1 Introduction

During the last two decades dynamic processes simulation has become an indispensable tool for the design and operation of complex chemical plants. The rigorous modeling of the chemical processes results in large-scale systems of differential and algebraic equations (DAE). Using an appropriate modeling the differential index of the resulting DAE systems can be restricted to index 1 in many cases [BP1]. For details about the numerical solution of DAE systems and the index problem we refer to [BC1, GH1].

For large-scale systems cost–effective numerical methods are needed. Under special modeling assumptions waveform iteration methods can be used for the concurrent dynamic process simulation [SM1]. These methods, also called dynamic iteration methods or Picard–type methods are well suited for the implementation on parallel computers.

Since the beginning of the 80'th the main application field for waveform iteration methods has been the circuit simulation of MOS digital integrated circuits [LRS]. Investigations of waveform iteration methods for systems of ordinary differential equations (ODE) [WS1, JP1, Br1, BB1] as well as for systems of differential algebraic equations [LRS, Mi1, SL1, SM1] are known. Convergence under certain conditions on the mathematical problem has been proven in [Br1] for explicit ODE systems and in [Mi1] for linear DAE systems of arbitrary index. Lelarasmee et al. [LRS] and Schneider [Sc1] proved convergence for a semiexplicit type of waveform iteration for semiexplicit DAEs of Index 1.

In this paper we consider the application of block waveform iteration methods to initial value problems for implicit DAE systems of index 1 arising in chemical process simulation. Block waveform iteration methods permit the concurrent treatment of blocks of subsystems of the entire system with multirate integration techniques gaining a coarse granular parallelism. Their convergence properties strongly depend on the assignment of variables to equations and the partitioning of the system into subsystem blocks.

First we proof convergence for waveform iteration methods applied to semiexplicit DAE sytems of index 1. The convergence conditions are given in a blocksystem oriented manner, i.e. only the blocksystems have to satisfy some corresponding conditions. Then we show that the convergence conditions are fulfilled for a simplified modeling of distillation columns. An assignment and partitioning algorithm is given, which takes the requirements of the convergence theorems into account.

Based on this investigations a prototype of a waveform–iteration code has been implemented and tested by means of examples included in the user package of the chemical process simulator SPEEDUP [PS1].

2 Waveformiteration

We consider the initial value problem (IVP) for a semiexplizit DAE system:

$$
\begin{aligned}
\dot{x}_1 &= \tilde{f}(x_1, x_2, t) \\
0 &= \tilde{h}(x_1, x_2, t) \\
x(t_0) &= x_0, \qquad t \in [t_0, t_e]
\end{aligned}
\tag{2.1}
$$

with $x = (x_1, x_2)^T$, x_0 the consistent initial value, $\tilde{f} : \mathbb{R}^k \times \mathbb{R}^l \times [t_0, t_e] \to \mathbb{R}^k$, $\tilde{h} : \mathbb{R}^k \times \mathbb{R}^l \times [t_0, t_e] \to \mathbb{R}^l$ and $n := k + l$.

Let the time interval be denoted by $T := [t_0, t_e]$.

For index 1 problems (2.1) the inverse $(\tilde{h}_{x_2})^{-1}$ exists in a neighbourhood of the solution of the IVP. In the following we assume that $(\tilde{h}_{x_2})^{-1}$ exists in the whole domain.

Definition 1 *Let $f : \mathbb{R}^k \times \mathbb{R}^l \times \mathbb{R}^k \times \mathbb{R}^l \times T \to \mathbb{R}^k$, $h : \mathbb{R}^k \times \mathbb{R}^l \times \mathbb{R}^k \times \mathbb{R}^l \times T \to \mathbb{R}^l$ be functions with $f(x_1, x_2, x_1, x_2, t) \equiv \tilde{f}(x_1, x_2, t)$, $h(x_1, x_2, x_1, x_2, t) \equiv \tilde{h}(x_1, x_2, t)$. The general form of the continuous waveform iteration for the problem (2.1) is then given by*

$$
\begin{aligned}
\dot{x}_1^k &= f(x_1^k, x_2^k, x_1^{k-1}(t), x_2^{k-1}(t), t) \\
0 &= h(x_1^k, x_2^k, x_1^{k-1}(t), x_2^{k-1}(t), t) \\
x^k(t_0) &= x_0
\end{aligned}
\tag{2.2}
$$

for $k = 1, 2, \ldots$ with $x^0 : T \to \mathbb{R}^n$ be any arbitrary approximation for the beginning of the iteration which satisfies $x^0(t_0) = x_0$.

For the discrete waveform iteration on subintervals, the so called "windows", we refer to [Br1].

After partitioning of (2.1) into a set of r semiexplicit index 1 problems with $x_1 = (x_{11}, \ldots, x_{1r})^T$, $x_{1i} \in \mathbb{R}^{k_i}$, $\sum k_i = k$, $x_2 = (x_{21}, \ldots, x_{2r})^T$, $x_{2i} \in \mathbb{R}^{l_i}$, $\sum l_i = l$, $n_i := k_i + l_i$, $\sum n_i = n$, $x_{\underline{i}} := (x_{1,i}, x_{2,i})^T$, $x = (x_{\underline{1}}, \ldots, x_{\underline{r}})^T$, one obtains the following block structured representation

$$
\begin{aligned}
\dot{x}_{1i} &= \tilde{f}_i(x_{11}, \ldots, x_{1r}, x_{21}, \ldots, x_{2r}, t) \\
0 &= \tilde{h}_i(x_{11}, \ldots, x_{1r}, x_{21}, \ldots, x_{2r}, t) \\
x_{\underline{i}}(t_0) &= x_{\underline{i},0}, \qquad i = 1(1)r\ .
\end{aligned}
\tag{2.3}
$$

The corresponding block waveform iteration is then given by

$$
\begin{aligned}
\dot{x}_{1i}^k &= f_i(x_1^k, x_2^k, x_1^{k-1}(t), x_2^{k-1}(t), t), \\
0 &= h_i(x_1^k, x_2^k, x_1^{k-1}(t), x_2^{k-1}(t), t), \\
x_{\underline{i}}^k(t_0) &= x_{\underline{i},0}, \qquad i = 1(1)r\ .
\end{aligned}
\tag{2.4}
$$

Two special cases are the block Gauss Seidel waveform iteration where f_i and g_i are given by

$$
\begin{aligned}
f_i(x_1, x_2, y_1, y_2, t) &:= \tilde{f}_i(x_{11}, x_{21}, \ldots, x_{1i}, x_{2i}, y_{1i+1}, y_{2i+1}, \ldots, y_{1r}, y_{2r}, t) \\
h_i(x_1, x_2, y_1, y_2, t) &:= \tilde{h}_i(x_{11}, x_{21}, \ldots, x_{1i}, x_{2i}, y_{1i+1}, y_{2i+1}, \ldots, y_{1r}, y_{2r}, t)
\end{aligned}
\tag{2.5}
$$

and the block Jacobi waveform iteration with

$$\begin{aligned} f_i(x_1,x_2,y_1,y_2,t) &:= \tilde{f}_i(y_{11},y_{21},\dots,y_{1i-1},y_{2i-1},x_{1i},x_{2i},y_{1i+2},y_{2i+2},\dots,y_{1r},y_{2r},t) \\ h_i(x_1,x_2,y_1,y_2,t) &:= \tilde{h}_i(y_{11},y_{21},\dots,y_{1i-1},y_{2i-1},x_{1i},x_{2i},y_{1i+1},y_{2i+1},\dots,y_{1r},y_{2r},t)\,. \end{aligned} \tag{2.6}$$

The block Jacobi waveform iteration is especially suitable for parallelization.

3 Convergence considerations

For problems (2.1) with index 1 the existence of an unique solution $x_2 = \tilde{g}(x_1,t)$ of the algebraic equations $0 = \tilde{h}(x_1,x_2,t)$ follows from the implicit function theorem. Because each blocksystem in (2.3) is assumed to have index 1, every $\tilde{h}_i$ is solvable for x_{2i} as well. Hence in the cases of block Gauss Seidel– and of block Jacobi waveform iteration the h_i are also sovable for x_{2i}.

Then (2.4) can formally be rewritten as

$$\begin{aligned} \dot{x}^k_{1i} &= f_i(x^k_1, x^k_2, x^{k-1}_1(t), x^{k-1}_2(t), t), \\ x^k_{2i} &= g_i(x^k_1, x^k_2, x^{k-1}_1(t), x^{k-1}_2(t), t), \\ x^k_{\lrcorner i}(t_0) &= x_{\lrcorner i,0}, \qquad i = 1(1)r, \end{aligned} \tag{3.1}$$

In the case of the block Jacobi waveform iteration the g_i are even independent of x_2, so that 3.1 has the representation

$$\begin{aligned} \dot{x}^k_{1i} &= f_i(x^k_1, x^k_2, x^{k-1}_1(t), x^{k-1}_2(t), t), \\ x^k_{2i} &= g_i(x^k_1, x^{k-1}_1(t), x^{k-1}_2(t), t), \\ x^k_{\lrcorner i}(t_0) &= x_{\lrcorner i,0}, \qquad i = 1(1)r. \end{aligned} \tag{3.2}$$

Let $C(T,\mathbb{R}^n)$ and $C^1(T,\mathbb{R}^n)$ be the spaces of the continuous and the continuous differentiable n dimensional functions defined on T.

The direct sum $\bar{Z} := C^1(T,\mathbb{R}^k) \oplus C(T,\mathbb{R}^l)$ is a set of ordered pairs defined by

$$\bar{Z} := \{(z_1,z_2)^T : z_1 \in C^1(T,\mathbb{R}^k), z_2 \in C(T,\mathbb{R}^l)\}.$$

Let $|.|_m$ be any norm in $\mathbb{R}^m$, then for $z_2 \in C(T,\mathbb{R}^l)$ and $z_1 \in C^1(T,\mathbb{R}^k)$ exponetially weighted norms for arbitrary but fixed $\alpha > 0$ are defined by

$$\begin{aligned} ||z_2||_{\alpha,l} &:= \sup_{t\in T}(e^{-\alpha(t-t_0)}|z_2(t)|_l) \\ ||z_1||_k &:= |x(t_0)|_k + \frac{1-e^{-\alpha(t_e-t_0)}}{\alpha}||\dot{z}_1||_{\alpha,k}. \end{aligned}$$

With this norms a norm for $z \in \bar{Z}$ is defined by

$$||z||_{\bar{Z}} := \max\{||z_1||_k, ||z_2||_{\alpha,l}\}.$$

Lemma 1 *$\{\bar{Z}, ||.||_{\bar{Z}}\}$ is a Banach–space.*

Proof:

It has to be shown, that the limit $z = (z_1, z_2)^T$ of an arbitrary Cauchy sequence $(z^i)_{i=1}^{\infty}$ in $\{\bar{Z}, \|.\|_{\bar{Z}}\}$ is an element of $\bar{Z}$.

$\forall \epsilon > 0$ there $\exists i_0$ such that $\|z^0 - z^p\|_{\bar{Z}} < \epsilon$ holds $\forall q, p > i_0$.

We have that

$$
\begin{aligned}
\epsilon &> \|z^q - z^p\|_{\bar{Z}} = \|(z_1^q, z_2^q)^T - (z_1^p, z_2^p)^T\|_{\bar{Z}} = \max\{\|z_1^q - z_1^p\|_k, \|z_2^q - z_2^p\|_{\alpha,l}\} \\
&= \max\left\{|z_1^q(t_0) - z_1^p(t_0)|_k + \frac{1 - e^{-\alpha(t_e - t_0)}}{\alpha}\|\dot{z}_1^q - \dot{z}_1^p\|_{\alpha,k}, \|z_2^q - z_2^p\|_{\alpha,l}\right\} \\
&= \max\left\{|z_1^q(t_0) - z_1^p(t_0)|_k + \frac{1 - e^{-\alpha(t_e - t_0)}}{\alpha}\sup_{t\in T}(e^{-\alpha(t-t_0)}|\dot{z}_1^q(t) - \dot{z}_1^p(t)|_k),\right. \\
&\qquad \left.\sup_{t\in T}(e^{-\alpha(t-t_0)}|z_2^q(t) - z_2^p(t)|_l)\right\} \\
&\geq \max\left\{|z_1^q(t_0) - z_1^p(t_0)|_k + \frac{1 - e^{-\alpha(t_e - t_0)}}{\alpha}e^{-\alpha(t_e-t_0)}\sup_{t\in T}|\dot{z}_1^q(t) - \dot{z}_1^p(t)|_k,\right. \\
&\qquad \left. e^{-\alpha(t_e-t_0)}\sup_{t\in T}|z_2^q(t) - z_2^p(t)|_l\right\}.
\end{aligned}
$$

Since $\epsilon \to 0$ for growing q and p it follows that

$$|z_1^q(t_0) - z_1^p(t_0)|_k \to 0, \qquad \sup_{t\in T}|\dot{z}_1^q(t) - \dot{z}_1^p(t)|_k \to 0 \quad \text{and} \quad \sup_{t\in T}|z_2^q(t) - z_2^p(t)|_l \to 0.$$

So we have uniform convergence for $\dot{z}_1^i \to \dot{z}_1$, $z_2^i \to z_2$ and thus $\dot{z}_1 \in C(T, \mathbb{R}^k)$, $z_2 \in C(T, \mathbb{R}^l)$. Because also $z_1^i(t_0) \to z_1(t_0)$ it follows the uniform convergence $z_1^i \to z_1$ and hence $z_1 \in C^1(T, \mathbb{R}^k)$.

□

With respect to the partitioned system (2.3) we have $z_1 = (z_{11}, \ldots, z_{1r})^T$ and $z_2 = (z_{21}, \ldots, z_{2r})^T$. With $z_{\_i} := (z_{1i}, z_{2i})^T$ we can define function sets Z_i corresponding to $\bar{Z}$ and norms $\|.\|_{Z_i}$ corresponding to $\|.\|_{\bar{Z}}$. Because of Lemma 1, the spaces $\{Z_i, \|.\|_{Z_i}\}$, $i = 1, \ldots, r$, are Banach–spaces. For $z = (z_{\_1}, \ldots, z_{\_r})^T \in Z$, $Z := Z_1 \oplus Z_2 \oplus \ldots \oplus Z_r$, a norm $\|.\|_Z$ is defined by

$$\|z\|_Z := \max_{i\in\{1,\ldots,r\}}\{\|z_{\_i}\|_{Z_i}\}.$$

One easily can show that $\{Z, \|.\|_Z\}$ is a Banach–space.

For $x, y \in Z$, an operator $O : Z \times Z \to Z$ is defined by

$$O(x, y)(t) = O(x_1, x_2, y_1, y_2)(t) := \begin{bmatrix} x_{1,0} + \int_{t_0}^{t} f(x_1, x_2, y_1, y_2, s)ds \\ g(x_1, x_2, y_1, y_2, t) \end{bmatrix}.$$

From the definition of the operator O we find that the block waveform iteration (3.1) has the formal representation

$$x^k = O(x^k, x^{k-1})$$

with $x^k(t_0) = x_0$ and an arbitrary starting function $x^0 \in Z$.

We now consider the operator equation

$$x = O(x, y).$$

If this equation is uniquely solvable for x, an operator

$$P : Z \to Z \tag{3.3}$$

is defined where x is determined by the equation $x = P(y)$.

In the following Lemma 2 the Banach space $\{Z, ||.||_Z\}$ and the operator O are more generally defined. The coinciding notation is chosen because the above defined Banach space $\{Z, ||.||_Z\}$ and operator O are applicable to this Lemma, what will be shown later.

The proof of the Lemma 2 also can be found in [Br1].

Lemma 2 *Let $\{Z, ||.||_Z\}$ be a Banach–space and let the operator $O : Z \times Z \to Z$ satisfy the following assumptions:*

a1 *O is globally Lipschitz continuous, i.e. there exist constants $K_x, K_y \geq 0$ such that for all $x, y, \bar{x}, \bar{y}$*

$$||O(x, y) - O(\bar{x}, \bar{y})||_Z \leq K_x ||x - \bar{x}||_Z + K_y ||y - \bar{y}||_Z,$$

a2 $0 < K_x + K_y < 1$.

Then

f1 *For each $y \in Z$ the equation $x = O(x, y)$ is uniquely solvable for x. The operator P defined in (3.3) is contractive with a Lipschitz–constant $M_y = \frac{K_y}{1-K_x}$.*

f2 *The sequence (x^k) defined by*

$$x^k = O(x^k, x^{k-1})$$

converges to a unique limit x for any starting function $x^0 \in Z$.

Proof:

Let $y \in Z$ be arbitrary but fixed. First it is shown, that the operator

$$O\_y := O(., y), \qquad O\_y : Z \to Z$$

is contractive and has a unique fixpoint. From **a1** it is known that O_y is Lipschitz continuous with the Lipschitz constant K_x and from **a2** we have that $K_x < 1$. Thus the fixpoint theorem of Banach is applicable to O_y which proofs the assertion.

The operator $P : Z \to Z$ is defined in that way, that P appoints to every $y \in Z$ the fixpoint of O_y.

For arbitrary $y, \bar{y} \in Z$ with $x := P(y)$ and $\bar{x} := P(\bar{y})$ we have

$$||x - \bar{x}||_Z = ||O(x, y) - O(\bar{x}, \bar{y})||_Z \leq K_x ||x - \bar{x}||_Z + K_y ||y - \bar{y}||_Z$$

and thus

$$||x - \bar{x}||_Z \leq \frac{K_y}{1 - K_x} ||y - \bar{y}||_Z.$$

Since

$$\|x - \bar{x}\|_Z = \|P(y) - P(\bar{y})\|_Z,$$

P is Lipschitz continuous. From **a2** it followes that the Lipschitz constant $\frac{K_y}{1-K_x}$ is smaller than 1, i.e. P is contractive. This proofs **f1**.

With $x := x^k$ and $y := x^{k-1}$, we have

$$x^k = O(x^k, x^{k-1})$$

and thus

$$x^k = P(x^{k-1}).$$

Because of **f1** the fixpoint theorem of Banach is applicable to P what proves **f2**.

□

If $\mathbb{R}^m = \mathbb{R}^{m_1} \oplus \mathbb{R}^{m_2} \oplus \ldots \oplus \mathbb{R}^{m_q}$, then an appropriate norm for $w = (w_1, \ldots, w_q)^T \in \mathbb{R}^m$ is defined by

$$|w| := \max_{i \in \{1,\ldots,q\}} |w_i|_{m_i}$$

Lemma 3 *Let the waveform iteration (3.1) for the partitioned system (2.3) be considered. If the functions f_i and g_i, $i = 1, \ldots, r$ fulfill Lipschitz conditions, i.e. for all $\xi = (\xi_1, \xi_2)^T, \bar{\xi} = (\bar{\xi}_1, \bar{\xi}_2)^T, \eta = (\eta_1, \eta_2)^T, \bar{\eta} = (\bar{\eta}_1, \bar{\eta}_2)^T \in \mathbb{R}^k \oplus \mathbb{R}^l$, $t \in T$ exist positiv constants $f_{ix}, f_{iy}, g_{ix}, g_{iy}$ with*

$$|f_i(\xi, \eta, t) - f_i(\bar{\xi}, \bar{\eta}, t)|_{k_i} \leq f_{ix}|\xi - \bar{\xi}| + f_{iy}|\eta - \bar{\eta}| \tag{3.4}$$

$$|g_i(\xi, \eta, t) - g_i(\bar{\xi}, \bar{\eta}, t)|_{l_i} \leq g_{ix}|\xi - \bar{\xi}| + g_{iy}|\eta - \bar{\eta}| \tag{3.5}$$

then the following estimations hold for $x, y, \bar{x}, \bar{y} \in Z$:

$$\begin{aligned} &\|f_i(x_1(.), x_2(.), y_1(.), y_2(.), .) - f_i(\bar{x}_1(.), \bar{x}_2(.), \bar{y}_1(.), \bar{y}_2(.), .)\|_{\alpha,k_i} \\ \leq\ & f_{ix}\|x - \bar{x}\|_Z + f_{iy}\|y - \bar{y}\|_Z, \end{aligned} \tag{3.6}$$

$$\begin{aligned} &\|g_i(x_1(.), x_2(.), y_1(.), y_2(.), .) - g_i(\bar{x}_1(.), x_2(.), \bar{y}_1(.), \bar{y}_2(.), .)\|_{\alpha,l_i} \\ \leq\ & g_{ix}\|x - \bar{x}\|_Z + g_{iy}\|y - \bar{y}\|_Z. \end{aligned} \tag{3.7}$$

Proof: With $x, y, \bar{x}, \bar{y} \in Z$ one obtains from (3.4)

$$\begin{aligned} &|f_i(x_1(t), x_2(t), y_1(t), y_2(t), t) - f_i(\bar{x}_1(t), \bar{x}_2(t), \bar{y}_1(t), \bar{y}_2(t), t)|_{k_i} \\ \leq\ & f_{ix} \max_{i \in \{1,\ldots,r\}} \{\max\{|x_{1i}(t) - \bar{x}_{1i}(t)|_{k_i}, |x_{2i}(t) - \bar{x}_{2i}(t)|_{l_i}|\}\} + \\ & f_{iy} \max_{i \in \{1,\ldots,r\}} \{\max\{|y_{1i}(t) - \bar{y}_{1i}(t)|_{k_i}, |y_{2i}(t) - \bar{y}_{2i}(t)|_{l_i}|\}\} \end{aligned}$$

Let j be the index i which yields the maximum for the x-component. Then we have

$$
\begin{aligned}
& f_{ix} \max_{i\in\{1,\dots,r\}} \{\max\{|x_{1i}(t)-\bar{x}_{1i}(t)|_{k_i}, |x_{2i}(t)-\bar{x}_{2i}(t)|_{l_i}|\}\} \\
\leq\ & f_{ix}\max\left\{|x_{1j}(t_0)-\bar{x}_{1j}(t_0)+\int_{t_0}^{t}(\dot{x}_{1j}(s)-\dot{\bar{x}}_{1j}(s))ds|_{k_j}, |x_{2j}(t)-\bar{x}_{2j}(t)|_{l_j}\right\} \\
\leq\ & f_{ix}\max\left\{|x_{1j}(t_0)-\bar{x}_{1j}(t_0)|+\int_{t_0}^{t}e^{\alpha(s-t_0)}e^{-\alpha(s-t_0)}|\dot{x}_{1j}(s)-\dot{\bar{x}}_{1j}(s)|_{k_j}ds,\right. \\
& \left. e^{\alpha(t-t_0)}e^{-\alpha(t-t_0)}|x_{2j}(t)-\bar{x}_{2j}(t)|_{l_j}\right\} \\
\leq\ & f_{ix}\max\left\{|x_{1j}(t_0)-\bar{x}_{1j}(t_0)|_{k_j}+\int_{t_0}^{t}e^{\alpha(s-t_0)}\sup_{s\in T}\left\{e^{-\alpha(s-t_0)}|\dot{x}_{1j}(s)-\dot{\bar{x}}_{1j}(s)|_{k_j}\right\}ds,\right. \\
& \left. e^{\alpha(t-t_0)}\sup_{t\in T}\left\{e^{-\alpha(t-t_0)}|x_{2j}(t)-\bar{x}_{2j}(t)|_{l_j}\right\}\right\} \\
=\ & f_{ix}\max\left\{|x_{1j}(t_0)-\bar{x}_{1j}(t_0)|_{k_j}+\|\dot{x}_{1j}-\dot{\bar{x}}_{1j}\|_{\alpha,k_j}\int_{t_0}^{t}e^{\alpha(s-t_0)}ds, e^{\alpha(t-t_0)}\|x_{2j}-\bar{x}_{2i}\|_{\alpha,l_j}\right\} \\
=\ & f_{ix}\max\left\{|x_{1j}(t_0)-\bar{x}_{1j}(t_0)|_{k_j}+\frac{e^{\alpha(t-t_0)}-1}{\alpha}\|\dot{x}_{1j}-\dot{\bar{x}}_{1j}\|_{\alpha,k_j}, e^{\alpha(t-t_0)}\|x_{2j}-\bar{x}_{2j}\|_{\alpha,l_j}\right\} \\
\leq\ & f_{ix}e^{\alpha(t-t_0)}\max\left\{|x_{1j}(t_0)-\bar{x}_{1j}(t_0)|_{k_j}+\frac{1-e^{-\alpha(t-t_0)}}{\alpha}\|\dot{x}_{1j}-\dot{\bar{x}}_{1j}\|_{\alpha,k_j}, \|x_{2j}-\bar{x}_{2j}\|_{\alpha,l_j}\right\} \\
=\ & e^{\alpha(t-t_0)}f_{ix}\max\left\{\|x_{1j}-\bar{x}_{1j}\|_{k_j}, \|x_{2j}-\bar{x}_{2j}\|_{\alpha,l_j}\right\}.
\end{aligned}
$$

Because the same estimate holds for the $y-$component we obtain

$$
\begin{aligned}
& |f_i(x_1(t),x_2(t),y_1(t),y_2(t),t)-f_i(\bar{x}_1(t),\bar{x}_2(t),\bar{y}_1(t),\bar{y}_2(t),t)|_{k_i} \\
\leq\ & e^{\alpha(t-t_0)}\left(f_{ix}\|x-\bar{x}\|_Z+f_{iy}\|y-\bar{y}\|_Z\right).
\end{aligned}
$$

Using the norm definition of $\|.\|_{\alpha,k_i}$ one obtains (3.6).
Going for g through the same procedure as for f one gets (3.7).

□

Theorem 1 *Let the assumptions of Lemma 3 be satisfied. If further the Lipschitz constants g_{ix}, g_{iy} of g_i fulfill for every i the condition*

$$g_{ix}+g_{iy}<1,$$

then the sequence (x^k) obtained by the block waveform iteration (3.1) converges in $\{Z,\|.\|_Z\}$ to the solution of (2.1).

Proof:
We show that the operator O is globally Lipschitz continuous and the Lipschitz constants satisfy the condition **a2** of Lemma 2. Then **f1, f2** can be followed.
We have

$$\|O(x,y)-O(\bar{x},\bar{y})\|_Z=\|z-\bar{z}\|_Z=\max_{i\in\{1,\dots,r\}}\{\max\{\|z_{1i}-\bar{z}_{1i}\|_{k_i}, \|z_{2i}-\bar{z}_{2i}\|_{\alpha,l_i}\}\}.$$

Let j be the maximal i. Using the result of Lemma 3, it follows that

$$
\begin{aligned}
&\|O(x,y)-O(\bar{x},\bar{y})\|_Z = \\
&= \max\left\{|z_{1j}(t_0)-\bar{z}_{1j}(t_0)| + \frac{1-e^{-\alpha(t_e-t_0)}}{\alpha}\|\dot{z}_{1j}-\dot{\bar{z}}_{1j}\|_{\alpha,k_j}, \|z_{2j}-\bar{z}_{2j}\|_{\alpha,l_j}\right\} \\
&= \max\left\{\frac{1-e^{-\alpha(t_e-t_0)}}{\alpha}\|f_j(x_1(.),x_2(.),y_1(.),y_2(.),.)-f_j(\bar{x}_1(.),\bar{x}_2(.),\bar{y}_1(.),\bar{y}_2(.),.)\|_{\alpha,k_j},\right. \\
&\qquad \left.\|g_j(x_1(.),x_2(.),y_1(.),y_2(.),.)-g_j(\bar{x}_1(.),x_2(.),\bar{y}_1(.),\bar{y}_2(.),.)\|_{\alpha,l_j}\right\} \\
&\le \max\left\{\frac{1-e^{-\alpha(t_e-t_0)}}{\alpha}\left(f_{jx}\|x-\bar{x}\|_Z+f_{jy}\|y-\bar{y}\|_Z\right), g_{jx}\|x-\bar{x}\|_Z+g_{jy}\|y-\bar{y}\|_Z\right\}.
\end{aligned}
$$

Hence for large enough chosen α the Lipschitz constants of O are

$$K_x = g_{jx}, \quad K_y = g_{jy}.$$

Because the assumption $g_{jx}+g_{jy}<1$ satisfies the condition **a2** of Lemma 2 the proof is completed.

$\square$

Let $z_{\_i} = (z_{1i}, z_{2i})^T \in Z_i$. Then norms $|.|_0$, $|.|_1$ usually used for the continuous and continuous differentiable functions are defined by

$$
\begin{aligned}
|z_{2i}|_0 &:= \sup_{t\in T}\{|z_{2i}(t)|\}, \\
|z_{1i}|_1 &:= |z_{1i}|_0 + |\dot{z}_{1i}|_0 \ .
\end{aligned}
$$

Further a norm $|.|_{Z_i}$ for $z_{\_i} \in Z_i$ is defined by

$$|z_{\_i}|_Z := \max\{|z_{1i}|_1, |z_{2i}|_0\}.$$

Another norm $|.|_Z$ for $z = (z_{\_1}, \dots, z_{\_r})^T \in Z$ is then defined by

$$|z|_Z := \max\{|z_{\_i}|_{Z_i}\}.$$

With this definitions $\{Z, |.|_Z\}$ is a Banach space.

Theorem 2 *With the assumptions of theorem 1 the sequence (x^k) obtained by the block waveform iteration (3.1) converges in $\{Z, |.|_Z\}$ to the solution of (2.1).*

Proof:

Let the fixpoint of P be denoted by x^*. To show that the block waveform iteration (3.1) converges to $z^* \in \{Z, |.|_Z\}$ for $k \to \infty$ we look for a constant $K > 0$ such that

$$|x^k - x^*|_Z \le K\|x^k - x^*\|_Z.$$

For $z = (z_{\_1}, \dots, z_{\_r})^T \in Z$ it holds by definition

$$|z|_Z = \max_{i\in\{1,\dots,r\}}\{\max\{|z_{1i}|_1, |z_{2i}|_0\}\}.$$

With

$$z_{1i}(t) = z_{1i}(t_0) + \int_{t0}^{t} \dot{z}_{1i}(s)ds$$

we have

$$\begin{aligned}
|z_{1i}(t)|_{k_i} &\leq |z_{1i}(t_0)|_{k_i} + \int_{t0}^{t} e^{-\alpha(s-t_0)} \|\dot{z}_{1i}\|_{\alpha,k_i} ds \\
&\leq e^{\alpha(t-t_0)} \left(|z_{1i}(t_0)|_{k_i} + \frac{1-e^{-\alpha(t_e-t_0)}}{\alpha} \|\dot{z}_{1i}\|_{\alpha,k_i} \right)
\end{aligned}$$

and hence

$$|z_{1i}|_0 \leq e^{\alpha(t_e-t_0)} \|\dot{z}_{1i}\|_{k_i}.$$

Further it is

$$\begin{aligned}
|\dot{z}_{1i}(t)|_{k_i} &= e^{\alpha(t-t_0)} e^{-\alpha(t-t_0)} |\dot{z}_{1i}(t)|_{k_i} \\
&\leq e^{\alpha(t-t_0)} \|\dot{z}_{1i}\|_{\alpha,k_i} \\
&\leq \frac{\alpha}{1-e^{-\alpha(t_e-t_0)}} e^{\alpha(t-t_0)} \left(|z_{1i}(t_0)|_{k_i} + \frac{1-e^{-\alpha(t_e-t_0)}}{\alpha} \|\dot{z}_{1i}\|_{k_i} \right)
\end{aligned}$$

and hence

$$|\dot{z}_{1i}|_0 \leq \frac{\alpha}{1-e^{-\alpha(t_e-t_0)}} e^{\alpha(t_e-t_0)} \|z_{1i}\|_{k_i}.$$

Finally one has

$$|z_{2i}(t)|_{l_i} \leq e^{\alpha(t-t_0)} \|z_{2i}\|_{\alpha,l_i}$$

and thus

$$|z_{2i}|_0 \leq e^{\alpha(t_e-t_0)} \|z_{2i}\|_{\alpha,l_i}$$

what results in

$$|z|_Z \leq \left(1 + \frac{\alpha}{1-e^{-\alpha(t_e-t_0)}}\right) e^{\alpha(t_e-t_0)} \|z\|_Z. \tag{3.8}$$

Then replacing z by $x^k - x^*$ in (3.8) leads to the assertion.

□

In summary, for the convergence of the block waveform iteration (3.1) for semiexplicit DAE systems of index 1 the Lipschitz continuity of f_i and g_i, $i = 1, \dots, r$, is required, where the Lipschitz constants of g_i satisfy the inequality

$$g_{ix} + g_{iy} < 1.$$

A local approximation for the Lipschitz constants g_{ix}, g_{iy} can be determined by means of the Jacobians $\frac{\partial g_i}{\partial x}$, $\frac{\partial g_i}{\partial y}$ evaluated in a fixed point $(x_1(t^*), x_2(t^*), y_1(t^*), y_2(t^*), t^*)$. In the following these arguments are left away.

We remember that the blocksystems h_i were solved for $x_{2i} = g_i(x_1, x_2, y_1, y_2)$ with g_i independent of x_{2i}. A deduction from the implizit function theorem yields

$$\left[\frac{\partial g}{\partial x_1} \frac{\partial g}{\partial x_2} \frac{\partial g}{\partial y_2} \frac{\partial g}{\partial y_2}\right] = \left[\frac{\partial h}{\partial x_{2i}}\right]^{-1} \left[\frac{\partial h}{\partial x_1} \frac{\partial h}{\partial x_2} \frac{\partial h}{\partial y_1} \frac{\partial h}{\partial y_2}\right] . \tag{3.9}$$

The constants g_{ix} and g_{iy} are then evaluated for the block Jacobi waveform iteration by

$$\begin{aligned} g_{ix} &= \left|\frac{\partial g_i}{\partial x_1}\right| = \left|\left[\frac{\partial h_i}{\partial x_{2i}}\right]^{-1} \frac{\partial h_i}{\partial x_{1i}}\right|_{n_{1i}} && (3.10)\\ g_{iy} &= \left|\frac{\partial g_i}{\partial y}\right| = \sum_{j\neq i}\left|\left[\frac{\partial h_i}{\partial x_{2i}}\right]^{-1} \frac{\partial h_i}{\partial y_{1j}}\right|_{n_{1j}} + \sum_{j\neq i}\left|\left[\frac{\partial h_i}{\partial x_{2i}}\right]^{-1} \frac{\partial h_i}{\partial y_{2j}}\right|_{n_{2j}}. && (3.11)\end{aligned}$$

and for the block Gauss Seidel waveform iteration by

$$\begin{aligned} \bar{g}_{ix} &= \left|\frac{\partial g_i}{\partial x}\right| = \sum_{j=1}^{i}\left|\left[\frac{\partial h_i}{\partial x_{2i}}\right]^{-1} \frac{\partial h_i}{\partial x_{1j}}\right|_{n_{1j}} + \sum_{j=1}^{i-1}\left|\left[\frac{\partial h_i}{\partial x_{2i}}\right]^{-1} \frac{\partial h_i}{\partial x_{2j}}\right|_{n_{2j}}\\ \bar{g}_{iy} &= \left|\frac{\partial g_i}{\partial y}\right| = \sum_{j=i+1}^{r}\left|\left[\frac{\partial h_i}{\partial x_{2i}}\right]^{-1} \frac{\partial h_i}{\partial y_{1j}}\right|_{n_{1j}} + \sum_{j=i+1}^{r}\left|\left[\frac{\partial h_i}{\partial x_{2i}}\right]^{-1} \frac{\partial h_i}{\partial y_{2j}}\right|_{n_{2j}}.\end{aligned}$$

Here the matrix norm $|.|$ is induced by the vector norm $|.|$. The coinciding notation for the norms is used for simplicity.

These conditions just require the Jacobian of the discretized problem (2.1) to be block diagonal dominanat because the diagonal elements of the Jacobian in the hyperrows, belonging to the differential part $\dot{x}_i - \tilde{f}_i = 0$ of the DAE system, get arbitrary large with reduction of the stepsize. This comes from the stepsize in the denominator of the discretized $\dot{x}$.

Definition 2 *A matrix $A \in \mathbb{R}^{n\times n}$, $A = (A_{ij})_{i,j=1}^{M}$, $A_{ij} \in \mathbb{R}^{n_i \times n_j}$, $\sum_{i=1}^{M} n_i = n$, is called block diagonal dominant if*

$$\sum_{i\neq j} |A_{ii}^{-1} A_{ij}| \leq 1, \qquad i = 1, \ldots, M$$

holds.

For an implementation on a computer the evaluation of these Lipschitz constants is still to expansive. In chapter 5 we give a strategy for the partitioning of implicit index 1 problems, which is related to the results of this chapter but requieres less computation time due to some heuristics.

4 Mathematical modeling of distillation columns

The modeling of distillation columns like it has been done in [Wo1], [Re1] leads to linear DAE systems of index 1:

$$\begin{aligned} D\dot{u} &= \tilde{f}(u, v, t)\\ 0 &= \tilde{h}(u, v, t)\\ (u(t_0), v(t_0))^T &= (u_0, v_0)^T\end{aligned}$$

where D is a diagonal matrix with constant coefficients.

If the modeling is done with the following restrictions,

- constant molar hold–up HU^L of the liquid phase,
- neglectable hold–up HU^V of the vapor phase,
- temporal constant pressure profile over column hight,
- ideal mixing in liquid phase,
- phase equilibrium between vapor and liquid phase with constant tray efficiency coefficient,
- no excessive enthalpy,

one obtains for each tray of the distillation column, except for the bottom tray, the following system of equations:

Material balance for each component $i = 1(1)N$:

$$\begin{aligned}
\frac{d(u_{i,j}HU_j^L)}{dt} &= (L_j + U_j + U_{j,n}^R)u_{i,j} - L_{j-1}u_{i,j-1} \\
&\quad +(V_j + W_j + W_{j,m}^R)v_{i,j} - V_{j+1}v_{i,j+1} - F_j^L u_{i,j}^F \\
&\quad -F_j^V v_{i,j}^F - U_{k,j}^R u_{j,k} - W_{l,j}^R v_{i,l}
\end{aligned}$$

Energy balance:

$$\begin{aligned}
\frac{d(H_j^L HU_j^L)}{dt} &= (L_j + U_j + U_{j,n}^R)H_j^L - L_{j-1}H_{j-1}^L \\
&\quad +(V_j + W_j + W_{j,m}^R)H_j^L - V_{j+1}H_{j+1}^V - F_j^L H_{F,j}^L \\
&\quad -F_j^V H_{F,j}^V - U_{k,j}^R H_k^L - W_{l,j}^R H_l^V + Q_j
\end{aligned}$$

with

$$H_j^L = \sum_{i=1}^{N} u_{i,j}h_{i,j}^L, \quad H_j^V = \sum_{i=1}^{N} v_{i,j}h_{i,j}^V,$$
$$H_{F,j}^L = \sum_{i=1}^{N} u_{i,j}^F h_{i,j}^{L,F}, \quad H_{F,j}^V = \sum_{i=1}^{N} v_{i,j}^F h_{i,j}^{V,F}.$$

Phase equilibrium relation for $i = 1(1)N$:

$$\eta_j k_{i,j}u_{i,j} - v_{i,j} + (1-\eta_j)v_{i,j+1} = 0.$$

The tray efficiency coefficients η_j of tray j are smaller than 1 and calculated from

$$\eta_j = \frac{v_{i,j} - v_{i,j+1}}{v_{i,j}^* - v_{i,j+1}}.$$

The equilibrium constants $k_{i,j}$ are evaluated by

$$k_{i,j} = \gamma_{i,j}\frac{p_{i,j}^0}{p_j},$$

where the activity coefficients $\gamma_{i,j}$ are given by

$$v_{i,j}^* p_j = u_{i,j}\gamma_{i,j}p_{i,j}^0.$$

The following quantities are for the liquid and vapor phase respectively:

for liquid	for vapor	explanation
F_j^L	F_j^V	feed streams
U_j	W_j	side stripping streams
$U_{j,m}^R$	$W_{j,m}^R$	recycle streams
HU_j^L	HU_j^V	hold–ups
H_j^L	H_j^V	specific enthalpies
$h_{i,j}^L$	$h_{i,j}^V$	specific enthalpies of component i
$u_{i,j}$	$v_{i,j}$	mol fraction of component i
$u_{i,j}^*$	$v_{i,j}^*$	mol fraction of component i in equilibrium
	$p_{i,j}^0$	vapor pressure of component i in tray j
	p_j	vapor pressure in tray j

Now each variable is assigned to an equation, namely

- $u_{i,j}$ to the material balance equation i,
- H_j^L to the energy balance equation,
- $v_{i,j}$ to the phase equilibrium equation i.

The given DAE system consists of subsystems corresponding to the trays. Now we have to find a partitioning which ensures the index 1 property for each blocksystem. This requirement is already satisfied if each subsystem builds one blocksystem. Other partitionings can be obtained by merging several subsystems together. As the result we obtain semiexplicit DAE systems of index 1 for each blocksytem. If using the block Jacobi waveform iteration the convergence property $g_{jx_1} + g_{jy} < 1$ still has to be verified. For this we assume that each tray j builds the blocksystem j, for the other above given partitionings the convergence property can be proved analogously. To obtain the (x_1, x_2, y_1, y_2) notation for the arguments of the functions f_j and h_j in (2.6) we define the vectors $u_j := (u_{1,j}, \dots, u_{N,j})^T$, $v_j := (v_{1,j}, \dots, v_{N,j})^T$. With the identity transformations $u_j \mapsto x_{1j}$, $v_j \mapsto x_{2j}$ and $u_l \mapsto y_{1l}$, $v_l \mapsto y_{2l}$ for $l \neq j$ we can proceed with the evaluation of g_{jx_1} and g_{jy}.

From the phase equilibrium relations one obtains for the Jacobian matrix

$$
\begin{aligned}
\left[\frac{\partial h_j}{\partial x_j}\frac{\partial h_j}{\partial y}\right] &= \left[\frac{\partial h_j}{\partial x_{1,j}}\frac{\partial h_j}{\partial x_{2,j}} 0 \dots 0 \frac{\partial h_j}{\partial y_{2,j+1}} 0 \dots 0\right] \\
&= \begin{bmatrix} \eta_j k_{1j} & & & -1 & & & 1-\eta_j & & \\ & \ddots & & & -1 & 0 & & 1-\eta_j & & 0 \\ & & \eta_j k_{Nj} & & & -1 & & & 1-\eta_j & \end{bmatrix}
\end{aligned}
$$

Trivially $\left[\frac{\partial h_j}{\partial x_{2,j}}\right]^{-1} = \mathrm{diag}(-1)$ and hence

$$\begin{aligned}
g_{jx_1} + g_{jy} &= \left|\left[\frac{\partial h_j}{\partial x_{2j}}\right]^{-1} \frac{\partial h_j}{\partial x_{1j}}\right|_{n_j} + \left|\left[\frac{\partial h_j}{\partial x_{2j}}\right]^{-1} \frac{\partial h_j}{\partial y_{2,j+1}}\right|_{n_j} \\
&= \left\|\begin{bmatrix} -\eta_j k_{1j} & & \\ & \ddots & \\ & & -\eta_j k_{Nj} \end{bmatrix}\right\| + \left\|\begin{bmatrix} \eta_j - 1 & & \\ & \ddots & \\ & & \eta_j - 1 \end{bmatrix}\right\| \\
&= \eta_j k_{_j} + 1 - \eta_j < 1,
\end{aligned}$$

for $\max_{i\in\{1,\dots,N\}}\{k_{ij}\} =: k_{\_j} < 1$.

Hence the following theorem is proved.

Theorem 3 *For the described mathematical model of a distillation column the block Jacobi waveform iteration (3.2) converges for any partitioning given above.*

5 Implementation

The mathematical modeling of chemical processes in chemical plants leads usually [AT1] to initial value problems for implicit DAE systems

$$\begin{aligned}
&F(t, y(t), \dot{y}(t), u(t)) = 0,\ y(t_0) = y_0, \\
&F : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^q \to \mathbb{R}^n, t \in [t_0, t_e],
\end{aligned} \tag{5.1}$$

with $F = (f_1, \dots, f_n)^T$, a given parameter vector function $u(t)$ and the unknown vector function $y(t) = (v_1(t), \dots, v_n(t))^T$.

In many cases during the process of modeling it can be made sure that the index of the system (5.1) is 1. Usually the arising systems are stiff, and their discretization and linearization yield systems of equations with sparse nonsymmetric Jacobian matrices. The systems can comprise several 10 000 equations (e.g. distillation columns) and are structured into subsystems

$$\begin{aligned}
&F_i(t, y, \dot{y}, u) = 0,\ y(t_0) = y_0, \\
&F_i : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^q \to \mathbb{R}^{n_i},\ \sum n_i = n,\ i = 1, \dots, m
\end{aligned} \tag{5.2}$$

in accordance with the functional units of the chemical plant.

To apply the block Jacobi waveform iteration there has to be done a one to one assignment of variables to the equations and a partitioning of the system (5.1) in such a way that the waveform iteration is convergent. Because (5.1) is a fully–implicit problem the convergence condition for semiexplicit problems is not applicable. For this we use some heuristic. Like observed before, in case of block Jacobi waveform iteration for semiexplicit index 1 problems the convergence condition $g_{(ix_i)} + g_{(iy)} < 1$ implies the block diagonal dominance of the Jacobian of the discretized problem. So our partitioning algorithm puts priority to getting the Jacobian of the partitioned discretized problem (5.1) block diagonal dominant.

We assume that the hyperrows of the Jacobian $\frac{\partial \tilde{F}_i}{\partial y} = \frac{\partial F_i}{\partial y} + c_i * \frac{\partial F_i}{\partial \dot{y}}$ can be computed separately. $\tilde{F}_i$ is a discretized subsystem from (5.2) and c_i the corresponding discretization constant dependent on the integration method and stepsize used.

Assigning variables to equations, system (5.2) can be rewritten to

$$F_i(t, x_i(t), \dot{x}_i(t), y_i(t), \dot{y}_i(t), u(t)) = 0,\ x_i(t_0) = x_{i,0},\ i = 1(1)m, \tag{5.3}$$

where x_i is the vector of variables assigned to the subsystem F_i and y_i is the vector remaining if the components x_i are removed from y.

The system is then partitioned by merging subsytems F_i to blocksytems $\mathcal{F}_j = (F_{j1}, ..., F_{jm_j})^T$, $\sum m_j = m$. With the notations $X_j = (x_{j1}, \ldots, x_{jm_j})^T$ and the corresponding Y_j, the partitioning leads to

$$\mathcal{F}_j(t, X_j(t), \dot{X}_j(t), Y_j(t), \dot{Y}_j(t), u(t)) = 0,\ X_j(t_0) = X_{j,0},\ j = 1(1)M.$$

The waveform iteration is done over time windows $[t_p, t_{p+1}] \subseteq [t_0, t_e]$, $p = 1, \ldots, p_e$, $\cup[t_p, t_{p+1}] = [t_0, t_e]$ [GB1] to speed up the convergence. Here the blocksystems can be solved concurrently using general known methods. We use BDF, Newton's method and sparse matrix solver.

The algorithm reads as

do for $p = 0, 1, 2, ...$
set Y_j^0 on $[t_p, t_{p+1}]$ for $j = 1(1)M$
do for $k = 1, 2, ...$
  do for $j = 1(1)M$
    solve for $t \in [t_p, t_{p+1}]$

$$\begin{aligned} \mathcal{F}_j(t, X_j^k(t), \dot{X}_j^k(t), Y_j^{k-1}(t), \dot{Y}_j^{k-1}(t), u(t)) &= 0 \\ Y_j^k(t_p) &= \tilde{Y}_j(t_p) \end{aligned}$$

    enddo
  until $\|Y^k - Y^{k-1}\|_{n_j,[t_p,t_{p+1}]} < \epsilon$
enddo

For assigning variables to equations as well as merging strongly connected subsystems into blocks we define "weights" for the couplings between equations and subsystems respectively using the Jacobian matrix

$$A := \frac{\partial \tilde{F}(y)}{\partial y} \mid_{y=\tilde{y}},\ A = (a_{pq}) \in \mathbb{R}^{n \times n}$$

of the nonlinear system

$$\tilde{F}(y) \ = \ 0,\ \tilde{F} : \mathbb{R}^n \to \mathbb{R}^n,$$

obtained by the discretization of the DAE system at the time point $t = \tilde{t}$, $\tilde{y} \sim y(\tilde{t})$. During the assignment process each variable v_q is assigned to one and only one equation f_p, such that the resulting assignment $x_i \longrightarrow F_i$ is consistent with respect to the state variables for each subsystem i and the $n_i \times n_i$ Jacobians $\frac{\partial \tilde{F}_i}{\partial x_i}$ are at least non singular.

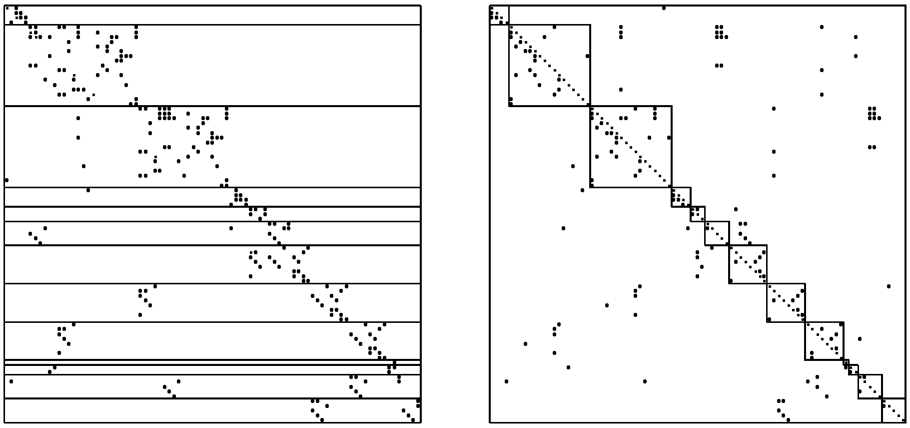

Figure 1: DYNEVAP: Jacobian matrix before and after assignment

To treat this problem we consider the linear weighted matching problem

$$\sum_{p=1}^{n}\sum_{q=1}^{n} w_{pq}s_{pq} \longrightarrow max, \ \sum_{k=1}^{n} s_{pk} = 1, \ \sum_{k=1}^{n} s_{kq} = 1,$$

$$s_{pq} = \begin{cases} 1 & : \text{if variable } v_q \text{ is assigned to equation } f_p \\ 0 & : \text{else} \end{cases}$$

$$w_{pq} = \begin{cases} 0 & : f_p \text{ depends neither on } v_q \text{ nor on } \dot{v}_q \\ 1 + \frac{|a_{pq}|}{\sum_{r=1}^{n}|a_{pr}|} & : f_p \text{ depends on } v_q\text{, but not on } \dot{v}_q \\ 3 + \frac{|a_{pq}|}{\sum_{r=1}^{n}|a_{pr}|} & : f_p \text{ depends on } \dot{v}_q \end{cases}$$

Starting from the original Jacobian we generate a parametrized directed graph and solve the matching problem with graph algorithms from the package LEDA [Nä1]. In Figure 1 the structure of the Jacobi matrix of the example DYNEVAP is given before and after the assignment of the variables to the equations. To merge tightly coupled subsystems to blocks we define "strong" connections between equations and subsystems respectively. We call a row p of the matrix A with $f_p \in F_i$ *dominant with respect to subsystem* i, if

$$\sum_{q \notin K_i} |a_{pq}|/|a_{pp}| < 1, \text{ with index set } K_i = \{r \mid f_r \in F_i\}.$$

Then the subsystem i is called *strong input to subsystem* j, if there exists a

$p_j \in \{p \mid f_p \in F_j$, row p is <u>not</u> dominant with respect to subsystem $j\}$, so that

$$\frac{\sum_{k\in K_i} |a_{p_j k}|}{|a_{p_j p_j}|} \geq \beta_{p_j},\ 0 < \beta_{p_j} \leq 1.$$

After determining strong inputs for the subsystems, we initialize blocks with one subsystem each and merge blocks containing strong input subsystems successively. In general the block partitioning is done only once before the iteration process starts, but there is an option to repeat it for some $t > t_0$ if convergence problems appear.

Codes of block waveform iteration methods have been tested on sequential machines. Currently the block waveform algorithm uses a modified DASSL code [BC1] including our linear sparse matrix package [Gr1] for numerical integration of the block systems. A program, automatically creating an interface for our code out of the data supplied by SPEEDUP when simulating a process [Ho1], is used. The interface contains the DAE system in a structured representation, so it is possible to evaluate the function and the Jacobian-matrix subsystem–wise. At present the parallel case is simulated by these codes.

The numerical methods were run on two examples. The example DYNEVAP consisting of 87 equations within 13 subsystems represents a double effect evaporator. The second example BTX, a mathematical model of a Benzene-Toluene-Xylene distillation column, is made of 52 subsystems containing 1089 equations. For the example DYNEVAP an appropriate partitioning has been found, so that block waveform iteration method converges rapidly.

For BTX an appropriate partitioning, fulfilling all conditions for assignment and block generation, has not been found. Obviously the subsytems are strongly connected due to strong feedbacks between the stages (trays) of the column. For this reason possibilities to combine our iterative block methods with parallelizable direct block methods are investigated. A paper concerning this topic is in preparation.

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