Slow/fast kinetic scheme with slow diffusion

P. Rouchon
Centre Automatique et Systèmes, École des Mines de Paris
60 Bd. Saint Michel, 75272 Paris cedex 06, FRANCE.
Email: pierre.rouchon@ensmp.fr.

Internal Report A195
March 1997

This short note follows [3]. We consider here slow/fast chemical reactions with additional slow diffusions:

$$\frac{\partial x}{\partial t} = \eta \Delta x + v(x, \epsilon) \tag{1}$$

where $x = (x_1, \ldots, x_n)$ are the concentration profiles, $\Delta = \nabla \cdot \nabla$, ϵ is a small positive parameter, η ($\sim \epsilon$) is the diffusion matrix (symmetric and positive definite) and $v(x, \epsilon)$ corresponds to the kinetic scheme. As in [3], we assume the following slow/fast structure for v [4]:

A1 for $\epsilon = 0$, $\frac{\mathrm{d}x}{\mathrm{d}t} = v(x, 0)$ admits an equilibrium manifold of dimension n_s, $0 < n_s < n$, denoted by Σ_0.

A2 for all $x_0 \in \Sigma_0$, the Jacobian matrix, $\left.\frac{\partial v}{\partial x}\right|_{(x_0,0)}$ admits $n_f = n - n_s$ eigenvalues with a strictly negative real part (the eigenvalues are counted with their multiplicities).

Locally around Σ_0, there exists a partition of x into two groups of components, $x = (x_s, x_f)$, with $\dim(x_s) = n_s$ and $\dim(x_f) = n_f$, such that the projection of Σ_0 on the x_s-coordinates is a local diffeomorphism.

Using the approximation lemma of invariant manifold, and its version for slow/fast systems [2, theorem 5, page 32], we are looking for an asymptotic expansion versus ϵ,

$$x_f = h_0 + h_1 + \ldots,$$

of an invariant slow manifold of (1) closed to Σ_0 (h_0, h_1 , ... depend on the profiles x_s). The slow equations derived here below, and, in particular, the slow diffusion terms, admit a rather unexpected form that has, as far as we known, nether been derived elsewhere.

Following [2, 3], the zero order approximation h_0 is defined by the algebraic equation (in the sequel, we do not recall the dependence versus ϵ)

$$v_f(x_s, h_0) = 0.$$

h_1 is obtained by zeroing of the first order term in

$$\frac{\partial x_f}{\partial t} - \left(\frac{\partial h_0}{\partial x_s} + \frac{\partial h_1}{\partial x_s} + \dots\right)\frac{\partial x_s}{\partial t} = 0.$$

Using the shortcut notations $h_{0,s} = \dfrac{\partial h_0}{\partial x_s}$, ... we have

$$(v_{f,f} - h_{0,s}v_{s,f})h_1 = h_{0,s}(\eta_s \Delta x_s + \eta_{sf}\Delta h_0 + v_s) - \eta_{fs}\Delta x_s - \eta_f \Delta h_0$$

with

$$\eta = \begin{pmatrix} \eta_s & \eta_{sf} \\ \eta_{fs} & \eta_f \end{pmatrix}, \quad \Delta h_0 = h_{0,ss}(\nabla x_s, \nabla x_s) + h_{0,s}\Delta x_s$$

and where the functions are evaluated at $(x_s, x_f = h_0(x_s))$. Using

$$h_{0,s} = -v_{f,f}^{-1} v_{f,s},$$

we obtain the following first order approximation of the slow dynamics:

$$\begin{aligned} \frac{\partial x_s}{\partial t} &= C(x_s, h_0)(\eta_s \Delta x_s + \eta_{sf}\Delta h_0 + v_s(x_s, h_0)) \\ &\quad + E(x_s, h_0)(\eta_{fs}\Delta x_s + \eta_{ff}\Delta h_0) \end{aligned} \tag{2}$$

where the correction matrix C is identical to the one in [3],

$$C = 1 - v_{s,f}(v_{f,f}^2 + v_{f,s}v_{s,f})^{-1} v_{f,s}$$

and E is defined by

$$E = -v_{s,f}(v_{f,f}^2 + v_{f,s}v_{s,f})^{-1} v_{f,f}.$$

When the kinetics v is in Tikhonov normal form, i.e., $v = (\epsilon v_s, v_f)$, we recover (up to second order terms in ϵ) the classical reduced model

$$\frac{\partial x_s}{\partial t} = \eta_s \Delta x_s + \eta_{sf}\Delta h_0 + v_s(x_s, h_0), \quad v_f(x_s, h_0) = 0.$$

We will consider now the case, already pointed out in [1] and considered in [3], of affine fast fibers: the change of coordinates yielding to Tikhonov normal form is linear. Using notation of [3, section 4, equation (18)], (1) admits the special structure

$$\begin{aligned}\frac{\partial x_s}{\partial t} &= \eta_s \Delta x_s + \eta_{sf} \Delta x_f + A_{ss}\ \epsilon \tilde{v}_s(x_s, x_f) + A_{sf}\ \tilde{v}_f(x_s, x_f) \\ \frac{\partial x_f}{\partial t} &= \eta_{fs} \Delta x_s + \eta_f \Delta x_f + A_{fs}\ \epsilon \tilde{v}_s(x_s, x_f) + A_{ff}\ \tilde{v}_f(x_s, x_f).\end{aligned}$$

The change of coordinates

$$(x_s, x_f) \mapsto (\xi = x_s - A_{sf}(A_{ff})^{-1} x_f\ ,\ x_f).$$

leads to

$$\begin{aligned}\frac{\partial \xi}{\partial t} &= (\eta_s - A_{sf} A_{ff}^{-1} \eta_{fs}) \Delta x_s + (\eta_{sf} - A_{sf} A_{ff}^{-1} \eta_{ff}) \Delta x_f \\ &\quad + (A_{ss} - A_{sf}(A_{ff})^{-1} A_{fs})\ \epsilon \tilde{v}_s \\ \frac{\partial x_f}{\partial t} &= \eta_{fs} \Delta x_s + \eta_f \Delta x_f + A_{fs} \epsilon \tilde{v}_s + A_{ff} \tilde{v}_f.\end{aligned}$$

Assuming that eigenvalues of

$$A_{ff} \left(v_{f,f} + A_{sf} A_{ff}^{-1} v_{f,s} \right)$$

have strictly negative real parts, then the quasi-steady-state method can be applied and leads to the following slow system

$$\begin{aligned}\frac{\partial \xi}{\partial t} &= (\eta_s - A_{sf} A_{ff}^{-1} \eta_{fs}) \Delta x_s + (\eta_{sf} - A_{sf} A_{ff}^{-1} \eta_{ff}) \Delta x_f + \dots \\ &\quad \dots + (A_{ss} - A_{sf}(A_{ff})^{-1} A_{fs})\ \epsilon \tilde{v}_s \\ 0 &= \tilde{v}_f.\end{aligned}$$

Pulling back into the original coordinates (x_s, x_f) yields:

$$\begin{aligned}\frac{\partial x_s}{\partial t} &= \left[1 - A_{ss}(A_{ff})^{-1} v_{f,f}^{-1} v_{f,s}\right]^{-1} \Big((\eta_s - A_{sf} A_{ff}^{-1} \eta_{fs}) \Delta x_s + \dots \\ &\quad \dots + (\eta_{sf} - A_{sf} A_{ff}^{-1} \eta_{ff}) \Delta x_f + (A_{ss} - A_{sf}(A_{ff})^{-1} A_{fs})\ \epsilon \tilde{v}_s \Big) \\ 0 &= \tilde{v}_f(x_s, x_f).\end{aligned}$$

Let us finish with a small example derived from [3, equation (1)] by adding slow diffusion:

$$\begin{aligned}\frac{\partial x_1}{\partial t} &= \eta_1 \Delta x_1 - k_1 x_1 + k_2 x_2 - \epsilon k x_1 x_2 \\ \frac{\partial x_2}{\partial t} &= \eta_2 \Delta x_2 + k_1 x_1 - k_2 x_2.\end{aligned} \tag{3}$$

Setting $\dfrac{\partial x_2}{\partial t}$ to zero et neglecting η_2 yields an incorrect slow model (diffusion and kinetics)

$$\frac{\partial x_1}{\partial t} = \eta_1 \Delta x_1 - \epsilon (k k_1 / k_2) x_1^2$$

whereas reduction via the above computations provides the correct slow equation

$$(1 + k_1/k_2)\frac{\partial x_1}{\partial t} = (\eta_1 + \eta_2 k_1/k_2)\Delta x_1 - \epsilon (k k_1/k_2) x_1^2.$$

References

[1] V. Van Breusegem and G. Bastin. A singular perturbation approach to the reduced order dynamical modelling of reaction systems. Technical Report 92.14, CESAME, University of Louvain-la-Neuve, Belgium, 1993.

[2] J. Carr. *Application of Center Manifold Theory.* Springer, 1981.

[3] P. Duchêne and P. Rouchon. Kinetic scheme reduction via geometric singular perturbation techniques. *Chem. Eng. Science*, 51:4661–4672, 1996.

[4] N. Fenichel. Geometric singular perturbation theory for ordinary differential equations. *J. Diff. Equations*, 31:53–98, 1979.