Continuation Techniques with Parameter Step Control

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Abstract: *We examine Proportional-Integral-Derivative (PID) feedback control to enhance algorithm performance via parameter adaption. Of particular interest is use in branch-following algorithms applicable to turning point and bifurcation problems. Results of numerical experiments are described for finite element approximation of a benchmark Navier-Stokes problem and for the classical Bratu reaction-diffusion problem.*

Continuation techniques provide a means of extending the range of flows for which a solution can be computed using a given nonlinear iterative method [5, 10, 2, 12]. A variety of finite difference and finite element methods has been developed for approximate solution of nonlinear applications. The system of nonlinear equation resulting from the approximation is usually solved using an iterative method such as Picard, successive approximations or Newton. In the vicinity of a solution, Newton's method converges quadratically and the method can produce results very efficiently. However, the range of convergence is small for many flows considered on important applications, so that the benefits of a high rate of convergence are difficult to obtain [4]. To solve this problem, we need an appropriate starting guess which can be obtained using some kind of continuation technique. An simple continuation technique is to incrementally increase the parameter (e.g. the Reynolds (Re) number in the stationary Navier-Stokes equations) from zero to the final value of interest, using successive intermediate solutions as starting iterates for the next problem in sequence (*incremental Newton*). The essential idea is to compute solutions to a sequence of problems as a parameter is varied along a continuation path [4]. Such a set of solutions is also said to define a "solution branch". Provided the step in Re is not larger this procedure assists in providing a starting iterate that is in the domain of attraction of Newton method for each successive nonlinear solve along the path. A bad initial guess for the Newton method may not converge or may converge to the wrong solution (i.e. a solution on a different branch). By differentiating the nonlinear problem with respect to the continuation parameter, we can construct an associated initial-value problem which may be integrate numerically with an Euler scheme to determine the solution at successive values of the parameter [4]. This scheme is an variant of the continuation scheme defined a *Euler-Newton method*. However, although these methods works well when the continuation path consists of regular points, they may fail when turning and bifurcation points lie on the path. In this case, the Jacobian matrix in the Newton solver becomes increasingly ill conditioned as the singular point is approached. One method to circumvent this problem is to use arc length as an alternative parameterization for the continuation method. One popular method of this type is the *arclength continuation* technique described by Keller [10]. Now one must solve a larger "bordered" Jacobian system at each Newton iteration. Splitting this system alleviates this difficulty, but the singularity then persists, necessitating adaption of the arclength step near the singular point [5, 9, 1, 2]. To adapt the arclength for overall efficiency of the continuation techniques and to maintain convergence near the singular point, a PID feedback control algorithm is introduced based on controlling accuracy as determined by truncation error estimates [15, 13, 16]. Of particular interest is use in branch-following algorithms applicable to turning point and bifurcation problems. Results of numerical experiments are described for finite element approximation of the lid driven cavity problem and the Bratu reaction-diffusion problem.

Method

Consider the nonlinear parameterized boundary value problem for the steady-state behavior of a physical system in an abstract notation as

$$G(u, \lambda) = 0 \tag{1}$$

where G is the residual operator for the boundary value problem, $u \in V$ is the state variable solution and $\lambda \in R^m$ is a vector of parameters. In this work, we focus on two classes of stationary problems: incompressible Navier-Stokes problems for different values of the Reynolds number (Re) and the Bratu reaction-diffusion problem with parameter continuation along a solution branch. A finite element discretization is introduced in the weak formulation of the problem and a Newton method is then formulated for the resulting nonlinear system. For the viscous flow equation we use a penalty finite element formulation and for the reaction-diffusion problem we use a Galerkin formulation.

The implicit function theorem specifies sufficient criteria guaranteeing that a branch can be parameterized by λ. For a specific stationary solution of (1) the criterion basically requires nonsingularity of the Jacobian matrix G_u. If a path consists of regular points, we can use the incremental Newton method to increase the parameter, using successive intermediate solutions as starting iterates for the next problem in sequence. By differentiating the nonlinear system (1) with respect to the continuation parameter, we obtain the linear system

$$G_u \frac{\partial u_h}{\partial \lambda} = -G_\lambda \tag{2}$$

to be solved for $\frac{\partial u_h}{\partial \lambda}$. Equation (2) involves the calculation of Jacobian matrix G_u as for the original Newton's method, but has a different right-hand side. The benefit of solving this extra system of equations is an improved initial guess for the finite element solution u_h. This solution can be used in the forward integration rule (Euler's method),

$$u_h(\lambda + d\lambda) = u_h(\lambda) + d\lambda \frac{\partial u_h}{\partial \lambda}(\lambda) \tag{3}$$

to obtain a good starting vector in Newton iteration of the nonlinear system (1). This scheme is termed *Euler-Newton* continuation method and is suitable provided that there are no limit points. If this is not the case, the problem may parameterized with respect to arclength than λ, as suggested by Keller. In the arclength continuation method, (1) is augmented with a constrained equation as

$$P(u, \lambda, s) = \begin{bmatrix} G(u, \lambda) \\ N(u, \lambda, s) \end{bmatrix} = 0 \tag{4}$$

where s is the arclength parameter, defined as the distance along the solution branch (i.e. s is non-decreasing even if λ is decreasing along the branch). In this work we use a linearized arclength constrained or a "pseudo arclength" given by

$$\begin{aligned} N(u, \lambda, s) \quad = \quad & (u - u(s_i))^t \frac{\partial u}{\partial s}|_{s_i} + \\ & (\lambda - \lambda(s_i)) \frac{\partial \lambda}{\partial s}|_{s_i} - \\ & (s - s_i) = 0 \end{aligned} \tag{5}$$

where s_i is some arbitrary point in the path. Now we must to consider the augmented Jacobian system associated with the nonlinear system (4) to obtain the solution (u, λ) via Newton method

$$\begin{bmatrix} G_u & G_\lambda \\ N_u^t & N_\lambda \end{bmatrix}^k \begin{bmatrix} \delta u \\ \delta \lambda \end{bmatrix}^{k+1} = \begin{bmatrix} -G \\ -N \end{bmatrix}^k \tag{6}$$

where $k = 0, 1, \cdots$. Here for convenience (in terms of reuse of existing computational tools) we use a two-solve procedure. At each Newton step, we need to perform the following computations:

1. Solve $G_u y = G_\lambda$ (first solve).
2. Solve $G_u z = -G$ (second solve).
3. Calculate $\delta\lambda = \frac{-N - N_u^t z}{N_\lambda - N_u^t y}$.
4. Calculate $\delta u = z - (\delta\lambda) y$.

Note that this algorithm is roughly twice as expensive as a normal Newton solve, and therefore only attractive to use near turning points or regions of rapid change in the solution relative to the parameter λ. Observe also that the initialization of the arclength continuation algorithm requires the solution and parameter derivatives with respect to s from the previous step, since we are using the linearized arclength constrained (5). So, we assume that two previous solutions, $\{u_0, \lambda_0\}$ and $\{u_1, \lambda_1\}$, have been computed without requiring arclength continuation, but the incremental Newton with small increments of the parameter λ.

To generate an initial guess for the Newton iterations we use an extension of the Euler-Newton approach described before. The main idea is to assume in (4) that the "derivative" of $P(x(s))$, $x = [u, \lambda]$, with respect to s is the zero vector. By chain-differentiation of P one arrives at

$$\begin{bmatrix} G_u & G_\lambda \\ N_u^t & N_\lambda \end{bmatrix} \begin{bmatrix} \frac{\partial u}{\partial s} \\ \frac{\partial \lambda}{\partial s} \end{bmatrix} = \begin{bmatrix} 0 \\ -N_s \end{bmatrix} \quad (7)$$

which is an equation for determining the tangent vector. Then a predictor or initial guess for Newton's method can be obtained by

$$u_2^* = u_1 + \frac{\partial u}{\partial s}\Delta s, \quad \lambda_2^* = \lambda_1 + \frac{\partial \lambda}{\partial s}\Delta s \quad (8)$$

Observe that (7) conveniently involves the same matrix as the augmented Jacobian system of (6). So, to estimate the initial guess we also use the same two-step algorithm described before. This retains monotonicity in the continuation variable and greatly simplifies the implementation, because of the close similarity to the incremental scheme for non-singular problems. To adapt the arclength for overall efficiency and to maintain convergence near the singular point, a PID feedback control algorithm is introduced based on controlling accuracy as determined by truncation error estimates. More specifically, the arclength stepsize can be defined as follows

$$\triangle s_{n+1} = \left(\frac{e_{n-1}}{e_n}\right)^{k_P} \left(\frac{1}{e_n}\right)^{k_I} \left(\frac{{e_{n-1}}^2}{e_n e_{n-2}}\right)^{k_D} \triangle s_n \quad (9)$$

where

$$e_n = \frac{e_n^*}{\text{tol}} \qquad e_n^* = \frac{\| \frac{\partial u}{d\lambda}|_n - \frac{\partial u}{d\lambda}|_{n-1} \|}{\| \frac{\partial u}{d\lambda}|_n \|} \quad (10)$$

k_P, k_I and k_D are the PID parameters and *tol* is a supplied tolerance corresponding to the normalized changes of the most recent solution tangents with respect to the parameter λ. For the incremental Newton, a similar PID algorithm is used to choose the parameter increment, based on controlling the changes in the variables of interest between two consecutive solutions in the continuation process. The efficiency of this kind of control was demonstrated by Valli, Carey and Coutinho in [15, 13, 16]. Further, the computational overhead of the selection procedure is insignificant compared to solver operations, since the arclength stepsize selection involves only storing a few extra vectors and computation of associated norms.

Numerical Results

Numerical experiments were conducted for the "lid driven cavity" problem for a range of Reynolds (Re) numbers and for the Bratu reaction-diffusion problem with parameter continuation along a solution branch.

Lid Driven Cavity Problem: The lid-driven cavity flow is a standard test case for steady Navier-Stokes computations and there are numerous published results that can be used for comparison purposes [6, 14, 8]. The domain of analysis is a unit square. Both velocity components are prescribed to be zero, except at the top boundary (the lid) where the horizontal velocity component has a unit value. However, this problem is complicated by the presence of two corner singularities. As described in [6] and [11], this problem can be regularized. Prabhakar and Reddy [11] specify a hyperbolic tangent

u-velocity distribution on the top wall:

$$u(x) = \begin{cases} tanh(\beta x), & 0 \le x \le 0.5, \\ -tanh(\beta(x-1)), & 0.5 < x \le 1.0 \end{cases} \quad (11)$$

with $\beta > 0$. In the present study $\beta = 100$ is used, which give a smooth but at the same time sharp transition form $u = 0.0$ to $u = 1.0$ near the walls of the driven surface. For representative problems with Reynolds numbers of moderate order (up to 10^3), solutions can be achieved in few iterations using successive approximations or Newton-Raphson iterations. Figure 1 (top) shows how successive approximation and Newton iterations perform as problem Reynolds number increases. Results are for bilinear elements on a fixed uniform mesh ($h = \frac{1}{16}$) with initial zero velocities. As we can see, Newton iterations fail to converge for $Re > 10^3$. As the Re increases the convective term becomes more significant and the mesh size must be reduced accordingly to prevent oscillations and retain accuracy and convergence. To obtain a solution for much higher Re numbers we need an appropriate starting guess which can be obtained using some kind of continuation technique.

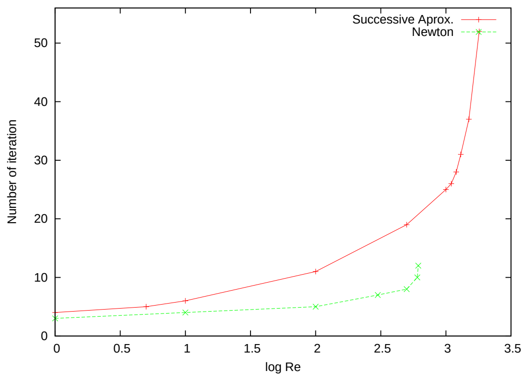

Figura 1: Total number of iterations as Re increases using successive approximations and Newton iterations.

For $Re = 12500$, we compare incremental Newton for fixed and adaptive Re number increments using bilinear elements on a 128×128 grid. For fixed step sizes, the initial Re number is 500 (the maximum Re number that we can achieved convergence) and then we use fixed increments of 1000. For the PID approach, the minimum and maximum Re increments are 500 and $3,000$, respectively, and the tolerance for changes in two consecutive velocities in the continuation process is $tol = 1$. Figure 2 (bottom) shows the number of total iterations when the Re number increases using fixed and adaptive increments. For $Re > 10^3$ standard Newton iteration from zero velocity fails to converge whereas PID continuation techniques permit more efficient solution for much higher Re numbers. The PID incremental solution for $Re = 12500$ is obtained in 46 Newton iterations, reducing the computational cost by about 31% when compared with fixed increments of $Re = 1000$. Figure 3 shows the horizontal velocity u along the vertical centerline (left) and the vertical velocity v along the horizontal centerline (right) for the lid driven cavity problem with $Re = 12500$ and the agreement is favorable when compared with the results in [3, 7]. We also compare the value of the stream function at the primary vortex center and the result shows difference of 5.e-3 with [3]. The method used there is a p-type finite element scheme for the fully coupled stream function-vorticity formulation and for $Re = 12,500$ they use a high resolution mesh $h = 1/32$, $p = 8$.

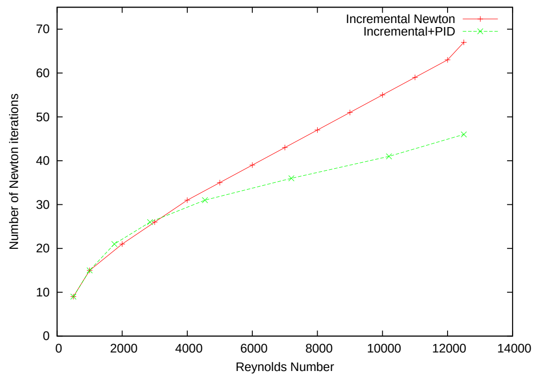

Figura 2: Total number of Newton iterations using incremental Newton and PID-incremental Newton.

Bratu Problem: The Bratu reaction-diffusion problem [5],

$$-\nabla^2 u = \lambda e^u \quad (12)$$
$$u = 0 \quad (13)$$

defined at the unit square domain, has a turning point near to the parameter $\lambda = 6.81$. The arclength approach with PID control is applied to follow the main branch of solutions with minimum and a maximum arclength stepsizes of 0.5 and 1.0 respectively and a tolerance of 0.1

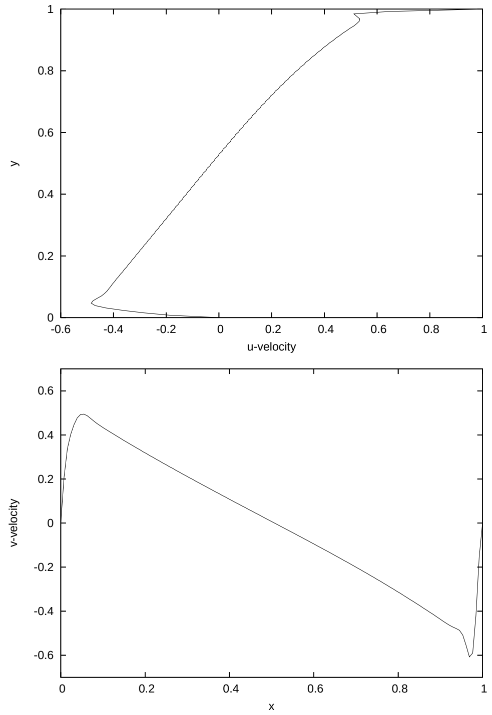

Figura 3: Computed u-velocity along the vertical centerline (top) and v-velocity along the horizontal centerline (bottom) for $Re = 12500$.

in the changes of the solution tangents with respect to the parameter λ. We consider 4-node isoparametric quadrilateral elements on a uniform 32×32 mesh. The algorithm uses the Newton-Euler approach to generate an initial guess for the Newton iterations, the maximum number of Newton iterations allowed is 20 and the Newton tolerance is 10^{-10}. Figure 4 shows the main branch of solutions and the arclength stepsize variation. With PID feedback, the arclength stepsize rapidly grows from the initial value to the maximum value until λ reaches approximately 5 (corresponding to an arclength parameter greater than 10). Following this, the PID controller reduces the arclength step to the minimum value to follow the solution branch through the turning point and then allows the stepsize to increase again. Using the PID control we are also able to estimate the turning point as $\lambda = 6.81278399$. Figure 5 shows the concentration solutions for two values of the parameter: $\lambda = 5.704$ and $\lambda = 0.904$ after the turning point.

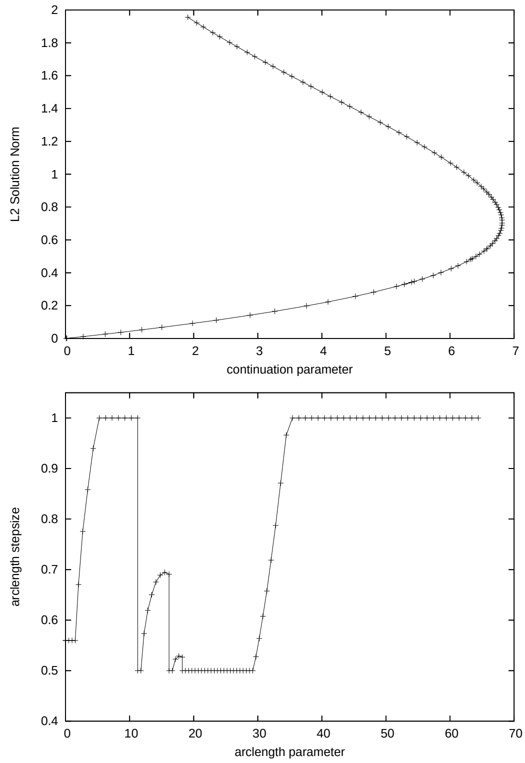

Figura 4: The main brach of the solutions (top) and the arclength stepsize variation (bottom).

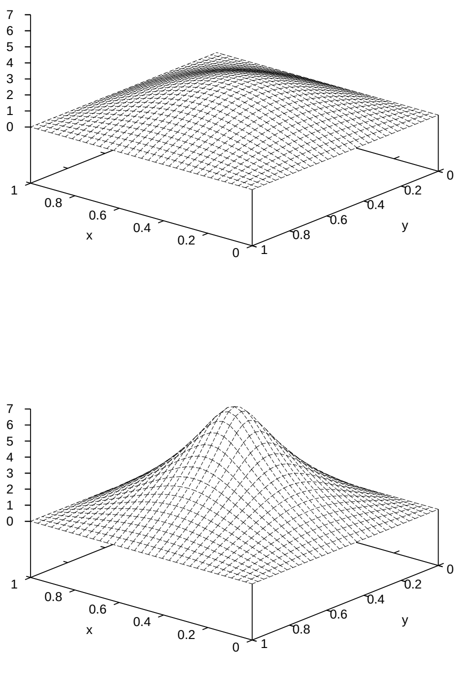

Figura 5: The concentration for the Bratu problem: $\lambda = 5.704$ (top) and $\lambda = 0.904$ (bottom) after the turning point.

Conclusion

Continuation methods with a PID control algorithm are developed to adapt the parameter stepsize and the arclength for branch tracing algorithms and are applied to representative flow and reaction-diffusion problems. The improved performance of the PID algorithm is verified in numerical experiments for the driven cavity problem and the Bratu reaction-diffusion problem. The PID continuation techniques permit more efficient solution for much higher *Re* numbers in the driven cavity problem, reducing the the computational cost by about 31% when compared with fixed increments. The PID feedback control algorithm is also a good technique to adapt the arclength for overall efficiency and to maintain convergence near the singular point in the Bratu problem.

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