Deflated Hermitian Lanczos Methods

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BAYLOR ***HPC systems***

Outline

- *Deflation basics; model systems*
- *Two methods for the solution of hermitian systems with multiple right-hand sides:*

  - Lan-DR(m,k)/D-CG
  - Minres-DR(m,k)/D-Minres

  Will use *M^+M to model pos. def. spectrum and $\gamma_5 M$ to model indefinite one.*

  See: ***arXiv: 0806.3477***

- *Not covered here:* Seed CG – pos. definite spectrum (see our poster)

Deflation basics

Krylov subspace:

$$Span\{r_0, Ar_0, A^2 r_0, \ldots, A^{m-1} r_0\}$$

Starting, residual vectors:

$$r_0 = \sum \beta_i z_i \quad r = r_0 - A\hat{x}$$

$$r = q(A) r_0 = \sum \beta_i q(\lambda_i) z_i$$

q is poly of degree m or less that has value 1 at 0.

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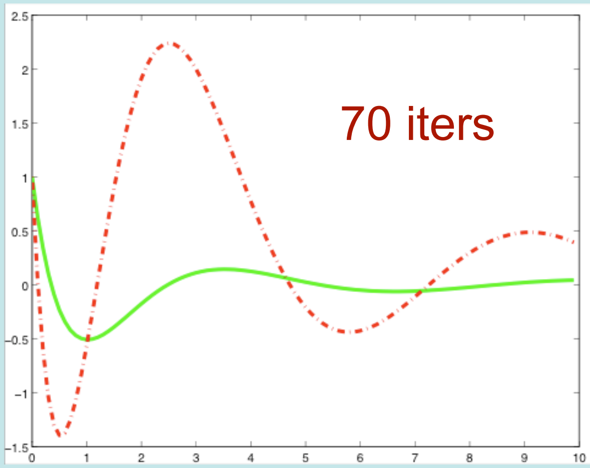
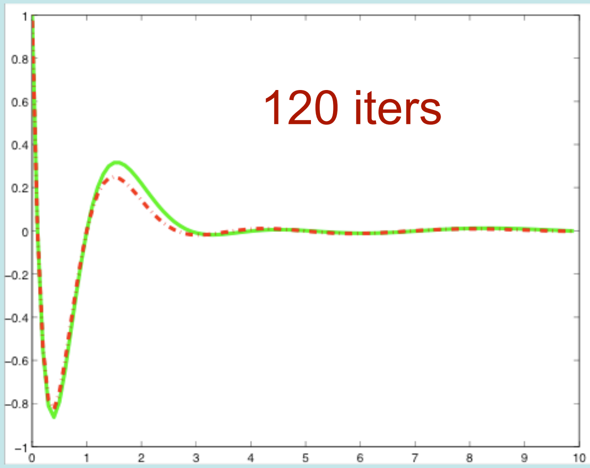
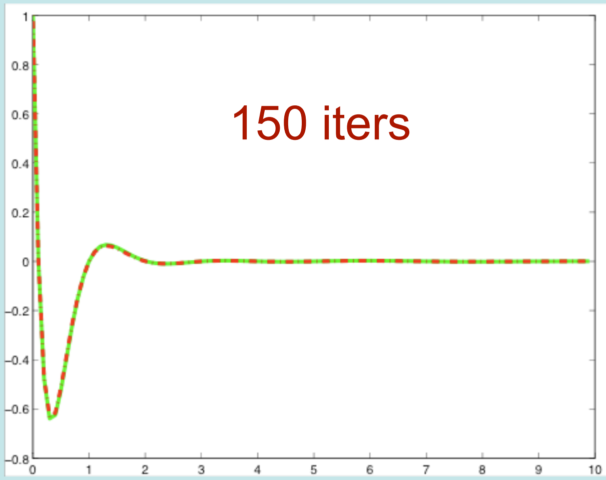
Minres and CG Polynomials (pos. def. spectrum)





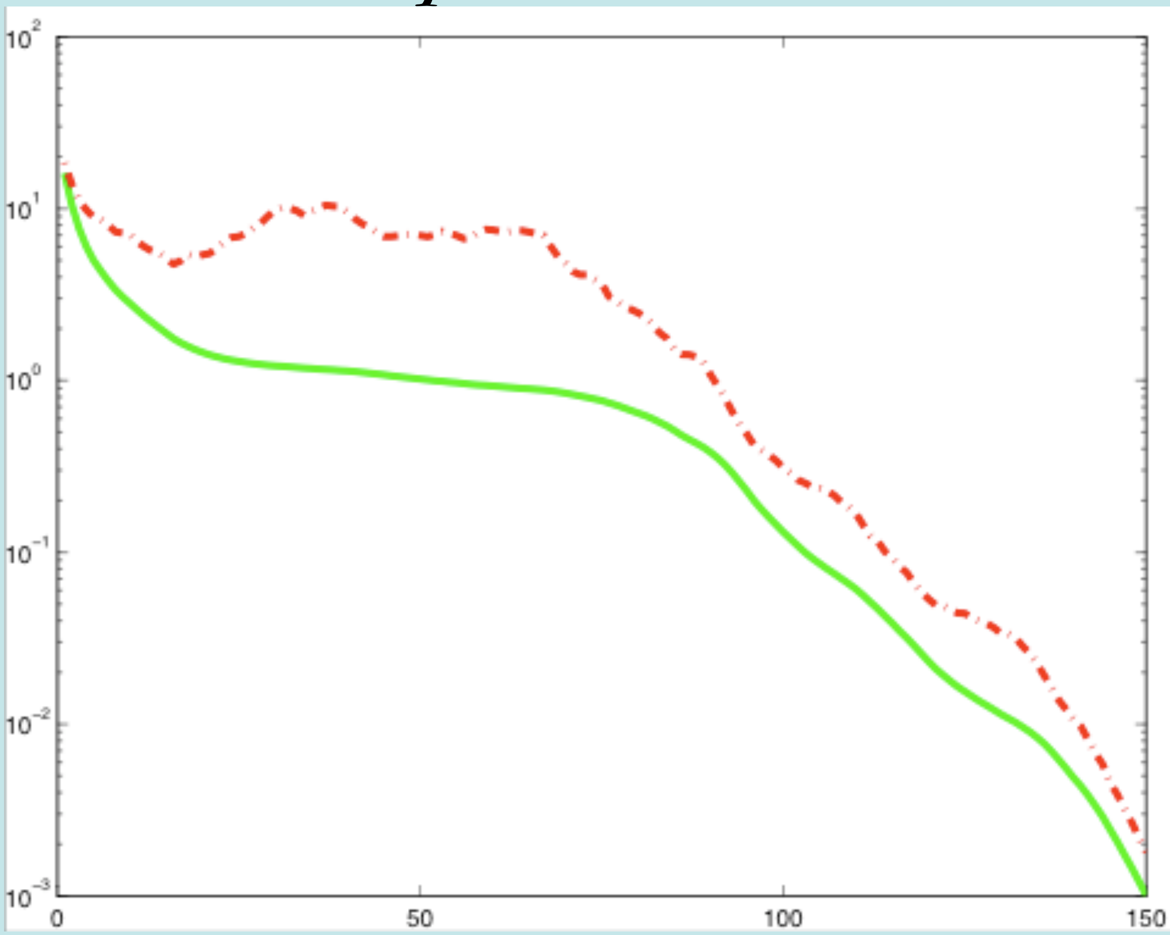


Eigenvalues .1, 1, 2, 3,…, 999;

MinRes and CG polynomials of various degrees

Minres - green; CG - dotted

Minres and CG Convergence (pos. def. spectrum)



Eigenvalues .1, 1, 2, 3,…, 999;

Minres - green; CG - dotted

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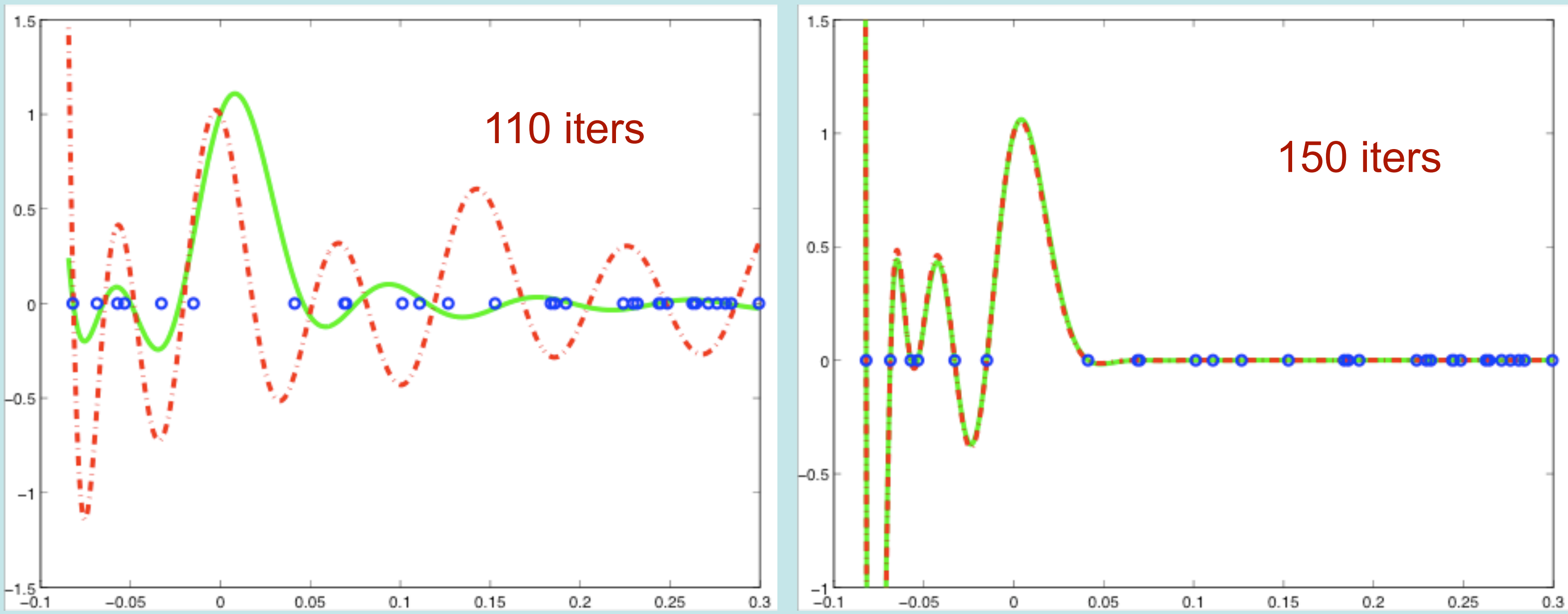
Minres and CG Polynomials (indef. spectrum)

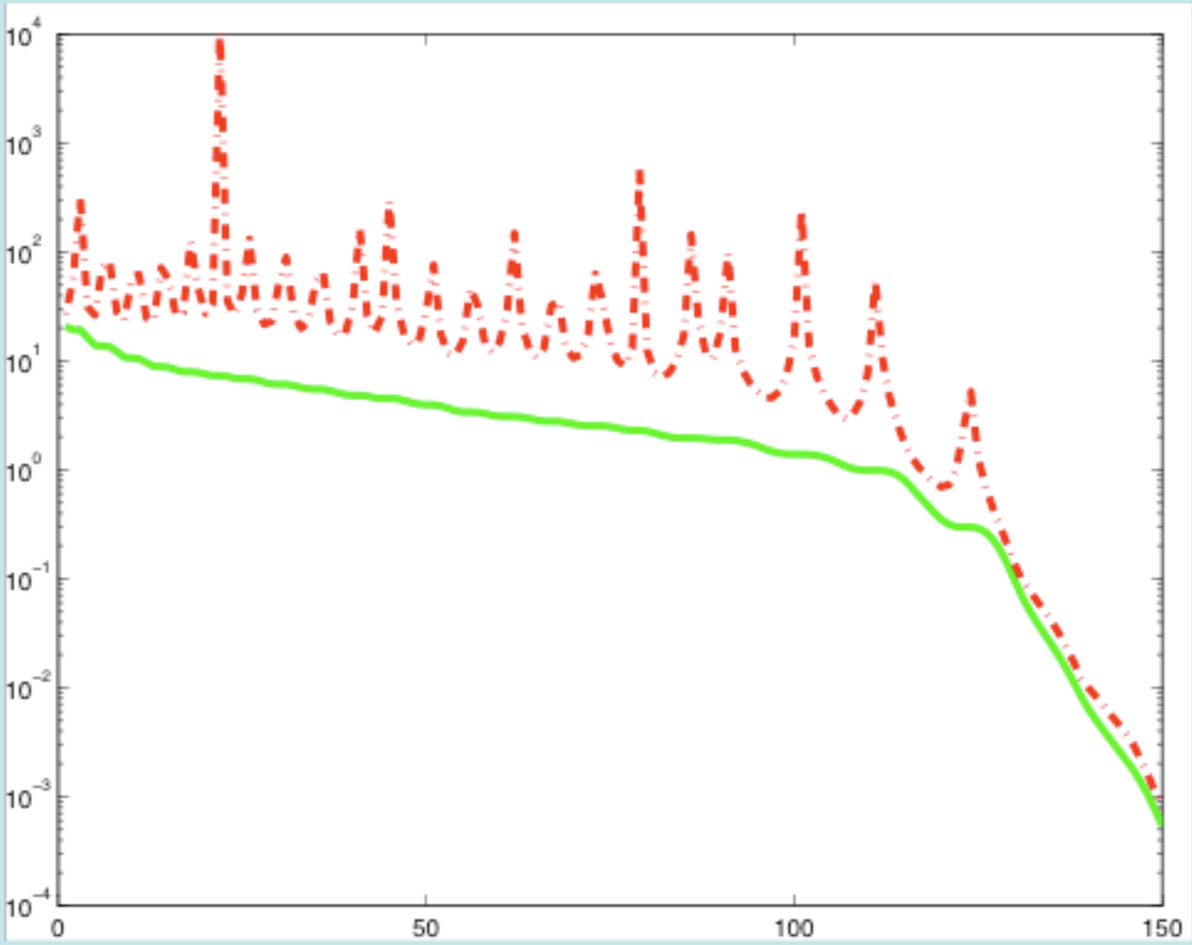


Indefinite problem of dimension 1000.

Entries are random with 22 negative eigenvalues.

Minres - green; CG - dotted

Minres and CG Convergence (indef. spectrum)

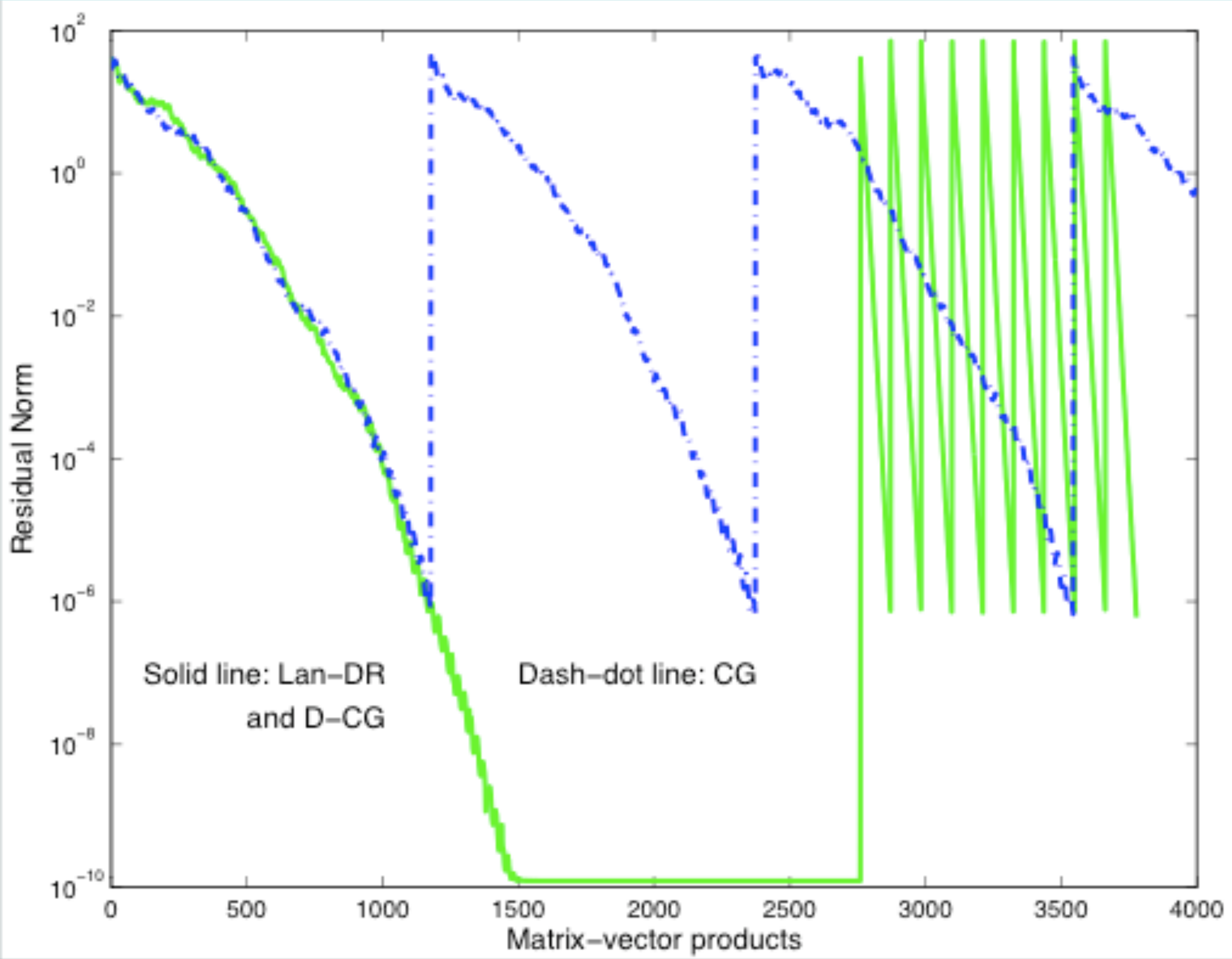


Indefinite problem of dimension 1000.

Entries are random with 22 negative eigenvalues.

Minres - green; CG - dotted

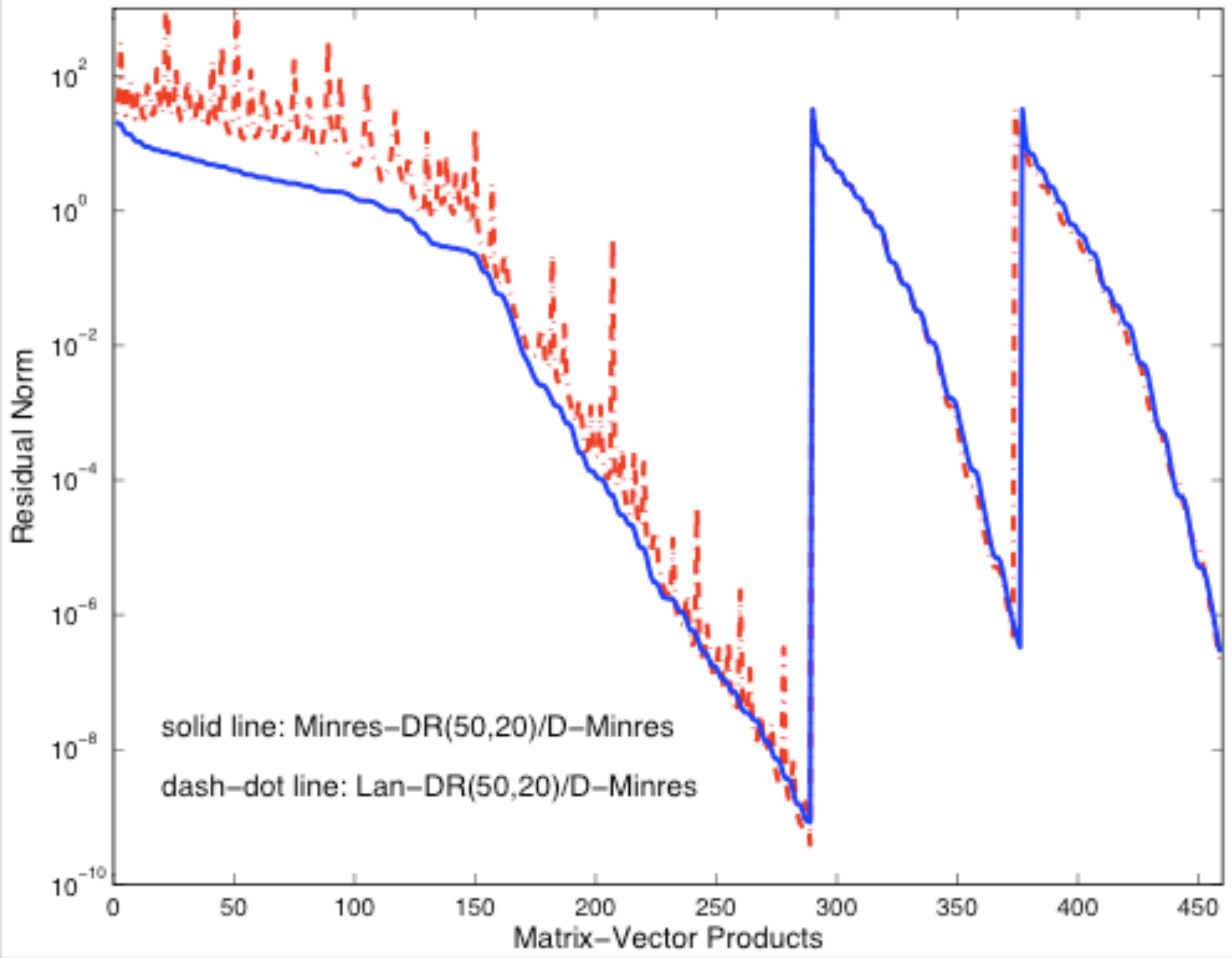
Lan-DR/D-CG vs. regular CG



Eigenvalues .1, .2, …., 9.8,9.9,10,11,12,…, 4910.

44 cycles of *Lan-DR*(180,120)

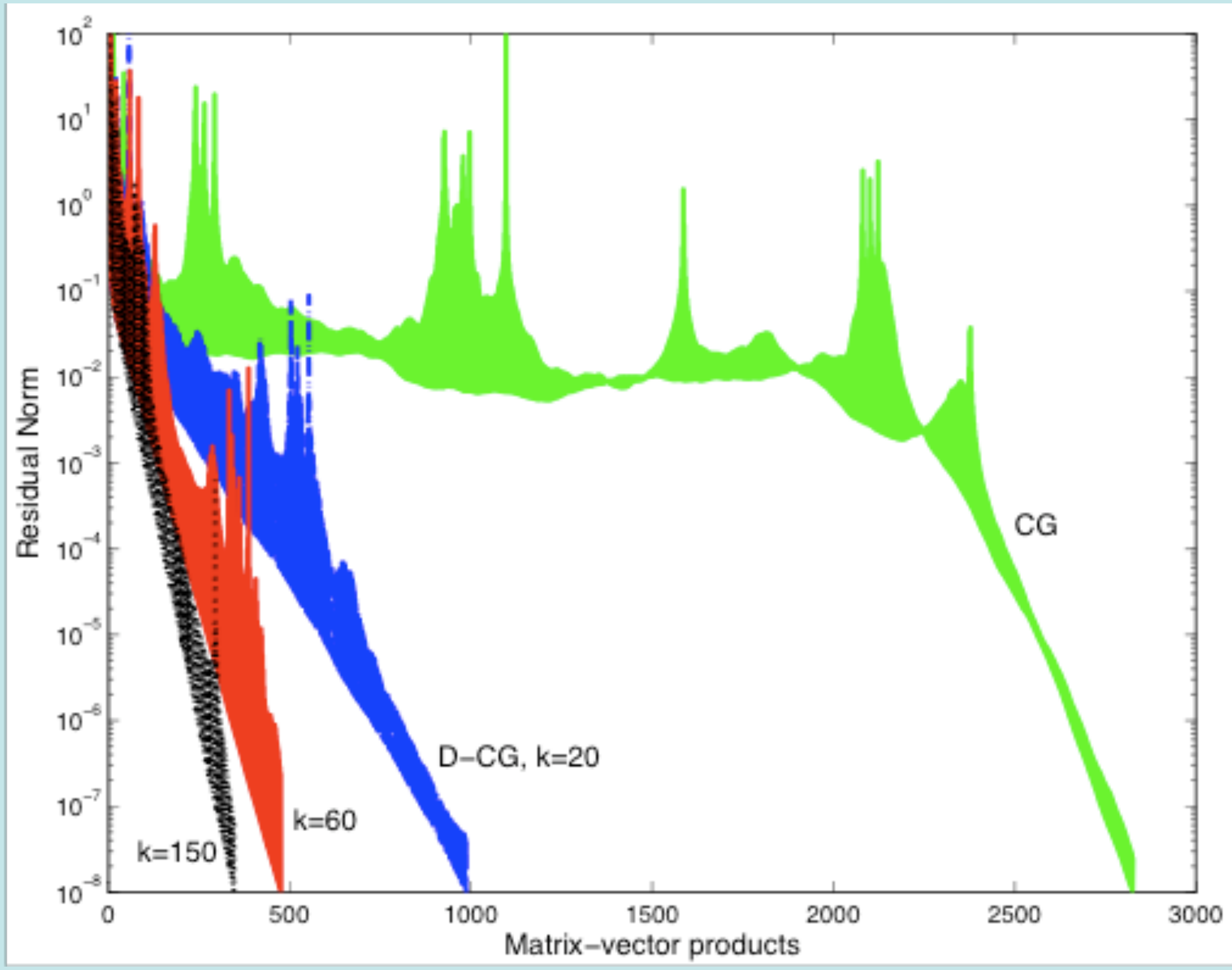
Minres-DR vs. Lan-DR



Indefinite problem of dimension 1000.

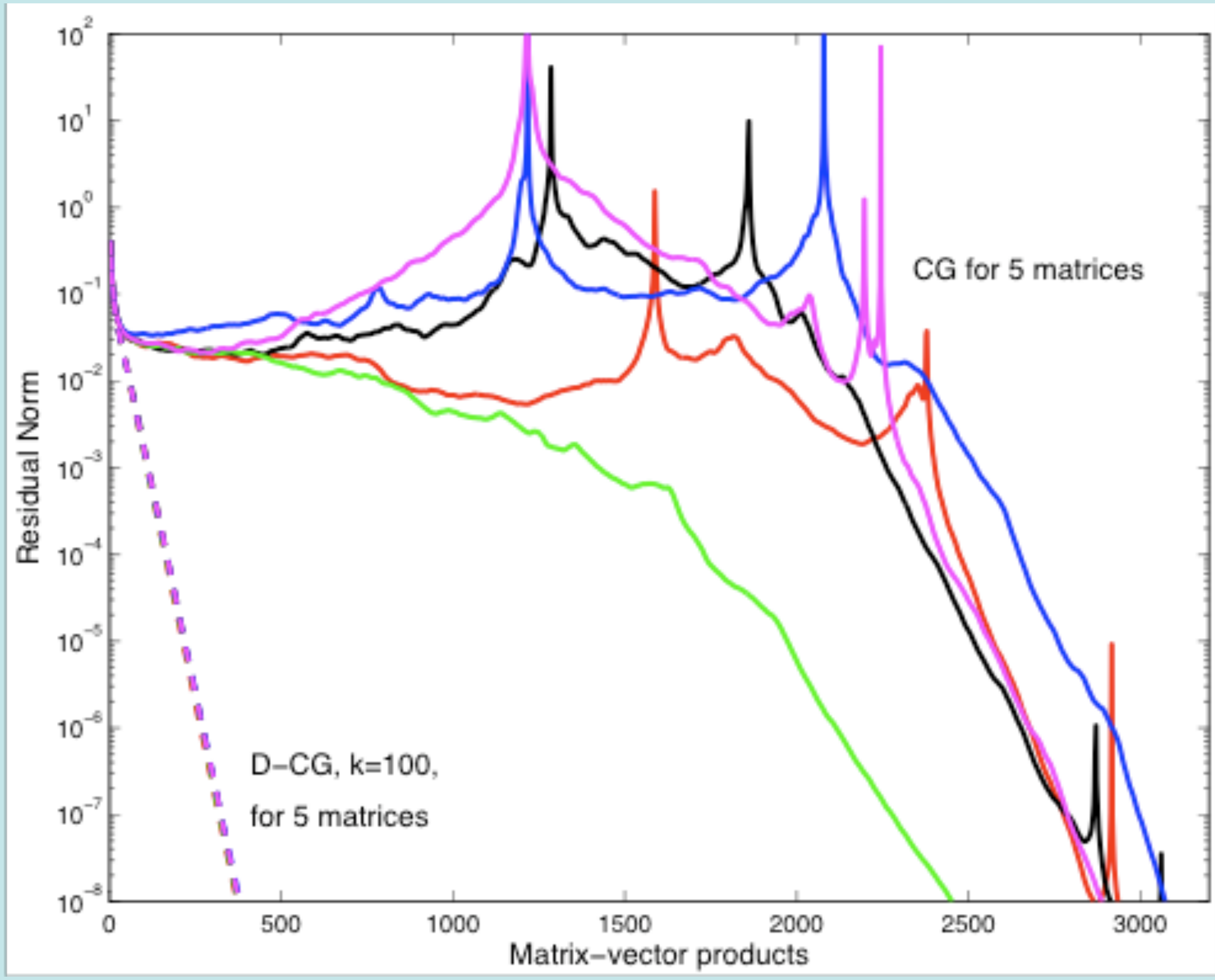
Entries are random with 22 negative eigenvalues.

CG vs. D-CG ($\gamma_5 M$)



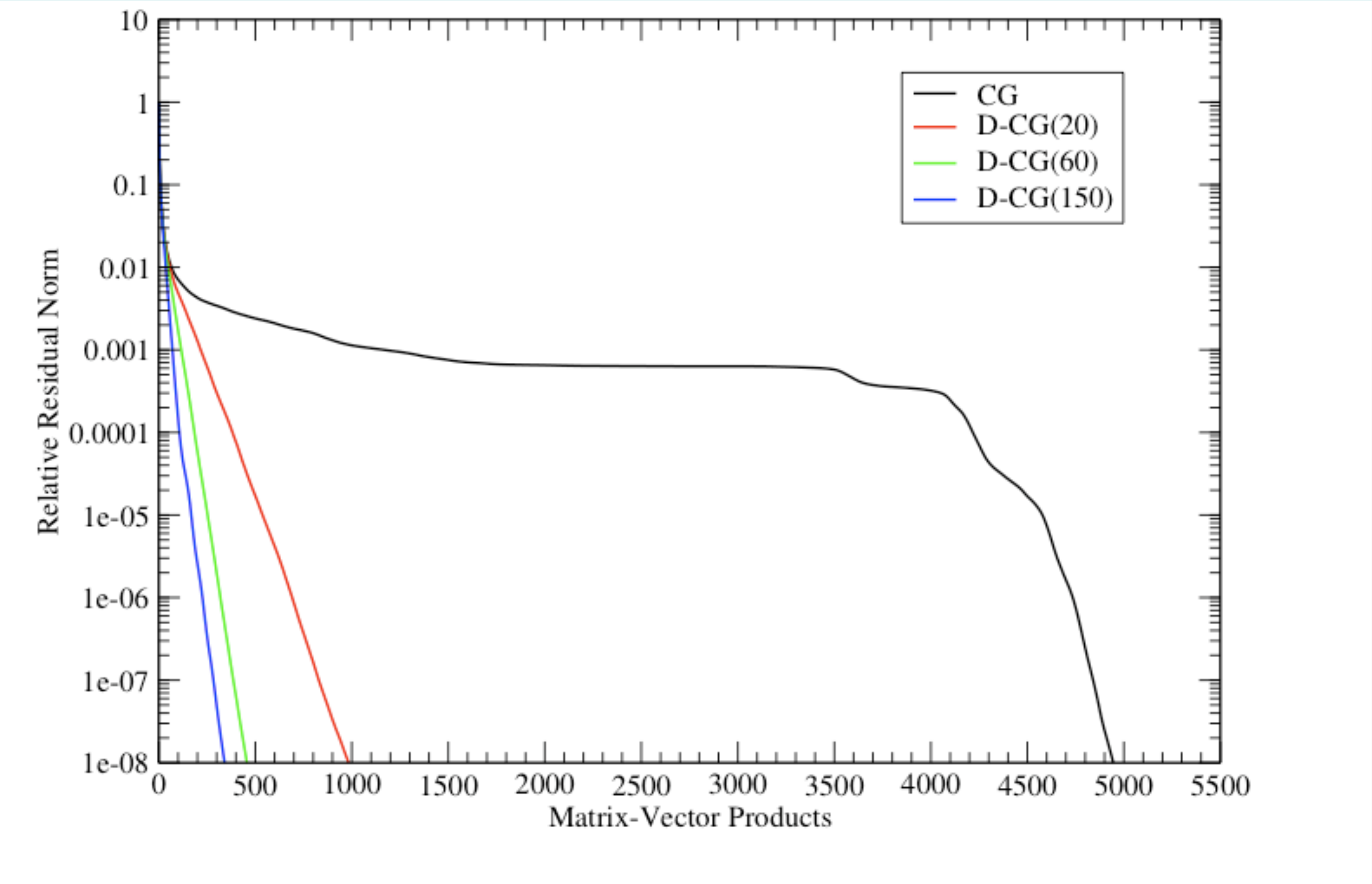
Using deflated *Lan-DR(200,k)* eigenvectors near K_{cr}, 20^3 x 32 lattice (config #1; r for M, on even/odd system).

More on CG vs. D-CG ($\gamma_5 M$)



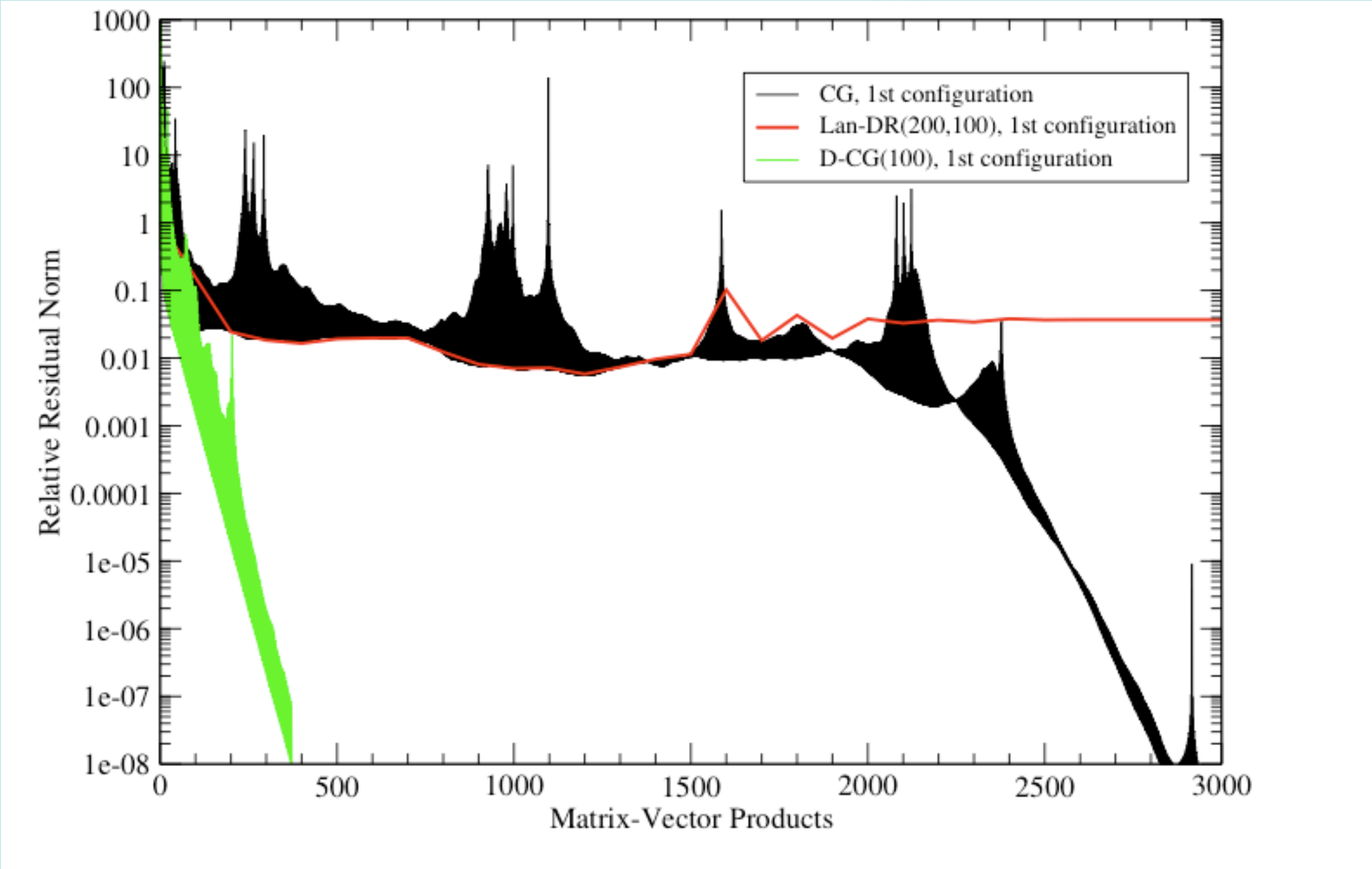
Insensitivity of lattice systems after deflation with *Lan-DR(200,k)*.

D-CG ($M^{+}M$)



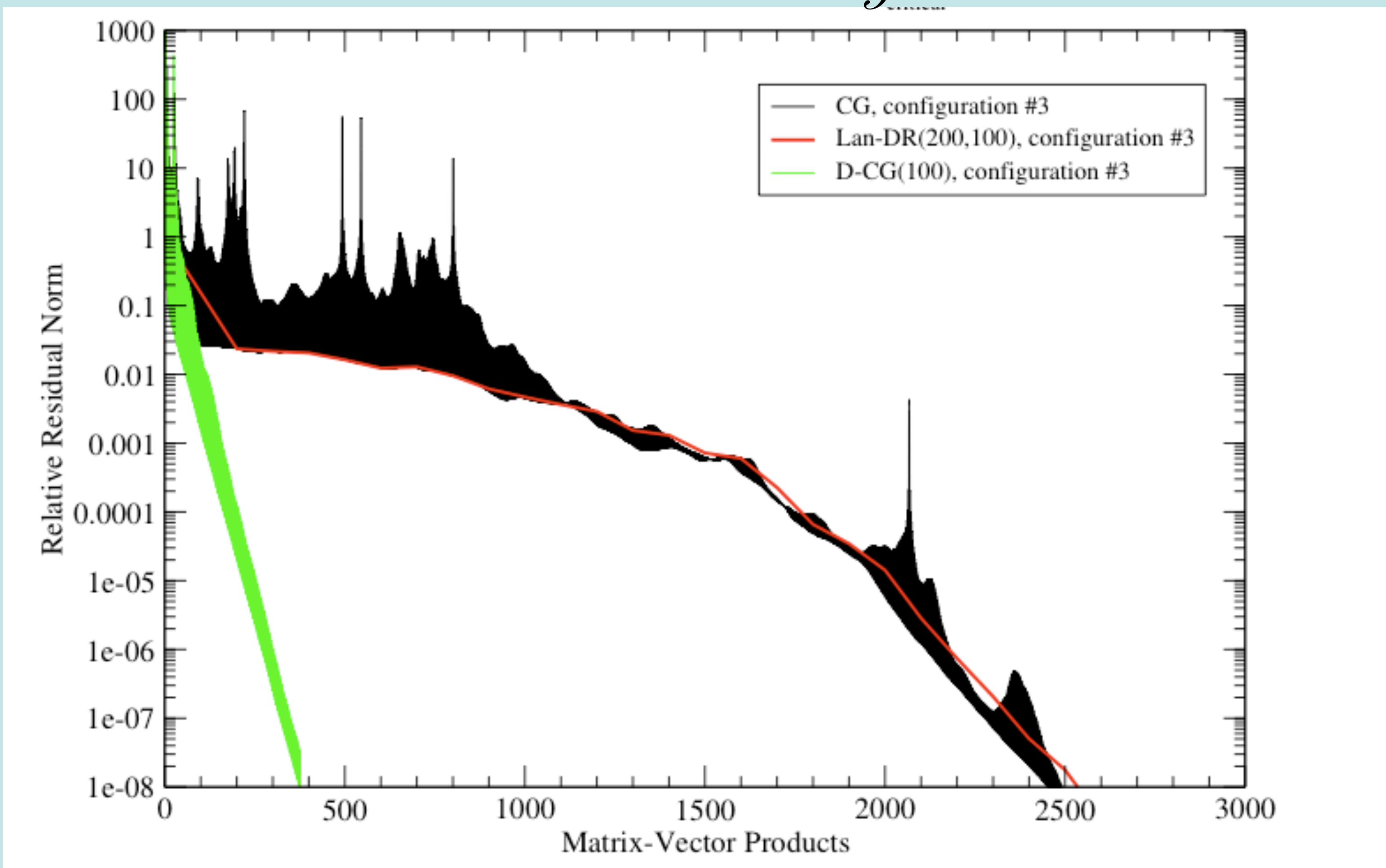
Getting M from $M^{+}M$ (pos. def. spectrum, config. #1; even/odd residual). 1st rhs: *Lan-DR(200,k).*

Lan-DR/D-CG ($\gamma_5 M$)



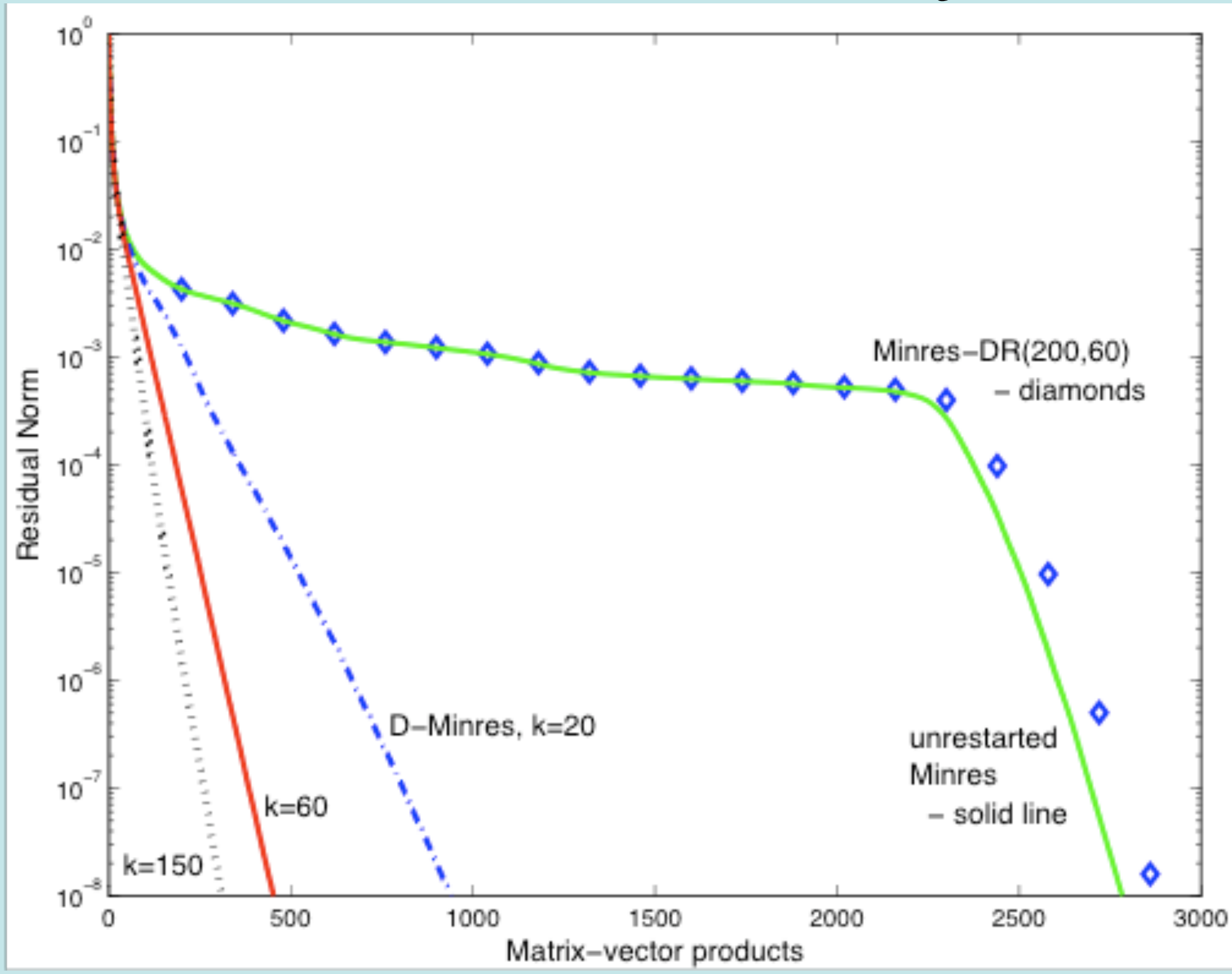
Non-convergence of initial *Lan-DR*(200,100) on config. #1- but eigenvectors are useful! (see also slide 11)

Lan-DR/D-CG ($\gamma_5 M$)



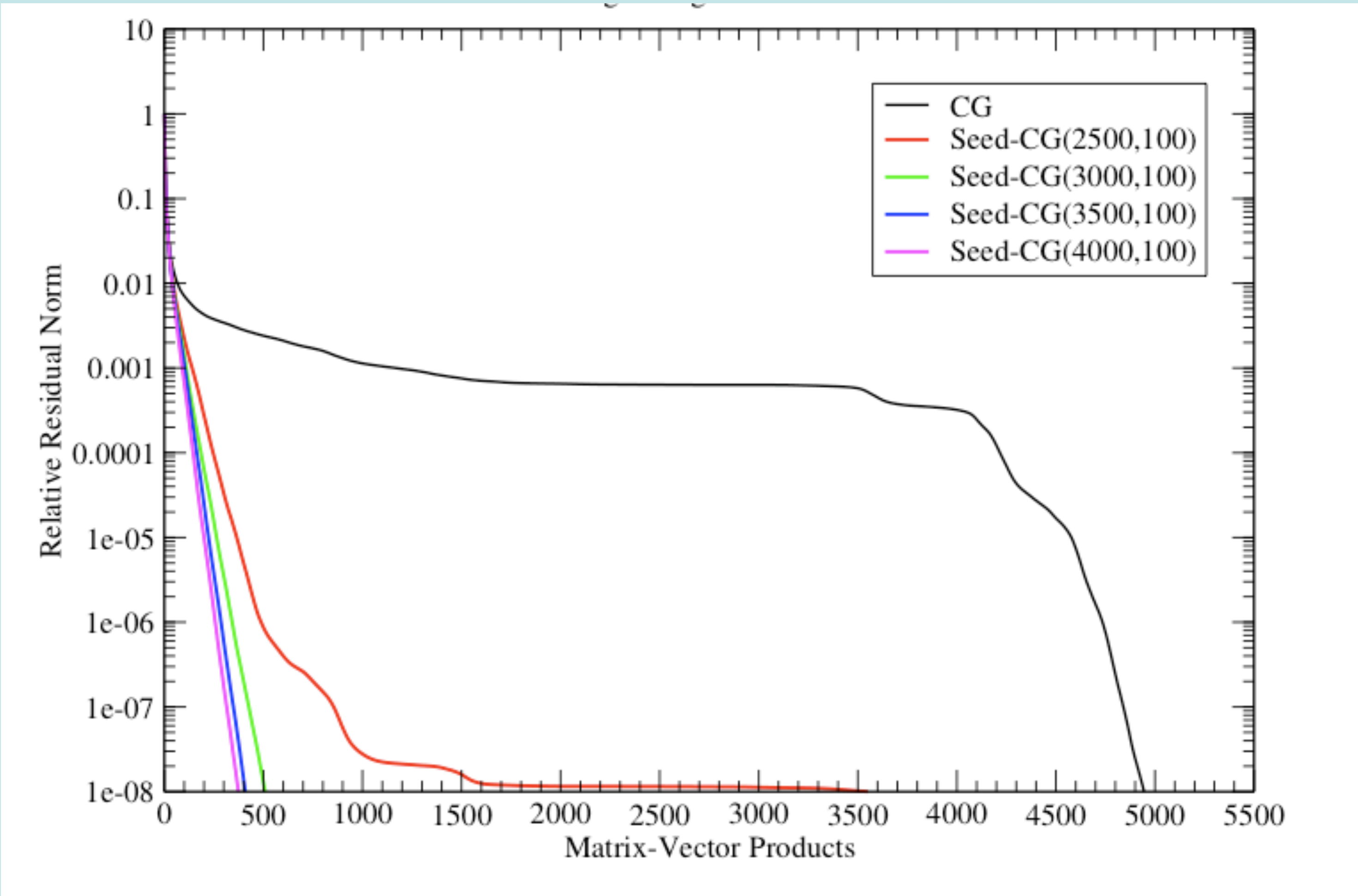
Convergence of initial *Lan-DR*(200,100) for this configuration (#3).

Minres vs. D-Minres ($\gamma_5 M$)



Using γ_5 *M* to get *M* from config.#1 using *D-Minres*.
(Compare with slide 13 for M^+M case.)

Advertisement: Seed-CG vs. CG



Using $M^{+}M$ to get M from config.#1 using *Seed-CG*.
(Compare with slide 13.)

Summary

- *Lan-DR*(*m,k*) combines the solution of linear equations with the calculation of *k* Ritz eigenvectors for hermitian systems. If calculated to sufficient precision, provides *D-CG* an efficient starting point for multiple rhs's.
- *Minres-DR*(*m,k*)/*D-Minres* does the same for systems with an indefinite spectrum using harmonic Ritz vectors. D-Minres on $\gamma_5 M$ was about as fast as D-CG on M^+M.