

orbits are close to the exact orbits, even after an unlimited number of timesteps. The equivalence between the discrete-time and continuous-time dynamics holds only for sufficiently small of the timestep Δ . For intermediate values of Δ (sufficiently large that the conservation law does not hold, but sufficiently small that the numerical orbits are not chaotic) a new "super-adiabatic" invariant A is derived, and it is shown that conservation of A forces the numerical orbits to lie on smooth closed curves. If the potential energy varies rapidly over a small region, it is shown that very high-order resonances between the timestep and the orbital period T , (i.e., $T/\Delta = n$, where n is a large integer) produce large deviations of these closed curves from the exact orbit. Such resonances also cause extreme sensitivity of the numerical orbit to the timestep.

BOUNDARY ELEMENT SOLUTION OF HEAT CONVECTION-DIFFUSION PROBLEMS. B. Q. Li, *Massachusetts Institute of Technology, Cambridge, Massachusetts, USA*; J. W. Evans, *University of California, Berkeley, California, USA*.

A boundary element method is described in detail for the solution of two-dimensional steady-state convective heat diffusion problems in homogeneous and isotropic media with both linear and nonlinear boundary conditions. Through an exponential variable transformation, the introduction of fundamental solutions and the use of Green's theorem, the problem is reduced to one involving values of temperature and/or heat flux in the form of an integral only along the boundary. The integral is solved numerically for three examples. Two of them have linear boundary conditions and their numerical results are compared with the corresponding analytical solutions. The other has a nonlinear boundary condition due to heat radiation and an iterative procedure is applied to obtain the numerical solution. The fictitious source formulation leading to the boundary element solution of the same problems is discussed as an alternative. The extension of the method to formulate transient and/or three-dimensional convective heat diffusion problems is also described, and the relevant fundamental solutions are given. Finally, the exponential variable transformation is applied to construct a functional of variational principle which leads to developing a finite element formulation of the problems with a banded, symmetric stiffness matrix.

CLOSED FORM SOLUTION FOR LOCALIZED MODES ON A POLYMER CHAIN WITH A DEFECT. V. K. Saxena, *Universidade Federal de Santa Catarina, Florianopolis, SC, BRAZIL*; L. L. Van Zandt and W. K. Schroll, *Purdue University, West Lafayette, Indiana, USA*.

The problem of localized vibration modes on a polymer chain with a symmetry breaking defect is formulated as a finite sum of exponentially decaying waves on the polymer. Applying a set of similarity and unitary transformations, and using the singular value decomposition technique, the size of the problem is reduced to relatively small dimensions as compared to the large size of the original set of equations for propagating modes on the chain. A modification of the polynomial eigenvalue problem converts the algebraic system to a simple eigenvalue problem which may be diagonalized to give eigenvectors of different decaying waves for an expansion set to describe general localized excitations. Application of proper boundary conditions at the site of broken symmetry leads to determination of the frequencies of the localized modes and corresponding eigenvector expansion. Possible applications of the algorithm to various defect problems on a polymer chain are discussed and some preliminary results on a particular defect are presented.

RUNGE-KUTTA SMOOTHER FOR SUPPRESSION OF COMPUTATIONAL-MODE INSTABILITY OF LEAP FROG SCHEME. Akira Aoyagi, *Kyushu Industrial University, Fukuoka, JAPAN*; Kanji Abe, *The University of Tokyo, Tokyo, JAPAN*.

The Runge-Kutta smoother is applied to suppress nonlinear numerical instabilities in the leap-frog scheme for time integration of the Korteweg-de Vries equation. The accuracy of integration is compared

with one using a second-order smoother. The Runge–Kutta smoother enables us to make long-time integration of the Korteweg–de Vries equation for large amplitudes.

NUMERICAL SOLUTION OF A HYPERBOLIC SYSTEM OF CONSERVATION LAWS WITH SOURCE TERM ARISING IN A FLUIDIZED BED MODEL. I. Christie and G. H. Ganser, *West Virginia University, Morgantown, West Virginia, USA*; J. M. Sanz-Serna, *Universidad de Valladolid, Valladolid, SPAIN*.

A model of a gas fluidized bed is considered which leads to a hyperbolic system of conservation laws with a source term. The system is solved numerically by a second order operator splitting technique based on a Roe approximate Riemann solver. Numerical experiments demonstrate the ability of the model to reproduce qualitatively the slugging phenomenon in the case when the bed is subject to a relatively large gas flux.

APPROXIMATING THE DIRAC DISTRIBUTION FOR FOURIER ANALYSIS. Stuart B. Cohen and Ivan N. Krischner, *University of Michigan, Ann Arbor, Michigan, USA*.

For some boundary or initial value problems, the presence of a Dirac distribution on the boundary or in the field results in finite solutions at some points in the domain. However, its presence leads to difficulties if the problem is solved analytically using a Fourier decomposition, since computation and presentation of the solution usually necessitate some sort of truncation. To circumvent this problem, the Dirac distribution is often approximated by a Gaussian distribution, which results in a very simple Fourier transform on an infinite domain. On a finite domain the transform is not as simple, but may still be computed. However, the derivative of the Gaussian is discontinuous on the finite domain, since the smooth function has been truncated. Thus a different approximation, the β_π -distribution, is proposed. This function satisfies the same criteria which make the Gaussian applicable as an approximation of the Dirac distribution on the infinite domain, but its derivative is continuous everywhere on the finite domain. This article presents a procedure for computing the Fourier coefficients of the β_π -distribution. Since a large value of the order of the distribution is chosen to approximate the singular behavior, the integral for the Fourier coefficients must be evaluated using a Fourier–Bessel decomposition, which allows the computation to be carried out over large values of the Fourier index. The technique is illustrated with application to a simple two-dimensional boundary value problem containing a singularity in the boundary condition. Convergence is significantly improved if the proposed distribution is used. Values of some Fourier coefficients of the β_π -distribution are provided in an appendix for several values of its order.

ON THE NATURE OF BOUNDARY CONDITIONS FOR FLOWS WITH MOVING FREE SURFACES. Michael Renardy and Yuriko Renardy, *Virginia Polytechnic Institute & State University, Blacksburg, Virginia, USA*.

We consider small perturbations of plane parallel flow between a wall and a moving free surface. The problem is posed on a rectangle with inflow and outflow boundaries. The usual boundary conditions are posed at the wall and the free surface, and the fluid satisfies the Navier–Stokes equations. We examine the nature of boundary conditions which can be imposed at the inflow and outflow boundaries in order to yield a well-posed problem. This question turns out to be more delicate than is generally appreciated. Depending on the precise situation and on the regularity required of the solution, boundary conditions at just one or both endpoints of the free surface need to be imposed. For example, we show that if the velocities at the inflow and outflow boundaries are prescribed, then the position of the free surface at the inflow boundary can be prescribed, but not at the outflow if an H^1 -solution is desired. Numerical simulations with the FIDAP package are used to illustrate our analytical results.