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Abstracts of Papers to Appear

A CARTESIAN GRID FINITE-VOLUME METHOD FOR THE ADVECTION–DIFFUSION EQUATION IN IRREGULAR GEOMETRIES. Donna Calhoun* and Randall J. LeVeque.*,† **Department of Applied Mathematics, and* †*Department of Mathematics, University of Washington, Box 352420, Seattle, Washington 98195-2420.* E-mail: calhoun@amath.washington.edu, rjl@amath.washington.edu.

We present a fully conservative, high-resolution, finite volume algorithm for advection–diffusion equations in irregular geometries. The algorithm uses a Cartesian grid in which some cells are cut by the embedded boundary. A novel feature is the use of a "capacity function" to model the fact that some cells are only partially available to the fluid. The advection portion then uses the explicit wave-propagation methods implemented in CLAWPACK, and is stable for Courant numbers up to 1. Diffusion is modeled with an implicit finite volume algorithm. Results are shown for several geometries. Convergence if verified and the 1-norm order of accuracy is found to between 1.2 and 2, depending on the geometry and Peclet number. Software is available on the web.

A TIME-SPLITTING TECHNIQUE FOR THE ADVECTION–DISPERSION EQUATION IN GROUNDWATER. Annamaria Mazzia, Luca Bergamaschi, and Mario Putti. *Dipartimento di Metodi e Modelli Matematici per le Scienze Applicate, Università degli Studi di Padova, via Belzoni 7, 35131 Padova, Italy.* E-mail: mazzia@dmsa.unipd.it, berga@math.unipd.it, putti@dmsa.unipd.it.

In this paper a time-splitting technique for the two dimensional advection–dispersion equation is proposed. A high resolution in space Godunov method for advection is combined with the RT0 Mixed Finite Element for the discretization of the dispersion term. Numerical tests on an analytical one-dimensional example ascertain the convergence properties of the scheme. At different Peclet numbers, the choice of optimal timestep size used for the two equations is discussed, showing that with accurate selection of the timestep sizes, the overall CPU time required by the simulations can be drastically reduced. Results on a realistic test case of groundwater contaminant transport confirm that the proposed scheme does not suffer from Peclet limitations, and always displays only small amounts of numerical diffusion across the entire range of Peclet numbers.

NUMERICAL SIMULATIONS FOR RADIATION HYDRODYNAMICS. II. TRANSPORT LIMIT. W. Wenlong Dai and Paul R. Woodward. *School of Physics and Astronomy/Laboratory for Computational Science and Engineering, University of Minnesota, 116 Church Street S.E., Minneapolis, Minnesota 55455.*

A finite difference scheme for two-dimensional radiation hydrodynamical equations in the transport limit is proposed . The scheme is of Godunov-type, in which the set of time-averaged flux needed in the scheme is calculated through Riemann problems solved. In the scheme, flow signals are explicitly treated, while radiation signals are implicitly treated. Flow fields and radiation fields are updated simultaneously. An iterative approach is proposed to solve the set of nonlinear algebraic equations arising from the implicitness of the scheme. The sweeping method used in the scheme significantly reduces the number of iterations or computer CPU time needed. A new approach to further accelerate the convergence is proposed, which further reduces the number of iterations needed by more than one order. No matter how many cells radiation signals propagate in one timestep, only an extremely small number of iterations are needed in the scheme, and each iteration costs only about 0.8% of computer CPU time which is needed for one timestep of a second-order accurate and fully explicit scheme. Two-dimensional problems are treated through a dimensionally split technique. Therefore, iterations for solving the set of algebraic equations are carried out only in each one-dimensional sweep. Through numerical examples

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it is shown that the scheme keeps the principle advantages of Godunov schemes for flow motion. In the timescale of flow motion numerical results are the same as those obtained from a second-order accurate and fully explicit scheme. The acceleration of the convergence proposed in this paper may be directly applied to other hyperbolic systems.

MULTISYMPLECTIC RUNGE–KUTTA COLLOCATION METHODS FOR HAMILTONIAN WAVE EQUATIONS. Sebastian Reich. *Department of Mathematics and Statistics, University of Surrey, Guildford GU2 5XH, United Kingdom.*

A number of conservative PDEs, like various wave equations, allow for a multisymplectic formulation which can be viewed as a generalization of the symplectic structure of Hamiltonian ODEs. We show that Gauss–Legendre collocation in space and time leads to multisymplectic integrators, i.e., to numerical methods that preserve a symplectic conservation law similar to the conservation of symplecticity under a symplectic method for Hamiltonian ODEs. We also discuss the issue of conservation of energy and momentum. Since time discretization by a Gauss–Legendre method is computational rather expensive, we suggest several semi-explicit multisymplectic methods based on Gauss–Legendre collocation in space and explicit or linearly implicit symplectic discretizations in time.

EFFICIENT CALCULATION OF JACOBIAN AND ADJOINT VECTOR PRODUCTS IN WAVE PROPAGATIONAL INVERSE PROBLEM USING AUTOMATIC DIFFERENTIATION. Thomas F. Coleman,* Fadil Santosa,† and Arun Verma.‡ **Computer Science Department and Center for Applied Mathematics, Cornell University, Ithaca, New York 14850; †Minnesota Center for Industrial Mathematics, School of Mathematics, University of Minnesota, Minneapolis, Minnesota 55455; and ‡Cornell Theory Center, Cornell University, Ithaca, New York 14850.* E-mail: coleman@tc.cornell.edu, santosa@math.umn.edu, verma@cs.cornell.edu.

Wave propagational inverse problems arise in several applications including medical imaging and geophysical exploration. In these problems, one is interested in obtaining the parameters describing the medium from its response to excitations. The problems are characterized by their large size, and by the hyperbolic equation which models the physical phenomena. The inverse problems are often posed as a nonlinear data-fitting where the unknown parameters are found by minimizing the misfit between the predicted data and the actual data. In order to solve the problem numerically using a gradient-type approach, one must calculate the action of the Jacobian and its adjoint on a given vector. In this paper, we explore the use of automatic differentiation (AD) to develop codes that perform these calculations. We show that by exploiting structure at two scales, we can arrive at a very efficient code whose main components are produced by AD. In the first scale we exploit the time-stepping nature of the hyperbolic solver by using the "Extended Jacobian" framework. In the second (finer) scale, we exploit the finite difference stencil in order to make explicit use of the sparsity in the dependence of the output variables to the input variables. The main ideas in this work are illustrated with a simpler, one-dimensional version of the problem. Numerical results are given for both one- and two-dimensional problems. We present computational templates that can be used in conjunction with optimization packages to solve the inverse problem.