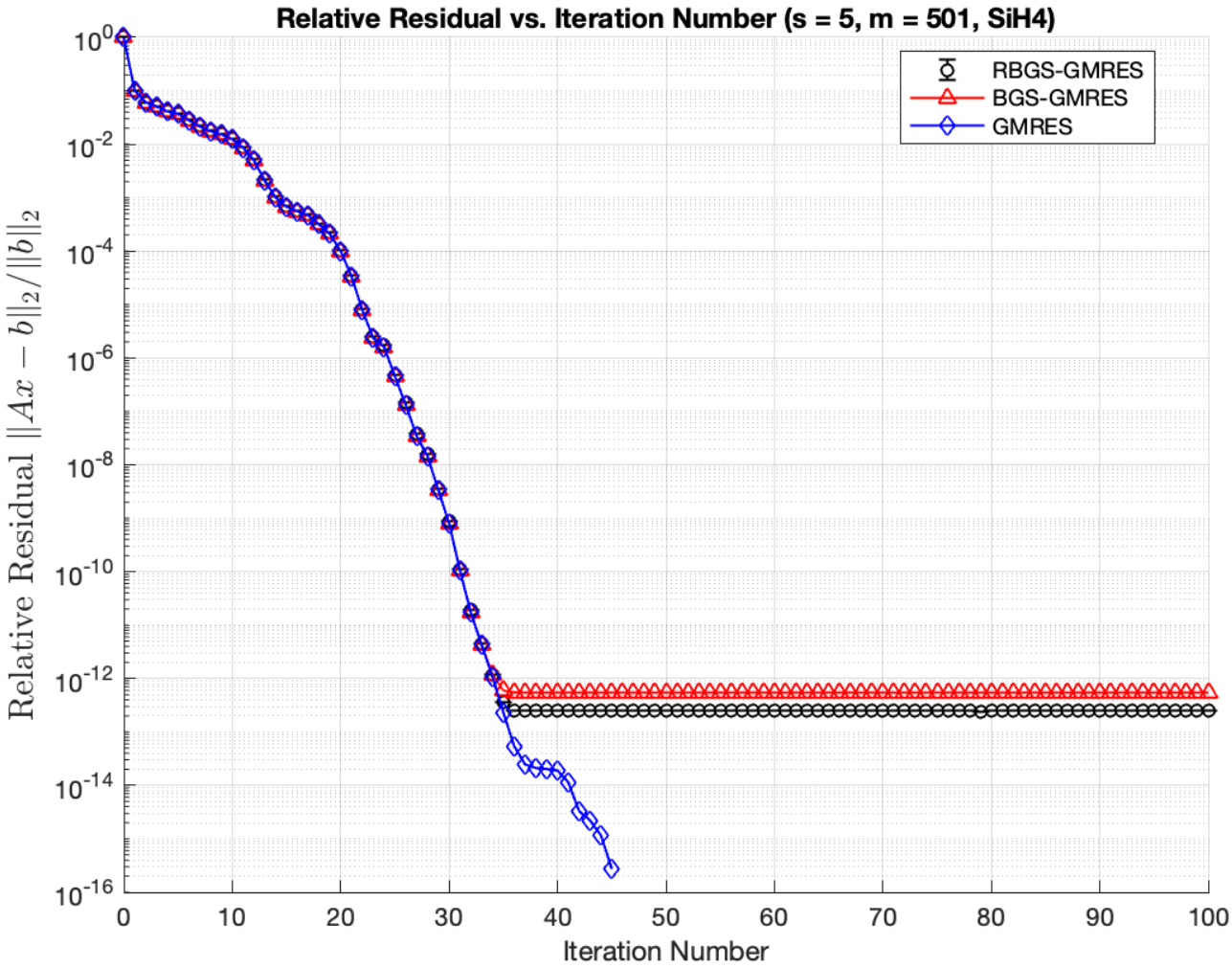
2.1 SiH4

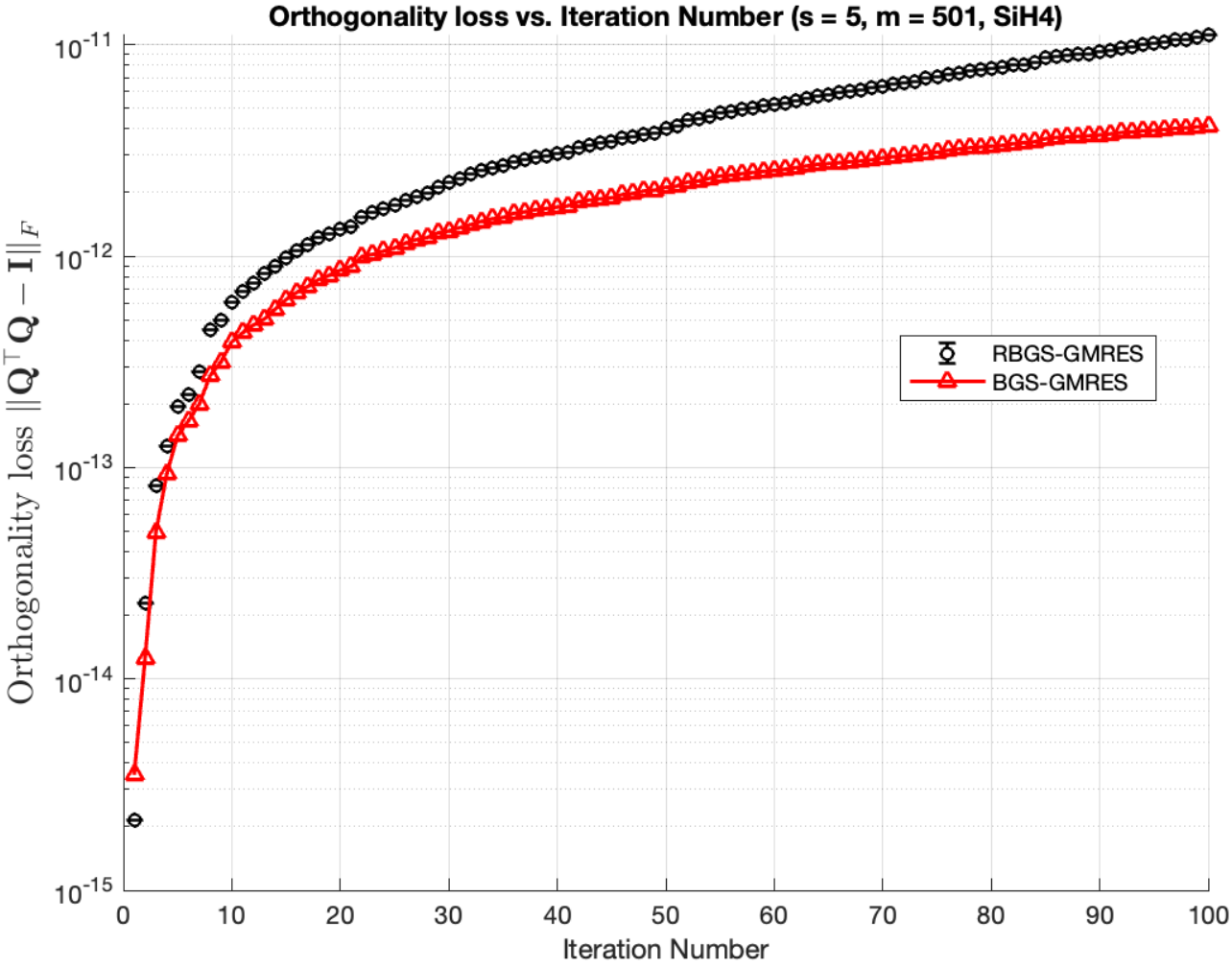
Matrix info: (n = 5041)
condition number: (1.065536e+03)
Sketch info: (m = 501, d = 2 * m)
Converge info: (ctol = 1e-16)
Krylov basis: (monomial basis and newton basis)

➤ Results for Step Sizes

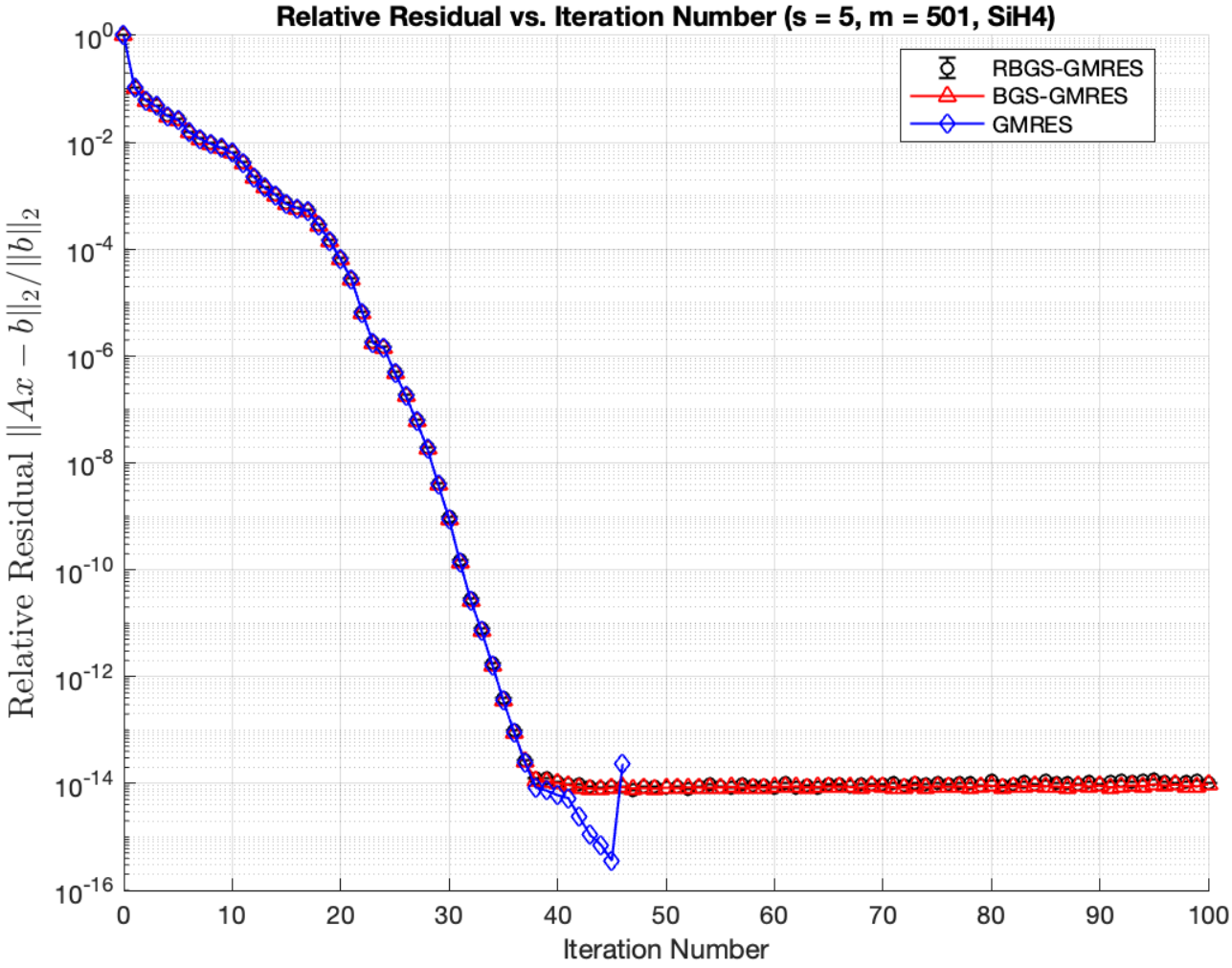
relative residual (after reorthogonalization)

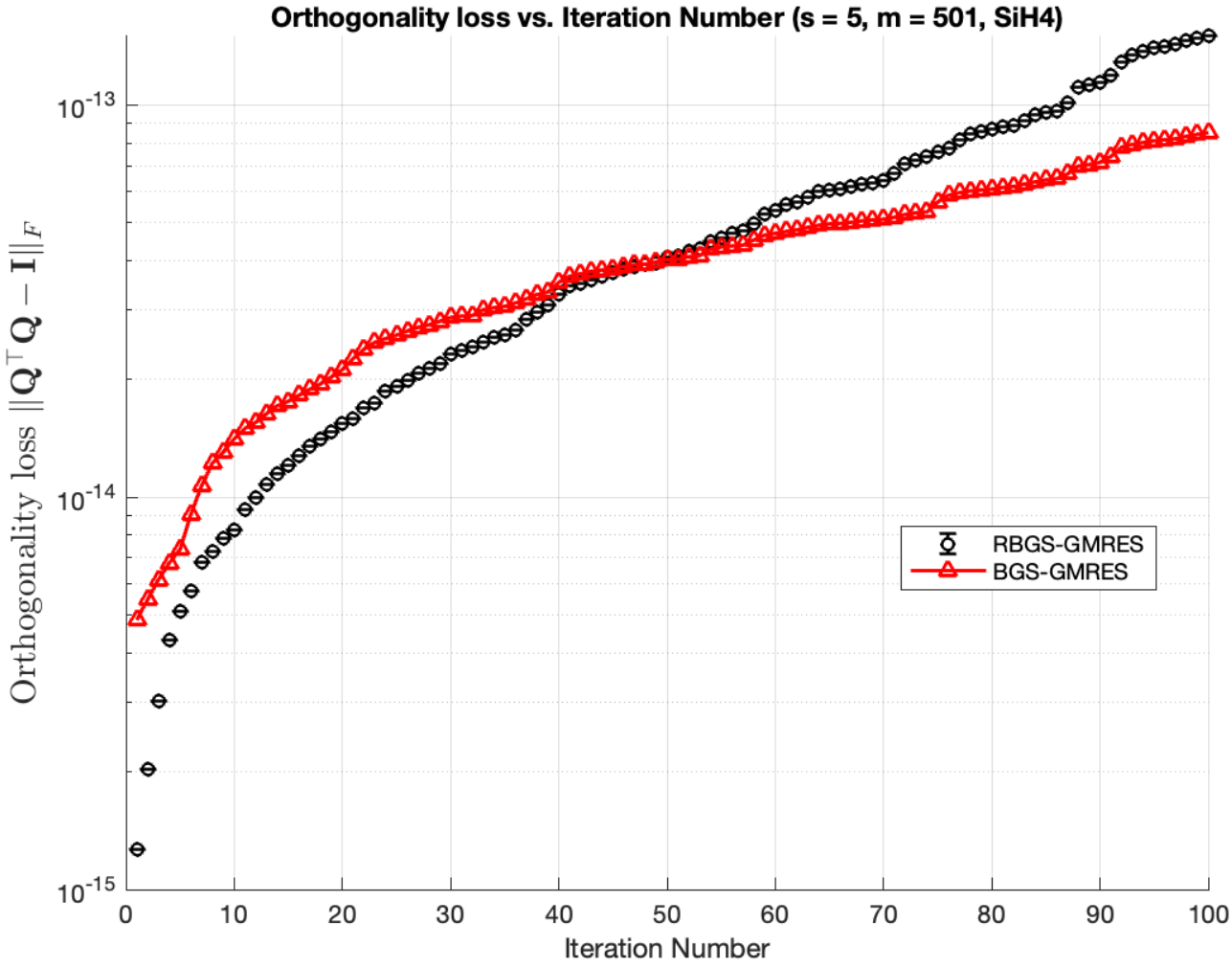
- s=5


Relative Residual vs. Iteration Number (s = 5, m = 501, SiH4)
RBGS-GMRES
BGS-GMRES
GMRES
Relative Residual $||Ax - b||_2/||b||_2$
Iteration Number
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
0
10
20
30
40
50
60
70
80
90
100

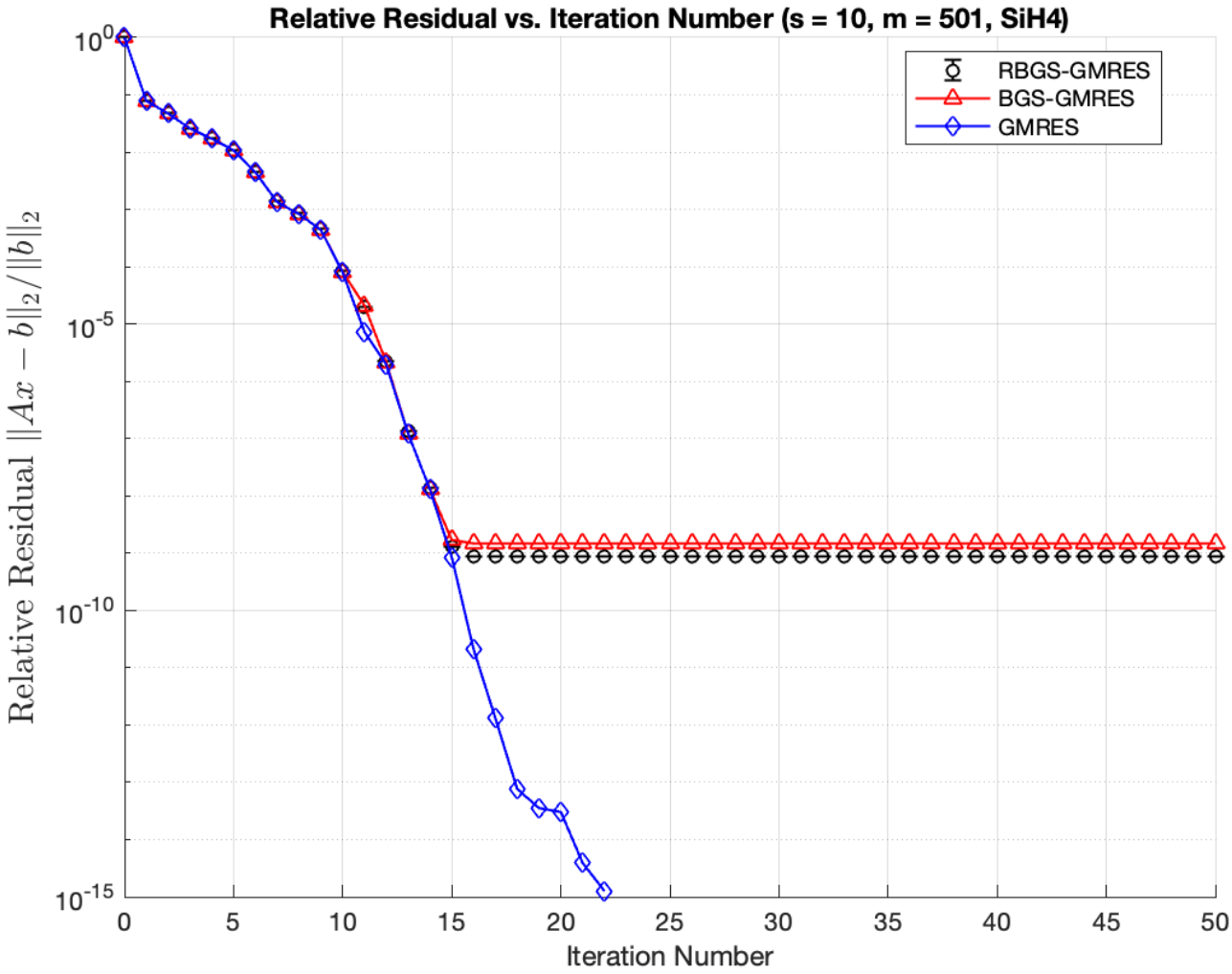


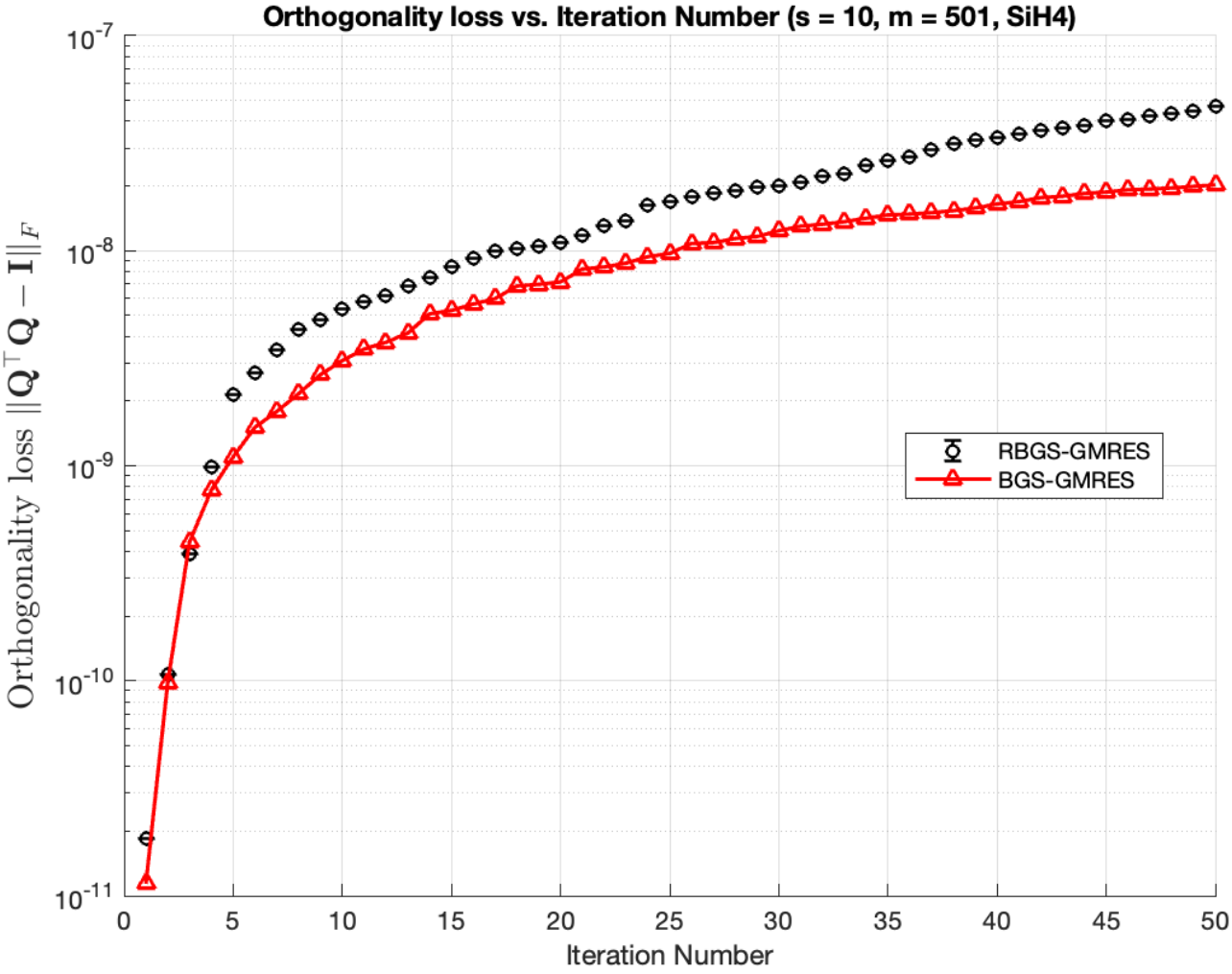
| Newton basis


Relative Residual vs. Iteration Number (s = 5, m = 501, SiH4)
RBGS-GMRES
BGS-GMRES
GMRES
Relative Residual $||Ax - b||_2/||b||_2$
Iteration Number

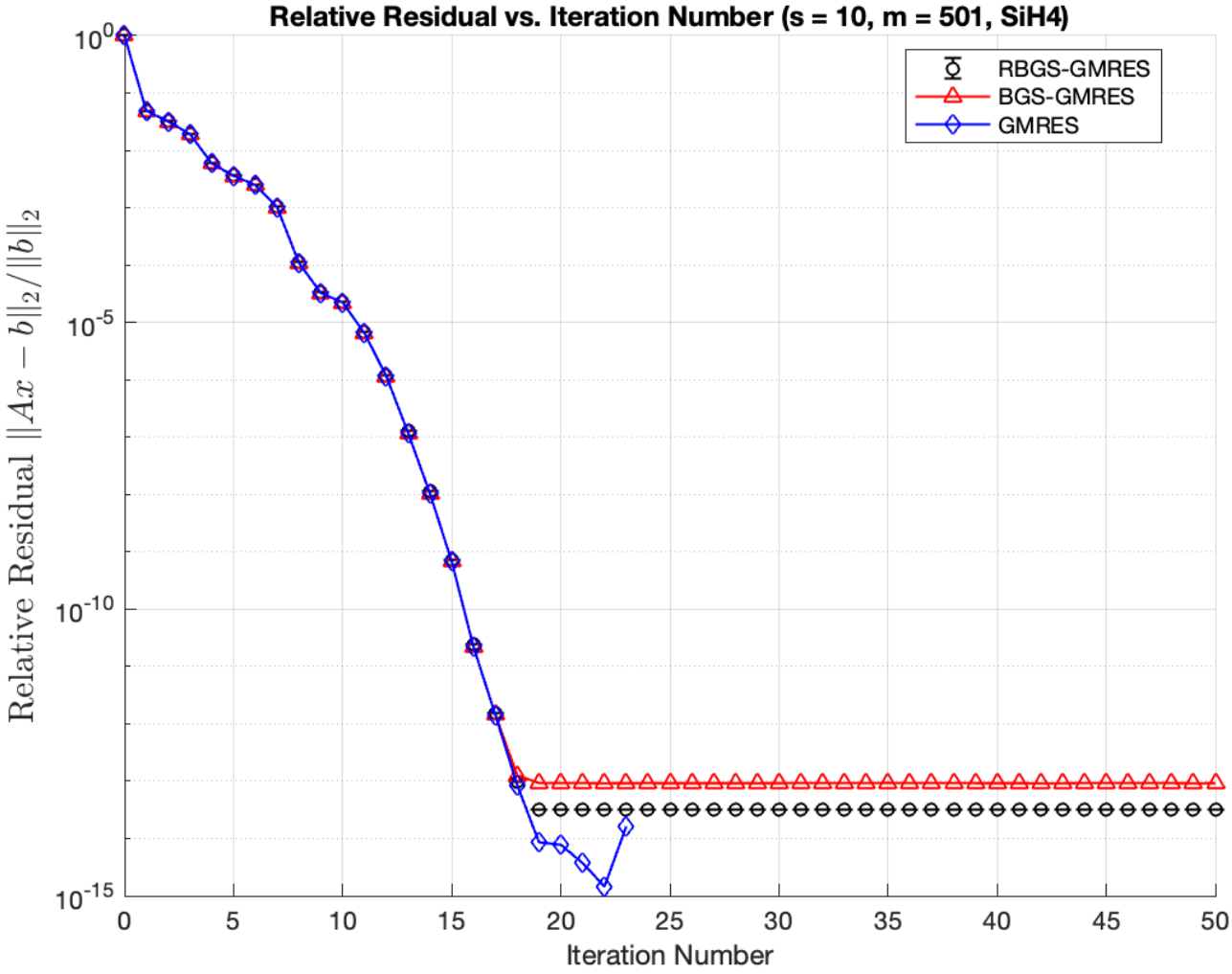

Orthogonality loss vs. Iteration Number (s = 5, m = 501, SiH4)
RBGS-GMRES
BGS-GMRES
Orthogonality loss $||\mathbf{Q}^\top \mathbf{Q} - \mathbf{I}||_F$
Iteration Number

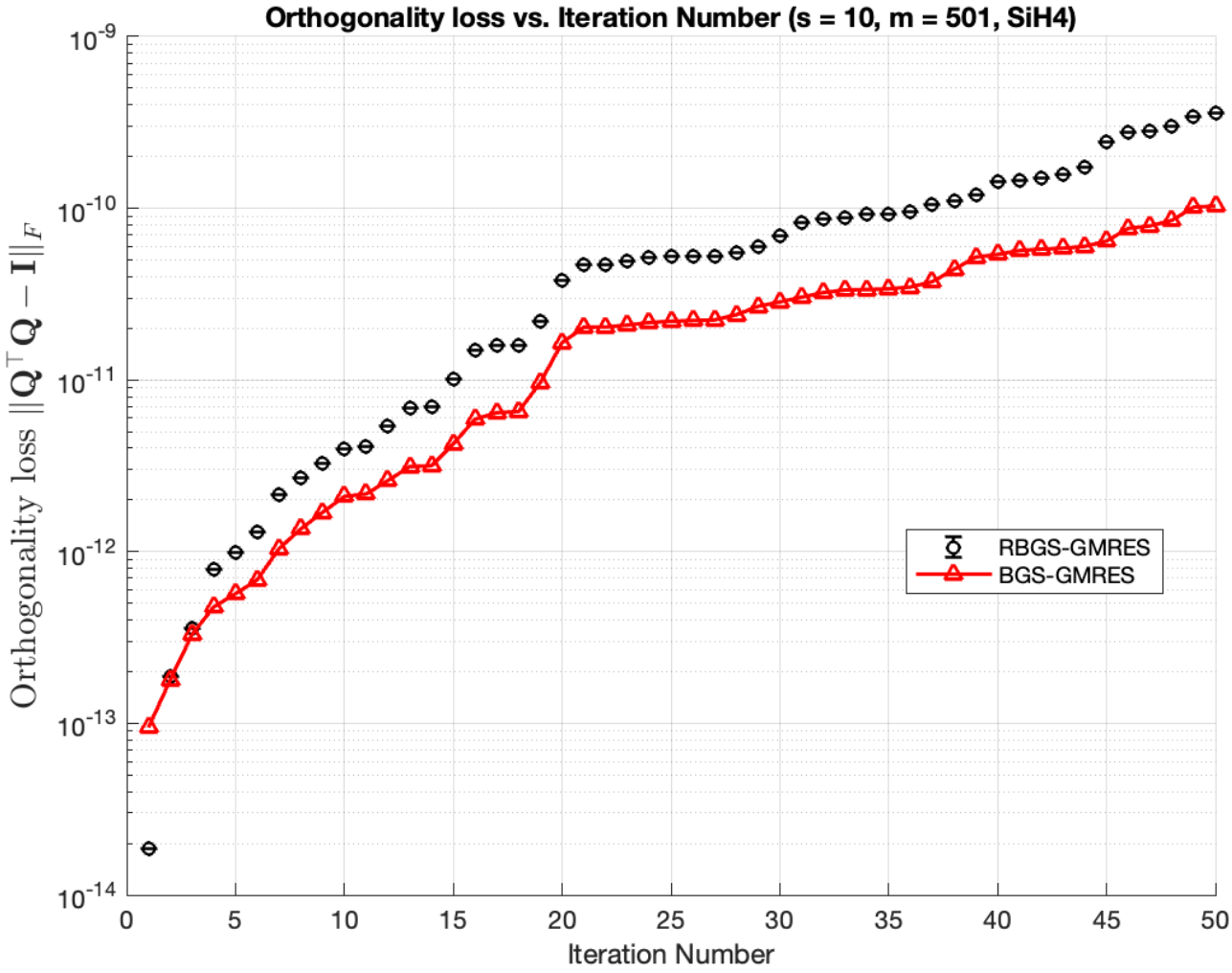
- s=10


Relative Residual vs. Iteration Number (s = 10, m = 501, SiH4)
RBGS-GMRES
BGS-GMRES
GMRES
Relative Residual $\|Ax-b\|_2/\|b\|_2$
Iteration Number
10^{0}
10^{-5}
10^{-10}
10^{-15}
0
5
10
15
20
25
30
35
40
45
50

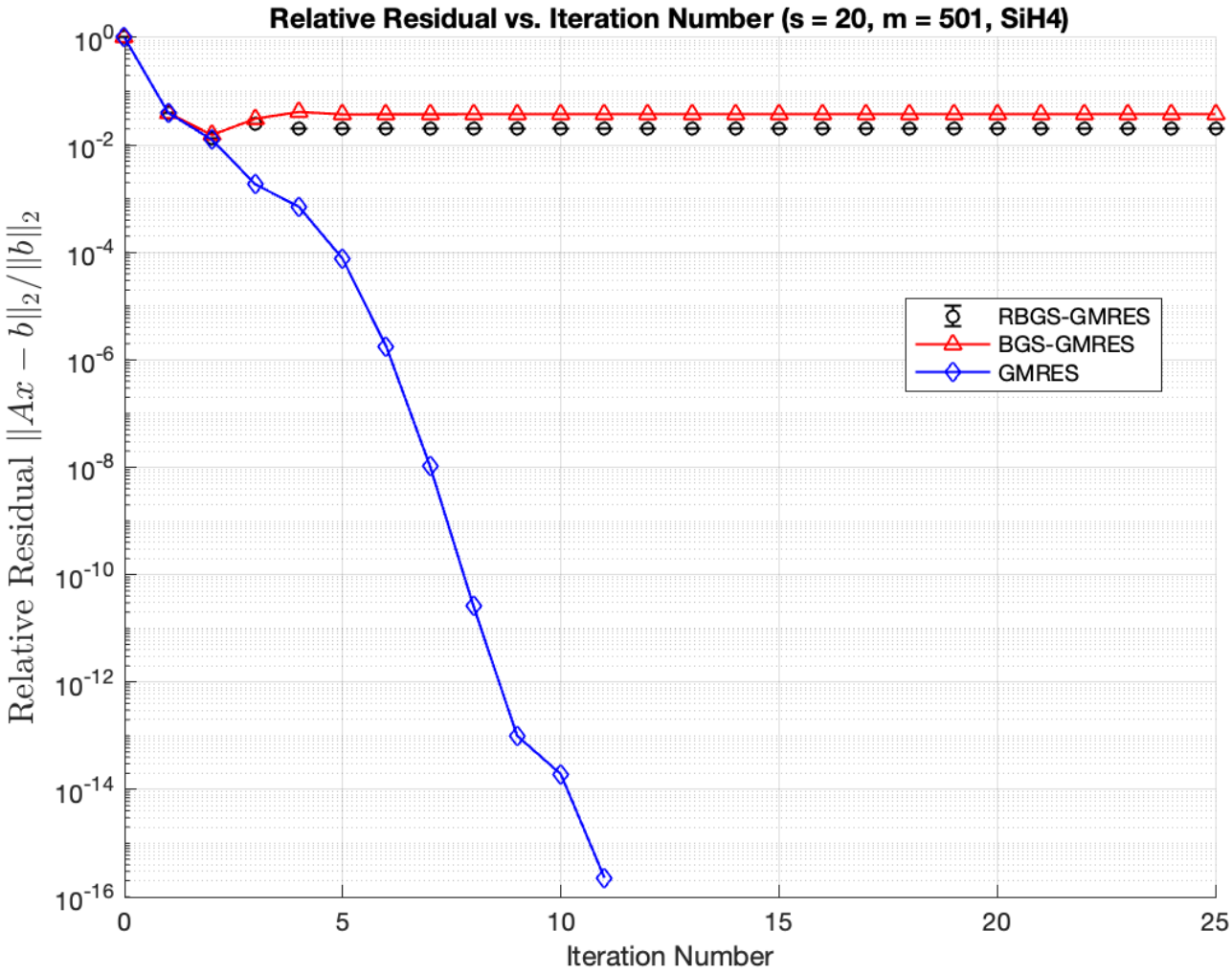


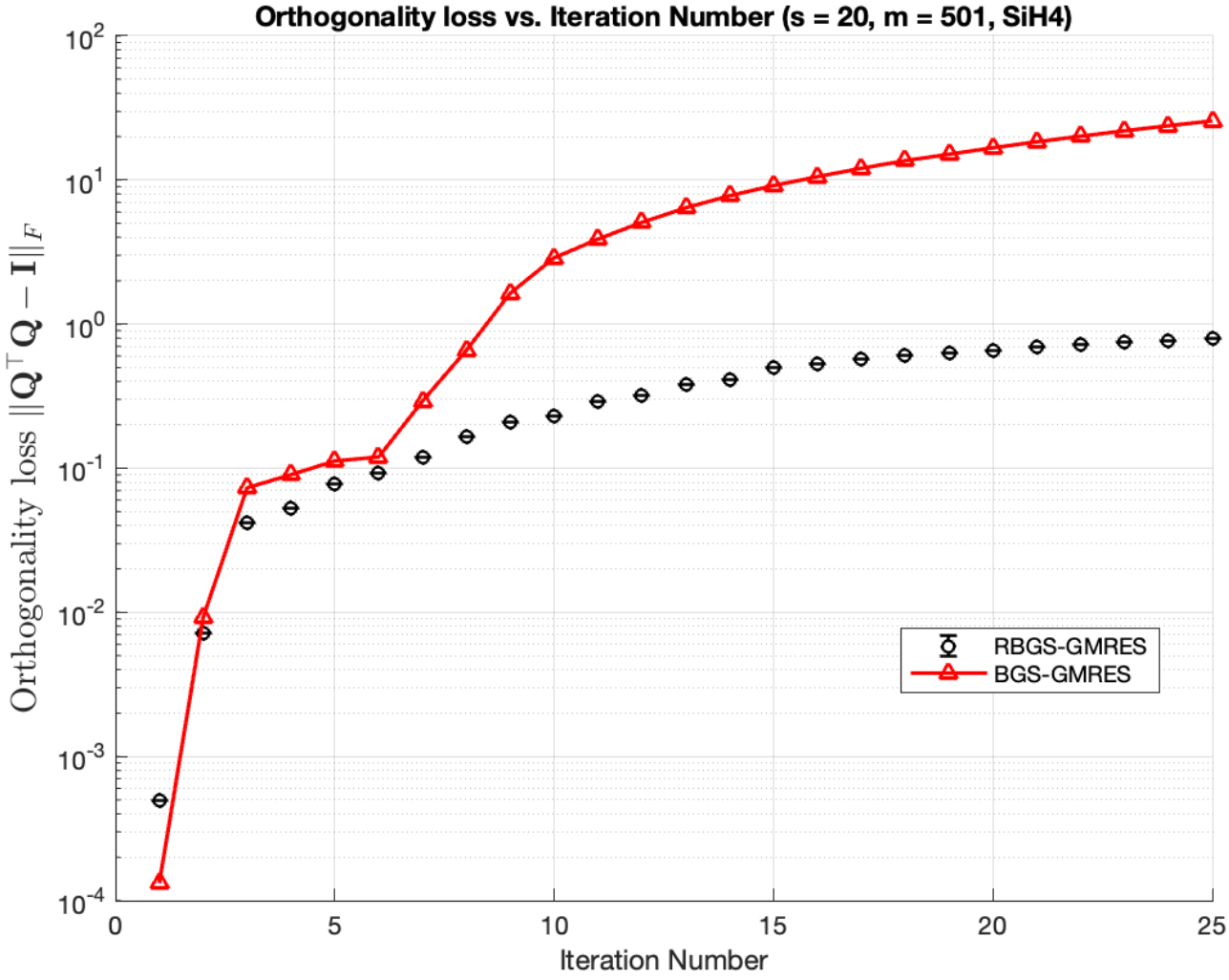
| Newton basis


Relative Residual vs. Iteration Number (s = 10, m = 501, SiH4)
RBGS-GMRES
BGS-GMRES
GMRES
Relative Residual $||Ax - b||_2/||b||_2$
Iteration Number

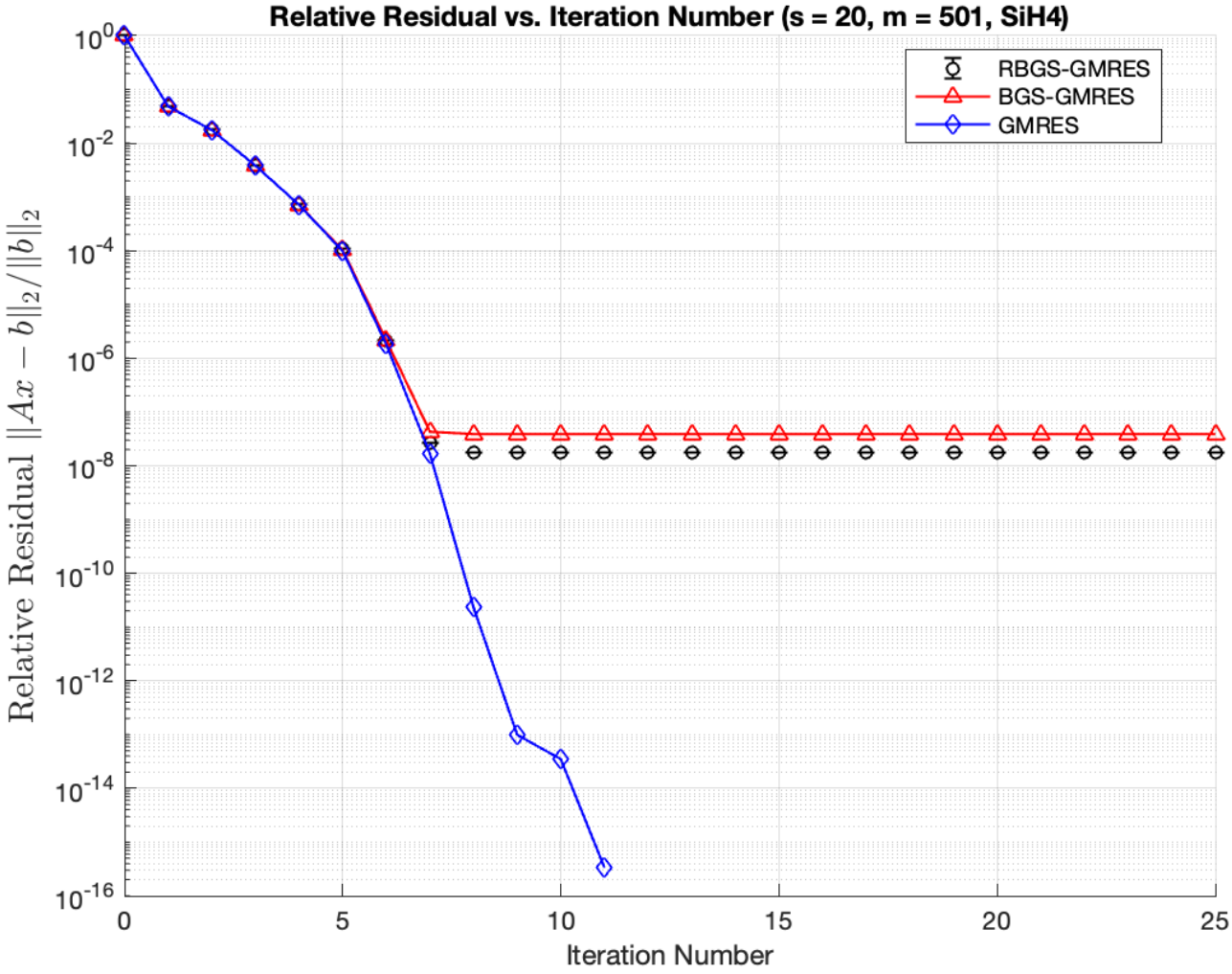

Orthogonality loss vs. Iteration Number (s = 10, m = 501, SiH4)
RBGS-GMRES
BGS-GMRES
Orthogonality loss $||\mathbf{Q}^\top\mathbf{Q} - \mathbf{I}||_F$
Iteration Number

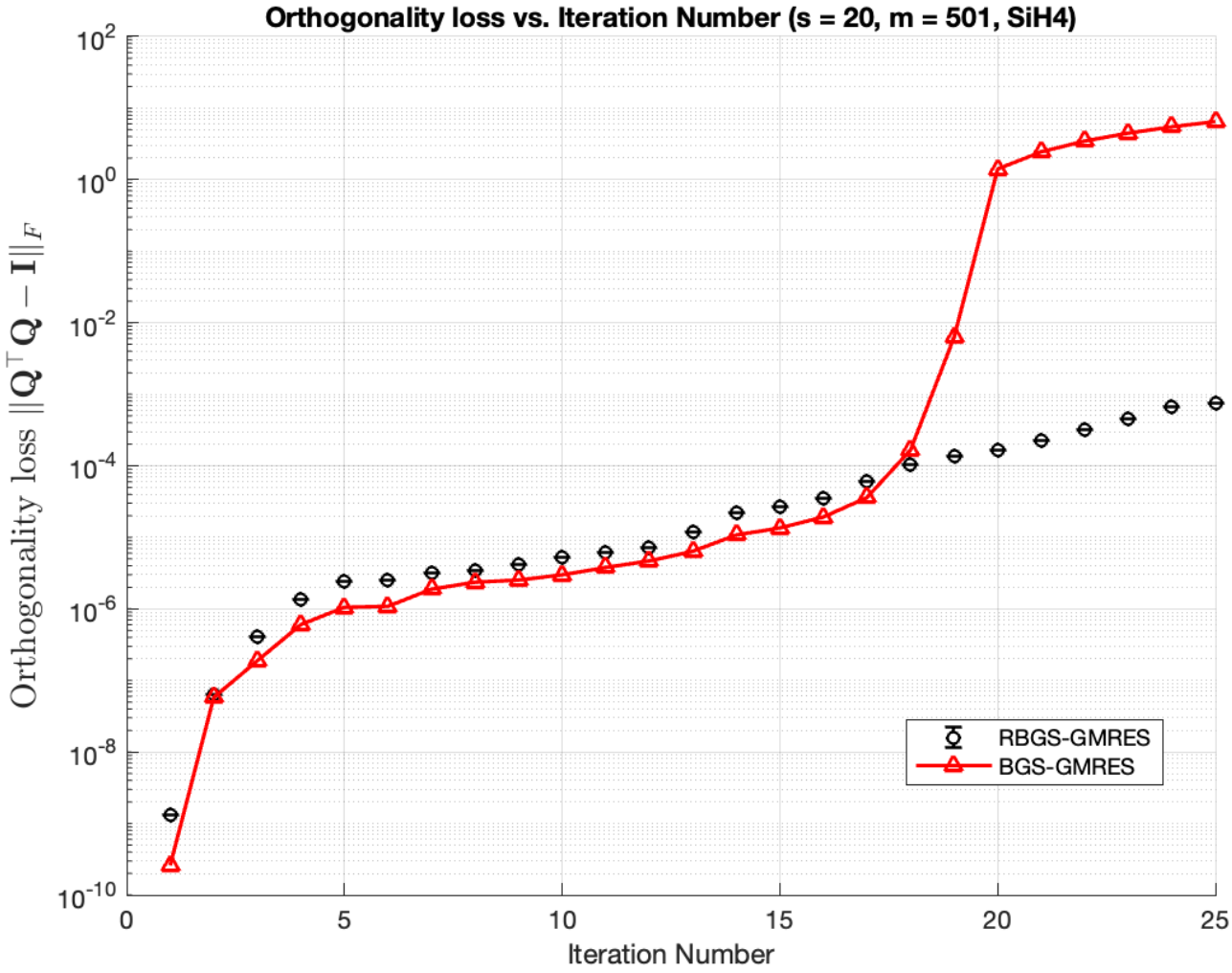
- s=20


Relative Residual vs. Iteration Number (s = 20, m = 501, SiH4)
Relative Residual $||Ax - b||_2 / ||b||_2$
Iteration Number
RBGS-GMRES
BGS-GMRES
GMRES
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
0
5
10
15
20
25



| Newton basis


Relative Residual vs. Iteration Number (s = 20, m = 501, SiH4)
RBGS-GMRES
BGS-GMRES
GMRES
Relative Residual $||Ax - b||_2/||b||_2$
Iteration Number


Orthogonality loss vs. Iteration Number (s = 20, m = 501, SiH4)
RBGS-GMRES
BGS-GMRES
Orthogonality loss $||\mathbf{Q}^\top\mathbf{Q} - \mathbf{I}||_F$
Iteration Number

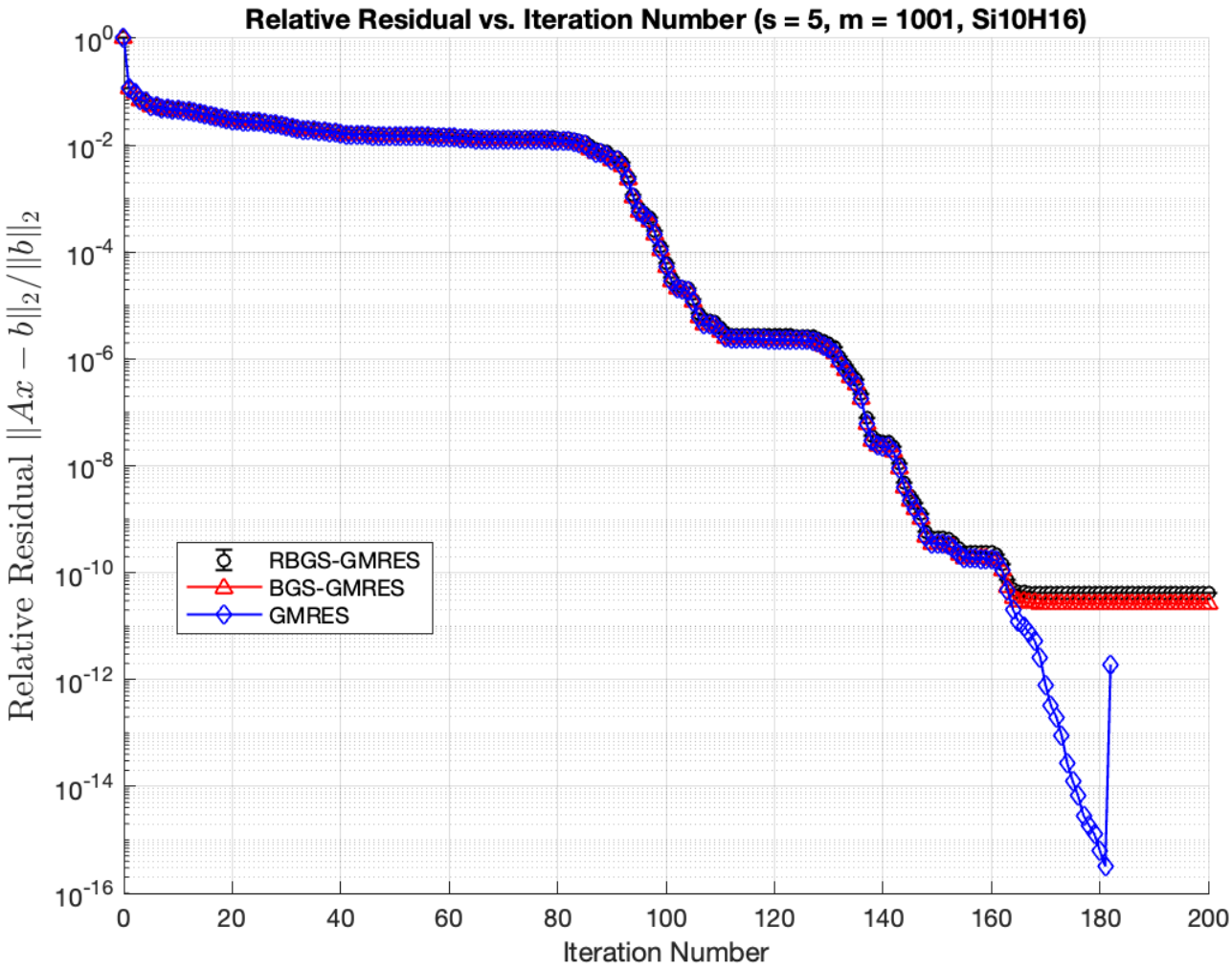
2.2 Si10H16

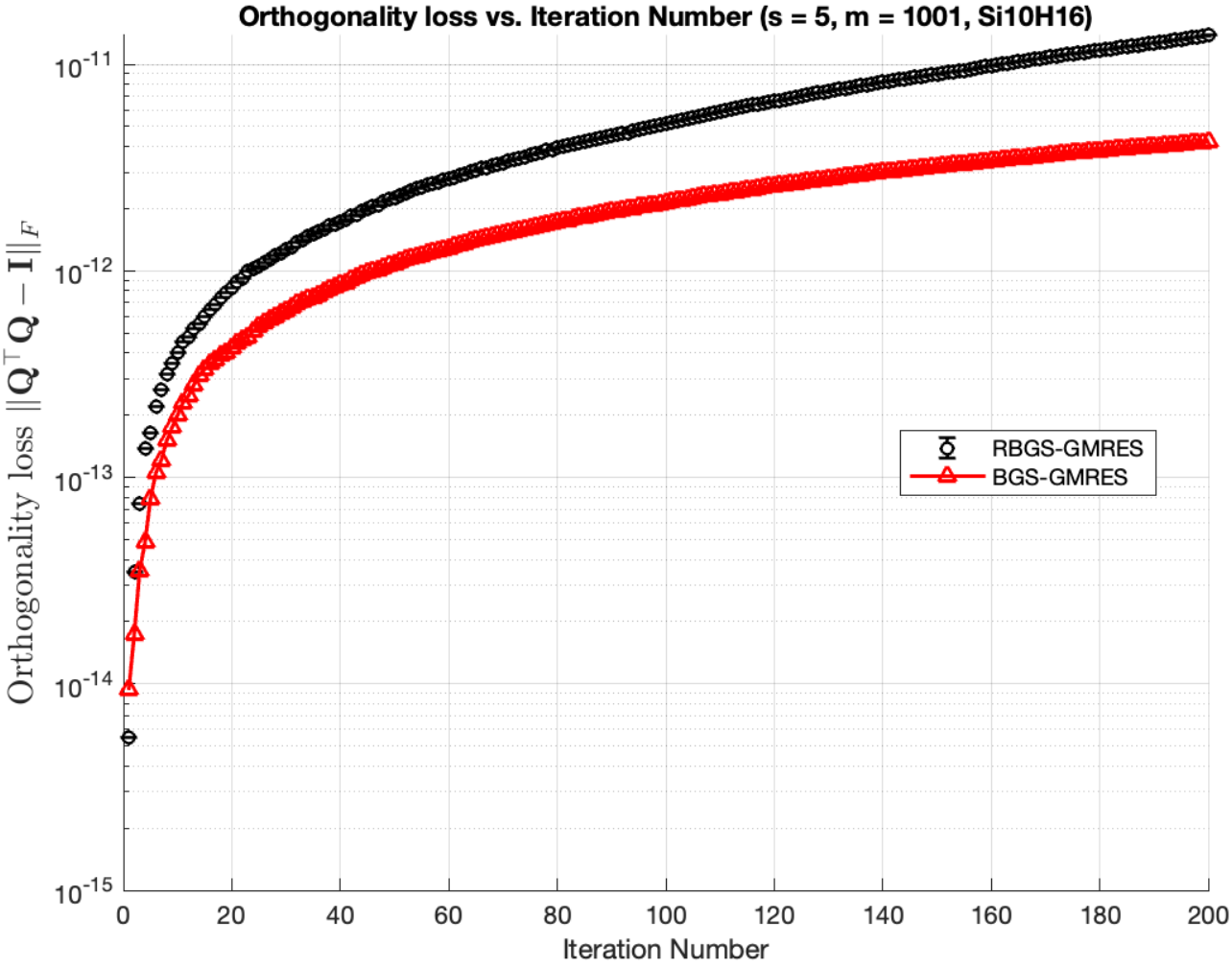
Matrix info: (n = 17077)
Condition number: (5.633416e+04)
Sketch info: (m = 1001, d = 2 * m)
Converge info: (ctol = 1e-16) **Krylov basis:** monomial basis

➤ Results for Step Sizes

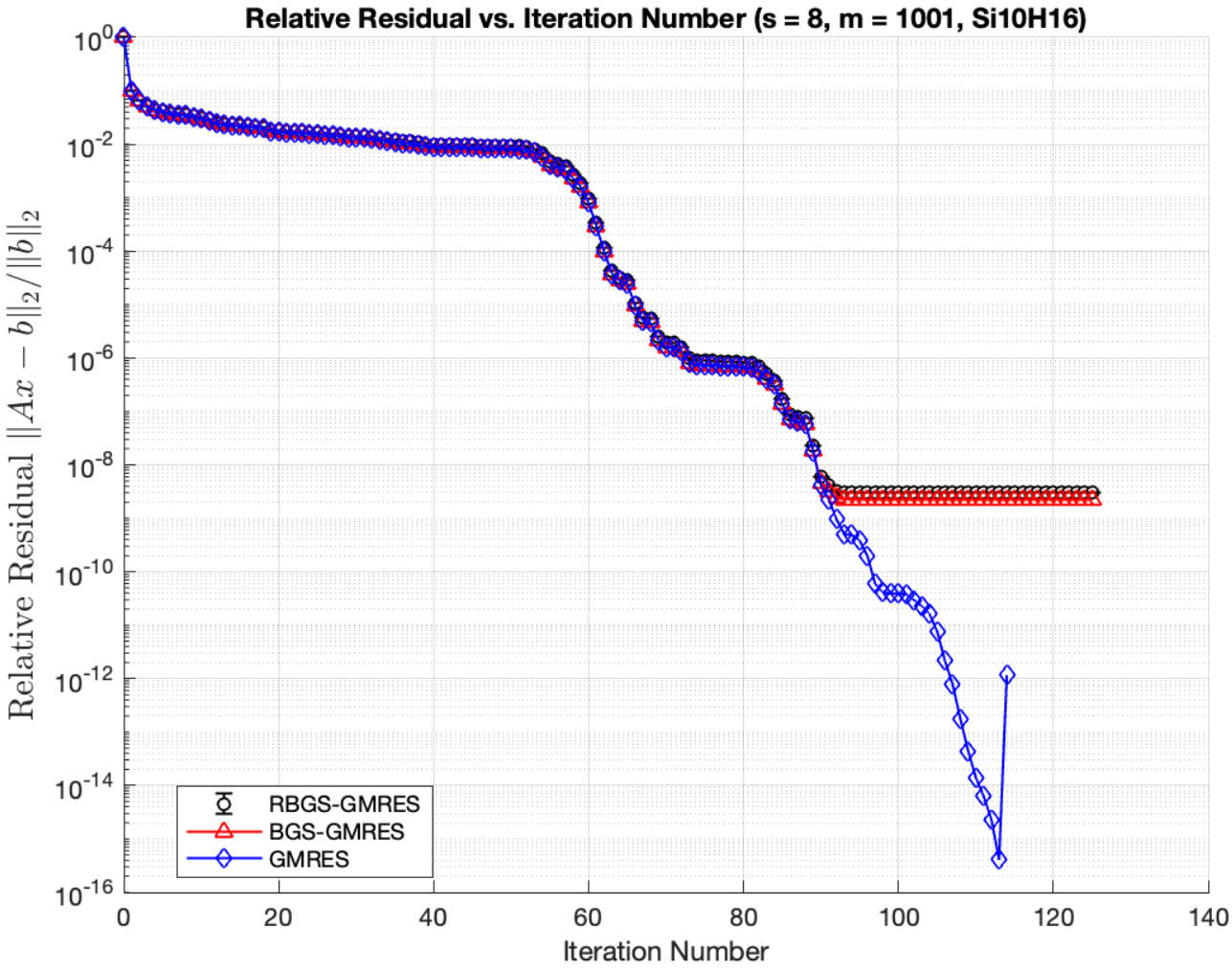
relative residual (after reorthogonalization)

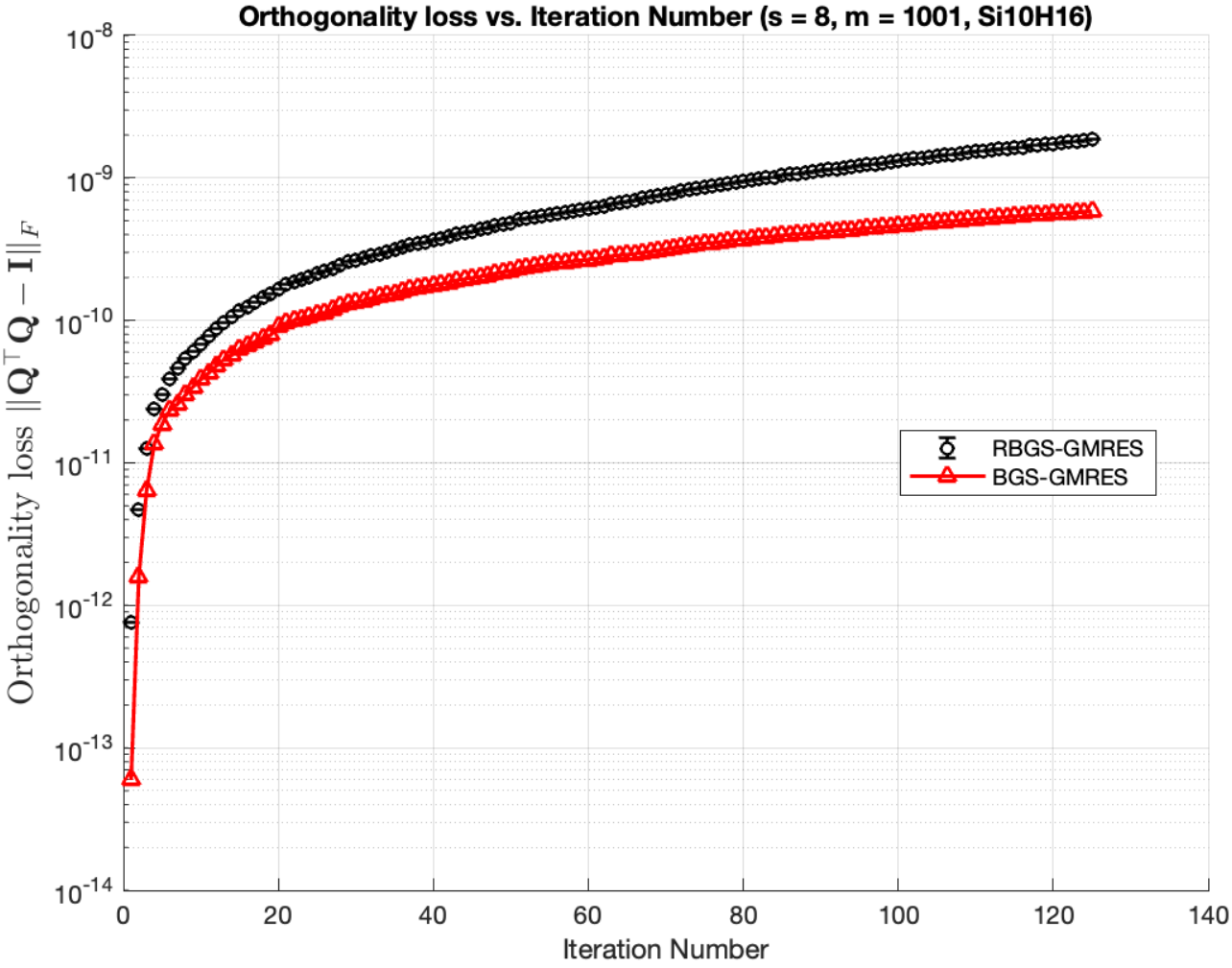
- s=5



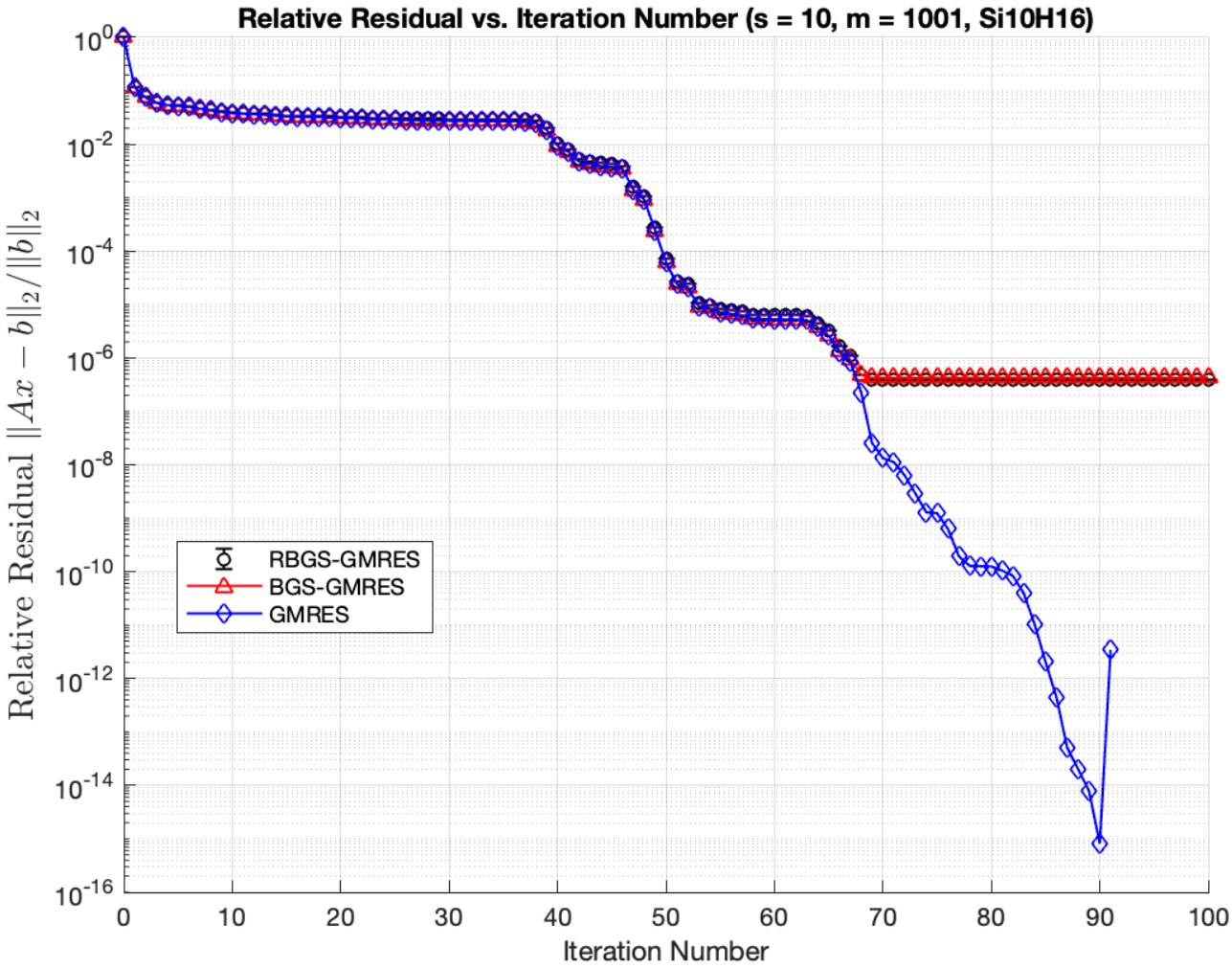

Orthogonality loss vs. Iteration Number (s = 5, m = 1001, Si10H16)
Orthogonality loss $\|\mathbf{Q}^\top\mathbf{Q}-\mathbf{I}\|_F$
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
0
20
40
60
80
100
120
140
160
180
200
Iteration Number
RBGS-GMRES
BGS-GMRES

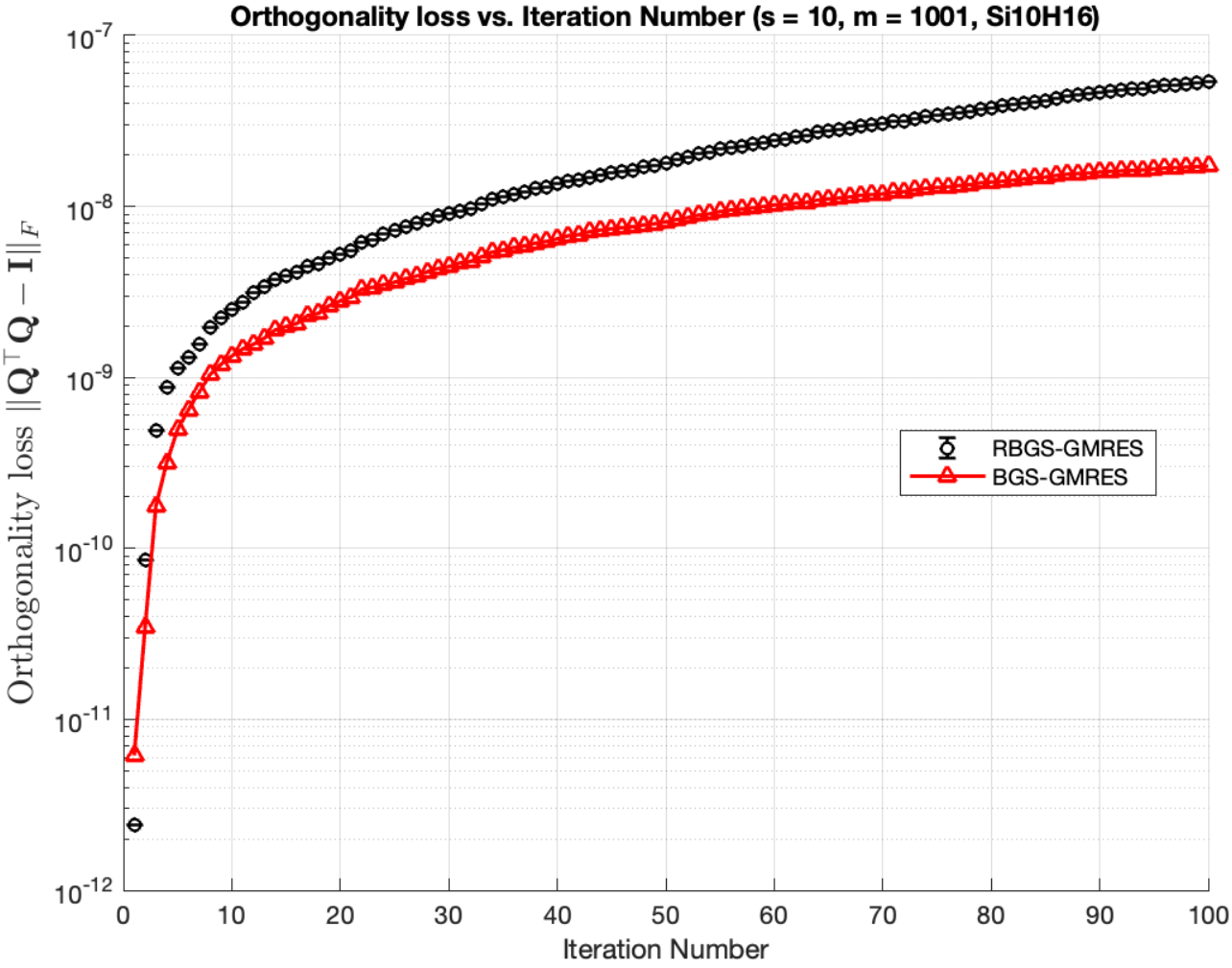
- s=8


Relative Residual vs. Iteration Number (s = 8, m = 1001, Si10H16)
Relative Residual $||Ax - b||_2/||b||_2$
Iteration Number
RBGS-GMRES
BGS-GMRES
GMRES
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
0
20
40
60
80
100
120
140

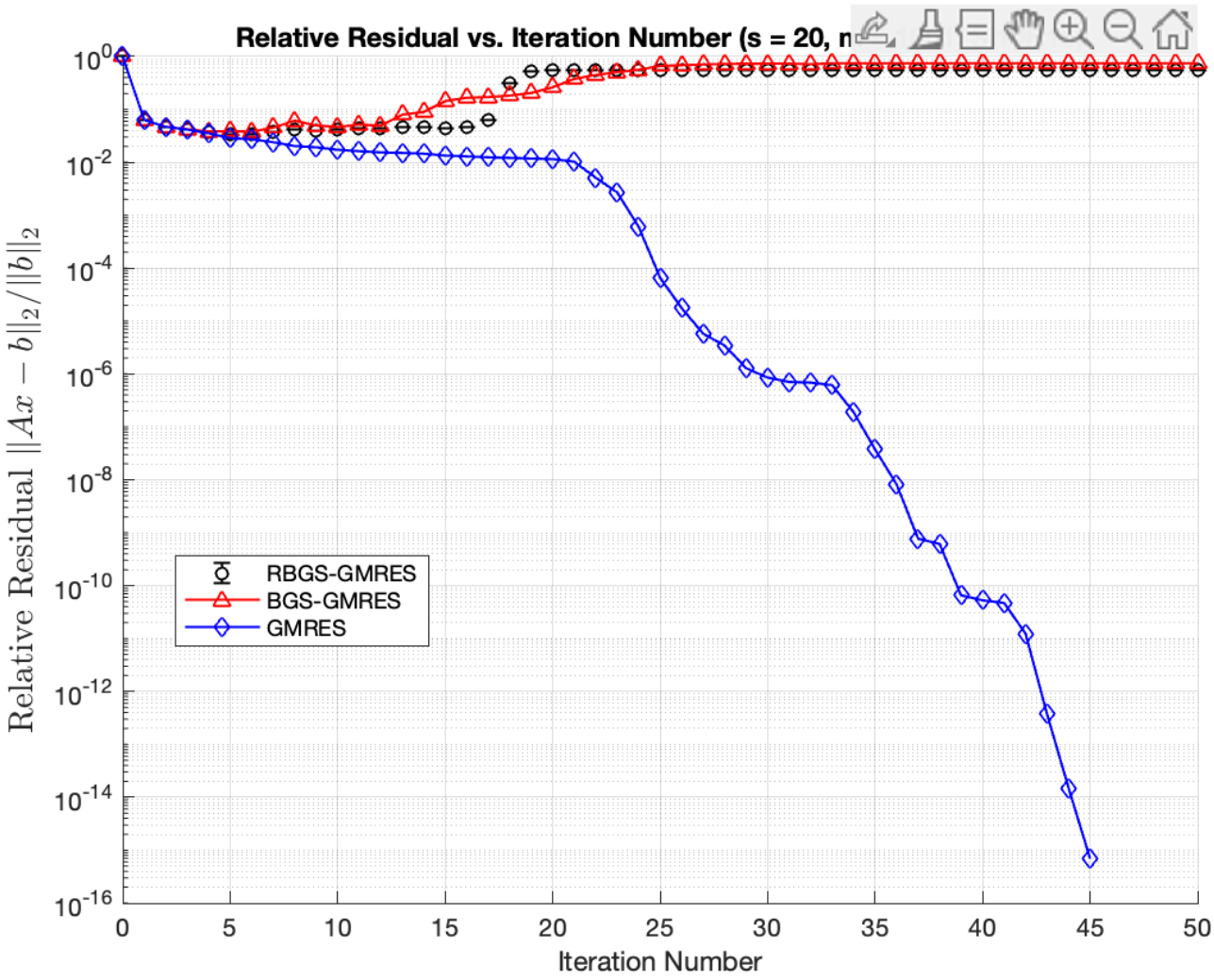

Orthogonality loss vs. Iteration Number (s = 8, m = 1001, Si10H16)
Orthogonality loss $\|\mathbf{Q}^\top\mathbf{Q}-\mathbf{I}\|_F$
Iteration Number
RBGS-GMRES
BGS-GMRES
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
0
20
40
60
80
100
120
140

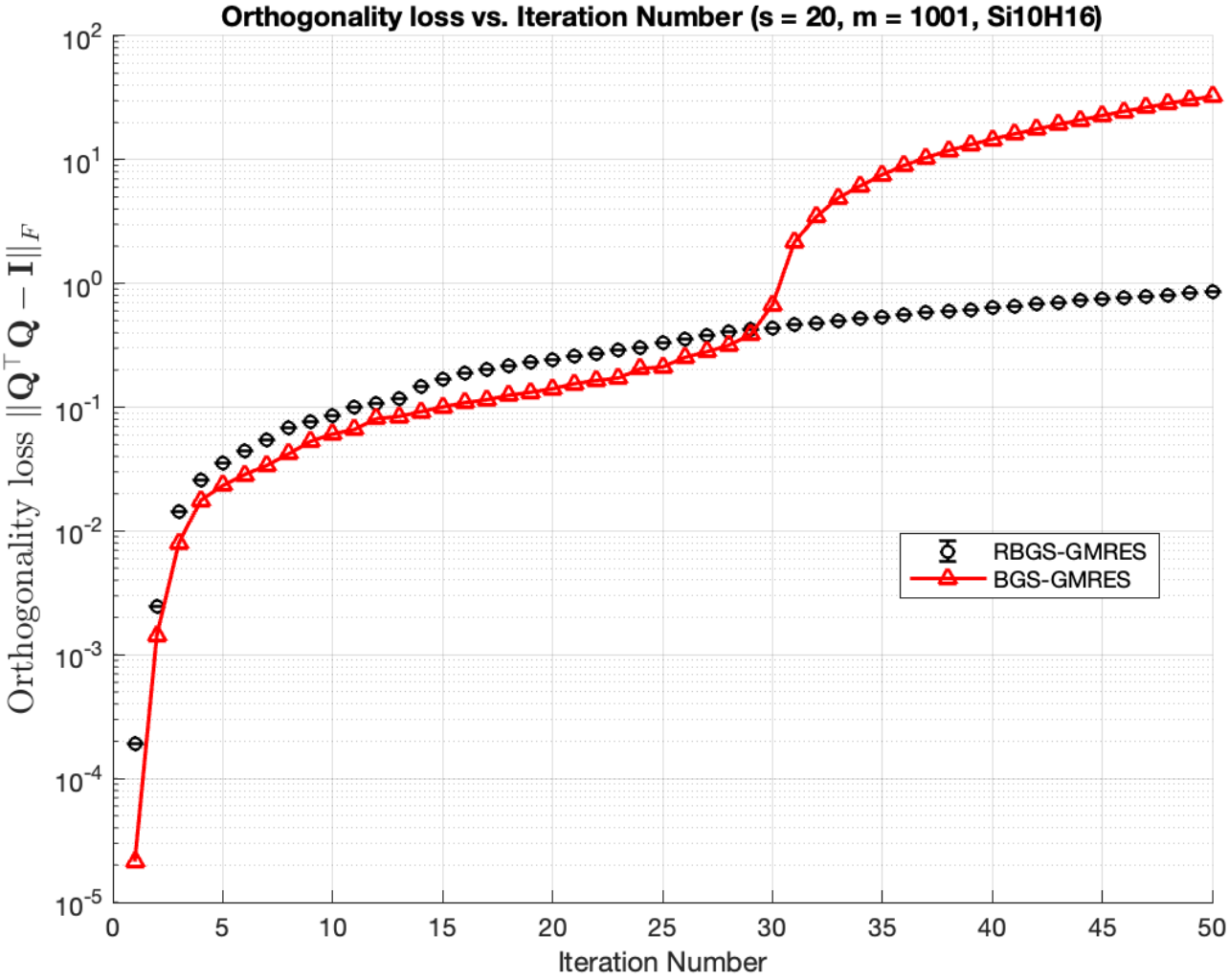
- s=10


Relative Residual vs. Iteration Number (s = 10, m = 1001, Si10H16)
Relative Residual $||Ax - b||_2/||b||_2$
Iteration Number
RBGS-GMRES
BGS-GMRES
GMRES
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
0
10
20
30
40
50
60
70
80
90
100


Orthogonality loss vs. Iteration Number (s = 10, m = 1001, Si10H16)
Orthogonality loss $\|\mathbf{Q}^\top\mathbf{Q}-\mathbf{I}\|_F$
Iteration Number
RBGS-GMRES
BGS-GMRES
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
0
10
20
30
40
50
60
70
80
90
100

- s=20


Relative Residual vs. Iteration Number (s = 20, n
Relative Residual $||Ax - b||_2/||b||_2$
Iteration Number
RBGS-GMRES
BGS-GMRES
GMRES
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
0
5
10
15
20
25
30
35
40
45
50



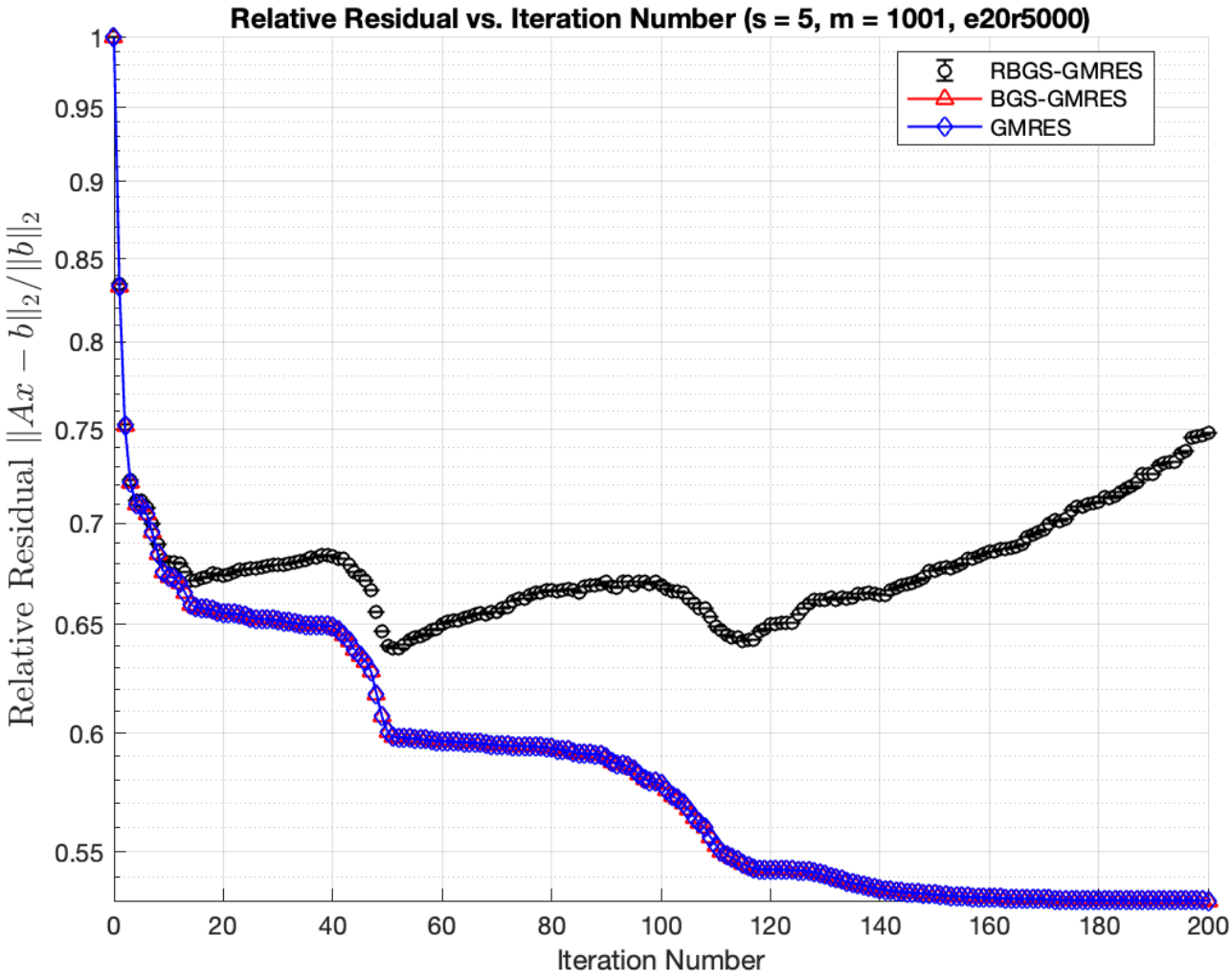
2.3 e20r5000 - tested in Adaptive s-step GMRES with randomized and truncated low-synchronization orthogonalization

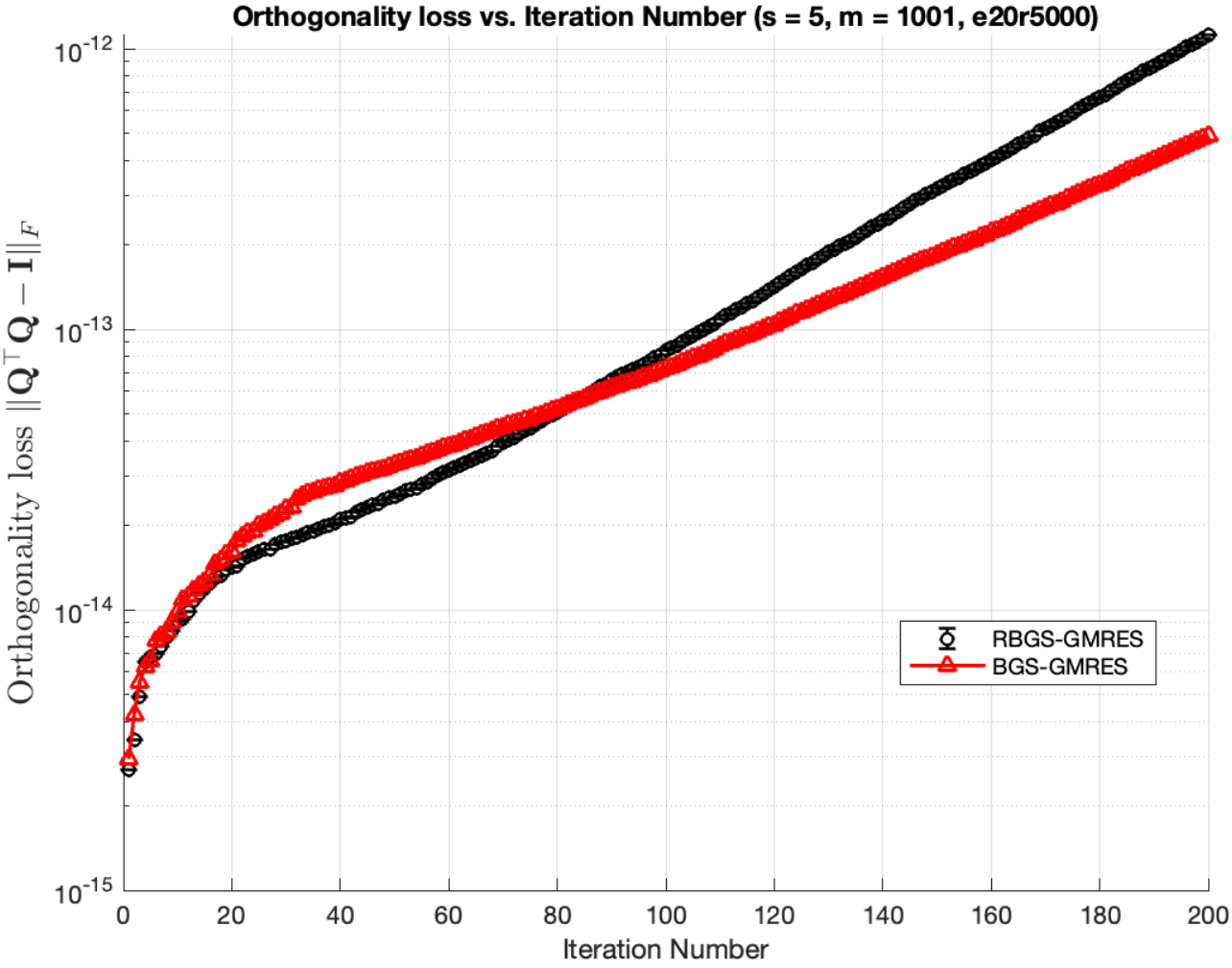
Matrix info: (n = 4241)
Condition number: (4.44e+10)
Sketch info: (m = 1001, d = 2 * m)
Converge info: (ctol = 1e-16)

➤ Results for Step Sizes

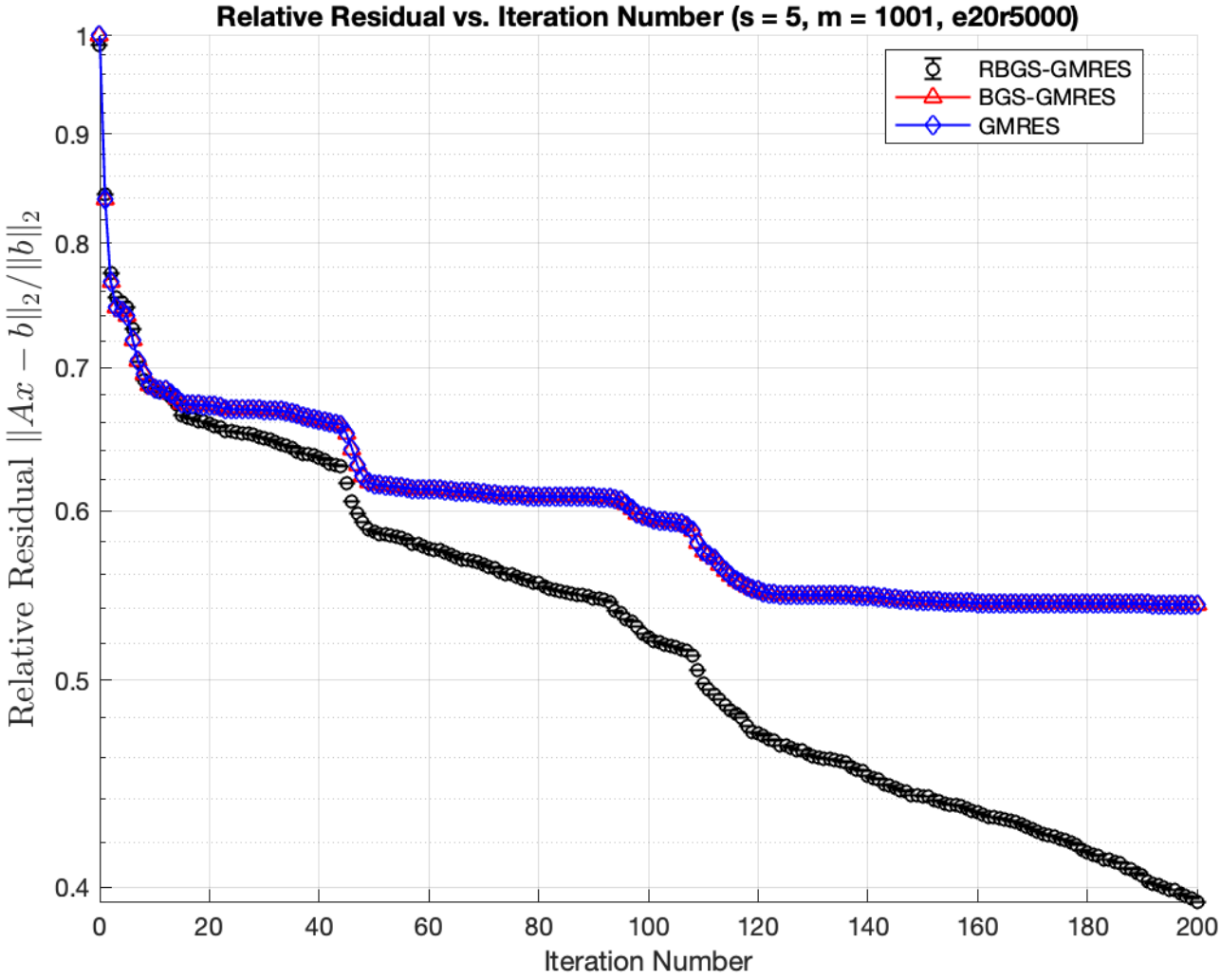
relative residual (after reorthogonalization)

- s=5


Relative Residual vs. Iteration Number (s = 5, m = 1001, e20r5000)
RBGS-GMRES
BGS-GMRES
GMRES
Relative Residual $\|Ax-b\|_2/\|b\|_2$
Iteration Number
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0
20
40
60
80
100
120
140
160
180
200



| Sketched residual



➤ **Results in the paper, s=5, monomial basis**

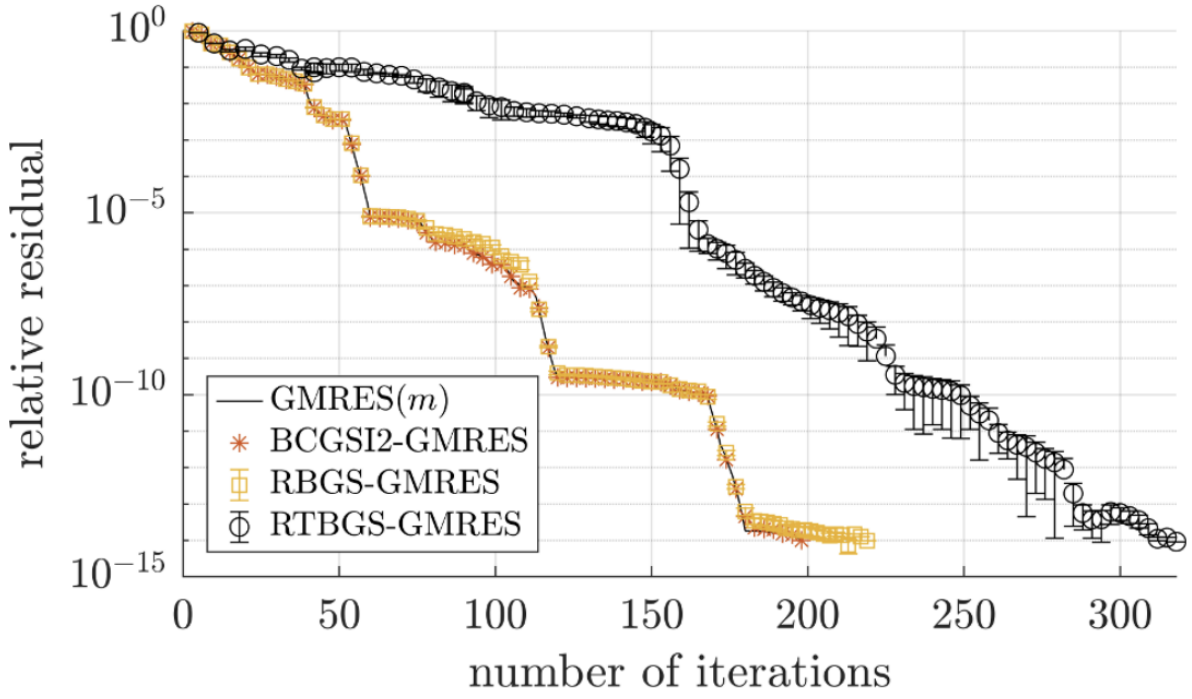
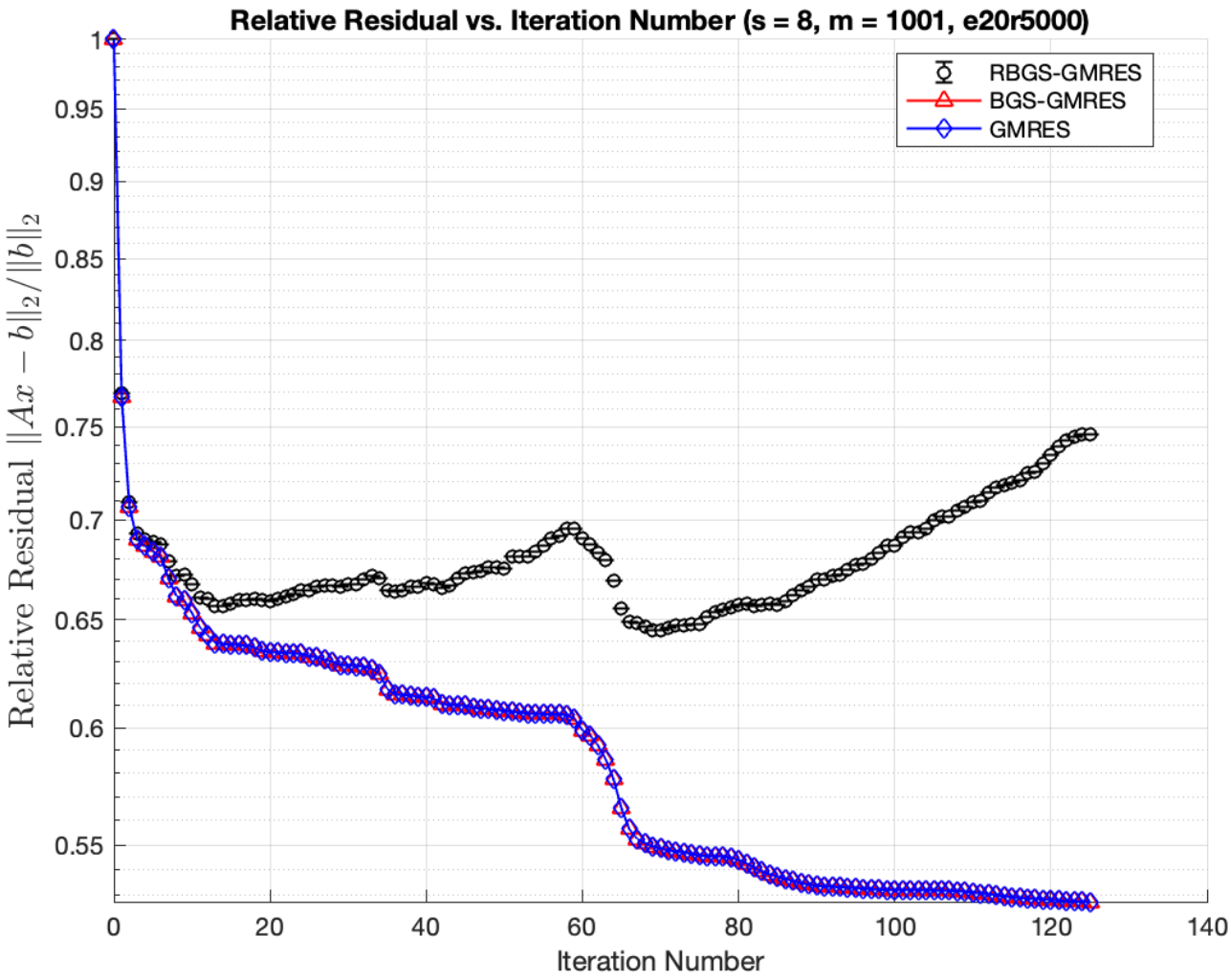
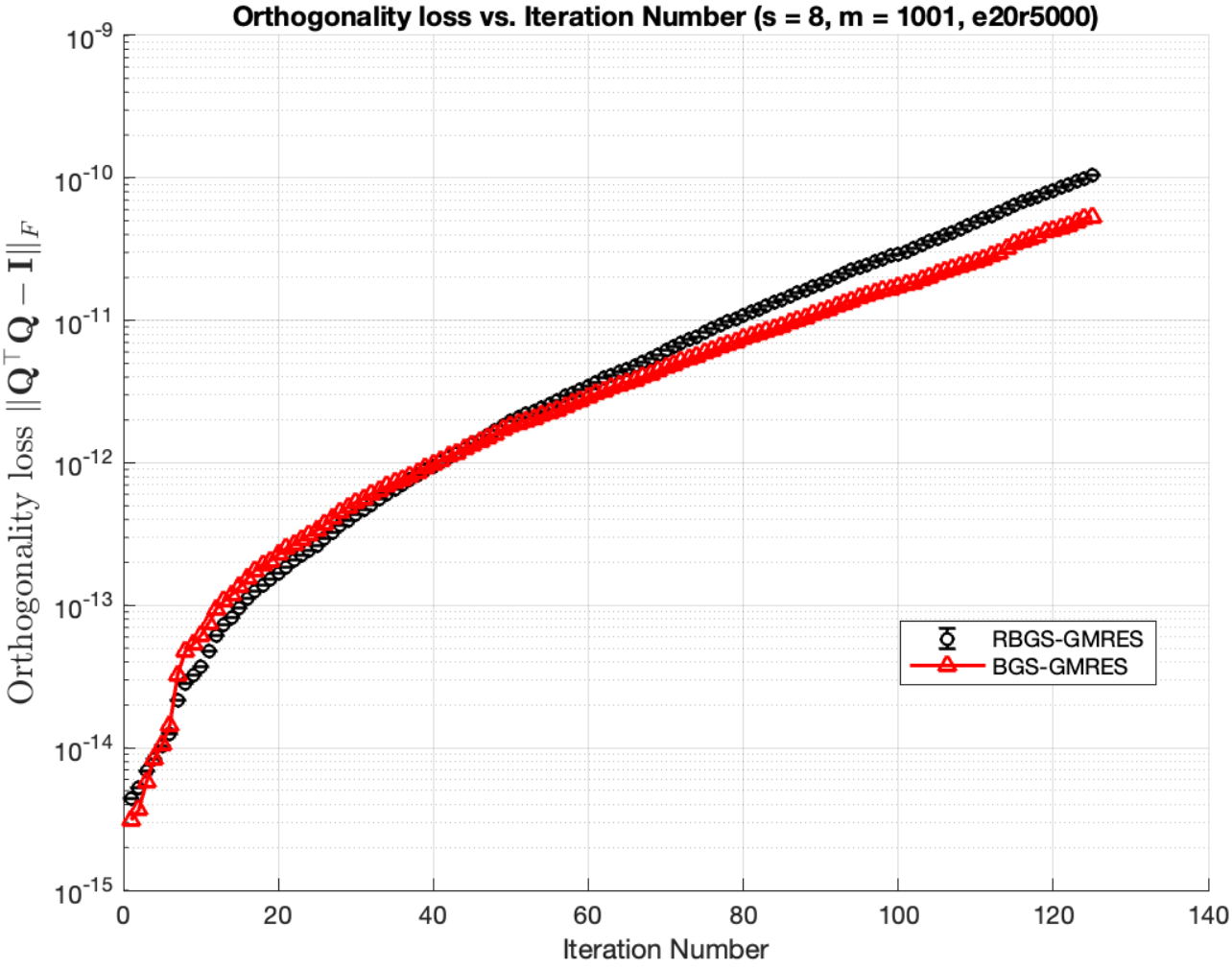


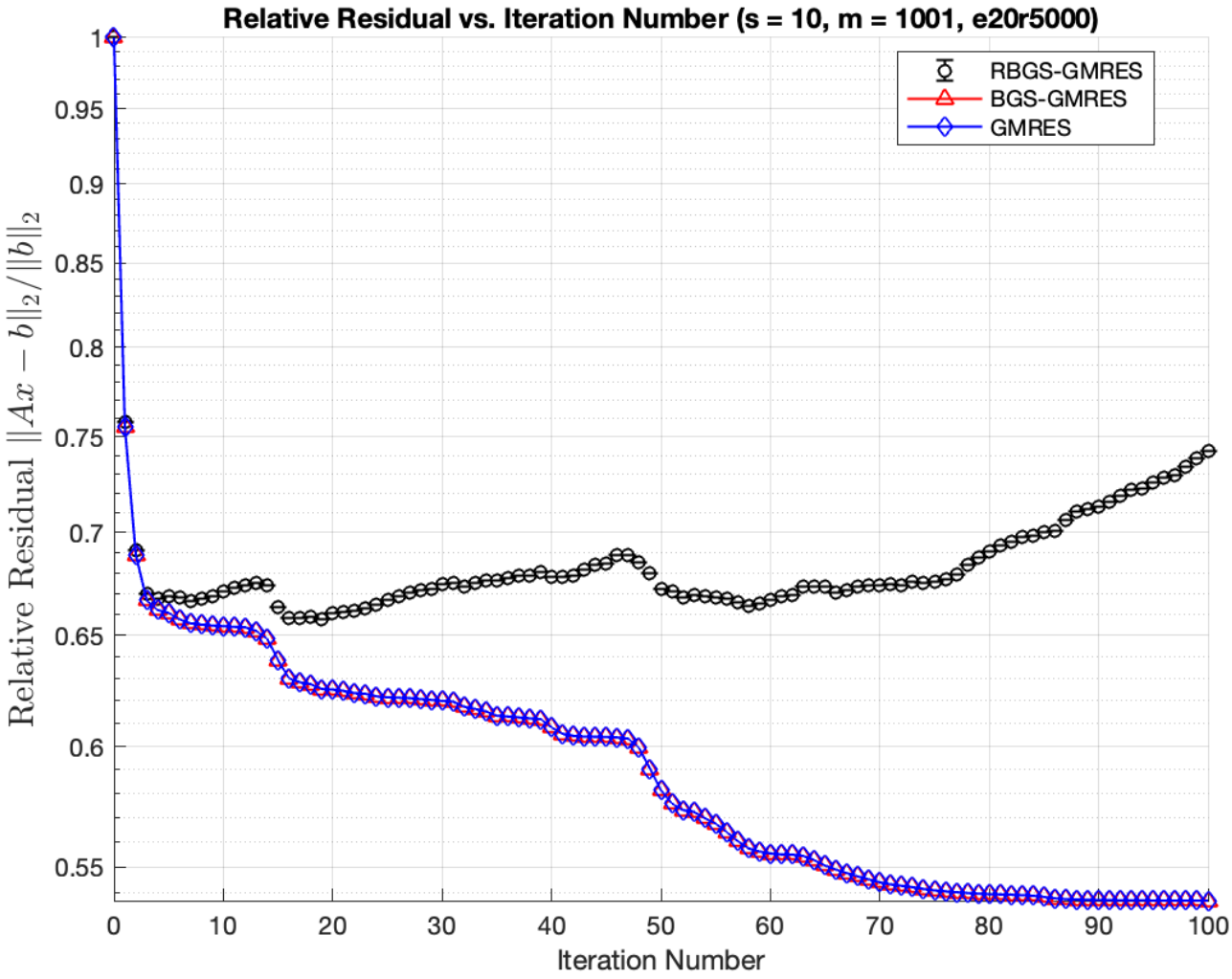
Fig. 1. Convergence histories for `e200`. The randomized methods show residual means with 95% confidence intervals based on 20 runs. BCGSI2-GMRES used the ICE with a condition number bound of $\Omega = 10^{-1}u^{-1/2}$ for Krylov basis orthogonalization, while the randomized methods used $\Omega = 10^{-2}u^{-1/2}$. With an initial step size of $s = 5$, the ICE restricted all s-step methods to three steps per iteration.

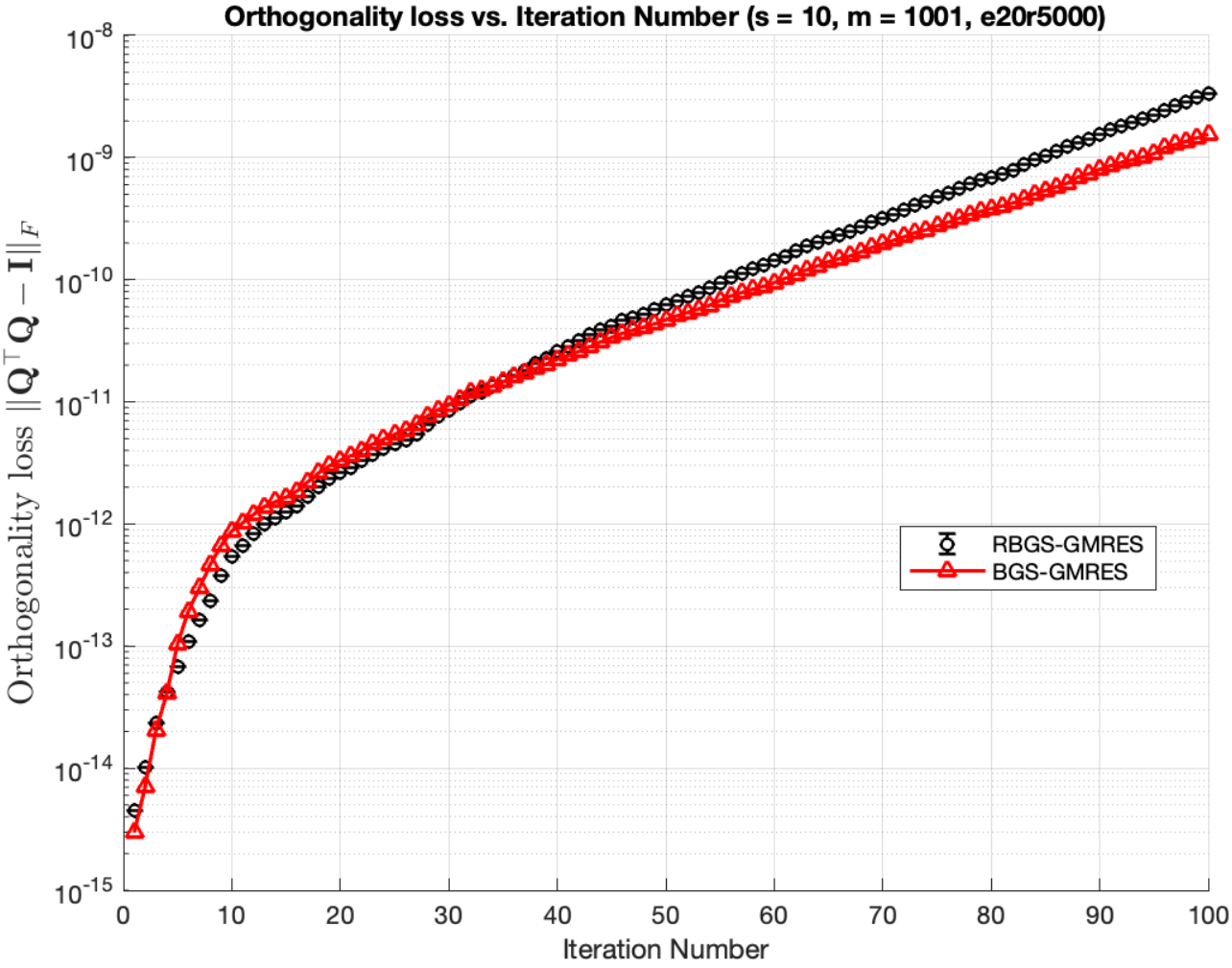
- s=8


Relative Residual vs. Iteration Number (s = 8, m = 1001, e20r5000)
RBGS-GMRES
BGS-GMRES
GMRES
Relative Residual $\|Ax-b\|_2/\|b\|_2$
Iteration Number
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0
20
40
60
80
100
120
140

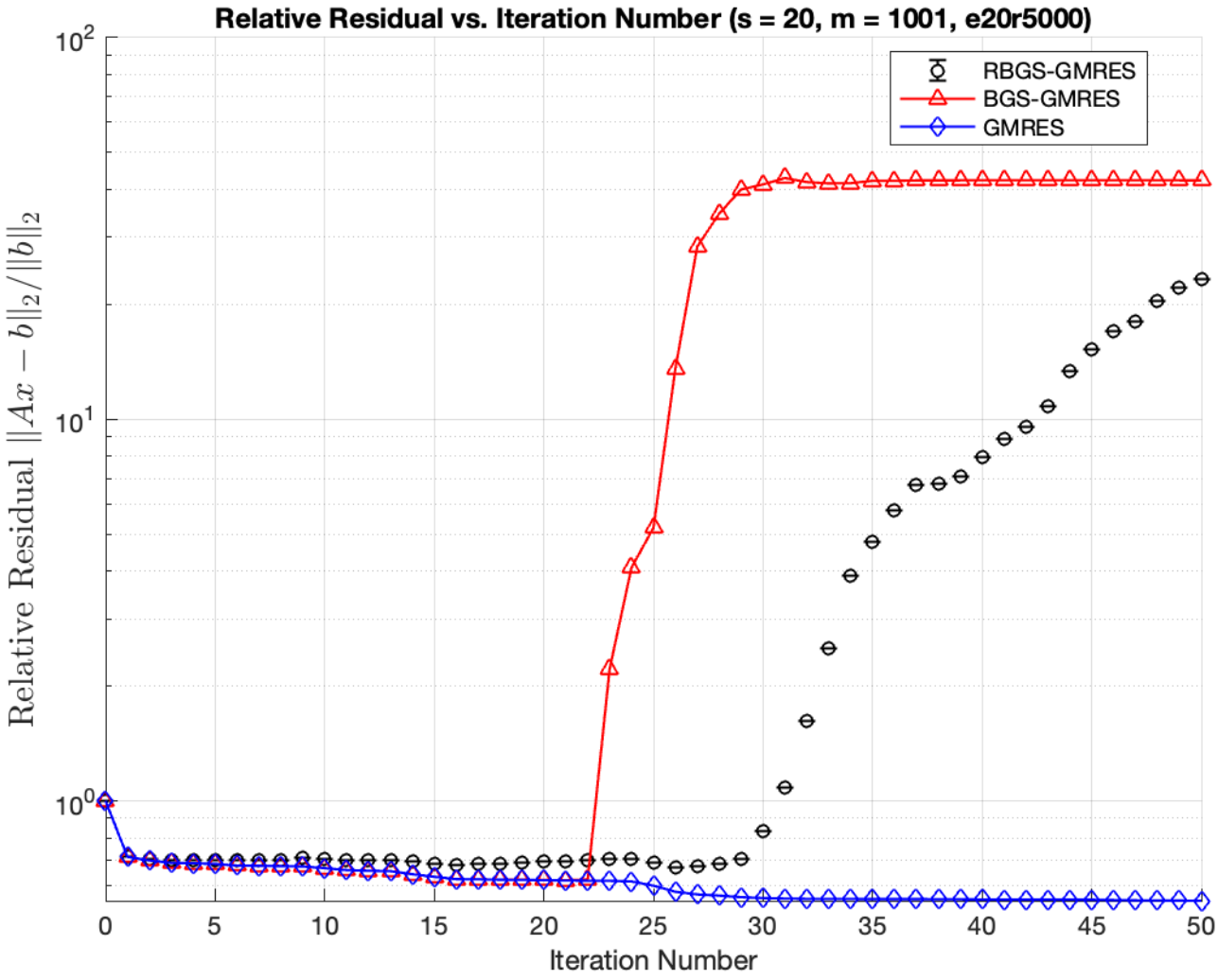

Orthogonality loss vs. Iteration Number (s = 8, m = 1001, e20r5000)
Orthogonality loss $\|\mathbf{Q}^\top\mathbf{Q} - \mathbf{I}\|_F$
Iteration Number
RBGS-GMRES
BGS-GMRES
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
0
20
40
60
80
100
120
140

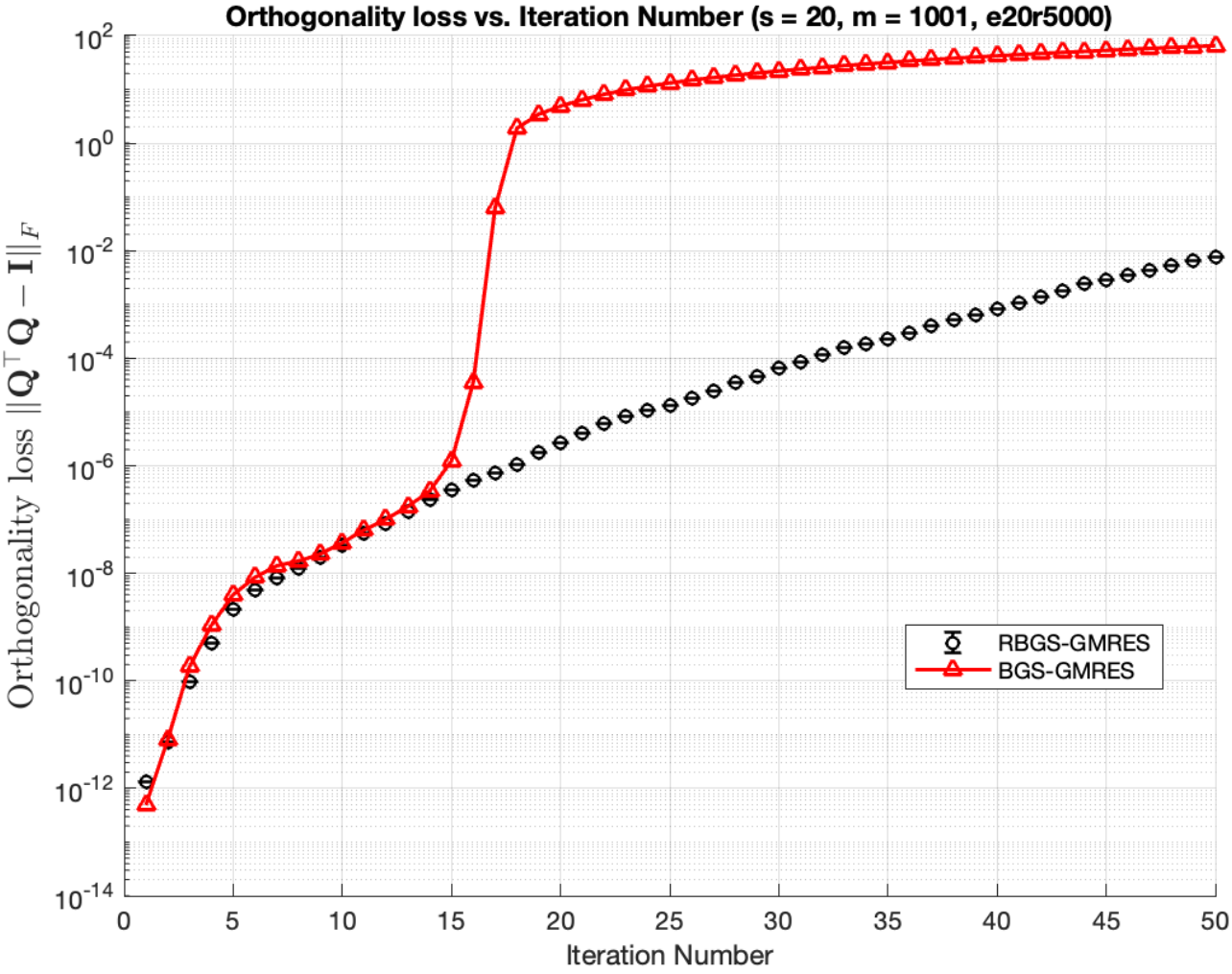
- s=10


Relative Residual vs. Iteration Number (s = 10, m = 1001, e20r5000)
RBGS-GMRES
BGS-GMRES
GMRES
Relative Residual $\|Ax-b\|_2/\|b\|_2$
Iteration Number
1
0.95
0.9
0.85
0.8
0.75
0.7
0.65
0.6
0.55
0
10
20
30
40
50
60
70
80
90
100


Orthogonality loss vs. Iteration Number (s = 10, m = 1001, e20r5000)
Orthogonality loss $\|\mathbf{Q}^\top\mathbf{Q}-\mathbf{I}\|_F$
Iteration Number
RBGS-GMRES
BGS-GMRES
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
0
10
20
30
40
50
60
70
80
90
100

- s=20


Relative Residual vs. Iteration Number (s = 20, m = 1001, e20r5000)
RBGS-GMRES
BGS-GMRES
GMRES
10^2
10^1
10^0
Relative Residual $||Ax - b||_2/||b||_2$
0
5
10
15
20
25
30
35
40
45
50
Iteration Number


Orthogonality loss vs. Iteration Number (s = 20, m = 1001, e20r5000)
Orthogonality loss $\|\mathbf{Q}^\top\mathbf{Q} - \mathbf{I}\|_F$
Iteration Number
RBGS-GMRES
BGS-GMRES
10^{2}
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
0
5
10
15
20
25
30
35
40
45
50