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Optimization of Flexible Coupling in Domain Decomposition for a System of PDEs

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1 Introduction

Domain decomposition (DD) may be applied to boundary-value problems for various reasons, ranging from the wish to solve the discretized problem on a (massively) parallel machine or a cluster of scalar machines, to the necessity to use different mathematical or numerical models in different parts of the domain of definition, or the need of a flexible modeling technique on complex domains. In any case, the performance of domain decomposition methods is of utmost importance. For an application running on a parallel architecture, computing time may be duly saved, in spite of the overhead imposed by the domain decomposition method. The performance of a DD method becomes especially a factor of importance when such a method is to be used in a non-parallel environment. In that case there is no gain in wall-clock time for the method, which could compensate for the method's overhead. Then, the benefits of possible gain in modeling-flexibility or possibly a higher accuracy of results obtained with a DD method, must compensate for the DD method's overhead cost.

In the present paper we report on the optimization of a flexible coupling technique for a system of PDEs.

Optimization of Interface Conditions

We consider a two-grid DD method for a system of partial differential equations. For our analysis the domain of definition is divided into two disjoint subdomains, on each of which a subproblem is defined. The subproblems are artificially decoupled. The coupling between the subproblems, such that the substructured problem becomes equivalent to the original problem, is restored in the iteration scheme applied on the level of the subproblems. The convergence of this iteration scheme and hence the performance of the DD method, depends strongly on the equations (interface conditions) that are used to restore the coupling of the subproblems. The proposed

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method features the optimization of a set of parameters which appear in the interface conditions. Optimization is considered w.r.t. the convergence rate of the additive Schwarz method used in the subproblem iteration scheme.

The Generalized Schwarz Coupling and Convergence

A flexible coupling mechanism is obtained by introducing a set of free parameters in the interface conditions. An optimal set of values for the parameters in a given problem is obtained when the best convergence rate of the subproblem-iteration, over all possible values that these parameters can take, is achieved. The optimal values depend on the specific problem at hand, as well as on the choices made for the substructuring, the discretization used to obtain a set of algebraic equations and the iteration scheme on the level of subproblems to solve this set of equations.

Our starting point is the optimization of a flexible coupling technique proposed by Tan and Borsboom [TB93] and Tan [Tan95]. This method is based on a generalization of the classical Schwarz algorithm, known as 'Generalized Schwarz Splitting' by Tang [Tan92]. For a one-dimensional two-point boundary-value problem Tang obtained an increase in convergence rate, with the asymptotic convergence factor changing from 0.91 for the classical Alternating Schwarz Method (requiring 60 iterations to satisfy his convergence criterion) to 10^{-4} (requiring only 3 iterations to satisfy his criterion) for Tang's generalized Schwarz method. Tan and Borsboom applied Tang's generalized Schwarz to a two-dimensional advection-diffusion problem and obtained an asymptotic convergence factor of 0.3. Their even-more-generalized Schwarz method, with interface conditions including second-order cross-derivatives, gives an asymptotic convergence factor of 0.05. The latter method is the generalized Schwarz method that we adopt as a starting point for our method and which we will extend for use with a set of PDEs.

We consider a DD method for a system of n linear partial differential equations, discretized with a finite-difference scheme. The domain of definition Ω is divided in two parts denoted by Ω_i, $i = 1, 2$, with a common boundary Γ. For the interface conditions on iteration level m of the subproblem defined on Ω_i, we use a discretization of the general interface condition

$$
\begin{aligned}
u_i^{(m)} + \alpha \frac{\partial u_i^{(m)}}{\partial n} + \beta \frac{\partial u_i^{(m)}}{\partial t} + \gamma \frac{\partial^2 u_i^{(m)}}{\partial t \partial n} &= \\
u_i^{(m-1)} + \alpha \frac{\partial u_i^{(m-1)}}{\partial n} &+ \beta \frac{\partial u_i^{(m-1)}}{\partial t} + \gamma \frac{\partial^2 u_i^{(m-1)}}{\partial t \partial n}.
\end{aligned}
$$

Here n and t denote normal and tangential directions on Γ, respectively. The discretized interface conditions involve the values the unknown function variables across the interface Γ.

A local mode analysis is applied to reveal the relation between the interface parameters α, β, and γ on the one hand and the asymptotic convergence rate of the iteration process on the other hand. From this analysis the sensitivity of the convergence rate as depending on the interface parameters can be studied, which seems to be an important issue for the practical application of the proposed DD method.

Finally an optimization algorithm is applied, which is used to obtain an optimal set of values for the parameters in each of the interface equations. Unfortunately, it appears that for the cases considered, the optimal set of interface parameters and the corresponding asymptotic convergence factors are very close to the classical Dirichlet-Dirichlet domain coupling of Schwarz' original method.

2 Model Equations and Discretization

The area of application that we will concentrate on in the future, is part of the field of viscous CFD for ship hydrodynamics. Therefore, our target is the incompressible, steady Navier-Stokes equations.

The Reduced Navier-Stokes Equations

The method for the Navier-Stokes equations that we consider is based on a finite-difference discretization of the steady equations in generalized coordinates. This method features the neglect of diffusion in the 'main stream' direction (parabolization) and a *downwind* discretization of the pressure derivative in this direction. The result is called *partially parabolized* or *reduced* discretization of the Navier-Stokes equations. In a Cartesian coordinate system (x, y) in R^2 and for $(x, y) \in \Omega \subset R^2$, they are given by

$$\begin{aligned}
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} &= 0, \\
u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial p}{\partial x} - D\frac{\partial^2 u}{\partial y^2} &= 0, \\
u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial p}{\partial y} - D\frac{\partial^2 v}{\partial y^2} &= 0,
\end{aligned}$$

where $u : \Omega \to R$ and $v : \Omega \to R$ are Cartesian velocity components in x and y direction, respectively and where $p : \Omega \to R$ denotes the (generalized) pressure. The constant $D > 0$ is the diffusion coefficient. The above set of equations is supplemented with an appropriate set of boundary conditions.

In this paper we consider a model for the reduced Navier-Stokes equations. This model will be used in a local mode analysis for a domain-decomposition method which requires the model to be linear. Since the discretization of the pressure gradient plays an important role in our Navier-Stokes method, we will not adhere to the usual set of convection-diffusion equations as a model for analysis. The linearization of the reduced Navier-Stokes equations that we use includes convection and diffusion of momentum, driven by a *known* convection field with a constant diffusion coefficient and driven by the unknown pressure gradient. Furthermore, the continuity equation is kept in the model. From the physical point of view this equation will act as a constraint on the pressure field. The model equations considered are then given by

$$\begin{aligned}\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y} &= 0,\\ a\frac{\partial u}{\partial x}+b\frac{\partial u}{\partial y}+\frac{\partial p}{\partial x}-D\frac{\partial^2 u}{\partial y^2} &= 0,\\ a\frac{\partial v}{\partial x}+b\frac{\partial v}{\partial y}+\frac{\partial p}{\partial y}-D\frac{\partial^2 v}{\partial y^2} &= 0,\end{aligned}$$

again supplemented with an appropriate set of boundary conditions. Here, $a:\Omega\rightarrow R$ and $b:\Omega\rightarrow R$ are the Cartesian components of the convection field in x and y direction, respectively. Without loss of generality we will assume $a,b>0$. The main stream direction is chosen to be in the x direction, which leads to the property $a>b$. For physical relevance, we will assume that (a,b) is divergence-free. The domain is assumed to be subdivided in two subdomains, with a common boundary Γ. In his paper Γ is assumed to be perpendicular to the main stream direction x.

The Discretized Equations

The discretization that we use is a standard finite-difference discretization. In this paper the first derivatives of velocity components are discretized with the first-order upwind finite-difference formula. Second-order derivatives are discretized with standard second-order finite-differences. The pressure derivative is discretized with the first-order accurate, downwind finite-difference. See Hoekstra [Hoe92] for more information on the particular choice for the discretization.

The domain Ω is divided in two domains Ω_i, $i=1,2$. A discrete approximation of a function $u_k:\Omega_k\rightarrow R$, $k=1,2$, is denoted by $u_k^{i,j}=u_k(i\Delta x, j\Delta y)$, $0\le i\le I_k+1$ and $0\le j\le J+1$. Here, Δx and Δy denote constant step sizes in x and y direction, respectively. Following this scheme, the discretized equations are given by

$$\begin{aligned}\frac{u_k^{i,j}-u_k^{i-1,j}}{\Delta x}+\frac{v_k^{i,j}-v_k^{i,j-1}}{\Delta y} &= 0,\\ a\frac{u_k^{i,j}-u_k^{i-1,j}}{\Delta x}+b\frac{u_k^{i,j}-u_k^{i,j-1}}{\Delta y}+\frac{p_k^{i+1,j}-p_k^{i,j}}{\Delta x}-D\frac{u_k^{i,j+1}-2u_k^{i,j}+u_k^{i,j-1}}{\Delta y^2} &= 0,\\ a\frac{v_k^{i,j}-v_k^{i-1,j}}{\Delta x}+b\frac{v_k^{i,j}-v_k^{i,j-1}}{\Delta y}+\frac{p_k^{i,j+1}-p_k^{i,j}}{\Delta y}-D\frac{v_k^{i,j+1}-2v_k^{i,j}+v_k^{i,j-1}}{\Delta y^2} &= 0.\end{aligned}$$

The general interface conditions are discretized using central finite differences. Following Tan and Borsboom in [TB93], the coefficient γ for the cross-derivative terms in the interface conditions is taken equal to $\beta\Delta x$, thus reducing the number of free parameters, while we may still be confident to obtain a considerable increase in convergence rate for an optimal set of parameters. For the model problem the interface equations on Γ are given by

$$\begin{aligned}
&\frac{1}{2}(u_2^{1,j}+u_2^{0,j})+\frac{\alpha_1}{\Delta x}(u_2^{1,j}-u_2^{0,j})+\frac{\beta_1}{2\Delta y}(u_2^{0,j+1}-u_2^{0,j-1})= \\
&\qquad \frac{1}{2}(u_1^{I_1+1,j}+u_1^{I_1,j})+\frac{\alpha_1}{\Delta x}(u_1^{I_1+1,j}-u_1^{I_1,j})+\frac{\beta_1}{2\Delta y}(u_1^{I_1,j+1}-u_1^{I_1,j-1}), \\
&\frac{1}{2}(v_2^{1,j}+v_2^{0,j})+\frac{\alpha_2}{\Delta x}(v_2^{1,j}-v_2^{0,j})+\frac{\beta_2}{2\Delta y}(v_2^{0,j+1}-v_2^{0,j-1})= \\
&\qquad \frac{1}{2}(v_1^{I_1+1,j}+v_1^{I_1,j})+\frac{\alpha_2}{\Delta x}(v_1^{I_1+1,j}-v_1^{I_1,j})+\frac{\beta_2}{2\Delta y}(v_1^{I_1,j+1}-v_1^{I_1,j-1}), \\
&\frac{1}{2}(p_1^{I_1+1,j}+p_1^{I_1,j})+\frac{\alpha_3}{\Delta x}(p_1^{I_1+1,j}-p_1^{I_1,j})+\frac{\beta_3}{2\Delta y}(p_1^{I_1+1,j+1}-p_1^{I_1+1,j-1})= \\
&\qquad \frac{1}{2}(p_2^{1,j}+p_2^{0,j})+\frac{\alpha_3}{\Delta x}(p_2^{1,j}-p_2^{0,j})+\frac{\beta_3}{2\Delta y}(p_2^{1,j+1}-p_2^{1,j-1}).
\end{aligned}$$

3 Fourier Analysis

For the set of algebraic equations defined above and an additive Schwarz iteration scheme, we perform a local mode analysis. Therefore, we supplement the set of equations with Dirichlet boundary conditions on the inlet and outlet parts of the domain boundary.

Denote an approximation after m iterations with $u_k^{(m)} = \bigcup_{i,j} u_k^{i,j(m)}$. Similar notations will be used for other grid functions. We assume solutions which are periodic in y. Discrete Fourier transformation in the direction along the interface Γ gives for the error components after the mth iteration

$$\begin{aligned}
e_k^{i,j(m)} &= u_k^{i,j(m)} - u_k^{j,k(*)} &&= \sum_{s=0}^{J-1} \rho_{i,s,k}^{(m)} \mathrm{e}^{\mathrm{i}j\theta_s}, \\
f_k^{i,j(m)} &= v_k^{i,j(m)} - v_k^{j,k(*)} &&= \sum_{s=0}^{J-1} \sigma_{i,s,k}^{(m)} \mathrm{e}^{\mathrm{i}j\theta_s}, \\
g_k^{i,j(m)} &= p_k^{i,j(m)} - p_k^{j,k(*)} &&= \sum_{s=0}^{J-1} \tau_{i,s,k}^{(m)} \mathrm{e}^{\mathrm{i}j\theta_s},
\end{aligned}$$

where $\theta_s = \frac{2\pi s}{J}$, $s = 0, \ldots, J-1$ and $\rho_{i,s,k}$, $\sigma_{i,s,k}$ and $\tau_{i,s,k}$ are the discrete Fourier transforms. The superscript $(*)$ indicates exact solution of the algebraic equations.

For each Fourier mode s the transformed equations for the Fourier transforms $\rho_{i,s,k}$, $\sigma_{i,s,k}$ and $\tau_{i,s,k}$ of the errors $e_k^{i,j}$, $f_k^{i,j}$ and $g_k^{i,j}$ can be written as

$$\begin{pmatrix} \rho_i \\ \sigma_i \\ \tilde{\tau}_i \end{pmatrix}_{s,k} = \begin{pmatrix} 1 & -a\frac{H_s}{G_s}\mathrm{e}^{-\mathrm{i}\theta_s} & \frac{H_s^2}{G_s}\mathrm{e}^{-\mathrm{i}\theta_s} \\ 0 & \frac{a}{G_s} & -\frac{H_s}{G_s} \\ a-G_s & aH_s\mathrm{e}^{-\mathrm{i}\theta_s} & 1-H_s^2\mathrm{e}^{-\mathrm{i}\theta_s} \end{pmatrix} \begin{pmatrix} \rho_{i-1} \\ \sigma_{i-1} \\ \tilde{\tau}_{i-1} \end{pmatrix}_{s,k},$$

where

$$G_s = a + b\frac{\Delta x}{\Delta y}(1 - \mathrm{e}^{-\mathrm{i}\theta_s}) - 2D\frac{\Delta x}{\Delta y^2}(\cos\theta_s - 1),$$

$$H_s = \frac{\Delta x}{\Delta y}(\mathrm{e}^{\mathrm{i}\theta_s} - 1),$$

and where we used $\tilde{\tau}_i = \tau_{i+1}$, $i = 0, \ldots, I_k$. The above recurrence relation has a general solution, which can be written as

$$\begin{pmatrix} \rho_i \\ \sigma_i \\ \tilde{\tau}_i \end{pmatrix}_{k,s} = R_{k,s}\lambda_{s,1}^i e_1 + S_{k,s}\lambda_{s,2}^i e_2 + T_{k,s}\lambda_{s,3}^i e_3.$$

Here $\lambda_{s,n}$ denotes the nth eigenvalue of the recurrence matrix, with a corresponding eigenvector e_n, $n = 1, 2, 3$.

If we now make Fourier transforms of the boundary conditions and interface equations, the iteration index m for the additive Schwarz iteration enters the equations, and we can readily derive an iteration equation for $z_s^{(m)} = (R_{1,s}^{(m)}, S_{2,s}^{(m)}, T_{2,s}^{(m)})^T$. Here the derived algebraic relations between $S_{1,s}$, $T_{1,s}$ and $R_{1,s}$ and between $R_{2,s}$ and $S_{2,s}$ and $T_{2,s}$ are used to eliminate $S_{1,s}$, $T_{1,s}$ and $R_{2,s}$. The iteration can be written as

$$Mz^{(m)} = Nz^{(m-1)}.$$

The 3×3 matrix M has a very simple structure and can be easily inverted analytically. The eigenvalues $\chi_i(M^{-1}N)$, $i = 1, 2, 3$, of the iteration matrix $M^{-1}N$, the spectral radius $\rho(M^{-1}N) = \max_i |\chi_i(M^{-1}N)|$ and asymptotic convergence factor $\rho_\infty(M^{-1}N) = \max_{\theta_s} \rho(M^{-1}N)$ can be determined. The asymptotic convergence factor depends on the free parameters in the interface conditions.

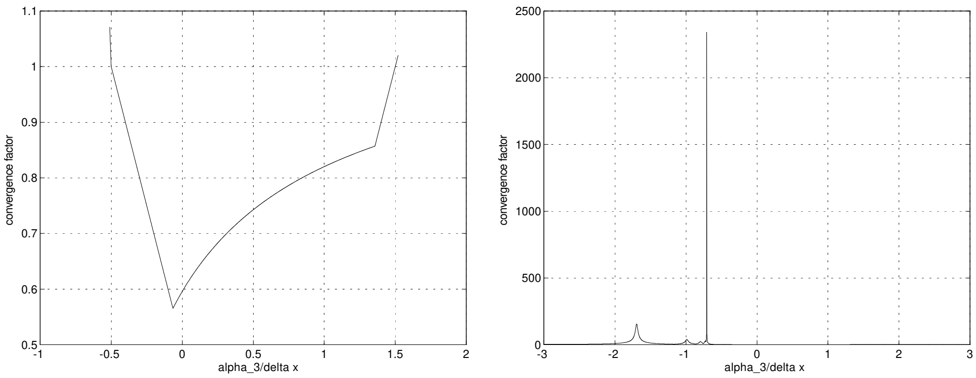
4 Optimization of the Interface Conditions

The asymptotic convergence rate as a function of the free parameters in the interface conditions can be studied. In order to choose an optimization algorithm to find the best possible asymptotic convergence rates, a better understanding of and insight in the asymptotic convergence rate as a function of the free parameters is a prerequisite.

Convergence Factor

The convergence factor is the maximum over all Fourier modes and the three eigenvalues of the iteration matrix. While changing the free parameters, the asymptotic convergence factor may be reached at a different eigenvalue and/or at a different Fourier mode. So, even if the eigenvalues for a fixed Fourier mode depend C^1 continuously on the free parameters, ρ_∞ is not necessarily a C^1 continuous function of the parameters. The discrete set of Fourier modes may be extended to include all modes $0 < \theta < 2\pi$. Then, in general, the asymptotic convergence factor as a function of the free parameters will only be non-differentiable at the intersection points $\chi_i = \chi_j$, $i \neq j$. Therefore, any technique used for the optimization of the free parameters in the interface conditions with respect to convergence factor should not require the derivative of the asymptotic convergence factor with respect to the free parameters. An example of the convergence factor as a function of a free parameter is given in Figure 1. Here the coefficient of the x component of the pressure gradient is varied, while the coefficients are fixed (at there optimal values). It appears that the convergence factor

Figure 1 Asymptotic convergence factor as a function of $\alpha_3/\Delta x$.



is quite strongly dependent on the interface parameters, which makes a sensible choice for these parameters even more important.

Optimization

The optimal values of the free parameters can be computed by applying an appropriate minimization algorithm. However, any of the classical minimization schemes will fail in general, unless the starting value is chosen sufficiently close to the solution. This is particularly so for the present case, since the asymptotic convergence factor as a function of the free parameters appears to have a number of local minima.

We apply a minimization algorithm by Powell [Pow64], which is based on a one-dimensional or line minimization algorithm. The line minimizations are consecutively applied in mutually conjugate directions, which are constructed during the minimization process. As a line minimization an inverse parabolic interpolation scheme is used.

As an example, we present in Table 1 the results of a numerical optimization of the free parameters and their corresponding (optimal) convergence factors for the model problem, as predicted by the Fourier analysis presented in this paper. We considered

Table 1 Optimal parameters and convergence factors.

I	$\alpha_1/\Delta x$	$\beta_1/\Delta y$	$\alpha_2/\Delta x$	$\beta_2/\Delta y$	$\alpha_3/\Delta x$	$\beta_3/\Delta y$	ρ_∞	ρ^c_∞
10	−0.3941	0.0986	−0.2022	10.67	−0.0672	−0.0012	0.567	0.594
100	−0.0799	0.2937	0.0607	17.47	−0.0607	0.0576	0.561	0.594

a domain $\Omega = (0,2) \times (0,1)$ and used a constant convection field with $\frac{b}{a} = 0.1$, Péclet number $\mathrm{Pe} = \frac{a\Delta x}{D} = 10^4$ and number of steps in i direction $I_1 = I_2 = I$. The table also contains the asymptotic convergence factor ρ^c_∞ for the classical Schwarz method, as predicted with the Fourier analysis. Unfortunately, it appears that the optimal value of the asymptotic convergence factor is not significantly different from that of the classical Schwarz method. In an experiment which numerically solves the discretized problem in the present DD context, using the optimal interface parameters from Table 1, the convergence factor was found to be 0.60. This is in good agreement with the theoretical convergence factors presented in Table 1.

5 Concluding Remarks

The DD method presented involves optimization of interface conditions with respect to the convergence rate of the additive Schwarz iteration scheme used on the level of the subproblem blocks. As such, the method may be considered a generalized Schwarz splitting method. We considered a first-order accurate discretization of a model for the reduced Navier-Stokes equations and an interface perpendicular to the main stream direction. The interface equations involve the unknown function values, first-order derivatives in normal and tangential direction and the second-order cross-derivative term.

For the rather simple discretization used, a Fourier analysis for the additive Schwarz iteration can be done analytically with the aid of modern tools from computer algebra.

The Fourier analysis revealed the relation between the asymptotic convergence rate and the free parameters in the interface conditions.

In general, the asymptotic convergence rate is a non-smooth function of the free parameters. The minimization of Powell may be used to obtain a local minimum in the asymptotic convergence factor as a function of the parameters. However, this function may have a substantial number of local minima, and such a minimization method is not suited for general application.

Unfortunately, the minimum convergence factor for the generalized interface conditions as obtained by the optimization, is only slightly smaller than the convergence factor for the classical Dirichlet-Dirichlet coupling of the original Schwarz method. This is contrary to the expectations, based on results obtained by Tang [Tan92] and Tan and Borsboom [TB93].

The reason for this may be the one-sided upwind and downwind discretization of the various terms in the PDEs considered. Furthermore, early in our analysis we decided to make the coefficient of the cross-derivative term in the interface conditions equal to the coefficient of the tangential-derivative term in the interface conditions. This choice was based on the results obtained by Tan and Borsboom, who with the same choice for a scalar advection-diffusion equation have been rather successful. For the present case this choice may be less appropriate.

The minimum convergence factor seems to be quite sensitive to the choice of the parameters in the interface condition. However, further research has shown that, in the case considered and the specific choices that we made, the optimal convergence rate itself is not very sensitive for problem parameters such as convection angle, the mesh Péclet number or the number of grid cells used.

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