Iterirani Ritzov postupak

počela, trenutačno stanje, budući razvoj

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Mini – simpozij *Numerički postupci* u okviru projekta *Novi, učinkoviti iteracijski postupak proračuna konstrukcija – poopćenje suvremenih postupaka*

YODA, IP – 2014 – 09 – 2899

10. lipnja 2019.

Hrvatska zaklada za znanost

Iteracijski pristupamo realnom, simetričnom sustavu

$$\mathbf{A}\,\mathbf{x} = \mathbf{b},$$

reda n. Trenutačno rješenje i rezidual su:

$$\begin{aligned} \mathbf{x}_{(i+1)} &= \mathbf{x}_{(i)} + \mathbf{p}_{(i)}, \\ \mathbf{r}_{(i+1)} &= \mathbf{b} - \mathbf{A}\,\mathbf{x}_{(i+1)}. \end{aligned}$$

Prirast rješenja prikažemo diskretiziranim Ritzovim postupkom:

$$\mathbf{p}_{(i)} = \mathbf{\Phi}_{(i)}\,\mathbf{a}_{(i)},$$

gdje su

$$\begin{aligned} \mathbf{\Phi}_{(i)} &= \begin{bmatrix} \phi_{1,(i)} & \phi_{2,(i)} & \ldots & \phi_{m,(i)} \end{bmatrix}, \\ \mathbf{a}_{(i)} &= \begin{bmatrix} a_{1,(i)} & a_{2,(i)} & \ldots & a_{m,(i)} \end{bmatrix}^{\mathrm{T}}. \end{aligned}$$

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Ako su poopćena Ritzova matrica i vektor opterećenja

$$\overline{\mathbf{A}}_{(i)} = \mathbf{\Phi}_{(i)}^{\mathrm{T}} \mathbf{A} \mathbf{\Phi}_{(i)} \quad \text{i} \quad \overline{\mathbf{r}}_{(i)} = \mathbf{\Phi}_{(i)}^{\mathrm{T}} \mathbf{r}_{(i)},$$

oboje reda m, funkcional opadanja energije unutar koraka jest:

$$\Delta f(\mathbf{a}_{(i)}) = \frac{1}{2} \mathbf{a}_{(i)}^{\mathrm{T}} \overline{\mathbf{A}}_{(i)} \mathbf{a}_{(i)} - \mathbf{a}_{(i)}^{\mathrm{T}} \overline{\mathbf{r}}_{(i)}.$$

Iz uvjeta najvećeg opadanja dobivamo mali sustav $(m \ll n)$

$$\overline{\mathbf{A}}_{(i)} \mathbf{a}_{(i)} = \overline{\mathbf{r}}_{(i)},$$

koji treba riješiti u svakom koraku. Potom odredimo

$$\mathbf{p}_{(i)}, \quad \mathbf{x}_{(i+1)} \quad \text{i} \quad \mathbf{r}_{(i+1)}.$$

Prekid postupka: $\|\mathbf{r}_{(i)}\|_2 \leqslant \varepsilon \|\mathbf{r}_{(0)}\|_2$.

Proširenja:

$$\mathbf{x}_{(i+1)} = \mathbf{x}_{(i)} + \omega_{(i)}\,\mathbf{p}_{(i)},$$
$$\mathbf{r}_{(i+1)} = \mathbf{r}_{(i)} - \omega_{(i)}\,\mathbf{A}\,\mathbf{p}_{(i)},$$

gdje je $\omega_{(i)} \in (0, 2)$ faktor relaksacije poznat iz postupka SOR.

Dvornik, J.: *Generalization of the CG Method Applied to Linear and Nonlinear Problems*, Trends in computerized structural analysis and synthesis; Proceedings of the Symposium (urednici Noor, A. K. i Mccomb, H. G. Jr.), NASA, Langley Research Center, Washington D. C., 30. X – 1. XI 1978., Pergamon Press, str. 217. – 223.

Dvornik, J.: *Generalization of the CG Method Applied to Linear and Nonlinear Problems*, Computers & Structures, **10** (1979) 1/2, str. 217.–223.

Kratki teorijsko – povijesni uvod

Computers & Structures Vol 10, pp. 217–223
0045-7949/79/0401-0217/$02.00/0

GENERALIZATION OF THE CG METHOD APPLIED TO LINEAR AND NONLINEAR PROBLEMS

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(*Received* 19 *May* 1978)

Abstract—A method of solving a set of linear equations through iteration process is described. In every step of the process the Ritz method is applied. With a suitably chosen procedure for generating coordinate vectors, the process is efficient when applied to nonlinear and in some cases even to linear problems. Present experience is limited, and no objective criteria have been developed for an *a priori* judgment of coordinate vectors what would very probably contribute to the efficiency. Some standard iterative algorithms can be interpreted as special cases of this procedure.

- povratak postupku: rane devedesete
- motivacija: rad S. Polića na pločama umjerene debljine
- pristup metodom konačnih razlika
- riješeno $1,6 \cdot 10^6$ jednadžbi

```
PROGRAM GCGMETHOD

c##############################################################
c     iterativni algoritam za rjesavanje velikih sustava
c     linearnih algebarskih jednadzbi oblika 'Ax=b' sa
c     simetricnom i pozitivno definitnom matricom sustava 'A'

c     izradili:      Prof.dr. Josip Dvornik   dipl.ing.gradj.
c                             Damir Lazarevic dipl.ing.gradj.
c###############################################################

IMPLICIT DOUBLE PRECISION (A-H,O-Z)

c########################################
c     NM - broj koordinatnih vektora
c     sve potrebne vektore smjestamo u
c     dinamicki alocirani vektor 'L'
c########################################

PARAMETER (NM=5, NMAX=100000000)
COMMON L(NMAX)
```

```
I1=2*K+1
I2=I1+K
I3=I2+N+1
I4=I3+2*N
I5=I4+2*N
I6=I5+2*N
I7=I6+2*N
I8=I7+2*N*NM
I9=I8+2*N*NM
I10=I9+2*N
I11=I10+2*NM*NM
I12=I11+2*NM
I13=I12+2*NM
I14=I13+NM-1

CALL INPUT ( N,K,I14,L(1),L(I1),L(I2),L(I3),OM1,OM2,EPS1,EPS2 )

CALL SOLVER ( N,NM,OM1,OM2,EPS1,EPS2,L(1),L(I1),L(I2),L(I3),
     *          L(I4),L(I5),L(I6),L(I7),L(I8),L(I9),L(I10),L(I11),
     *          L(I12),L(I13) )
```

O koordinatnim vektorima

- povremena primjena kroz stručni rad zavoda
- povratak drugi put: 2014. godine
- istraživački projekt HRZZ–a: 2015. godine
- poboljšana inačica: IRM (*Iterated Ritz Method*)
- nije riječ o iteraciji po potprostorima
- najbliži su projektivni postupci

Sve je u koordinatnim vektorima

Uvjet konvergencije:

$$\mathbf{\Phi}_{(i)} = \left[\phi_{1,(i)}\right] \not\angle \left[\mathbf{r}_{(i)}\right].$$

Može ih biti i više, samo moraju biti linearno nezavisni:

$$\mathbf{\Phi}_{(i)} = \left[\mathbf{P}\,\mathbf{r}_{(i)} \quad \mathbf{p}_{(i-1)} \quad \phi_{3,(i)} \quad \phi_{4,(i)} \quad \cdots \quad \right].$$

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O koordinatnim vektorima

- matrica $\mathbf{P}$: „jeftina” i dobro aproksimira $\mathbf{A}^{-1}$
- tvorba: SOR, SSOR, ICC, AMG, SAI, čak i loši postupci, ...
- preduvjetovanje: $\mathbf{P} = \mathbf{M}^{-1}$, $(\mathbf{M}^{-1}\mathbf{A}\,\mathbf{x} = \mathbf{M}^{-1}\mathbf{b})$
- realizacija: različiti redoslijedi nepoznanica

Ovisno o $\mathbf{\Phi}_{(i)}$ neki su postupci posebni slučajevi IRM–a:

- Gauß–Seidel: $\mathbf{\Phi}_{(i)} = \left[\mathbf{e}_{(i)}\right]$ i $\omega_{(i)} = 1$
- SOR: kao GS ali $\omega_{(i)} \neq 1$
- najstrmiji silazak: $\mathbf{\Phi}_{(i)} = \left[\mathbf{r}_{(i)}\right]$
- Jacobi: $\mathbf{\Phi}_{(i)} = \left[\mathbf{D}^{-1}\,\mathbf{r}_{(i)}\right]$
- konjugirani gradijenti: $\mathbf{\Phi}_{(i)} = \left[\mathbf{r}_{(i)} \quad \mathbf{p}_{(i-1)}\right]$
- Krilovljevi postupci: $\mathbf{\Phi}_{(i)} = \left[\mathbf{r}_{(0)} \quad \mathbf{A}\,\mathbf{r}_{(0)} \quad \mathbf{A}^2\,\mathbf{r}_{(0)} \quad \dots \quad \right]$
- projektivni postupci,...

Trenutačno stanje postupka

- jedan ili dva vektora vjerojatno premalo
- više vektora: veće smanjenje energije, ali „skuplji” korak
- težnja: mali broj učinkovitih vektora ($m \leqslant 10$)
- skup potencijalno dobrih vektora je golem
- teorija i kriteriji izbora optimalnog potprostora nepoznati

Trenutačno stanje postupka

Vektori generirani postupkom SSOR ($2 \leqslant m \leqslant 10$):

$$
\begin{aligned}
\phi_{1,(i)} &= \mathbf{L}_\Omega^{-1}\,\mathbf{D}\,\mathbf{U}_\Omega^{-1}\,\mathbf{r}_{(i)}, \\
\phi_{j,(i)} &= \mathbf{L}_\Omega^{-1}\,\mathbf{D}\,\mathbf{U}_\Omega^{-1}\,(\mathbf{A}\,\phi_{j-1,(i)}), \qquad j = 2,\ldots,m-1, \\
\phi_{m,(i)} &= \mathbf{p}_{(i-1)},
\end{aligned}
$$

gdje je $\Omega \notin (0,2)$ lokalni faktor relaksacije.

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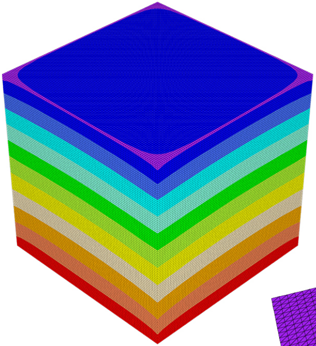
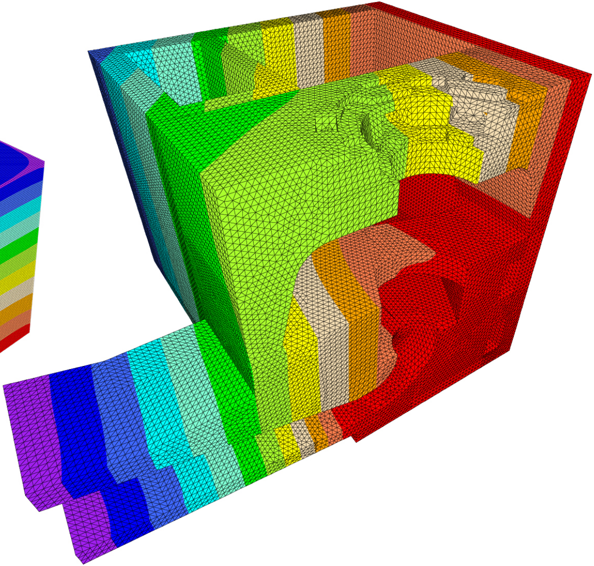
Ukratko o realizaciji i testiranju

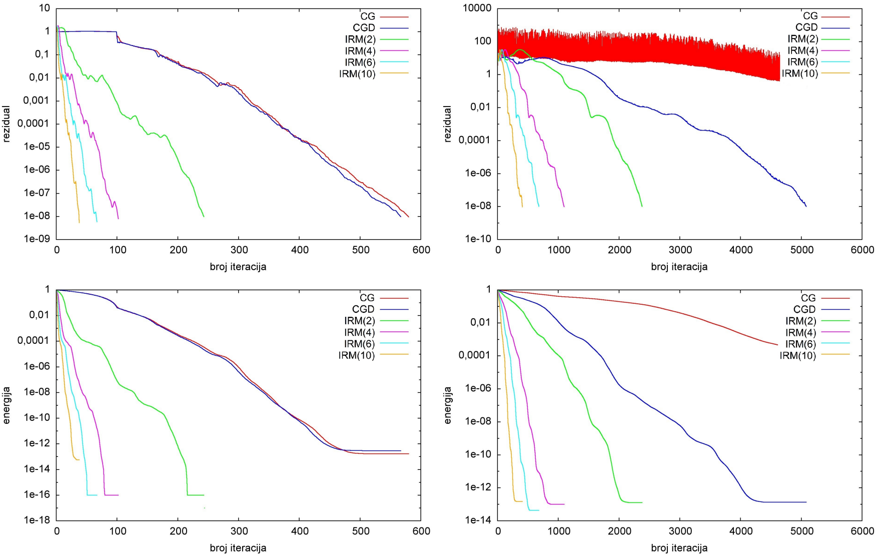
- gfortran, 64-bitne inačice: Ubuntu (5.3.1) i OS X (6.1.0)
- štedni zapisi matrice: CSC ili CSR, adresirano 512 GB RAM–a
- spajanje s FEAP–om (8.4.1)
- provjere na:
  - vrlo malim modelima (korak po korak)
  - različito generiranim ravninskim i prostornim rešetkama
  - raznovrsnim modelima iz naše prakse
- nužno: poznata je ovisnost o naravi problema
- konvergencija ovisi o razdiobi krutosti, ležajeva i opterećenja
- riješeno preko 10^7 (ekstrem $1,9 \cdot 10^8$) jednadžbi
- broj uvjetovanosti $10^3 \leqslant \kappa(\mathbf{A}) \leqslant 10^{11}$
- popunjenost matrice: od 10^{-4} do 10^{-7}

Realizacija i testiranje





Realizacija i testiranje



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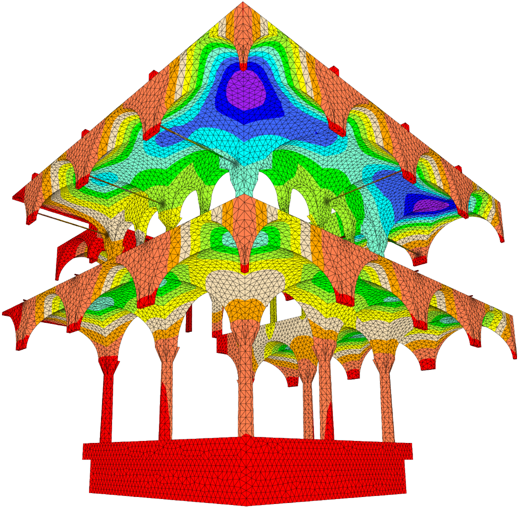
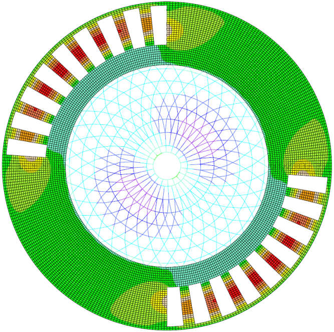
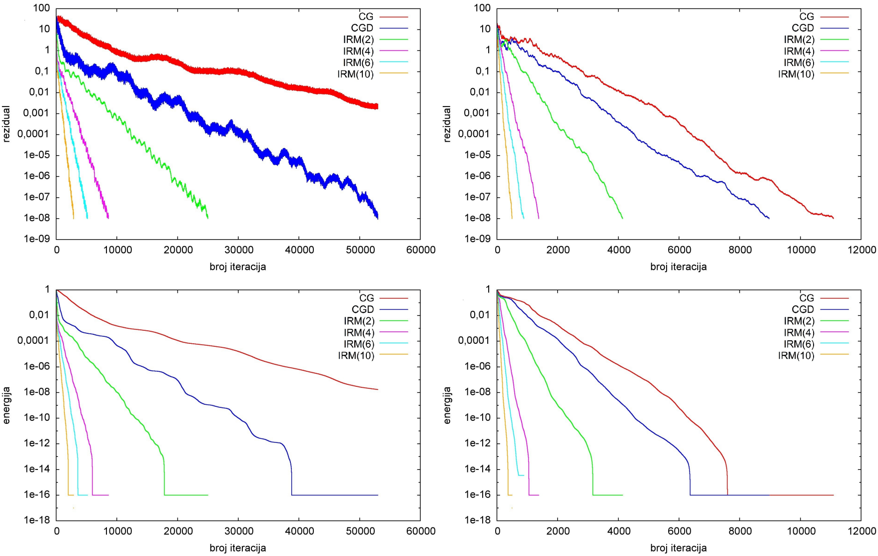




Realizacija i testiranje



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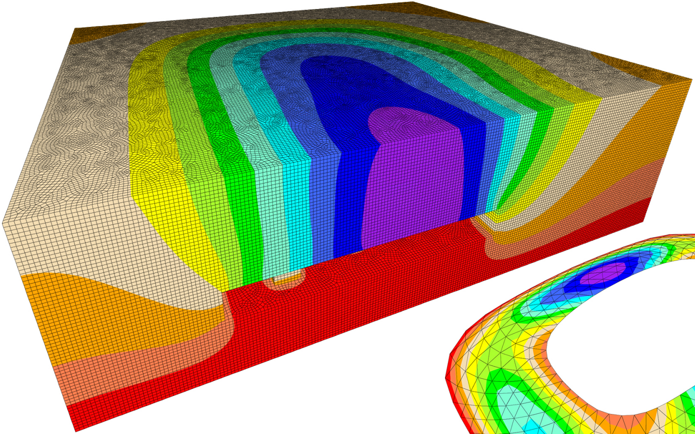

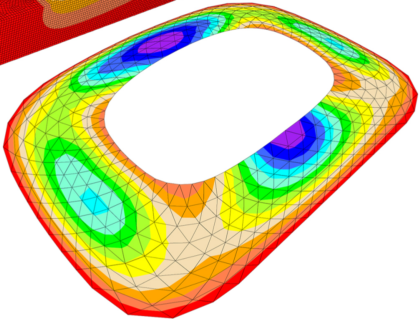

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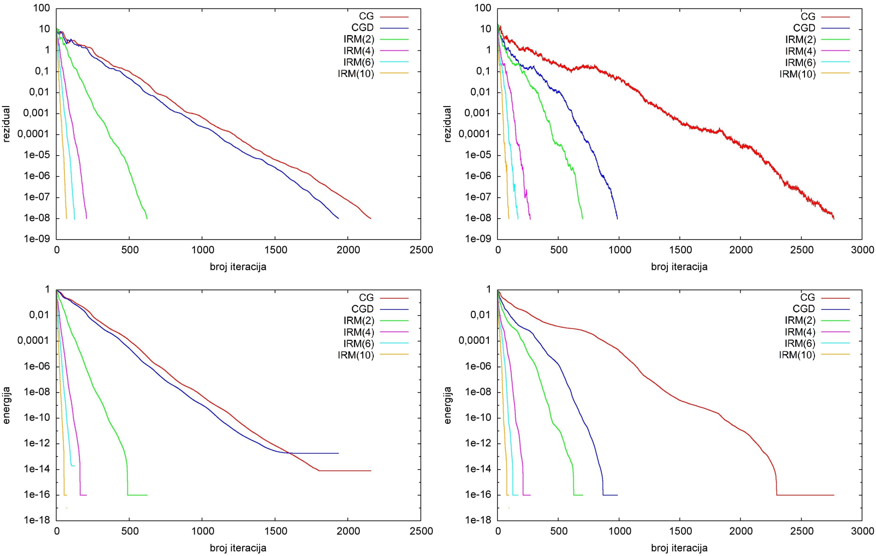

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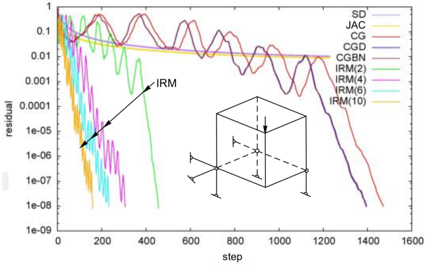

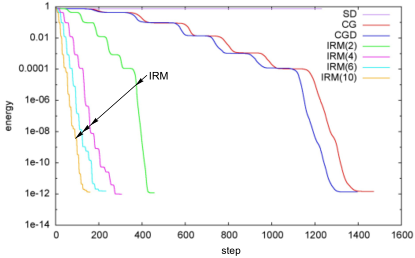

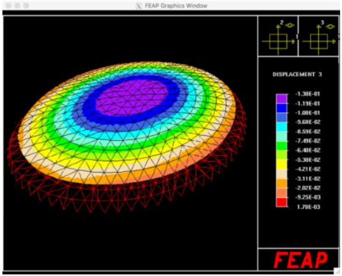

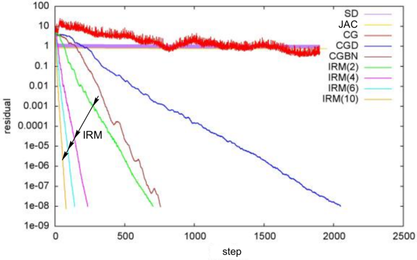

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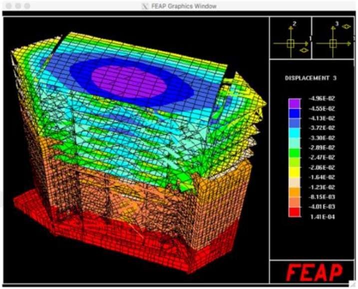

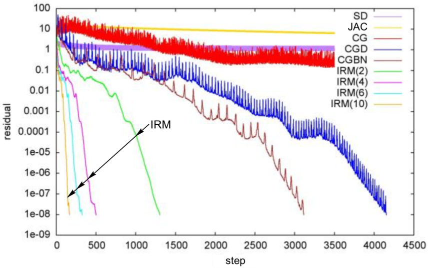

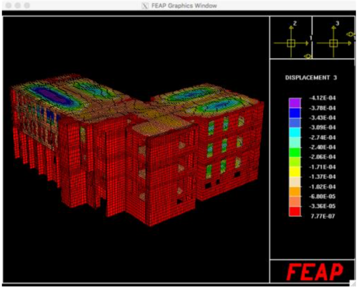

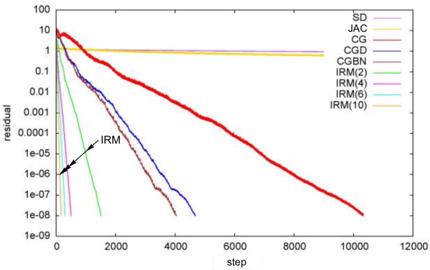

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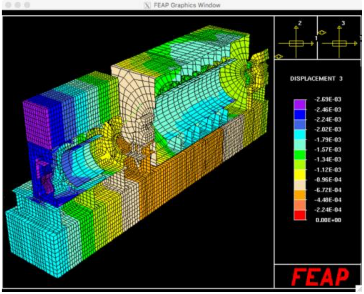
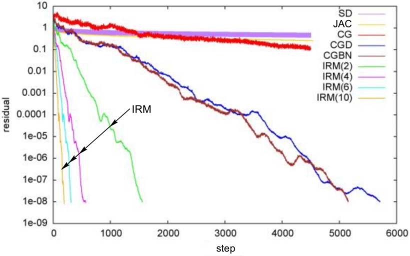
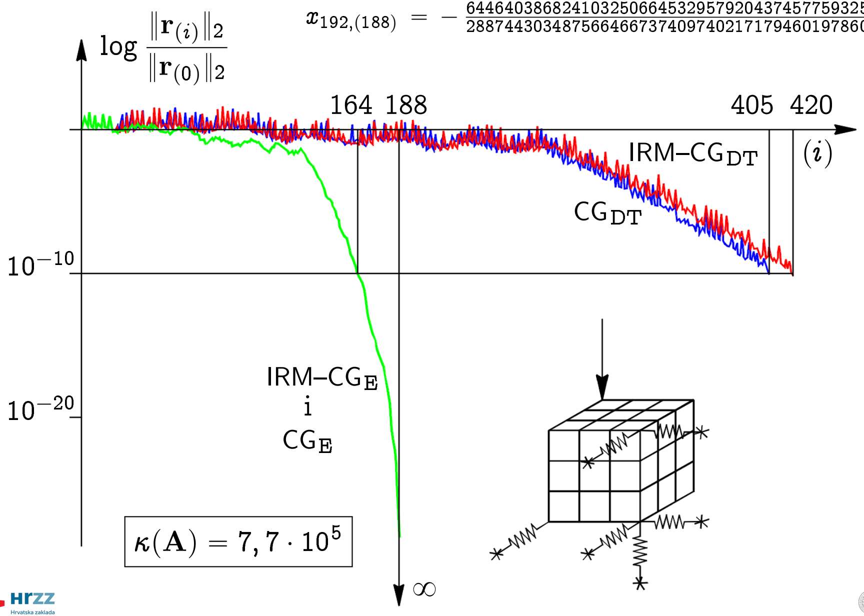


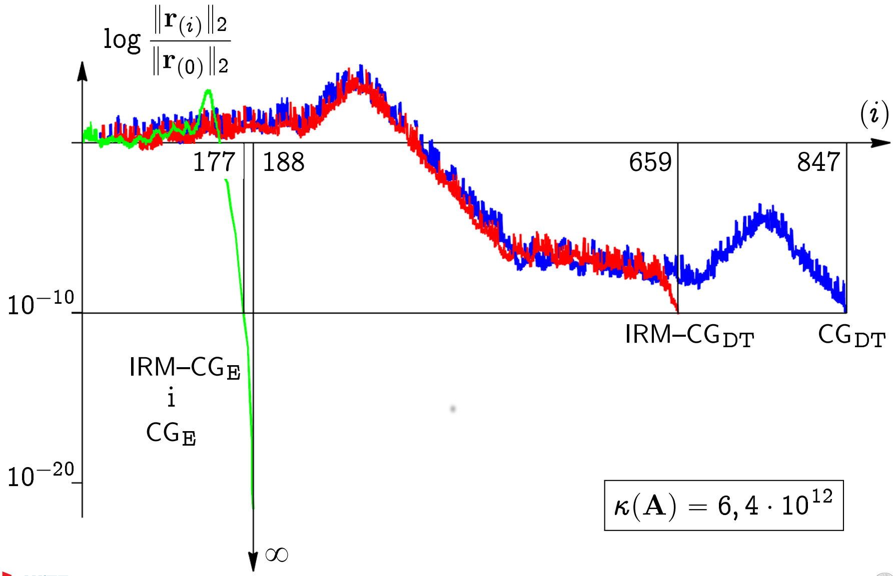


- temeljna prednost: vrlo stabilan postupak
- dobri rezultati za veliki $\kappa(\mathbf{A})$ i mali ε
- razlog: ne primjenjuje se rekurzivna $\mathbf{A}$–ortogonalizacija
- manja osjetljivost na gomilanje pogrešaka zaokruživanja
- provjere uz primjenu egzaktne aritmetike (Mathematica)
- ulazni podaci i tijek proračuna: cijeli brojevi i razlomci

Primjena egzaktne aritmetike

$$x_{192,(188)} = -\frac{6446403868241032506645329579204374577593254 13}{2887443034875664667374097402171794601978600 00}$$

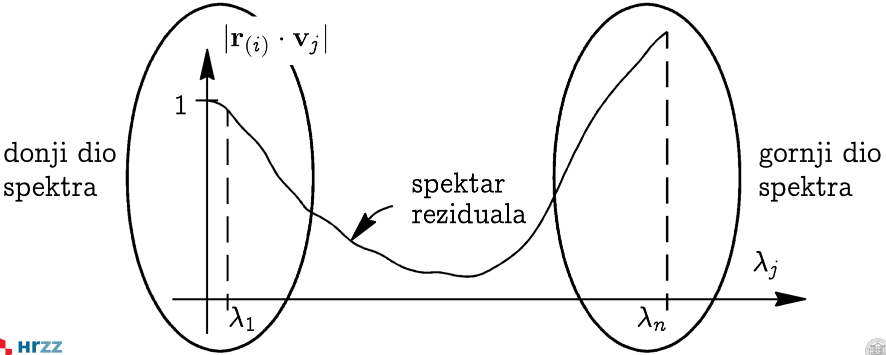



log $\frac{\|\mathbf{r}_{(i)}\|_2}{\|\mathbf{r}_{(0)}\|_2}$
(i)
177
188
659
847
10^{-10}
10^{-20}
IRM–CG$_{\mathrm{DT}}$
CG$_{\mathrm{DT}}$
IRM–CG$_{\mathrm{E}}$
i
CG$_{\mathrm{E}}$
∞
$\kappa(\mathbf{A}) = 6,4 \cdot 10^{12}$

Težnja: povećati omjer $\Delta \mathbf{r}_{(i)} / \Delta t_{(i)}$ (malo brzih koraka)

Putovi napretka

- traganje za boljim vektorima (zapravo matricom $\mathbf{P}$)
- primjena zamisli *spektra reziduala*



Hrvatska zaklada za znanost

Minimizacija kvadrata reziduala

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathbf{A}\,\mathbf{x} - \mathbf{x}^T \mathbf{b}.$$

$$\mathbf{r}^T\mathbf{r} = (\mathbf{b} - \mathbf{A}\,\mathbf{x})^T(\mathbf{b} - \mathbf{A}\,\mathbf{x}) = \mathbf{b}^T\mathbf{b} - 2\,\mathbf{x}^T\mathbf{A}\,\mathbf{b} + \mathbf{x}^T\mathbf{A}^2\,\mathbf{x}$$

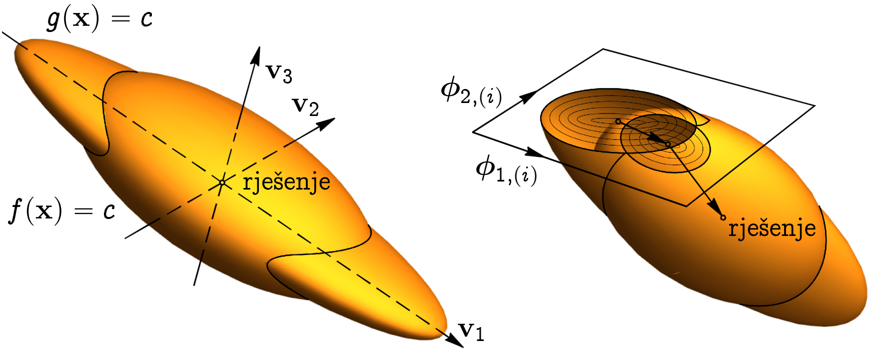
$$g(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{A}^2\,\mathbf{x} - \mathbf{x}^T\mathbf{A}\,\mathbf{b}$$

$$\mathbf{A}^2\,\mathbf{x} = \mathbf{A}\,\mathbf{b},$$

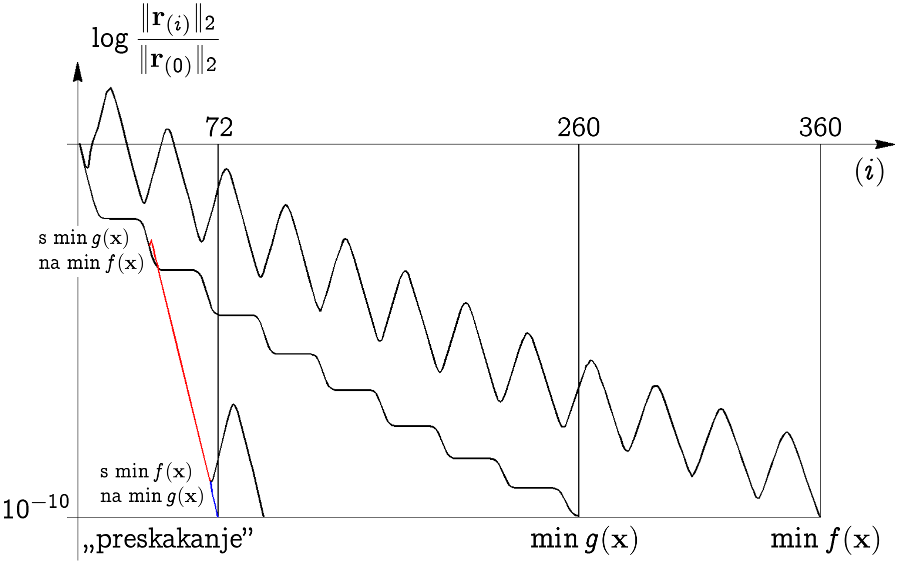
- polazni sustav loše preduvjetovan s $\mathbf{A}$: $\kappa(\mathbf{A}^2) = \kappa(\mathbf{A})^2$
- $\mathbf{A}^2$ više popunjena od $\mathbf{A}$
- isti $\mathbf{v}_j$ i $(\lambda_j)_{\mathbf{A}^2} = (\lambda_j^2)_{\mathbf{A}}$

HRZZ Hrvatska zaklada za znanost

Budući razvoj



- min $f(\mathbf{x})$: energija pada monotono, rezidual nepravilno
- min $g(\mathbf{x})$: oboje pada monotono (IRM stabilniji i često brži)
- ne primjenjujemo rezidual $\mathbf{A}\,\mathbf{r}$, nego $\mathbf{r}$
- istoznačno preduvjetovanju s $\mathbf{A}^{-1}$
- vraća uvjetovanost izvornoga sustava



$\log \frac{\|\mathbf{r}_{(i)}\|_2}{\|\mathbf{r}_{(0)}\|_2}$
72
260
360
(i)
s min $g(\mathbf{x})$
na min $f(\mathbf{x})$
s min $f(\mathbf{x})$
na min $g(\mathbf{x})$
10^{-10}
„preskakanje”
min $g(\mathbf{x})$
min $f(\mathbf{x})$

Optimizacija koda

- prof. Fresl sa suradnicama
- brižljivo programiranje (20% brži korak)
- bitni načini programskog prevođenja i povezivanja
- i učinci optimizacijskih opcija
- ponešto u posebnom članku

Što još?

- brojna testiranja i usporedbe s drugim postupcima
- paralelizacija: svakom koordinatnom vektoru procesor
- obećava primjena na nelinearne probleme

Kratica projekta: **YODA**.

Hard to see, the dark side is.

YODA
Georg Lucas: Star Wars, Episode I:
The Phantom Menace (1999.)