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# FINAL REPORT ON 

 AFOSR CONTRACT F49620-83-C-0064Steven A. Orszag, Principal Investigator<br>Department of Mathematics MIT

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# FINAL REPORT ON AFOSR CONTRACT F49620-83-C-0064 

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Cambridge, MA 02139
-In the attactred-papers, we summarize work done on this research project. The major results include:

1. Development of renormalization group techniques for large-eddy simulations of turbulent flows.
2. The first direct numerical simulation of turbulent spots in channel and boundary layer flows.
3. The further development of spectral methods for turbulence simulations.
4. The identification of secondary instability modes in free shear layers.
5. The development of an efficient multi-grid marching method for solution of the parabolized Navier-Stokes equations.
6. A mathematical analysis of boundary conditions for the parabolized compressible Navier-Stokes equations.
7. The further development of a method to improve numerical solu tion of singular perturbation problems by use of asymptotic approximations.

Further details are given in the attached papers.

## List of Papers

M. Israeli and P. Bar-Yoseph, Numerical Solution of Multi-Dimensional Diffusion-Convection Problems by Asymptotic Corrections, in Proc. Fifth GAMM-Conference on Num. Meth. in Fl. Mech., Friedr. Vieweg \& Sohn, 1984.
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# Maurizio Pandolfi/Renzo Piva (Eds.) 

# Proceedings of the Fifth GAMM-Conference on Numerical Methods in Fluid Mechanics 

Rome, October 5 to 7, 1983

With 263 Figures

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NUMERICAL SOLUTION OF MULTI-DIMENSIONAL DIFFUSION-CONVECTION PROBLEMS
BY ASYMPTOTIC CORRECTIONS

M. Israeli* and P. Bar-Yoseph**<br>Technion - Israel Institute of Technology<br>Haifa, Israel

## SUMMARY


#### Abstract

The Booster Method for improvement of the numerical solution of partial differential equations by the addition of asymptotic corrections to the right hand side is presented. It is applied here to the diffusionconvection equation for the case of 'small' diffusion. The correction terms were used in finite difference and finite element schemes. The finite element results were used as reference for checking the performance of the finite difference schemes. Excellent results were obtained without the use of upstreaming or artificial diffusion. Theoretical expectations were confirmed.


## 1. INTRODUCTION

Singularly perturbed initial and boundary value problems for partial differential equations appear in various fields of application such as fluid dynamics, heat transfer, transport of atmospheric pollution, etc. In particular, such equations appear in diffusion-convection processes. often the (normalized) diffusion coefficient $\varepsilon$ becomes small, and thin boundary or interior layers appear within the region of interest. Consequently, these problems become increasingly difficult to solve numerically by discretization methods.

We would like to avoid the use of a prohibitively large number of grid points, as required for resolution by straightforward numerical methods when $\varepsilon$ decreases. To this end, several approaches are possible, such as the use of nonuniform meshes, adaptive techniques, positive type schemes. etc. The question of applicability of such schemes to multi-dimensional problems is presently open.

A different approach is motivated by classical singular perturbation methods where 'inner' and 'outer' solutions are combined to give approximate solutions. These solutions become more accurate as the equations become stiffer, howaver, the error is fixed for a given $\varepsilon$ and cannot be improved or estimated reliably in most cases of interest.

The Booster Method attempts to combine the asymptotic approach, with known discretization methods, in order to obtain a numerical method which improves when $\varepsilon$ becomes smaller. At the same time, it keeps the property that the error can be made arbitrarily small for any fixed $\varepsilon$ by refining the computational mesh (Israeli and Ungarish [1],[2]). For the onedimensional cage, we were able to prove that an improvement by a factor of $\varepsilon^{n+1}$ can be obtained where $\varepsilon$ is the 'small' parameter and $n$ is the order of the asymptotic approximation used (Israeli and Ungarish [2]). We expect similar behaviour in the multidimensional case [1].

In the present paper, we investigate a multi-dimensional application to diffusion-convection problems.

[^0]
## 2. FORMULATION

We consider the transport of a quantity $q$ in a rectangular region. The normalized partial differential equation is

$$
\begin{equation*}
L(q) \equiv-E \nabla^{2} q+\vec{V} \cdot \nabla q=0 \tag{1}
\end{equation*}
$$

In the present application the velocity field $\vec{V}$ is assumed to be known and $q$ is specified on the boundaries. This problem was often used as a test case for various finite difference and finite element methods of solution and it is well known that most methods fail as the cell Reynolds number $(|\vec{V}| h) / \varepsilon$ becomes larger than $O(1)$ (here $h$ is a representative mesh size). For example centered schemes develop unphysical oscillations in space, while uncentered schemes have unacceptable artificial diffusion and are of lower order over the same computational stencil.

The Booster Method uses an asymptotic approximation $\tilde{q}(x, y)$ to the solution $q(x, y)$ in order to reduce the truncation error in the numerica: scheme.

The 'usual' numerical solution $Q(x, y)$ (defined only at grid points) is obtained from

$$
\begin{equation*}
L_{N}(Q)=f \tag{2}
\end{equation*}
$$

where $L_{N}$ is the discrete approximation to the differential operator $L$. The improved numerical solution $\bar{\phi}$ is obtained from

$$
\begin{equation*}
L_{N}(\bar{Q})=E+L_{N}(\tilde{q})-L(\bar{q}) \tag{3}
\end{equation*}
$$

Here $L(\bar{q})$ is the differential operator applied to the approximate solution. Thus the Booster Method applies an asymptotic correction to the right hand side of the equation and therefore requires a negligible amount of extra work. It can be used with any numerical scheme without modification in the method of solution.

The same basic approach of using asymptotic corrections to the right hand side can be used to improve the Standard Finite Element (SFE) method. The resulting Asymptotic Finite Element (AFE) method is described briefly in the following; for details see Bar-Yoseph and Israeli [4].[5].

Suppose that the unit square is divided into elements and that the variation of $q$ within the given region is approximated by

$$
\begin{equation*}
Q(\vec{x})=N_{i}(\vec{x}) Q_{i} \tag{4}
\end{equation*}
$$

where $Q_{i}$ is the value of the approximate solution at the $i$-th nodal point and $N_{i}$ is the corresponding global trial function (we use the sumation convention, with sumation over the nodes within the given region). The Bubnov-Galerkin finite element scheme of eq. (1) is given by

$$
\begin{equation*}
\varepsilon\left(\nabla^{T} N_{j}, \nabla N_{i} Q_{i}\right)_{h}+\left(N_{j} \cdot \vec{v} \cdot \nabla N_{i} Q_{i}\right)_{h}=\left(N_{j}, f\right)_{h}, \quad j=1,2, \ldots m \tag{5}
\end{equation*}
$$

where $m$ is the number of inner nodal points and (., $m$ denotes the usual inner product in $L_{2}(\Omega)$. The subscript $h$ in $(\cdot, \cdot) h$ denotes an approximation to (•..) obtained by a quadrature rule.

Our corresponding asymptotic finite element (AFE) scheme for eq. (1) is the following

$$
\begin{align*}
& \varepsilon\left(\nabla^{T} N_{j}, \nabla N_{i} \bar{Q}_{i}\right)_{h}+\left(N_{j}, \vec{V} \cdot \nabla N_{i} \bar{Q}_{i}\right)_{h}=\left(N_{j}, f\right)_{h} \\
+ & \left\{\varepsilon\left(\nabla^{T} N_{j}, \nabla N_{i} \tilde{q}_{i}\right)_{h}+\left(N_{j}, \vec{v} \cdot \nabla N_{i} \tilde{q}_{i}\right)_{h}-\left(N_{j}, L \tilde{q}\right) j, j=1,2, \ldots, m,\right. \tag{6}
\end{align*}
$$

where $\tilde{\mathrm{q}}_{i}$ is the value of the asymptotic solution at the $i$-th nodal point. Here the terms included in the first line coincide with the SFE scheme, eq. (5), while the terms in the second line (in curled brackets) represent the correction term which is the essence of the present AFE scheme. This AFE scheme can also improve the pointwise error estimate of the SFE scheme by a factor of the $O\left(\varepsilon^{n+1}\right)$ [4].

Usually the finite element solution supplies values everywhere inside the elements via the interpolation (4). Applying the same interpoiation using $\bar{Q}_{i}$ instead of $Q_{i}$ will not give good results within the elements especially when there are no nodal points inside the boundary layers. One should use instead the interpolation

$$
q(\vec{x})=\tilde{q}(\vec{x})+N_{i}(\vec{x})\left(\bar{Q}_{i}-\tilde{q}_{i}\right)
$$

which recovers the proper boundary layer behaviour.
3. ASYMPTOTIC SOLUTION

The approximation $q(x, y)$ can be obtained by the method of matched asymptotic expansions (Cole [3]). Such approximations usually satisfy the boundary conditions and become increasingly accurate as $\varepsilon$ decreases. Often the error decreases like some power of $\varepsilon$ depending on the number of terms used in the construction of the solution (see Table I).

We first construct the zeroth order asymptotic approximation from the outer solution $q_{0}$, where

$$
\begin{equation*}
\overrightarrow{\mathrm{v}} \cdot \nabla q_{0}=0 \tag{7}
\end{equation*}
$$

and from the boundary layer $q_{b}$ satisfying a one-dimensional boundary layer equation in the direction normal to the boundaries (where the flow exits the computational region). A complete zeroth order solution should also include corner regions, tangential regions, and boundary layers developing from discontinuities in boundary conditions. Restricting ourselves for now to continuous boundary conditions and constant velocity field not tangent to any boundary, we find that only the exit corner layer has to be included.

Equation (7) implies that the solution remains constant along streamlines, consequently it carries with it the q-values entering the computational region. The difference between these values and the values encountered at the exit forces the boundary layers.

We consider the flow in the unit square with vertices $(0,0),(0,1)$, $(1,0),(1,1)$. Let the components of $v$ be $u$ and $v$ (both positive) and the differences of the exit boundary $x=1$ and $y=1$ be $f(y)$ and $g(x)$ respectively. Then the structure of the boundary layers will be

$$
\begin{equation*}
q_{b}=f(y) e^{u(x-1) / \varepsilon}+g(x) e^{v(y-1) / \varepsilon}-p e^{u(x-1) / \varepsilon} e^{v(y-1) / \varepsilon} \tag{8}
\end{equation*}
$$

where $p=f(1)=g(1)$ and $f(0)=g(0)=0$ by assumption.
The third term in (8) is the corner boundary layer and it satisfies the differential equation exactly (in this particular case). The approximation $\tilde{q}$ is obtained by adding $q_{0}$ from (7) to $q_{b}$ from (8). It is a
uniformly valid approximation in the square, and is easily adapted to particular cases. In our example $u=v=\sqrt{2} / 2$ and the outer solution is

$$
\begin{equation*}
q_{0}=\sin \pi(x-y), \tag{9}
\end{equation*}
$$

corresponding to the boundary conditions

$$
\begin{equation*}
q(x, 0)=\sin \pi x ; q(0, y)=-\sin \pi y \tag{10}
\end{equation*}
$$

On the other hand we take

$$
\begin{equation*}
q(x, 1)=\sin \pi(x-1)+x, \quad q(1, y)=\sin \pi(1-y)+y, \tag{11}
\end{equation*}
$$

giving rise to $f(y)=y$ and $g(x)=x$, which satisfy the requirement of continuity on the boundary.

## 4. RESULTS

We solved the differential equation (1) in the unit square with the boundary conditions (10) and (11) on a net with 6,12 and 24 equal intervals in the $x$ and $y$ directions. We used centered three-point differences for the first and second derivatives. As we do not have the exact solution for this problem, we used as reference a solution obtained with the AFE scheme employing a uniform mesh of $24 \times 24$ biquadratic Lagrangian elements (more details appear in (5]). The range of $\varepsilon$ reproduced in the tables was $\varepsilon=0.01, \varepsilon=0.02, \varepsilon=0.05$.
As a seminorm we used a weighted average of the absolute value of the errors. A proper mix of interior and boundary layer points was obtained by taking only the 25 mesh points contained in a square near the corner (1,1).
We observe that (Table I) the error in the asymptotic approximation $A(\varepsilon, h)$ decreases roughly like $\varepsilon$. The error in the regular (Table III) numerical salution $N(\varepsilon, h)$ decreases very slowly with $h$ and increases as $\varepsilon$ decreases.
We note first that the errors in Table II are in all cases smaller than the corresponding errors in Tables I and III. Moreover the analysis of [2] indicates that the error in the improved solution $B(\varepsilon, h)$ should decrease with $\varepsilon$ and $h$ (Table II). In fact it should be proportional to the product of the previous errors. Table IV presents the ratio $K(\varepsilon, h)=B(\varepsilon, h) /((A(\varepsilon, h) N(\varepsilon, h)))$. We expect it to approach a constant, the fact that the values in Table IV are not far from unity makes the booster method quite attractive.
We note that the centered method is quite useless by itself. Our experience shows that the Booster Method works equally well with other schemes and other discretization methods.

## ACKNOWLEDGEMENT

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$1$
transition and turbullence
renormalization group formulation of large eddy smulation
v. yakhot, s.a. orszag

1. introduction
Perheps the most distinguishing charecteristic of high Reynolds numbr turbulent flows is their large range of excited space and time scales. i. homoganeous turbulence, diutipation-scale eddies are of order $R^{3 / 4}$ time order to solve the Navier-Stokea equations accurately for such a turbulen order to solve the Navier-Stokes equations accurately for such and it is necessary to retain order $\left(R^{3 / 4}\right)^{3}$ spatial degrees of freedom Also. inc the time scale for aignificant evolution of homogeneous turbu lence is of the order of the turnover time of an energy containing eddy, i is necessary to perform order $\boldsymbol{n}^{3 / 4}$ time steps to calculate for aignif
icant evolution time of the flow. Even if these calculations require onl o(1) arithmetic operations per degree of freedom per time step. the tota computational work involved would be order $R^{3}$, while the computer etorag requirement vould be $\mathrm{R}^{9 / 4}$. In thia case, doubling the Reynolde numbe
would require an order of magnitude 1 mprovement in computer capability would require an order of magnitude improvement in computer capability With this kind of operation and ztorage count, it it unlikely that forser able advances in computere will allow the full numerical $\quad$ tumulation achieved (see bRACHET et al. (21).
This pessimistic operation and storage count for solution of $t$ Navier-stokes equations is the origin of interest in the so-calle large-eddy-simulation method. Here. excitations on scales amaller the those resolvable on the numerical grid are modelled, usualiy by an ed
 Iffective grid on the large eddies (defined as those motions adequate)
represented on the numerical grid). The most common form for this sGs edr represented on the numerical grid). The most
visconity coefficient is due to smacorinsky

## 11. <br> $$
v_{\text {edd } y}=c \Delta^{2}\left|\left[\frac{\partial v_{1}}{\partial x_{j}}+\frac{\partial v_{i}}{\partial x_{i}}\right]^{2}\right|^{1 / 2}
$$

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atione scale with the outer variables. i. e. Channel height (ConTE-BEI. 31). Transport-eddy modelling does allow simulation of flows at somew, higher Reynolds numbers
(MOIN \& KIM $|14|$ achieve $R_{*}=640(R=13000)$ by transport-e $: ~$ modelifing, while the direct numerical simulations of orszac \& patera l: are restricted to $R_{*}=200$ ), but bursts at mean-flow Reynolds numbers $R$. 20000-100000 (in plane Poiseuille flow) are beyond subgrid scale mois as now implemented in cray-2 ciesty simulation of well-bounded flow is to fare significan' better than direct simulation, the dependence of required degrees freedom must acale less rapidily than $R_{*}^{3}$ as $R_{*}$, becomes large. At present
no such method exists.

A second problem with current transport-eddy schemes stems from the : the mall seales are modelled in the wall layer. In particular, the apf KIM (14)) is not fuliy futified. While this correction (VAN DRIEST II wat originally intended to model the effect of fluctuations within viscous sublayer in modulating the interaction of molecular and eddy
cosities, applying it to subgrid scale model could eliminate significantly alter fluctuations in the supergrid or resolvable scales third problem it that existing schemes rely upon evailability of exp.
 velocity profile in turbulent channel flow. To achieve agreement experiment, they chose parameters that differ from those that seen.
work best for homogeneous turbulence. Other chotces of parameters 9 work best for homogeneous turbulence.

In this paper, we use renormalization group (RNG) methods to address solution of the latter two difficulties encountered by transport- -
modelifing. The RNG SGS clocures obtalned below seem to model properiy interaction of turbuient motions in the vall region without ad hoc damp factors. and also appar to account for the generetion of random burats
the buffer layer, without requiring extensive experimental dat to the buffer layer. Without requiring extensive experimental dats an will be addressed once again in the conclusion of this paper. but remain
subject of current investigation.


 no such method exists

## 


I one is interested in the physics of wall turbulence, neglect of the wall
 ' ansport-eddy simulation. However. transport-eddy simimiations (as curantly implemented) are much more severaly limited than the earlier
at - piesentiy practiced, transport-eddy subgrid scale simulations is that,
 art hursts (whach muat be done to capture the turbulence product
oprity). Che number of required degraes of freedom scales as $R_{*}^{3}$. This

Where $\Delta$ is the grid scale and $v_{i}$ is the large-eddy volocity. It has been sionsl grounds with the kolmogorov theory of the inertial range. For the
 The banic action of the eddy viacosity ( 1.1 ) on large scales seema corroct :ies in this formulation of large-eddy simulationa. First, large-eddy simulations based on (1.1) alone neqlect the effect of random forcing of The eddy viscosity (1.1) is non-stochastic (at the subgrid leval, though it is still random due to supergrid fluctuations), while the action of should be expected that in addition to eddy viscous offects of sminis. scalas on large scales. there should 1 lo bo a random forcing effect, giving
ise to an eddy diffusion process and production of turbulent anergy his point vill be discussed laters. Second, the eddy viscosity (1.1) does iot properly model interfarence effects between eddy and molecular vis-
cosity. which is essential in turbulent processes uhere eddy effecte mit = inhibited (for example. near rigid walis). The simple superposition of Idy and molecular wiscosity near walls does not lead to correct results
see moin \& KIM (14)। see MOIN \& KIM (141).
EARDORFF 14.6 .71 made pioneer1ng studzes of turbulent shear flows using ated only up to the edge of the buffer layer between the viscous sublayer ad the logarithmic reqion of the velocity profile. A boundary condition A Which the turbulent fluctuating stress is assumed known. Molecular vissity plays no role in DEARDORFF' scalculations. Which are performed at asst formally, at infinite R. Clearly such a simulation does not give a
aithful representation of the wall region and accompanying burats. $\longrightarrow$ —
${ }^{6} 5$
elsmination of these modes involves modified interaction coeffici,
 method, the resulting equations are then transformed to look as mur possible like the original syatem (2.1) - (2.2).

To illustrate the technical details of the RNG method, consider fou tranuform of (2.1):
where $\hat{k}=(\vec{k}, w)$ and
$G^{0}=\left(-1 \omega+v_{0} k^{2}\right)$
$P_{\ell m}(k)=\delta_{\ell m}-\frac{k_{\ell^{k} m}}{k^{2}}$

$P_{t m}(k)=\delta_{t m}-\frac{k^{2}}{k}$
 effect of the modes from the strip $A_{e^{-t}<k<A \text {. The velocity ficid is: }}$ into the two components: $v^{\wedge}(\hat{k})$ with $O<k<A e^{k}$ and $v^{\prime}(\hat{k})$ with $A e^{-Q}$ into the two components:
$\times \int\left[v^{\prime}(\hat{q}) v_{n}^{\prime}(\hat{k}-\hat{q}) \cdot 2 v_{m}^{\prime}(\hat{q}) v_{n}^{*}(\hat{k}-\hat{q})+v_{m}^{\prime}(\hat{q}) v_{n}(\hat{k}-\hat{q})\right] d \dot{q}$
In order to eliminate modes from the interval $A e^{-1}<k<A$, $a l l$ terms $v_{n}$ in (2.5) should be removed by repested substitution of ( 2.5 ) for $v$ ' into (2.5). Thia generates an infinite expansion for $v$ in powers of
which $v^{\prime}$ does not formally appear. Next, averages are taken over the of zandom force $\boldsymbol{f}^{\prime}$ helonging to the strip $A e^{-8}<k \times A$. Thit procedure mally eliminates the modes $A 0^{-l}$ " $k$. Afrow the problem; the result.
represented diagrammaticaliy in Fig. 1 . where the thick slashed
 line denotes
denote $-\frac{1 \lambda_{0}}{2} P_{\text {smn }}(k)$ and random force $f(k)$. respectively.

It follow from Fig. i, that after removing the modes $N e^{-\ell} k$ a
$\left(-1 \omega * v_{0} k^{2}\right) v_{i}^{\prime}(\hat{k})=f_{l}(\hat{k})-\frac{{ }^{\prime} \hat{o}_{0}}{2} P_{e m n}(\hat{k}) / f_{n}^{\prime}(\dot{q}) f_{m}^{\prime}(\hat{k}-\dot{q}) d \dot{q}$



## 


 $\qquad$
 FOURNIER $\&$ FRISCH 191, and YAKHOT 1191, showed that the large-acile spectium of an incompreasible fluid governed by the Navier-Stoken equatione - pectrum proportional to $k^{-3}($ see $(2.2)$ below). generates the kolmogorov $k^{-5,3}$ energy spectrus in the infrared $(k \cdot 0)$ limit
Tre problem treated by the above authors is:
with

$$
-\frac{\nabla R}{0} \cdot 1 \cdot v_{0} \nabla^{2} \dot{v}
$$ the random driving force (2.2) in the equationa of motion for the small

icales
In this section. we rework the infrared RNG method for the problem (2.1)subgrid scale closura. However. before proceeding to this task lat us give some further fustification for the inclusion of the random force (2.2) at
n the one hand, the random force (2.2) is justified by earlier work on the infrared renormalizetion group because of ite consistency with the $k^{-5 / 3}$
spectrum at smalik. However, for our preaent purposes thia ie but veak justificstion. because we are interested in eliminating only the vory smallest scales (highest $k$ ) of motion that represent the SGS motiona. YAK-
!ot $|19|$ generalized the RNG mothods to the ultraviolet case, in which the largest scales of motion are removed by the RNG procedure, and thowed that
 hus turbalence is driven by a force confined to if band of wave numbers. :hen the ultraviolet RNC procedure inducea andom force at high wave
numbere of the form (2.2). The assumptione leading to the latter conclu--ions have recently been weakened (Yakhot, unpublished). in any case, if


- 

$G_{n}(k)=\left(-1 w+v(l) k^{2}\right)^{-1}$







# Lectures on Spectral Methods for Turbulence Computations. 

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## 1. - Introduction to spectral methods.

Spectral methods are based on representing the solution to a problem as a truncated series of smooth functions of the independent variables. Whereas finite-element methods are based on expansions in local basis functions, spectral methods are based on expansions in global functions. Spectral methods are the extension of the standard technique of separation of variables to the solution of arbitrarily complicated problems.

Let us begin by illustrating spectral methods for the simple one-dimensional heat equation. Consider the mired initial-boundary-value problem

$$
\begin{array}{ll}
\frac{\partial u(x, t)}{\partial t}=K \frac{\partial^{2} u(x, t)}{\partial x^{2}} & (0<x<\pi, t>0), \\
u(0, t)=u(\pi, t)=0 & (t>0), \\
u(x, 0)=f(x) & (0<x<\pi) . \tag{1.3}
\end{array}
$$

The solution to this problem is

$$
\begin{align*}
& u(x, t)=\sum_{n=1}^{\infty} a_{n}(t) \sin n x,  \tag{1.4}\\
& a_{n}(t)=f_{n} \exp \left[-K_{n}: t\right], \tag{1.5}
\end{align*}
$$

where

$$
\begin{equation*}
f_{n}=\frac{2}{x} \int_{0}^{x} f(x) \sin n x d x \tag{1.6}
\end{equation*}
$$

are the coefficients of the Fourier sign series expansion of $f(x)$.

[^1]A sportal apmeximation to (1.1)-(1.3) is wotten by simply tumatint (1.1) t 0

$$
\begin{equation*}
\boldsymbol{u}_{v}(x, f)==\sum_{n=1}^{n} a_{n}(f) \sin u \cdot x \tag{1.7}
\end{equation*}
$$

and replating (1.5) by the rolution equation

$$
\begin{equation*}
\frac{d a_{n}}{d t}=-K n^{2} a_{n} \quad(n=1, \ldots . y) \tag{1.8}
\end{equation*}
$$

with the initial conditions $a_{n}(0)=f_{n}\left(n=1, \ldots, v^{\prime}\right)$.
The spectral approximation (1.7), (1.8) to (1.1)-(1.3) is an exceedingly good approximation for any time $t$ greater than zero as $N \rightarrow \infty$. In fact, the error $u(x, t)-u_{v}(x, t)$ satisfies

$$
\begin{equation*}
u(x, t)-u_{v}(x, t)=\sum_{n=x^{\prime}+1}^{\infty} f_{n} \exp \left[-K n^{2} t\right] \sin n x=O\left(\exp \left[-K_{1} y^{2} t\right]\right) \tag{1.9}
\end{equation*}
$$

$$
(N \rightarrow \infty)
$$

for any $t>0$. In contrast to (1.9), fnite-difference approximations to the heat equation using $N$ grid points in $x$ lead to errors that decay only algebraically with $\boldsymbol{N}$ as $\boldsymbol{V} \rightarrow \infty$. Furthermore, this spectral method for the solution of the heat equation is efficiently implementable by the fast Fourier transform (FFT) in $O(N \log N)$ operations.

There are several significant difficulties in extending the simple spectral method employed for (1.1)-(1.3) to more general problems. Among these difficulties are those caused by imposition of nontrivial boundary conditions, nonlinear and nonconstant coefficient terms, and complex geometries. These difficulties and their solutions will be discussed below (see also [1, 2]).

The Fourier series (1.4) converges fast if $u(x, t)$ is infinitely differentiable and $u(x, t)$ satisfies the boundary conditions

$$
\begin{gather*}
\hat{c}^{2 n} u(x, t)  \tag{1.10}\\
\hat{c} x^{2 n}
\end{gather*}=0
$$

$$
(x=0, \pi)
$$

for all nomegative integers $n$. Under these conditions, the error after $\mathcal{N}$ terms

$$
\varepsilon_{N}(x, t)=u(x, t)-\sum_{n=1}^{\stackrel{\rightharpoonup}{2}} a_{n}(t) \sin n \cdot r
$$

 other hamd, if $u(r, t)$ is not infinitely differentiable or if any of the conditions (1.10) is violated, then $\varepsilon_{s}(r \cdot f)=O(1: N r)$ as $N-\infty$ for nome finite $p$. For
"xample.

$$
1=\sum_{n=0}^{\infty}(-1)^{x} \begin{gather*}
\sin (\because n+1) r  \tag{1.11}\\
2 n+1
\end{gather*}
$$

$$
\text { ( } 11 \cdot: x \text { : } x \text { ) }
$$

but the error inemred by truncating after $N$ terms is of order $1 / X$ for anc tixed $x, 0<x<\pi$. Furthermore, the convergence of (1.11) is not uniform in $r$; (1.11) exhibits Gibbs' phenomenon, namely

$$
\varepsilon_{x}(\xi / N)=O(1) \quad(N \rightarrow \infty, \xi \text { fixed })
$$

For any fixed $\boldsymbol{V}$, there are points $x$ at which the error after $\boldsymbol{N}$ terms of (1.11) is not small. The poor convergence of (1.11) is due to the violation of (1.10) for $n=0$.

More generally, most eigenfunction expansions of a function $f(x)$ converge faster than algebraically (i.e. the error incurred by truncating after $\bar{V}$ terms goes to zero faster than any finite power of $1 / N$ as $N \rightarrow \infty$ ) only if $f(x)$ is infinitely differentiable and $f(x)$ satisfies an infinite number of special boundary conditions. For example, the Fourier-Bessel expansion

$$
f(x)=\sum_{n=0}^{\infty} a_{n} J_{0}\left(\lambda_{n} x\right)
$$

$$
(0<x \leqslant 1)
$$

Where $\lambda_{n}$ is the $n$-th smallest root of $J_{0}(\lambda)=0$, converges faster than algebraically only if $f$ is infinitely differentiable and

$$
\begin{equation*}
\left[\frac{1}{x} \frac{\mathrm{~d}}{\mathrm{~d} x} x \frac{\mathrm{~d}}{\mathrm{~d} x}\right]^{k} f(x)=0 \quad \text { at } x=1 \tag{1.12}
\end{equation*}
$$

for $k=0,1,2, \ldots$.
When a spectral expansion converges only algebraically fast, spectral methods based on these eigenfunction expansions cannot offer significant advantages over more conventional (finite-difference, finite-element) methods. Eigenfunction expansions of this kind should not normally be used unless the boundary conditions of the problem imply all the extra boundary constraints like (1.10) or (1.12). For example, if periodic boundary conditions are compatible with the differential equation to be solved, complex Fourier series are suitable to develop efficient spectral approximations.

In the development of spectral methods for general problems, it is important that the rate of convergence of the eigenfunction expansion being used does not depend on special properties of the eigenfunctions, like boundary conditions, but rather depend only on the smoothness of the function being expanded. Of course, if the solution to the problem being solved is not smooth, one should not expert errors that decrease faster than algebraically with $1 / \mathrm{s}$ when global
 may be achieved for these problems by either patehing the solution at diserntinuities or pre- and post-processing of the solution (see [ $\because=3$ ).

There is an easy way to ensure that the rate of convergence of a spertalat expansion of a function $f(x)$ depends only on the smoothess of $f(x)$, not on its boundary properties. The idea is to expand in terms of suitable elasies of orthogonal polynomials, including Chebyshev and Legendre polynomials for all those problems in which constraints like (1.10) and (1.12) are unrealistic. These polynomial expansions avoid all difficulties asscciated with the Gibbs phenomenon provided the solution $f(x)$ is smcoth.

From the mathematical point of view, the classical orthogonal polynomials are eigenfunctions of singular Sturm-Liouville problems. It is not hard to show [1] that expansions using eigenfunctions of such singular Sturm-Liouville problems converge at a rate that depends only on the smoothness of $f(x)$, in contrast to eigenfunction expansions based on nonsingular Sturm-Liouville problems that lead to additional boundary constraints like (1.10) on $f(x)$.

These results for orthogonal polynomial expansions are easily demonstrated in the case of Chebysher polynomial expansions. The $\boldsymbol{n}$-th-degree Chebyshev polynomial $T_{n}(x)$ is defined by

$$
\begin{equation*}
T_{n}(\cos \theta)=\cos n \theta \tag{1.13}
\end{equation*}
$$

Therefore, if

$$
\begin{equation*}
f(x)=\sum_{n=0}^{\infty} a_{n} T_{n}(x) \tag{1.14}
\end{equation*}
$$

then

$$
\begin{equation*}
g(\theta)=f(\cos \theta)=\sum_{n=0}^{\infty} a_{n} \cos n \theta \tag{1.15}
\end{equation*}
$$

Thus the Chebyshev polynomial expansion coefficients $a_{n}$ of $f(x)$ are just the Fourier cosine expansion coefficients of the even, periodic function $g(\theta)$. A simple integration-by-parts argument then shows that

$$
n^{y} a_{n} \rightarrow 0
$$

$$
(n \rightarrow \infty)
$$

provided $g(\theta)$ (or, equivalently, $f(x)$ ) has $p$ continuous derivatives. Since

$$
\left|f(x)-\sum_{n=0}^{N} a_{n} T_{n}(x)\right|<\sum_{n=x+1}^{\infty}\left|a_{n}\right| \quad \quad(|x|<1)
$$

it follows that the rate of convergence of (1.14) is faster than algebraic if $f$ is smooth.

In summary, spectral expansions shoubl be made using series of orthogomal polynomials unfess the beundary conditions of the woblem are fully compatible with some other class of eigenfunctions. In practire, Chebyshev and degendre polynomial expansions are recommended for most appliations, supplemented by Fourier series and surface harmonie series when boundary conditions premit.

Another difficulty with general kinds of spectral metheds is their application to problems with nonlinear and nonconstant cofficient terms. Before explaining the solution to this problem, let us illustrate the difficulty.

Suppose we wish to solve the partial differential equation

$$
\begin{equation*}
\frac{\hat{c} u}{\hat{c} t}=\mathscr{N}(u, u)+\mathscr{L} u \tag{1.16}
\end{equation*}
$$

where $u=u(x, t)$ and $\mathscr{N}$ is a bilinear (nonlinear) operator that involves only spatial derivatives and $\mathscr{L}$ is a linear operator that involves only spatial derivatives. The operators $\mathscr{N}$ and $\mathscr{L}$ may depend on both $x$ and $t$. A spectral method for the solution of (1.16) is obtained by seeking the solution as a finite spectral expansion:

$$
\begin{equation*}
u(x, t)=\sum_{n=1}^{x} a_{n}(t) \psi_{n}(x) \tag{1.17}
\end{equation*}
$$

where we assume for now that $\psi_{n}(x)(1<n<\infty)$ are a complete set of orthogonal functions. If we introduce the re-expansion coefficients $c_{n m}$, and $d_{n m}$ so that

$$
\begin{aligned}
& \mathscr{N}\left(\psi_{m}, \psi_{s}\right)=\sum_{n=1}^{\infty} c_{n m s}(t) \psi_{n} \\
& \mathscr{L}\left(\psi_{m}\right)=\sum_{n=1}^{\infty} d_{n m}(t) \psi_{n}
\end{aligned}
$$

and equate coefficients of $\psi_{m}(x)(n=1, \ldots, S)$ in (1.16), we obtain

$$
\begin{equation*}
\frac{\mathrm{d} a_{n}}{\mathrm{~d} t}=\sum_{m=1}^{N} \sum_{p=1}^{N} c_{n m p}(t) a_{m}(t) a_{9}(t)+\sum_{m=1}^{N} d_{n m}(t) a_{m}(t) \quad(n=1, \ldots, N) . \tag{1.18}
\end{equation*}
$$

Equations (1.18) are the spectral evolution equations for the solution of (1.16). They have one very serious drawback. In general $c_{n m}$, and $d_{n m}$ are nonzero for typical $n, m, p$, so that evaluation of $d a / d t$ from (1.18) for all $n=1, \ldots, N$ requires $O\left(N^{2}\right)$ arithmetic operations for the bilinear term and $O\left(N^{2}\right)$ operations for the linear term. Thus solution of (1.18) requires order $\lambda^{3}$ operations per time step. Since operational spectral calculations now involve $N>10^{\circ}$, the computational cost of the direct solution of (1.18) is prohibitive (even if only linear terms are present).

The preblem hare is one of computational complexity. Finite edinerence mothook for the solution of (1.16) on $X$ arid points may require mily onder $\therefore$ operations per time step. If the spectral method really reguites onder fos oprations per time step, it ramot compete when $V$ is large.

Another example illustrating the computational complexity of nertab methods is given by the nonline:r difusion equation

$$
\begin{equation*}
\frac{\hat{c} u(r, t)}{\hat{c} t}=\operatorname{cxp}[u] \frac{\hat{c}^{2} u}{\hat{c} x^{2}}(x, t) \tag{1.19}
\end{equation*}
$$

If we reck the solution as

$$
\begin{equation*}
\psi(x, t)=\sum_{n=1}^{N} \|_{n}(f) \psi_{n}(x) \tag{1.20}
\end{equation*}
$$

in terms of the orthonormal functions $\psi_{n}(x)$, then

$$
\begin{equation*}
\frac{\mathrm{d} a_{n}}{\mathrm{~d} t}=\int \psi_{m}(x) \exp \left[\sum_{m=1}^{N} a_{m}(t) \psi_{m}(x)\right] \sum_{p=1}^{N} a_{p} \psi_{p}^{\prime \prime}(x) \mathrm{d} x \tag{1.21}
\end{equation*}
$$

for $n=1, \ldots, N$. These evolution equations for $\left\{a_{n}(t)\right\}$ have an exponential degree of computational complexity as they are expressed as an integral functional oi $\left\{a_{n}(t)\right\}$.

The solution to the problem of computational complexity is to use the author's transform methods. Let us illnstrate the technique for a pseudospectral (or collocation) approximation to (1.19). First, we introduce $\boldsymbol{N}$ suitable collocation points $x_{1}, x_{2}, \ldots x_{N}$ lying within the computational domain. Then the approximate solution (1.20) is forced to satisfy the partial differential cquation (1.19) (or its boundary conditions) exactly at these discrete points at every time $t$. More specifically, the following three steps are done at each time step $t$ :
i) Determine $N$ coefficients $a_{n}(t)(n-1, \ldots, N$ ) so that

$$
\begin{equation*}
u\left(x_{j}, t\right)=\sum_{n=1}^{N} a_{n}(t) \psi_{n}\left(x_{j}\right) \quad(j=1, \ldots, N) \tag{1.22}
\end{equation*}
$$

ii) Evaluate $u_{c x}\left(x_{i}, t\right)$ by

$$
\begin{equation*}
u_{c z}(x, t)=\sum_{n=1}^{x} a_{n}(t) \psi_{n}^{\prime \prime}\left(x_{j}\right) \quad(j=1, \ldots, \lambda) \tag{1.23}
\end{equation*}
$$

iii) Finally, evaluate $\hat{c} u(x, t), \hat{c} t \quad b y$

$$
\begin{equation*}
\frac{\hat{c} u(x, t)}{\hat{c} t}=\operatorname{cxp}[u(, r, t)] u_{x x}(x, t) \quad(j=1, \ldots . N) \tag{1.24}
\end{equation*}
$$

and march forward to the next time step.

The ide: of the pseudespertral transform method can le restated as follow:
 ind each term in whatever representation that term is most accurately, and simply, evaluated. Thus, in (1.21), we evaluate exp [u] in the physical represell tation while we compute $u_{s x}$ in the spectral representation by (1.22) berause it is most accurately done there.

It should be apparent to the reader that pseudospectral transform methods can be applied to any problem that can be treated by finite-difference methods regardless of the technical complexity of nonlinear and nonconstant coefficient terms.

For the expressions of interest, computation of derivatives of a $\boldsymbol{N}$-term spectral expansion requires order $I$ arithmetical operations. For the Fourier series (1.i), this fact is obvious:

$$
\begin{aligned}
& \frac{\mathrm{d}}{\mathrm{~d} x} \sum_{n=1}^{N} a_{n} \sin n x=\sum_{n=1}^{N} n a_{n} \cos n x, \\
& \mathrm{~d}^{2} \sum^{2} x_{n=1}^{N} a_{n} \sin n x=-\sum_{n=1}^{x} n^{2} a_{n} \sin n x .
\end{aligned}
$$

For the Chebyshev polynomial expangion (1.14), the computational complexity: of differentiation is a little less apparent. Since $T_{n}(\cos \theta)=\cos n \theta$,

$$
\frac{T_{n+1}^{\prime}(x)}{n+1}-\frac{T_{n-1}^{\prime}(x)}{n-1}=\frac{2}{c_{n}} T_{n}(x)
$$

$(n>0)$,
where $c_{0}=2, c_{n}=1(n>1)$ and $T_{0}^{\prime}=T_{-1}^{\prime}=0$. Therefore, if

$$
\frac{d}{d x} \sum_{n=0}^{r} a_{n} T_{n}(x)=\sum_{n=0}^{N} b_{n} T_{n}(x),
$$

then

$$
\because \sum_{n=1}^{\infty} a_{n} T_{n}^{\prime}(x)=\sum_{n-9}^{\Gamma} r_{n} b_{n}\left[\begin{array}{c}
\left.T_{n+1}^{\prime}-\frac{T_{n-1}^{\prime}}{n+1}-1\right]=\sum_{n=1}^{n+1}\left[c_{n-1} b_{n-1}-b_{n+1}\right] T_{n}^{\prime}(x) \cdot n . ~ . n . ~
\end{array}\right.
$$

Equating coefficients of $T_{n}^{\prime}(x)$ for $n=1, \ldots, N+1$ gives the recurrence relation

$$
\begin{cases}c_{n-1} b_{n-1}-b_{n+1}=2 n a_{n} & (1<n<N)  \tag{1.25}\\ b_{n}=0 & (n>N)\end{cases}
$$

The solution of (1.25) for $b_{n}$ given $a_{n}$ requires only order $\mathcal{V}$ arithmetic operation. Similar recurreuce relations can be obtained for differentiation of spertal sorice based on other sets of orthogonal polyommals and functions.

In the rase of Fondier series, the transurm (1.7) and it, inverae rall the
 form. However, most of the computational efliciency of tratisform methods comes not from the FFT but from the separability of multidimensional transforms. Thus a three-dimensional diserete Fourier transform can be expresed as three one-dimensional Fourier transforms

$$
\begin{align*}
& \sum_{i=0}^{J-1} \sum_{i=0}^{\pi-1} \sum_{i=0}^{2-1} a(j, k, l) \exp \left[2 \pi i\left(\frac{j m}{J}+\frac{l n}{\hbar}+\frac{l p}{P}\right)\right]=  \tag{1.26}\\
& \left.\quad=\sum_{j=0}^{J-1} \exp \left[\because \pi i j m^{\prime} J\right]_{k=0}^{s-1} \exp \left[2 \pi i h_{i}^{\prime} h^{\prime}\right] \sum_{i=0}^{t-1} a(j, l, l) \exp [\because \pi i] p / L\right]
\end{align*}
$$

The left-hand side of (1.26) requires roughly $(J K L)^{2}$ operations to evaluate at all the points $0<m<J, 0<n<K, 0<p<L$. On the other hand, even without the FFT, the right-hand side of (1.26) requires only about ( $J K L$ ). $\cdot(J+K+L)$ operations to evaluate at all the points. When the FFT is applied to the one-dimensional transforms on the right-hand side of (1.26), the number of operations necessary to evaluate (1.26) is reduced further to ( $J K L$ ). $\cdot\left(\log _{2} J+\log _{2} K+\log _{2} L\right)$ if $J, K, L$ are powers of 2.

Spectral approximations to general boundary-value problems lead to full $\boldsymbol{N} \times \boldsymbol{V}$ matrix equations for the $\boldsymbol{N}$ expansion coefficients $a_{n}$. It would seem that solution of these equations requires $O\left(N^{3}\right)$ arithmetic operations, while storage of the matrix requires $O\left(N^{2}\right)$ memory locations. Since typical problems now involve $N \sim 10^{6}$, the direct solution (or even the direct formulation) of such problems would seem unworkable now.

Consider the solution of a general linear differential equation $L_{u}=f$. Let a $N$-term spectral approximation to this problem be giren by

$$
\begin{equation*}
L_{1 p} u_{s}=f_{s}, \tag{1.2i}
\end{equation*}
$$

Where $f_{s}$ is a suitable $N$-term approximation to $f$. As mentioned several times earlier, the matrix representation of (1.27) is generally a full $N \times N$ matrix, so that direct solution of (1.27) by Gauss elimination methods would require order $\lambda^{2}$ storage (for the matrix reprecentation of $L_{08}$ ) and order $N^{3}$ arithmetic operations.

Here we shall describe a method that permits the solution of (1.2\%) using order $\mathcal{N}$ storage locations with the number of arithmetic operations of order the larger of $N \log N^{\circ}$ and the number of oncrations requircd to solve $I_{4}=f$ by a first-order finite-difference method. The important conclusion is that spectial methods for general problems in general geometries ran be implemented efficiently with operation costs and storage not much larger than that of the simplest finitr-differener approrimation to the problem with the some mumber of degrees of frocilom. Since nectand methuds require many fewer degrees of frealem to


 ciencies result from th: new methond.

The ideat of the itrastion method is :as follows: Supluse we ise able to com-
 properties:
i) $L_{a b}$ has a sparse matrix representation so that it ran be represented using only $O(N)$ storage locations.
ii) $L_{a b}$ is efficiently invertible in the sense that the equation

$$
\begin{equation*}
L_{\Delta D}{ }^{1}{ }_{x}=f_{s} \tag{1.28}
\end{equation*}
$$

is solvable as efficiently as a first-order fnite-difference approximation to the problem.
iii) $L_{A D}$ approximates $L_{A D}$ in the sense that

$$
\begin{equation*}
0<m<\left\|_{u}^{1 /} L_{a p}^{-1} L_{\mathrm{ab}}\right\|_{1}<M<\infty \tag{1.29}
\end{equation*}
$$

for suitable constants $m, J$ as $N \rightarrow \infty$. Roughly speaking, (1.29) requires that the eigenvalues of $L_{a p}^{-2} L_{i}$, be bounded from above and below as $\boldsymbol{N} \rightarrow \infty$.

We propose to construct $L_{\mathrm{ap}}$ from $L_{a p}$ by changing the discretization operator either in addition to or in place of approximating the differential operator. Thus we construct $L_{\Delta p}$ by a suitable low-order finite-differcnec approximation to $L$.

A simple example is given by the second-order differential equation

$$
\begin{equation*}
L u=f(x) u^{\prime \prime}(x)+g(x) u^{\prime}(x)+h(x) u(x)=r(x) \quad(0<x<9 \boldsymbol{\pi}) \tag{1.30}
\end{equation*}
$$

with periodic boundary conditions $u(x+\Omega \boldsymbol{\tau})=\boldsymbol{q}(x)$ and $f(r)>0$. A spectral approximation is approximately sought as the finite Fourier series

$$
\begin{equation*}
u(r)=\sum_{i k<K} a_{k} \exp [i k, r] . \tag{1.31}
\end{equation*}
$$

If the Fourier ceefficients of $f(x), g(x), h(x), r(x)$ are dencted $f_{b}, g_{b}, h_{i}, r_{h}$. respectively, then the spectral (Galeikin) equations for $a_{b}$ are

$$
\begin{equation*}
I_{a v} d=\sum_{\substack{i p, x \\ i b^{n}, k}}\left[-p^{2} j_{k-p}+i p g_{k-p}+h_{k}\right] a_{p}=r_{k} \tag{1.3:}
\end{equation*}
$$

( 'learly, these equations hawe, in qeneral, a full matrix representation that


 represtatation, we use the finite-diflerence approximation
where $u_{j}=u(x)$ and $\Delta x=9 \boldsymbol{\pi} / \boldsymbol{N}$. Obviously, $L_{a p}$ is parse and efficjently invertible. To verify ( 1.29 ) we use the following elementary argument (that may be made more rigorous but no more correct by more involved whis-like arguments). If $\lambda$ is an eigenvalue of $L_{a p}^{-1} L_{a p}$, then there exists a function $\boldsymbol{u}(r)$ such that

$$
\begin{equation*}
L_{0 \mathrm{p}} u=\lambda L_{2 \mathrm{p}} u \tag{1.34}
\end{equation*}
$$

If $u(x)$ is a smooth function of $x$ (in the limit $N \rightarrow \infty$ ), then both $L_{a p} u$ and $L_{01}$ t should be good approximations to $L u(x)$, so (1.3t) implies $i \sim 1$. On the other hand, if $u(x)$ is a highly oscillatory function of $r$ (in the limit $N \rightarrow \infty$ ), then

$$
\begin{equation*}
u^{\prime \prime} \gg u^{\prime} \gg v \quad(N \rightarrow \infty) \tag{1.35}
\end{equation*}
$$

Therefore,

$$
\begin{equation*}
L_{\Delta p} u \sim f\left(x_{j}\right) \frac{u_{j+1}-2 u_{j}+u_{j-q}}{(\Delta x)^{2}} \tag{1.36}
\end{equation*}
$$

and, if transform (pseudospectral) methods are used to evaluate $L_{0 p}{ }^{1}$,

$$
\begin{equation*}
L_{s p} u \sim f\left(x_{j}\right) \sum_{k i<x}\left(-k^{2}\right) a_{k} \exp \left[i k x_{1}\right] \tag{1.37}
\end{equation*}
$$

so (6.18) gives

$$
\begin{equation*}
f(r,) \sum_{k=k}\left(-k^{2}\right) a_{k} \exp \left[i k r_{1}\right] \sim i f\left(r_{2}\right)^{u_{i+1}-\Omega n, \div u_{j-1}}(\Delta r)^{2} . \tag{1.3s}
\end{equation*}
$$

The eirenfunctions of (1.38) are

$$
u_{,}=\exp \left[i q_{2}, r_{2}\right]
$$

and the assoriated eigenvatue is

$$
i==\begin{gathered}
(1 / \operatorname{Lr})^{2} \\
\left\{\sin ^{2} \vdots \eta \lambda r\right.
\end{gathered} .
$$



$$
1 ; \frac{x^{2}}{1}
$$

Thus (1.:! ! holds with $m=1$ and $M=. \boldsymbol{\tau}^{2} ; 1 \approx \because .5$.
There are sereral extensions of the above method for construeting $I_{20}$ that are important in practice. First, in the ase of Chebsinev spectral methots, it is appropriate to construct $L_{\text {ap }}$ using finite-difference approximations based on the collocation points $x,=\cos \pi j / \boldsymbol{N}$. In this case, the operator bounds (1.99) continue to hold with $M=2.5, m=1$ for a wide variety of operators $L$. Second, higher-order equations are best treated by writing them as a system of lower-order equations. Thus direct construction of $L_{\text {ap }}$ for $L=\Gamma^{4}$ gives

$$
1 \leqslant V_{\Delta R}^{-1} L_{a D}^{\|} \approx 6 \approx\left(\frac{\pi^{2}}{4}\right)^{2}
$$

However, if we introduce $v=\Gamma^{2} u$ and define the second-order operator $\mathcal{K}^{\circ}$ by

$$
K\binom{u}{v}=\left\{\begin{array}{l}
\Gamma^{2} u-v, \\
\Gamma^{2} v,
\end{array}\right.
$$

then direct construction of $K_{\text {ap }}$ as a finite-difference operator gives

$$
1 \leqslant\left\|K_{a D}^{-1} K_{t D}\right\| \leqslant 2.5
$$

Third, odd-order operators, initial-value problems and problems of mixed type are best treated by constructing $L_{a 0}$ on a grid that is roughly $50 \%$ finer than that used in construction of $L_{0 p}$ by collocation. In this case the spectral bounds (1.29) with $M \leqslant 2.5$ continue to hold for most problems. For example, the operator $\hat{c} / \hat{c} x$ with periodic boundary conditions has spectrum ik; while its centered finite-difference approximation has spectrum $i \sin (k \Delta x) / \Delta x$, so

$$
L_{\Delta p}^{-1} L_{\mathrm{aD}}{ }^{\eta}=O(k \Delta x / \sin k \Delta x),
$$

which is unbounded for $|k \Delta x|<\pi$, but bounded br $4 \pi / 3 \sqrt{3} \approx 2.4$ if $|k \Delta x|<2 \pi / 3$.

## 2. - Applications.

21. Introduction. - Over the last few years, there has been progress in understanding fundamental nonlinear processes in shear flows. In this section, I shall survey some results that have emerged from numerical studies of tran-
 problems. First, I shall summarize results on the basie matahitites that aerm
 to be universal in charatere and may explat mathy of the unifyine features of tramsition. Seromd. I shatl give some exampies of progress in the numerial simalation of high-Reyolds-number thows. Finally, I will give a syopsis of new ideas for subgrid scale chosures of huge-Reynolds-humber turbandere.

Full details of the ideas discussed here are given in the referencen.
$2 \because$ A transitional instability. - The processes by which laminar flows undergo transition to turbulence remain basically unsolved. However, recent numerical studies have provided some insights into transition, including:
$2 \div .1$. Nonclassical character of transitional instabilities. The primary linear (exponential) instability of classical plane parallel shear flows with noninflectional velocity profiles, as described by the Orr-Sommerfeld (or related) equations, is much too weak to describe transition. For example, linear instability of plane Poiseuille flow $\left(C(z)=1-z^{2},|z|<1\right.$ ) occurs for Reynolds numbers $R_{\mathrm{c}}>5758$, while Squire's theorem implies that the critical disturbance is two-dimensional. The fact that this instability is induced by a subtle interplay of viscosity and shear implies that its growth rates are quite small on convective time scales. For example, the most rapidly growing exponential mode of the Orr-Sommerfeld equation is obtained at $R_{\text {odt }}=48000$; its growth rate is only 0.0076 ; it is so feeble that perturbations grow by a factor 10 in a time of about 300 , in which time a point on the centerline moves about 150 channel widths. In contrast, transition is observed to occur explosively over a few channel widths at Reynolds numbers as low as roughly 1000. A transitional instability that affects noninflectional plane parallel shear flows must have a characteristic convective time scale.
2.2.2. Three dimensionality of transition. Tro-dimensional fluids do not appear to exhibit the kind of strong chaos that is characteristic of turbulent shear flows. In thermal convection, ClRry et al. [3] shor that twodimensional flows do not appear to act in a strongly chaotic war, but threedimensional flows may be strongly chaotic at large enough Reynolds number. Even for inflectional free shear flows, in which there are strong inviscid twodimensional instabilities, Brachet and Orszag [4] show that the flows that develop from tro-dimensional finite-amplitude disturbances are not strongly chaotic, in contrast to the flows that develop three-dimensionally.

2:3. Instability of twodimensional nonlinear travelling waves. Perhaps the simplest instability that has the character of a transitional instability is the dinear threedimensional instability of two-dimensional finite-amplitude fows. Orszag and Kells [5] and Onszig and l'itera [6]


Fig. 1. - Streamlines of the steady (stable) finite-amplitude twodimensional travel. ling wave for plane Poiseulle flow at $R=4000$, ploted in the rest frame of the wave (from [6]).
show how such an instability fits the basic features of transition in classical shear flows, including their convective growth rates, inherent three-dimensionality, onset at Reynolds numbers in accord with experimental observations and flow features in accord with early transitional flows. These instabilities have been analyzed both by direct numerical simulation of the evolving threedimensional flow and by a linear perturbation analysis of the nonparallel twodimensional (nonlinear travelling wave) flow. In tig. 1, we show the streamlines of a typical twodimensional base state (here for plane Poiseuille flow at $R=4000$ ). The nonparallel character of the base flow leads to considerable complication in its linear stability analysis (see [6] for the formulation of these large-matrix eigenvalue problems). A topic of much current research interest js the development of efficient numerical methods for finding eigenvalues of the very large matrices encountered in problems of this sort. In fig. $\because$. ne give a stability diaram for this transitional instability ; here we plot contours of constant growth rate as a function of the amplitude of the two-dimensional base state and the levolds mumber. The arowth rates of this instability are $1 \div 2$ orders of magnitude larger thatn these of orresommerfeld modes. The


Fig. 2. - Contours of constant growth rate (labelled by growth rate) as a function of $R$ and the amplitude of the background two.dimensional nonlinear wave (see right. hand scale).
development of this three-dimensional secondary instability seems to be consistent with available experimental data on early transitional flows. In fig. 3, we compare contours of the $x$ velocity at the so-called one-spike stage of transition in plane Poiseuille flow obtained a) experimentally by Nishroka, Iida and Kanbayashi [7] and b) numerically by Kletger and Schimaxn [8]. The


Fig. 3. - Contours of $x$ velocity in the $(x, y)$-plane at the one-spike stare in the laboratory experiments of Vishioka et al. (a)) and in the numerical simulation of Kleiser and Schumann (b)) (from [8]).




20.4. Comperition between two-dimensional latitng ant there dimensional instabilities. Inflertional free shear flows. like mixing laters and jats, are invisidly unstable to two-dimensinabl disturbances. squins theorem implies that these instabilities are strougent when twodimensional: when these twodimensional instabilities evolve in time, they saturate into ordered laminar-flow states characterized by large-seale vortical flow structures. These vortical flows may themselves be unstable to subharmonic (paring) instabilities, in which two (or more) vortices are paired and generate a new larger-scale vortex motion [9]. In these fows, the three-dimensional instability discussed above is also present [10], but it is not necessarily stronger than the pairing instability. However, the three-dimensional secondary instability is effective at much smaller spanwise spatial scales than is the inviscid primary instability and seems to lead directly to chaotic flows [4].


Fig. 4. - Time evolution of the Fourier component $b_{02}$ of the temperature field in two-dimensional Benard convection at $R_{\mathrm{a}}=120 R_{\text {ac. }} \mathrm{Ir}=20[3]$. The numbers labelling each plot give the wave number cut-off used to derive the Galerin approximation to the Bonssinesq equations. Thus $1 \times 2$ gives the Lorentz equations, white the higher-order models are higher-order Galerkin approximations. Ohserve that as the resolution increases the chaos disappears.
 that, whike bow-omer dymamal statems derived by Galerkios approximation

 (ser tig. f). Similarly, it was shown by OBszate and Kebls [a] that underresolved humerical calculations of transitional phanar shear flows may be spuriously chatic. Cinder-resolved computations do not have decrees of frectom associated with small spatial scales available to act as an eddy viscosity on well-resolved large scales.
23. Computer simulations of turbulence. - In this subsection, I shall give three examples of numerical simulations of turbulent flows. The first two examples, turbulent channel flow and the simulation of a turbulent spot, are of the nature of numerical experiments in which the numericist uses the computer in much the same way as the experimentalist uses the laboratory, namely as a source of data about flows in a controlled environment. The final example, the Taylor-Green vortex, is an example in which the computer is being used to try to uncover fundamental physical laws of turbulence.
23.1. Turbulent channel flow. Turbulent channel flows have been simulated numerically three ways: a) large-eddy simulation with a subgrid scale turbulence closure for eddies outside the wall layer and a heuristic boundary condition applied at the edge of the viscous sublayer by Deardorff [11] and Schumaxi [12], b) large-eddy simulation with a subgrid scale turbulence closure applied to eddies of all scales including those in the wall layer by Mors and Kar [13] and c) full numerical solution of the Navier-Stokes equations by Orszag and Patera [14]. The really crucial differences are, as we again note in subsect. 24 below, between $a$ ) and $b$ )-c). Simulations of type a) have much smaller computational requirements at a given Reynolds number $R$ than either of types $b$ ) or $c$, the latter requiring asymptotically similar computational work at large $R$. The deficiency of simulations of type $a$ ) is that they require modelling of wall layer effects in terms of an over-simplified boundary condition; the deficiencies of types $b$ ) and $c$ ) are that, with currently available computer resolution (say $64 \times 64 \times 65$ on a Cray-1 computer), Reynolds numbers are limited to about 10000 (type b)) or 5000 (type c)). For simulations of types $b$ ) or $c$ ), the computational work scales as $R^{2}$, so future increases in computer power do little to increase the effective Reynolds number of the computations.

Nevertheless, it is possible to achieve interesting results with full numerical solutions of the Navier-Stokes equations. In fig. 5, we plot the mean velocity profle found in the channel flow computations of Orszag and Patera [14]. The fit to a logarithmic wall layer velocity profle is only marginal, but the resulting von Karmán constant 0.45 is within experimental bounds, so this calenation does give the first computation of a wall layer from the basic prin-


Fig. 5. - Mean turbulent profile obtained by full numerical simulation of plane Poiseuille flow at $R=5000$ using a $64 \times 64 \times 65$ spectral simulation. Note the viscous sublayer, buffer region and logarithmic laver of $8 \div 9$ data points (from [14]).


Fig. 6. - A plot of the turbulent wall pressure spectrum as a function of frequency (from [15]).
ciples of fluid dynamics. Another more recent result from computations of this type is given in fig. 6 , in which we plot the wall pressure spectrum in a moderate-resolution ( $32 \times 32 \times 33$ ) run compared with available experimental data (see [15]). Despite the moderately low Reynolds number ( $R=5000$ ) of the simulation, agreement is achieved because flow features that do not depend explicitly on the boundary wall layer structure tend to be Reynolds number independent.



 recently，we have begran at study of spots using full hamerical selutions of the Navierstokes equations at moderate Reynolds numbers［1s］．The latter simn－ bations are perfermed ber foring the intial tow using at leatized force to drive a jet of flad vertically，then atlowing the disturbatce to evolve naturally． In fig． $\bar{i}$ and $x$ ，we plot contours of maximum vertio：l－z veleaty in the（ $\because$, ， 1 ） and（ $r, z$ ）plathes at various times of evolution of plane Poiseuille Hon．Tha character of this spot evolution is similar to that observed experimentally： the spot seems to spread in the spanwise direction by＂transwere contami－ mation⿻，in agreement with the dye injertion experiments of Gad－el－Hak ct al．［19］；the greatest turbulent activity is near the edres of the spot．the ＂spreading＊angle of the spot relative to its source is about $10^{\circ}$ ，in agreement with the channel flow experiments of Carison et al．［20］；the vertical structure of the spot is in qualitative agreement with that observed experiment．．lly． Further numerical experiments are under way that should elucidate det：ils of the flow in spots and the surrounding floid．


Fig．7．－Contours of the maximum $z$－velocity in the $(x, y)$－plane at $t=12,18$ after initializing a turbulent－spot computation by imposed vertical forcing．These computa－ tions are performed using a spectral code with $128(x) \times 32(y) \times 32(z)$ resolution．Fonrier series are used in $x$ and $y$ ；Chebrshev polynomial expansions are used in $z$ ．Here $R=6000$ ．


Fig．8．－Same as fig． 7 ，except $x-z$ contours of maxy $\mid r_{2}$ ．

23．3．TayIor－Green vortex．In order to gain understanding of the basic physies of the generation of small－scale turbulent flow features，a nice
 that whith develops in time from intial eomblions that empsist af exatation
 Doromes strongly thred dimmsional and dovelops rxatation at all spatial salev. The TG vortex las been wed to st uly subll fundamental gurstions as the wahancement of vortieity by vortex line stretehing, the aproach to inotrope of the mall sales. possible singular behatior of the Euler equations, formation of all inertial rance and anelysis of the peomotry and intermittence of highvortioty recions. The TG tlow is advantageons for these studies brause its sperial symmetry has allowed the development of numerical algorithms that are a factor 64 more efficient in both memory and storage than conventional periodir- germetry spectral methods. For a three-dimensional flow, this factor 64 translates into a factor 4 increased rance of apatial scale:-it is now pessible to compute the TG vortex flow with $512 \times 512 \times 512$ Fourier modes for each velocity component on the Cray-1 computer (or more than $4 \cdot 10^{8}$ effective degrees of freedom:).


Fig. 9. - A plot of the distribution of harge-vorticity regions in the TG vortex flow as a function of time $t$ and distance $d$ away from the side-walls of the impermeable cuhe in which the How takes place. Whserve how vorticity explodes in towards the



 Indeed, we find that the development of the turhulent thow serems to 1 engute viscosity to imbue instabilities of varticel haructure in which the imitial herere scale nonturbukent verticity maderges an raplesive redistabution in ghae (ser fig. 9). These visecsity-indued instabilities are probatly efiective berame viscosity allows vortex line recommetions prohibited in invised thow. Nimila diffusional instabilities have now been shown to be rexponsible for the generation of small-scale structures in two-dimensional magnetohydrodynamie [:3] and kinetic [24] turbulence. Further study of viscesity-indued instabilities shouht clarify the development of intermittent flow strurtures in turbulence.
24. Subgrid scale turbulence closures. - Perhaps the most distinguishing characteristic of high-Reynolds-number turbulent Hows is their lirge range of excited space and time scales. In homogeneous turbulence, dissipation scale eddies are of order $R^{\mathbf{d}}$ times smaller than entrg-ontaining eddies. Including the effect of this range of spatial scales on the allowable time step in a numerical solution of the Navier-Stokes equations gives the estimete that order $R^{2}$ operations are required to simulate a turbulent flow. This is the reason for interest in the large-eddy simulation method in which excitations on scales smaller than those resolvable numerically are modelled, usually by an eddy riscosity coefficient (see [11, 12]). The basic action of an eddy viscosity on large eddies is reasonable, although it cannot reproduce the random character of the action of small-scale eddies. However, in order to model properly wall turbulence, it is necessary to extend the subgrid modelling ideas of Deardorff and schumann and treat the turbulence all the way up to a rigid wall, as in recent work by Mois and Kisy [13]. Unfertunately, in order for Mors and Kis to rezolve motions down to the seale of turbulent bursts, which is necessary in order to capture the mechaninm producing the turbulence, the work restriction $O\left(R^{3}\right)$ remains. Thus the Reynolds-number restrictions are similar for large-pddy and full numerical solutions of the Navier-Stokes equations that attempt to integrate all the way through the wall layer region.

In ref at work, Yakhot and Orszag [25] have used dynamic renormalization group (RNG) methods to treat wall-bounded turbulence. The idee of the infra-red RNG method is to use perturbation methods based cn the direct. interaction approximation [ 26 ] to eliminate all small spatial scales up to the resolvable grid scale from the Navier-Stokes equations. This is done perturbitively by eliminating narrew bands of wave vecters from the dynamies foce fig. 10), renormatizing the resulting reduced dynamical equation to la ve the form of the Navier-Stokes equation with moditied viseosity and randem foreing terms, and then repeating the process iteratively until all the reguiral small seales are remosed. The revilting dyamical ropations involve a moditied

 Sentmans and Mons and kint in the wall redions in which there is interfereme
 to obtaming a faithfol representation of the wall region. . Ano, the indured


Fig. 10. - A selienatic representation of the modial structure of the dyamic renormalization group. Here $k_{0}$ represents wave numbers within the energy containing range, while 1 gives the high-wave-number (viscous) cut-off. Modes in the hatched band are removed at each step of the $\mathrm{R} \boldsymbol{\mathrm { N }} \mathrm{G}$ procedure.
random furce is large in the butfer layer between the viscous sublayer and the logarithmic layer, giving a turbulence source in this region. Further work is now under way applying these KNG -based closures to both large-eddy simulations of turbulent shear flows and to the derivation of new classes of turbulence transport (Reynolds averaged) equations that should be useful in engineering applications.

## 3. - Conclusion.

I have reviewed several areas of activity in the numelical simulation of transition and turbulence in which I have been intimately involved recently. In this short space, it has not been possible to do justice to all of the large number of researchers involved in these fields; the references do a more complete job of surreying the literature. The principal conclusions from our studies are:
i) Sumerical methods now provide essential information complementary to that available from experiment and mathematical analysis.
ii) Computational fluid mechanics has now matured, so that there are techniques that can be reliably applied to the mest difficult of fluid-mechanical problems. In contrast to 10 years ago, it is no longer mainly a question of how to compute a complicated flow, rather, now, it is a question of which flow to compute in order to extract the most useful information.
iii) It is crurial, especially in our studies of transitional flows, that we hare used spectral numerical methods (see sect. 1 above). Spectral methods are so arcurate for these problems that we can confidently conclude the: properly tested mumerical results are true fluid-medianical results. In contrast to finite-diflorence or finite-element methods in which an increase in spatial resolution by a factor $\because$ leads to an error decreare by a factor 4 or 8 or so, with spectral



 with experiment on wave sperels．The confidence in these results hat permithed new amalytial insights into the character of the onset of wave instabilitios of Taylon vortices in Courte flow［zi？］．
iv）Sen menerations of bigree and faster computers（an most protitably be ured to extend the range of applimation of computational fluid dyamics． Transition and turbulence problems in complex geometries with complex physies，like multiphase flows，will surely be the subject of studies in the near fiture．

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