Manifold Reduction

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1 Computational Singular Perturbation Basics

1.1 The Projected System

Consider the dynamical system:

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{F}(\boldsymbol{x}) \tag{1a}$$

$$\boldsymbol{x}(0) = \boldsymbol{x}_\circ \tag{1b}$$

where $\boldsymbol{x} \in \mathbb{R}^N$. When the system develops a broad separation of time scales, the source term can be separated into slow and fast lower-dimensional modes:

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{F}(\boldsymbol{x}) \tag{2a}$$

$$= \boldsymbol{F}_s(\boldsymbol{x}) + \boldsymbol{F}_f(\boldsymbol{x}) \tag{2b}$$

$$= \mathbf{V}_s(\boldsymbol{x}) \cdot \boldsymbol{\varphi}_s + \mathbf{V}_f(\boldsymbol{x}) \cdot \boldsymbol{\varphi}_f \tag{2c}$$

where $\boldsymbol{\varphi}_s \in \mathbb{R}^{N_s}$, $\boldsymbol{\varphi}_f \in \mathbb{R}^{N_f}$, $N_s + N_f = N$, and:

$$\boldsymbol{\varphi}_s(\boldsymbol{x}) = \mathbf{U}_s(\boldsymbol{x}) \cdot \boldsymbol{F}(\boldsymbol{x}), \tag{3a}$$

$$\boldsymbol{\varphi}_f(\boldsymbol{x}) = \mathbf{U}_f(\boldsymbol{x}) \cdot \boldsymbol{F}(\boldsymbol{x}) \tag{3b}$$

such that

$$\mathbf{U}_s(\boldsymbol{x}) \cdot \mathbf{V}_s(\boldsymbol{x}) = \mathbf{I}_{ss}, \tag{4a}$$

$$\mathbf{U}_f(\boldsymbol{x}) \cdot \mathbf{V}_f(\boldsymbol{x}) = \mathbf{I}_{ff}. \tag{4b}$$

A typical choice for the basis vectors is the eigendecomposition of the Jacobian $\mathbf{J} = \partial_{\boldsymbol{x}} \boldsymbol{F}$, i.e.

$$\mathbf{J} = \begin{pmatrix} \mathbf{V}_s & \mathbf{V}_f \end{pmatrix} \begin{pmatrix} \boldsymbol{\Lambda}_{ss} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Lambda}_{ff} \end{pmatrix} \begin{pmatrix} \mathbf{U}_s \\ \mathbf{U}_f \end{pmatrix}. \tag{5}$$

The fast modes will quickly exhaust, imposing the following algebraic constraint on the dynamics of the system:

$$\boldsymbol{\varphi}_f(\boldsymbol{x}) = \mathbf{U}_f(\boldsymbol{x}) \cdot \boldsymbol{F}(\boldsymbol{x}) = \mathbf{0}. \tag{6}$$

Using the above in (1), we arrive at a system where the dynamics have been projected onto the slow invariant manifold (SIM):

$$\begin{aligned} \frac{d\boldsymbol{x}}{dt} &= \boldsymbol{F}_s(\boldsymbol{x}) \\ &= \boldsymbol{F}(\boldsymbol{x}) - \boldsymbol{F}_f(\boldsymbol{x}) \\ &= \boldsymbol{F}(\boldsymbol{x}) - \mathbf{V}_f(\boldsymbol{x}) \cdot \boldsymbol{\varphi}_f \\ &= \boldsymbol{F}(\boldsymbol{x}) - \mathbf{V}_f(\boldsymbol{x}) \mathbf{U}_f(\boldsymbol{x}) \cdot \boldsymbol{F}(\boldsymbol{x}) \\ &= [\mathbf{I} - \mathbf{V}_f(\boldsymbol{x}) \mathbf{U}_f(\boldsymbol{x})] \cdot \boldsymbol{F}(\boldsymbol{x}) \\ &= \mathbf{P}(\boldsymbol{x}) \cdot \boldsymbol{F}(\boldsymbol{x}), \end{aligned} \tag{7}$$

i.e. the projector $\mathbf{P}(\boldsymbol{x})$ filters the source term's fast components.

1.2 Estimating the Distance to the SIM

We might find that the state $\boldsymbol{x}^*$ is not on the manifold. We therefore seek a nearby state $\boldsymbol{x}^* + \Delta\boldsymbol{x}$ that satisfies the algebraic constraint in eq. (6). To leading order and ignoring the rotation of the basis vectors, this is:

$$\begin{aligned}\boldsymbol{\varphi}_f(\boldsymbol{x}^* + \Delta\boldsymbol{x}) &\approx \boldsymbol{\varphi}_f(\boldsymbol{x}^*) + \nabla\boldsymbol{\varphi}_f|_{\boldsymbol{x}^*} \cdot \Delta\boldsymbol{x} \\ &= [\mathbf{U}_f \cdot \boldsymbol{F}]\,|_{\boldsymbol{x}^*} + [\mathbf{U}_f\mathbf{J}]\,|_{\boldsymbol{x}^*} \cdot \Delta\boldsymbol{x} \\ &= [\mathbf{U}_f \cdot \boldsymbol{F}]\,|_{\boldsymbol{x}^*} + [\mathbf{U}_f\mathbf{J}\mathbf{V}_f\mathbf{U}_f]\,|_{\boldsymbol{x}^*} \cdot \Delta\boldsymbol{x} \\ &= \mathbf{0}\end{aligned} \tag{8}$$

which leads to

$$\mathbf{U}_f|_{\boldsymbol{x}^*} \cdot \Delta\boldsymbol{x} = -\left[\left(\mathbf{U}_f\mathbf{J}\mathbf{V}_f\right)^{-1}\mathbf{U}_f \cdot \boldsymbol{F}\right]\Big|_{\boldsymbol{x}^*} \tag{9}$$

and using the orthogonal complement of $\mathbf{U}_f$:

$$\Delta\boldsymbol{x}(\boldsymbol{x}^*) = -\left\{\left[\mathbf{V}_f\left(\mathbf{U}_f\mathbf{J}\mathbf{V}_f\right)^{-1}\mathbf{U}_f\right] \cdot \boldsymbol{F}\right\}\Big|_{\boldsymbol{x}^*}. \tag{10}$$

Note that, since $\mathbf{V}_f$ and $\mathbf{U}_f$ are chosen to be the fastest eigenmodes of the Jacobian $\mathbf{J}$, the above becomes:

$$\begin{aligned}\Delta\boldsymbol{x}(\boldsymbol{x}^*) &= -\left[\left(\mathbf{V}_f\boldsymbol{\Lambda}_{ff}^{-1}\mathbf{U}_f\right) \cdot \boldsymbol{F}\right]\Big|_{\boldsymbol{x}^*} \\ &= -\mathbf{R}(\boldsymbol{x}^*) \cdot \boldsymbol{F}(\boldsymbol{x}^*).\end{aligned} \tag{11}$$

1.3 Integrating the Projected System

The system is advanced from state $\boldsymbol{x}^n$ at time instant t^n to state $\boldsymbol{x}^{n+1}$ at $t^{n+1} = t^n + \Delta t$ in a two-stage process. The first stage advances the projected system using a standard explicit time integrator to an intermediate state $\boldsymbol{x}^*$. The second stage restores the state of the system back to the SIM, which has drifted away during the previous stage due to the choice of eigenvectors as basis of the slow/fast subspaces, which neglects coupling between slow and fast modes.

1. Explicit integration:
$$\boldsymbol{x}^* = \boldsymbol{x}^n + \int_{t^n}^{t^{n+1}} \mathbf{P}(\boldsymbol{x}) \cdot \boldsymbol{F}(\boldsymbol{x})dt \tag{12}$$

2. Fast correction:
$$\boldsymbol{x}^{n+1} = \boldsymbol{x}^* - \mathbf{R}(\boldsymbol{x}^*) \cdot \boldsymbol{F}(\boldsymbol{x}^*) \tag{13}$$

1.4 The Slow System

Even though the projected system is no longer stiff, it is still of the same size as the original system. A reduced system can be obtained by focusing only on slow modes only instead. First, consider the state of the system $\boldsymbol{x}^n$ at a time instant t^n. Any changes to the state vector within a small time interval $\left[t^n, t^{n+1}\right]$ can be decomposed into fast and slow components. Therefore, the state of the system at a time instant $t = t^n + \tau$ can be written as:

$$\boldsymbol{x}(t) = \boldsymbol{x}^n + \mathbf{V}_s(\tau) \cdot \boldsymbol{\vartheta}_s(\tau) + \mathbf{V}_f(\tau) \cdot \boldsymbol{\vartheta}_f(\tau) \tag{14}$$

where $\tau \in (0, \Delta t]$ and $\Delta t = t^{n+1} - t^n$. Now, we assume the fast modes have exhausted, i.e.

$$\boldsymbol{\vartheta}_f = \mathbf{0}. \tag{15}$$

Furthermore, the rotation of the basis vectors can be deemed negligible, i.e.

$$\mathbf{V}_s(\tau) = \mathbf{V}_s^n, \tag{16a}$$
$$\mathbf{V}_f(\tau) = \mathbf{V}_f^n, \tag{16b}$$
$$\mathbf{U}_s(\tau) = \mathbf{U}_s^n, \tag{16c}$$
$$\mathbf{U}_f(\tau) = \mathbf{U}_f^n. \tag{16d}$$

With these assumptions in mind, we can arrive at the following system of differential equations for the slow modes:

$$\frac{d\boldsymbol{\vartheta}_s}{d\tau} = \mathbf{U}_s^n \cdot \boldsymbol{F}(\boldsymbol{x}^n + \mathbf{V}_s^n \cdot \boldsymbol{\vartheta}_s) \tag{17a}$$
$$\boldsymbol{\vartheta}_s(0) = \mathbf{0} \tag{17b}$$

1.5 Integrating the Slow System

The system is advanced from state $\boldsymbol{x}^n$ at time instant t^n to state $\boldsymbol{x}^{n+1}$ at $t^{n+1} = t^n + \Delta t$ in a three-stage process. The first stage advances the reduced slow system using a standard explicit time integrator to an intermediate state $\boldsymbol{\vartheta}_s^*$. During the second stage, the intermediate state of the original system is reconstructed from the slow modes. The last stage restores the state of the system back to the SIM, which has drifted away during the previous stage due to the choice of eigenvectors as basis of the slow/fast subspaces, which neglects coupling between slow and fast modes.

1. Explicit integration:
$$\boldsymbol{\vartheta}_s^* = \int_{t^n}^{t^{n+1}} \mathbf{U}_s^n \cdot \boldsymbol{F}(\boldsymbol{x}^n + \mathbf{V}_s^n \cdot \boldsymbol{\vartheta}_s) dt \tag{18}$$

2. Reconstruction:
$$\boldsymbol{x}^* = \boldsymbol{x}^n + \mathbf{V}_s^n \cdot \boldsymbol{\vartheta}_s^* \tag{19}$$

3. Fast correction:
$$\boldsymbol{x}^{n+1} = \boldsymbol{x}^* - \mathbf{R}(\boldsymbol{x}^*) \cdot \boldsymbol{F}(\boldsymbol{x}^*) \tag{20}$$

1.6 Chemical Kinetics

As an example, consider the adiabatic, isobaric, homogeneous combustion of an ideal gas mixture with M species. The evolution of the mixture is described by the following system of differential equations:

$$\frac{d\boldsymbol{z}}{dt} = \frac{1}{\rho}\dot{\boldsymbol{\omega}} \tag{21a}$$

$$\frac{dT}{dt} = -\frac{1}{\rho c_p}\boldsymbol{h}^T\dot{\boldsymbol{\omega}} \tag{21b}$$

where $\boldsymbol{z}$ is the vector of species' specific moles, T is the mixture's temperature, ρ and c_p its density and specific heat at constant pressure respectively, $\boldsymbol{h}$ is the vector of species' molar enthalpies and $\dot{\boldsymbol{\omega}}$ is the species' net molar production rate. These equations are supplemented by the ideal gas equation of state:

$$pW = \rho RT \tag{22}$$

where R is the universal gas constant and the mean molecular weight is given by:

$$W = \left[\sum_{i=1}^{M} z_i\right]^{-1}. \tag{23}$$

The set of chemical processes chosen to model $\dot{\boldsymbol{\omega}}$ is the San Diego mechanism, which consists of 9 species and 21 reversible reactions. The system was evolved in time using a time integrator based on the CSP concepts described above. Results are shown in 1.

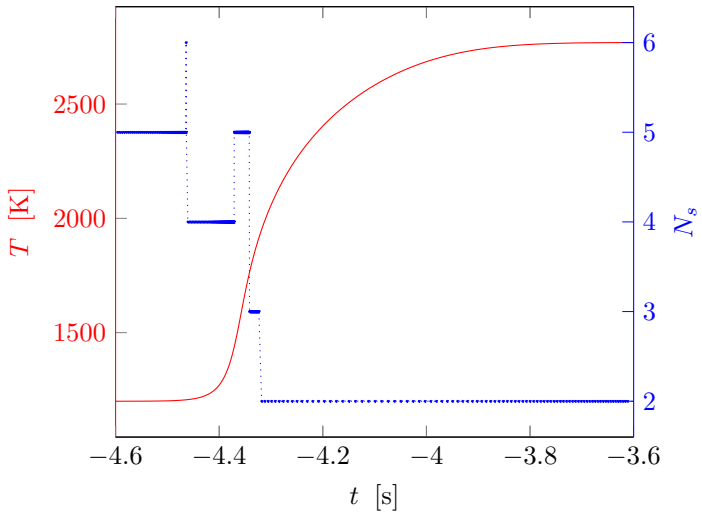

Figure 1: Temperature T and dimension of the slow subspace N_s against time. Only two modes, corresponding to temperature and a composition progress variable, are active after ignition.