FINITE ELEMENT SIMULATION AND CONTROL OF NONLINEAR FLOW AND REACTIVE TRANSPORT

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ABSTRACT

In this work we develop a decoupled scheme and finite element model for incompressible viscous flow with control for multi species reactive transport and thermal processes. The finite element flow formulation is based on a penalty Galerkin method and the nonlinear reactive transport application utilizes a Galerkin approach. One interesting aspect of the work is the introduction of adaptive active control for the timestep algorithm and for the boundary conditions in the transport processes, e.g., we investigate the suitability of a PID control scheme (for timestep control) and compare its efficiency with another time-stepping strategy. Supporting numerical studies are presented to demonstrate the approach.

1 INTRODUCTION

Since the early 1970's there has been a rapid expansion of research and applications for finite element simulations of fluid flow and transport processes. The subject area has matured to a point where the method is now applied to a wide variety of flow problems ranging from viscous incompressible non-newtonian flows to chemically reacting compressible high speed aerodynamic flows. Similarly, there are diverse applications to heat and species transport and to complex fluid flow and transport processes. For general treatments of these see, for instance, Carey and Oden [1]. There are now several commercial analysis programs that are based on this methodology.

With the evolution of the methodology and its extension to more complex classes of coupled problems there has been an increasing need for improved algorithms and other enhancements such as adaptive grid refinement and coarsening. For example, several adaptive timestepping strategies have been studied as a means to provide stable accurate transient (and steady state) solutions more efficiently. This adaptive timestepping selection process is usually approached by means of local truncation error analysis.

In like fashion, the adaptive grid schemes use feedback from the computed solution on a given intermediate grid to ascertain where the grid should be locally refined. We remark that both of these processes (adaptive timestep selection and adaptive grid refinement) can be viewed as examples of feedback control problems. This brings us to the main theme of the present work - the utilization of feedback control algorithms in conjunction with finite element analysis.

Of course, control theory has been extensively developed, particularly in electrical engineering and is also used widely in chemical engineering applications. Its potential in conjunction with an analysis technique such as finite elements is obvious, and yet there have been relatively few focussed studies in this direction. We argue that this situation is about to change dramatically as analysis software continuous to evolve and become more "fully automated". The focus in our work is two-fold: (1) the use of a control approach for automatic timestep selection; (2) the treatment of chemically reacting systems through automatic feedback control applied to boundary conditions. Only the first case will be consider in this short paper.

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The outline of the treatment is as follows. In the next section we briefly state the class of coupled flow and transport problems under investigation. The finite element formulation and solution approach is also given. Then in section 3 we describe a simple PID control approach and indicate how it can be applied to timestep control. Following this, a representative test problem for 2D coupled viscous flow and reactive transport is stated and results compared for fixed timestep, an adaptive timestep scheme in the literature and our PID control approach. Flow and species concentration results at the final time are also given.

2 COUPLED VISCOUS FLOW AND TRANSPORT

We are investigating applications arising in analysis of coupled incompressible viscous flow and heat or mass transfer. The present work will be restricted to steady viscous flow and coupled transient reaction-convection-diffusion processes. Accordingly, the flow is determined by approximate solution of the stationary incompressible Navier Stokes equations

$$-\nu\Delta\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla p = \mathbf{f} \quad (1)$$

$$\nabla\cdot\mathbf{u} = 0 \quad (2)$$

where $\mathbf{u}$ is velocity, p is pressure, $\mathbf{f}$ is the applied body force, $\nu > 0$ is the kinematic viscosity. Boundary conditions complete the stationary flow problem in (1), (2).

The transient transport equation is

$$\frac{\partial\mathbf{c}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{c} - \nabla\cdot(\mathbf{k}\nabla\mathbf{c}) = \mathbf{g}(\mathbf{c}) \quad (3)$$

where $\mathbf{c}$ is the concentration vector of component species (including temperature), $\mathbf{u}$ is the velocity tensor and $\mathbf{g}(\mathbf{c})$ is the chemical reaction source/sink term. From (3) it is clear that the time rate of change (evolution) of the species component fields depends on advection, diffusion and chemical reaction, respectively. Boundary conditions for species concentration or flux and initial conditions for concentrations complete the mathematical statement of the problem for (3). Of particular interest in the present work are time dependent boundary conditions to which control can be applied to achieve a desired behavior in the solution at a later time. For example, we may wish to adjust the boundary data so that the maximum concentration fluctuates within a certain range.

For simplicity and convenience we use a penalty method to enforce the incompressibility constraint. Introducing a finite element discretization and basis on Ω_h the variational boundary value problem reduces to solving for the velocity approximation $\mathbf{u}_h \in H^h$ satisfying

$$\int_{\Omega_h} \nu\nabla\mathbf{u}_h{:}\nabla\mathbf{v}_h\; dx + \int_{\Omega_h} \mathbf{u}_h\cdot\nabla\mathbf{u}_h\cdot\mathbf{v}_h\; dx - \frac{1}{\epsilon}\mathbf{I}\,(\nabla\cdot\mathbf{u}_h)(\nabla\cdot\mathbf{v}_h)\; dx = \int_{\Omega_h} \mathbf{f}\cdot\mathbf{v}_h\; dx,\;\; \forall\mathbf{v}_h \in {H_0}^h \quad (4)$$

where we have assumed essential boundary data for $\mathbf{u}_h$ such that $\mathbf{v}_h$ vanishes on the boundary, and $\mathbf{I}$ denotes reduced numerical integration. This leads to the nonlinear algebraic system

$$\mathbf{A}\mathbf{u} + \mathbf{b}(\mathbf{u}) + \frac{1}{\epsilon}\mathbf{C}\mathbf{u} = \mathbf{F} \quad (5)$$

which is solved by Newton's method in the present study.

Similarly, introducing a Galerkin finite element scheme for transport component c_i

$$\int_{\Omega_h} \left(\frac{\partial c_{h_i}}{\partial t}\omega_h + \mathbf{u}_h\cdot\nabla c_{h_i}\,\omega_h + \mathbf{k}\nabla c_{h_i}\cdot\nabla\omega_h \right)\; dx = \int_{\Omega_h} g_i(\mathbf{c})\,\omega_h\; dx,\;\; \forall\omega_h \in {V_0}^h \quad (6)$$

where again we have assumed essential data for convenience. The resulting semi-discrete ODE system for the nodal vector $\mathbf{c}_i$ (component i) has the form

$$\mathbf{M}\frac{d\mathbf{c}_i}{dt} + \mathbf{B}(\mathbf{u})\,\mathbf{c}_i + \mathbf{D}\,\mathbf{c}_i = \mathbf{g}_i \quad (7)$$

where $\mathbf{g_i}$ depends on the unknown species solution. We integrate the ODE system implicitly using a Crank-Nicolson scheme with timestep $\triangle t$. That is, at each timestep $\triangle t$ we solve systems of the form

$$\mathbf{P}\mathbf{c}^{n+1} = \mathbf{d} \tag{8}$$

where n denotes the timestep index. The timestep may be chosen adaptively and in the next section we describe one possible strategy that utilizes a PID control scheme based on the approach in Coutinho and Alves [2].

3 ADAPTIVE CONTROL

One of the most widely used algorithms for closed-loop control is the three-term control, known as the Proportional-Integral-Differential (PID) control loop. The popularity of PID controllers can be attributed to their functional simplicity and to their robust performance in a large range of operating conditions. The objective in using PID control algorithms is to control the output along a smooth curve (vs. time) towards the set-point while minimizing overshoot, the amount the system output response proceeds beyond the desire response.

Stepsize selection algorithms in most integration methods are based on control of the maximum change in the key variables (pressure, saturation/concentration, etc.). According to Hairer and Wanner [4], stepsize selection can be viewed as an automatic control problem with a PID controller defined as

$$\triangle t_{n+1} = (\frac{e_{n-1}}{e_n})^{k_P} (\frac{tol}{e_n})^{k_I} (\frac{{e_{n-1}}^2}{e_n e_{n-2}})^{k_D} \ \triangle t_n, \tag{9}$$

where tol is some input tolerance, e_n is the measure of the change of the quantities of interest in time step $\triangle t_n$, and k_P, k_I and k_D are the PID parameters.

An estimate of the solution change is compared with the specified accuracy requirement, and the result is fed back to calculate the new time step. The controller tries to select the stepsize such that e_n comes as close as possible to the input tolerance, tol, along a smooth curve. For time step n = 2, 3, ... we may proceed sequentially as follows:

1. Given $(\triangle t)_{min}$, $(\triangle t)_{max}$, k_p, k_I, k_D, and tol, and starting with $\frac{e_{n-2}}{tol} = \frac{e_{n-1}}{tol} = 1.0$, and $\triangle t_{n+1}$ = $\triangle t_n$ = some initial timestep value.

2. calculate e_n.

3. if $e_n > tol$ reject the timestep:

   - t^{n+1} = t^n - $\triangle t_n$
   - $\triangle t_{n+1}$ = max ($\frac{tol}{e_n}\triangle t_n$, $\triangle t_{min}$)
   - $c^{n-1} \leftarrow c^n$

   else

   - calculate $\triangle t_{n+1}$ using (9)
   - $\triangle t_{n+1}$ = max ($\triangle t_{n+1}$, $\triangle t_{min}$)
   - $\triangle t_{n+1}$ = min ($\triangle t_{n+1}$, $\triangle t_{max}$)

4. $e_{n-2} = e_{n-1}$, $e_{n-1} = e_n$.

In the present work the measure of the relative change e_n of the concentration over a timestep is evaluate by computing $\frac{\|\mathbf{c}^{n+1}-\mathbf{c}^n\|}{\|\mathbf{c}^{n+1}\|}$, where c^n is the approximate concentration at time t^n, and $\|\cdot\|$ denotes the Euclidean norm. We supply timestep limiters, $(\triangle t)_{min}$ and $(\triangle t)_{max}$, to prevent an excessive growth or reduction of the time step ("anti_windup effect").

If a timestep gives an unacceptable value of e_n, the step is rejected. Then the step is repeated with a scaled timestep size based on the magnitude of the error relative to the tolerance. However, we find

in numerical experiments that the number of rejections is very small, producing a smooth sequence of timesteps. In our algorithm, if the sequence of iterates of the nonlinear system is converging at a slow rate, the timestep is also rejected.

Although feedback control theory provides sophisticated techniques to choose the PID parameters, robustness is required when a general finite element method is used for a wide range of different simulations. We perform parametric studies of the PID controller for values similar to those used by Gustaffson et al. [5] and also by Coutinho and Alves [2]. Subsequent numerical experiments demonstrate that the PID controller is very robust for the reaction-diffusion application studied here.

4 NUMERICAL RESULTS

To test the approach, we first construct a problem on the unit square domain and $t > 0$ having analytic solution

$$c(x, y, t) = 10^2(t+1)^2 x(x-1)y(y-1)$$

for the concentration. The velocity field for Stokes flow is

$$\mathbf{u}(x, y, t) = ((x^2(1-x)^2(2y - 6y^2 + 4y^3),\ y^2(1-y)^2(2x + 6x^2 - 4x^3)),$$

We assume coefficients of dispersion in the x and y directions have been normalised so that, $k_{11} = k_{22} = 1$, and $k_{12} = k_{21} = 0$. The reaction term is taken to be $-c^2 + f$, where f is a function of (x, y, t). The initial condition is taken as the exact solution at the initial time t = 0, and we specify essential boundary conditions, $c(t, x, y) = 0$, on the unit square domain. Since we are interested in the time integration error control we select for this study biquadratic basis functions and a mesh with 2×2 elements. Therefore, the solution at any time t is exactly represented in the finite element basis so that the approximation error is associated with time discretization.

First we calculate the solution at $t = 0.1$ for a fixed time step $\Delta t = 10^{-04}$, and then we compare this with the PID timestep control approach. We also include a comparison with another heuristic adaptive stepsize selection scheme by Winget and Hughes [6]. Table 1 shows the L^2-norm of the error in the concentration solution, the number of time iterations, *ntstep*, the number of rejected steps, *nrejec*, and the number of Newton iterations, *newt*, for different values of the PID parameters.

case	k_p, k_I, k_D	error	*ntstep*	*nrejec*	*newt*
1	0.1 0.3 0.015	$.39033754E-05$	62	0	124
2	0.075 0.175 0.01	$.38654828E-05$	62	0	124
3	0.1 0.16 0.011	$.38823761E-05$	63	0	126
4	0.06 0.13 0.008	$.38599892E-05$	63	0	126
5	0.08 0.216 0.0116	$.38827800E-05$	62	0	124
6	0.15 0.32 0.017	$.38890713E-05$	63	1	128
7	No control	$.13885237E-05$	100	0	200
8	Winget & Hughes	$.33119825E-05$	66	0	132

Table 1: Results for the PID controller using bilinear elements on a 2×2 grid.

With the PID control strategy we find the approximate solutions with a much smaller number of steps without any significant loss of accuracy (Table 1). We also find that the PID controller is very robust. The timestep size is plotted against time for Cases 2 and 8 in Figures 1 and 2, respectively. We see in Figure 1 that the PID controller produce a smooth sequence of time steps. The approach of Winget and Hughes also shows good results for this particular example.

The next problem is nonisothermal reaction on a catalyst section $\Omega = (0, 1) \times (0, 1)$ defined by [3]

$$-\nabla^2 T \quad = \quad \beta\phi^2 c\ exp(\gamma(1 - \frac{1}{T}))$$

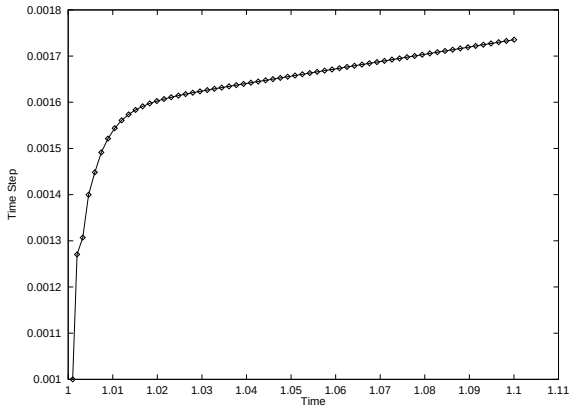

Figure 1: Time step variation for case 2 on a 2×2 grid using PID controller.

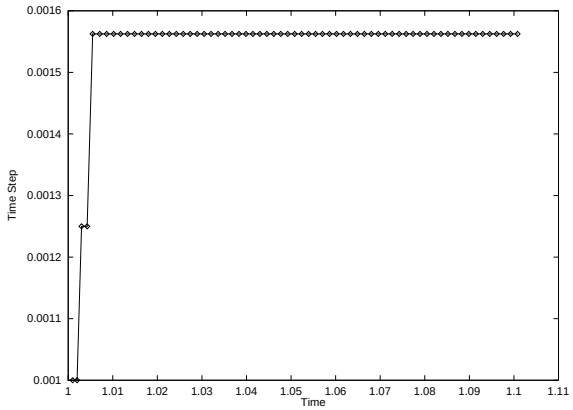

Figure 2: Time step variation on a 2×2 grid using Winget and Hughes approach.

$$-\nabla^2 c \quad = \quad -\phi^2 c \; exp(\gamma(1 - \frac{1}{T})),$$

where T is the temperature, c is the concentration, ϕ is the Thiele modulus, and β and γ are dimensionless variables. We assume $T = c = 1$ on the right side of the unit square, and no flux on the rest of the boundary. The initial conditions are taken as $T = c = 1 + sin(\pi x)sin(\pi y)$.

The approximate solution was calculated for $\beta = 0.6$, $\gamma = 20$, $\phi = 0.5$, and a grid with 8×8 bilinear elements. We first obtain the approximate solution for a fixed time step of 10^{-04}. In the PID control we assume parameters $k_p = 0.075$, $k_I = 0.175$, and $h_D = 0.01$, an initial timestep of 10^{-04}, and a tolerance of 10^{-06} for changes in nodal temperature and concentration. We allow a minimum and a maximum time step of 10^{-04} and 10^{-03}, respectively. Table 2 shows the performance results for each case studied, and Figures 3 and 4 show plots of timestep size for PID controller and Winget and Hughes approach, respectively.

Since we have a much stronger nonlinearity in this problem than in the previous one, we can better observe the advantage of using timestepping control. In this problem the PID control also shows better results than the approach used by Winget and Hughes.

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case	*ntstep*	*nrejec*	*newt*
No Control	936	0	2065
PID Control	166	0	563
Winget&Hughes	178	8	623

Table 2: Results for the steady state catalyst problem using time control.

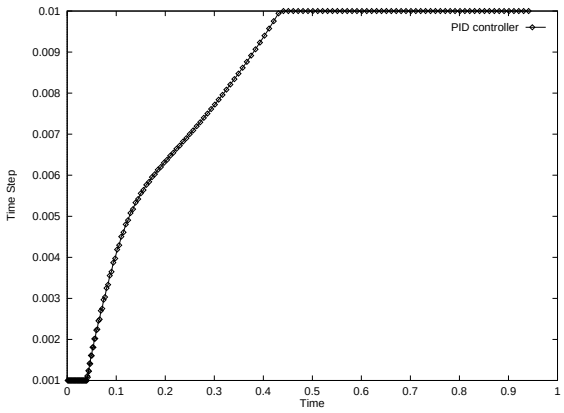

Figure 3: The time step variation for the steady state catalyst problem using PID controller.

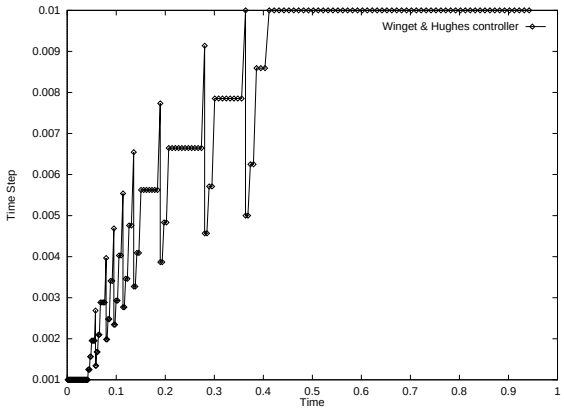

Figure 4: The time step variation for the steady state catalyst problem using Winget&Hughes approach.