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CONVERGENCE OF THE GALERKIN METHOD FOR NONLINEAR PROBLEMS INVOLVING CHEMICAL REACTION*

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Abstract. Convergence of the Galerkin method applied to a nonlinear parabolic partial differential equation has been proved by Ladyzhenskaja, Solonnikov and Ural'ceva. That proof is extended to a system of second order semilinear parabolic differential equations arising in nonisothermal, chemically reacting systems. The proof by Visik for nonlinear systems of parabolic equations is not valid in this case. Boundary conditions of the first, second, and third kinds are included for many different forms of the reaction expression.

1. Introduction. We prove below the convergence of the Galerkin method for systems of semilinear parabolic partial differential equations of a special type. The parabolic equations are those used frequently in mathematical models of chemical reactors. The existence of classical and generalized solutions has been proved for nonlinear parabolic equations by Ladyzhenskaja and Ural'ceva [6], Browder [1] and Dubinskii [3] using the Leray–Schauder fixed-point theorem. Such proofs do not, however, give a method of finding the solution as a by-product. In contrast, the existence proofs for systems by Visik [8], [9] and for a single equation by Ladyzhenskaja, Solonnikov and Ural'ceva [5] use the Galerkin method to construct a generalized solution. These proofs thus imply that an approximate solution generated using Galerkin's method converges as the number of terms in the series is increased. Unfortunately, Visik's proof for systems of equations is not applicable to the equations of interest because of the form of the reaction rate expression. We use Galerkin's method to extend the proof of Ladyzhenskaja et al. [5] to include systems of equations. (Ladyzhenskaja et al. [5] treat systems of equations using the Leray–Schauder fixed-point theorem.) We first prove the extended theorem for boundary conditions of the first kind and then outline the corresponding results for more general boundary conditions of the second and third kinds. We conclude with a discussion of the practical cases for which the theorems are applicable.

2. Convergence of the Galerkin method. The problem is

$$(1)\qquad \begin{gathered} \frac{\partial u_j(x,t)}{\partial t} - \alpha_j \nabla_x^2 u_j(x,t) + R_j(u(x,t),x,t) = 0, \qquad j = 1,\cdots,M, \\ u_j|_s = 0, \quad u_j|_{t=0} = \psi_{j0}(x), \quad \psi_{j0}|_s = 0, \end{gathered}$$

where $u(x,t) = (u_1(x,t),\cdots,u_M(x,t))$, $x = (x_1,\cdots,x_n)$ is a point in an n-dimensional Euclidean space E_n, Ω is a bounded domain in E_n, S is the boundary of Ω, $\bar{\Omega} = \Omega \cup S$, $Q_T = \{x \in \Omega, 0 < t \leqq T\}$, $S_T = \{x \in S,\ 0 < t \leqq T\}$, and ∇_x^2 is the Laplacian operator in E_n. The $\alpha_j > 0$ are real-valued constants, and the $\psi_{j0}(x)$ are

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given, real-valued functions. The function $R(u(x,t),x,t)$ is a given real-valued continuous function of its arguments.

The function spaces follow those defined by Ladyzhenskaja et al. [5], although the notation is simplified. $L_q(\Omega)$ is the Banach space consisting of all real-valued measurable functions on Ω that are qth power summable on Ω. The norm is

$$\|u\|_{q,\Omega} = \left(\int_\Omega |u(x)|^q\,dx\right)^{1/q}, \qquad \|u\|_{\infty,\Omega} = \mathrm{vrai}_\Omega \max |u|.$$

The space $L_q(Q_T)$ is the Banach space consisting of all real-valued measurable functions on Q_T that are qth power summable on Q_T. The norm is

$$\|u\|_{q,Q_T} = \left(\int_{Q_T} |u(x,t)|^q\,dx\,dt\right)^{1/q}.$$

$W(\Omega)$ is the Banach space consisting of all elements $L_2(\Omega)$ having generalized derivatives of all forms up to order one, inclusively, that are second power summable on Ω. $\mathring{W}(\Omega)$ is the subspace of $W(\Omega)$ with elements which vanish on S. $W_{q'}(Q_T)$ is the space of functions ϕ for which $\phi_t \in L_{q'}(Q_T)$ and $\phi_x \in L_2(Q_T)$, i.e.,

$$\|\phi_x\|_{2,Q_T} \equiv \left(\int_{Q_T} \nabla\phi\cdot\nabla\phi\,dx\,dt\right)^{1/2} < \infty,$$

and $\nabla\phi$ is the gradient in the Euclidean space E_n. $\mathring{V}(Q_T)$ is the space of all real-valued measurable functions $\phi(x,t)$ that equal zero on S_T and have the finite norm

$$|\phi|_{Q_T} = \operatorname*{vrai\,max}_{0\le t\le T} \|\phi\|_{2,\Omega} + \|\phi_x\|_{2,Q_T}.$$

The inner product (ϕ, v) is defined over Ω:

$$(\phi, v) = \int_\Omega \phi v\,dx.$$

The space $\mathring{V}'(Q_T)$ is obtained by completion in this norm of all smooth functions that are equal to zero on S_T. $V'(Q_T)$ is the completion of $V(Q_T)$ whose functions are not required to vanish on S_T. A function $u(x,t)$ is in a space if each element $u_j(x,t)$ is in the space.

Basically we extend the following theorem of Ladyzhenskaja, Solonnikov and Ural'ceva [5, p. 466] which is stated here in a simplified form applicable to this problem. (Here $u = u_1$.)

THEOREM 1. *The problem*

$$u_t - \frac{\partial}{\partial x_i} a_i(x,t,u,u_x) + a(x,t,u,u_x) = 0,$$

$$u|_{S_T} = 0, \qquad u|_{t=0} = \psi_0(x)$$

for any $\psi_0 \in L_2(\Omega)$ has at least one generalized solution u in $\mathring{V}'(Q_T)$ such that

$$\int_0^T h^{-2}\|u(x,t+h) - u(x,t)\|^2_{2,Q_{T-h}}\,dh < \infty$$

if the following conditions are satisfied:

(i) *For* $(x, t, u, p) \in \{\bar{\Omega} \times [0, T] \times E_1 \times E_n\}$ *the functions* $a_i(x, t, u, p)$ *and* $a(x, t, u, p)$ *are measurable in* (x, t, u, p) *and continuous in* (u, p) *for almost all* (x, t) *in* Q_T; *the functions* a_i *and* a *satisfy the inequalities*

$$|a_i(x, t, u, p)| \leqq \phi_1(x, t) + c|u|^{q^*/2} + c|p|, \qquad \phi_1 \in L_2(Q_T), \tag{2}$$

$$|a(x, t, u, p)| \leqq \phi_2(x, t) + c|u|^{q^*/q'} + c|p|^{m^*/q'}, \qquad \phi_2 \in L_{q'}(Q_T), \tag{3}$$

where

$$q^* < q = 2(n + 2)/n, \quad q' = q/(q - 1), \quad m^* < 2.$$

(ii) *For any function* $u(x)$ *from* $\mathring{W}(\Omega)$,

$$\int_\Omega [a_i(x, t, u, u_x)u_{x_i} + a(x, t, u, u_x)u]\,dx \geqq \nu\|u_x\|^2_{2,\Omega} - c(t)\int_\Omega (1 + u^2)\,dx, \tag{4}$$

$$\nu > 0, \qquad \int_0^T c(t)\,dt \leqq c.$$

(iii) *A monotonicity condition is valid*:

$$\int_\Omega [a_i(x, t, v, v_x) - a_i(x, t, v, u_x)](v_{x_i} - u_{x_i})\,dx \geqq \int_\Omega \nu(|v_x|, |u_x|)|v_x - u_x|\,dx, \tag{5}$$

where $\nu(\tau_1, \tau_2)$ *is a continuous positive function for* $\tau_1 \geqq 0$ *and* $\tau_2 \geqq 0$, *while* u *and* v *are arbitrary elements of* $\mathring{W}(\Omega)$.

For (1) it is clear that conditions analogous to (2) and (5) are automatically satisfied, whereas (3) and (4) place restrictions on $R(u(x, t), x, t)$. We prove here the following extension of Theorem 1.

THEOREM 2. *The problem* (1) *for any* $\psi_{j0} \in L_2(\Omega)$ *has at least one generalized solution* $u(x, t)$ *in* $\mathring{V}'(Q_T)$ *if the following conditions are valid*:

(i) *For* $(x, t, u) \in \{\bar{\Omega} \times [0, T] \times E_M\}$ *the function* $R(u, x, t)$ *is measurable in* (x, t, u) *and continuous in* u *for almost all* (x, t) *from* Q_T; *the function* R *satisfies the inequality*

$$|R_j(u, x, t)| \leqq \phi_j(x, t) + c|\mathbf{u}|^{q^*/q'}, \qquad \phi_j \in L_{q'}(Q_T),$$

where

$$q' = q/(q - 1), \quad q = 2(n + 2)/n, \quad q^* < q, \quad |\mathbf{u}| = \left(\sum_{j=1}^M u_j^2\right)^{1/2}.$$

(ii) *For any functions* $u(x)$ *from* $\mathring{W}(\Omega)$,

$$\sum_{j=1}^M u_j R_j \geqq -c(t)\left(1 + \sum_{j=1}^M u_j^2\right), \tag{6}$$

$$\int_0^T c(t)\,dt \leqq c.$$

By a generalized solution we mean one satisfying

$$\int_{Q_T} [-u_j\phi_t + \alpha_j \nabla u_j \cdot \nabla \phi + R_j \phi]\, dx\, dt + \int_\Omega u_j(x,t)\phi(x,t)\, dx - \int_\Omega \psi_{j0}(x)\phi(x,0)\, dx = 0$$

for $j = 1, \cdots, M$ and any smooth ϕ in $W_{q'}(Q_T)$ which vanishes on S_T. Since the proof basically follows that of Ladyzhenskaja, Solonnikov and Ural'ceva, we present only the essential details which differ.

We take a fundamental system $\{\psi_k(x)\}$ in the space $\mathring{W}(\Omega)$ such that $(\psi_k, \psi_l) = \delta_{lk}$, $\max_\Omega (|\psi_k|, |\psi_{kx}|) = c_k < \infty$. An approximate solution $u_j^N(x,t)$ is sought in the usual form:

$$u_j^N = \sum_{k=1}^N c_{jk}^N(t)\psi_k(x),$$

where the c_{jk}^N are determined from the system of ordinary differential equations

$$(u_{jt}^N, \psi_k) + \alpha_j \int_\Omega \nabla u_j^N \cdot \nabla \psi_k\, dx + (R_j, \psi_k) = 0, \qquad \begin{array}{l} j = 1, 2, \cdots, M, \\ k = 1, 2, \cdots, N, \end{array} \tag{7}$$

and initial conditions

$$c_{jk}^N(0) = (\psi_{j0}, \psi_k), \qquad \begin{array}{l} j = 1, 2, \cdots, M, \\ k = 1, 2, \cdots, N. \end{array}$$

From the properties of the fundamental system and the hypotheses of the theorem all terms in (7) are summable functions of t on $[0, T]$ and are continuous in the c_{jk}^N. For the existence of at least one solution of problem (1) on $[0, T]$ it is sufficient to know that all possible solutions c_{jk}^N are uniformly bounded on $[0, T]$. Since

$$\max_{0 \leqq t \leqq T} \sum_{k=1}^N (c_{jk}^N(t))^2 = \max_{0 \leqq t \leqq T} \|u_j^N\|_{2,\Omega}^2 \leqq |u_j^N|_{Q_T}^2,$$

we must bound the last term independently of N,

$$|u_j^N|_{Q_T} \leqq c, \qquad j = 1, \cdots, M. \tag{8}$$

Consider (7) for some j. Multiply the kth equation by c_{jk}^N and sum over k from 1 to N. Integrate the result with respect to t. Do this for each j, add and apply (6).

$$\begin{aligned} &\sum_{j=1}^M \{\tfrac{1}{2}\|u_j^N(x,t)\|_{2,\Omega}^2 + \alpha_j \|u_{jx}^N\|_{2,Q_t}^2\} \\ &\quad \leqq \int_0^t \left\{c(t) + (c(t) + \tfrac{1}{2})\left(\sum_{j=1}^M \|u_j^N\|_{2,\Omega}^2\right)\right\} dt + \tfrac{1}{2}\sum_{j=1}^M \|\psi_{j0}\|_{2,\Omega}^2. \end{aligned} \tag{9}$$

We can rewrite (9) in the form

$$\frac{dy(t)}{dt} \leqq d(t)y(t) + F(t),$$

with

$$y(t) = \sum_{j=1}^{M} \{\tfrac{1}{2}\|u_j^N(x,t)\|_{2,\Omega}^2 + \alpha_j \|u_{jx}^N\|_{2,Q_T}^2\},$$

$$d(t) = 1 + 2c(t), \qquad F(t) = c(t).$$

Since $d(t)$ and $F(t)$ are nonnegative and integrable on $[0, T]$, it is easy to prove that

$$y(t) \leqq \exp\left\{\int_0^t d(\tau)\,d\tau\right\}\left[\int_0^t F(\tau)\,d\tau + y(0)\right],$$

and this implies (8) for each j. The inequality is proved by multiplying the differential inequality by the integrating factor $\exp\{-\int_0^t d(\tau)\,d\tau\}$, integrating with respect to t, and using the fact that $d(t)$ and $F(t)$ are nonnegative.

The remainder of the proof follows the proof of Theorem 1 and is not repeated here: $l_{N,k,j}(t) = (u_j^N(x,t), \psi_k(x))$, $j = 1, \cdots, M$, $k = 1, \cdots, N$, is shown to be continuous in t and equicontinuous for any fixed $k \leqq N$. This guarantees the weak convergence in $L_2(\Omega)$, which is uniform in $t \in [0, T]$, of u_j^N to u_j. The limit function is an element of $\mathring{V}(Q_T)$. It may be necessary to select a convergent subsequence. Finally u_j is shown to be a generalized solution.

3. Boundary conditions of the third kind. As Ladyzhenskaja et al. point out [5, p. 475], Theorem 1 can be generalized to include boundary conditions of the second and third kind. We state here the corresponding generalization of Theorem 2.

THEOREM 3. *The problem*

$$\frac{\partial u_j(x,t)}{\partial t} - \alpha_j \nabla_x^2 u_j(x,t) + R_j(u(x,t), x, t) = 0,$$

(10)
$$[\mathbf{n}\cdot\nabla u_j + \delta_j(s,t)u_j]_{S_T} = \psi_j(s,t), \qquad s \in S,$$

$$u_j|_{t=0} = \psi_{j0}(x), \qquad j = 1, \cdots, M,$$

has at least one generalized solution $u(x,t)$ in $V'(Q_T)$ if the conditions of Theorem 2 are valid with $\mathring{W}(\Omega)$ replaced by $W(\Omega)$, the boundary S is piecewise smooth, and (for $n = 1$)

$$\|\delta_j\|_{2,S_T} \leqq \mu_j, \qquad \|\psi_j\|_{4/3,S_T} \leqq \mu_j, \qquad j = 1, \cdots, M.$$

By a generalized solution we mean one satisfying

(11)
$$\int_{Q_T} [-u_j\phi_t + \alpha_j \nabla u_j\cdot\nabla\phi + R_j\phi]\,dx\,dt + \int_\Omega u_j(x,t)\phi(x,t)\,dx$$
$$- \int_\Omega \psi_{j0}(x)\phi(x,0)\,dx + \alpha_j\int_{S_T}(\delta_j u_j - \psi_j)\phi\,ds\,dt = 0$$

for any smooth ϕ in $W_{q'}(Q_T)$. The functions $\psi_k(x)$ must form a fundamental system in $W(\Omega)$ but not $\mathring{W}(\Omega)$. Clearly Theorems 2 and 3 can be combined if boundary conditions (1) are valid on S_1 and (10) on S_2, $S = S_1 \cup S_2$. The fundamental system ψ_k must vanish on S_1.

4. Application. We present here two problems arising in chemical engineering for which the above theorems are useful. Consider unsteady-state diffusion and chemical reaction inside a catalyst pellet, which is governed by the set of equations for $c = c(r, t)$ and $T = T(r, t)$:

$$\begin{aligned}
&\frac{\partial c}{\partial t} = \alpha_1 \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c}{\partial r}\right) + \beta_1 R(c, T),\\
&\frac{\partial T}{\partial t} = \alpha_2 \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) + \beta_2 R(c, T), \qquad 0 \leqq r \leqq 1,\\
&-\left.\frac{\partial c}{\partial r}\right|_{r=1} = \mathrm{Sh}\,(c(1, t) - c_1(t)), \qquad -\left.\frac{\partial T}{\partial r}\right|_{r=1} = \mathrm{Nu}\,(T(1, t) - T_1(t)),\\
&c = c_0(r), \quad T = T_0(r) \quad \text{at } t = 0, \qquad \frac{\partial c}{\partial r} = \frac{\partial T}{\partial r} = 0 \quad \text{at } r = 0.
\end{aligned} \tag{12}$$

The functions $c_1(t)$ and $T_1(t)$ represent the concentration and temperature outside the catalyst pellet, and the various terms in the equation can be identified as the accumulation, diffusion, and generation of species or energy. The terms α_j, Sh, Nu are positive constants with Sh being called the Sherwood number and Nu the Nusselt number. For continuity we require $c_1(0) = c_0(1)$, $T_1(0) = T_0(1)$. Oftentimes the conditions are $c_0 = 0$, $c_1 = 1$, which do not satisfy the compatibility conditions. This discontinuity is not handled by the mathematics but it is not realistic physically either. A continuous change of $c_1(t)$ from 0 at $t = 0$ to 1 at $t = \varepsilon$ is handled mathematically and is more realistic physically. For this problem $n = 1$, $q = 6$, $q' = 1.2$, so that Theorem 2 requires $q^*/q' < 5$.

The second problem of interest is that governing diffusion and reaction in a tubular, packed bed reactor in plug flow.

$$\begin{aligned}
&\frac{\partial c}{\partial z} = \alpha_1 \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial c}{\partial r}\right) + \beta_1 R(c, T),\\
&\frac{\partial T}{\partial z} = \alpha_2 \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial T}{\partial r}\right) + \beta_2 R(c, T),\\
&\left.\frac{\partial c}{\partial r}\right|_{r=1} = 0, \qquad -\left.\frac{\partial T}{\partial r}\right|_{r=1} = \mathrm{Nu}\,(T - T_1(z)) \quad \text{at } r = 1,\\
&c = T = 1 \quad \text{at } z = 0, \qquad \frac{\partial c}{\partial r} = \frac{\partial T}{\partial r} = 0 \quad \text{at } r = 0.
\end{aligned} \tag{13}$$

Here the problem is steady state and the variable time is replaced by the variable z representing the distance down the reactor bed.

In both problems the reaction rate term takes many forms. One example corresponds to an irreversible, first order reaction $A \to B$.

$$R(c, T) = c \exp\{\gamma(1 - 1/|T|)\} \equiv cK(\gamma, T), \qquad \gamma > 0.$$

Since $0 \leqq K(\gamma, u_2) \leqq e^\gamma$,

$$|R_j| \leqq e^\gamma |\beta_j||u_j|,$$
$$\beta_1 u_1^2 K + \beta_2 u_1 u_2 K \geqq -c(u_1^2 + u_2^2),$$
$$c = e^\gamma(|\beta_1| + \sqrt{\beta_1^2 + \beta_2^2})/2,$$

as required by Theorem 2. Another example is provided by a reaction governed by a Langmuir–Hinshelwood form of the reaction rate

$$R = K(\gamma, u_2)u_1/[1 + K(\gamma, u_2)|u_1|],$$
$$|R_j| \leqq |\beta_j|,$$
$$\frac{\beta_1 u_1^2 K + \beta_2 u_2 u_1 K}{1 + K|u_1|} \geqq -c(u_1^2 + u_2^2),$$

with the same choice of c as before. For the reversible reaction $A \rightleftarrows B$ the rate of reaction of species A can be represented by

$$R = e^{\gamma_1}[(1 - c)e^{-\gamma_1/|T|} - \kappa c e^{-\gamma_2/|T|}]$$

which satisfies the conditions of Theorem 2 since $\kappa > 0$ is a constant and

$$|R| \leqq |\beta_j| e^{\gamma_1}[1 + (1 + \kappa)|u_1|].$$

Equation (6) is satisfied if

$$c = e^{\gamma_1}[|\beta_1| + \sqrt{\beta_1^2 + 4\beta_2^2}][1 + \kappa + \sqrt{(1 + \kappa)^2 + 1}]/2.$$

5. Construction of solution. We next use Theorem 3 to construct a solution to (12) or (13) when R takes one of the forms in § 4.

THEOREM 4. *A generalized solution to* (12) *or* (13) *can be constructed in the following manner, provided* $c_0 = \psi_{10}$ *and* $T_0 = \psi_{20}$ *are real-valued functions of* x *which are in* $L_2(\Omega)$, $\Omega = \{x|0 < x < 1\}$, *the functions* $c_1 = \psi_1$ *and* $T_1 = \psi_2$ *are square integrable, the reaction rate* $R(c, T)$ *satisfies the conditions of Theorem* 2, *and* α_1, α_2, $\mathrm{Sh} = \delta_1$, $\mathrm{Nu} = \delta_2 > 0$. *The solution is expanded in the form*

$$u_j^N(x, t) = \sum_{k=0}^{N-1} c_{jk}^N(t) P_k(x),$$

where $P_k(x)$ *are orthonormal polynomials of degree* k, *and* $c_{jk}^N(t)$ *and* $c_{jk}^N(0)$ *are determined from the following equations*:

$$\text{(14)}\quad \begin{aligned} &\int_0^1 (u_{jt}^N P_k + \alpha_j \nabla u_j^N \cdot \nabla P_k + \beta_j R P_k) x^{a-1}\, dx + \alpha_j[(\delta_j u_j - \psi_j)P_k]_{x=1} = 0, \\ &c_{jk}^N(0) = (\psi_{j0}, P_k). \end{aligned}$$

We first note that Theorem 3 is applicable for $x \in E_n$ and it is thus also applicable for $x \in E_1$ with

$$\nabla_x^2 u = \frac{1}{x^{a-1}} \frac{\partial}{\partial x}\left(x^{a-1} \frac{\partial u}{\partial x}\right)$$

with $a = 1, 2, 3$ corresponding to planar, cylindrical, and spherical geometry, respectively. The conditions of Theorem 3 on δ_j and ψ_j and the conditions of Theorem 2 on R, $c(x, 0)$, and $T(x, 0)$ are satisfied by hypothesis. We thus need only find a fundamental system $P_k(x)$ satisfying

$$\int_0^1 P_k(x)P_j(x)x^{a-1}\,dx = \delta_{kj}, \qquad \int_0^1 \frac{dP_k}{dx}\frac{dP_j}{dx}x^{a-1}\,dx < \infty.$$

One possibility is the Jacobi polynomials (see Courant and Hilbert [2, p. 90]), which are a complete set of functions on the interval (0, 1), are orthogonal and can be normalized, and satisfy the differential equation

$$x(1-x)\frac{d^2G_n(x)}{dx^2} + [a-(a+1)x]\frac{dG_n(x)}{dx} + (a+n)nG_n(x) = 0.$$

Each $G_n(x)$ is a polynomial in x of degree n, and the first derivatives are square integrable. Other orthogonal polynomials are equally suitable. The conditions of Theorem 4 are therefore satisfied. The integration of (14) is usually performed numerically.

For computational purposes, the Galerkin method requires calculation of the integrals

$$\int_0^1 R(u_1, u_2)P_k(x)x^{a-1}\,dx.$$

For the $R(u_1, u_2)$ functions listed above this is clearly impossible to do analytically. One alternative is to use the quadrature formula corresponding to the orthogonal polynomials

$$\int_0^1 f(x)x^{a-1}\,dx = \sum_{i=1}^{m} W_i^{(m)}f(x_i),$$

where $m \geqq n$ and the x_i are the roots to $P_m(x) = 0$.

This formula is exact when $f(x)$ is a polynomial of degree $2m - 1$ and the error decreases to zero as $m \to \infty$ for continuous functions $f(x)$. Another alternative, and the one employed in computations, is to use the collocation method rather than the Galerkin method. The differential equation is satisfied at the roots to the $P_n(x)$ polynomial. An example of the computations and comparison to finite difference methods is presented elsewhere [4].

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