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Letter to the Editor

A Further Comment on "A Resolution of the Stiffness Problem of Reactor Kinetics" or "It's All About Nothing?"

In his recent letter,[1] G. Van den Eynde provided a correction to a reactor kinetics solution published by Chao and Attard[2] some 20 yr ago. With the computer algebra package MAPLE, version 9.51, Van den Eynde revisited the following fundamental reactor kinetics equations (RKEs) written in vector form:

$$\frac{d\vec{n}(t)}{dt} = \underline{A}(t)\vec{n}(t) + \vec{q}(t) \ , \tag{1a}$$

where

$$\vec{n}(t) \equiv \begin{bmatrix} N(t) \\ C_1(t) \\ \cdots \\ C_6(t) \end{bmatrix} \ , \quad \vec{q}(t) \equiv \begin{bmatrix} Q(t) \\ 0 \\ \cdots \\ 0 \end{bmatrix}$$

$$\underline{A}(t) \equiv \begin{bmatrix} \frac{\beta}{\Lambda}(\rho_\$(t) - 1) & \lambda_1 & \lambda_2 & \cdots & \lambda_6 \\ \frac{\beta_1}{\Lambda} & -\lambda_1 & 0 & & 0 \\ \cdots & 0 & -\lambda_2 & & \cdots \\ & & & \cdots & 0 \\ \frac{\beta_6}{\Lambda} & 0 & \cdots & 0 & -\lambda_6 \end{bmatrix} \tag{1b}$$

with the initial condition

$$\vec{n}(0) \equiv \begin{bmatrix} 1 \\ \frac{\beta_1}{\lambda_1 \Lambda} \\ \cdots \\ \frac{\beta_6}{\lambda_6 \Lambda} \end{bmatrix} \ . \tag{1c}$$

For completeness, the required data are given in Table I. Van den Eynde demonstrated the inaccuracy of the published values of Chao and Attard beyond $t = 4s$. Apparently, Chao and Attard never meant their solution to be a reference solution, but it was considered so by Sanchez,[3] Aboanber and Hamada,[4] and Kinard and Allan[5] in their development of new point-kinetics numerical methods. The inaccurate results published could have led to inappropriate conclusions concerning the numerical methods used by these and other authors.

Like the popular Seinfeld sitcom, some readers of Van den Eynde's letter would consider it "a letter about nothing"—after all, as pointed out by Chao and Attard, the discrepancy probably did not have "[a] significant impact to any author's conclusion."[2] Some readers like myself, however, may view the value of Van den Eynde's letter in a slightly different way. In particular, the approaches of Van den Eynde and Chao and Attard are at extreme ends of the numerical spectrum. On the one hand, the Chao and Attard approach represents the "old world" of a basic application of a standard finite difference algorithm. On the other hand, Van den Eynde's approach represents the "new world" of relatively sophisticated computer algebra combined with an efficient Rosenbrock-type differencing scheme. This letter addresses the question—Is there a middle ground where old solutions can be considered in a new light to provide reliable reference solutions? While what is to be presented here pertains only to the above case, the general concept is applicable to any discrete solution, practical limitations notwithstanding. The basic idea involves nothing less than a new concept of "a solution."

Development of a Benchmark Solution via Simple Forward Finite Difference

Equation (1a) can be discretized by simply integrating over the interval $h \equiv t_{j+1} - t_j$, which is assumed to be uniform over the times of interest $[0, T]$. After application of the trapezoidal rule for the integral over $\vec{n}$, the following discretization results:

TABLE I
Point-Kinetics Data of Chao and Attard

	$\beta = 0.007$	$\Lambda = 0.00002$
i	β_i	λ_i
1	0.000266	0.0127
2	0.001491	0.0317
3	0.001316	0.1150
4	0.002849	0.3110
5	0.000896	1.4000
6	0.000182	3.8700

TABLE II
Romberg and We Converged Powers

t (s)	MAPLE	Romberg	We
2.00E+00[a]	1.3382001E+00	1.3382001E+00	1.3382001E+00
4.00E+00	2.2284419E+00	2.2284419E+00	2.2284419E+00
6.00E+00	5.5820524E+00	5.5820524E+00	5.5820524E+00
8.00E+00	4.2786296E+01	4.2786296E+01	4.2786296E+01
9.00E+00	4.8752002E+02	4.8752002E+02	4.8752002E+02
1.00E+01	4.5116363E+05	4.5116362E+05	4.5116362E+05
1.10E+01	1.7922136E+16	1.7922136E+16	1.7922137E+16

[a]Read as 2.00×10^{00}.

TABLE IV
Nine-Digit Accuracy

t (s)	Romberg and O/We
2.00E+00[a]	1.338200050E+00
4.00E+00	2.228441897E+00
6.00E+00	5.582052449E+00
8.00E+00	4.278629573E+01
9.00E+00	4.875200217E+02
1.00E+01	4.511636239E+05
1.10E+01	1.792213607E+16

[a]Read as 2.00×10^{00}.

$$\left[\underline{I} - \frac{h}{2}\underline{A}_{j+1}\right]\vec{n}_{j+1} = \left[\underline{I} + \frac{h}{2}\underline{A}_j\right]\vec{n}_j + \frac{h}{2}\left[\vec{q}_{j+1} + \vec{q}_j\right] \ , \quad (2a)$$

where

$$\vec{n}_j \cong \vec{n}(t_j) \ ,$$

$$\underline{A}_j \equiv \underline{A}(t_j) \ ,$$

and

$$\vec{q}_j \equiv \vec{q}(t_j) \ . \quad (2b)$$

This is a forward difference approximation where the exact solution at t_j is known to be of the form

$$\vec{n}(t_j) = \vec{n}_j + \sum_{k=1}^{\infty} a_{jk} h^{2k} \ . \quad (3)$$

The particular error tail suggests the application of a Romberg[6] convergence acceleration of the solution. In the Romberg algorithm, even higher error orders are sequentially eliminated by halving the interval h until convergence. Thus, rather than choose a single h that is considered sufficiently small enough by some ad hoc intuitive standard, several h's are considered allowing the solution to be extrapolated toward zero discretization. The solution, therefore, is now a sequence of solutions tending toward their limit. In this regard, the Wynn-epsilon[7] (We) extrapolation can also be applied in addition. The We filter is well known to accelerate the convergence of a sequence to its limit under relatively general conditions. In applying either acceleration, no longer does one discretization provide the desired result. The solution now becomes an extrapolation of a sequence of solutions on a path in the space of discretized solutions. This procedure defines a new way of defining a numerical solution.

Table II gives the results of both the Romberg and the We convergence acceleration applied to the above RKEs with a reactivity ramp of

$$\rho_\$(t) \equiv 0.1t \ .$$

All digits of the MAPLE results, save one in the Romberg acceleration and two in the We acceleration (highlighted), are matched requiring $0.5s$ on a 0.7-GHz Dell INSPIRON/4000 laptop. The mesh spacing at convergence is 0.000244, which is nearly 2.5 times that of Chao and Attard's original calculation but yielding much greater accuracy with acceleration. An additional convergence scenario can be devised by filtering the Romberg results through the We. All three accelerated solutions are shown in Table III with the discrepant digits relative to the converged solution highlighted. The efficiency of the R/We accelerated sequence is essentially the same as the We acceleration of the original sequence.

In the interest of scholarly pursuit, Table IV is included pushing the accuracy two additional digits. As can be observed, the discrepant "2" in the Romberg solution seems not to be so.

TABLE III
Original Sequence and the Three Convergence Scenarios

t (s)	Original(O)	O/R	O/We	R/We
2.00E+00[a]	1.3382001E+00	1.3382001E+00	1.3382001E+00	1.3382001E+00
4.00E+00	2.2284419E+00	2.2284419E+00	2.2284419E+00	2.2284419E+00
6.00E+00	5.5820525E+00	5.5820524E+00	5.5820524E+00	5.5820524E+00
8.00E+00	4.2786299E+01	4.2786296E+01	4.2786296E+01	4.2786296E+01
9.00E+00	4.8752025E+02	4.8752002E+02	4.8752002E+02	4.8752002E+02
1.00E+01	4.5116873E+05	4.5116362E+05	4.5116362E+05	4.5116362E+05
1.10E+01	1.7929727E+16	1.7922136E+16	1.7922137E+16	1.7922135E+16

[a]Read as 2.00×10^{00}.

The Conclusion

While the Van den Eynde approach, producing what is claimed to be the undisputedly accurate solution, couples sophisticated numerical methods with modern day and, most probably, the-way-of-the-future analytical software, there is an associated intellectual cost. What has been shown here is that the same level of accuracy was indeed available when the incorrect results of Chao and Attard were first published simply by including acceleration. It should be rather gratifying to us "old timers" that the simplest of numerical methods, even implemented in FORTRAN 77, can give (nearly) identical results to today's sophisticated computational machinery. This is certainly a very small point—but after all—"it's all about nothing" anyway.

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