

Asymptotics with Variable Fast Time Scales

S. H. Lam*

Department of Mechanical and Aerospace Engineering
Princeton University, Princeton, NJ 08544, U.S.A.

Abstract

The interesting features of the five benchmark problems to be discussed in the *International Workshop on Model Reduction in Reacting Flow*, (Rome, Italy, September 3-5, 2007) can all be attributed to the strong dependence of the relevant fast time scales on the state variables.

1 Introduction

We shall first use conventional singular perturbation methodology to analyze the benchmark problems, then follow up by a brief summary of the CSP methodology [1, 2, 3, 4].

The time interval of interest is $t = O(1)$. All state variables here are assumed to be non-negative.

2 Conventional asymptotics

Conventional asymptotics depends on the “insights” and skills of the investigator, who is responsible for the identification and the exploitation of the small singular perturbation parameter. Only the leading order results will be presented here.

2.1 The Williams problem

The original ODE system [5] is ($\epsilon > 0$):

$$\frac{dx}{dt} = -x - xy, \quad (1)$$

$$\frac{dy}{dt} = \frac{1}{\epsilon}(x + (\alpha - 1)xy - \gamma y). \quad (2)$$

Exploiting insights from experience, we can rewrite the above exactly as follows:

$$\frac{dx}{dt} = x \left\{ \mathcal{Y}(x) - y + \tau_W(x)\mathcal{S}(x)\frac{d\mathcal{Y}(x)}{dx} \right\} - \left(1 + \tau_W(x)x\frac{d\mathcal{Y}(x)}{dx} \right) \mathcal{S}(x), \quad (3)$$

$$\frac{dy}{dt} = \frac{1}{\tau_W(x)} \left\{ \mathcal{Y}(x) - y + \tau_W(x)\mathcal{S}(x)\frac{d\mathcal{Y}(x)}{dx} \right\} - \left(\frac{d\mathcal{Y}(x)}{dx} \right) \mathcal{S}(x). \quad (4)$$

where

$$\mathcal{Y}(x) \equiv \frac{x}{\gamma - (\alpha - 1)x}, \quad (5)$$

$$\mathcal{S}(x) \equiv x(1 + \mathcal{Y}(x)), \quad (6)$$

$$\tau_W(x) \equiv \frac{\epsilon}{\gamma - (\alpha - 1)x}. \quad (7)$$

When $\tau_W(x) > 0$ (it has the physical unit of time) is asymptotically small, this is a very straightforward singular perturbation problem. The sign of $\tau_W(x)$ is overwhelmingly important. For asymptotically small and positive $\tau_W(x)$, the leading order slow manifold is $y \approx \mathcal{Y}(x) + O(\tau_W)$. Once the solution is inside the slow manifold, the leading order reduced model is obtained by simply neglecting all $O(\tau_W)$ terms. The two curly brackets—they are identical—can be shown to be $O(\tau_W^2)$. Either one of the reduced model ODEs can be replaced by the approximate algebraic relation provided by setting the curly bracket to $O(\tau_W^2)$. When a previously small and positive $\tau_W(x)$ is no longer small and positive, solutions already inside the slow manifold would emerge from the slow manifold.

2.2 The Lindemann problem

The original ODE system [6] is ($\epsilon > 0$):

$$\frac{dy}{dt} = \frac{z}{\epsilon}(z - y) - y, \quad (8)$$

*Professor emeritus. Email: lam@princeton.edu

$$\frac{dz}{dt} = -\frac{z}{\epsilon}(z-y). \quad (9)$$

When both y and z are $O(1)$, this singular perturbation problem for small ϵ is trivial. Exploiting insights from experience, we can rewrite the above exactly as follows:

$$\frac{dy}{dt} = \frac{1}{\tau_L(z)} \left\{ (z-y) - \frac{\tau_L(z)}{2}y \right\} - \frac{1}{2}y, \quad (10)$$

$$\frac{dz}{dt} = -\frac{1}{\tau_L(z)} \left\{ (z-y) - \frac{\tau_L(z)}{2}y \right\} - \frac{1}{2}y, \quad (11)$$

where $\tau_L(z)$ has the physical unit of time and is defined by:

$$\tau_L(z) \equiv \frac{\epsilon}{z}. \quad (12)$$

When $\tau_L(z)$ is positive and small, this is a classical problem for the partial equilibrium approximation (note that the quasi-steady state approximation (QSSA) does *not* work for this problem when y and z are the dependent variables). The leading order slow manifold is $z \approx y + O(\tau_L)$. Once the solution is inside this slow manifold, the leading order reduced model is obtained by neglecting the two curly brackets (which can be shown to be $O(\tau_L^2)$). Note that $z \approx y + O(\tau_L)$ cannot be used in Eq.(8) nor in Eq.(9). When a previously small $\tau_L(z)$ is no longer small, solutions already inside the slow manifold would emerge from it. When $\tau_L(z) > 0$ is asymptotically large and $y \approx z/\tau_L(z)$, a new gap of time scales shows up.

2.3 The Semenov (ODE) problem

The original ODE system [7] is ($D_a > 0, \gamma > 0, B > 0$):

$$\frac{dx}{dt} = -x + D_a(1-x)e^{f(y)}, \quad (13)$$

$$\frac{dy}{dt} = -(1+\beta)y + BD_a(1-x)e^{f(y)}, \quad (14)$$

where

$$f(y) \equiv \frac{y}{1+y/\gamma}. \quad (15)$$

Following [4], we define $R(x, y)$ by:

$$R(x, y) \equiv D_a(1-x)e^{f(y)}. \quad (16)$$

The original two dependent variables problem can be restated as a three dependent variables problem governed by the following exact ODE system:

$$\frac{dx}{dt} = -x + R, \quad (17)$$

$$\frac{dy}{dt} = -(1+\beta)y + BR, \quad (18)$$

$$\frac{dR}{dt} = -\frac{1}{\tau_S(x, y)}(R - R_\infty(x, y)), \quad (19)$$

where the new ODE for R is obtained by differentiating Eq.(16) with respect to time, and $R_\infty(x, y)$ and $\tau_S(x, y)$ are shorthand notations for:

$$R_\infty(x, y) \equiv \frac{x(1+y/\gamma)^2 - (1+\beta)(1-x)y}{(1+y/\gamma)^2 - B(1-x)}, \quad (20)$$

$$\tau_S(x, y) \equiv \frac{(1+y/\gamma)^2}{D_a e^{f(y)} [(1+y/\gamma)^2 - B(1-x)]}. \quad (21)$$

The exact solution of Eq.(19) is Eq.(16).

The magnitude of $\tau_S(x, y)$ depends strongly on the magnitude of $f(y) > 0$ and its sign depends on the values of x and y . When $\tau_S(x, y)$ is positive and very small (in comparison to the currently active time scale) along the solution trajectory, Eq.(19) says R rapidly relaxes toward $R_\infty(x, y)$. The leading order “slow manifold”—an approximate relation between y and x —can be obtained by applying QSSA to Eq.(19) using Eq.(16) for $R(x, y)$ and Eq.(20) for $R_\infty(x, y)$. When $\tau_S(x, y) > 0$ is no longer small but is $O(1)$, the QSSA for Eq.(19) fails. Solutions then emerge from the slow manifold. Interestingly, when $\tau_S(x, y)$ is not small but is *comparable* to the currently active time scale, its being negative has *no* mathematical (i.e. instability or explosiveness) significance.

It is also possible to introduce curly brackets which can be neglected once the solution is inside the slow manifold. Such niceties are omitted here.

For the sample cases with $D_a = 0.1$ and $0.2, \gamma = 35, \beta = 1.8, B = 10$ (for initial conditions $0 \leq x(0) \leq 1$ and sufficiently large positive $y(0)$), the early value of $\tau_S(x, y)$ along the solution trajectory is small and negative—conveying the message that the chemistry term is locally “explosive.” Then as time marches on, the value of $1/\tau_S(x, y)$ turns positive while $\tau_S(x, y)$ itself stays small for a while. During the time $\tau_S(x, y)$ is both positive and small, R approaches $R_\infty(x, y)$ rapidly while x approaches 1 from below (this is the leading order slow manifold). At some finite t later $1/\tau_S(x, y)$ changes sign again and stays $O(1)$, and R no longer follows $R_\infty(x, y)$ and x moves away from 1 as the solution emerges from the slow manifold (see Eq.(19)). The stability of the final equilibrium point is controlled by the value of D_a . (The two relevant eigenvalues there could be complex conjugates). Additional remarks on this problem can be found in §3.

2.4 The Semenov (PDE) problem

The original PDE system [7] is ($\beta > 0, \gamma > 0, L_e > 0$):

$$\frac{\partial c}{\partial t} = L_e \frac{\partial^2 c}{\partial x^2} - \phi^2 e^{-\gamma/T} c, \quad (22)$$

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \beta \phi^2 e^{-\gamma/T} c. \quad (23)$$

The above PDEs can be rewritten exactly as:

$$\frac{\partial c}{\partial t} = L_e \frac{\partial^2 c}{\partial x^2} - \frac{c}{\tau_{chem}(T)}, \quad (24)$$

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \beta \frac{c}{\tau_{chem}(T)}, \quad (25)$$

where

$$\tau_{chem}(T) \equiv \frac{e^{\gamma/T}}{\phi^2} = e^{(\gamma/T - 2 \ln \phi)} > 0. \quad (26)$$

The physical unit of τ_{chem} is time, is always positive, and it depends on T . Note that the value of $\tau_{chem}(T)$ can be “small” only if $T > \gamma/(2 \ln \phi)$. When $c > 0$, the chemistry term is active when $\tau_{chem}(T)$ is comparable to (or much smaller than) the current time interval of interest. It is important to note that the spatial independent variable, x , has the physical unit of the square root of time—because it had been divided by the square root of the thermal conductivity coefficient. When the global extent of the x domain of interest (in this physical unit) is large compared to the square root of $\tau_{chem}(\bar{T})$ where \bar{T} is some representative temperature, the effects of wall boundary conditions are confined to thin boundary layers.

In the absence of diffusion, $T + \beta c$ is conserved for fixed x , and the *steady state* solution is simply $c_{ss}(x) = 0$ and $T_{ss}(x) = T(t = 0, x) + \beta c(t = 0, x)$. The amount of time needed to reach (chemical) steady state is $O(\tau_{chem}(\bar{T}))$. When diffusion is present and $L_e = 1$, the PDE of linear combination $T + \beta c$ is independent of the chemistry term, and the diffusion problem is very simple. For $L_e > 0$ in the steady state, we expect a net diffusion in-flux of c and a net heat conduction out-flux of energy from the x -domain of interest, and that the final $T + L_e \beta c$ will be strictly linear with respect to x . When there are many chemical species in the problem and diffusion is locally important, there is no “slow manifold” to reduce the number of chemical species, and the diffusion terms in the reduced model are modified by the reduced chemistry approximations. See Lam [4] for additional discussions on the coupling of chemistry and diffusions.

2.5 The Davis-Skodje problem

The original ODE system [8] is ($\gamma > 0$):

$$\frac{dy_1}{dt} = -y_1, \quad (27)$$

$$\frac{dy_2}{dt} = -\gamma y_2 + \frac{(\gamma - 1)y_1 + \gamma y_1^2}{(1 + y_1)^2}. \quad (28)$$

Eq.(28) can be rewritten exactly as:

$$\frac{d}{dt} \left(y_2 - \frac{y_1}{1 + y_1} \right) = -\frac{1}{\tau_{DS}} \left\{ y_2 - \frac{y_1}{1 + y_1} \right\}. \quad (29)$$

For $\tau_{DS} = 1/\gamma = \text{constant}$, the exact solutions are readily available. In the small $\tau_{DS} > 0$ limit (even if τ_{DS} depends on y_1 and y_2), this is an especially simple singular perturbation problem.

When diffusion is present, the CSP analysis for this class of “toy problems” can be found in [4].

3 CSP Methodology

CSP is computational. It does not need *a priori* identification of the singular perturbation parameter, nor insights of the investigators on the problem. No intuition, experience, or estimations of order of magnitudes are needed. In fact, dimensional formulation can be used since the concept of “order unity” is not involved. The desired time resolution, the error tolerance of the approximate solutions and the time domain of interest are assumed specified.

The CSP methodology provides a two-step refinement procedure to find the (column and row) CSP basis vectors of the fast subspace. A CSP mode is considered fast if its time scale is much smaller than those in a group of the “currently active” modes—i.e. there is a gap in the fast/slow time scales. An arbitrary “trial set” of the fast basis vectors can be used to initiate the CSP refinement procedure, and at least one complete two-step refinement cycle is required—except when the trial set is the set of fast eigenvectors of the Jacobian matrix of the chemistry term. This trial set is special because it does provide the leading order approximation without undergoing refinement. Further refinements merely improve it quality. Conventional asymptotics methodology uses intuition and experience to *guess* at the CSP fast basis vectors.

The CSP methodology uses the CSP-refined fast basis vectors to compute a matrix of the time scales of

the fast modes numerically (see §4). The magnitude of the eigenvalues of this matrix are the time scales of the set of fast modes. For each of the $N = 2$ problems here, there is at most one fast time scale. The entities $\tau_W(x)$, $\tau_L(z)$, $\tau_S(x, y)$, $\tau_{chem}(T)$, and τ_{DS} used in §2 were the *educated guesses* of the fast time scales.

For a general N -dimensional problem, CSP refines the fast basis vectors and computes the time scale matrix on the fly. Attention is paid to the contribution of the M fast components on the right hand sides (including diffusion terms) of these N equations. When the reciprocal of the the negative real part of the eigenvalues of the $M \times M$ time scale matrix are all small (compared to the currently active time scale of the problem), the amplitudes of all the fast mode components of the right hand sides decrease rapidly. When their contributions drop below the user-specified error tolerance thresholds for all N components of the state vector, they are said to be exhausted, and can thus be justifiably neglected. The surviving $N - M$ slow components of the right hand sides of the equations is then the *reduced model* of the original problem.

The amplitudes of the “exhausted fast modes” should continue to be monitored after their exhaustion. It is possible for an exhausted fast mode to be revived (when the time scale gap is disappearing). The “initial” conditions to be used as the solutions emerge from the slow manifold have some innate uncertainty, and the handling of this uncertainty is not straightforward. When solutions with different original initial conditions enter and then emerge from a slow manifold, the “effective initial conditions” for the subsequent trajectories are very close to each other. Thus plots of the subsequent trajectories in state variable space are initially bunched together, and such bunching could be misinterpreted as evidence that a slow manifold exists there. Asymptotics based on time scales separation, either analytical or computational, offers no advantage in identifying limit cycles.

For the Semenov ODE problem (§2.3), the educated guess of the fast (column and row) basis vectors were: $\mathbf{a}_1 = [1, B]^{transpose}$ and $\mathbf{b}^1 = [(1+\beta)y, -x]/((1+\beta)y - Bx)$. The quality of this guessed set can be improved by CSP refinements.

4 Remarks

In fast/slow problems with an identified small parameter $\epsilon(\mathbf{y}) > 0$ (where \mathbf{y} here represents the state vector

of the dependent variables), the leading order conventional singular perturbation approximation after the rapid transients have decayed is independent of $\epsilon(\mathbf{y})$ in the asymptotic limit of $\epsilon \rightarrow 0$. Thus for any small $\epsilon(\mathbf{y}) > 0$ —the details of its \mathbf{y} dependence is irrelevant in the leading approximation.

In general, the fast subspace is M -dimensional, and is spanned by M pairs of CSP refined (orthonormal) column and row basis vectors $\mathbf{a}_m^o(\mathbf{y})$ and $\mathbf{b}_m^o(\mathbf{y})$, $m = 1, \dots, M$. The $M \times M$ fast time scales matrix $\tau_{m'}^m(\mathbf{y})$ is the inverse of $(d\mathbf{b}_o^m/dt + \mathbf{b}_o^m \cdot \mathbf{J}) \odot \mathbf{a}_m^o$, where $\mathbf{J}(\mathbf{y})$ is the $N \times N$ Jacobian of the chemistry term with respect to \mathbf{y} . With CSP methodology, the “complications” of $\tau_{m'}^m(\mathbf{y})$ being \mathbf{y} dependent is handled in strides—*so long there is a gap in the fast/slow time scales*.

References

- [1] Lam, S. H., The CSP method to understand complex chemical kinetics, *Combustion Science and Technology*, **89**, 5-6, (1993).
- [2] Lam, S. H. and Goussis, D. A., The CSP method of simplifying kinetics, *International Journal of Chemical Kinetics*, **26**, April, (1994).
- [3] Lam, S. H., Reduced Chemistry modeling and sensitivity analysis, *Aerothermochemistry for Hypersonic Technology*, Von Karman Institute of Fluid Dynamics, 1994-1995 Lecture Series Programme. (1995). Available at <http://www.princeton.edu/~lam/vki.html>.
- [4] Lam, S. H., Reduced Chemistry-Diffusion Coupling, *Combustion Science and Technology*, **179**, 4, (2007).
- [5] Williams, F. A., *Combustion Theory*, 2nd ed., Appendix B, 2.5.3, page 520, (1985).
- [6] Laidler, K. J., *Theories of Chemical Reaction Rates*, McGraw Hill series in advanced chemistry, (1969).
- [7] Uppal, A., Ray, W. H., and Poore, A., On the dynamic behavior of continuous stirred tank reactors, *Chemical Engineering Science*, **29**, pp. 967-985, (1974).
- [8] Davis, M. J. and Skodje, R. T., *J. Chem. Phys.* **111**, p. 859, (1999).