IDR(s)

A family of simple and fast algorithms for solving large nonsymmetric systems of linear equations

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Outline

- Introduction
- The Induced Dimension Reduction Theorem
- The IDR(s) algorithm
- Numerical experiments
- Conclusions

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Product Bi-CG methods

Bi-CG solves nonsymmetric linear systems using (short) CG recursions but needs extra matvec with $\boldsymbol{A}^H$.

Idea of Sonneveld: use 'wasted' matvec in a more useful way.
Result: transpose-free methods:

- CGS (Sonneveld, 1989)
- Bi-CGSTAB (Van der Vorst, 1992)
- BiCGSTAB2 (Gutknecht, 1993)
- TFQMR (Freund, 1993)
- BiCGstab(ℓ) (Sleijpen and Fokkema, 1994)
- Many other variants

Historical remarks

Sonneveld first developed IDR (1980).

Analysis showed that IDR was Bi-CG combined with linear minimal residual steps.

The fact that IDR is transpose free, combined with the relation with Bi-CG led to the development of a now famous algorithm: CGS.

Later Van der Vorst proposed another famous method: Bi-CGSTAB, which is mathematicaly equivalent with IDR.

As a result of these developments, the basic IDR idea was abandoned for the Bi-CG approach. IDR is now forgotten.

The IDR idea

The IDR-idea is to generate a sequence of subspaces $\mathcal{G}_0 \cdots \mathcal{G}_j$ with the following operations:

- Intersect $\mathcal{G}_{j-1}$ with fixed subspace $\mathcal{S}$,
- Compute $\mathcal{G}_j = (\boldsymbol{I} - \omega_j \boldsymbol{A})(\mathcal{G}_{j-1} \cap \mathcal{S})$.

The subspaces $\mathcal{G}_0 \cdots \mathcal{G}_j$ are nested and of shrinking dimension.

The IDR theorem

Theorem 1 (IDR) *Let $\boldsymbol{A}$ be any matrix in $\mathbb{C}^{N\times N}$, let $\boldsymbol{v}_0$ be any nonzero vector in $\mathbb{C}^N$, and let $\mathcal{G}_0$ be the complete Krylov space $\mathcal{K}^N(\boldsymbol{A}, \boldsymbol{v}_0)$. Let $\mathcal{S}$ denote any (proper) subspace of $\mathbb{C}^N$ such that $\mathcal{S}$ and $\mathcal{G}_0$ do not share a nontrivial invariant subspace of $\boldsymbol{A}$, and define the sequence $\mathcal{G}_j$, $j = 1, 2, \ldots$ as*

$$\mathcal{G}_j = (\boldsymbol{I} - \omega_j \boldsymbol{A})(\mathcal{G}_{j-1} \cap \mathcal{S})$$

where the ω_j's are nonzero scalars. Then

(i) $\mathcal{G}_j \subset \mathcal{G}_{j-1}$ for all $j > 0$.

(ii) $\mathcal{G}_j = \{\boldsymbol{0}\}$ for some $j \leq N$.

Making an IDR algorithm

The IDR theorem can be used to construct solution algorithms.

This is done by constructing residuals $\boldsymbol{r}_n \in \mathcal{G}_j$.

According to the IDR theorem ultimately $\boldsymbol{r}_n \in \mathcal{G}_M = \{\mathbf{0}\}$.

In order to generate residuals and corresponding solution approximations we first look at the basic recursions.

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Krylov methods: basic recursion (1)

A Krylov-type solver produces iterates $\boldsymbol{x}_n$, for which the residuals $\boldsymbol{r}_n = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_n$ are in the Krylov spaces

$$\mathcal{K}^n(\boldsymbol{A}, \boldsymbol{r}_0) = \boldsymbol{r}_0 \oplus \boldsymbol{A}\boldsymbol{r}_0 \oplus \boldsymbol{A}^2\boldsymbol{r}_0 \oplus \cdots \oplus \boldsymbol{A}^n\boldsymbol{r}_0 \ ,$$

The next residual $\boldsymbol{r}_{n+1}$ can be generated by

$$\boldsymbol{r}_{n+1} = -\alpha \boldsymbol{A}\boldsymbol{r}_n + \sum_{j=0}^{\widehat{j}} \beta_j \boldsymbol{r}_{n-j} \ .$$

The parameters α, β_j determine the specific method and must be such that $\boldsymbol{x}_{n+1}$ can be computed.

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Krylov methods: basic recursion (2)

By using the difference vector

$$\Delta \boldsymbol{r}_k = \boldsymbol{r}_{k+1} - \boldsymbol{r}_k = -\boldsymbol{A}(\boldsymbol{x}_{n+1} - \boldsymbol{x}_n),$$

an explicit way to satisfy this requirement is

$$\boldsymbol{r}_{n+1} = \boldsymbol{r}_n - \alpha \boldsymbol{A} \boldsymbol{r}_n - \sum_{j=1}^{\widehat{j}} \gamma_j \Delta \boldsymbol{r}_{n-j} \ ,$$

which leads to the following update for the x estimate:

$$\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \alpha \boldsymbol{r}_n - \sum_{j=1}^{\widehat{j}} \gamma_j \Delta \boldsymbol{x}_{n-j} \ ,$$

Computation of a new residual (1)

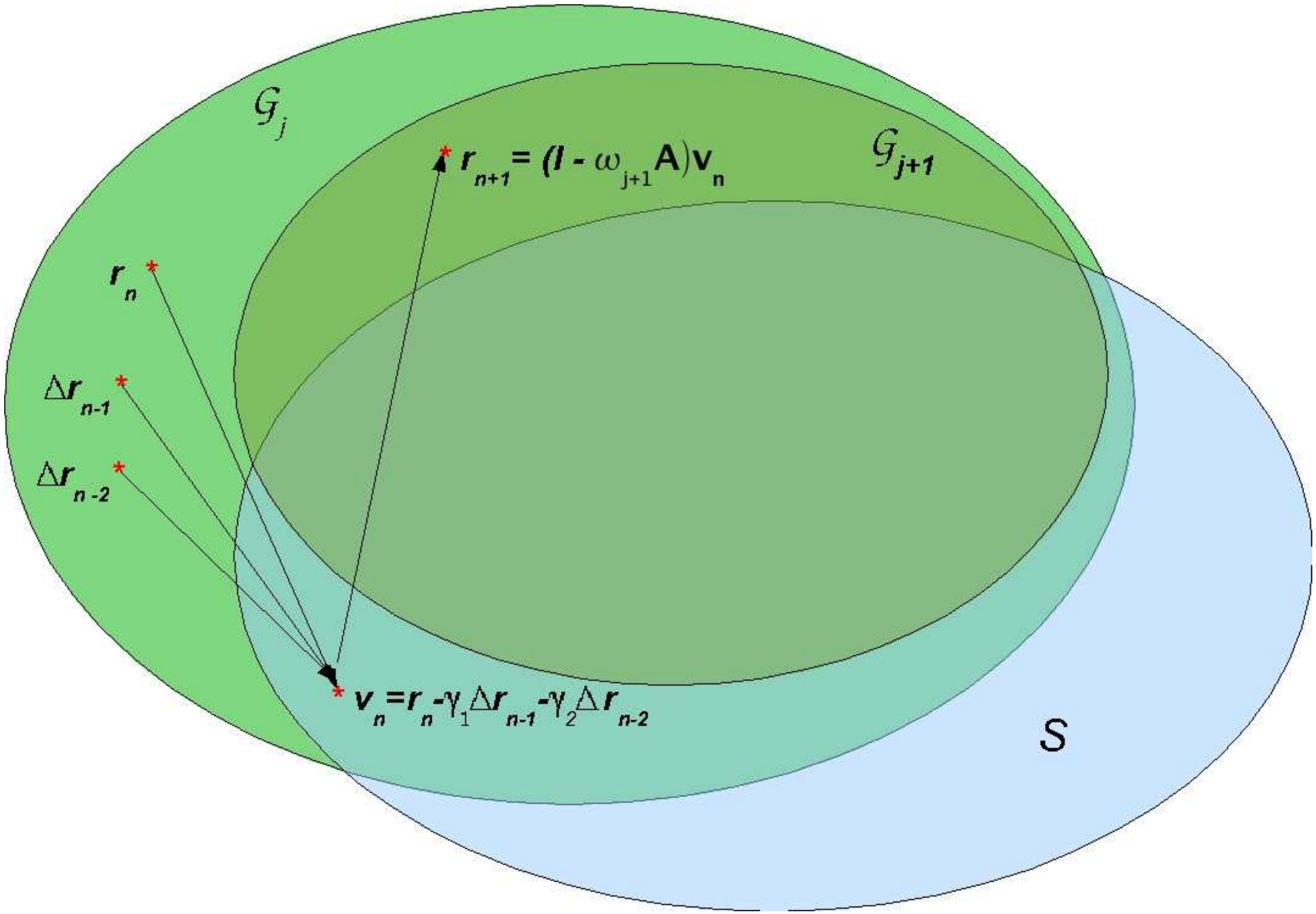
Residuals are computed that are forced to be in the subspaces $\mathcal{G}_j$, by application of the IDR-theorem.

The residual $\boldsymbol{r}_{n+1}$ is in $\mathcal{G}_{j+1}$ if

$$\boldsymbol{r}_{n+1} = (\boldsymbol{I} - \omega_{j+1}\boldsymbol{A})\boldsymbol{v} \quad \text{with } \boldsymbol{v} \in \mathcal{G}_j \cap \mathcal{S} \; .$$

The main problem is to find $\boldsymbol{v}$.

Computation of a new residual (2)



Computation of a new residual (3)

The vector $\boldsymbol{v}$ is a combination of the residuals $\boldsymbol{r}_l$ in $\mathcal{G}_j$.

$$\boldsymbol{v} = \boldsymbol{r}_n - \sum_{j=1}^{\widehat{j}} \gamma_j \Delta \boldsymbol{r}_{n-j} \ .$$

Let the space $\mathcal{S}$ be the left null space of some $N \times s$ matrix $\boldsymbol{P}$:

$$\boldsymbol{P} = (\boldsymbol{p}_1 \ \boldsymbol{p}_2 \ \ldots \ \boldsymbol{p}_s), \quad \mathcal{S} = \mathcal{N}(\boldsymbol{P}^H) \, .$$

Since $\boldsymbol{v}$ is also in $\mathcal{S} = \mathcal{N}(\boldsymbol{P}^H)$, it must satisfy

$$\boldsymbol{P}^H \boldsymbol{v} = \boldsymbol{0} \, .$$

Combining these two yields an $s \times \widehat{j}$ linear system for the coefficients γ_j that (normally) is uniquely solvable if $\widehat{j} = s$.

Computation of a new residual (4)

Hence with the residual $\boldsymbol{r}_n$, and a matrix $\Delta \boldsymbol{R}$ consisting of the last s residual differences:

$$\Delta \boldsymbol{R} = (\Delta \boldsymbol{r}_{n-1} \; \Delta \boldsymbol{r}_{n-2} \; \ldots \; \Delta \boldsymbol{r}_{n-s})$$

a suitable $\boldsymbol{v}$ can be found by

Solve $s \times s$ system $\qquad (\boldsymbol{P}^H \Delta \boldsymbol{R})\boldsymbol{c} = \boldsymbol{P}^H \boldsymbol{r}_n$

Calculate $\qquad \boldsymbol{v} = \boldsymbol{r}_n - \Delta \boldsymbol{R}\boldsymbol{c}$

Building $\mathcal{G}_{j+1}$ (1)

Assume $\boldsymbol{r}_n$ and all columns of $\Delta\boldsymbol{R}$ are in $\mathcal{G}_j$, and let $\boldsymbol{r}_{n+1}$ be calculated as

$$\boldsymbol{r}_{n+1} = \boldsymbol{v} - \omega_{j+1}\boldsymbol{A}\boldsymbol{v}$$

Then $\boldsymbol{r}_{n+1} \in \mathcal{G}_{j+1}$.
Since $\mathcal{G}_{j+1} \subset \mathcal{G}_j$ (theorem) we automatically have

$$\boldsymbol{r}_{n+1} \in \mathcal{G}_j$$

Now the next $\Delta\boldsymbol{R}$ is made by repeating the calculations.

In this way we find $s+1$ residuals in $\mathcal{G}_{j+1}$

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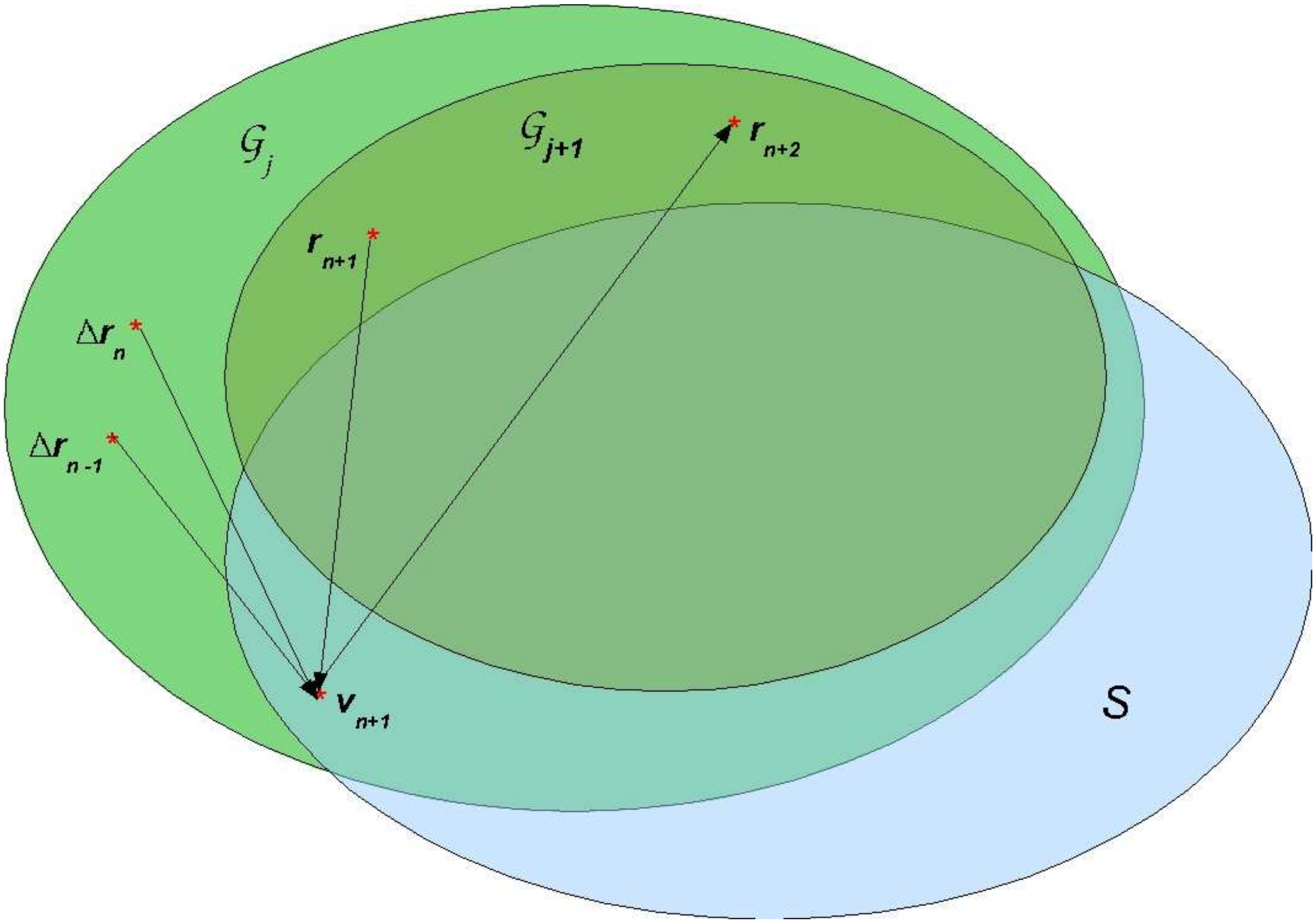
Building $\mathcal{G}_{j+1}$ (2)



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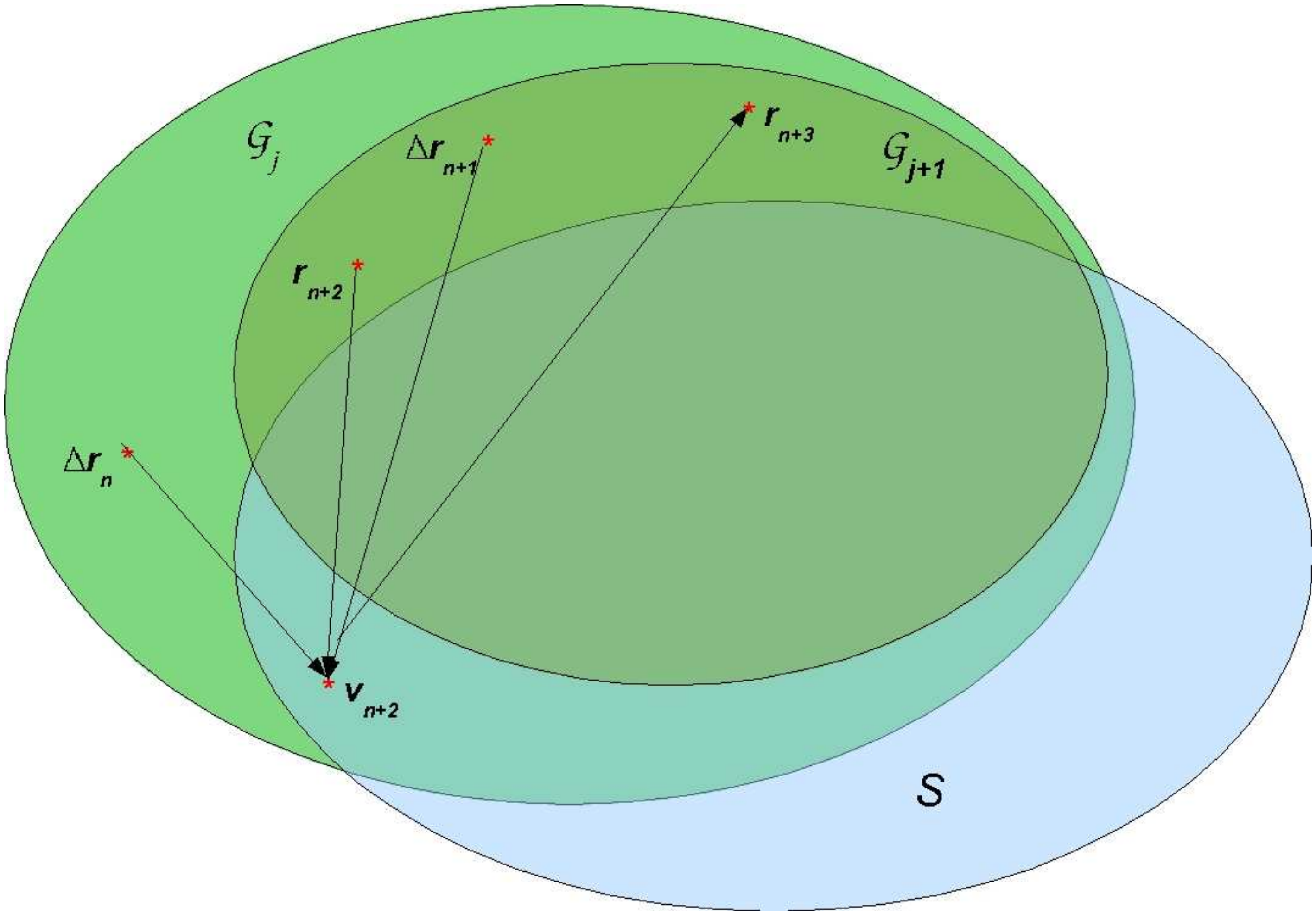
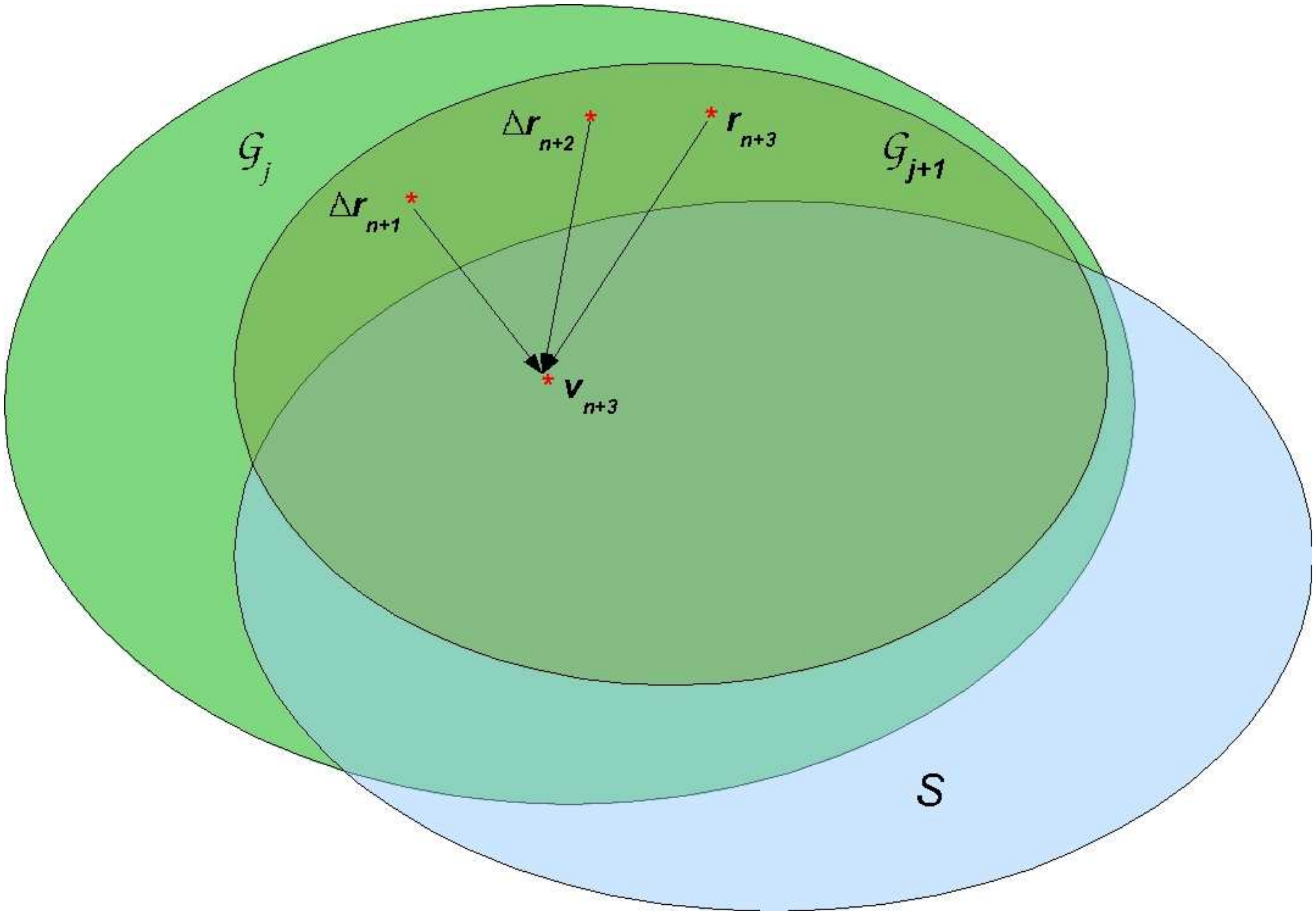
Building $\mathcal{G}_{j+1}$ (3)



Building $\mathcal{G}_{j+1}$ (4)



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A few details

1. The first $s+1$ residuals, starting with $\boldsymbol{r}_0$ can be constructed by any Krylov-based iteration, such as a local minimum residual method.
2. In our actual implementation, all steps are identical. However, in calculating the first residual in $\mathcal{G}_{j+1}$, a new value ω_{j+1} may be chosen. We choose ω_{j+1} such that $\|\boldsymbol{v} - \omega_{j+1}\boldsymbol{A}\boldsymbol{v}\|$ is minimal.

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Basic IDR(s) algorithm.

while $\|\boldsymbol{r}_n\| > TOL$ **or** $n < MAXIT$ **do**

  for $k = 0$ to s **do**

    Solve $\boldsymbol{c}$ from $\boldsymbol{P}^H d\boldsymbol{R}_n \boldsymbol{c} = \boldsymbol{P}^H \boldsymbol{r}_n$

    $\boldsymbol{v} = \boldsymbol{r}_n - d\boldsymbol{R}_n \boldsymbol{c}$; $\boldsymbol{t} = \boldsymbol{A}\boldsymbol{v}$;

    if $k = 0$ **then**

      $\omega = (\boldsymbol{t}^H \boldsymbol{v})/(\boldsymbol{t}^H \boldsymbol{t})$;

    end if

    $d\boldsymbol{r}_n = -d\boldsymbol{R}_n \boldsymbol{c} - \omega \boldsymbol{t}$; $d\boldsymbol{x}_n = -d\boldsymbol{X}_n \boldsymbol{c} + \omega \boldsymbol{v}$;

    $\boldsymbol{r}_{n+1} = \boldsymbol{r}_n + d\boldsymbol{r}_n$; $\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + d\boldsymbol{x}_n$;

    $n = n + 1$;

    $d\boldsymbol{R}_n = (d\boldsymbol{r}_{n-1} \cdots d\boldsymbol{r}_{n-s})$; $d\boldsymbol{X}_n = (d\boldsymbol{x}_{n-1} \cdots d\boldsymbol{x}_{n-s})$;

  end for

end while

Vector operations per MATVEC

Method	DOT	AXPY	Memory Requirements
IDR(1)	2	4	8
IDR(2)	$2\frac{2}{3}$	$5\frac{5}{6}$	11
IDR(4)	$4\frac{2}{5}$	$9\frac{7}{10}$	17
IDR(6)	$6\frac{2}{7}$	$13\frac{9}{14}$	23
Full GMRES	$\frac{n+1}{2}$	$\frac{n+1}{2}$	$n+2$
BiCGSTAB	2	3	7

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Relation with other methods

Although the approach is different, IDR(s) is closely related to some Bi-CGSTAB methods:

- IDR(1) and Bi-CGSTAB yield the same residuals at the even steps.
- ML(k)BiCGSTAB (Yeung and Chen, 1999) seems closely related to IDR(s), BUT
  - IDR(s) is MUCH simpler (both conceptually and its implementation)
  - Other, more natural extensions are possible, e.g. to avoid breakdown.

Performance of IDR(s)

The IDR theorem states that

- it is possible to generate a sequence of nested subspace $\mathcal{G}_j$ of shrinking dimension,
- but does not say how fast the dimension shrinks

It can be proven that the dimension reduction is (normally) s,
So $dim(\mathcal{G}_{j+1}) = dim(\mathcal{G}_j) - s$.
IDR(s) requires at at most $N + \frac{N}{s}$ matrix-vector multiplications to compute the exact solution.

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Numerical experiments

We will present two typical numerical examples

- A 2D Ocean Circulation Problem
- A 3D Helmholtz Problem

A 2D Ocean Circulation Problem

We compare IDR(s) with Full GMRES, restarted GMRES and Bi-CGSTAB.

This ocean example is representative for a wide class of CFD problems.

We will compare:

- Rate of convergence
- Stagnation level (of the true residual norm)

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Stommel's model for ocean circulation

Balance between bottom friction, wind stress and Coriolis force.

$$-r\,\Delta\psi - \beta\,\frac{\partial\psi}{\partial x} = (\nabla \times \mathbf{F})_z$$

plus circulation condition around islands k

$$\oint_{\Gamma_k} r\,\frac{\partial\psi}{\partial n}\,ds = -\oint_{\Gamma_k} \mathbf{F}\cdot\mathbf{s}\,ds.$$

- ψ: streamfunction
- r: bottom friction parameter
- β: Coriolis parameter
- $\mathbf{F}$: Wind stress

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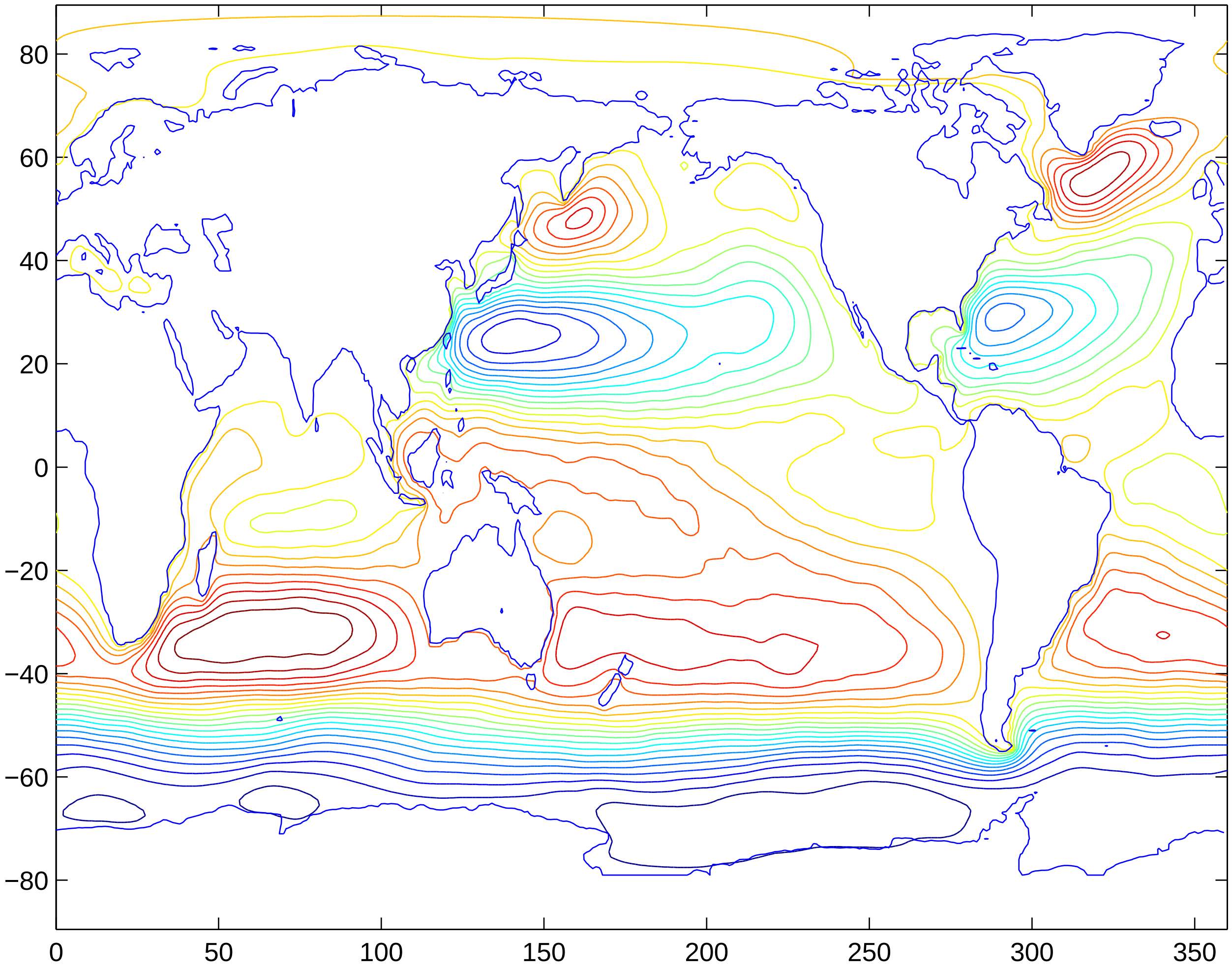
Discretization of the ocean problem

- Discretization with linear finite elements
- Results in nonsymmetric system of 42248
- Eigenvalues are (almost) real

Solution parameters:

- ILU(0) preconditioning
- $\boldsymbol{P}$: $s-1$ random vectors plus $\boldsymbol{r}_0$ (for comparison with Bi-CGSTAB)

Solution of the ocean problem



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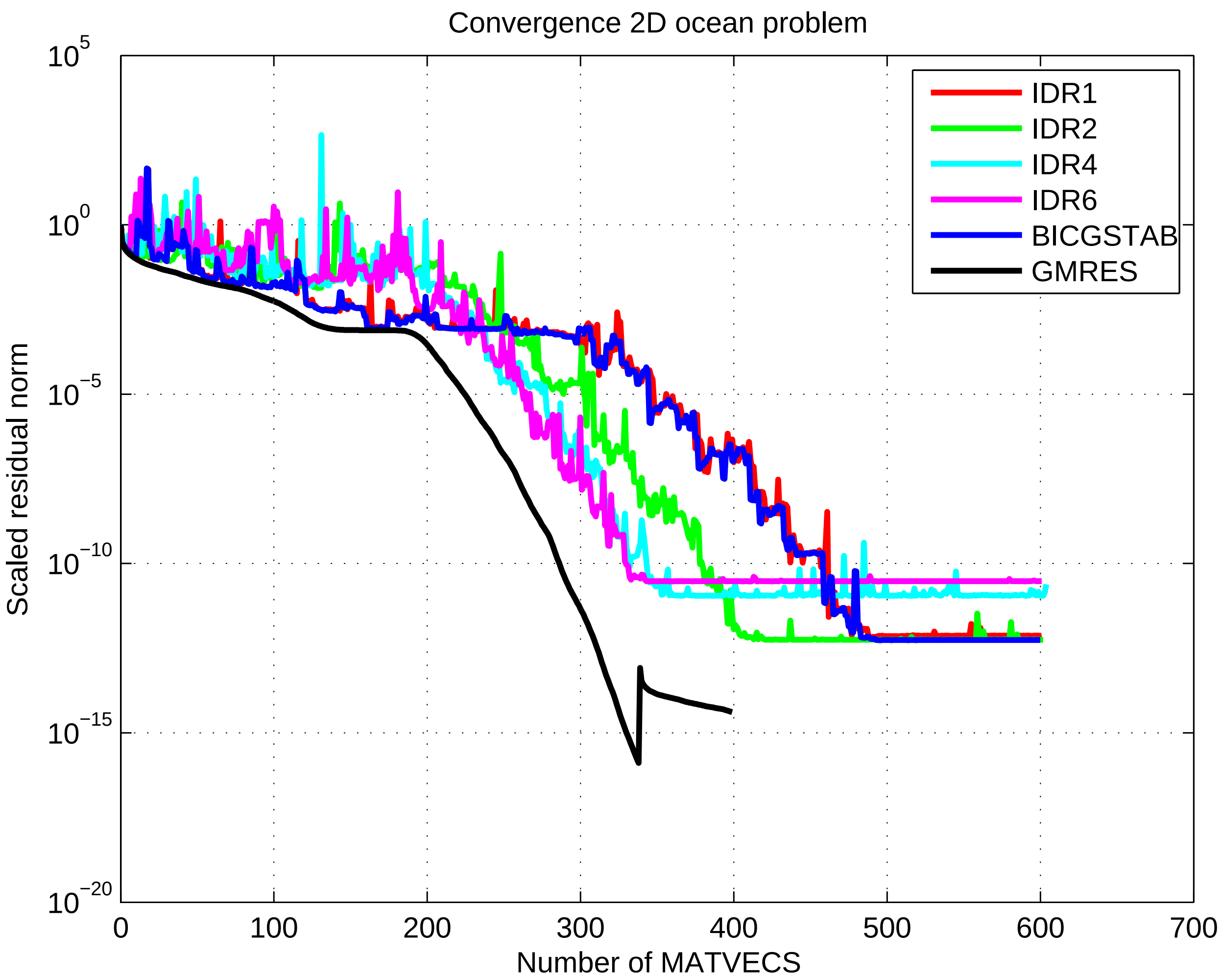
Convergence for the ocean problem



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Some observations

- Required number of MATVECS decreases if s is increased. IDR(4) and IDR(6) are close to the optimal convergence curve of full GMRES.
- Convergence curves of IDR(1) and Bi-CGSTAB coincide.
- Stagnation levels of IDR(s) comparable with Bi-CGSTAB.

Required number of MATVECS

Method	Number of MATVECS	Vectors
Full GMRES	265	268
GMRES(20)	> 10000	23
GMRES(50)	4671	53
Bi-CGSTAB	411	7
IDR(1)	420	8
IDR(2)	339	11
IDR(4)	315	17
IDR(6)	307	23

Tolerance: $\|\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_n\| < 10^{-8}\|\boldsymbol{b}\|$

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A 3D Helmholtz Problem

Example models sound propagation in a room of $4 \times 4 \times 4m^3$.

A harmonic sound source gives acoustic pressure field

$$\boldsymbol{p}(\boldsymbol{x}, t) = \widehat{p}(\boldsymbol{x})e^{2\pi i f t}.$$

The pressure function $\widehat{p}$ can be determined from

$$\frac{-(2\pi f)^2}{c^2}\widehat{p} - \Delta\widehat{p} = \delta(\boldsymbol{x} - \boldsymbol{x}_s) \quad \text{in } \Omega.$$

in which

- c: the sound speed (340 m/s)
- $\delta(\boldsymbol{x} - \boldsymbol{x}_s)$: the harmonic point source, in the center of the room.

Boundary conditions

Five of the walls are reflecting, modeled by

$$\frac{\partial \widehat{p}}{\partial n} = 0 \; ,$$

and the remaining wall is sound absorbing,

$$\frac{\partial \widehat{p}}{\partial n} = -\frac{2\pi i f}{c}\widehat{p} \; \text{on } \Gamma_3 .$$

Discretization

Discretization with FEM yields linear system

$$[-(2\pi f)^2 \boldsymbol{M} + 2\pi i f \boldsymbol{C} + \boldsymbol{K}]\boldsymbol{p} = \boldsymbol{b}$$

- Frequency $f = 100Hz$.
- System matrix complex, symmetric (but not Hermitian) and indefinite: difficult for iterative methods
- gridsize $h = 8\ cm$: 132651 equations

Solution parameters:

- ILU(0) preconditioning
- $\boldsymbol{P}$: Initial residual plus $s-1$ real random vectors
- Only comparison with BiCGstab(ℓ)

Results Helmholtz Problem

Method	Number of MATVECS	Elapsed time [s]
IDR(1)	1500	3322
IDR(2)	598	1329
IDR(4)	353	783
IDR(6)	310	698
BiCGstab(1)	1828	3712
BiCGstab(2)	1008	2045
BiCGstab(4)	656	1362
BiCGstab(8)	608	1337

Tolerance: $\|\boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_n\| < 10^{-8}\|\boldsymbol{b}\|$

Conclusions

- The IDR-theorem offers a new approach for the development of iterative solution algorithms
- The IDR(s) algorithm presented here is quite promising and seems to outperform state-of-the-art Bi-CG-type methods for important classes of problems.

More information:

http://ta.twi.tudelft.nl/nw/users/gijzen/software.html

- Report: IDR(s): a family of simple and fast algorithms for solving large nonsymmetric linear systems, submitted
- Matlab code, (includes preconditioning and deflation)