Working Notes on a Reaction Diffusion Model: a Finite Element Formulation http://people.sc.fsu.edu/∼jburkardt/presentations/... ...fem_neumann.pdf

Jeffrey Borggaard, John Burkardt, John A. Burns & Eugene M. Cliff

28 October 2008

1 Motivation

We describe an algorithm and some simple computer codes for a reaction-diffusion problem in one space dimension

2 Reaction-Diffusion Problem

We consider a one-dimensional reaction/diffusion model

$$w_t(t,\xi) = w_{\xi\xi}(t,\xi) + N\left(w(t,\xi)\right), \quad 0 \le \xi \le 1, \quad 0 < t \le T \ , \tag{1}$$

with homogeneous Neumann boundary conditions

$$w_x(t,0) = 0, \qquad w_x(t,1) = 0 \ , \tag{2}$$

and prescribed initial condition

$$w(0,\xi) = f(\xi) \ . \tag{3}$$

The (nonlinear) functions N and f are given.

3 Finite Element Formulation

3.1 Weak Formulation

The weak formulation of the problem (1-3) is constructed by the usual integration-by-parts procedure:

$$\begin{aligned}\int_0^1 w_t(t,\xi)\psi(\xi)\mathrm{d}\xi &= \int_0^1 w_{\xi\xi}(t,\xi)\psi(\xi)\mathrm{d}\xi + \int_0^1 N\left(w_\xi(t,\xi)\right)\psi(\xi)\mathrm{d}\xi \\ &= w_\xi(t,\xi)\psi(\xi)|_0^1 - \int_0^1 w_\xi(t,\xi)\psi_\xi(\xi)\mathrm{d}\xi + \int_0^1 N\left(w_\xi(t,\xi)\right)\psi(\xi)\mathrm{d}\xi \\ &= -\int_0^1 w_\xi(t,\xi)\psi_\xi(\xi)\mathrm{d}\xi + \int_0^1 N\left(w_\xi(t,\xi)\right)\psi(\xi)\mathrm{d}\xi\ .\end{aligned}$$

4 Galerkin Approximation

The solution $w(t,\xi)$ is approximated by a finite sum of basis functions, *viz*: $\mathcal{B} = \{\phi_1, \phi_2, ..., \phi_m\}$

$$w(t,\xi) \approx \sum_{\jmath=1}^{m} w_\jmath^m(t)\ \phi_\jmath(\xi)\ .$$

The basis functions are used as test functions in the weak form to obtain

$$\sum_\jmath \langle \phi_\jmath, \phi_\imath \rangle \dot{w}_\jmath^m = -\sum_\jmath \langle \phi'_\jmath, \phi'_\imath \rangle\, w_\jmath^m(t) + \int_0^1 N\left(\sum_{\jmath=1}^{m} w_\jmath^m(t)\ \phi_\jmath(\xi)\right)\phi_\imath(\xi)\,\mathrm{d}\xi\ , \quad \imath = 1,2,...,m \tag{4}$$

The term on the left and the first term on the right can be conveniently written in matrix terminology as

$$M\dot{w}^m(t) \quad \text{and} \quad Kw^m(t)\ , \quad \text{respectively}\ ,$$

where $w^m(t)$ is the column vector $(w_1^m(t), w_2^m(t), ..., w_m^m(t))^T$. The $m \times m$ matrices M and K are given by

$$M_{\imath\jmath} = \langle \phi_\imath, \phi_\jmath \rangle\ , \qquad K_{\imath\jmath} = \langle \phi'_\imath, \phi'_\jmath \rangle\ .$$

The initial condition for the approximation follows from

$$\sum_\jmath w_\jmath^m(0)\phi_\jmath(\xi) \approx w_0(\xi) \implies Mw^m(0) = \langle \phi, w_0 \rangle\ . \tag{5}$$

It remains to characterize the nonlinear term $N(\cdot)$.

4.1 Linear Splines

As a specific instance of these ideas consider the case wherein the basis ($\mathcal{B}$) consists of *hat functions*. More precisely, we consider a uniform grid of $n+1$ points on the interval $[0,1]$ and define $\phi_\imath$ as the continuous, piecewise linear function that is unity at $\xi_\imath = \frac{(\imath-1)}{n}$, $\imath = 1, 2, ..., n+1$ and zero at the other grid points. Simple calculations show that:

$$M = \frac{1}{6n} \begin{bmatrix} 2 & 1 & 0 & \dots & 0 & 0 \\ 1 & 4 & \ddots & & 0 & 0 \\ 0 & \ddots & \ddots & & \vdots & \vdots \\ \vdots & & & & \ddots & 0 \\ 0 & & & \ddots & 4 & 1 \\ 0 & \dots & & \dots & 1 & 2 \end{bmatrix}, \tag{6}$$

$$K = n \begin{bmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 & \ddots & & 0 & 0 \\ 0 & \ddots & \ddots & & \vdots & \vdots \\ \vdots & & & & \ddots & 0 \\ 0 & & & \ddots & 2 & -1 \\ 0 & \dots & & \dots & -1 & 1 \end{bmatrix} \tag{7}$$

4.2 Nonlinear Term

There are several methods for approximating the nonlinear term in the model. We begin by considering some specific nonlinearities and carry out the calculations indicated in Equation (4).

4.2.1 Quadratic

First consider a quadratic nonlinearity

$$N^{[2]}(w) = w^2 \ .$$

In this case we are able to exploit the local support of our basis functions. Note that for any $\imath = 1, ..., n$, the basis function $\phi_\imath$ is supported on the interval $[\xi_{\imath-1}, \xi_{\imath+1}]$. Thus we define

$$\mathcal{N}_\imath^{[2]}(w) \triangleq \int_0^1 \left(\sum_{\jmath=1}^{n} w_\jmath \, \phi_\jmath(\xi) \right)^2 \phi_\imath(\xi) \, \mathrm{d}\xi$$

$$\langle (w_{\imath-1}\phi_{\imath-1}(\xi) + w_\imath \phi_\imath(\xi) + w_{\imath+1}\phi_{\imath+1}(\xi))^2 , \ \phi_\imath(\xi) \rangle$$

$$= w_{\imath-1}^2 \langle \phi_{\imath-1}^2, \phi_\imath \rangle + w_\imath^2 \langle \phi_\imath^2, \phi_\imath \rangle + w_{\imath+1}^2 \langle \phi_{\imath+1}^2, \phi_\imath \rangle$$

$$+ \, 2 \, w_{\imath-1} w_\imath \langle \phi_{\imath-1}\phi_\imath, \phi_\imath \rangle + 2 \, w_{\imath-1} w_{\imath+1} \langle \phi_{\imath-1}\phi_{\imath+1}, \phi_\imath \rangle + 2 \, w_\imath w_{\imath+1} \langle \phi_\imath \phi_{\imath+1}, \phi_\imath \rangle \ .$$

Calculations with the linear spline basis functions lead to

$$\begin{aligned}
\langle \phi_\imath^2, \phi_\imath \rangle &= \frac{1}{2\,n} \\
\langle \phi_{\imath-1}\phi_{\imath+1}, \phi_\imath \rangle &= 0 \\
\langle \phi_{\imath-1}\phi_{\imath-1}, \phi_\imath \rangle &= \frac{1}{12\,n} \\
\langle \phi_{\imath+1}\phi_{\imath+1}, \phi_\imath \rangle &= \frac{1}{12\,n} \\
\langle \phi_{\imath-1}\phi_\imath, \phi_\imath \rangle &= \frac{1}{12\,n} \\
\langle \phi_\imath \phi_{\imath+1}, \phi_\imath \rangle &= \frac{1}{12\,n} \ ,
\end{aligned}$$

so that

$$\mathcal{N}_\imath^{[2]}(w) = \left[(w_{\imath-1} + w_\imath)^2 + 4\, w_\imath^2 + (w_{\imath+1} + w_\imath)^2 \right] / (12\, n) \ , \quad \imath = 2, ..., n-1 \ . \tag{8}$$

Since ϕ_1 (and ϕ_n) has support on a single interval we have:

$$\langle \phi_1^2, \phi_1 \rangle = \frac{1}{4n} \ , \quad \text{and} \quad \langle \phi_1 \phi_2, \phi_1 \rangle = \langle \phi_2^2, \phi_1 \rangle = \frac{1}{12n} \ ,$$

along with

$$\langle \phi_n^2, \phi_n \rangle = \frac{1}{4n} \ , \quad \text{and} \quad \langle \phi_n \phi_{n-1}, \phi_n \rangle = \langle \phi_{n-1}^2, \phi_n \rangle = \frac{1}{12n} \ ,$$

so that

$$\mathcal{N}_1^{[2]}(w)) = \left[2\, w_1^2 + (w_1 + w_2)^2 \right] / (12\, n) \tag{9}$$

$$\mathcal{N}_n^{[2]}(w)) = \left[(w_{n-1} + w_n)^2 + 2\, w_n^2 \right] / (12\, n) \ . \tag{10}$$

4.2.2 Cubic

For a cubic nonlinearity similar analysis leads to

$$\begin{aligned}
\langle \phi_{\imath-1}^3, \phi_\imath \rangle &= \frac{1}{20\,n} \\
\langle \phi_{\imath}^3, \phi_\imath \rangle &= \frac{2}{5\,n} \\
\langle \phi_{\imath+1}^3, \phi_\imath \rangle &= \frac{1}{20\,n} \\
\langle \phi_{\imath-1}^2 \phi_\imath, \phi_\imath \rangle &= \frac{1}{30\,n} \\
\langle \phi_{\imath-1}^2 \phi_{\imath+1}, \phi_\imath \rangle &= 0 \\
\langle \phi_{\imath-1} \phi_\imath^2, \phi_\imath \rangle &= \frac{1}{20\,n} \\
\langle \phi_{\imath-1} \phi_{\imath+1}^2, \phi_\imath \rangle &= 0 \\
\langle \phi_\imath^2 \phi_{\imath+1}, \phi_\imath \rangle &= \frac{1}{20\,n} \\
\langle \phi_\imath \phi_{\imath+1}^2, \phi_\imath \rangle &= \frac{1}{30\,n} \\
\langle \phi_{\imath-1} \phi_\imath \phi_{\imath+1}, \phi_\imath \rangle &= 0 \,,
\end{aligned}$$

so that

$$\mathcal{N}_\imath^{[3]}(w) = \left[(w_{\imath-1} + w_\imath)^3 + 6\,w_\imath^3 + (w_\imath + w_{\imath+1})^3 - w_\imath (w_{\imath-1}^2 + w_{\imath+1}^2) \right] / (20\,n) \,, \qquad \imath = 2, ..., n-1 \,. \quad (11)$$

Here again, since ϕ_1 (and ϕ_n) has support on a single interval we have:

$$\mathcal{N}_1^{[3]}(w)) = \left[3\,w_1^3 + (w_1 + w_2)^3 - w_1 w_2^2 \right] / (20\,n) \quad (12)$$

$$\mathcal{N}_n^{[3]}(w)) = \left[(w_{n-1} + w_n)^3 + 3\,w_n^3 - w_{n-1}^2 w_n \right] / (20\,n) \,. \quad (13)$$

4.2.3 Constant and Linear

For completeness the expressions for constant and linear forcing terms are, respectively

$$\mathcal{N}^{[0]}(w) = \left(\frac{1}{n} \right) \begin{bmatrix} 1 \\ 2 \\ \vdots \\ 2 \\ 1 \end{bmatrix} \,, \quad (14)$$

and

$$\mathcal{N}^{[1]}(w) = M\,w \ , \tag{15}$$

where M is the mass matrix.

Clearly, this direct analytical approach becomes tedious for high-order nonlinearities and is not practical on non-uniform meshes, nor in higher space dimensions.

5 ODE Model

In summary, using finite elements (specifically, linear splines) the reaction-diffusion model (1 - 3) is approximated by the ordinary-differential equation system:

$$M\dot{w}(t) = -Kw(t) + \sum_{\jmath=0}^{3} c_\jmath \mathcal{N}^{[\jmath]}\left(w(t)\right) \ , \tag{16}$$

with initial condition given by (5). Representations for the nonlinear (through 3^{rd}-order) terms have been given in Equations (8 - 15). The resulting ODE system (16) with initial condition (5) can be *solved* numerically in a variety of ways.

5.1 Numerical Results

The ODE model (16) was implemented in a MATLAB code. After brief experimentation the initial-value problem was solved using the implicit solver `ode15s`. Our numerical results use the initial condition

$$w_0(x) = \sin(\pi\, x) \ .$$

Our first problem uses the nonlinear reaction term

$$N(w) = -w\left(1 - w^2\right) \ ,$$

and was solved using spatial discretization $n = 32$ on the time interval $[0, 4]$. Initial results are shown in Figures 1. Note that the initial *sine* distribution quickly evolves to a (seemingly)uniform one and then uniformly decays to zero. To better display the initial response a second run was made on the time interval $[0, 0.1]$ and is shown in Figure 2. It seems that by $t = 0.1$ the spatial distribution is nearly uniform at $w \approx 0.6$. With w uniform in space, the associated ODE for the time evolution is

$$\frac{\mathrm{d}\,w}{\mathrm{d}t} = -w(t)\left(1 - w(t)^2\right) \ ,$$

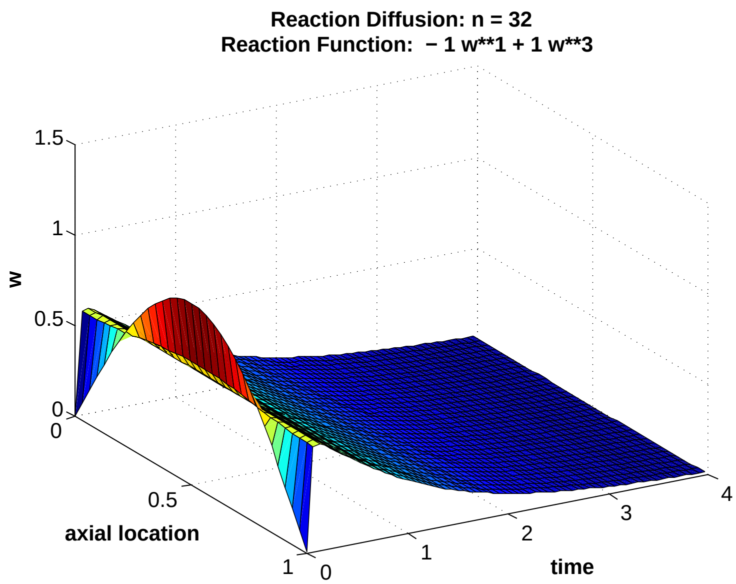

Figure 1: Time/space evolution $N(w) = -w(1-w^2),\ w(0,x) = \sin(\pi\, x)$

with solution characterized by

$$w^2(t) = \frac{\exp\left(2\,(c-t)\right)}{1+\exp\left(2\,(c-t)\right)}\ , \quad \text{where} \quad c = t_0 + \frac{1}{2}\log\left(\frac{w_0^2}{1-w_0^2}\right)\ . \qquad (17)$$

Figure 3 displays the decay of the (square of) the L_2 norm of the finite-element solution, along with the prediction from Equation (17).

A second problem uses the nonlinear reaction term

$$N(w) = w\left(1-w^2\right)\ ,$$

and was solved using spatial discretization $n = 32$ on the time interval $[0, 4]$. Results are shown in Figures 4 and 5. In this case the fem solution approaches a uniform constant at $w \approx 1$.

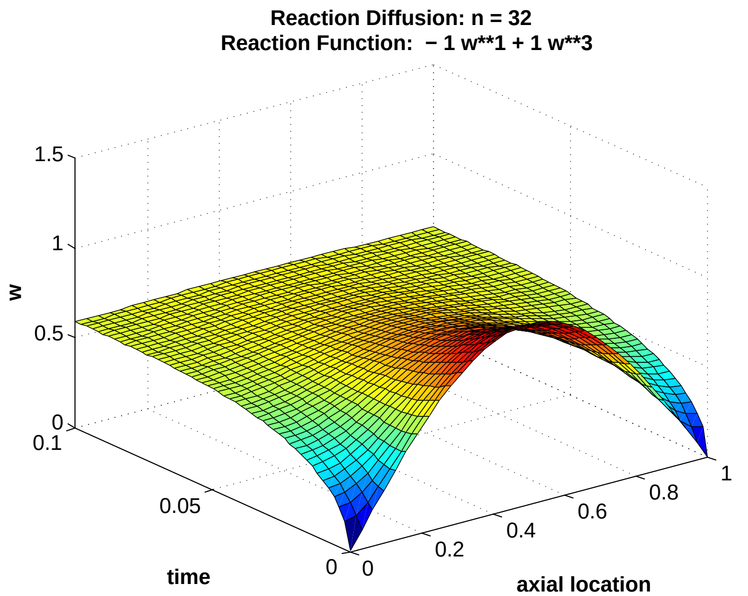

Figure 2: Initial time/space evolution $N(w) = -w(1 - w^2)$, $w(0, x) = \sin(\pi\, x)$

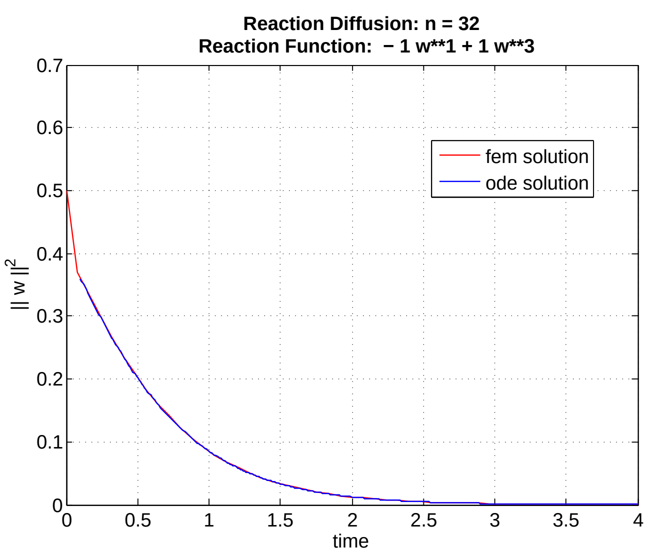

Figure 3: Evolution of the norm: $N(w) = -w(1 - w^2)$, $w(0, x) = \sin(\pi\, x)$

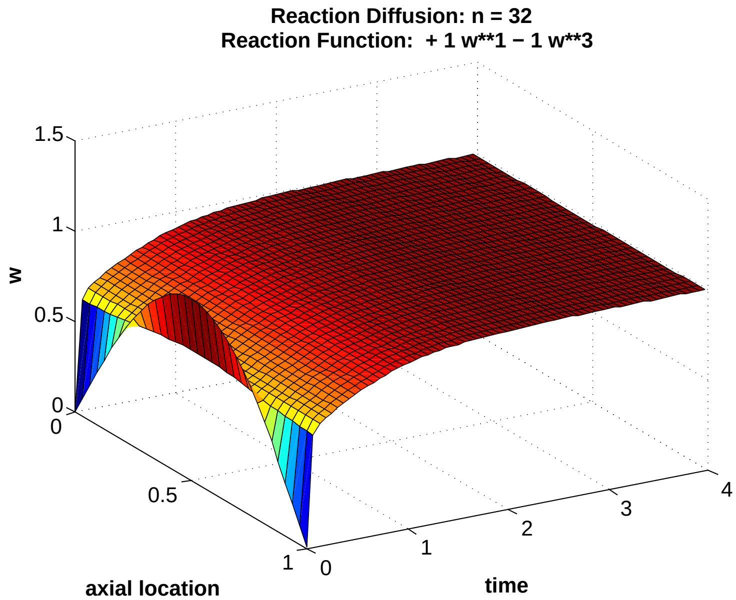

Figure 4: Time/space evolution $N(w) = w(1 - w^2),\ w(0, x) = \sin(\pi\, x)$

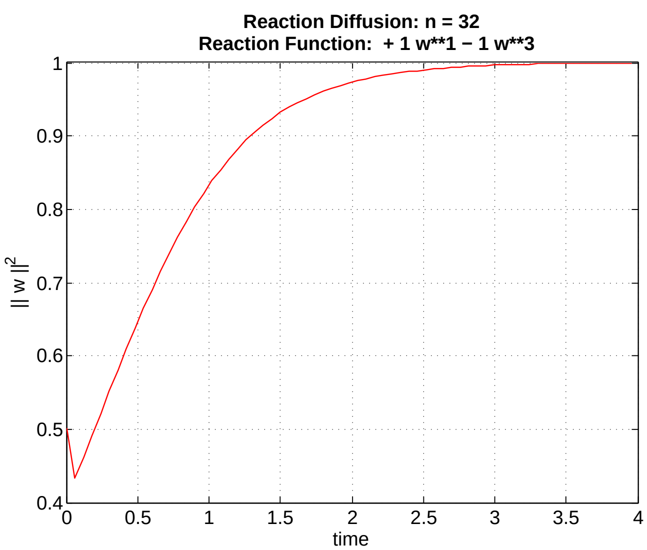

Figure 5: Evolution of the norm: $N(w) = w(1 - w^2),\ w(0, x) = \sin(\pi\, x)$