A Pre–Conditioned Spectral Collocation Method For Two Dimensional Nonlinear Elasticity

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Abstract

In this paper we discuss a pre-conditioned spectral-collocation method for the computation of minimizers of the calculus of variations in the context of two dimensional elasticity. The spectral collocation method is used in conjunction with a Richardson extrapolation iteration. We compare the performance of the pre-conditioned method with the one without pre–conditioning.

Key words: pre–conditioning, spectral–collocation, Richardson extrapolation, nonlinear elasticity

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1 Introduction

The phenomena of void formation on bodies in tension have been observed among others by [7]. Ball [1] showed in the context of nonlinear elasticity, that void formation or "cavitation" can decreased the (potential) energy of a body in tension when the tension is sufficiently large. The numerical aspects of cavitation and other singular minimizers in elasticity are very delicate. It has been observed that because of the so called Lavrentiev phenomena [8], that the usual finite element methods can fail to compute both the minimizer and the minimum energy. A numerical method for overcoming the Lavrentiev phenomenon has been proposed in [2] and [9]. This method uses a decoupling on the deformation gradient that works quite well for one dimensional problems, but for higher dimensional problems, after discretization, yields a large scale constrained optimization problem. To handle numerically this problem effectively one would need to use for instance multigrid methods and exploit the sparsity of the resulting discrete equations. Instead of taking this approach in this work we proceed by discretizing the energy functional using a spectral method (finite differences in the radial direction and a truncated Fourier series for the angular variable).

Our approach here is similar to that of [10] but we present some preliminary results for a preconditioning method that renders a scheme with a rate of convergence essentially independent of the mesh size. We employ a formulation of the problem using the invariants of the Cauchy-Green deformation tensor (cf. (3.4)-(3.6)) instead of the principal stretches (the square root of the eigenvalues of the Cauchy-Green tensor) as done in [10]. This renders a system of partial differential equations, the Euler-Lagrange equations, without the singularity when the two principal stretches are equal and as a consequence leads to a more stable numerical scheme. We still have a singularity at the center of the body due to the use of polar coordinates.

The structure of the paper will be as follows. In Section 2 we discuss a numerical method for finding local minima of our discrete problems. The method we use is an iterative scheme based on a second order Richardson extrapolation technique (see [6]). In Section 3 we describe a two dimensional model for nonlinear elasticity and define a class of stored energy functions which allows for cavitation according to the results in [1]. In Section 4 we discuss the discretization of the two dimensional energy functional of Section 3. We describe the spectral collocation method which is used in conjunction with the Richardson extrapolation iteration. In Section 5 we describe a preconditioning method for the scheme of Section 4 and finally in Section 6, we compare the pre–conditioned method with the one without pre-conditioning.

2 An Accelerated Steepest Descent Method

In this section we describe an accelerated steepest descent method based on a second order Richardson extrapolation formula. We consider the problem of minimizing the

functional

$$I(u) = \int_\Omega f(x, \nabla u(x))\, dx, \tag{2.1}$$

where u belongs to some space of smooth functions and is subjected, for simplicity, to Dirichlet boundary conditions. The steepest descent method for minimizing (2.1) would then take the form

$$\begin{aligned} u^{k+1} &= u^k - \lambda L(u^k) \quad , \quad k = 0, 1, 2, \ldots, \\ u^0 &\qquad \text{given,} \end{aligned} \tag{2.2}$$

where $\lambda > 0$, and $L(\cdot)$ is the first variation of I, i.e., $L(u) = 0$ are the Euler-Lagrange equations of (2.1).

Let L_h, for a given mesh size h, denote a discretization of L (by finite differences say). Let u_h denote a mesh function and in (2.2) write $\Delta t = \lambda$. Then (2.2) becomes

$$\begin{aligned} \frac{u_h^{k+1} - u_h^k}{\Delta t} &= L_h(u^k) \quad , \quad k = 0, 1, 2, \ldots, \\ u_h^0 &\qquad \text{given.} \end{aligned} \tag{2.3}$$

Thus the iteration step "k" can be viewed as a discretization of an artificial time variable "t" and (2.3) is the discretization of the parabolic equation $w_t = L(w)$. The Courant-Friedrichs-Lewy stability condition for (2.3) requires in general that $\Delta t = O(h^2)$, which makes the convergence in (2.3) slow when h is small. To overcome this problem one considers instead the hyperbolic equation

$$w_{tt} + \varepsilon w_t = L(w) \ \text{ in } \ \Omega. \tag{2.4}$$

The Courant-Friedrichs-Lewy stability condition for (2.4) requires that $\Delta t = O(h)$ which makes the convergence in "t" faster than in (2.3). We can now discretize (2.4) as

$$\begin{aligned} \frac{u_h^{k+1} - 2u_h^k + u_h^{k-1}}{(\Delta t)^2} + \varepsilon \frac{u_h^{k+1} - u_h^k}{\Delta t} &= L_h(u_h^k) \quad , \quad k = 1, 2, \ldots, \\ u_h^0, u_h^1 \ \text{ given,} & \end{aligned} \tag{2.5}$$

which is referred to as the *second order Richardson method.*

3 A Two Dimensional Model for Nonlinear Elasticity

We consider a body which in its reference configuration occupies the unit disk Ω in $\mathbb{R}^2$. Let $p : \Omega \to \mathbb{R}^2$ denote a deformation of the body. Let $F(x)$ be the 2×2 matrix of partial derivatives of p at x. The requirement that $p(\cdot)$ *preserves orientation* takes the form

$$\det F(x) > 0 \quad , \quad x \in \Omega. \tag{3.1}$$

Let $W : M^{2\times 2}_+ \to \mathbb{R}$ be the *stored energy function* of the material of the body. The *total stored energy* on the body due to the deformation p is given by

$$I(p) = \int_\Omega W(F(x))\, dx. \tag{3.2}$$

If Ω is subject to a deformation g on the boundary, i.e.,

$$p(x) = g(x) \quad , \quad x \in \partial\Omega, \tag{3.3}$$

then the equilibrium configuration satisfying (3.3), minimizes (3.2) among all functions satisfying (3.1) and belonging to some appropriate Sobolev space.

A physically reasonable model for W for an isotropic material is as follows. Let $\mathbf{C} = F^t F$ be the *Cauchy-Green deformation tensor* and $(i_1(\mathbf{C}), i_2(\mathbf{C}))$ be the principal invariants of $\mathbf{C}$, i.e,

$$i_1(\mathbf{C}) = \operatorname{trace} \mathbf{C} \quad , \quad i_2(\mathbf{C}) = \det \mathbf{C}. \tag{3.4}$$

We take

$$W(F) = \frac{1}{2}\Phi(i_1(\mathbf{C}), i_2(\mathbf{C})) \quad , \quad F \in M^{2\times 2}_+, \tag{3.5}$$

where

$$\Phi(i_1, i_2) = A i_1^{\alpha/2} + B\left(\frac{i_1}{i_2}\right)^{\beta/2} + C i_2^{\gamma/2} + D i_2^{-\delta/2}, \tag{3.6}$$

and $A, B, C, D \geq 0$ and $\alpha, \beta, \gamma, \delta > 1$. Let (r, θ) be polar coordinates for Ω and $(R(r,\theta), \Theta(r,\theta))$ the polar coordinates for $p(\Omega)$. An elementary computation now shows that the principal invariants $(i_1(\mathbf{C}), i_2(\mathbf{C}))$ are given by

$$\operatorname{trace} \mathbf{C} = R_r^2 + \frac{R_\theta^2}{r^2} + \left(\Theta_r^2 + \frac{\Theta_\theta^2}{r^2}\right) R^2 \quad , \quad \det \mathbf{C} = \frac{R^2}{r^2}\left(\Theta_\theta R_r - \Theta_r R_\theta\right)^2. \tag{3.7}$$

4 A Spectral Collocation Method

Consider the problem of minimizing (3.2) subject to (3.1), (3.3), (3.4), (3.5), and (3.6). In this section we discuss how the method of Section (2) is used to solve numerically this problem. The Euler-Lagrange equations for (3.2), (3.5) are given by

$$\begin{aligned} &-\frac{\partial}{\partial r}\left(r\Phi_1 R_r + \Phi_2 \frac{R^2}{r}\left(\Theta_\theta R_r - \Theta_r R_\theta\right)\Theta_\theta\right) \\ &\quad - \frac{\partial}{\partial \theta}\left(\Phi_1 \frac{R_\theta}{r} - \Phi_2 \frac{R^2}{r}\left(\Theta_\theta R_r - \Theta_r R_\theta\right)\Theta_r\right) \\ &\quad + r\Phi_1 R\left(\Theta_r^2 + \frac{\Theta_\theta^2}{r^2}\right) + \Phi_2 \frac{R}{r}\left(\Theta_\theta R_r - \Theta_r R_\theta\right)^2 = 0, \end{aligned} \tag{4.1}$$

$$-\frac{\partial}{\partial r}\left(r\Phi_1 R^2\Theta_r - \Phi_2\frac{R^2}{r}\left(\Theta_\theta R_r - \Theta_r R_\theta\right)R_\theta\right)$$
$$-\frac{\partial}{\partial\theta}\left(\Phi_1\frac{R^2}{r}\Theta_\theta + \Phi_2\frac{R^2}{r}\left(\Theta_\theta R_r - \Theta_r R_\theta\right)R_r\right) = 0. \tag{4.2}$$

where the arguments of $\Phi_1 = \partial\Phi/\partial i_1$, etc., are $(i_1(\mathbf{C}), i_2(\mathbf{C}))$. For the boundary condition (3.3), we take

$$R(1,\theta) = \lambda(\theta) \quad , \quad \Theta(1,\theta) = g(\theta) \quad , \quad \theta \in [0, 2\pi), \tag{4.3}$$

where $\lambda(\theta), g(\theta) - \theta$ are periodic functions, e.g., $\lambda(\theta) = \text{constant}$, $g(\theta) = \theta$. We consider also the problem in which (4.3a) is the only one specified. This corresponds to a *slip* boundary condition at the edge $s = 1$. The natural boundary conditions for (4.1) and (4.2) are given by

$$\lim_{r\longrightarrow 0^+} -\left(r\Phi_1 R_r + \Phi_2\frac{R^2}{r}\left(\Theta_\theta R_r - \Theta_r R_\theta\right)\Theta_\theta\right) = 0, \tag{4.4}$$

$$\lim_{r\longrightarrow 0^+} -\left(r\Phi_1 R^2\Theta_r - \Phi_2\frac{R^2}{r}\left(\Theta_\theta R_r - \Theta_r R_\theta\right)R_\theta\right) = 0, \tag{4.5}$$

These equations represent the free-boundary condition that determines the shape of the possible inner cavity at the center of the plate. When (4.3a) is the only one specified, we have instead of (4.3b) the condition

$$\left(r\Phi_1 R^2\Theta_r - \Phi_2\frac{R^2}{r}\left(\Theta_\theta R_r - \Theta_r R_\theta\right)R_\theta\right)\Big|_{r=1} = 0, \tag{4.6}$$

which states that on the outer boundary the tangential component of the stress is zero. We also have the periodicity conditions

$$R, R_r, R_\theta, \Theta - \theta, \Theta_r, \Theta_\theta \quad \text{are periodic in} \quad \theta. \tag{4.7}$$

For any integers $n, m \geq 1$, let

$$h = \frac{1}{n} \quad , \quad r_i = ih \quad , \quad 0 \leq i \leq n, \tag{4.8}$$

$$k = \frac{2\pi}{m} \quad , \quad \theta_j = jk \quad , \quad 0 \leq j \leq m, \tag{4.9}$$

$$r_{i+1/2} = \frac{r_{i+1} + r_i}{2} \quad , \quad 0 \leq i \leq n-1. \tag{4.10}$$

For any function u of (r,θ), we let u_{ij} denote an approximation of $u(r_i,\theta_j)$. We now approximate $u_r(r_{i+1/2},\theta_j)$ by

$$u_r(r_{i+1/2},\theta_j) \approx \delta u_{ij} = \frac{u_{i+1,j} - u_{ij}}{h} \quad , \quad 0 \leq i < n \ , \ 0 \leq j \leq m. \tag{4.11}$$

For the derivatives in the θ direction we use a truncated Fourier series. More specifically, let $\{u_{ij}\}$, $0 \le i \le n, 0 \le j \le m$ be a mesh function defined over (4.8–4.9) and let

$$u_{ij} = \sum_{|\alpha| \le N} a_\alpha(r_i) \mathrm{e}^{\imath \alpha \theta_j} \quad , \quad 0 \le i < n \ , \ 0 \le j < m, \tag{4.12}$$

be its discrete Fourier representation ($\imath^2 = -1$). We now compute

$$u_{\theta,ij} = \sum_{|\alpha| \le N} \imath \alpha a_\alpha(r_i) \mathrm{e}^{\imath \alpha \theta_j} \quad , \quad 0 \le i < n \ , \ 0 \le j < m. \tag{4.13}$$

Numerically, to compute (4.13), one first computes the $\{a_\alpha\}$ in (4.12) using an FFT routine, then compute the $\{\imath\alpha a_\alpha\}$, and finally use an inverse FFT routine to get the mesh representation of u_θ. Expressions like $u_{\theta,i+1/2,j}$ now have the following meaning:

$$u_{\theta,i+1/2,j} = \frac{1}{2}\left(u_{\theta,i+1,j} + u_{\theta,ij}\right) \quad , \quad 0 \le i < n \ , \ 0 \le j < m, \tag{4.14}$$

where $u_{\theta,i+1,j}$ and $u_{\theta,ij}$ come from (4.13). With the formulas (4.11), (4.13), and (4.14) we discretize (3.2), (3.5) by

$$I_h(R_h, \Theta_h) = hk \sum_{i=0}^{n-1} \sum_{j=0}^{m-1} r_{i+1/2} \Phi^{i+1/2,j}, \tag{4.15}$$

where

$$\Phi^{i+1/2,j} = \Phi(i_1^{i+1/2,j}, i_2^{i+1/2,j}), \tag{4.16}$$

$$i_1^{i+1/2,j} = \delta R_{ij}^2 + \left(\frac{R_{\theta,i+1,j}^2 + R_{\theta,ij}^2}{2r_{i+1/2}^2}\right) + \left(\delta\Theta_{ij}^2 + \left(\frac{\Theta_{\theta,i+1,j}^2 + \Theta_{\theta,ij}^2}{2r_{i+1/2}^2}\right)\right) R_{i+1/2,j}^2, \tag{4.17}$$

$$i_2^{i+1/2,j} = \left(\frac{R_{i+1/2,j}}{r_{i+1/2}}\right)^2 \left(\Theta_{\theta,i+1/2,j}\delta R_{ij} - \delta\Theta_{ij} R_{\theta,i+1/2,j}\right)^2, \tag{4.18}$$

$0 \le i < n$, $0 \le j < m$ and $R_h = \{R_{ij}\}$, $\Theta_h = \{\Theta_{ij}\}$.The combination of (4.11), (4.13), (4.14) with the method of Section 2, applied to (4.15) and (4.16–4.18) is called a *spectral-collocation method* (see [3], [4], and [5].)

5 A Pre-Conditioning Scheme

Define L_R, L_Θ as the left sides of (4.1), (4.2) respectively. Then the first variation of (3.2) is given by

$$\delta I(p) \cdot (\delta R, \delta\Theta) = \int_\Omega \left(L_R \delta R + L_\Theta \delta\Theta\right) \mathrm{d}r \, \mathrm{d}\theta. \tag{5.1}$$

Let $\hat{L}_R$, $\hat{L}_\Theta$ be negative definite approximations of $-L_R$, $-L_\Theta$, which are *easily* invertible. Consider the equations

$$\hat{L}_R \cdot \delta R = L_R \quad , \quad \hat{L}_\Theta \cdot \delta\Theta = L_\Theta. \tag{5.2}$$

Upon substitution of (5.2) into (5.1) we get that

$$\delta I(p) \cdot (\delta R, \delta\Theta) = \int_\Omega \left(\delta R(\hat{L}_R \cdot \delta R) + \delta\Theta(\hat{L}_\Theta \cdot \delta\Theta) \right) \mathrm{d}r \, \mathrm{d}\theta, \tag{5.3}$$

which is less than zero because $\hat{L}_R$, $\hat{L}_\Theta$ are negative definite. For any function $f(\theta)$, we use the notation

$$\langle f(\theta) \rangle = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) \, \mathrm{d}\theta \approx \frac{1}{m} \sum_{j=0}^{m-1} f(\theta_j). \tag{5.4}$$

To construct $\hat{L}_R$, $\hat{L}_\Theta$, we let

$$a(r) = \left\langle r\Phi_1 + \Phi_2 \frac{R^2}{r} \Theta_\theta^2 \right\rangle, \tag{5.5}$$

$$b(r) = \frac{1}{r} \left\langle \Phi_1 + \Phi_2 R^2 \Theta_r^2 \right\rangle, \tag{5.6}$$

$$c(r) = \left\langle r\Phi_1 \left(\Theta_r^2 + \frac{1}{r^2} \Theta_\theta^2 \right) + \frac{\Phi_2}{r} \left(\Theta_\theta R_r - \Theta_r R_\theta \right)^2 \right\rangle, \tag{5.7}$$

$$d(r) = \left\langle \left(r\Phi_1 + \frac{\Phi_2}{r} R_\theta^2 \right) R^2 \right\rangle, \tag{5.8}$$

$$e(r) = \frac{1}{r} \left\langle \left(\Phi_1 + \Phi_2 R_r^2 \right) R^2 \right\rangle, \tag{5.9}$$

(cf. (4.7)). We define

$$\hat{L}_R = \frac{\partial}{\partial r} \left(a(r) \frac{\partial}{\partial r} \right) + b(r) \frac{\partial^2}{\partial \theta^2} - c(r), \tag{5.10}$$

$$\hat{L}_\Theta = \frac{\partial}{\partial r} \left(d(r) \frac{\partial}{\partial r} \right) + e(r) \frac{\partial^2}{\partial \theta^2}. \tag{5.11}$$

To solve the first equation in (5.2), we write

$$\delta R = \sum_{|\alpha| \le N} v_\alpha(r) \mathrm{e}^{\imath\alpha\theta} \quad , \quad L_R = \sum_{|\alpha| \le N} g_\alpha(r) \mathrm{e}^{\imath\alpha\theta}. \tag{5.12}$$

Upon substituting (5.12) in (5.2) and equating the coefficients of $\mathrm{e}^{\imath\alpha\theta}$ we get the following equations for the Fourier coefficients of δR:

$$\frac{\mathrm{d}}{\mathrm{d}r} \left(a(r) \frac{\mathrm{d}}{\mathrm{d}r} v_\alpha(r) \right) - (c(r) + \alpha^2 b(r)) v_\alpha(r) = g_\alpha(r) \quad , \quad 0 < r < 1, \tag{5.13}$$

$$v_\alpha(0) = 0 = v_\alpha(1) \quad , \quad |\alpha| \leq N. \tag{5.14}$$

If we let $v_{\alpha,i}$ denote an approximation of $v_\alpha(r_i)$ and $g_{\alpha,i}$ denote an approximation of $g_\alpha(r_i)$, then we can approximate (5.13)–(5.14) by

$$a_{i+1/2}v_{\alpha,i+1} - (a_{i+1/2} + a_{i-1/2} + h^2(c_i + \alpha^2 b_i))v_{\alpha,i} + a_{i-1/2}v_{\alpha,i-1} = h^2 g_{\alpha,i}, \tag{5.15}$$

$$v_{\alpha,0} = 0 = v_{\alpha,n} \quad , \quad 1 \leq i \leq n-1 \quad , \quad |\alpha| \leq N. \tag{5.16}$$

We now have to solve N tridiagonal systems each of which can be solved in time proportional to n. In this way we get an approximation of δR, and we can repeat this process with the second equation in (5.2), to approximate $\delta\Theta$. We now use these *preconditioned* $\delta R, \delta\Theta$ in (2.5) instead of L_h.

6 Numerical Results and Conclusions

We tested the preconditioned spectral-collocation method described on Sections 2,4, and 5 on a test problem for the model of Section 3. We used $n = 20$ and $m = 32$ in the calculations and the parameters in (3.5) are set to $A = B = C = D = 1.0$, $\alpha = \beta = \gamma = \delta = 1.5$. For our test runs, we used as initial configuration for the numerical schemes, functions of the form:

$$\begin{aligned} R_0(r,\theta) &= u_0 + (\lambda_0 - u_0)(1 + d_1\cos n_1\theta + d_2 \sin n_2\theta)r^b \\ &\quad + (d_3\cos n_3\theta + d_4 \sin n_4\theta)r(1-r), \end{aligned} \tag{6.1}$$

$$\Theta_0(r,\theta) = \theta, \tag{6.2}$$

where u_0 represents the radius of the initial inner cavity (always circular in this case) and λ_0 is proportional to the outer displacement which need not be circular. It follows from (6.1)–(6.2) that the functions in (4.3) are given by $\lambda(\theta) = R_0(1,\theta)$ and $g(\theta) = \theta$. In Figure (1) we show the initial configuration used in (2.5) which corresponds to (6.1)–(6.2) with $u_0 = 1.0$, $\lambda_0 = 1.0$, $d_1 = d_2 = d_3 = d_4 = 1.0$, $n_1 = n_2 = n_3 = n_4 = 2$. This configuration has discrete energy (cf. (4.15)) of 15.78. In Figure (2) we show the final configuration computed by the pre–conditioned method which has discrete energy of 14.50.

In Figure (3) we compare the performance of the preconditioned method with that without preconditioning. The vertical axis is the discrete L_2 norm of the error as measured by the first variation of (4.15). (This first variation corresponds to a discretization of the Euler-Lagrange equations (4.1),(4.2).) The horizontal axis is just the index k in (2.5). We can appreciate the superior performance of the preconditioned method in this problem achieving an error of the order of 10^{-10} in approximately 10000 iterations. We can see a similar behavior in Figure (4) for the boundary iteration where now the vertical axis is the maximum norm of the boundary error as measured by the corresponding discretizations of (4.4-4.5). The computations corresponding to the preconditioning represented an overhead in the execution time per iteration of approximately 6% over the

no–preconditioning in this problem. Note however that according to Figures (3) and (4), the preconditioned scheme achieves the same performance as the no–preconditioned scheme at approximately 4000 iterations which represents an improvement in performance of about 60%.

Figures (5,6) show different runs of the preconditioned method for $n = 20, 30$, and 40. The vertical axis is as in Figure (3). Since $\Delta t = O(h)$, by the Courant-Friedrichs-Lewy stability condition, the horizontal axis in Figure (5) is $k\Delta t$, where k is as in (2.5), to take into account the factors of two in Δt as we double n. The results in Figure (5) show that for this particular problem the convergence rate is essentially independent of the mesh size. In Figure (6) we show the same runs but with k as in (2.5) on the horizontal axis.

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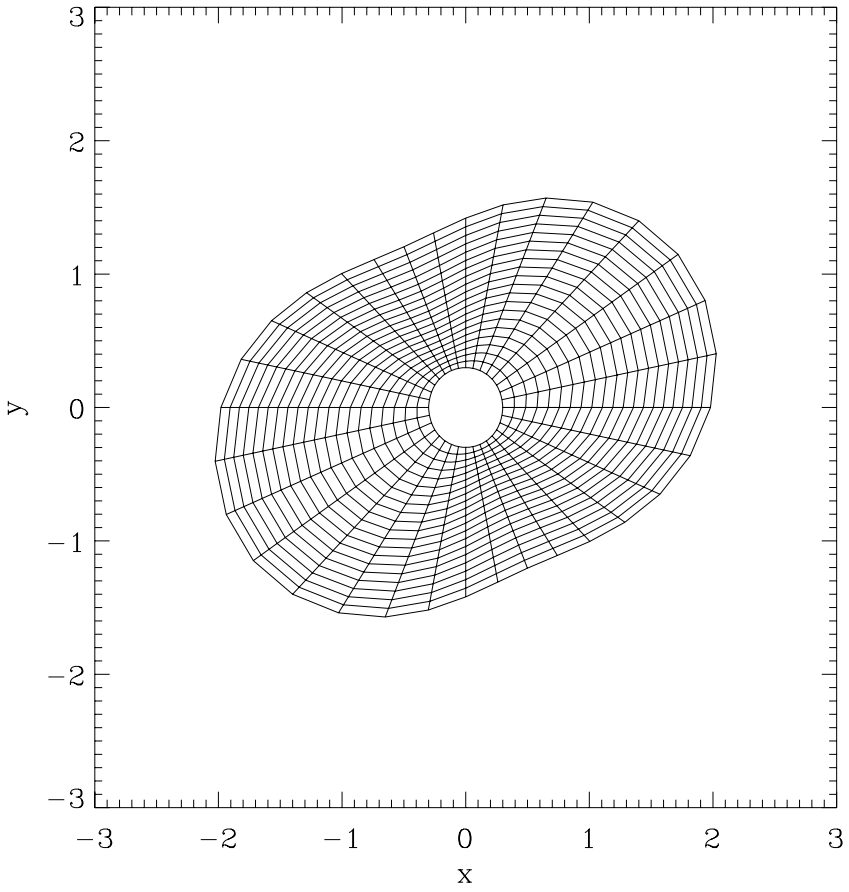

Figure 1: Initial configuration (6.1) for the data $u_0 = 1.0$, $\lambda_0 = 1.0$, $d_1 = d_2 = d_3 = d_4 = 1.0$, $n_1 = n_2 = n_3 = n_4 = 2$.

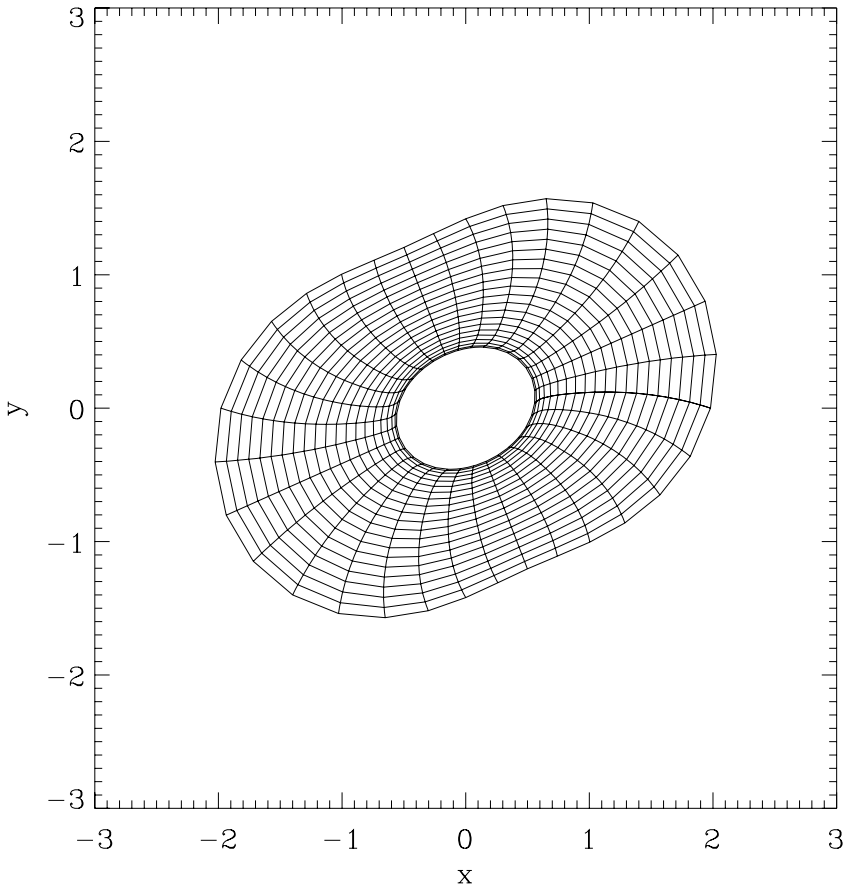

Figure 2: Final computed configuration by the pre–conditioned spectral collocation method using the initial configuration (6.1) with data $u_0 = 1.0$, $\lambda_0 = 1.0$, $d_1 = d_2 = d_3 = d_4 = 1.0$, $n_1 = n_2 = n_3 = n_4 = 2$.

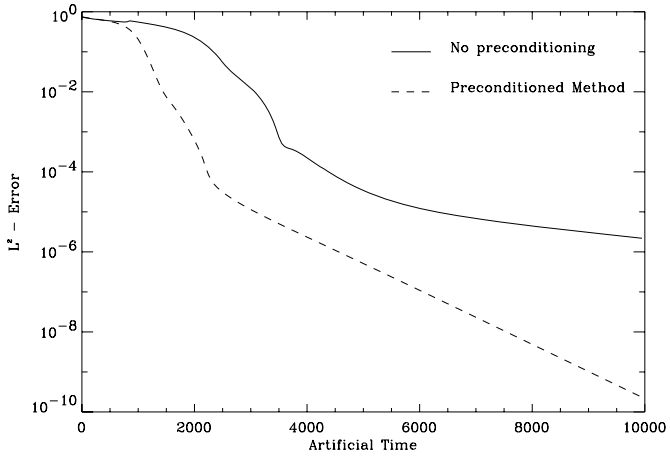

Figure 3: A comparison between pre–conditioning and no conditioning for the L_2 interior error.

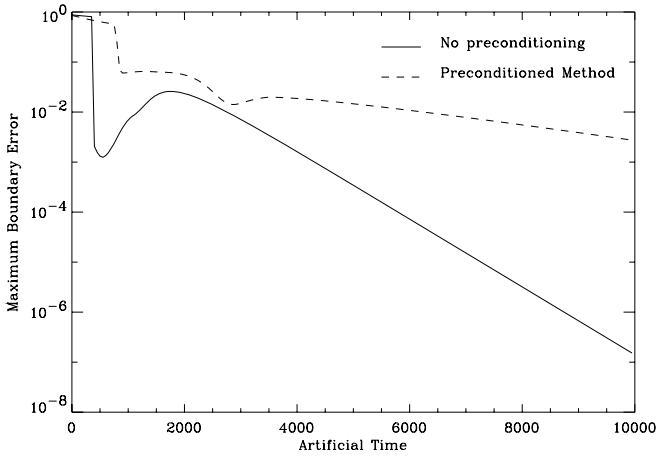

Figure 4: A comparison between pre–conditioning and no conditioning for the inner boundary.

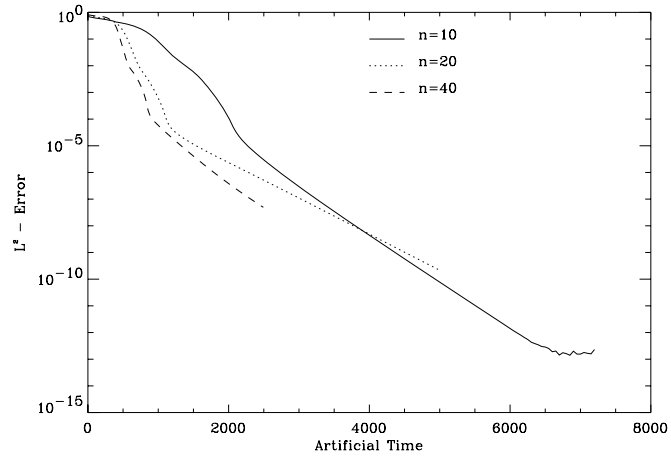

Figure 5: A comparison of the performance of the pre–conditioned scheme with respect to the artificial time for different values of n.

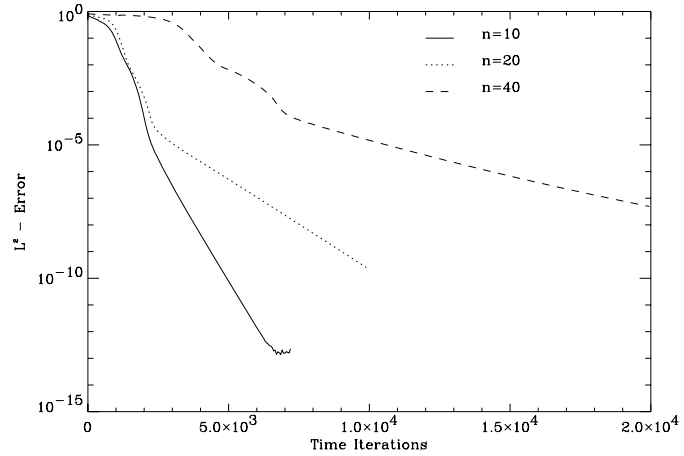

Figure 6: A comparison of the performance of the pre–conditioned scheme with respect to the time iterations for different values of n.