A PARALLELIZABLE AND FAST ALGORITHM FOR VERY LARGE GENERALIZED EIGENPROBLEMS

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Example: MHD

- interaction plasma and magnetic field

- Fluid eqns + Maxwell

- <u>**applications**</u>:
  stability tokamak plasmas
  coronal loops, solar flares

LINEAR MHD

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\nabla \cdot (\rho \mathbf{V}) \\
\rho \frac{\partial \mathbf{V}}{\partial t} &= -\rho (\mathbf{V} \cdot \nabla) \mathbf{V} - \nabla p \\
& \quad + (\nabla \times \mathbf{B}) \times \mathbf{B} \\
\frac{\partial p}{\partial t} &= -(\mathbf{V} \cdot \nabla) p - \gamma p \nabla \cdot \mathbf{V} + \\
& \quad (\gamma - 1) \eta (\nabla \times \mathbf{B})^2 \\
\frac{\partial \mathbf{B}}{\partial t} &= \nabla \times (\mathbf{V} \times \mathbf{B}) - \nabla \times (\eta \nabla \times \mathbf{B}) \\
\text{with} & \quad \nabla \cdot \mathbf{B} = 0
\end{aligned}
$$

- linearise around an equilibrium

- assume solutions of the form $e^{\lambda t}$:
  generalized eigenproblem

LINEAR MHD

• block tridiagonal matrices:
$100 - 2000$ blocks of size $80 - 320$
$\Rightarrow$ matrices of order $8,000 - 640,000$

For smallest systems:
• Shift-and-Invert IRA
(Sorensen)
• Shift-and-Invert Lanczos
(Cullum et al)
• Jacobi-Davidson, no inversion
(Booten, Fokkema, Sleijpen, van der Vorst)

PROBLEM AND APPROACH

PROBLEM: find one or more eigenvalues of $Ax = \lambda Bx$

A and B unsymmetric, large

CONVENTIONAL APPROACH:
Shift-and-Invert

$$(A - \sigma B)^{-1} Bx = \tilde{\lambda} x$$

$$\tilde{\lambda} = \frac{1}{\lambda - \sigma}, \ \lambda = \sigma + \frac{1}{\tilde{\lambda}}$$

Apply Arnoldi, convergence to eigenvalues closest to σ

Problem: $(A - \sigma B)^{-1}$

QZ METHOD

Compute orthogonal Q and Z:

$$AQ = ZS, \ \ BQ = ZT$$

such that S and T are
upper triangular.

Columns q_i:
Generalized Schur vectors

generalized Schur pair:

$$S_{i,i}/T_{i,i}$$

Iterative approach based upon
Jacobi-Davidson method

PROJECTION

$$(A - \lambda B)x = 0$$

Petrov-Galerkin conditions:
Find $x_m \in \{v_1, \ldots, v_m\}$, such that

$$(A - \theta B)x_m \perp \{w_1, \ldots, w_m\}$$

With
$V_m \equiv [v_1|v_2|\cdots|v_m]$,
$W_m \equiv [w_1|w_2|\cdots|w_m]$,
and $x_m = V_m y$:

$$(W_m^* A V_m - \theta W_m^* A V_m)y = 0$$

Apply standard QZ (LAPACK) for projected matrices $W_m^* A V_m$, and $W_m^* A V_m$

STANDARD QZ

Find orthogonal U_L and U_R:

$$U_L^*(W_m^* A V_m) U_R = S_A$$

$$U_L^*(W_m^* B V_m) U_R = S_B$$

S_A and S_B are upper-triangular ordered such that leading elements define eigenvalue closest to σ

Eigenpair approximation (x_m, θ);

$$\theta = S_B(1,1)/S_A(1,1)$$

$$x_m = V_m U_R(:,1)$$

At convergence we have have
x: the first column of Q
$(AQ = ZS,\ BQ = ZT)$
$z_1 \in span\{Aq_1, Bq_1\}$
Therefore, W_m taken as $AV_m - \sigma BV_m$

JACOBI-DAVIDSON

How to expand V_m (and W_m)?

Compute *residual vector*

$$r \equiv (A - \theta B)x_m$$

Also compute auxiliary vector:

$$\gamma z \equiv (A - \sigma B)x_m$$

Find correction v for x_m with

$$x_m^* v = 0$$

and

$$(I - zz^*)(A - \theta B)(I - x_m x_m^*)v = -r$$

Approximately solved with
few steps of GMRES

$v_{m+1} \equiv v \Rightarrow V_{m+1}$
$w_{m+1} \equiv (A - \sigma B)v \Rightarrow W_{m+1}$

HOW TO CONTINUE?

Expansion of Schur Form:

$$A\,[Q_k, q] = [Z_k, z] \begin{bmatrix} S_k & s \\ & \alpha \end{bmatrix}$$

and

$$B\,[Q_k, q] = [Z_k, z] \begin{bmatrix} T_k & t \\ & \beta \end{bmatrix}$$

with $Q_k^* q = 0$, $Z_k^* z = 0$.

This leads to

$$(I - Z_k Z_k^*)(\beta A - \alpha B)(I - Q_k Q_k^*)q = 0$$

$(q, \lambda \equiv \alpha/\beta)$ eigenpair of:

$$(I - Z_k Z_k^*)(A - \lambda B)(I - Q_k Q_k^*)$$

Apply "JD - algorithm with Schur form" for this matrix pair: q and z.

PROJECTED MATRICES

The projected matrices in JD satisfy:

$$W_m^*(I - Z_k Z_k^*)A(I - Q_k Q_k^*)V_m = W_m^* A V_m$$

and

$$W_m^*(I - Z_k Z_k^*)B(I - Q_k Q_k^*)V_m = W_m^* B V_m$$

EXPLICIT RESTART

For projected matrices we compute the generalized Schur form

$$W_m^* A V_m \, U_R = U_L S_A$$

and

$$W_m^* B V_m \, U_R = U_L S_B$$

S_A and S_B are ordered so that $|S_B(i,i)/S_A(i,i) - \sigma|$ form a nondecreasing row

The first few of columns of reordered V_m represent best eigenvector appox's can be used for restart

SOME PRACTICAL NOTES

1. After convergence of some eigenvectors:
   solution of correction eq. easier

2. Corr. eq. with precond. solver:
   preconditioning can be used more often:
   pays to make better preconditioning

3. For standard eigenproblems
   JD + QR-reduction

4. Numerical examples:
   maximum dimension of V: 15
   after restart: 10

PARALLELISM

Computational elements:

1. Given $V_m = [v_1|v_2|\cdots|v_m]$
and $W_m = [w_1|w_2|\cdots|w_m]$
compute $M_A \equiv W_m^* AVm$, $M_B \equiv W_m^* AVm$

requires Av_m, Bv_m,
$2m$ inner products
for last row and column of M_A and M_B

2. QZ-algorithm for M_A and M_B
negligible if $m \ll n$

3. Form $x_m = V_m y$: multiple update

PARALLELISM(2)

4. compute $r = (A - \theta B)x_m$, $\|r\|_2$
and $z = (A - \sigma B)x_m$, $z := z/\|z\|_2$

requires 2 updates, 2 norms

5. Solve approximately

$$(I - zz^*)(I - Z_k Z_k^*)$$

$$(A - \theta B)(I - Q_k Q_k^*)(I - x_m x_m^*)v = -r$$

with few steps of (prec.) GMRES

most expensive part:
requires inner products, updates
matrix vector products for A and B

6. Orthogonalize v wrt V_m, and
$w = (A - \sigma B)v$ wrt W_m

PARALLEL PERFORMANCE

For problem coming from acoustics:
A and B 19-diagonal, $n = 136,161$

Results for interior isolated eigenvalue, on the CRAY T3D:

Processors	Elapsed time (sec)
16	206.4
32	101.3
64	52.1

For $n = 274,625$, 64 processors:
93.3 seconds, 1.0 Gflops
(1 shift-invert step 600 sec. at peak-perf.)

MORE DETAILS

JD-algorithm:
Sleijpen and van der Vorst
SIMAX, 17 (2), March 1996

JD: general problems
Sleijpen et al
BIT, 36, Dec. 1996

JDQR and JDQZ
Fokkema et al, Preprint 941
UU, January 1997 (revised)
to appear in SISC

Parallel perf
Sleijpen et al, SIAM News, Aug. 96

these papers and others:
`http://www.math.ruu.nl/people/vorst`