An efficient implementation of CSP ∗

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Abstract

We consider initial-value problems governed by a system of autonomous ordinary differential equations (ODEs). When the required integration stepsizes of the ODE system is very very small in comparison to the time domain of interest. Then the initial-value problem is said to be stiff.

1 Introduction

This paper presents a new formulation of CSP (Computational Singular perturbation) to deal with large and complicated chemical kinetics problems. [3] The main feature of the new CSP is that no expensive eigen computation is needed.

1.1 A demonstration problem

Consider the following toy initial-value problem for three unknowns x, y, z.

\[
\frac{dx}{dt} = \mathcal{X}(x, y, z). \tag{1a}
\]
\[
\frac{dy}{dt} = Y(x, y, z). \tag{1b}
\]
\[
\frac{dz}{dt} = Z(x, y, z). \tag{1c}
\]

For chemical kinetics, the unknowns are usually the concentrations of the chemical species in the reaction system, but the reaction system’s temperature may also be one of the unknowns. The right hand side of each of the ODEs depends on the stoichiometric coefficients and the reaction rates of all the included chemical reactions.

The initial conditions are:

\[
x(t = 0) = x_0, \quad y(t = 0) = y_0, \quad z(0) = z_0. \tag{1d}
\]

where \(x_0, y_0, z_0\) are arbitrary positive numbers, and \(X(x,y,z), Y(x,y,z)\) and \(Z(x,y,z)\) are some completely general algebraic functions of \(x, y,\) and \(z.\)

It is assumed that subroutines for their evaluations can be and have been coded and are available.

In order to compute solutions for such initial-value problems by numerical integration, one must first choose an integration time step \(\Delta t.\) It is well-known that the computed solutions are meaningful only if the chosen \(\Delta t\) is sufficiently small. The crucial question is, how small is sufficiently small?

1.2 Characteristic timescales of all the unknowns in the problem.

We define \(\tau_x, \tau_y\) and \(\tau_z\) by:

\[
\tau_x \equiv -\frac{1}{\partial X(x, y, z)/\partial x}, \quad \tau_y \equiv -\frac{1}{\partial Y(x, y, z)/\partial y}, \quad \tau_z \equiv -\frac{1}{\partial Z(x, y, z)/\partial z}. \tag{2}
\]

It is easy to show that the physical unit of all the \(\tau\)’s as defined above is time. It is important to note that these \(\tau\)’s are the negative reciprocals of the diagonal elements of the problem’s Jacobian. See Eq.(10) of [8]. Since subroutines for \(X((x,y,z)) Y((x,y,z))\) and \(Z((x,y,z))\) are available, partial derivatives can be computed using the definition of partial derivative using just two subroutine calls. For example:

\[
\frac{\partial X}{\partial x} = \frac{X(x + \delta x, y, z) - X(x, y, z)}{\delta x}. \tag{3}
\]
where $\delta x$ is some small number. Thus, given $x(t), y(t)$ and $z(t)$ at any time $t$, the current values of $\tau_x(t), \tau_y(t)$ and $\tau_z(t)$ can be computed on the fly. We limit our attention to problems for which all eigenvalues of the current Jacobian are expected to be real (in the time epoch of interest) and that all the current $\tau(t)$’s are positive. When any one of the $\tau$’s is currently negative, the system is currently explosive. When all the $\tau$’s are currently positive, the system is currently stable and is expected to decay to some partial equilibrium or quasi-steady state value $O(\tau)$ seconds later. Thus if $\tau_x$ is currently the smallest positive $\tau$, then variable $x$ is currently the fastest variable (often referred to as the radical of the reaction system. The value of $x(t)$ is expected to decay exponentially from its initial value $x_o$ to its current partial equilibrium or quasi-steady state value $x_{qs}$ in $O(\tau_x)$ seconds. Inside this thin initial transient layer, the slower variables ($y, z$) are approximately constant and can be approximated by their initial values. It is clear that the $\Delta t$ used to numerically integrate the whole ODE system must be small in comparison to the current $\tau_x$. Otherwise, all solutions computed using unacceptable $\Delta t$ to do the numerical integrations are meaningless.

1.3 Alternative representations

Let $\hat{X}(x, y, z)$ denote an alternative representation of $X(x, y, z)$ as shown by the righthand side of the equation below.

$$X(x, y, z) \approx \hat{X}(x, y, z) \equiv X(x = 0, y, z) - \frac{x}{\tau_x(y, z)}.$$  \hspace{1cm} (4)

Note that the partial $x$ derivative of $X(x, y, z)$ and that of $\hat{X}(x, y, z)$ are the same provided the $x$-dependence of $\tau_x(x, y, z)$ computed from Eq.(3) is sufficiently weak. The $x$ dependence of $\tau_x(x, y, z)$ (weak or strong?) can be computationally determined. Note that $dx/dt=\hat{X}(x, y, z)$ is a linear ODE for $x(t)$ and its exact analytical solution (for given $y$ and $z$) is known. The mathematical meaning of $\tau_x$ for species $x$ is obvious, when the analytical solution of $dx/dt=\hat{X}(x, y, z)$ is examined carefully. When $x(t)$ reaches quasi-steadiness (i.e. $\hat{X} \approx 0$). Eq.(4) can be solved to yield the quasi-steady value of $x(y, z)$.

$$x_{qs}(y, z) \equiv \tau_x X(x = 0, y, z).$$  \hspace{1cm} (5)
Hence Eq(1a), the ODE for \( x(t) \), can now be discarded and replaced by the algebraic equation \( x(t) = x_{qs}(y(t), z(t)) \). Consequently, the upper bound of acceptable integration timestep \( \Delta t \) to integrate the resulting DAE system numerically is no longer set by the value of the current \( \tau_x \). The assumption that \( \tau_x \) has weak \( x \)-dependence is the crucial enabling step of this new CSP formulation. In addition, the upper bound of acceptable integration timestep \( \Delta t \) to integrate the resulting DAE system numerically is no longer set by the value of the current \( \tau_x \). The assumption that \( \tau_x \) has weak \( x \)-dependence is the crucial enabling step of this new CSP formulation. In addition, The accuracy and validity of \( X(x, y, z) \approx \hat{X}(x, y, z) \) with \( \hat{X}(x, y, z) \) defined by Eq.(4) can be and should be computationally established.

2 The Euler algorithm

This algorithm asserts that inside one single integration timestep, the right hand side of an ODE can be approximated by its value at the initial instant. Thus, to march \( x(t) \) forward in time starting at \( t = t_0 \) where \( x(t_0) = x_o \), one Euler timestep \( \Delta t \) later, we have:

\[
\frac{x(t_0 + \Delta t) - x(t_0)}{\Delta t} = \hat{X}(x(t_0), y(t_0), z(t_0))
\]  

We denote the ratio \( \Delta t/\tau_x \) by \( \sigma \) The above equation can be rewritten in terms of \( \sigma \) as follows:

\[
x(t_0 + \Delta t) = (1 - \sigma)x(t_0) + \sigma x_{qs}(t_o).
\]

Note that when \( \sigma = 1 \), the value of \( x \) decays linearly from its initial value \( x_o \) to \( \sigma x_{qs}(y(t_0), z(t_0)) \) in one Euler step. This is equivalent to doing a ” CSP radical correction”. see §6.5 of [2]. The precise details of the jump trajectory inside the one thin step is usually not of interest. Note that when \( \mathcal{X}(x = 0, y, z) \) is \( O(1) \), then according to Eq.(5), \( x_{qs}(t) \) is \( O(\tau_x) \) (in other words, it is negligibly small in the small \( \tau_x \) limit). It can be shown rigorously that the Euler algorithm does recover the correct exponential (rather than linear) decay inside the thin layer in the small \( \sigma \) limit.

2.1 The Quasi-Steady approach

1. It is important to note that we do not assume \( \tau_x \), the current smallest computed \( \tau \), is the negative reciprocal of the
largest eigenvalue of the system’s current Jacobian. However we do tacitly assumed that the order of magnitudes and the signs of these two numbers are the same. The smallness of the ratio of the current smallest $\tau$ over any of the current larger $\tau$’s is the small parameter to be exploited by conventional singular perturbation (SP) analysis. The most crucial enabling step of the present approach is the introduction of a ”CSP-data-inspired” and computationally verifiable alternative representation of $\mathcal{X}(x,y,z)$, see Eq.(4). CSP takes full advantage of the verifiable linearity of $dx/dt = \hat{\mathcal{X}}(x,y,z)$.

2. Let us introduce $\eta \equiv t/\tau_x$ and use $\eta$ to replace $t$ as the independent variable. When $\eta = O(1)$, it is easy to show that $y(\eta) \approx y_0$, and $z(\eta) \approx z_0$. (i.e. the slow unknowns are approximately constant inside the very thin initial transient layer.) Moreover, The ODE for $x(\eta)$ is no longer stiff in the $\tau_x \to 0$ limit.

3. The $\eta$ formulation is even useful when there is no $\tau$ gap among the fast $\tau$’s.

4. When $\eta \gg 1$, the algebraic Eq.(5) says $x_{qs}(t)$ is O($\tau_x$) and most importantly, it depends only on the slow variables. We can now replace the $x(t)$ ODE by the algebraic Eq.(5). Consequently, the extreme stiffness of the original ODE problem in the $\tau_x \to 0$ limit is removed. Since Eq.(5) played a dominant role in the above description, This model reduction strategy is called the quasi-steady approach. This approach only works if the determinant of the fast Jacobian is not zero. Otherwise, the set of algebraic Eq(5)’s has redundancy issues, and the partial equilibrium approach described in Section 2.2 below must be used.

5. When the details of the rapid transients inside the thin transient layer is not of interest, the Euler explicit integration algorithm with $\sigma = 1$ is recommended to handle the ODE of the current radical.

6. Non-linearity in any non-stiff ODE system is not an issue,
because it is being dealt with routinely and correctly by numerical integrations.

7. When there are *more than one* very fast species (e.g. x and y), and there is *no* large tau-gap between them, such problems are more difficult, and they need special considerations. See §2.2 below. A probable cause of the special difficulties is that one of the fast reactions inside the thin transient layer is reversible. It is possible to show that for such problems, some linear combination of the fast variables is a slow variable (i.e. it is approximately constant inside a thin transient layer. See Eq.(2.16) in §2.3 of [2].

2.2 The Partial Equilibrium approach

Consider the following special initial-value problem:

\[
\frac{dx}{dt} = \mathcal{X}(x, y, z) \equiv f(z) - \frac{x-Ky}{\tau}, \quad (8a)
\]

\[
\frac{dy}{dt} = \mathcal{Y}(x, y, z) \equiv g(z) + \frac{x-Ky}{\tau}, \quad (8b)
\]

\[
\frac{dz}{dt} = \mathcal{Z}(x, y, z) = O(1). \quad (8c)
\]

where $K$ and $\tau$ are positive slow parameters. Note that when $K=O(1)$, both $x$ and $y$ are nearly equally fast species in the small $\tau$ limit, while $z$ is always a slow species. Thus for this toy problem, the number of fast species is larger than the number of fast reactions. In addition, the determinant of its $2 \times 2$ fast Jacobian is zero. Thus zero is one of the eigenvalues of this Jacobian. It was noted previously that the quasi-steady approach will have ”redundency” problems under such conditions. Subtracting $K$ dy/dt from dx/dt, we obtain:

\[
\frac{d(x-Ky)}{dt} = f(z) - Kg(z) - \frac{(1+K)(x-Ky)}{\tau}. \quad (9)
\]

The above ODE says when the sole fast reversible reaction reaches *partial equilibrium*, the equilibrated value of $x - Ky$ is $\frac{[f(z)-Kg(z)]\tau}{(1+K)}$, which is an $O(\tau)$ number for any finite initial value $(x_o - Ky_o)$. 
After some intelligent examination of the stoichiometric coefficients of the fast reversible reaction. A most interesting and useful new variable $u$, defined by $u \equiv x + y$, would suggest itself. Adding Eq.(8a) and Eq.(8b), an exact ODE for $u$ is obtained:

$$\frac{du}{dt} = \mathcal{U}(z) \equiv \mathcal{X}(x, y, z) + \mathcal{Y}(x, y, z) = f(z) + g(z), \quad (10)$$

Note that as defined above, the new variable $u$ is a slow variable (inspite of the fact that both $x$ and $y$ are fast variables). Most importantly, $\mathcal{U}(z)$ is a function of $z$ only, and is independent of both $x$ and $y$. Note also that we can now use $y = u - x$ to eliminate $y$ from Eq.(2.2) to obtain:

$$x - Ky = -Ku + (1 + K)x = \frac{[f(z) - g(z)]\tau}{(1 + K)}, \quad (11)$$

$$(1 + K)x = Ku + \frac{[f(z) - g(z)]\tau}{(1 + K)}. \quad (12)$$

Let $N$ denote the total number of species, and let $M$ denote the number of fast species. Usually, $M$ is much smaller than $N$. An eigenanalysis can easily be done (using computations) on the small $M \times M$ Jacobian of the $M$ fast species. Viewed from the vantage point of elementary eigenanalysis, the scalar $u$, as defined above, is the amplitude of the zero-eigenvalue-mode of the $M \times M$ fast Jacobian.

In the small $\tau$ limit, the major result of the above singular perturbation analysis is:

$$x \approx \frac{Ku}{1 + K} \approx Ky. \quad (13)$$

Using this algebraic partial equilibrium equation in Eq.(8c), we obtain:

$$\frac{dz}{dt} = \mathcal{Z}(x = Ku/(1 + K), y = u/(1 + K), z) \quad (14)$$

This ODE and Eq.(10) are two non-stiff ODEs for the two slow variables $z(t)$ and $u(t)$, Thus they can be integrated numerically together using generous timesteps. Once the slow $u(t)$ has been found, The values of the two fast variables are given by: $x(t) = K$.
u(t)/(1+K), and y(t)=u(t)/(1+K). Note that the ODEs for the current pair of fast species x and y and the current values of $\tau_x$ and $\tau_y$ are totally out of the game. Since $K = x_{qs}/y_{qs}$, thus the current numerical value of $K$ can easily be computationally determined on the fly. The above singular perturbation (SP) approaches are strictly conventional when carried out by hand. Their logic is simple and clearly programable.

2.3 Conclusions

• Generalization of the above 3 unknowns toy demonstration problems to N unknowns real problems, is straightforward.

• The new CSP provides insights which can be and should be exploited when the goal is to derive "reduced models" or to numerically integrate very stiff ODE systems.

• The new CSP also provides the mathematical rationale on how to choose and update the current acceptable timestep when doing numerical integration on very stiff ODE systems. The onestep Euler algorithm is the same as doing a CSP "radical correction". See §6.5 of [2].

This paper is is a followup of a 2013 CSP paper[5] [9] The most outstanding feature of the new CSP is that no expensive eigenvalues and eigen-vectors calculations are needed or involved. For reacting flow problems, the governing PDEs may include diffusion terms, CSP can deal with the interesting couplings between reduced chemistry and diffusion. See [9].

References


