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Improving Convergence Behavior of Nonlinear Equation Systems in Intensified Process Models by Decomposition Methods

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Abstract

Modelling and simulating intensified processes can be a rather demanding task, since convergence problems occur frequently and force the numerical algorithm to abort before a solution for the related equation system is found. These systems are mostly large-scaled, they contain a high number of nonlinear terms and their equations are strongly coupled through certain variables. A promising way to eliminate the convergence problems is presented here in the form of two decomposition methods alias Dulmage-Mendelsohn decomposition and bordered block transformation that arise from linear algebra. They divide the overall equation system into lower dimensional subsystems which can be solved separately in sequence. This is said to reduce the numerical costs and improve the condition in most cases. To check these assertions the decomposition methods were applied on the equation system of a reactive distillation column. Subsequently the original and the decomposed versions were iterated by a simultaneous solver. Their performance during iteration concerning condition, numerical costs and convergence were compared and validated by the condition number, the function counts and the number of successful iterations starting from systematically chosen initial values out of the solution environment. Based on the results we discuss use cases for the decomposed and the original versions and close this work by presenting some ideas about how the efficiency of the decomposition methods could be further improved.

Keywords: Numerical methods, Efficiency, Robustness, Condition

1. Introduction and Motivation

The number of intensified processes in chemical industry is steadily increasing due to the significant associated economic potential compared to standard process concepts. As in conventional processes a model is needed for design and control which has to describe the process performance adequately. The strong interrelation of multiple unit operations within a single apparatus causes difficulties for both physical modeling and the applied numerical algorithms to solve the resulting nonlinear equation system. In this contribution, the focus is laid on the numerical aspects of intensified processes.

Certain variables link the unit operations in an intensified equipment, so that the equation system can only be solved simultaneously. Typically, Newton-based algorithms are used, which do not always converge for large-scale systems with a high number of nonlinear terms.

A strategy to overcome these problems is to subdivide the overall system into subsystems, which can be solved independently in sequence. Two of these decomposition methods, the Dulmage-

Mendelsohn (DM) decomposition and the bordered block transformation (BBTF) are examined here. In the worst case, each subsystem is theoretically as ill-conditioned as the original system. Consequently, for most cases the condition number of the subsystems will improve greatly. Apart from that, the computational effort is reduced due to solving lower dimensional systems in sequence. Two decomposed versions of a reactive distillation column will exemplary be investigated based on these assertions.

2. Solving Nonlinear Equation Systems

The solution of nonlinear systems is divided among three different classes of algorithms: Direct substitution methods (e.g. Wegstein, Dominant Eigenvalue) typically suffer from stability issues in case of ill-conditioned systems; residual minimization techniques (e.g. MATLAB's fsolve) face issues with the nonuniqueness of solutions of squared nonlinear systems. Next to those, the (quasi-)Newton-type class of algorithms combined with globalizing line search techniques is the workhorse for many difficult nonlinear systems. They solve equation systems of the form:

$$0 = F(x) \tag{1}$$

by calculating a Newton step Δx_k to the next iteration point x_{k+1} via:

$$J(x_k) \cdot \Delta x_k = -F(x_k) \tag{2}$$

While the various Newton implementations differ in how the Jacobian matrix J is computed (e.g. Broyden's approximation, analytic Jacobian) and whether the full Newton step is performed (dampening and line search techniques), they almost all have to solve a linear system for each Newton step.

Therefore, well-known techniques, which improve the condition of linear systems such as row and column scaling or those which reduce numerical costs by permuting rows and columns can also enhance the iteration performance of Newton-type algorithms.

In this study, the numerical performance is evaluated by the number of equation calls also called function count until a solution is found and the condition of the initialized system is measured by the condition number based on the Euclidean norm.

2.1. Decomposition Techniques

The core of most decomposition methods is the permutation of columns and rows. During the solution of a nonlinear systems the row and column order of the Jacobian matrix J is rearranged for the solution of each linear Newton step. Given that J contains the first derivatives of all equations with respect to all variables a permutation of the rows implies a rearrangement of the equations and a permutation of columns changes the order of all variables.

2.1.1. Dulmage-Mendelsohn Decomposition

In DM the original Jacobian is converted to an upper block triangular matrix by maximizing the number of blocks along the diagonal Dulmage and Mendelsohn (1958). Fig. 1 shows the incidence matrix of the Jacobian belonging to a tray-based column model. Starting from the first block on the bottom right of J the blocks are solved in sequence. Already calculated variables from former blocks act as constants values in the following. Thus, all entries above the diagonal are previously determined quantities. Obviously the number of variable dependencies within the equations increases from the bottom left to the top right, causing highly dependent equations to be solved last.

2.1.2. Bordered Block Transformation

In contrast to DM, BBTF turns the Jacobian to a lower block triangular form as shown in Fig. 1 for the examined example. Erisman et al. (1985) present the principle of the method in greater detail. During the restructuring highly linked variables called "tearing variables" are separated and shifted to the right of J. Hence, the dimension of the blocks can be further reduced. The solution process is divided into an inner and an outer loop. It starts with the inner iteration from the block in the upper left corner of J. All blocks are then solved in sequence for a constant set of tearing variables. During the outer iteration the tearing variables are iterated within the "tearing equations", wherein all other variables from the inner loop are kept constant. The algorithm converges on satisfying a certain tolerance for the outer loop.

3. Decomposition of a reactive distillation model

Representatively a model for the production of Methyl-Tert-Butylether (MTBE) in a reactive distillation column has been built and used for investigations on both decomposition methods.

MTBE appears as additive in fuels and as solvent or extracting agent in the chemical industry. As discussed by Taylor and Krishna (2000) the conventional process requires a reactor followed by three extraction columns to cope with the arrising azeotropes of the reaction mixture. Through the combination of reaction and distillation the extend of the process reduces to only one column. Nevertheless this leads to a more complex process model and a higher challenge in solving the related equation system.

3.1. Model description

MTBE is synthesized by the reaction of Methanol with Isobutene at the presence of another olefin, which is N-Butene in this case. Neglecting the side reactions, following reaction:

$$CH_3OH + C_4H_8 \Longleftrightarrow C_5H_{12}O \tag{3}$$

is considered in the liquid phase of the model. Amberlist 15 acts as a solid caterlyst in the reactive part of the column.

The classical equilibrium stage approach is applied which involves thermal, mechanical and chemical equilibrium between liquid and vapor phase on all stages. Nevertheless the reaction kinetics are considered in th liquid phase based on data from Rehfinger and Hoffmann (1989) and Sundmacher and Hoffmann (1994). The real fluid behavior of the liquid phase is described by UNIFAC, while the vapor phase is assumed to behave as ideal gas. All thermo-physical and component-dependent properties are taken from CHEMCAD (2017).

Since the focus of this work is the observation of the decomposition methods the model validation through experimental data is not amplified here. Beside this the model consists of only two rectifying and one reactive stage to keep the restructuring comprehensible.

The entire model encompasses 664 nonlinear algebraic equations. It has been implemented in our department's modeling and code generation software MOSAICmodeling, that is presented by Merchan et al. (2016).Both decomposition methods are already integrated in MOSAICmodeling and could be used on the test system. Subsequently the original and decomposed versions were exported to MATLAB and iterated with the Netwon-based Trust-region-dogleg-solver.

3.2. Observation of the decomposed systems

Figure 1 presents the incidence Jacobian matrices of the original and the decomposed systems. The DM decomposition retains a quite large block with the dimension of 576. This block contains

the whole UNIFAC-model and conservation balances which are both strongly coupled through the mole fractions and stage temperatures.

The BBTF identifies the mole fractions of all three components that take part in reaction 3 and the stage temperatures as tearing variables. This sums up to 12 tearing variables. As a result the block dimension along the diagonal can be drastically reduced to a dimension of 3 at maximum.

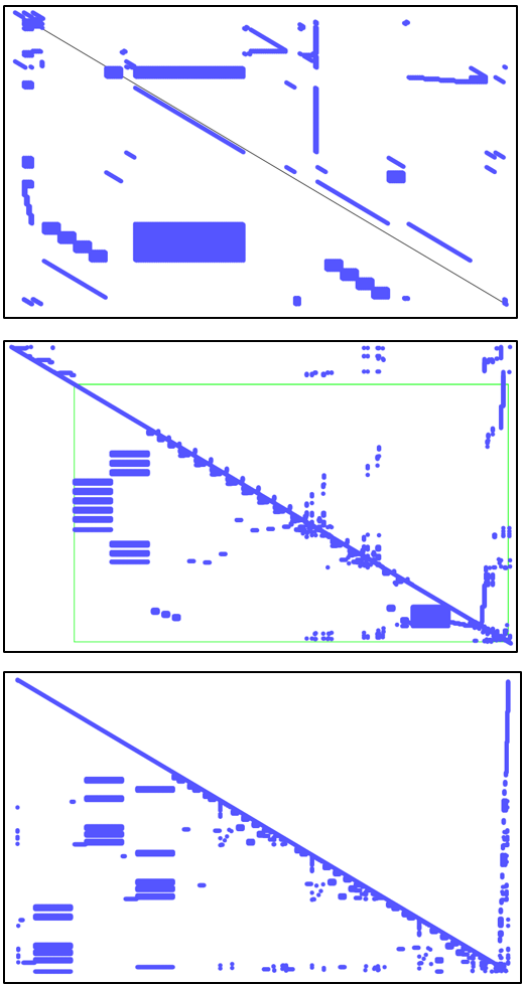

Figure 1: Incidence Jacobian matrices of the original equation system (top), the DM decomposed system (center) and the BBTF decomposed system (bottom)

3.3. Test methods and results

Starting at the solution of the equation system each iteration variable is separately varied between $\pm$ 5 and 30 % while keeping the other variables at their solution value. This is done for the original and the decomposed systems. Figure 2 shows the ratio of successful runs to performed runs over the perturbation of the variables for all three systems. Since the number of converging iterations does not differ much between increasing and decreasing the variable values by a certain percentage (the maximum difference is five iterations), only the average value is shown.

BBTF features the best convergence performance in this case. The ratio of successful iterations stays constant at 98 % in the examined range. The number of failed iterations refers to the perturbation of the tearing variables. Even for a perturbation of 5 % these iterations do not succeed. In contrast the perturbation of all other variables does not influence the convergence result at all. Hence the convergence of a BBTF decomposed system highly depends on the initial guess of the tearing variables, while the initial guess of the remaining variables can be arbitrary.

For the other two systems the number of successful iterations decreases with higher perturbations as expected. The DM seems to be a bit more robust than the original system. Interestingly in both versions the perturbation of certain variables leads to failing iterations for all tested perturbation values. These variables can be identified as quantities of the UNIFAC model, to be exact they are the van der Waals volumina and surfaces that determine the combinatorial component of the activity coefficient. Per definition they are both related to the molar fractions that were identified as highly linked variables and could spread any deviation directly into other parts of the equation system. On top they occur in exponential expressions that are strongly nonlinear and obviously not well described by any linear approximation of a Newton-based algorithm.

Next to the convergence performance the computational effort to iterate the three systems has been investigated. Therefore, all variables were perturbed at once by $\pm$ 3 %. Subsequently the systems were solved under the same solver settings (maximum number of function calls per block: 30000,

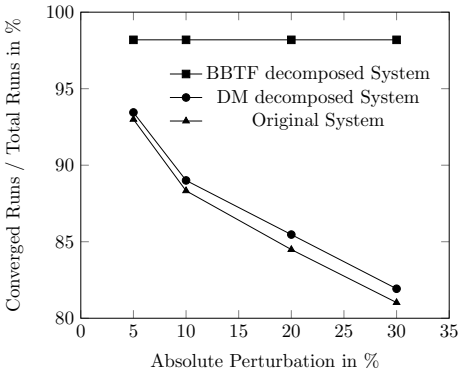

Figure 2: Ratio of converged to total iterations by variable wise perturbation at the initial point

Table 1: Function counts to solver termination at 3% pertubation of all variables

System	**Function Counts** (+3%)	(-3%)	**Solved**
BBTF	in: $> 10^6$ out: 693	in: $> 10^6$ out: 1078	no
BBTF (TV=const.)	in: 303054 out: 110	in: 121265 out: 44	yes
DM	14254	13094	yes
Original	15960	15295	yes

Step size tolerance:10^{-6}, function tolerance: 10^{-10}). During iteration the function calls have been tracked to finally calculate the total function count until the solver terminates. The results are presented in Table 1.

Although the residual series of the BBTF decomposed system seemed to converge, it could not be properly reduced after more than one million function calls within the inner iterations. Both outer iterations ($\pm$ 3% perturbation) were terminated by deceeding the set step size tolerance. When keeping the tearing variables at their solution values the solver needed a total sum of 303164 function calls to succeed at a perturbation of +3 % and less than half the number at a perturbation of -3 %. Hence in BBTF both the convergence and the efficiency of the solving procedure depend a lot on the tearing variable values.

The best performance shows the DM decomposed system closely followed by the original system. Presumably the performance of the decomposed system would be much better in a more decoupled system. For this example, 97 % of the function counts are used within the large block with its 576 equations.

Finally, the conditions of the systems along their iteration trajectories are examined by recording their condition numbers. It is started from the initial point where all variables exceed their solution by 3 %. Surprisingly, the condition number of the original and the decomposed system differ only marginally for their first 17 iteration steps. This encourages the suspicion that the DM decomposition cannot efficiently uncouple the overall system into lower dimensional blocks in this case. Hence the problematic terms causing the high condition numbers are probably still part of the large block. The iteration number until a solution is found equals 23 for both systems, although less functions calls are necessary to solve the lower dimensional large block of the decomposed system. From iteration step 17 to 23 the condition numbers vary by roughly $2 \cdot 10^{18}$. This could be the result of slightly differing final values of the iteration variables. Using the same solver settings the original version might be more accurate since both iterations finish by deceeding the

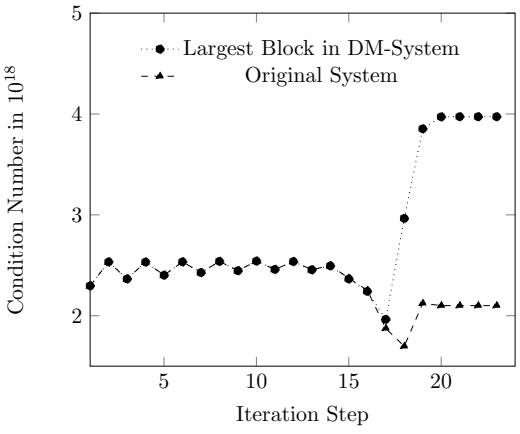

Figure 3: Condition numbers along iteration trajectories of the original system and the largest blocks of the DM decomposed system

function tolerance. In the iteration of the original system the quadratic sum of more function residuals has to fulfill this criterion.

The condition numbers of the outer iteration of the BBTF decomposed system do not change much and lie all within the range $4.879 \pm 0.0005 \cdot 10^{13}$. This is the best conditioned system of the three examined versions. The condition numbers of the inner blocks are negligibly small.

4. Conclusion and Outlook

The effect of the Dulmage-Mendelsohn decomposition and bordered block transformation on a nonlinear algebraic equation system referring to a stationary reactive distillation model has been examined concerning convergence, computational effort and conditioning.

The results show that the DM decomposed system features a small improvement to the original system regarding the convergence behavior and the decrease in numerical costs during iteration. Nevertheless, a large block remains, that probably hinders the efficiency to be further increased. This block is caused by the used UNIFAC model where mole fractions and temperatures induce a strong coupling between the equations in the system. A concept to eliminate this problem is to decompose the large block by DM as well and solve it in an inner iteration. This will be part of our future investigations.

For known solutions of the tearing variables the BBTF seems to be quite robust to any perturbation of the inner iteration variables. Due to the low dimensional blocks the condition can be improved by five orders of magnitude to the original system. Still the numerical costs are quite high. Even when the tearing variables are initialized with their solution values the solver requires roughly 20 times more function calls than the other system modifications. This is the result of a very low convergence velocity. When the tearing variables differ only slightly from their solution the low convergence velocity can lead to a stagnating minimization of the function residuals. The BBTF gives a better numerical performance in systems with a lower number of tearing variables as discussed in Bublitz et al. (2017). Further test cases will be performed to identify a limit for the number of tearing variables where the numerical costs are still reasonable low. Beside this, methods as the one of Baharev et al. (2017) that systematically generate initial values close to the solution will be examined in order to provide a sufficient set of initial values for the tearing variables and achieve a certain level of efficiency during the iteration of a BBTF decomposed system.

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