CHAPTER 29

A Domain Decomposition Approach for the Computation of Incompressible Flow by the Pseudospectral Matrix Element Method and Its Parallel Implementation

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Abstract

A recently developed pseudospectral matrix element (PSME) method [1], which extended the formulation of the pseudospectral matrix (PSM) method to a multi-element scheme, has been applied by the authors to the solution of the incompressible, primitive variable, Navier-Stokes equations for complex geometries in two and three dimensions. This has been accomplished by a new implementation of the Schwarz alternating procedure (SAP), which allows computation of the flow field in such geometrical configurations. The SAP divides the computational domain into a number of overlapping subdomains, of simpler geometry with patched grid points, in which the solution is more easily obtained. With an iterative procedure between subdomains, the complete solution is found.

A new domain decomposition (DD) procedure follows the original PSM method and employs only the continuity equation as the subdomain pressure boundary condition (including the overlapped interfaces) that permits one to utilize the eigenfunction expansion of the resulting pressure operator to reduce the original multi-dimensional problem to a series of one-dimensional ones. Appropriate downstream boundary conditions have been developed for the PSME method in the domain decomposed solutions which makes this method very attractive for computing inflow-outflow problems on a truncated domain of fewer nodes.

The PSME method on the decomposed domains has been efficiently implemented in parallel without making any processor sit idle. This is accomplished by developing fully parallelizable code for each overlapping subdomain and solving for each in turn.

Computational results for both two- and three-dimensional flow over a backward facing step at different Reynolds numbers are presented in this paper. No pronounced three-dimensional effects are observed except in the boundary layer along in the spanwise direction.

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1 Introduction

The solution of boundary-value problems for complex geometries has been successfully implemented by exchanging data among the different zones (or subdomains), i.e. solving the problem on each subdomain separately and then updating the boundary values on the overlapped interface. The data exchange can been done in a straight forward manner, this is what is usually called SAP [2]. Fuchs [3] pointed out that one major difficulty with the SAP when solving the incompressible Navier-Stokes equations in streamfunction-vorticity form for a rigid body confined in a flow region is that the value of streamfunction is unknown on the surface of the rigid body. In primitive variables the question arises of how the boundary conditions for the pressure are handled on the interatively solved subdomains even with the prescribed velocity components. Instead of directly imposing conditions on both the pressure and its first derivatives at the edge of each overlapped region [4], the consistent use of the continuity equation to generate the subdomain pressure boundary conditions (including the overlapped interfaces) should be preferable. This is mainly because the former definitely creates non divergence-free velocity fields along the imaginary overlapped interfaces while the latter still guarantees differential mass conservation there.

Flow over a backward step is always presented as the standard test problem for different numerical schemes. Some investigators [5,6] assumed that the fully developed velocity profile is established right at the step and some considered the upstream effect before the step. Recently Armaly [7] *et al.* have performed a careful experimental study of such a flow for a wide range of Reynolds number. Although great care was taken to ensure that the initial inlet flow was two-dimensional, in addition to the well-known entrance effects they also found that as the Reynolds number increased above 450 three-dimensional effects became gradually apparent downstream from the step. These results motivated us to do numerical experiments on three-dimensional flow over a backward step.

For the purpose of high-speed computation, the issue of how to map a numerical algorithm for the solution of each subdomain onto the specific architecture of parallel machines so as to achieve highly parallel performance remains an open question. There are roughly two approaches to this problem: (1) distribute processors proportional to the amount of cpu time required per subdomain or (2) allocate all the processors to a single subdomain and do different subdomains in sequence. The first one seems to be far reached due to the requirement of a complier smart enough to anticipate the cpu time difference among subdomains, otherwise some processors with their jobs done earlier hâve to be sit idle until other processors finish their jobs. On the contrary, there is no data communication constraint for the second one and it becomes more attractive if the computation of each subdomain can be highly parallelizeable. In this paper, authors would like to use this concept to apply PSME method to the solution of incompressible flows in complex geometries. Although originally designed for a shared memory parallel processor with a few computational elements, our code is written entirely in terms of the proposed Fortran 8x standard and can be run on any machine (parallel or not) for which a complier implementing the standard exists.

2 Calculation of derivatives by PSME method

For simplicity, the spatial domain is divided into NE elements each of which has $N+1$ collocations, $x_j = 1/2[(b^e - a^e)\cos\pi(j-1)/N + b^e + a^e]$ $(1 \le j \le N+1; 1 \le e \le NE)$. The derivatives of a function $f(x)$ in the interior of element e can be discretized as

$$f_x^e(x_i) = \frac{1}{L^e}\sum_{m=1}^{N+1} \hat{GX}_{i,m}^{(1)} f_m^e \tag{1a}$$

$$f_{xx}^e(x_i) = \frac{1}{(L^e)^2}\sum_{m=1}^{N+1} \hat{GX}_{i,m}^{(2)} f_m^e = \frac{1}{L^e}\sum_{m=1}^{N+1} \hat{GX}_{i,m}^{(1)} (f_x^e)_m \tag{1b}$$

here L^e is the length of eth element defined on the interval $[a^e, b^e]$; $f_m^e \equiv f^e(x_m)$ and $\hat{\mathbf{GX}}^{(1)}$, $\hat{\mathbf{GX}}^{(2)}$ are the invariant derivative matrices based on the domain [0,1].

The interfacial derivatives at the inter-element points, are approximated by weighting of the derivatives from each side, according to the relations

$$f_x|_{interface} = \alpha f_x^e + \beta f_x^{e+1} \tag{2a}$$

$$f_{xx}|_{interface} = \alpha f_{xx}^e + \beta f_{xx}^{e+1}, \quad \alpha + \beta = 1, \quad 1 \le e \le NE - 1 \tag{2b}$$

With the choice of $\alpha = L^e/(L^e + L^{e+1})$, the fraction of total length of two adjacent elements, Eqs. (2), in view of Eqs. (1), now become

$$f_x|_{interface} = \frac{1}{L^e + L^{e+1}} \sum_{m=1}^{N+1} (\hat{GX}_{N+1,m}^{(1)} f_m^e + \hat{GX}_{1,m}^{(1)} f_m^{e+1}) \tag{3a}$$

$$f_{xx}|_{interface} = \frac{1}{L^e + L^{e+1}} \sum_{m=1}^{N+1} (\hat{GX}_{N+1,m}^{(1)} (f_x^e)_m + \hat{GX}_{1,m}^{(1)} (f_x^{e+1})_m) \tag{3b}$$

In Eq. (3a), c^0 continuity is explicitly assumed whenever the calculation of interface values of the first derivative is required. However, c^0 continuity is only implicitly assumed for the second derivative calculation. We can expand Eq. (3b) using Eq. (1b) and impose c^1 continuity to get

$$\begin{aligned} f_{xx}|_{interface} = \; & \frac{1}{L^e + L^{e+1}} [\sum_{m=1}^{N+1} (BX_{N+1,m}^* f_m^e + BX_{1,m}^{**} f_m^{e+1}) + \\ & (\hat{GX}_{N+1,N+1}^{(1)} + \hat{GX}_{1,1}^{(1)}) f_x|_{interface}] \end{aligned} \tag{4}$$

where it has been implicitly assumed that $f_x^e(x_{N+1}) = f_x^{e+1}(x_1) = f_x|_{interface}$. As will be shown shortly, the explicit value of $f_x|_{interface}$ is never needed. This requirement is met by the finite element method employing variational or Galerkin procedures wisth trial functions that are c^0 across element boundaries, i.e., flux (first derivative) continuity is intrinsically satisfied through integration by parts. This is exactly the same for the PSME method because the second term in the bracket of Eq. (4) is automatically cancelled out since, $\hat{GX}_{1,1}^{(1)} = (2N^2 + 1)/3 = -\hat{GX}_{N+1,N+1}^{(1)}$. The elements of the modified matrices $\mathbf{BX}^*, \mathbf{BX}^{**}$ are

$$BX_{N+1,m}^* = \frac{1}{L^e} \sum_{n=1}^{N} \hat{GX}_{N+1,n}^{(1)} \hat{GX}_{n,m}^{(1)} \tag{5a}$$

$$BX_{1,m}^{**} = \frac{1}{L^{e+1}} \sum_{n=2}^{N+1} \hat{GX}_{1,n}^{(1)} \hat{GX}_{n,m}^{(1)} \tag{5b}$$

In order to set up a simple and efficient matrix operation for derivatives by the PSME method, an operator with global-type structure which combines each local element derivative can be constructed. Therefore, Eqs. (1a) and (3a) representing the first derivatives can be cast into the form

$$\mathbf{f}' = \mathbf{G}^{(1)} \mathbf{f} \tag{6}$$

where $\mathbf{G}^{(1)}$ has the diagonal form

$$\mathbf{G}^{(1)} = \begin{bmatrix} \mathbf{A}^{(1)} & & & & \\ & \mathbf{A}^{(2)} & & & \\ & & \mathbf{A}^{(3)} & & \\ & & & \ddots & \\ & & & & \mathbf{A}^{(NE)} \end{bmatrix} \tag{7}$$

The hatched area in Eq. (7) arises from the Eq. (3a) at the element-element interface while the non-overlapped area is simply Eq. (1a) in the interior of each element. The blocks $\mathbf{A}^{(n)}, n = 1, ..., NE$ are of size $(N+1)^2$ with one point overlaped region at the corners, and the overall size of matrix $\mathbf{G}^{(1)}$ is $(NX+1)^2$.

In an analogous manner, second derivative of Eqs. (1b) and (3b) can be plugged into the form

$$\mathbf{f}'' = \mathbf{G}^{(2)}\mathbf{f} \tag{8}$$

where $\mathbf{G}^{(2)}$ has the same diagonal form as $\mathbf{G}^{(1)}$.

The proposed PSME method has been tested on a standard one-dimensional convection-diffusion problem [1] as well as stationary shock wave of Burger's equation [8]. Spectral accuracy is observed for both cases.

3 Governing equations

The three-dimensional flow over a backward step (shown in Fig. 1) with an expansion ratio 2 in the vertical direction and an aspect ratio of 8 in the spanwise direction can be represented in a primitive variable formulation. In cartesian coordinates, the time-dependent Navier-Stokes equations in dimensionless form can be written as

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{\mathrm{Re}} \frac{\partial^2 u_i}{\partial x_j^2} \tag{9a}$$

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{9b}$$

Here u, v, w are the velocity components in the horizontal, vertical and spanwise direction, respectively, and Re is the Reynolds number, $\rho US/\mu$, where ρ is the density, U is the maxium velocity of inflow, S is the step height, and μ is the viscosity.

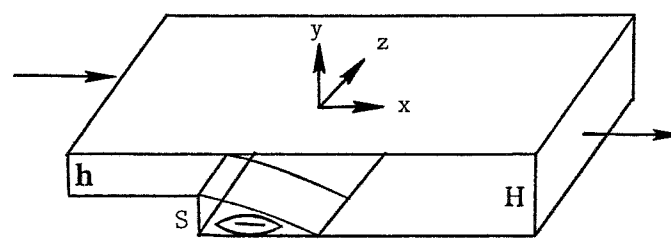

Figure 1: Three-dimensional configuration for flow over a backward step

Eqs. (9) are only solved for half of the domain due to the experimental results [7] of symmetry about the xy plane at $z = 0$, i.e., u, v, p are symmetric and w is anti-symmetric with respect to the central plane. Initially fully developed profiles are used for both the upstream and downstream regions. At the time $t > 0$, the boundary conditions are given

by

$$v = w = 0, u = 4(y - y^2) \quad \text{at } x = -2 \tag{10a}$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 v}{\partial x^2} = \frac{\partial^2 w}{\partial x^2} = 0 \quad \text{at } x = l \tag{10b}$$

$$u = v = w = 0 \quad \text{at } y = 1 \tag{10c}$$

$$u = v = w = 0 \quad \text{at } y = 0 \text{ for } x \leq 0 \tag{10d}$$

$$u = v = w = 0 \quad \text{at } y = -1 \text{ for } x \geq 0 \tag{10e}$$

$$u = v = w = 0 \quad \text{at } z = 4 \tag{10f}$$

$$\frac{\partial u}{\partial z} = \frac{\partial v}{\partial z} = \frac{\partial p}{\partial z} = 0, w = 0, \quad \text{at } z = 0 \tag{10g}$$

Appropriate outflow boundary conditions should have little influence on the upstream flow development. This is usually the case when the upstream continuously generates the disturbance which will be propagated into the downstream.

Note that different downstream boundary conditions are possible, for instance in the two-dimensional case

1. u, v both prescribed
2. $\frac{\partial u}{\partial x} = 0$, $v = 0$
3. $\frac{\partial v}{\partial x} = 0$, $\frac{\partial^2 u}{\partial x^2} = 0$
4. $\frac{\partial^2 u}{\partial x^2} = 0$, $\frac{\partial^2 v}{\partial x^2} = 0$

Conditions (1) & (2) seem too restrictive to be applied on the truncated domain, while conditions (3) & (4) yield the least effect upon the upstream flow development.

4 Primitive variable formulation

The method used for solving the Navier-Stokes equation is Chorin's [9] splitting technique. According to this scheme, the equations of motion, in tensor form, are

$$\frac{\partial u_i}{\partial t} + \frac{\partial p}{\partial x_i} = F_i \tag{11}$$

where $F_i = -u_j \partial u_i / \partial x_j + 1/\mathrm{Re} \partial^2 u_i / \partial x_j^2$.

The first step is to split the velocity into a sum of predicted and corrected value. The predicted velocity is determined by time integration of the momentum equations without the pressure term

$$\bar{u}_i^{n+1} = u_i^n + \Delta t F_i^n \tag{12}$$

The second step is developing the pressure and corrected velocity field that satisfies the continuity equation by using the following relationships

$$u_i^{n+1} = \bar{u}_i^{n+1} - \Delta t \frac{\partial p}{\partial x_i} \tag{13a}$$

$$\frac{\partial u_i^{n+1}}{\partial x_i} = 0 \tag{13b}$$

By taking the divergence operator to Eq. (13a) in order to satisfy the continuity equation, Eq. (13b), throughout the whole domain, and incorporating of prescribed velocity boundary conditions, it generates the pressure Poisson equations in the interior as well as the supplemental pressure equations at the boundaries. Neumann type boundary conditions rather than those derived from the continuity equation are used for the pressure in the z direction because the inflow is discontinuous in the z direction. This leads to non divergence-free velocity only at the solid wall in the z direction, while the continuity equation is still satisfied for the rest of the domain. This problem does not appear in the two dimensional case.

Following the eigenfunction expansion technique (see detailed procedure in Ref. [10], [12]), the original three-dimensional pressure equation is reduced to a simple one-dimensional matrix operator. Therefore, the overall solution of pressure can be obtained through the linear superposition of each eigenvalue and its associated eigenvectors.

5 Schwarz alternating procedure

The SAP for iterative solution of the incompressible Navier-Stokes equations in primitive variable form for the three-dimensional flow over a backward step is summarized as follows (see Figure 2):

1. First assume $u^{n+1}, v^{n+1}, w^{n+1}$ on □ABMN. Usually u^n, v^n, w^n would be a good initial guess.

2. Solve domain II ∪ III employing boundary conditions derived from the continuity of velocity field on □ABMN, i.e., $\partial u/\partial x = -\partial v/\partial y - \partial w/\partial z$ where the pressure Poisson equation is solved by an eigenfunction expansion technique.

3. With the solutions of $u^{n+1}, v^{n+1}, w^{n+1}$ on □NBEX from step (2), solve domain I ∪ II employing the same type boundary conditions as above for the pressure on □NBEX, i.e., $\partial v/\partial y = -\partial u/\partial x - \partial w/\partial z$, to update $u^{n+1}, v^{n+1}, w^{n+1}$ on □ABMN.

4. Repeat steps (2) & (3) until the convergence tolerance has been met for $u^{n+1}, v^{n+1}, w^{n+1}$ along □ABMN, □NBEX.

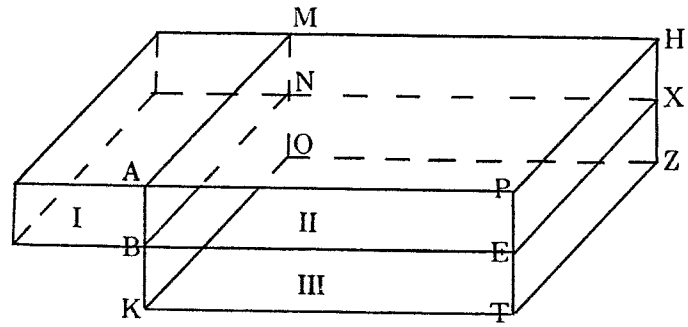

Figure 2: Three-dimensional configuration of domain decomposition

The novel features of this iteration scheme are: (i) for each iteration the divergence free condition is exactly satisfied everywhere except the boundary points in the direction where inflow carries the singular information; (ii) for every time step only a few iterations (usualy

$2 \sim 4$) are required to reach the converged solution for velocity components u, v, w; (iii) consistent mass conservation holds along $\overline{BN}$ despite a singular value for the vorticity and (iv) within each subdomain the eigenfunction expansion technique is still available to decompose the original three-dimensional problem into a simple one dimensional matrix operator.

6 Parallel implementation of N-S Equations

The method used to compute the solution of the Navier-Stokes equations in parallel performance is very important for the technique of domain decomposition with SAP. The basic idea is that in alternately performing steps (2) and (3) of section 5 all processors are used to update whichever subdomain II $\cup$ III or I $\cup$ II is current. Updating such a geometrically simple region can be performed efficiently in parallel [1] as we now sketch.

In our version of the time splitting approach for a single domain three steps account for most of the run time. These are computing the partial derivatives involved in updating the predicted velocity, transforming back and forth from physical to eigenfunctional space, and solving the sequence of reduced one-dimensional pressure equations in eigenfunction space.

The first two steps can be reduced to *dotproducts* and *matrix multiplications* between subsets of multimensional arrays - basic linear algebra operations defined in the proposed Fortran 8x standard and efficiently implementable on wide classes of vector, parallel and vector-parallel machines.

The key point of the last step is that instead of performing the whole backward substitution for each reduced pressure equation in turn, we perform one step of the backward substitution for all of the reduced pressure equations before going to the next step. Since the eigenfunction expansion has made each reduced equation independent, it is easy to parallelize each partial backward substitution.

Table I & II show some timings for the implementation of our program for the solution of both two- and three-dimensional flow over a backward step at Reynolds number 375 (four iterations of SAP) with $NX = 61$ (10 elements), $NY = 37$ (6 elements) at downstream, while NX=13 (2 elements), NY=19 (3 elements) atupstream and $NZ = 49$ (single element), running on an Alliant FX/8-series (eight processors) computer.

Table I. Cpu time in seconds per time step (2D)

number of processors	1	2	3	4	8
	4.07	2.10	1.48	1.18	0.74
speedup*	1	1.94	2.75	3.45	5.52

*: compared to 1 processor

Table II. Cpu time in seconds per time step (3D)

number of processors	1	2	3	4	8
	235.5	127.7	90.1	73.5	43.5
speedup*	1	1.84	2.61	3.20	5.42

*: compared to 1 processor

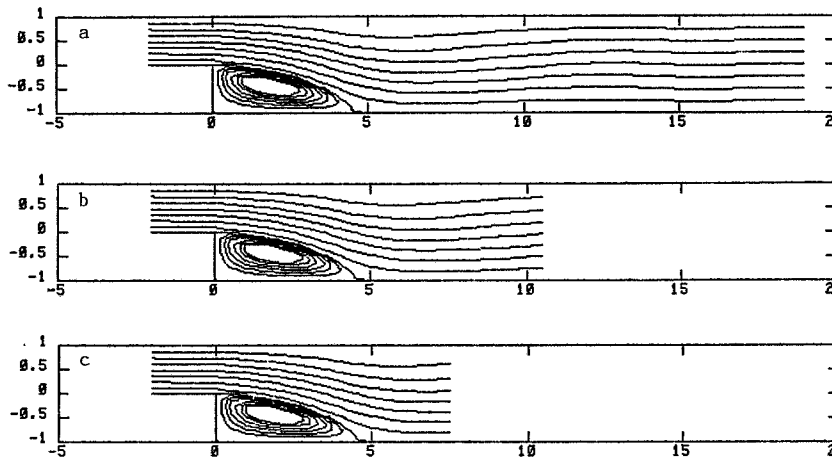

Fig. 3. Flow over a step, Re = 150, with downstream conditions at x/S = : a) 19.0, b) 10.5, c) 7.5

Note that using eight processors speeds the computation by a factor of 5.5, approximately 70% of the maximum possible value. It is worth emphasizing that our program is written entirely in terms of the proposed Fortran 8x standard and can be run on any machine for which a compiler implementing the standard exists.

7 Results and discussion

This section presents the results obtained by applying the present scheme, domain decomposition with SAP, to the two- and three-dimensional flow over a backward step. First, we will examine the effect of our downstream boundary conditions, the second derivative of velocity components vanishing in the streamwise direction, upon upstream flow development. Fig. 3 shows that the reattachment length at Re = 150 with downstream position X/S =19 (8 elements), 10.5 (5 elements) and 7.5 (4 elements) agrees very well with those found by Dirichlet boundary condition applied at infinity by the same method. Even the minimum streamfunction, i.e., ψ_{min}= -0.04421, -0.04434, -0.04425 for X/S = 19, 10.5 and 7.5, respectively, exhibits the same accuracy when compared to [11], ψ_{min}= -0.0436 by using 33*297 grid points. Fig. 4 provides streamline plots for the range of Reynolds number between Re =75 and Re = 375. As expected, with increasing Reynolds number, the downstream reattachment length of flow development increases up to Re = 375.

As Armaly *et al.* have pointed out, the deviation of the two-dimensional flow calculations from experimental results is due to three-dimensionality of the experimental flow observed above some certain Reynolds number. From the numerical results of three-dimensional flow, we find that the flow remains two-dimensional except in the boundary layers for Reynolds number, Re = 225, 300, 375, as is demonstrated by the plot of the spanwise location of the reattachment line shown in Fig. 5.

8 Conclusions

Domain decomposition with SAP has been used to solve the three-dimensional incompressible Navier-Stokes equations in primitive variable form in order to simulate flow over a

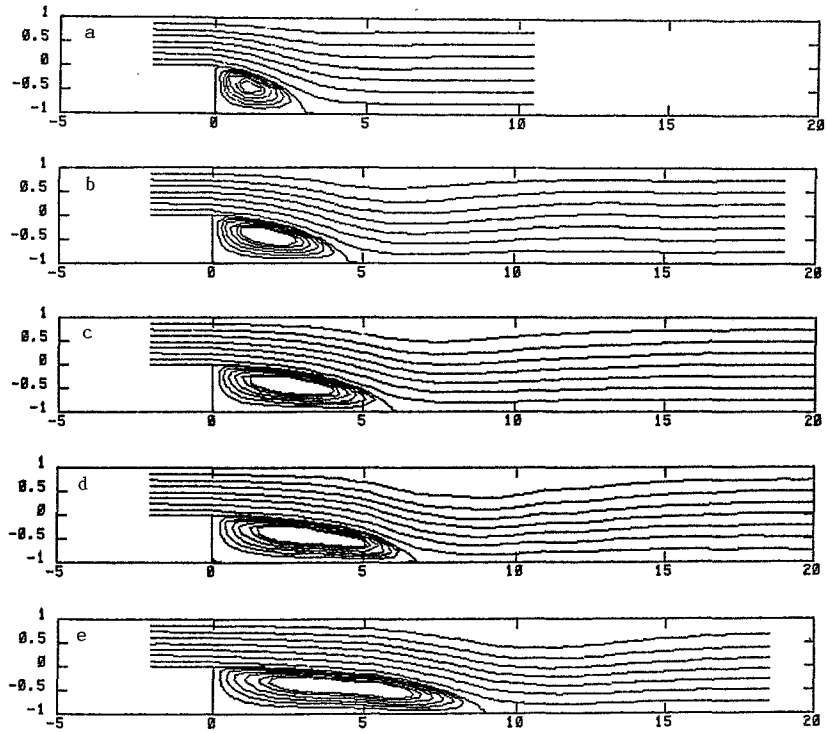

Fig. 4. Streamlines for flow over a step with Re = : a) 75, b) 150, c) 225, d) 300, e) 375

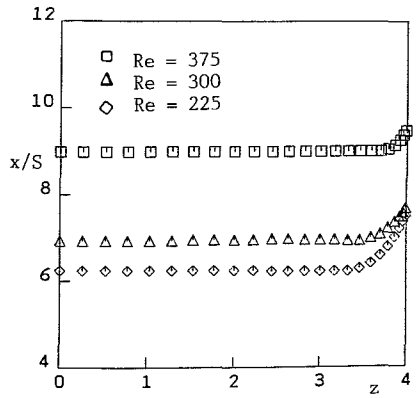

Fig. 5. Spanwise location of reattachment line with different Reynolds numbers

backward step. In the solution approach, the complex geometry is divided into a few subdomains, each of simple geometry, where the pressure solution can be easily obtained. With the continuity equation as the boundary conditions at the overlapped interfaces, an eigenfunction expansion technique can be applied to each subdomain to give the direct and fast solution of the three-dimensional pressure Poisson equations in one-dimensional form so that the parallel implementation of each subdomain could be easily achieved.

Numerical results computed by the PSME method are in good agreement with the two-dimensional experimental results. For Reynolds number up to 450, we found three-dimensional effects confined to the boundary layer region in the spanwise direction.

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