Journal of Computational Physics **163,** 548–549 (2000)
doi:10.1006/jcph.2000.6607, available online at http://www.idealibrary.com on IDEAL®

Abstracts of Papers to Appear

ADJOINT ERROR ESTIMATION AND GRID ADAPTATION FOR FUNCTIONAL OUTPUTS: APPLICATION TO QUASI-ONE-DIMENSIONAL FLOW. David A. Venditti and David L. Darmofal. *Department of Aeronautics and Astronautics, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Room 37-442, Cambridge, Massachusetts 02139.*

An error estimation and grid adaptation strategy for estimating and reducing simulation errors in functional outputs of partial differential equations is presented. The procedure is based on an adjoint formulation in which the estimated error in the functional can be directly related to the local residual errors of both the primal and adjoint solutions. This relationship allows local error contributions to be used as indicators in a grid-adaptive strategy designed to produce specially tuned grids for accurate estimation of the chosen functional. In this paper, attention is limited to one-dimensional problems, although the procedure is readily extendable to multiple dimensions. The error estimation procedure is applied to a standard, second-order, finite volume discretization of the quasi-one-dimensional Euler equations. Both isentropic and shocked flows are considered. The chosen functional of interest is the integrated pressure along a variable-area duct. The error estimation procedure, applied on uniform grids, provides superconvergent values of the corrected functional. Results demonstrate that additional improvements in the accuracy of the functional can be achieved by applying the proposed adaptive strategy to an initially uniform grid. The proposed adaptive strategy is also compared with a standard adaptive scheme based on the interpolation error in the computed pressure. The proposed scheme consistently yields more accurate functional predictions than the standard scheme.

REDUCTION OF CHEMICAL KINETICS IN AIR POLLUTION MODELING. Bruno Sportisse and Rafik Djouad. *Centre d'Enseignement et de Recherche Eau, Ville, Environnement, Ecole Nationale des Ponts et Chaussées (ENPC-CEREVE), rue Blaise Pascal, 77455 Champs sur Marne, France.*

We investigate in this article the use of reduction techniques in air pollution modeling. The reduction of chemical kinetics is performed on the basis of a time-scale analysis and of lumping. Lumping techniques are widely used in air pollution modeling and consist in replacing some *pure* chemical species with linear combinations of species. We focus here on the theoretical justification for such techniques. We propose an algorithm to build up lumped species in a systematic way. An application to three kinetic schemes coupled with diffusion is presented in a monodimensional case. This justifies the way we couple a reduced kinetic scheme with other processes.

ACCURATE AND EFFICIENT SIMULATION OF RIGID BODY ROTATIONS. Samuel R. Buss. *Department of Mathematics, University of California, San Diego.*

This paper introduces efficient and accurate algorithms for simulating the rotation of a three-dimensional rigid object and compares them to several prior methods. First, we introduce a second-order accurate method that incorporates a third-order correction; then a third-order accurate method; and finally a fourth-order accurate method. These methods are single-step and the update operation is only a single rotation. The algorithms are derived in a general Lie group setting. Second, we introduce a near-optimal energy-correction method which allows exact conservation of energy. This algorithm is faster and easier to implement than implicit methods for exact energy-conservation. Our third-order method with energy conservation is experimentally seen to act better than a fourth-order accurate method. These new methods are superior to naive Runge–Kutta or predictor–corrector methods, which are only second-order accurate for sphere-valued functions. The second-order symplectic

0021-9991/00 $35.00

McLachlan–Reich methods are observed to be excellent at approximate energy conservation, but are not as good at long-term accuracy as our best methods. Finally we present comparisons with fourth-order accurate symplectic methods, which have good accuracy but higher computational cost.

A NUMERICAL MODEL FOR TRICKLE BED REACTORS. Richard M. Propp, Phillip Colella, William Y. Crutchfield, and Marcus S. Day. *Lawrence Berkeley National Laboratory, Berkeley, California 94720.*

Trickle bed reactors are governed by equations of flow in porous media such as Darcy's law and the conservation of mass. Our numerical method for solving these equations is based on a total-velocity splitting sequential formulation which leads to an implicit pressure equation and a semiimplicit mass conservation equation. We use high-resolution finite difference methods to discretize these equations. Our solution scheme extends previous work in modeling porous media flows in two ways. First, we incorporate physical effects due to capillary pressure, a nonlinear inlet boundary condition, spatial porosity variations, and inertial effects on phase mobilities. In particular, capillary forces introduce a parabolic component into the recast evolution equation, and the inertial effects give rise to hyperbolic nonconvexity. Second, we introduce a modification of the slope limiting algorithm to prevent our numerical method from producing spurious shocks. We present a numerical algorithm for accommodating these difficulties, show the algorithm is second-order accurate, and demonstrate its performance on a number of simplified problems relevant to trickle bed reactor modeling.

A QUASI-STEADY-STATE SOLVER FOR THE STIFF ORDINARY DIFFERENTIAL EQUATIONS OF REACTION KINETICS. David R. Mott,* Elaine S. Oran,* and Bram van Leer.† **Laboratory for Computational Physics and Fluid Dynamics, Naval Research Laboratory, and* †*Department of Aerospace Engineering, The University of Michigan.*

A quasi-steady-state method that integrates stiff differential equations arising from reaction kinetics is presented. This predictor–corrector method is A-stable for linear equations and second-order accurate. The method is used for all species regardless of the timescales of the individual equations, and it works well for problems typical of hydrocarbon combustion. Start-up costs are low, making the method ideal for use in process-split reacting-flow simulations which require the solution of an initial-value problem in every computational cell for every global timestep. The algorithm is described, and error analysis and linear stability analysis are included. The algorithm is also applied to several test problems, and the results are compared to those of the stiff integrator CHEMEQ. The method, which we call α-QSS, is more stable, is more accurate, and costs less than CHEMEQ.