On computing eigenvalues of the discretized Navier Stokes equation

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Outline

- Physical problem
- Matrix transformations
  Shift-invert
  Cayley transformations
- Linear equation solver
- Purification
- Numerical experiments
- Future directions

This is very much work in progress!

Physical problem

Mixed finite element discretizations of time-dependent equations modelling incompressible fluid flow problems produce systems

$$\begin{aligned} M\dot{w} + H(w)w + Lw + Cy &= b, \\ C^T w &= c, \end{aligned}$$

where $w \in \mathcal{R}^n$, $y \in \mathcal{R}^m$ with $n > m$.

M, L symmetric positive definite $n \times n$ matrices,

$H(w)$ nonsymmetric $n \times n$ matrix,

C $n \times m$ matrix, full rank.

Rewriting

$$B\dot{v} + D(v)v = d,$$

where

$$B = \begin{pmatrix} M & 0 \\ 0 & 0 \end{pmatrix}, \quad D(v) = \begin{pmatrix} H(v) + L & C \\ C^T & 0 \end{pmatrix}$$

For linearised stability need eigenvalues of

$$Ax = \lambda Bx \qquad (1)$$

where

$$A = \begin{pmatrix} K & C \\ C^T & 0 \end{pmatrix}, \quad B = \begin{pmatrix} M & 0 \\ 0 & 0 \end{pmatrix}.$$

For discretized Navier Stokes, K is nonsymmetric

Steady state is linearly stable if

$$Re(\lambda_i) > 0, \quad i = 1, 2, ..., N = n + m$$

Need **left-most eigenvalues**

Theorem
The generalized eigenproblem (1) has $n - m$ finite eigenvalues and m infinite eigenvalues each of algebraic multiplicity 2. (Malkus 1981)

Infinite eigenvalues are zero eigenvalues of

$$\gamma Ax = Bx$$

ENTWIFE

- Finite element package, developed at Harwell Laboratory.
- Designed to solve discretized elliptic and parabolic pdes via the FEM and compute singular points e.g.
  - limit points
  - symmetry-breaking bifurcation points
  - Hopf bifurcation points of the steady solution set.
- Current interest is in
  - Stability of laminar flows in expanding channels and pipes
  - Stability of laminar flows past bluff bodies in pipes and channels

Our aim: to improve the reliability and efficiency of the eigencomputations within ENTWIFE.

Main concern is **robustness**.

Also need **efficiency**.... want to solve problems with 250,000 degrees of freedom.

Tradition has Arnoldi methods taking a back seat.
Subspace iteration codes are used.
Let's check it out !

Restriction: All matrix computations involving A and B must be performed using real arithmetic.

Our test problems were set up using ENTWIFE.

Matrix transformations

Original problem

$$Ax = \lambda Bx$$

Transform to standard problem

$$Tx = \nu x$$

and apply standard iterative technique.

Choose T so that

- Left-most eigenvalues of (A, B) transformed to well-separated extremal eigenvalues of T.
- Left-most eigenvalue λ_1 easily recovered from dominant eigenvalue ν_1 of T.
- $w = Tv$ is cheap.

For our problems, B is singular.

Shift-invert

Introduce a shift

$$(A - \sigma B)x = (\lambda - \sigma)Bx$$

and set

$$T_{SI} = (A - \sigma B)^{-1}B.$$

Relationship between finite eigenvalues of (A, B) and those of transformed problem is

$$\lambda = \sigma + \frac{1}{\nu}$$

Require the solution of

$$(A - \sigma B)x = By$$

- Finds eigenvalues close to σ.
- σ real:

  Eigenvalues close to σ mapped away from origin.

  Eigenvalues far from σ mapped close to zero.

- To find eigenvalues with arbitrary complex part, need σ complex.
- Can maintain real arithmetic but added costs.

Cayley transformation

Generalised Cayley transform

$$T_C(A, B; \sigma, \mu) = (A - \sigma B)^{-1}(A - \mu B)$$

$$\sigma < \mu$$

.

- Eigenvalues to the left of the line $(\sigma + \mu)/2$ mapped outside unit circle.
- Eigenvalues to the right of the line $(\sigma + \mu)/2$ mapped inside unit circle.
- Eigenvalues far from σ and μ mapped close to 1. Includes
  - eigenvalues with large real parts
  - eigenvalues with large imaginary parts

Relationship between finite eigenvalues of (A, B) and those of transformed problem is

$$\lambda = \frac{\sigma\nu - \mu}{\nu - 1}$$

Relation between λ and ν planes

Combine shift-invert and Cayley

- use shift-invert with zero shift to get initial approx. to spectrum
- switch to Cayley
- update σ and μ

To implement this with subspace or Arnoldi need a flexible reverse communication interface.

Linear equation solver

Efficiency of eigensolver depends on efficiency of solving

$$(A - \sigma B)x = y$$

For our problems, A, B are unassembled finite element matrices

$$A = \sum_{k=1}^{l} A^{(k)}, \quad B = \sum_{k=1}^{l} B^{(k)}.$$

It is important to exploit the element format ... do **not** assemble.

ENTWIFE uses the Harwell Subroutine Library code `MA42` (Duff and Scott, 93, 96)

`MA42` is a general frontal solver.

Complex and F90 versions available.

Frontal solvers

$$Ax = y, \quad A = \sum_{k=1}^{l} A^{(k)}.$$

Factorization proceeds **without** assembling A.

Assembly operation

$$a_{ij} \Leftarrow a_{ij} + a_{ij}^{(k)}.$$

Basic Gaussian elimination operation

$$a_{ij} \Leftarrow a_{ij} - a_{il}[a_{ll}]^{-1}a_{lj}$$

Interleave assembly and elimination.

Eliminations may be delayed by stability considerations.

Require

$$|a_{lk}| \geq u \cdot max_i |a_{ik}|$$

where stability threshold $u \in (0, 1]$ is a user set parameter.

Note: stability vs fill-in.

Key features:

- Factors stored in direct access files.
- Small amount of in-core memory.
- Dense linear algebra ... exploit Level 3 BLAS in factorization and in solution phase.
- Efficiency depends on element order.
  - Work involved in an elimination is quadratic in frontsize.
  - In-core storage depends on maximum frontsize.

  Order elements to keep **frontsize small.**

All our numerical experiments employ `MA42`.

Arnoldi with B semi-inner product

Consider the case B positive semi-definite. (Recall we have

$$B = \begin{pmatrix} M & 0 \\ 0 & 0 \end{pmatrix},$$

with M positive definite.)

Idea is to use B semi-inner product $x^T By$ rather than standard inner product $x^T y$.

Used by Nour-Omid, Parlett, Ericsson, & Jensen for Lanczos (1987) and Meerbergen & Spence for Arnoldi (1996).

Arnoldi plus purification

Consider the Arnoldi reduction

$$T_C V = (A - \sigma B)^{-1}(A - \mu B)V \; = \; VH + f e_m^T.$$

Assume $Hs = s\theta$, $\|s\| = 1$.
Set

$$y = Vs, \quad \hat{\lambda} = \frac{\sigma\theta - \mu}{\theta - 1}.$$

Using $(y, \hat{\lambda})$ as Ritz pair, can show residual is

$$\|(A - \hat{\lambda}B)y\| = \|(A - \mu B)f\| \frac{|e_m^T s|}{|\theta - 1|}.$$

Purify the Ritz vector using the correction:

$$T_C y = VHs + f(e_m^T s) = y\theta + f(e_m^T s).$$

Formally one step of the power method with T_C.

Arnoldi plus purification, cont.

Using $(y + f(e_m^T s)/\theta, \hat{\lambda})$ as Ritz pair gives

$$\|(A - \hat{\lambda}B)(y + f(e_m^T s)/\theta)\| = \|(A - \mu B)f\| \frac{|e_m^T s|}{|\theta(\theta - 1)|}.$$

Similar results with shift-invert (Ericsson & Ruhe 1980).
The bounds are

$$\|(A - \sigma B)f\| \frac{|e_m^T s|}{|\theta|} \quad \text{and} \quad \|Bf\| \frac{|e_m^T s|}{|\theta|^2}$$

No Purification   Purification

Numerical experiments

Software:

- Implicitly restarted Arnoldi: ARPACK Version 2.
- Subspace iteration: Modified SRRIT (Bai and Stewart).
- Linear solver: MA42.
- Tests performed on SUN Ultra 1 using double precision.
- All timings are CPU times in seconds.
- Convergence tolerance $tol = 1.0d - 05$.

SRRIT modified for reverse communication interface.

ARPACK allows standard inner product or B semi-inner product.

Also allows user to select the shifts used by implicitly shifted QR process.

Example: Flow of a Newtonian fluid past a cylinder in a channel.

First bifurcation is a Hopf bifurcation.

We request 2 left-most eigenvalues.

- Order of matrix is 6398
- 600 elements
- Maximum of 48 freedoms per element
- Left-most eigenvalue complex
  $\lambda_1 = 0.27 \pm 10.96i$
  $\lambda_3 = 2.38$
- `MA42` statistics:
  - factorize time 6.7 secs.
  - factorization take 10^8 flops.
  - real factor storage 907 Kwords.
  - integer factor storage 155 Kwords.
  - max. frontsize 168.
  - min. in-core storage 28 Kwords.
  - solve time single right-hand side 0.5 secs.
  - solve time 10 right-hand sides 1.5 secs.

Shift-invert

Shift $\sigma = -25$.

	`SRRIT`	`ARPACK`
Subspace dimension	10	20
No. of restarts	20	6
No. of linear solves	126	109
No. times $B * X$ computed	126	109
Time for linear solves	196	54
Time for $B * X$	91	54
Total time	316	121
Direct residuals	2.97d+00	6.98d-04

Notes:

- For `ARPACK`, $X = x$.
- `SRRIT` solving for multiple right-hand sides.
- Implicit shifts in IRA were all zero.
- Standard inner product used.
- Both codes returned 3 eigenvalues.

Reducing *tol* did **not** reduce residual for `SRRIT`.

ARPACK and shift-invert

Shift $\sigma = -25$.

	Inner product	
	B semi	Standard
No. of restarts	6	6
No. of linear solves	109	109
No. times $B * x$ computed	331	109
Time for linear solves	54	54
Time for $B * x$	173	54
Total time	243	121
Relative residuals:		
Before purification	1.13d-05	1.41d-05
After purification	3.11d-04	3.89d-04

Notes:

- `ARPACK` used subspace dim. 20
- Implicit shifts in IRA were all zero.

Results suggest:

- Use of B semi inner product expensive for little gain.
- Purification gives worse results ($|\theta| < 1$).

ARPACK and shift-invert

Shift $\sigma = -25$.

	Implicit shifts	
	Exact	Zero
No. of restarts	8	6
No. of linear solves	138	109
No. times $B * x$ computed	138	109
Time for linear solves	80	54
Time for $B * x$	66	54
Total time	161	121
Relative residuals:		
Before purification	3.47d-07	1.41d-05
After purification	9.56d-06	3.89d-04

Notes:

- `ARPACK` used subspace dim. 20.
- Standard inner product used.

Results suggest:

- Purification gives worse results ($|\theta| < 1$).
- Fewer restarts using zero implicit shifts.

Cayley

	`SRRIT`	`ARPACK`
Subspace dimension	10	20
No. of restarts	6	3
No. of linear solves	57	57
No. times $(A - \mu B) * X$ computed	57	57
Time for linear solves	85	34
Time for $(A - \mu B) * X$	74	52
Total time	178	95
Relative residuals:		
Before purification	7.10d-06	2.68d-07
After purification	5.74d-06	2.13d-07

Notes:

- Implicit shifts in IRA were all zero.
- Standard inner product used.

ARPACK and Cayley

	Inner product	
	B semi	Standard
No. of restarts	3	3
No. of linear solves	57	57
No. times $A * x$ computed	56	0
No. times $B * x$ computed	131	0
No. times $(A - \mu B) * x$ computed	1	57
Time for linear solves	34	34
Time for $A * x$	25	0
Time for $B * x$	61	0
Time for $(A - \mu B) * x$	1	52
Total time	129	95
Relative residuals:		
Before purification	1.92d-07	2.68d-07
After purification	1.58d-07	2.13d-07

Implicit shifts in IRA were all zero.

Results suggest:

- Use of B semi inner product expensive for little gain.
- Purification improves results slightly ($|\theta| > 1$).

ARPACK and Cayley

	Implicit shifts	
	Exact	Zero
No. of restarts	4	3
No. of linear solves	75	57
Time for $(A - \mu B) * x$	75	57
Time for linear solves	46	34
Time for $(A - \mu B) * x$	69	52
Total time	124	95
Relative residuals:		
Before purification	2.00d-06	2.68d-07
After purification	1.58d-06	2.13d-07

Standard inner product used.

Results suggest:

- Purification improves results slightly ($|\theta| > 1$).
- Fewer restarts using zero implicit shifts.

Future directions

- Modified Cayley transform (Cliffe, Garrett & Spence 1993)

  $$\begin{pmatrix} K - \sigma M & C \\ C^T & 0 \end{pmatrix}^{-1} \begin{pmatrix} K - \mu M & \beta C \\ \beta C^T & 0 \end{pmatrix} x = \nu x.$$

  $\beta = 1$ is standard Cayley.

  Eigenvalues are:

  ▷ $(\lambda_i - \mu)/(\lambda_i - \sigma)$, $i = 1, \ldots, n - m$

  ▷ m eigenvalues β, each with with algebraic multiplicity 2 and geometric multiplicity 1.

- Verification techniques
- Block Arnoldi
- Larger, harder problems!