Partitioning the ODE systems describing the chemical reactions

1. *Major assumptions*
2. *Partitioning into strong and week blocks*
3. *Advantages of the partitioned algorithms*
4. *"Local" error of the partitioned algorithms*
5. *"Global" error of the partitioned algorithms*
6. *Numerical values of some quantities involved in the partitioned algorithms*
7. *Computing times*
8. *Open problems*

References

1. **V. Alexandrov, A. Sameh, Y. Sidique and Z. Zlatev:** *"Numerical Integration of Chemical ODE Problems Arising in Air Pollution Modelling"*, Environmental Modeling & Assessment, Vol. 2 (1997), 365-377.
2. **Z. Zlatev:** *"Partitioning ODE Systems with an Application to Air Pollution Models"*, Computers and Mathematics with Applications, Vol. 42 (2001), 817-832.

No partitioning - results

Method	Computing time
QSSA-1	12.85
QSSA-2	11.72
Euler	15.11
Trapez.	15.94
RK-2	28.49

Better accuracy with the classical numerical methods

QSSA - once again

Backward Euler Formula

$$\frac{dy}{dt} = f(t, y), \quad y \in \Re^{NS}$$

$$y_{n+1} = y_n + \Delta t\, f_{n+1}, \qquad y_n \approx y(t_n), \quad f_n = f(t_n, y_n)$$

$$\left(I - \Delta t J_{n+1}^{[i-1]}\right)\Delta y_{n+1}^{[i]} = -y_{n+1}^{[i-1]} + y_n + \Delta t\, f(t_{n+1}, y_{n+1}^{[i-1]})$$

QSSA Method

$$\frac{dy_s}{dt} = f_s(t, y), \quad y_s \in \Re, \quad s = 1,2,..., NS$$

$$f_s(t, y) = P_s(t, y_1, y_2, ..., y_q) - L_s(t, y_1, y_2, ..., y_q)\, y_s$$

Steady state cases for different compounds

$$\frac{dy_s}{dt} = P_s(t, y_1, y_2, \ldots, y_q) - L_s(t, y_1, y_2, \ldots, y_q)\, y_s$$

$$s = 1, 2, \ldots, q, \qquad y_s \in \Re, \qquad y_s^{n+1} \approx y_s(t)$$

$$y_s^{n+1} = \frac{P_s}{L_s} \qquad \textit{for} \qquad \Delta t L_s > 10$$

$$y_s^{n+1} = \frac{P_s}{L_s} + \left(y_s^n - \frac{P_s}{L_s} \right) e^{-\Delta t L_s} \qquad 0.01 < \Delta t L_s \le 10$$

$$y_s^{n+1} = y_s^n + \Delta t \left(P_s - L_s y_s^n \right) \qquad \Delta t L_s \le 0.01$$

1. Major assumptions

It will be assumed that the components of the solution vector can be divided into several groups, so that the components belonging to different groups have different properties.

In the particular case where the chemical part of a large air pollution models is studied, the reactions are divided into fast reactions and slow reactions

2. Partitioning vector y_n

$$\frac{dy}{dt} = f(t,y), \quad y \in \Re^{NS}, \quad f \in \Re^{NS}$$

$$y_{n+1} = y_n + \Delta t\, f_{n+1}, \qquad y_n \approx y(t_n), \quad f_n = f(t_n, y_n)$$

$$\left(I - \Delta t J_{n+1}^{[0]}\right)\Delta y_{n+1}^{[i]} = -y_{n+1}^{[i-1]} + y_n + \Delta t\, f(t_{n+1}, y_{n+1}^{[i-1]})$$

Assume that:

y_n is partitioned to $NBLOCKS$ blocks

$r_1, r_2, \ldots, r_p \ \left(p < NS,\ 1 \le r_k \le NS, k = 1,2,\ldots,q\right)$ one of the blocks

The paritioning of y_n implies partitioning in $I - \Delta t J_{n+1}^{[0]}$

Two blocks of $I - \Delta t J_{n+1}^{[0]}$ correspond to each block of y_n

Strong and week blocks (the strong blocks are diagonal)

3. Forming the partitioned system

$$\left(A_{n+1}^{[0]}\right)\Delta y_{n+1}^{[i]} = -y_{n+1}^{[i-1]} + y_n + \Delta t\, f\left(t_{n+1}, y_{n+1}^{[i-1]}\right)$$

$$A_{n+1}^{[0]} = I - \Delta t J_{n+1}^{[0]}$$

$$A_{n+1}^{[0]} = S_{n+1}^{[0]} + W_{n+1}^{[0]} \qquad \textit{with} \qquad S_{n+1}^{[0]} = I - \Delta t\, \tilde{S}_{n+1}^{[0]}$$

Let $y_{n+1}^{[\mu]}$ *be the accepted solution obtained by the regular Newton method*

$$A_{n+1}^{[0]}\Delta y_{n+1}^{[\mu]} = -y_{n+1}^{[\mu-1]} + y_n + \Delta t\, f\left(t_{n+1}, y_{n+1}^{[\mu-1]}\right)$$

$$S_{n+1}^{[0]}\Delta z_{n+1}^{[i]} = -z_{n+1}^{[i-1]} + z_n + \Delta t\, f\left(t_{n+1}, z_{n+1}^{[i-1]}\right)$$

4. Why partitioned system?

Advantages:

1. It is not necessary to compute the non-zero elements of the weak blocks
2. Several small matrices are to be factorized instead of one big matrix
3. Several small systems of linear algebraic equations are to be solved at each Newton iteration (instead of one large system)

5. Requirements

$$A_{n+1}^{[0]}\Delta y_{n+1}^{[i]} = -y_{n+1}^{[i-1]} + y_n + \Delta t\ f\left(t_{n+1}, y_{n+1}^{[i-1]}\right)$$

$$S_{n+1}^{[0]}\Delta z_{n+1}^{[i]} = -z_{n+1}^{[i-1]} + z_n + \Delta t\ f\left(t_{n+1}, z_{n+1}^{[i-1]}\right)$$

It is desirable to find the conditions under which the approximate solution of the second problem is close to the approximate solution of the first one

$y_{n+1}^{[\mu]} - z_{n+1}^{[\nu]}$ is small

$\Delta z_{n+1}^{[\nu]} \to 0$ is not sufficient

Lemma 1

$$y_{n+1}^{[\mu]} - z_{n+1}^{[i]} = B_{n+1}^{[i-1]}\left(y_{n+1}^{[\mu]} - z_{n+1}^{[i-1]}\right) + C_{n+1}(y_n - z_n) + D_{n+1}^{[i-1]}\Delta y_{n+1}^{[\mu]}$$

where

$$C_{n+1} = \left(S_{n+1}^{[0]}\right)^{-1}$$

$$B_{n+1}^{[i-1]} = \Delta t\left(S_{n+1}^{[0]}\right)^{-1}\left(T_{n+1}^{[i-1]} - \tilde{S}_{n+1}^{[0]}\right)$$

$$D_{n+1}^{[i-1]} = \left(S_{n+1}^{[0]}\right)^{-1} W_{n+1}^{[0]} + B_{n+1}^{[i-1]}$$

$$T_{n+1}^{[i-1]} = \int_0^1 \frac{\partial f\left(t_{n+1,}\lambda y_{n+1}^{[\mu-1]} + (1-\lambda)z_{n+1}^{[i-1]}\right)}{\partial y} d\lambda$$

y_{n+1} exact solution of $y_{n+1} = y_n + \Delta t\, f(t_{n+1}, y_{n+1})$

$y_{n+1}^{[\mu]}$ approximat ion of y_{n+1} found by some numerical method

Lemma 2

$$y_{n+1}^{[\mu]} - z_{n+1}^{[i]} = \left(\prod_{j=1}^{i} B_{n+1}^{[i-j]} \right) \left(y_{n+1}^{[\mu]} - z_{n+1}^{[0]} \right)$$
$$+ \left[\sum_{k}^{i-1} \left(\prod_{j=1}^{k} B_{n+1}^{[i-j]} \right) \right] C_{n+1} \left(y_n - z_n \right)$$
$$- \left[\sum_{k}^{i-1} \left(\prod_{j=1}^{k} B_{n+1}^{[i-j]} \right) D_{n+1}^{[i-1-k]} \right] \Delta y_{n+1}^{[\mu]}$$

y_{n+1} exact solution of $y_{n+1} = y_n + \Delta t\, f(t_{n+1}, y_{n+1})$

$y_{n+1}^{[\mu]}$ approximation of y_{n+1} found by some numerical method

“Local” error

$$B_{n+1} = \max_{0 < j < i} \left(\left\| B^{[j]}_{n+1} \right\| \right)$$

$B_{n+1} < 1$ Major assumption

Theorem

$$\left\| y_{n+1} - z^{[i]}_{n+1} \right\| < \varepsilon$$

$$\left\| y^{[\mu]}_{n+1} - z^{[i]}_{n+1} \right\| < \varepsilon$$

1. if the number of iterations is sufficiently large and
2. if the error from the previous step is sufficiently small

“Global” error

$$B_k^{[\nu_k]} = \max_{0 \le i \le \nu_k} \left(\left\| B_k^{[i]} \right\| \right), \qquad 0 \le k \le n+1$$

$$E_k = \frac{C_k}{1 - B_k^{[\nu_k]}}, \qquad E = \max_{0 \le k \le n+1} (E_k)$$

Theorem

If $B_k^{[\nu_k]} < 1 \quad and \quad E < 1$ then the inequalities

$$\left\| y_{n+1} - z_{n+1}^{[\nu_{n+1}]} \right\| < \varepsilon \qquad and \qquad \left\| y_{n+1}^{[\mu]} - z_{n+1}^{[\nu_{n+1}]} \right\| < \varepsilon$$

will be satisfied when sufficiently many iterations are performed

“Global” error - continuation

If $E \neq 1$,

$$\left\| y_{n+1} - z_{n+1}^{[\nu_{n+1}]} \right\| < E^{n+1} \left(\left\| y_0 - z_0 \right\| \right) + \frac{1 - E^{n+1}}{1 - E} \delta$$

$$\left\| y_{n+1}^{[\mu]} - z_{n+1}^{[\nu_{n+1}]} \right\| < E^{n+1} \left(\left\| y_0 - z_0 \right\| \right) + \frac{1 - E^{n+1}}{1 - E} \delta$$

If $E = 1$,

$$\left\| y_{n+1} - z_{n+1}^{[\nu_{n+1}]} \right\| < \left\| y_0 - z_0 \right\| + n \delta$$

$$\left\| y_{n+1}^{[\mu]} - z_{n+1}^{[\nu_{n+1}]} \right\| < \left\| y_0 - z_0 \right\| + n \delta$$

Actual partitioning

1. Matrix S, which is obtained after the partitioning is a block-diagonal matrix containing 23 blocks.
2. The first diagonal block is a 13x13 matrix.
3. The next 22 clocks are 1x1 matrices (a Newton iteration procedure for scalar equations is used in this part).
4. This partitioning was recommended by the chemists (based on their knowledge of the chemical reactions)

Variation of the key quantities for different scenarios

Scenario	$\rho(B_N)$	E
1	[2.4E-4, 3.3E-2]	1.03425
2	[3.7E-4, 2.1E-2]	1.02179
3	[5.8E-3, 5.7E-2]	1.06040
4	[1.3E-3, 4.3E-2]	1.04606
5	[4.3E-3, 2.5E-2]	1.02522
6	[5.6E-3, 6.4E-2]	1.06882

$N = 1, 2, \ldots, 1260 \quad and \quad \Delta t = 30\,s$

$\rho(B_{n+1}) < \|B_{n+1}\|, \quad \|B_{n+1}\| = \rho(B_{n+1}) + \varepsilon$

Variation of the key quantities for different stepsizes

Stepsize	B	E
30	2.5E-2	1.025
10	1.4E-2	1.014
1	2.6E-3	1.0026
0.1	3.6E-4	1.00036
0.01	5.3E-5	1.000053

Scenario 5

Numerical Results

Method	Computing time	
QSSA-1	12.85	
QSSA-2	11.72	
Euler	15.11	
Trapez.	15.94	
RK-2	28.49	
Part. dense	10.09	Based on Euler

Better accuracy with the classical numerical methods

Accuracy results

Numer. Method	Scenario 2	Scenario 6
QSSA-1	3.20E-3	4.39E-1
QSSA-2	3.39E-3	3.86E-1
Euler	5.78E-4	3.57E-3
Trapez	5.78E-4	3.57E-3
Part. dense	5.72E-4	3.26E-3

$\Delta t = 30 s$

The chemical compound is ozone

Conclusions and open problems

1. We have shown that the physical arguments for achieving successful partitioning can be justified with clear algebraic requirements.
2. There is a drawback: if the chemical scheme is changed, then the whole procedure has to be carried out for the new chemical scheme.
3. Automatic partitioning is desirable.