

used in this sense to decompose the maximum memory working space required without affecting the results.

NUMERICAL MODELING OF ELECTROMAGNETIC CASTING PROCESSES. O. Besson, J. Bourgeois, P.-A. Chevalier, J. Rappaz, and R. Touzani, *Ecole Polytechnique Fédérale, Lausanne, SWITZERLAND*.

The main goal of this paper is to present a numerical model describing the major physical phenomena involved in electromagnetic casting industrial processes as precisely as possible. Under suitable physical assumptions, we derive the set of equations in the two-dimensional case; we describe in detail the numerical methods used to solve such equations and derive an iterative algorithm. Numerical results describing the case of an aluminium ingot are presented in order to show the efficiency of the method.

AN IMPROVEMENT OF FRACTIONAL-STEP METHODS FOR THE INCOMPRESSIBLE NAVIER-STOKES EQUATIONS. Hung Le and Parviz Moin, *Stanford University, Stanford, California, USA*.

A numerical method for computing three-dimensional, unsteady incompressible flows is presented. The method is a predictor-corrector technique combined with a fractional step method. Each time step is advanced in three sub-steps. The novel feature of the present scheme is that the Poisson equation for the pressure is solved only at the final sub-step resulting in substantial savings in computing time. It is shown that the method allows a larger CFL number and reduces the computing cost without loss of accuracy by satisfying the continuity equation only at the last sub-step. Numerical solutions for the decaying vortices and flow over a backward-facing step are obtained and compared with analytical and other numerical results.

NUMERICALLY INDUCED STOCHASTICITY. Alex Friedman, *Lawrence Livermore National Laboratory, Livermore, California, USA*; Steven P. Auerbach, *Science Applications International Corp., Emeryville, California, USA*.

The true motion of a particle in a one-dimensional potential well is regular, since conservation of energy constrains the velocity v at each value of the coordinate x . Nonetheless, when the orbit is computed numerically, stochastic behavior can result. We have considered simple integrators as mappings from (x, v) at one discrete time level to (x, v) at the next. In general, when the timestep size Δ is small enough, there are closed orbits, while for larger values there is chaos. Chaos can result for surprisingly small values of Δ in cases where the physical phase plane includes a separatrix. The behavior of the leapfrog mover as applied to motion in a particular double-well potential is examined in detail. Here, the onset of stochasticity occurs at step sizes much smaller than the stability threshold associated with the harmonic dependence of the potential at large $|x|$. Other one-dimensional wells and movers are also treated; implications of the area-preserving and energy conserving attributes possessed by some movers are discussed. A new variant of the standard map, displaying symmetry about both $x = 0$ and $v = 0$ in its phase plane, is introduced.

LONG-TIME BEHAVIOR OF NUMERICALLY COMPUTED ORBITS: SMALL AND INTERMEDIATE TIMESTEP ANALYSIS OF ONE-DIMENSIONAL SYSTEMS. Steven P. Auerbach, *Science Applications International Corporation, Emeryville, California, USA*; Alex Friedman, *Lawrence Livermore National Laboratory, Livermore, California, USA*.

The long-time behavior of numerically computed orbits in one-dimensional systems is studied by deriving a continuous-time "pseudo-dynamics" equivalent to the discrete-time numerical dynamics. The derivation applies to any numerical algorithm which conserves phase-space volume. A conservation law of the continuous-time system (conservation of the "pseudo-Hamiltonian") guarantees that the numerical

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