

ME 451C
Winter Quarter, 2004-05
Notes on the Final Exam

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March 20, 2005

Abstract

I am generally happy with your performances in this final exam. The following are notes which I hope you would find useful.

1 The Final Exam Problem

Consider the $N = 2$ reactive-diffusive PDE for $X_1(y, T)$ and $X_2(y, t)$:

$$\frac{\partial X_1}{\partial t} = W_1 + W_2, \quad (1)$$

$$\frac{\partial X_2}{\partial t} = -\gamma W_1 + W_3, \quad (2)$$

where

$$W_1 = \frac{X_2^2 - X_1^2}{\epsilon}, \quad (3)$$

$$W_2 = w_2(X_1, X_2) + D_{11} \frac{\partial^2 X_1}{\partial y^2} + D_{12} \frac{\partial^2 X_2}{\partial y^2}, \quad (4)$$

$$W_3 = w_3(X_1, X_2) + D_{21} \frac{\partial^2 X_1}{\partial y^2} + D_{22} \frac{\partial^2 X_2}{\partial y^2}. \quad (5)$$

Everything had been “intelligently” non-dimensionalized. The parameter γ may be a (differentiable) function of X_1 and X_2 . The domain

of interest is $0 \leq y \leq 1$ and $0 \leq t \leq 10$, and ϵ is some small positive number, most probably less than 0.01, but nobody knows the precise value (the error bar on ϵ is big, but it is quite certain that it is a small number). The chemistry terms are:

$$w_2 = 1 \tag{6}$$

$$w_3 = -2X_1^3. \tag{7}$$

The initial conditions are:

$$X_1(y, t = 0) = c_1(y), \tag{8}$$

$$X_2(y, t = 0) = c_2(y), \tag{9}$$

and $c_1(y) \neq c_2(y)$ and are $O(1)$ entities. The boundary conditions are:

$$X_1(y = 0, t) = b_1(t), \tag{10}$$

$$X_2(y = 0, t) = b_2(t), \tag{11}$$

$$\left(D_{11} \frac{\partial X_1}{\partial y} + D_{12} \frac{\partial X_2}{\partial y} \right) (y = 1, t) = 0, \tag{12}$$

$$\left(D_{21} \frac{\partial X_1}{\partial y} + D_{22} \frac{\partial X_2}{\partial y} \right) (y = 1, t) = 0, \tag{13}$$

and $b_1(t)$ and $b_2(t)$ are $O(1)$ entities.

The diffusion coefficients are:

$$D_{11} = 2D_{22} = D_{12} = D_{21} = \alpha, \tag{14}$$

where α is some $O(1)$ number.

1. Analytically derive the leading order reduced chemistry PDE using the conventional PE approximation—keeping in mind that $\gamma(X_1, X_2)$ is differentiable, $O(1)$ and independent of ϵ .

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The first step of a PE approximation (with M reactions being considered fast) is to find $N - M$ equations which do not have any contribution from the M fast reactions. Here we have $N = 2$ and $M = 1$, so we are looking for one such equation. Adding Eq.(1) times γ and Eq.(2), we have,

$$\gamma \frac{\partial X_1}{\partial t} + \frac{\partial X_2}{\partial t} = \gamma W_2 + W_3. \tag{15}$$

In the reduced chemistry region, W_1 is assumed to be $O(1)$ in the small ϵ limit. Hence, we have from Eq.(3):

$$X_2 = X_1 + \frac{\epsilon W_1}{X_2 + X_1} = X_1 + O(\epsilon). \quad (16)$$

Using this in Eq.(15), we have:

$$\frac{\partial X_1}{\partial t} = \frac{\gamma W_2 + W_3}{1 + \gamma} + O(\epsilon). \quad (17)$$

Or

$$\frac{\partial X_1}{\partial t} = \frac{\gamma(X_1, X_1) - 2X_1^3}{1 + \gamma} + D \frac{\partial^2 X_1}{\partial y^2} + O(\epsilon). \quad (18)$$

where D is shorthand for:

$$D = \frac{\gamma(D_{11} + D_{12}) + (D_{21} + D_{22})}{1 + \gamma}. \quad (19)$$

With the values given, we have $D \approx \alpha(2\gamma + 1.5)/(1 + \gamma)$.

Suppose $N = 173$ and $M = 8$. The above procedure remains valid. But you will agree that the algebra would be prohibitive. More importantly, how do you pick out the fast reactions (from the list of R elementary reactions)?

2. Analytically derive the once-refined (both steps) fast basis vector \mathbf{a}_1^o and \mathbf{b}_o^1 —under the assumption the $W_1 = O(1)$ in the small ϵ limit and γ is not a constant—starting with any choice for the initial guess. Show the fast and slow subspace projection matrices (under the $W_1 = O(1)$ assumption). Derive the CSP reduced chemistry PDEs (valid after the fast mode died) and compare the answer with the answer from (1).

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The Jacobian of the chemistry term is:

$$\mathbf{J} = \begin{bmatrix} \frac{\partial}{\partial X_1}(W_1 + w_2) & \frac{\partial}{\partial X_2}(W_1 + w_2) \\ \frac{\partial}{\partial X_1}(-\gamma W_1 + w_3) & \frac{\partial}{\partial X_2}(-\gamma W_1 + w_3) \end{bmatrix}, \quad (20)$$

Or

$$\mathbf{J} = \begin{bmatrix} -\frac{2X_1}{\epsilon} + \frac{\partial w_2}{\partial X_1} & \frac{2X_2}{\epsilon} + \frac{\partial w_2}{\partial X_2} \\ \frac{2\gamma X_1}{\epsilon} - W_1 \frac{\partial \gamma}{\partial X_1} + \frac{\partial w_3}{\partial X_1} & -\frac{2\gamma X_2}{\epsilon} - W_1 \frac{\partial \gamma}{\partial X_2} + \frac{\partial w_3}{\partial X_2} \end{bmatrix}. \quad (21)$$

To keep the algebra to a minimum, we choose the following as our trial fast basis vectors:

$$\mathbf{a}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \mathbf{b}^1 = [1, 0]. \quad (22)$$

The unrefined fast mode time scale

$$\tau_1^1 = -2X_1(1 + O(\epsilon))/\epsilon.$$

Step one refinement immediately yield

$$\mathbf{b}_o^1 = [1, -X_2/X_1] + O(\epsilon). \quad (23)$$

Using \mathbf{b}_o^1 along with \mathbf{a}_1 , we have the half-refined

$$\tau_{1o}^1 = -2X_1(1 + \gamma X_2/X_1 + O(\epsilon))/\epsilon.$$

Step two refinement now yields:

$$\mathbf{a}_1^o = \frac{1 + O(\epsilon)}{1 + \gamma X_2/X_1} \begin{bmatrix} 1 \\ -\gamma \end{bmatrix} \quad (24)$$

The fast subspace projection matrix \mathbf{Q}_{fast} is (neglecting the $O(\epsilon)$ terms in the refined basis vectors):

$$\mathbf{Q}_{fast} = \mathbf{a}_1^o \mathbf{b}_o^1 = \frac{1}{1 + \gamma X_2/X_1} \begin{bmatrix} 1 & -\frac{X_2}{X_1} \\ -\gamma & \gamma \frac{X_2}{X_1} \end{bmatrix} \quad (25)$$

The slow subspace projection matrix \mathbf{Q}_{slow} is:

$$\mathbf{Q}_{slow} = \mathbf{a}_1^o \mathbf{b}_o^1 = \frac{1}{1 + \gamma X_2/X_1} \begin{bmatrix} \gamma \frac{X_2}{X_1} & \frac{X_2}{X_1} \\ \gamma & 1 \end{bmatrix} \quad (26)$$

It is easily verified, as all of you did, that the reduced chemistry PDE derived using \mathbf{Q}_{slow} is the same as the one previously derived using the PE approximation.

The point I am trying to convey is: if $N = 173$ and $R = 289$ and everything has not been intelligently non-dimensionalized, the CSP methodology can still handle it routinely using computers. Just compute the N eigenvalues of the \mathbf{J} matrix, and decide for yourself, based on your personal choice of the time interval of interest, how many modes are considered fast (there is your M). Once these M fast modes are exhausted, your CSP-derived reduced chemistry PDE is applicable.

3. For $\gamma = \gamma(X_1, X_2)$ not being a constant, there is no approximate conserved scalar in general. Assume $\gamma = 1 + X_1 X_2$. Numerically compute the initial conditions for the reduced chemistry PDE for $c_1(y) = 1$, $c_2(y) = 0$.

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It is important to note that the initial condition for the reduced chemistry PDE must honor $X_1 = X_2 + O(\epsilon)$. Since $c_1(y) \neq c_2(y)$, there is a thin initial transient layer. And I cooked up a problem which has no approximate conserved scalars.

Everybody got this problem right.

4. Numerically compute the reduced chemistry ODE solution for the pure chemistry case for $\alpha = 0$, $\gamma = 1 + X_1 X_2$, $c_1(y) = 1$, $c_2(y) = 0$. We are interested for $0 \leq t \leq 10$.

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Everybody got this problem right.

5. Analytically derived the governing equations in the thin layer adjacent to $y = 0$ when $b_1(t) \neq b_2(t)$, and provide the appropriate boundary conditions (particularly at the “edge” of this thin layer). You can use classical asymptotic analysis, or CSP, or any good mathematics. Again, assumed $\gamma = \gamma(X_1, X_2)$ so that there is no approximate conserved scalars. You don’t need to do any computation, but need to provide a correctly posed mathematical problem for this layer.

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Everybody got the correct governing ODEs in the thin diffusion layer adjacent to the $y = 0$ boundary. The issue is how to come up with the “appropriate” boundary conditions at the edge of this layer. I cooked up a problem that has no approximate conserved scalars.

Let $\xi = y/\sqrt{\epsilon}$ where y is the original spatial coordinate. In the reduced chemistry region, we have

$$X_1 = X_2 + O(\epsilon) = \check{X}(y, t; \epsilon) + O(\epsilon). \quad (27)$$

In the thin side boundary layer ($\xi = O(1)$), we have:

$$X_1 = \hat{X}_1(\xi, t) + O(\epsilon), \quad X_2 = \hat{X}_2(\xi, t) + O(\epsilon). \quad (28)$$

What we want, in English, is this:

The thin layer solution as it approaches the edge of the thin layer should agree with the solution in the reduced chemistry region as it approaches the edge of the thin layer.

Writing this physical idea in terms of mathematics, we have:

$$\lim_{y \rightarrow 0} \check{X}_1(y, t) \leftrightarrow \lim_{\xi \rightarrow \infty} \hat{X}(\xi, t), \quad (29)$$

$$\lim_{y \rightarrow 0} \check{X}_2(y, t) \leftrightarrow \lim_{\xi \rightarrow \infty} \hat{X}(\xi, t) \quad (30)$$

Differentiating with respect to y , we have:

$$\lim_{y \rightarrow 0} \frac{\partial \check{X}_1(y, t)}{\partial y} \leftrightarrow \frac{1}{\sqrt{\epsilon}} \left(\lim_{\xi \rightarrow \infty} \frac{\partial \hat{X}(\xi, t)}{\partial \xi} \right), \quad (31)$$

$$\lim_{y \rightarrow 0} \frac{\partial \check{X}_2(y, t)}{\partial y} \leftrightarrow \frac{1}{\sqrt{\epsilon}} \left(\lim_{\xi \rightarrow \infty} \frac{\partial \hat{X}(\xi, t)}{\partial \xi} \right) \quad (32)$$

The major conclusion out of this is:

$$\lim_{\xi \rightarrow \infty} \frac{\partial \hat{X}_1}{\partial \xi} = O(\epsilon) \approx 0, \quad (33)$$

$$\lim_{\xi \rightarrow \infty} \frac{\partial \hat{X}_2}{\partial \xi} = O(\epsilon) \approx 0. \quad (34)$$

In English, this simply says: the thin layer solutions \hat{X}_1 and \hat{X}_2 approach constants (approximately) at the edge when ϵ is small. The reason is physically clear. If the ξ derivatives at the edge of the layer is finite, then the magnitude of the y derivatives would be huge (singular!) in the limit of small ϵ . But the leading order small ϵ solution in the reduced chemistry region is independent of ϵ .

After the proper boundary conditions are found, the problem is a two-point ODE boundary value problem. In general, this requires iterations. An interesting idea is to retain the time derivative term and proceed to solve numerically the parabolic PDEs with arbitrary initial condition along with the above derived boundary conditions (treating b_1 and b_2 as constants). When “steady state” arrives for the PDEs, you have got what you were looking for (for that pair of constant b_1 and b_2). The “time history” of this calculation is physically meaningless—they are merely the “iterants” for finding the solutions of your ODEs.

6. We are interested in the solution for the chemistry-diffusion coupled (reduced chemistry— $\epsilon \ll 1$) PDE. Use $\alpha = 1$, $\gamma = 2$, $c_1(y) = 1$, $c_2(y) = 0$ and $b_1(t) = b_2(t) = 0.1$. The time range of interest is $0 < t < 10$.

From what you have learn from the above studies, provide some sketches to show what the reduced chemistry solutions should look like qualitatively.

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After the initial transient, we have initially $X_1 \approx X_2 = 0.667$ (independent of y) as initial condition for the reduced chemistry region, and then it evolves with time with a y dependence as a consequence of the boundary condition ($X_1 = X_2 = 0.1$) for the parabolic PDE at the lower wall (for this particular boundary condition, reduced chemistry is good all the way to the wall). A thick diffusion boundary layer adjacent to the lower wall develops, and its thickness grows parabolically. Outside this diffusion layer, the chemistry term says everybody approaches $4^{-1/3} \approx 0.630$. For some $t = O(1)$, this diffusion layer will hit the top boundary and span the whole physical domain. Eventually, some steady-state distribution will be approached—governed by the ODEs obtained by dropping the time derivative term.

Again, I want to thank all of you for attending the course. I enjoyed it, and I wish the best for all your endeavors.