Iterative Methods for Linear Systems

Comparisons of methods for model problems

GMRES - Computational Cost

GMRES: $Ax = b$
choose x_0 (e.g. $x_0 = 0$) and tol
$r_0 = b - Ax_0;\ k = 0;\ v_1 = r_0 / \|r_0\|_2;$
while $\|r_k\|_2 > tol$
  $k = k + 1;$
  $w = Av_k;$
  Solve $P\tilde{v}_{k+1} = w;$
  for $j = 1 : k,$
    $h_{j,k} = v_j^H \tilde{v}_{k+1};$
    $\tilde{v}_{k+1} = \tilde{v}_{k+1} - h_{j,k} v_k;$
  end
  $h_{k+1,k} = \|\tilde{v}_{k+1}\|_2;\ v_{k+1} = \tilde{v}_{k+1} / h_{k+1,k};$
  update QR-dec: $\underline{H}_k = Q_{k+1} \underline{R}_k$
  $\|r_k\|_2 = |\tilde{q}_{k+1}^H e_1| \, \|r_0\|_2$
end
$y_k = R_k^{-1} \underline{Q}_k^H e_1 \|r_0\|_2;\ x_k = x_0 + V_k y_k;$
$r_k = r_0 - V_{k+1} \underline{H}_k y_k = V_{k+1}\left(I - \underline{Q}_k \underline{Q}_k^H\right) e_1 \|r_0\|_2;$ (or simply $r_k = b - Ax_k$)

4 kernels:
- matrix-vector product ($w = Av_k$)
- preconditioner ($P\tilde{v}_{k+1} = w$)
- inner product ($h_{j,k} = v_j^H \tilde{v}_{k+1}$)
- vector update ($\tilde{v}_{k+1} = \tilde{v}_{k+1} - h_{j,k} v_k$)
- (norm & vector scaling)

Computational Cost

Many cheap iterations vs minimum number of expensive iterations

Four main kernels

• matrix-vector product	comp: $2Nk_1$	comm: neighbor
• preconditioner	comp: $2Nk_2$	comm: neighbor (& global)
• vector update	comp: $2N$	comm: none
• inner product	comp: $2N$	comm: global (reduction)

Methods for non-Hermitian (nonsymmetric) problems:
- GMRES, GCR, FOM, BiCG, QMR, CGS, BiCGSTAB, TFQMR
- Short recurrence: cheap iteration / many iterations
- Full Orthogonalization: expensive iteration / minimum number

Matrix-vector product often linked to grid / domain partitioning
Partition scheme to minimize comm. volume / nr. of messages
Separate local/nonlocal references and overlap comm. with comp.

MINRES

MINRES: $Ax = b$

choose $x_0 \rightarrow r_0 = b - Ax_0$ and tol, set $k = 0$;
while $\|r_k\| > tol$ do
$k = k + 1$;
$\tilde{v}_{k+1} = Av_k - t_{k,k}v_k - t_{k-1,k}v_{k-1}$;
$t_{k+1,k} = \|\tilde{v}_{k+1}\|_2$; $v_{k+1} = \tilde{v}_{k+1}/t_{k+1,k}$;

Update QR: $Q_{k+1} = Q_k G_k; \underline{R}_k = G_k^H(Q_k^H \underline{T}_k); \hat{y}_{k,k} = q_k^H e_1 \|r_0\|_2$
$\rightarrow \underline{Q}_k, R_k, \hat{y}_k \equiv \underline{Q}_k^H e_1 \|r_0\|_2$;

$w_k = r_{k,k}^{-1}(v_k - w_{k-1}r_{k-1,k} - w_{k-2}r_{k-2,k})$;
$x_k = x_{k-1} + w_k \hat{y}_{k,k}$
end

Conjugate Gradients

(Easier form of) CG algorithm: $Ax = b$

Choose $x_0 \rightarrow r_0 = b - Ax_0$;

$p_1 = r_0$; $i = 0$

while $\|r_i\|_2 > tol$ do

$i = i + 1;$

$\alpha_i = \frac{\langle r_{i-1}, r_{i-1} \rangle}{\langle p_{i-1}, Ap_{i-1} \rangle};$

$x_i = x_i + \alpha_i p_i;$

$r_i = r_{i-1} - \alpha_i A p_i;$

$\beta_i = \frac{\langle r_i, r_i \rangle}{\langle r_{i-1}, r_{i-1} \rangle};$

$p_i = r_i - \beta_i p_{i-1};$

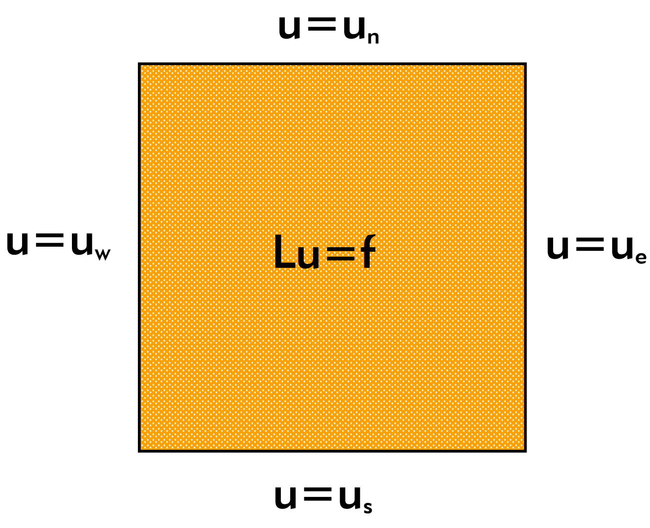
end

A Model Problem

Convection-Diffusion(-Reaction) Equation

Dirichlet boundary conditions

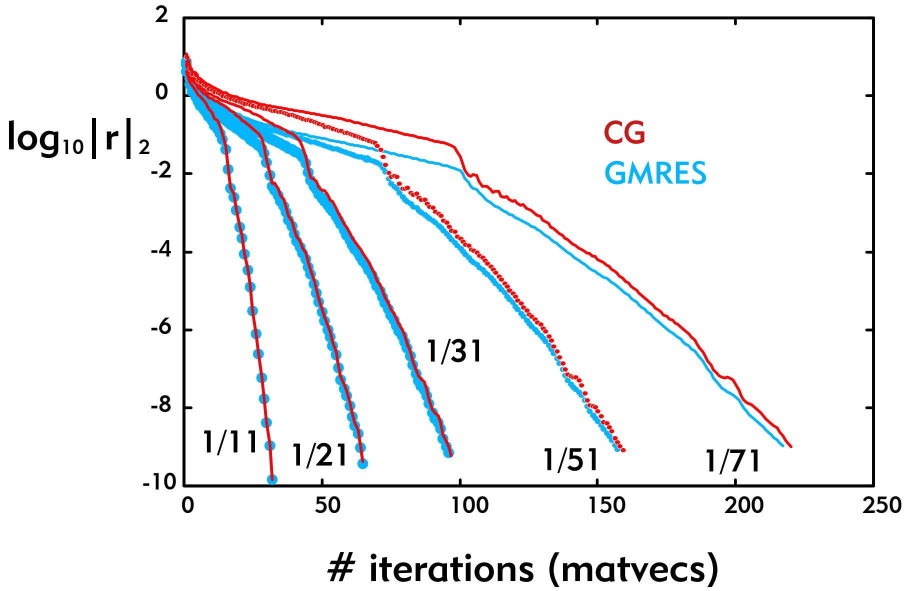
$$Lu = -(pu_x)_x - (qu_y)_y + ru_x + su_y + tu = f$$



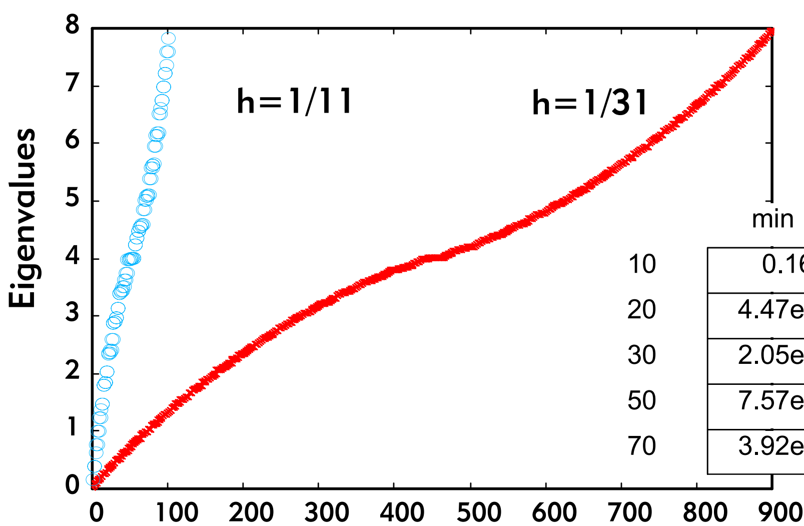
CG vs GMRES for various h

$p=q=1;\ t = 0;\ f = 0;$

$u_s = 0;\ u_w = 1;\ u_n = 1;\ u_e = 0;$



Eigenvalues for various h

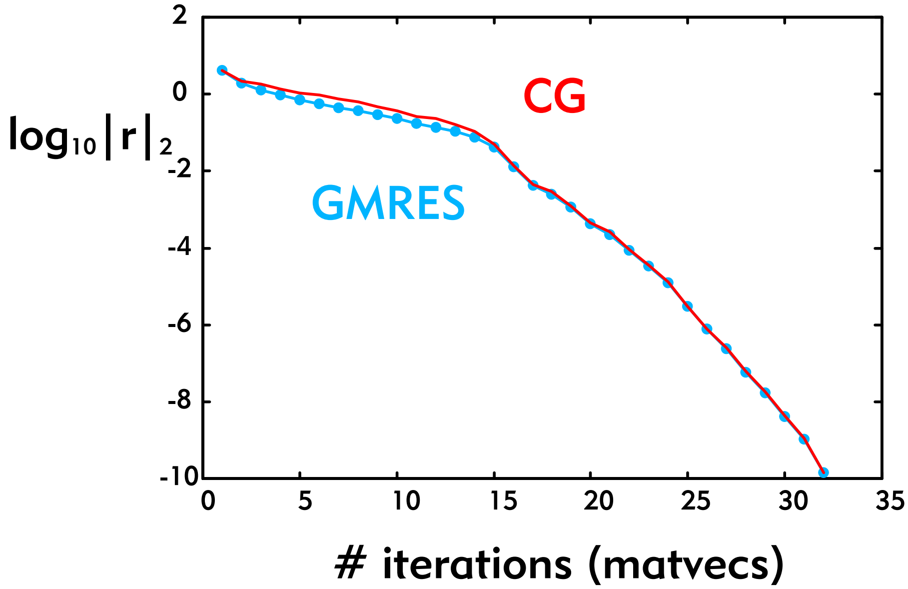


	min	max	cond. nr.
10	0.162	7.84	48.4
20	4.47e-2	7.95	178
30	2.05e-2	7.98	389
50	7.57e-3	7.99	1.06e3
70	3.92e-3	8.00	2.04e3

CG vs GMRES

$p = q = 1;\ t = 0;\ f = 0;\ h = 1/11;$

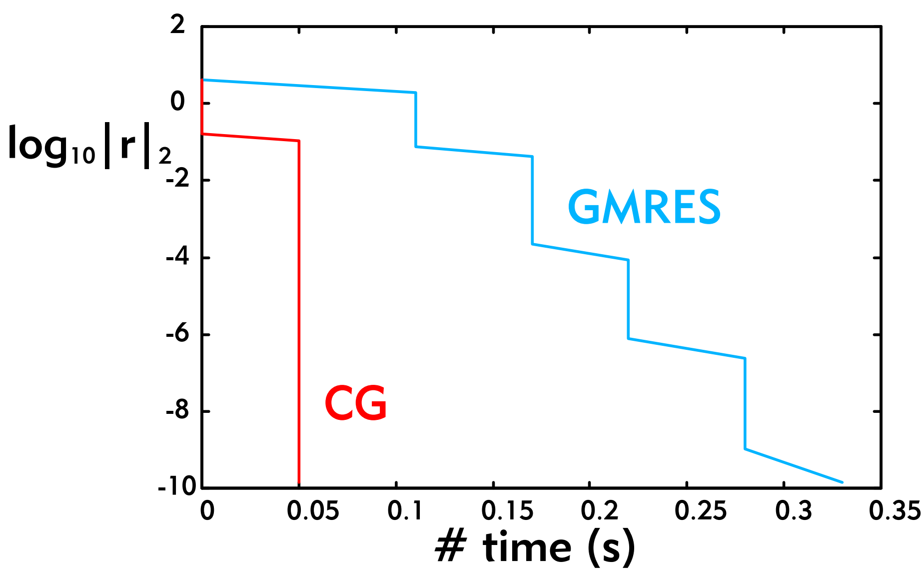
$u_s = 0;\ u_w = 1;\ u_n = 1;\ u_e = 0;$



CG vs GMRES

$p = q = 1;\ t = 0;\ f = 0;\ h = 1/11;$

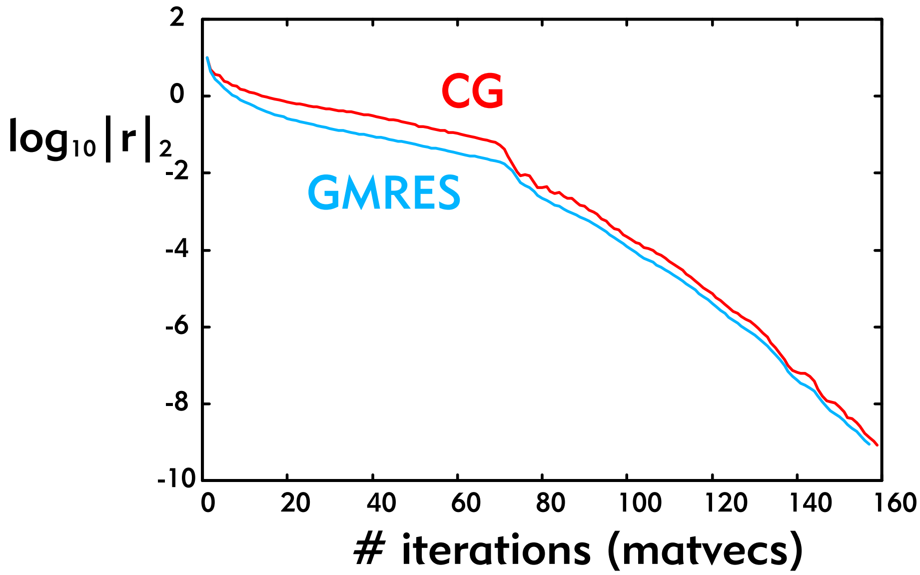
$u_s = 0;\ u_w = 1;\ u_n = 1;\ u_e = 0;$



CG vs GMRES

p=q=1; t = 0; f = 0; h=1/ 51;

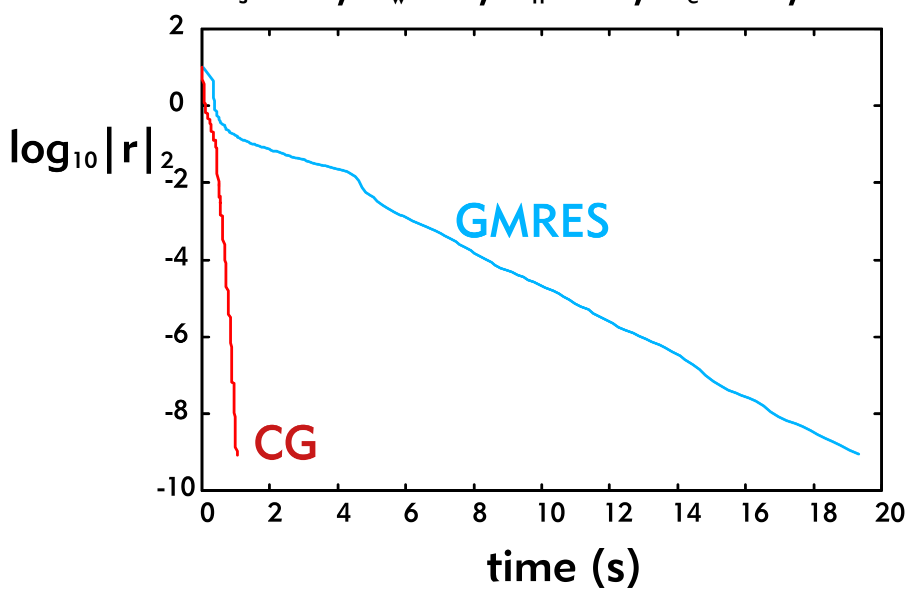
u_s = 0; u_w =1; u_n = 1; u_e = 0;



CG vs GMRES (time)

p=q=1; t = 0; f = 0; h=1/ 51;

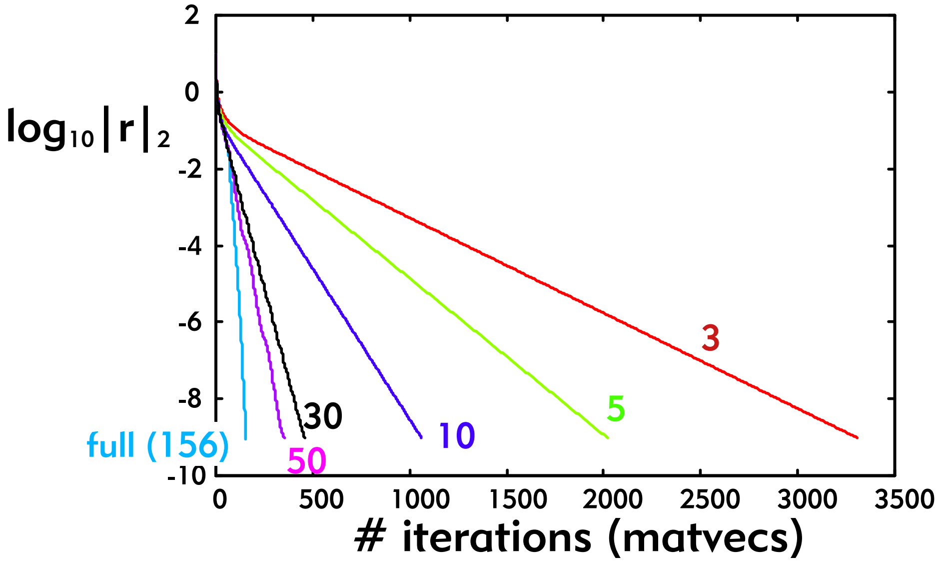
u_s = 0; u_w =1; u_n = 1; u_e = 0;



Iterations for GMRES(m)

$p = q = 1;\ t = 0;\ f = 0;\ h = 1/51;$

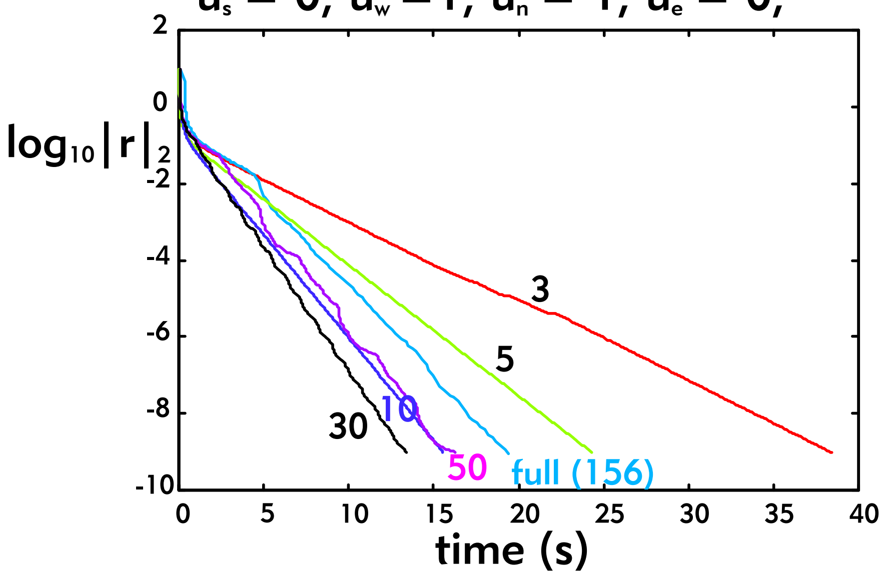
$u_s = 0;\ u_w = 1;\ u_n = 1;\ u_e = 0;$



Time for GMRES(m)

$p = q = 1;\ t = 0;\ f = 0;\ h = 1/51;$

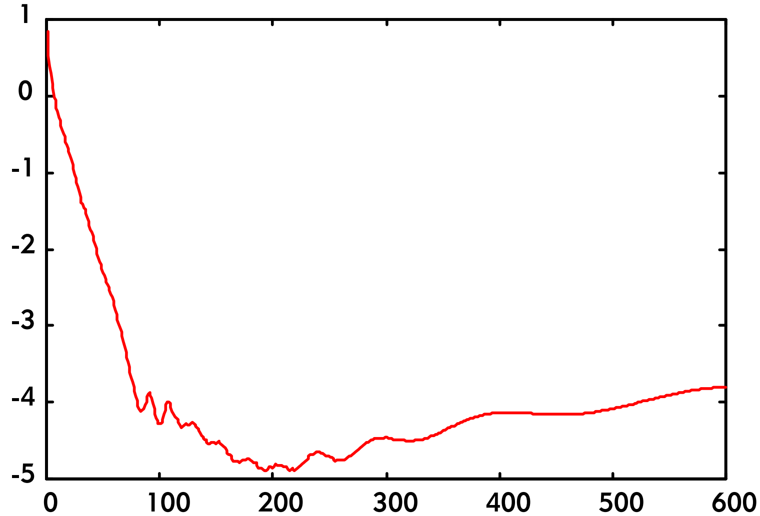
$u_s = 0;\ u_w = 1;\ u_n = 1;\ u_e = 0;$



CG for non-Hermitian Problem

p=q=1; r=s=5; h=1/31;

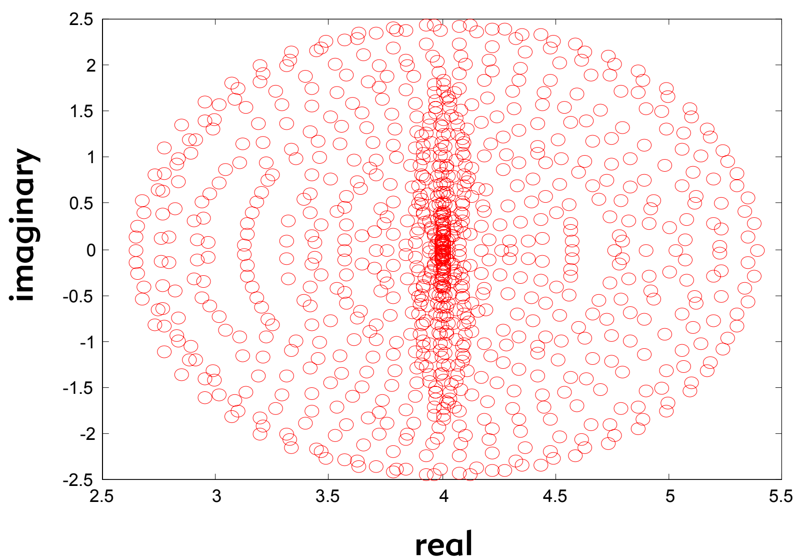
u_s=0; u_w=0; u_n=1; u_e=1;



Eigenvalues

p=q=1; r=s=70; h=1/31;

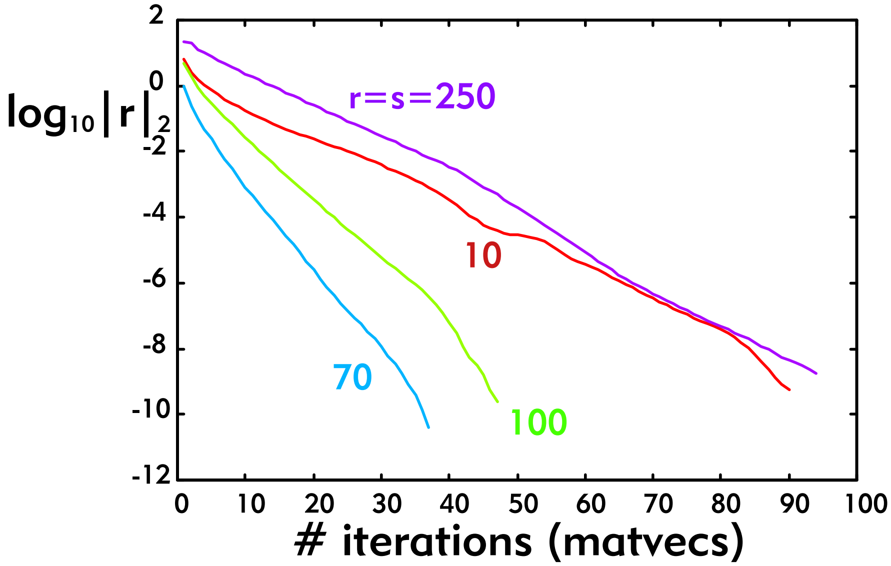
u_s=0; u_w=0; u_n=1; u_e=1;



GMRES for varying convection

p=q=1; r=s: given; h=1/31;

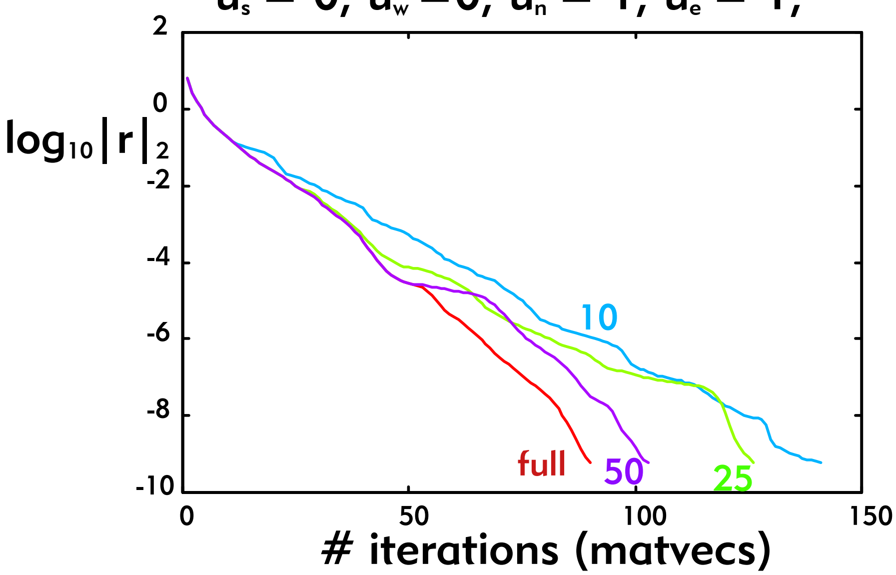
u_s = 0; u_w =0; u_n = 1; u_e = 1;



GMRES(m) with r=s=10

p=q=1; r=s=10; h=1/31;

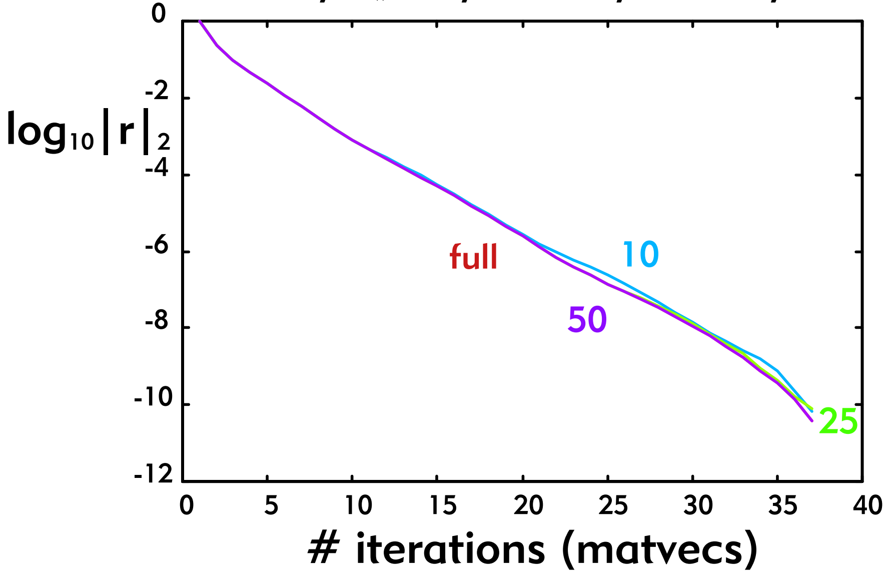
u_s = 0; u_w =0; u_n = 1; u_e = 1;



GMRES(m) with r=s=70

p=q=1; r=s=70; h=1/ 31;

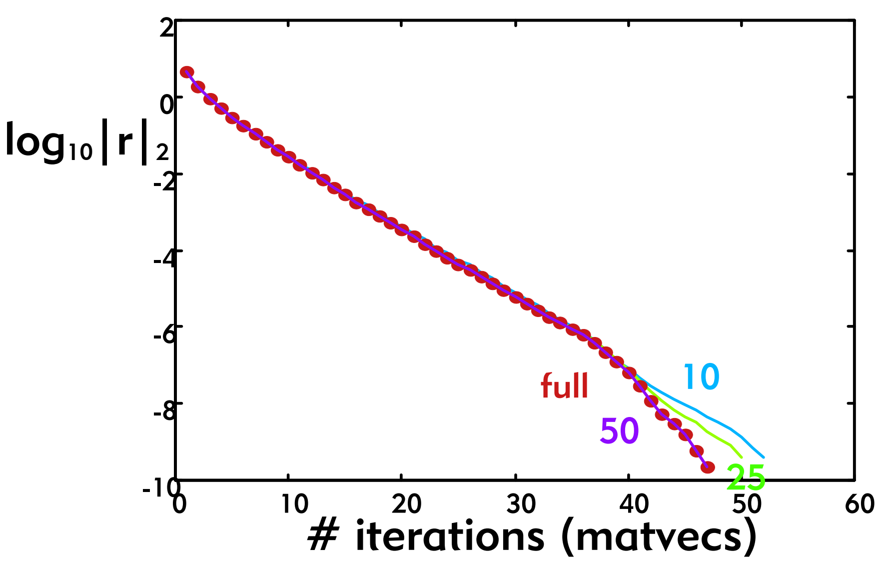
u_s = 0; u_w =0; u_n = 1; u_e = 1;



GMRES(m) with r=s=100

p=q=1; r=s=100; h=1/ 31;

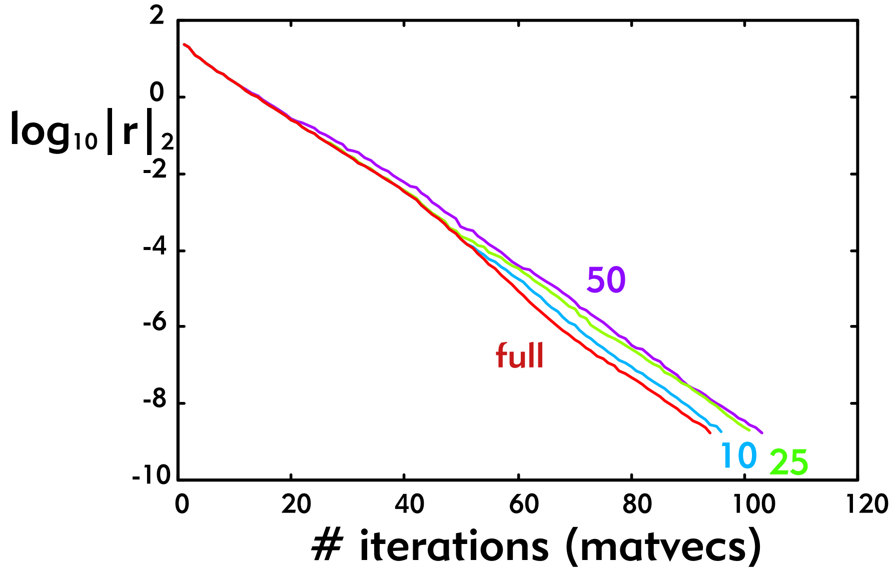
u_s = 0; u_w =0; u_n = 1; u_e = 1;



GMRES(m) with r=s=250

p=q=1; r=s=250; h=1/ 31;

u_s = 0; u_w =0; u_n = 1; u_e = 1;

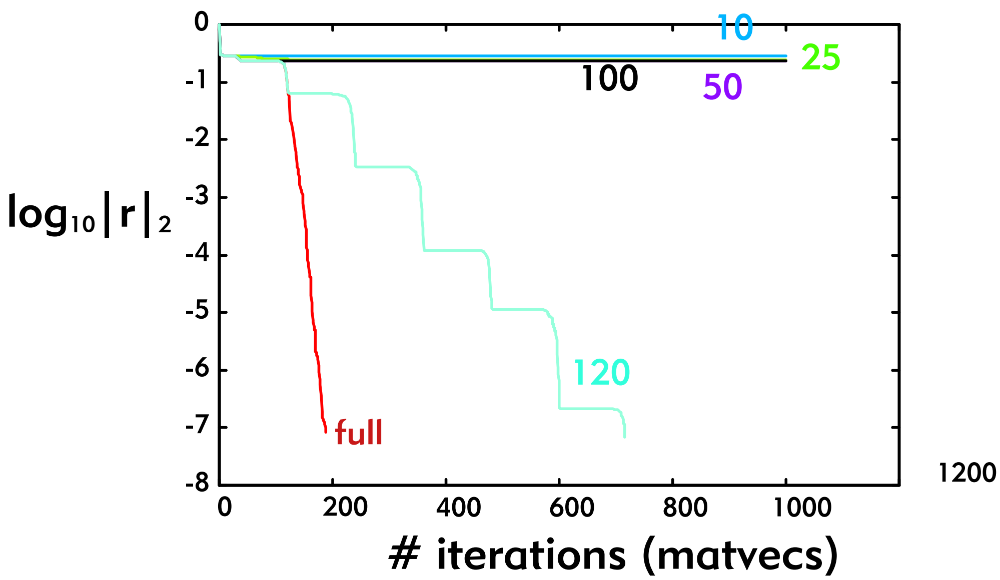


GMRES(m) after shifting spectrum

A=A-3.65*I

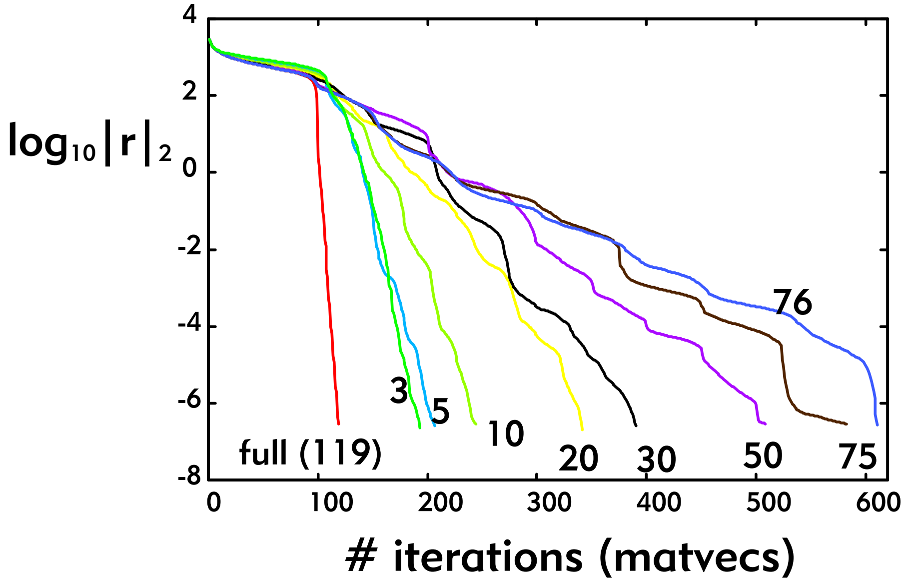
p=q=1; r=s=70; h=1/31;

u_s = 0; u_w =0; u_n = 1; u_e = 1;



Surprising Convergence of GMRES(m)

p=q=1; r=200; s=-200; t=0; f=0; h=1/51;
u_s = 0; u_w =100; u_n = 100; u_e = 0;



Surprising Convergence of GMRES(m)

p=q=1; r=200; s=-200; t=0; f=0; h=1/51;
u_s = 0; u_w =100; u_n = 100; u_e = 0;