An optimized Schwarz method in the Jacobi-Davidson method for eigenvalue problems

Abstract

The Jacobi-Davidson method [3] reduces a large linear eigenvalue problem to a small one by projecting it on an appropriate low dimensional subspace. The heart of the method lies in how the subspace is expanded: an expansion vector is computed from the so-called correction equation.
However the correction equation in itself poses a large linear problem, with size equal to the size of the originating large eigenvalue problem. Because of this, most of the computational work of the Jacobi-Davidson method arises from performing (approximate) solves for the correction equation.

This poster presents research [2, 1] about the question how a preconditioner based on a domain decomposition technique can be incorporated in the Jacobi-Davidson method to make it more efficient for PDE type of eigenvalue problems. The domain decomposition technique is an (locally) optimized additive Schwarz method based on earlier work from Tang [6] and Tan & Borsboom [4, 5] for linear systems.
In contrast to ordinary linear systems, the operator in the correction equation involves the matrix of the large eigenvalue problem, shifted by an approximate eigenvalue. Because of this, the operator in the correction equation is indefinite, for an internal eigenvalue even highly indefinite. Therefore, in case of the correction equation further investigation of this domain decomposition approach is needed. The situation is analyzed for constant coefficients. It turns out that the eigenvalue plays a critical role.

In many applications the eigenvalue problems exhibit coefficients that vary over the physical domain. For such a situation a strategy may be applied that is based on locally frozen coefficients. This strategy only requires knowledge of the constant coefficients case. As for the optimization only local behavior is taken into account, a generalization of the domain decomposition method to more complicated geometries is straightforward.
Once a preconditioner based on domain decomposition is constructed for the iterative computation of solutions to the correction equation (the "inner-loop"), one may take more advantage of it by considering the relationship between the "innerloop" and "outerloop" (the iterative computation of solutions to the eigenvalue problem with Jacobi-Davidson itself).

References

[1, 2, 3] See "more details" in bottom right corner.

[4] K. H. TAN AND M. J. A. BORSBOOM, *On generalized Schwarz coupling applied to advection-dominated problems*, in Domain decomposition methods in scientific and engineering computing **(DD7)** (University Park, PA, 1993), D. E. Keyes and J. C. Xu, eds., Amer. Math. Soc., Providence, RI, 1994, pp. 125–130.

[5] K. H. TAN, *Local coupling in domain decomposition*, Ph.D. thesis, Utrecht University, Utrecht, The Netherlands, 1995.

[6] W. P. TANG, *Generalized Schwarz splittings*, SIAM J. Sci. Stat. Comput., 13:573–595, 1992.

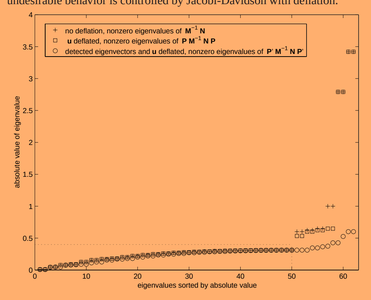

Menno Genseberger


Gerard Sleijpen


Henk van der Vorst

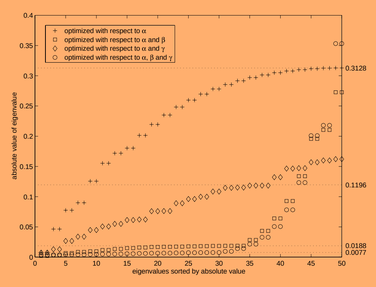
deflation

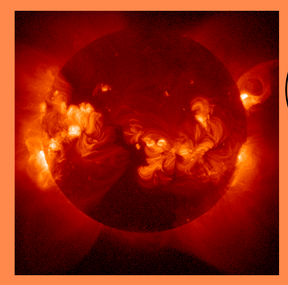
A number of components of the error for an internal eigenvalue are not confined to a neighborhood of the interface between the subdomains. This undesirable behavior is controlled by Jacobi-Davidson with deflation.

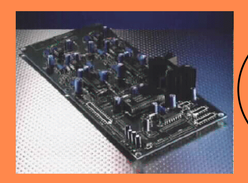


stronger coupling

More coupling parameters are introduced by inclusion of cross coupling, i.e. coupling parallel to the interface together with coupling perpendicular to the interface. This leads to stronger reduction of the errors.





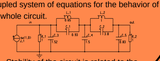


astrophysical processes

electric circuit design

One of the proposed mechanisms to explain the heating of the solar corona is resonant absorption of magnetic Alfven waves. Analysis of these magnetohydrodynamic waves in a coronal loop needs the solution of very large generalized eigensystems.

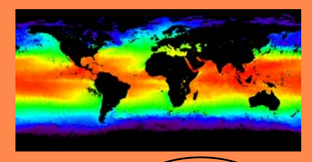
The behavior of each component (like coil, capacitor, ...) is described by one or more equations. Together with Kirchhoff's law this gives a coupled system of equations for the behavior of the whole circuit.



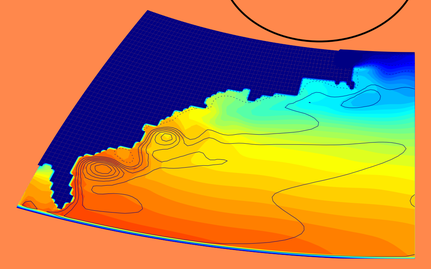
Stability of the circuit is related to the eigenfrequencies of this coupled system.

structural engineering

eigenvalue problem
Ax=λBx
in millions of unknowns



climate modelling



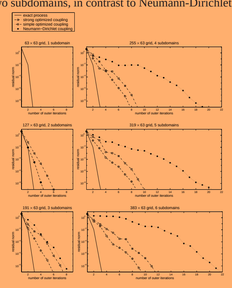
the origin of eigenvalue problems

Eigenvalue problems show up in a diversity of scientific discplines. In most situations the object of study is described by some partial differential equation. High resolution discretizations lead to (generalized) eigenvalue problems of very high dimension.

Conventional dense methods (like the QR-algorithm for the standard and the QZ-algorithm for the generalized eigenvalue problem) can not cope well with such high dimensions. In such a situation one may address a subspace method. Amongst these subspace methods the Jacobi-Davidson method offers many advantages and flexibility, amongst others good preconditioners as domain decomposition can be fully exploited.

more subdomains

The analysis for the determination of optimal coupling parameters was performed for a two subdomain decomposition. However, the results of this analysis also yield accurate estimates of optimal coupling parameters for more than two subdomains, in contrast to Neumann-Dirichlet coupling.



the Jacobi-Davidson method

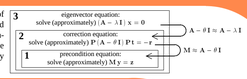
The correction equation describes an (inexact) Newton step. This special linear system has equal dimensions as the original eigenvalue problem. For not too low dimensional problems, most computational work of the Jacobi-Davidson method is therefore in this ingredient. However, Jacobi-Davidson is flexible and the correction equation doesn't need to be solved in high precision. Approximate solutions of the correction equation obtained with a preconditioned iterative solver may already result in fast convergence of Jacobi-Davidson.

The matrix in the correction equation is shifted by an approximate eigenvalue which makes it indefinite. This property prevents in general a succesfull application of an algebraic preconditioning technique (like ILU) to the correction equation.
A preconditioner based on domain decomposition might be suitable. Domain decomposition enables a subdivision of a large problem into smaller (coupled) subproblems. The kind of applications (see top-right corner) suit well in such an approach: they are described by partial differential equations on physical domains. Decomposition into smaller subproblems is also necessary as the corresponding problems are of very large scale. Because of the indefiniteness further investigation of the domain decomposition method is needed for the correction equation.

left preconditioning with $\mathbf{M} \approx \mathbf{B}$:

$$\mathbf{P}\,\mathbf{M}^{-1}\,\mathbf{B}\,\mathbf{P}\,\mathbf{t} = \mathbf{P}\,\mathbf{M}^{-1}\,\mathbf{r}$$
with $\mathbf{P} \equiv \mathbf{I} - \frac{\mathbf{M}^{-1}\,\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{M}^{-1}\,\mathbf{u}}$

Application of the domain decomposition method needs an adaption of the linear system. In the Jacobi-Davidson method this can be arranged for the eigenvalue problem, the correction equation or the preconditioning step. It turned out that once a preconditioner is constructed for the second option, even better (parallel) performance can be obtained by application of the same preconditioner to the first option.



For the computation of a solution $(\lambda, \mathbf{x})$ to the standard eigenvalue problem

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

in each iteration step Jacobi-Davidson [3]:

extracts an approximate solution $(\theta, \mathbf{u})$ from a search subspace by

- constructing $H \equiv \mathbf{V}^*\mathbf{A}\,\mathbf{V}$,
- solving $H\,s = \theta\,s$, and
- computing $\mathbf{u} = \mathbf{V}\,s$,

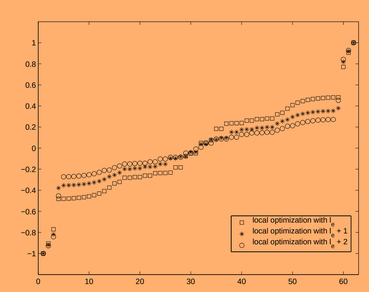
where the columns of $\mathbf{V}$ form an orthonormal basis for the search subspace,

corrects the approximate eigenvector $\mathbf{u}$ by computing a correction vector $\mathbf{t}$ from the *correction equation*:

$$\mathbf{t} \perp \mathbf{u}, \quad \mathbf{P}\,\mathbf{B}\,\mathbf{P}\,\mathbf{t} = \mathbf{r}$$

with $\mathbf{P} \equiv \mathbf{I} - \frac{\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{u}}$, $\mathbf{B} \equiv \mathbf{A} - \theta\,\mathbf{I}$ and $\mathbf{r} \equiv -\mathbf{B}\,\mathbf{u}$,

expands the search subspace with the orthogonal component $(\mathbf{I} - \mathbf{V}\,\mathbf{V}^*)\,\mathbf{t}$ of the correction vector $\mathbf{t}$.



Local optimization appears to be an efficient strategy for problems with variable coefficients. Such a strategy uses results from the analysis for the model problem with constant coefficients. Several variants have been tested.

variable coefficients

an optimized Schwarz method

example of enhancement in one direction

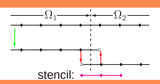
Let the PDE be defined on some domain Ω by the operator $\frac{\partial}{\partial x}\left(a\frac{\partial}{\partial x}\right) + b\frac{\partial}{\partial x}$ with constant a and b. Discretization by finite differences results in a grid covering the domain. The discretized operator may be represented for instance by the (coupling) stencil

$$\left(\frac{a}{h^2} - \frac{b}{2h}\right) \quad \left(-\frac{2a}{h^2}\right) \quad \left(\frac{a}{h^2} + \frac{b}{2h}\right)$$

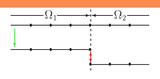
Now, the grid is decomposed into subgrids that cover the nonoverlapping subdomains Ω_1 and Ω_2. The differences between the approach of Tang [6] and Tan & Borsboom [4,5] are indicated in the pictures on the right. It can be observed that in Tang's approach the subgrids have one gridpoint in common at the interface between the subdomains. To prevent that for this gridpoint a splitting of the discretized operator (see the stencil) has to be made Tan and Borsboom refined the concept by defining a double set of additional gridpoints near the interface.
On the right, for the two subdomain case, this enhancement of $\mathbf{B}\,\mathbf{y} = \mathbf{d}$ is presented in an algebraic way. The blue part corresponds to the preconditioner $\mathbf{M}$, the red part to $\mathbf{N}$. Coupling between the unknowns y_l and y_r near the interface and corresponding additional unknowns $\tilde{y}_l$ and $\tilde{y}_r$ (at the "$\circ$") is defined by extra equations independently of the discretization via the coupling matrix

$$C \equiv \begin{bmatrix} C_{\ell\ell} & C_{\ell r} \\ C_{r\ell} & C_{rr} \end{bmatrix}.$$

Tan & Borsboom '93:



Tang '92:



stencil:

$\mathbf{B}\,\mathbf{y} = \mathbf{d} \longrightarrow \mathbf{B}_C\,\underline{\mathbf{y}} = \underline{\mathbf{d}}$.

$$\begin{bmatrix} \mathbf{B}_{1\ell} & \mathbf{B}_{1I} & \mathbf{B}_{1r} & 0 & 0 & 0 \\ \mathbf{B}_{I\ell} & \mathbf{B}_{II} & \mathbf{B}_{Ir} & 0 & 0 & 0 \\ 0 & C_{I\ell} & C_{Ir} & -C_{I\ell} & -C_{Ir} & 0 \\ 0 & -C_{I\ell} & -C_{Ir} & C_{I\ell} & C_{Ir} & 0 \\ 0 & 0 & 0 & \mathbf{B}_{Il} & \mathbf{B}_{Ir} & \mathbf{B}_{I2} \\ 0 & 0 & 0 & \mathbf{B}_{2l} & \mathbf{B}_{2I} & \mathbf{B}_{I2} \end{bmatrix} \begin{bmatrix} y_1 \\ y_I \\ y_r \\ \tilde{y}_l \\ \tilde{y}_r \\ y_2 \end{bmatrix} = \begin{bmatrix} d_1 \\ d_I \\ 0 \\ 0 \\ d_I \\ d_2 \end{bmatrix}$$

left preconditioning with $\mathbf{M} \approx \mathbf{B}_C$:

$$\mathbf{P}\,\mathbf{M}^{-1}\mathbf{B}_C\,\mathbf{P}\,\mathbf{t} = \mathbf{P}\,\mathbf{M}^{-1}\,\underline{\mathbf{r}},$$
with $\mathbf{P} \equiv \mathbf{I} - \frac{\mathbf{M}^{-1}\,\mathbf{u}\,\mathbf{u}^*}{\mathbf{u}^*\mathbf{M}^{-1}\,\mathbf{u}}$

For the computation of a solution to a linear system $\mathbf{B}\,\mathbf{y} = \mathbf{d}$ this optimized Schwarz method [4,5]

enhances the linear system:

$$\mathbf{B}\,\mathbf{y} = \mathbf{d} \longrightarrow \mathbf{B}_C\,\underline{\mathbf{y}} = \underline{\mathbf{d}}, \qquad (1)$$

splits $\mathbf{B}_C = \mathbf{M} - \mathbf{N}$ such that the preconditioner $\mathbf{M}$ is invertible locally on subdomains,

computes a solution of (1) by

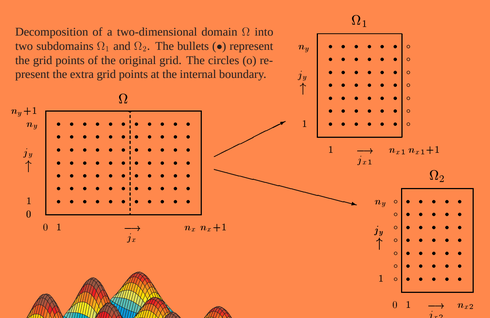
Richardson iteration $\underline{\mathbf{y}}^{(i+1)} = \underline{\mathbf{y}}^{(i)} + \mathbf{M}^{-1}\left(\underline{\mathbf{d}} - \mathbf{B}_C\,\underline{\mathbf{y}}^{(i)}\right)$

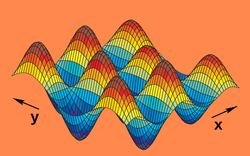
or

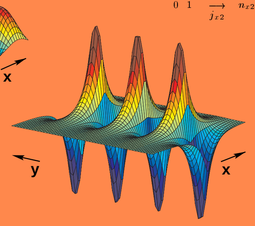
a more general Krylov method with $\mathcal{K}_m\left(\mathbf{M}^{-1}\,\mathbf{B}_C, \mathbf{M}^{-1}\,\underline{\mathbf{d}}\right) =$
$\text{span}\left(\mathbf{M}^{-1}\,\underline{\mathbf{d}},\ \mathbf{M}^{-1}\,\mathbf{B}_C\,\mathbf{M}^{-1}\,\underline{\mathbf{d}}, \ldots, \left(\mathbf{M}^{-1}\,\mathbf{B}_C\right)^{m-1}\,\mathbf{M}^{-1}\,\underline{\mathbf{d}}\right)$,

tunes C for "minimal" spectral radius of $\mathbf{M}^{-1}\,\mathbf{N}$. Then the errors for the Richardson iteration are damped "as much as possible" (as $\mathbf{M}^{-1}\,\mathbf{B}_C = \mathbf{I} - \mathbf{M}^{-1}\,\mathbf{N}$ each Richardson iteration step the error is amplified by the *error propagation matrix* $\mathbf{M}^{-1}\,\mathbf{N}$, general Krylov methods perform better since they accelerate the Richardson iteration).

Decomposition of a two-dimensional domain Ω into two subdomains Ω_1 and Ω_2. The bullets (•) represent the grid points of the original grid. The circles (o) represent the extra grid points at the internal boundary.

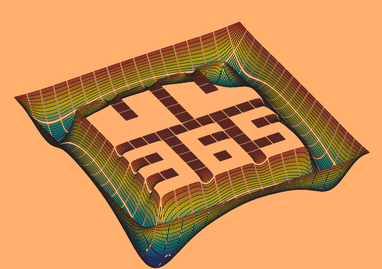






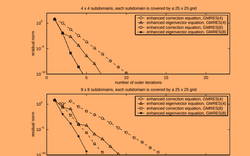
Eigenvectors of the error propagation matrix $\mathbf{M}^{-1}\,\mathbf{N}$ for the two-dimensional two subdomain case. In the x direction, the direction perpendicular to the interface between the subdomains, it typically behaves harmonic (top picture) or exponential (right picture).

For the determination of optimal coupling matrices C for a general problem the spectrum of the error propagation matrix $\mathbf{M}^{-1}\,\mathbf{N}$ is analyzed for a two-dimensional associated model eigenvalue problem. The results of this analysis yield (nearly) optimal C for the general two-dimensional case with more than two subdomains, variable coefficients and complicated geometries. The model eigenvalue problem is defined by an advection-diffusion operator with constant coefficients and the domain is decomposed in two subdomains.
After discretization, the advection-diffusion operator with constant coefficients can be written as a tensor product of two one-dimensional advection-diffusion operators. This tensor product notation facilitates the analysis: the situation in two dimensions can be seen as layered one-dimensional situations. In the one-dimensional situation for the component on a subdomain of an eigenvector of $\mathbf{M}^{-1}\,\mathbf{N}$ two typical situations occur: harmonic behavior and exponential behavior. The coupling of the components on the two subdomains for an eigenvector is expressed by the absolute value of the corresponding eigenvalue. Only in this expression the coupling matrix C can be found. For exponential behavior necessary estimations can be made without specific knowledge of the subdomain size. In the two-dimensional situation the problem of finding all eigenvectors of the error propagation matrix $\mathbf{M}^{-1}\,\mathbf{N}$ breaks up into layered one-dimensional problems. The one-dimensional problems are coupled by eigenvectors of a one-dimensional advection-diffusion operator. Now, for the coupling matrix C any linear combination of powers of this one-dimensional advection-diffusion operator can be taken. (With simple coupling we mean only zero powers, with stronger coupling also first powers.) This is used for the minimization of the absolute values of the eigenvalues that correspond to (a collection of) eigenvectors of the error propagation matrix $\mathbf{M}^{-1}\,\mathbf{N}$.



Eigenvalues and corresponding eigenvectors can efficiently be computed on more complicated geometries, with Jacobi-Davidson in combination with the preconditioner based on domain decomposition.

complicated geometry

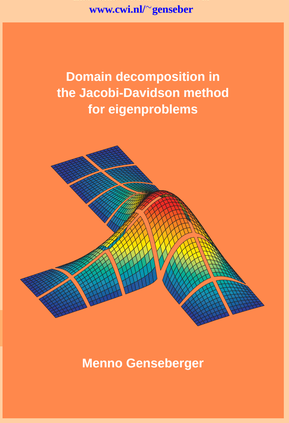


Even better performance can be obtained with the preconditioner because of the nested structure of the Jacobi-Davidson method. This aspect is not trivial for low accurate solutions of the correction equation and a large number of subdomains. Such a situation may occur if a large scale eigenvalue problem needs a massively parallel treatment.

nested method

more details

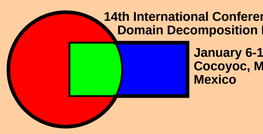
[1] M. GENSEBERGER, *Domain decomposition in the Jacobi-Davidson method for eigenproblems*, Ph.D. thesis, Utrecht University, 2001.
Hardcopy available here, see below.
Electronic version available via
www.cwi.nl/~genseber



[2] M. GENSEBERGER, G. L. G. SLEIJPEN, AND H. A. VAN DER VORST, *Using domain decomposition in the Jacobi-Davidson method*, preprint no. 1164 Mathematical Institute, Utrecht University, 2000, also appeared as report MAS-R0029, CWI, Amsterdam.

[3] G. L. G. SLEIJPEN AND H. A. VAN DER VORST, *A Jacobi-Davidson iteration method for linear eigenvalue problems*, SIAM J. Matrix Anal. Appl., 17:401–425, 1996. (Reappeared in SIAM Review 42:267–293, 2000.)

See also **www.math.uu.nl/people/sleijpen** and **www.math.uu.nl/people/vorst**



Mathematical Institute
Utrecht University
P.O. Box 80010
3508 TA Utrecht
The Netherlands
www.math.uu.nl

Modelling, Analysis & Simulation (MAS)
Centrum voor Wiskunde & Informatica (CWI)
(National Research Institute for Mathematics & Computer Science in the Netherlands)
P.O. Box 94079
1090 GB Amsterdam
The Netherlands
www.cwi.nl/mas