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Reacting Flows and Control Theory

S. H. Lam

Department of Mechanical and Aerospace Engineering, Princeton University

Corresponding Author:** ***S. H. Lam, *Department of Mechanical and Aerospace Engineering, Princeton University*

Abstract: *Model reduction of reacting flows looks for "slow manifolds"—by exploiting the fast/slow speed gap of the reaction system—so that some of the original ODEs can be replaced by algebraic equations. Control theory strives to determine some unknown control forces in a set of given ODEs in order to honor some user-specified behaviors— such as restricting the solutions to stay on some user-specified phase space surface (i.e. manifold). It is shown that some model reduction methodologies in reacting flows can be applied to control theory.*

1. INTRODUCTION

Reacting flows with active chemistry and control theory are distinct disciplines. They have mathematical similarities, and some of the similarities can be exploited.

2. REACTING FLOW PROBLEMS

Consider a generic initial value problem:

$$\frac{dy}{dt} = g(y), \tag{1a}$$

$$y(0) = y_0, \tag{1b}$$

where y and g are N -dimensional column vectors. For reacting flow problems, g(y) is usually the sum of contributions from many elementary chemical reactions—some very fast, and others not so fast. For the present purpose, g(y) is just any given differentiable function of y and may be arbitrarily non-linear. The relevant Jacobian $U(x_*u)$ is denoted by J—note that J is y-dependent when g(y) is non-linear.

Now consider the case when the eigenvalues of J have a wide gap, and that there are M "fast" modes (M < N) which are all known to be decaying modes. After the M fast modes decay away, the solution will then evolve in a slow manifold defined by:

$$f^m(y) \approx 0, 1 \le m \le M \tag{2}$$

for t >> T_M where T_M is the time scale (reciprocal of the magnitude of the real part of the eigenvalue) of the slowest fast mode. When solutions in the slow evolution period are of interest, finding the slow manifold—Eq.(2)—is a worthy objective, because knowledge of the slow manifold can be exploited to provide various insights and useful simplifications.

3. CSP ON REACTING FLOW PROBLEMS

Let a_n and b^n, n = 1, . . . , N be a full set of orthonormal (column and row) basis vectors spanning the full N -dimensional space. The right hand side of Eq.(1a) can always be expressed in terms of any full set of basis vectors:

$$g(y) = \sum_{N=1}^{N} a_n f^n \tag{3a}$$

Where

$$f^n(y) = b^n \odot g, \quad n = 1, \ldots, N, \tag{3b}$$

And $\odot$ is the N-dimensional inner product. For linear problems, the right and left eigenvectors of J are excellent choices for a^n and b^n. If the eigenmodes are ordered with the fastest modes first, then after the first M fast modes have sufficiently decayed, the solution will subsequently evolve in the slow manifold, Eq.(2). For non-linear problems, CSP provides a two-step refinement algorithm to improve the fast/slow decoupling of any trial basis vectors set [1, 2]. Each CSP refinement cycle improves the quality of the fast/slow decoupling—i.e. the smallness of the M $f^m(y)$'s—by a factor proportional to the eigenvalue gap between the fast and slow eigenmodes.

4. CONTROL PROBLEMS

Consider the following dynamics system:

$$\frac{dx}{dt} = A(x) + Bu, \tag{4}$$

where x and A are N-dimensional column vectors, A(x) is some given differentiable function of x and may be arbitrarily non-linear, u is a M-dimensional column vector $(M \le N)$ representing the to-be-determined "control forces," and B is a $N \times M$ known constant matrix. A typical control objective would be to find u(t) (or u(x)) such that the solution x(t)—after a brief transient—would evolve with acceptably small user-specified "tracking errors" i.e., the controlled x(t) trajectories would stay inside a manifold defined by:

$$F^m(X) \approx 0, \quad 1 \le m \le M, \tag{5}$$

Where the $F^m(x)$'s are M user-specified algebraic tracking errors from some desired trajectories. See Eq.(11) later for more general control objectives.

A control force program u(t) is called open-loop control while a control law $u(X_*)$ is called close-loop control, where X_* denotes sensor measurement of the actual true x to provide "feedback" to the controller. Asterisks shall be used to identify sensor measurements provided to the controller. It is assumed that good sensor measurements for all components of x are available.

5. RESTATING CONTROL PROBLEMS AS REACTING FLOW PROBLEMS

For the sake of simplicity (and to sidestep many complications), this exposition shall be limited to the special case of M = 1. So $F^1(x)$ is the sole user-specified algebraic function, and u is a scalar to be denoted by u. For this special case, the control problem can be restated in the form of reacting flow problems (with N + 1 species):

$$y = \begin{bmatrix} x \\ u \end{bmatrix}, \quad g(y) = \begin{bmatrix} A(x) + Bu \\ U(X_*, u) \end{bmatrix}, \quad f^1(y_*) = F^1(X_*). \tag{6}$$

Thus the species u has the new "kinetics" equation:

$$\frac{du}{dt} = U(X_*, u). \tag{7}$$

The problem now is to find $U(X_*, u)$ such that the tracking errors (as reported by the sensors)—starting with $f^1(y_*) = F^1(x_*) \ne 0$ initially—would decay toward $f^1(y_*) = F^1(X_*) \approx 0$ in some desirable manner after a brief transiet.

6. FAST REACTION AS UNIVERSAL DYNAMIC CONTROL LAW

To achieve the control objective $F^1(X_*) \approx 0$ for $t \gg T$, the following $U(x_* u)$ is recommended [3,4] for Eq.(7):

$$U(x_*, u) = -\frac{1}{K \Delta t}\left(\frac{dF^1(x_*)}{dt} + \frac{F^1(x_*)}{T}\right) \tag{8a}$$

Where

$$K = K(x_*) = \frac{\partial F^1}{\partial x} \odot B \tag{8b}$$

and K (x_*)=0 is assumed. Here, Tis an user-specified time constant of the "brief transient," and Δt is another user-specified positive time constant which must be smaller than T . Both are at the disposal of the user. While U (x_*, u) in Eq.(7) can be interpreted as the chemical kinetics term for the chemical species u, it is actually a close loop dynamic control law for the control force u. From the reacting flows point of view, the QSSA (quasi- steady-state approximation) is applicable to the species u only if (i) Eq.(7) is stable and (ii) U (x_*, u)'s "reaction rate" is "asymptotically large." Application of QSSA on Eq.(7) would yield an exponentially decaying F^1(x) toward zero (for t >> t)—with (user-specified) time constant T

The crucial question is then: how to ensure that QSSA is applicable to u (i.e. to Eq.(7) with Eq.(8a)) in the small Δt limit?

How does U (x_*,u) depend on u? Neither $F^1(X_*)/T$ nor K depends on but $(dF^1(x)/dt)_*$ does. Using straight forward mathematics, one obtains:

$$\begin{aligned}\left(\frac{dF^1(\mathrm{x})}{dt}\right)_* &= \frac{\partial F^1}{\partial \mathrm{x}_*} \odot \frac{d\mathrm{x}_*}{dt} \\ &= \frac{\partial F^1}{\partial \mathrm{x}_*} \odot \overbrace{(\mathbf{A}(\mathrm{x}_*) + \mathrm{B}u + O(\delta))}^{d\mathrm{x}_*/dt} \\ &= Ku + \frac{\partial F^1}{\partial \mathrm{x}_*} \odot (\mathbf{A}(\mathrm{x}_*) + O(\delta)),\end{aligned} \tag{9}$$

where O(δ) represents the measurement errors of dx_*/dt and they are assumed small (with zero mean). Thus, Eq.(8a) and Eq.(9) say that U (x_*, u) contains—through dx_*/dt provided by sensor measurements—a first order chemical reaction for species u, and its forward reaction rate (which is at the disposal of the user) is inversely proportional to Δt. It is now totally straight forward to show that QSSA is indeed a valid approximation for *u* in the small Δt limit. Thus Δt should be as small as possible.

To achieve control objective Eq.(5) with M =1for dynamic system Eq.(4), the recommended close loop dynamic control law is:

$$\frac{du}{dt} = \frac{1}{K\Delta t}\left(\frac{\partial F^1}{\partial X_*} \odot \frac{dx_*}{dt} + \frac{F^1(x_*)}{T}\right) \tag{10}$$

It is assumed that good quality sensor measurements of both x_*(t) and dx_*/dt are available to the controller to evaluate the right hand side. The initial condition for u(0) is quite irrelevant—any convenient value will do.

In actual implementation, the real world integrates Eq.(4)—using real world physics—while the "controller" (which is a microprocessor-based black box) integrates Eq.(10) numerically in real time—assuming that good quality real time sensor measurements of both x_* and dx_*/dt are available. Note that the precise numerical values of (small but finite) Δt used is irrelevant to the $F^1(X_*) \approx 0$ control objective (for $t \gg T$). The smallness of Δt is limited by practical hardware considerations of the finite turn-around time of sensor measurements and the software computational time inside the black box.

7. CAN YOU CONTROL X IF YOU DON'T KNOW A(X)?

It is important to note that this dynamics close loop control law Eq.(10) needs no information whatever on A(x), the open-loop dynamics of the original system—provided real time sensor measurements of both x_* and $(dx/dt)_*$ are available. It does need some information on the column vector B—its role here is merely to determine the sign of K. It is very easy to do computer simulations with this dynamics control law to confirm numerically that the same control law (for one specified control objective) can be used for any reasonable (unknown) A(x)—its nonlinearity is quite irrelevant so long as its (open loop) time scale is much larger than the very small Δt.

Hence Eq.(10) is a robust universal dynamic control law.

The exposition above was for the special control objective: $F^1(X) \approx 0$ after $t \gg T$ Generalizat- ion to the more general control objective:

$$\frac{dF^1}{dt} + H(F^1, X; t) \approx 0, \; t \gg \Delta t \tag{11}$$

is completely straight forward—where H (F ^{1}, x; t) is free to be chosen by the users. Just replace F ^{1}(x$_*$)/T in Eq.(10) by the desired $H(F^1, X_*; t)$.

8. Optimal Control

It is well known that optimal control theory usually generates two-point boundary value problems which are more cumbersome to solve than initial value problems. The methodology discussed here can be used to deal with the two-point boundary value issues, and was found successful [4] for a particular simple class of optimal control problems.

9. Concluding Remarks

When $M \geq 1$, B is a $N \times M$ matrix, and there are M control objectives in Eq.(5). The important matrix for control theory is then the $M \times M$ matrix K defined by:

$$K = \frac{\partial F^m}{\partial X} \odot B, m = 1, ..., M \tag{12}$$

When K is non-singular the control problem is said to have unity relative degree [5]—it was so assumed in the M =1case presented earlier. For problems with higher relative degrees (including the M = 1 case with K = 0), sensor measurements of higher time derivatives of x are needed.

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