Computational Singular Perturbation for Chemical Kinetics

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Abstract

Many interesting problems are governed by a system of ODEs:

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y};\mathbf{k}) \tag{1}$$

where $\mathbf{y}$ and $\mathbf{g}$) are N-dimensional column vectors, $\mathbf{k}$ is a vector of K elements, and t is time. The $\mathbf{y}$ vector is the unknown variable, while $\mathbf{g}(\mathbf{y};\mathbf{k})$ is explicitly given (and $\mathbf{k}$ represents all the parameters of the problem). Usually, everything is dimensional. When the problem is properly non-dimensionalized and a small dimensionless parameter ϵ is found, a skillful applied mathematician can do *paper and pencil perturbation analysis* (by exploiting the smallness of ϵ) to produce useful and insightful approximate theories.

I shall present the methodology of *Computational Singular Perturbation* (CSP) *which does not require non-dimensionalization of variables and parameters* and can provide—using numerical computation—useful and insightful approximate theories for massively complex problems (which are beyond the reach of paper and pencil analysis). Specifically, I shall present some very recent *new* CSP results on reacting flow problems involving complex chemical kinetics. The generality of the CSP methodology will be emphasized.

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