Supporting information for: Numerical Integration of the Chemical Rate Equations via a Discretized Adomian Decomposition

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Abstract

Included in this document are the following: 1) derivations connecting the Adomian polynomials to the Taylor series; 2) separation of the time dimension from the Adomian polynomials; 3) derivations equating the classical and modified Adomian polynomials; and 4) numerical results for ADM4, ADM6, ADM8, and ADM10 for the bimolecular and chloroperoxidase reactions. C++ class code and adaptive t_q details can be obtained from the author.

Contents

Derivations

Given the equation:

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$$L(t)y_i(t) = f_i(\vec{y}(t)) \tag{1}$$

where $L(t)$ is a linear differential operator.

Two coupled equations: $p = 2$

Adomian decomposition may be used to solve for $y_i(t)$ by applying the inverse of $L(t)$, where $i = 1, 2, ..., p$ are the individual solutions. Adomian decomposition can be shown to be a rearrangement of a Taylor expansion. Given that the Taylor series is familiar to most chemists, it is instructive to show the connection between ADM and Taylor series. To this end, we derive the Adomian polynomials $A_{(i,n)}$ and the solution $y_i(t)$ from the Taylor series. Expanding $f_i(\vec{y}(t))$ to third order for $p = 2$ (i.e., two coupled equations) around the point $y_1(0), y_2(0)$ yields:

$$\begin{aligned}
L(t)y_i(t) = f_i(y_1(t), y_2(t)) = \\
f_i(y_1(0), y_2(0)) + \\
\left((y_1(t) - y_1(0))\frac{\partial f_i(y_1(0), y_2(0))}{\partial y_1}\right) + \left((y_2(t) - y_2(0))\frac{\partial f_i(y_1(0), y_2(0))}{\partial y_2}\right) + \\
\left(\frac{(y_1(t) - y_1(0))^2}{2!}\frac{\partial^2 f_i(y_1(0), y_2(0))}{\partial y_1^2}\right) + \left((y_1(t) - y_1(0))(y_2(t) - y_2(0))\frac{\partial^2 f_i(y_1(0), y_2(0))}{\partial y_1 \partial y_2}\right) + \\
\left(\frac{(y_2(t) - y_2(0))^2}{2!}\frac{\partial^2 f_i(y_1(0), y_2(0))}{\partial y_2^2}\right) + \\
\left(\frac{(y_1(t) - y_1(0))^3}{3!}\frac{\partial^3 f_i(y_1(0), y_2(0))}{\partial y_1^3}\right) + \left(\frac{(y_1(t) - y_1(0))^2(y_2(t) - y_2(0))}{2!}\frac{\partial^3 f_i(y_1(0), y_2(0))}{\partial y_1^2 \partial y_2}\right) + \\
\left(\frac{(y_1(t) - y_1(0))(y_2(t) - y_2(0))^2}{2!}\frac{\partial^3 f_i(y_1(0), y_2(0))}{\partial y_1 \partial y_2^2}\right) + \left(\frac{(y_2(t) - y_2(0))^3}{3!}\frac{\partial^3 f_i(y_1(0), y_2(0))}{\partial y_2^3}\right) + \\
O(f_i(y_1(0), y_2(0))^4)
\end{aligned} \tag{2}$$

Adomian postulated that the solution $y_i(t)$ could be written as a series: $y_i(t) = y_i(0) + \sum_{n=1}^{\infty} y_{(i,n)}(t)$.

Substitution of this series into the Taylor expansion yields:

$$
\begin{aligned}
L(t)(y_{(i,1)}(t)+y_{(i,2)}(t)+...) = f_i(y_1(t),y_2(t)) = \\
f_i(y_1(0),y_2(0)) + \\
\left((y_{(1,1)}(t)+y_{(1,2)}(t)+...)\frac{\partial f_i(y_1(0),y_2(0))}{\partial y_1}\right) + \left((y_{(2,1)}(t)+y_{(2,2)}(t)+...)\frac{\partial f_i(y_1(0),y_2(0))}{\partial y_2}\right) + \\
\left(\frac{(y_{(1,1)}(t)+y_{(1,2)}(t)+...)^2}{2!}\frac{\partial^2 f_i(y_1(0),y_2(0))}{\partial y_1^2}\right) + \\
\left((y_{(1,1)}(t)+y_{(1,2)}(t)+...)(y_{(2,1)}(t)+y_{(2,2)}(t)+...)\frac{\partial^2 f_i(y_1(0),y_2(0))}{\partial y_1 \partial y_2}\right) + \\
\left(\frac{(y_{(2,1)}(t)+y_{(2,2)}(t)+...)^2}{2!}\frac{\partial^2 f_i(y_1(0),y_2(0))}{\partial y_2^2}\right) + \\
\left(\frac{(y_{(1,1)}(t)+y_{(1,2)}(t)+...)^3}{3!}\frac{\partial^3 f_i(y_1(0),y_2(0))}{\partial y_1^3}\right) + \\
\left(\frac{(y_{(1,1)}(t)+y_{(1,2)}(t)+...)^2(y_{(2,1)}(t)+y_{(2,2)}(t)+...)}{2!}\frac{\partial^3 f_i(y_1(0),y_2(0))}{\partial y_1^2 \partial y_2}\right) + \\
\left(\frac{(y_{(1,1)}(t)+y_{(1,2)}(t)+...)(y_{(2,1)}(t)+y_{(2,2)}(t)+...)^2}{2!}\frac{\partial^3 f_i(y_1(0),y_2(0))}{\partial y_1 \partial y_2^2}\right) + \\
\left(\frac{(y_{(2,1)}(t)+y_{(2,2)}(t)+...)^3}{3!}\frac{\partial^3 f_i(y_1(0),y_2(0))}{\partial y_2^3}\right) + \\
O(f_i(y_1(0),y_2(0))^4)
\end{aligned}
\tag{3}
$$

We are interested in the solution of chemical rate equations. These are initial-value problems where only $y_1(0)$ and $y_2(0)$ are known. We need to find $y_{(i,1)}(t)$, $y_{(i,2)}(t)$, etc. These may be obtained by a judicious rearrangement of the terms in Eq. (3). We group the terms such that each $y_{(i,n)}(t)$ depends only upon previous terms in the solution expansion. By design, this recursive procedure yields the Adomian polynomials. Each $y_{(i,n)}(t)$ is constructed from only those terms in the Taylor series whose second-indices sum to $n-1$. For example, $y_{(i,3)}(t)$ would contain

$$\underbrace{y_{(1,1)}(t)y_{(2,1)}(t)}_{1+1=2}\frac{\partial^2 f_i(y_1(0),y_2(0))}{\partial y_1 \partial y_2} \tag{4}$$

but not

$$\underbrace{y_{(1,2)}(t)y_{(2,1)}(t)}_{2+1=3}\frac{\partial^2 f_i(y_1(0),y_2(0))}{\partial y_1 \partial y_2} \tag{5}$$

Returning to the solution $y_i(t)$, we assign $y_{(i,1)}(t)$ thus:

$$L(t)y_{(i,1)}(t) = f_i(y_1(0),y_2(0)) = A_{(i,0)} \tag{6}$$

Here we have also introduced the Adomian polynomial, $A_{(i,0)}$, which is equal to $f_i(y_1(0),y_2(0))$. Multiplication by $L^{-1}(t)$ (i.e., integration with respect to t) yields $y_{(i,1)}(t)$ of the series solution.

$$y_{(i,1)}(t) = L^{-1}(t)(f_i(y_1(0),y_2(0)) = L^{-1}(t)A_{(i,0)} \tag{7}$$

Now that we have $y_{(i,1)}(t)$ in the integrated solution $y_i(t) = y_i(0) + y_{(i,1)}(t) + y_{(i,2)}(t) + ...$, we must find $y_{(i,2)}(t)$. Grouping the appropriate terms and equating them to $L(t)y_{(i,2)}(t)$ and followed by integration yields $y_{(i,2)}(t)$:

$$y_{(i,2)}(t) = L^{-1}(t)\left(y_{(1,1)}(t)\frac{\partial f_i(y_1(0),y_2(0))}{\partial y_1} + y_{(2,1)}(t)\frac{\partial f_i(y_1(0),y_2(0))}{\partial y_2}\right) = L^{-1}(t)A_{(i,1)} \tag{8}$$

The same procedure is followed with every term in the series solution of $y_i(t)$. Each subsequent term in the solution of $y_i(t)$ (i.e. $y_{(i,3)}(t)$, $y_{(i,4)}(t)$, etc.) is obtained by collecting terms from the Taylor expansion which depend on previously determined $y_{(i,n)}(t)$ and integrating. Finally, the series is summed in order to yield the integrated equation $y_i(t) = y_i(0) + y_{(i,1)}(t) + y_{(i,2)}(t) + ... = y_i(0) + L^{-1}(t)\sum_{n=0}^{\infty} A_{(i,n)}$ (Equation 8 in the article).

p coupled equations

The same procedure can be followed for any number of equations p:

$$
\begin{aligned}
L(t)y_i(t) = f_i(\vec{y}(t)) = \\
f_i(\vec{y}(0)) + \\
\sum_{j=1}^{p}\left((y_j(t)-y_j(0))\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right) + \\
\sum_{j=1}^{p}\sum_{k=1}^{j}\left(\frac{(y_j(t)-y_j(0))(y_k(t)-y_k(0))}{(1+\delta_{jk})!}\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j \partial y_k}\right) + \\
\sum_{j=1}^{p}\sum_{k=1}^{j}\sum_{l=1}^{k}\left(\frac{(y_j(t)-y_j(0))(y_k(t)-y_k(0))(y_l(t)-y_l(0))}{(1-\delta_{jk}\delta_{jl}+\delta_{jk}+\delta_{jl}+\delta_{kl})!}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j \partial y_k \partial y_k}\right) + \\
O(f_i(\vec{y}(0))^4)
\end{aligned} \tag{9}
$$

Substitution of the Adomian series solutions $y_i(t) = y_i(0) + \sum_{n=1}^{\infty} y_{(i,n)}(t)$:

$$
\begin{aligned}
L(t)(\sum_{n=1} y_{(i,n)}(t)) = \sum_{n=0} A_{(i,n)} = \\
f_i(\vec{y}(0)) + \\
\sum_{j=1}^{p}\left((\sum_{n=1}^{\infty} y_{(j,n)}(t))\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right) + \\
\sum_{j=1}^{p}\sum_{k=1}^{j}\left(\frac{(\sum_{n=1}^{\infty} y_{(j,n)}(t))(\sum_{n=1}^{\infty} y_{(k,n)}(t))}{(1+\delta_{jk})!}\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j \partial y_k}\right) + \\
\sum_{j=1}^{p}\sum_{k=1}^{j}\sum_{l=1}^{k}\left(\frac{(\sum_{n=1}^{\infty} y_{(j,n)}(t))(\sum_{n=1}^{\infty} y_{(k,n)}(t))(\sum_{n=1}^{\infty} y_{(l,n)}(t))}{(1-\delta_{jk}\delta_{jl}+\delta_{jk}+\delta_{jl}+\delta_{kl})!}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j \partial y_k \partial y_k}\right) + \\
O(f_i(\vec{y}(0))^4)
\end{aligned} \tag{10}
$$

The mapping of Taylor terms to the Adomian polynomials is summerized in Table 1. The Adomian polynomials can be cast as Equation 12 from the the article for any order of Adomian polynomial.

Table 1: Assignment of Taylor terms to Adomian polynomials

Adomian	Taylor line[a]	Taylor term
$A_{(i,0)}$	1	$f_i(\vec{y}(0))$
$A_{(i,1)}$	2	$\sum_{j=1}^{p}\left(y_{(j,1)}(t)\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right)$
$A_{(i,2)}$	2	$\sum_{j=1}^{p}\left(y_{(j,2)}(t)\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right)$
$A_{(i,2)}$	3	$\sum_{j,k=1,j\neq k}^{p}\left(y_{(j,1)}(t)y_{(k,1)}(t)\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j\partial y_k}\right)+\sum_{j=1}^{p}\left(\frac{y_{(j,1)}^2(t)}{2!}\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j^2}\right)$
$A_{(i,3)}$	2	$\sum_{j=1}^{p}\left(y_{(j,3)}(t)\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right)$
$A_{(i,3)}$	3	$\sum_{j,k=1}^{p}\left(y_{(j,2)}(t)y_{(k,1)}(t)\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j\partial y_k}\right)$
$A_{(i,3)}$	4	$\sum_{j,k=1,j\neq k}^{p}\left(\frac{y_{(j,1)}^2(t)y_{(k,1)}(t)}{2!}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j^2\partial y_k}\right)+\sum_{j=1}^{p}\left(\frac{y_{(j,1)}^3(t)}{3!}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j^3}\right)$
$A_{(i,3)}^*$	-	$\sum_{j,k,l=1,j\neq k\neq l}^{p}\left(y_{(j,1)}(t)y_{(k,1)}(t)y_{(l,1)}(t)\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j\partial y_k\partial y_l}\right)$

Mapping of Taylor terms from Eq. (10) to Adomian polynomials. [a]The Taylor line refers to the line number in Eq. (10) where line 1 is $f_i(\vec{y}(0))$. *From the fourth-order expansion.

Separation of variables

This section has two purposes. One, to show how separation of variables (i.e., the time dimension) is possible for the chemical rate equations, and two, to detail how the classical and modified approaches are equivalent. Starting with the following equation:

$$y_{(i,n+1)}(t)=L^{-1}(t)\left[A_{(i,n)}(\vec{y}(t))+\sum_{j=1}^{p}k_{(i,j)}y_{(j,n)}(t)\right] \tag{11}$$

For $n=0$:

$$
\begin{aligned}
y_{(i,1)}(t) &= L^{-1}(t)\left[A_{(i,0)}(\vec{y}(t)) + \sum_{j=1}^{p} k_{(i,j)} y_{(j,0)}(t)\right] \\
&= L^{-1}(t)\left(g_i(\vec{y}(0)) + \sum_{j=1}^{p} k_{(i,j)} y_{(j,0)}(t)\right) && (12)\\
&= L^{-1}(t)\left[f_i(\vec{y}(0))\right] && (13)\\
&= t\underbrace{\left[f_i(\vec{y}(0))\right]}_{Y_{(i,0)}=\hat{Y}_{(i,0)}} && (14)
\end{aligned}
$$

It is trivial to show that Eq. (12) and Eq. (13) are equivalent (see Equations 4 and 5 from the article). Given that $f_i(\vec{y}(t))$ has no dependence on t, operation of $L^{-1}(t)$ yields Eq. (14). Here we have introduced the time-separated polynomial $\hat{Y}_{(i,n)}$, which for $n = 0$ is equivalent to the general polynomial $Y_{(i,n)}$. Moving on to $n = 1$,

$$
\begin{aligned}
y_{(i,2)}(t) &= L^{-1}(t)\left[A_{(i,1)}(\vec{y}(t)) + \sum_{j=1}^{p} k_{(i,j)} y_{(j,1)}(t)\right] \\
&= L^{-1}(t)\left[\sum_{j=1}^{p}\left(y_{(j,1)}(t)\frac{\partial g_i(\vec{y}(0))}{\partial y_j}\right) + \sum_{j=1}^{p} k_{(i,j)} y_{(j,1)}(t)\right] && (15)\\
&= L^{-1}(t)\left[\sum_{j=1}^{p}\left(y_{(j,1)}(t)\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right)\right] && (16)\\
&= L^{-1}(t)\left[t\sum_{j=1}^{p}\left(\hat{Y}_{(j,0)}\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right)\right] \\
&= \frac{t^2}{2!}\underbrace{\left[\sum_{j=1}^{p}\left(\hat{Y}_{(j,0)}\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right)\right]}_{Y_{(i,1)}=\hat{Y}_{(i,1)}} && (17)
\end{aligned}
$$

Eq. (15) and Eq. (16) are equivalent given that,

$$
\begin{aligned}
\frac{\partial f_i(\vec{y}(0))}{\partial y_j} &= \frac{\partial g_i(\vec{y}(0))}{\partial y_j} + \frac{\partial h_i(\vec{y}(0))}{\partial y_j} \\
&= \frac{\partial g_i(\vec{y}(0))}{\partial y_j} + k_{(i,j)}
\end{aligned}
\tag{18}
$$

The same holds for all n. Likewise, all $g_i(\vec{y}(0))$ can be replaced with $f_i(\vec{y}(0))$ with no fear of contamination from additional linear terms $h_i(\vec{y}(0))$. All other terms in the polynomial contain partial derivatives (i.e., $\partial^l f_i(\vec{y}(0)) = \partial^l g_i(\vec{y}(0))$ for $l > 2$) and as such $\partial^l h_i(\vec{y}(0))$ will be zero . We can see this for $n = 2$:

$$
\begin{aligned}
y_{(i,3)}(t) &= L^{-1}(t)\left(A_{(i,2)}(\vec{y}(t)) + \sum_{j=1}^{p} k_{(i,j)} y_{(j,2)}(t)\right) \\
&= L^{-1}(t)\left[\sum_{j=1}^{p}\left(y_{(j,2)}(t)\frac{\partial g_i(\vec{y}(0))}{\partial y_j}\right) + \sum_{j=1}^{p} k_{(i,j)} y_{(j,2)}(t)\right. \\
&\left. + \sum_{j,k=1, j\neq k}^{p}\left(y_{(j,1)}(t)y_{(k,1)}(t)\frac{\partial^2 g_i(\vec{y}(0))}{\partial y_j \partial y_k}\right) + \sum_{j=1}^{p}\left(\frac{y_{(j,1)}^2(t)}{2!}\frac{\partial^2 g_i(\vec{y}(0))}{\partial y_j^2}\right)\right] \\
&= L^{-1}(t)\left[\sum_{j=1}^{p}\left(y_{(j,2)}(t)\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right)\right. \\
&\left. + \sum_{j,k=1, j\neq k}^{p}\left(y_{(j,1)}(t)y_{(k,1)}(t)\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j \partial y_k}\right) + \sum_{j=1}^{p}\left(\frac{y_{(j,1)}^2(t)}{2!}\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j^2}\right)\right] \\
&= L^{-1}(t)\left[\frac{t^2}{2!}\sum_{j=1}^{p}\left(\hat{Y}_{(j,1)}\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right)\right) \\
&+ t^2 \sum_{j,k=1, j\neq k}^{p}\left(\hat{Y}_{(j,0)}\hat{Y}_{(k,0)}\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j \partial y_k}\right) + \frac{t^2}{2!}\sum_{j=1}^{p}\left(\hat{Y}_{(j,0)}^2\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j^2}\right)\Bigg] \\
&= L^{-1}(t)\frac{t^2}{2!}\left[\sum_{j=1}^{p}\left(\hat{Y}_{(j,1)}\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right)\right. \\
&\left. + 2\sum_{j,k=1, j\neq k}^{p}\left(\hat{Y}_{(j,0)}\hat{Y}_{(k,0)}\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j \partial y_k}\right) + \sum_{j=1}^{p}\left(\hat{Y}_{(j,0)}^2\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j^2}\right)\right] \qquad (19) \\
&= \frac{t^3}{3!}\underbrace{\left[\sum_{j=1}^{p}\left(\hat{Y}_{(j,1)}\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right) + 2\sum_{j,k=1, j\neq k}^{p}\left(\hat{Y}_{(j,0)}\hat{Y}_{(k,0)}\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j \partial y_k}\right) + \sum_{j=1}^{p}\left(\hat{Y}_{(j,0)}^2\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j^2}\right)\right]}_{\hat{Y}_{(i,2)}}
\end{aligned}
$$

(20)

It is important to note the factor of two introduced when separating $t^2/2!$ from Eq. (19). For $n \geq 2$, the time-separated polynomial $\hat{Y}_{(i,n)}$ must be used. This polynomial will be introduced shortly, but first, for $n = 3$

$$
\begin{aligned}
y_{(i,4)}(t) &= L^{-1}(t)\left[A_{(i,3)}(\vec{y}(t)) + \sum_{j=1}^{p} k_{(i,j)} y_{(j,3)}(t)\right] \\
&= L^{-1}(t)\left[\sum_{j=1}^{p}\left(y_{(j,3)}(t)\frac{\partial g_i(\vec{y}(0))}{\partial y_j}\right) + \sum_{j,k=1}^{p}\left(y_{(j,2)}(t)y_{(k,1)}(t)\frac{\partial^2 g_i(\vec{y}(0))}{\partial y_j \partial y_k}\right)\right. \\
&+ \sum_{j,k=1,j\neq k}^{p}\left(\frac{y^2_{(j,1)}(t)y_{(k,1)}(t)}{2!}\frac{\partial^3 g_i(\vec{y}(0))}{\partial y_j^2 \partial y_k}\right) + \sum_{j=1}^{p}\left(\frac{y^3_{(j,1)}(t)}{3!}\frac{\partial^3 g_i(\vec{y}(0))}{\partial y_j^3}\right) \\
&+ \left.\sum_{j,k,l=1,j\neq k\neq l}^{p}\left(y_{(j,1)}(t)y_{(k,1)}(t)y_{(l,1)}(t)\frac{\partial^3 g_i(\vec{y}(0))}{\partial y_j \partial y_k \partial y_l}\right) + \sum_{j=1}^{p} k_{(i,j)} y_{(j,3)}(t)\right] \\
&= L^{-1}(t)\left[\sum_{j=1}^{p}\left(y_{(j,3)}(t)\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right) + \sum_{j,k=1}^{p}\left(y_{(j,2)}(t)y_{(k,1)}(t)\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j \partial y_k}\right)\right. \\
&+ \sum_{j,k=1,j\neq k}^{p}\left(\frac{y^2_{(j,1)}(t)y_{(k,1)}(t)}{2!}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j^2 \partial y_k}\right) + \sum_{j=1}^{p}\left(\frac{y^3_{(j,1)}(t)}{3!}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j^3}\right) \\
&+ \left.\sum_{j,k,l=1,j\neq k\neq l}^{p}\left(y_{(j,1)}(t)y_{(k,1)}(t)y_{(l,1)}(t)\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j \partial y_k \partial y_l}\right)\right] \\
&= L^{-1}(t)\left[\frac{t^3}{3!}\sum_{j=1}^{p}\left(\hat{Y}_{(j,2)}\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right) + \frac{t^3}{2!}\sum_{j,k=1}^{p}\left(\hat{Y}_{(j,1)}\hat{Y}_{(k,0)}\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j \partial y_k}\right)\right. \\
&+ \frac{t^3}{2!}\sum_{j,k=1,j\neq k}^{p}\left(\hat{Y}^2_{(j,0)}\hat{Y}_{(k,0)}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j^2 \partial y_k}\right) + \frac{t^3}{3!}\sum_{j=1}^{p}\left(\hat{Y}^3_{(j,0)}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j^3}\right) \\
&+ \left. t^3\sum_{j,k,l=1,j\neq k\neq l}^{p}\left(\hat{Y}_{(j,0)}\hat{Y}_{(k,0)}\hat{Y}_{(l,0)}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j \partial y_k \partial y_l}\right)\right] \\
&= L^{-1}(t)\frac{t^3}{3!}\left[\sum_{j=1}^{p}\left(\hat{Y}_{(j,2)}\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right) + 3\sum_{j,k=1}^{p}\left(\hat{Y}_{(j,1)}\hat{Y}_{(k,0)}\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j \partial y_k}\right)\right. \\
&+ 3\sum_{j,k=1,j\neq k}^{p}\left(\hat{Y}^2_{(j,0)}\hat{Y}_{(k,0)}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j^2 \partial y_k}\right) + \sum_{j=1}^{p}\left(\hat{Y}^3_{(j,0)}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j^3}\right) \\
&+ \left. 3!\sum_{j,k,l=1,j\neq k\neq l}^{p}\left(\hat{Y}_{(j,0)}\hat{Y}_{(k,0)}\hat{Y}_{(l,0)}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j \partial y_k \partial y_l}\right)\right] \\
&= \frac{t^4}{4!}\left[\sum_{j=1}^{p}\left(\hat{Y}_{(j,2)}\frac{\partial f_i(\vec{y}(0))}{\partial y_j}\right) + 3\sum_{j,k=1}^{p}\left(\hat{Y}_{(j,1)}\hat{Y}_{(k,0)}\frac{\partial^2 f_i(\vec{y}(0))}{\partial y_j \partial y_k}\right)\right. \\
&+ 3\sum_{j,k=1,j\neq k}^{p}\left(\hat{Y}^2_{(j,0)}\hat{Y}_{(k,0)}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j^2 \partial y_k}\right) + \sum_{j=1}^{p}\left(\hat{Y}^3_{(j,0)}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j^3}\right) \\
&+ \left. 3!\sum_{j,k,l=1,j\neq k\neq l}^{p}\left(\hat{Y}_{(j,0)}\hat{Y}_{(k,0)}\hat{Y}_{(l,0)}\frac{\partial^3 f_i(\vec{y}(0))}{\partial y_j \partial y_k \partial y_l}\right)\right] \qquad (21)
\end{aligned}
$$

The same follows for $n = 4, 5, ...$, and so on. In conclusion, for time-independent first-order differential equations, like the chemical rate equations, we have:

$$y_i(t) = y_i(0) + \sum_{n=0} \frac{t^{n+1}}{(n+1)!} \hat{Y}_{(i,n)} \tag{22}$$

For equations with explicit polynomial time-dependence $dy_i(t)/dt = kt^{\bar{n}} y_i$ (such as the quantum harmonic oscillator), $b_n(t)$ is appropriately modified. The current implementation of this method can only handle direct polynomial time-dependence (i.e., $\bar{n} \geq 0$).

$$b_n(t) = \frac{\bar{n}! t^{\bar{n}+n+1}}{(\bar{n}+n+1)!} : \qquad \bar{n} \geq 0 \tag{23}$$

The time-separated polynomial is given as:

$$\hat{Y}_{(i,n\neq 0)}(\vec{y}(t)) = \sum_{l_{(1,1)}, l_{(1,2)}, \cdots, l_{(2,1)}, \cdots, l_{(p,n)}=0}^{n} \left(\delta_{(n, \sum_{j=1}^{p} (l_{(j,1)} + 2l_{(j,2)} + \ldots + (n-1) l_{(j,n-1)} + n l_{(j,n)}))} \frac{y_{(1,1)}^{l_{(1,1)}}}{l_{(1,1)}!} \cdots \frac{y_{(p,n)}^{l_{(p,n)}}}{l_{(p,n)}!} \right)$$
$$\times \frac{n!}{l_{(1,1)}! \ldots l_{(p,n)}! 1^{l_{(1,1)}} 2^{l_{(1,2)}} \ldots (n-1)^{l_{(p,n-1)}} n^{l_{(p,n)}}} \times \frac{\partial^{l_{(1,1)} + \ldots + l_{(p,n)}} f_i(\vec{y}(0))}{\partial y_i^{l_{(1,1)} + \cdots + l_{(1,n)}} \cdots \partial y_p^{l_{(p,1)} + \cdots + l_{(p,n)}}} \tag{24}$$

Results for ADM4, ADM6, ADM8, ADM10

Scheme 1: Bimolecular Reaction

Table 2: ADM results for Scheme 1

			ADM10		ADM8		ADM6		ADM4	
modification	h	m	τ	$l1/m$	τ	$l1/m$	τ	$l1/m$	τ	$l1/m$
eddd	0.1	1001	489.59	0.00	489.51	0.00	318.90	0.00	201.03	0.00
eedd	0.1	1001	6.43	29.72	6.28	0.35	4.33	1.99	3.08	12.02
eeed	0.1	1001	4.49	42.15	4.32	0.46	3.06	2.82	2.16	18.58
eeee	0.1	1001	2.84	42.15	2.92	0.46	2.05	2.82	1.52	18.58
eddd	0.2	501	245.12	0.00	244.34	0.00	159.26	0.00	100.25	0.00
eedd	0.2	501	5.67	29.70	5.72	0.35	3.75	1.98	2.48	12.01
eeed	0.2	501	3.73	41.88	3.64	0.46	2.48	2.79	1.68	18.40
eeee	0.2	501	2.09	41.88	2.21	0.46	1.49	2.79	1.07	18.40
eddd	0.5	201	97.34	0.00	97.14	0.00	63.36	0.00	39.86	0.00
eedd	0.5	201	5.36	29.62	5.34	0.35	3.43	1.98	2.20	11.98
eeed	0.5	201	3.27	41.88	3.24	0.46	2.15	2.80	1.40	18.44
eeee	0.5	201	1.69	41.88	1.83	0.46	1.09	2.80	0.81	18.44
eddd	1	101	48.23	0.02	48.12	0.00	31.39	0.00	19.71	0.00
eedd	1	101	5.06	29.52	5.07	0.35	3.31	1.97	2.10	11.95
eeed	1	101	3.12	40.24	3.12	0.43	2.03	2.62	1.30	17.37
eeee	1	101	1.55	40.24	1.53	0.43	0.98	2.62	0.67	17.37
eddd	2	51	23.57	0.15	23.63	0.00	15.37	0.00	9.60	0.01
eedd	2	51	4.99	29.40	4.99	0.35	3.24	1.97	2.05	11.91
eeed	2	51	3.05	39.05	3.04	0.42	1.98	2.53	1.37	16.69
eeee	2	51	1.47	39.05	1.47	0.42	0.93	2.53	0.63	16.69

The first column designates which modifications are enabled (e) and disabled (d): first letter → capping derivative, second → propagator (t_q=10 s), third → adaptive discrete axis (tolerance=1E-2), fourth → initial zero derivatives excluded. h is the step-size in s, m is the number of integration points, τ is the computational duration in ms, and $l1/m = \frac{1}{m}\sum_i^m |y_i - \hat{y}_i|$is scaled by 1E7.

Scheme 2: Chloroperoxidase

Table 3: ADM results for Scheme 2

			ADM10		ADM8		ADM6		ADM4	
modification	h	m	τ	$l1/m$	τ	$l1/m$	τ	$l1/m$	τ	$l1/m$
eddd	0.001	10001	23436.65	0.64	23433.68	0.64	13526.49	0.64	7607.05	0.64
eedd	0.001	10001	2621.93	0.64	2619.86	0.64	1514.65	0.66	855.08	0.76
eeed	0.001	10001	271.98	0.63	269.95	0.64	159.39	0.68	92.93	0.95
eeee	0.001	10001	92.58	0.64	90.17	0.65	50.22	0.68	32.25	0.95
eddd	0.002	5001	11720.82	0.64	11715.17	0.64	6768.12	0.64	3807.00	0.64
eedd	0.002	5001	2352.01	0.63	2351.70	0.64	1358.28	0.67	766.28	0.84
eeed	0.002	5001	265.78	0.63	264.05	0.65	154.48	0.69	88.52	0.99
eeee	0.002	5001	84.39	0.64	83.47	0.65	44.35	0.70	27.20	0.99
eddd	0.005	2001	4689.72	0.64	4687.54	0.64	2704.09	0.64	1520.56	0.64
eedd	0.005	2001	2350.64	0.63	2347.70	0.64	1356.92	0.67	763.24	0.84
eeed	0.005	2001	267.46	0.63	266.69	0.64	154.60	0.69	87.37	0.96
eeee	0.005	2001	81.24	0.64	81.99	0.65	41.38	0.69	24.46	0.96
*eddd	0.01	1001	2342.95	0.63	2340.89	0.64	1348.37	0.67	760.18	0.85
eeed	0.01	1001	2341.34	0.63	2341.87	0.64	1349.34	0.67	760.32	0.85
eeee	0.01	1001	256.39	0.63	256.31	0.64	148.06	0.69	83.65	0.96

The first column designates which modifications are enabled (e) and disabled (d): first letter → capping derivative, second → propagator (t_q=0.01 s), third → adaptive discrete axis (tolerance=1E-4), fourth → initial zero derivatives excluded. h is the step-size in s, m is the number of integration points, τ is the computational duration in ms, and $l1/m = \frac{1}{m}\sum_i^m |y_i - \hat{y}_i|$ is scaled by 1E8. *eddd and eedd are equivalent for $h = 0.01$ s.