Enhanced Elliptic Grid Generation

Decay parameters that govern grids near boundaries are determined automatically.

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An enhanced method of elliptic grid generation has been invented. Whereas prior methods require user input of certain grid parameters, this method provides for these parameters to be determined automatically.

"Elliptic grid generation" signifies generation of generalized curvilinear coordinate grids through solution of elliptic partial differential equations (PDEs). Usually, such grids are fitted to bounding bodies and used in numerical solution of other PDEs like those of fluid flow, heat flow, and electromagnetics. Such a grid is smooth and has continuous first and second derivatives (and possibly also continuous higher-order derivatives), grid lines are appropriately stretched or clustered, and grid lines are orthogonal or nearly so over most of the grid domain. The source terms in the grid-generating PDEs (hereafter called "defining" PDEs) make it possible for the grid to satisfy requirements for clustering and orthogonality properties in the vicinity of specific surfaces in three dimensions or in the vicinity of specific lines in two dimensions.

The grid parameters in question are decay parameters that appear in the source terms of the inhomogeneous defining PDEs. The decay parameters are characteristic lengths in exponential-decay factors that express how the influences of the boundaries decrease with distance from the boundaries. These terms govern the rates at which distance between adjacent grid lines change with distance from nearby boundaries.

Heretofore, users have arbitrarily specified decay parameters. However, the characteristic lengths are coupled with the strengths of the source terms, such that arbitrary specification could lead to conflicts among parameter values. Moreover, the manual insertion of decay parameters is cumbersome for static grids and infeasible for dynamically changing grids.

In the present method, manual insertion and user specification of decay parameters are neither required nor allowed. Instead, the decay parameters are determined automatically as part of the solution of the defining PDEs. Depending on the shape of the boundary segments and the physical nature of the problem to be solved on the grid, the solution of the defining PDEs may provide for rates of decay to vary along and among the boundary segments and may lend itself to interpretation in terms of one or more physical quantities associated with the problem.

The limiting form of the defining equations used in this method is partly analogous to boundary-value PDEs for heat transfer over long, thin fins governing convection and conduction of heat across the boundary segments and heat generated or lost within the volume to be enclosed by the grid. Each limiting form of the defining equations is deemed to be valid near at least one boundary segment. Each such equation includes at least two independent Cartesian coordinate variables and at least one generalized coordinate as a dependent variable, the integral form of which constitutes a boundary constraint. Boundary conditions analogous to temperature and thermal conductivity prescription can be specified by the user. In addition, as an essential element of the method, a selected power of at least one heat-transfer coefficient must correspond to at least one decay parameter (which, as stated above, the user does



A **Grid in an Annulus** between relatively rotating inner and outer circles was generated by the present method.

not specify) near at least one boundary segment, and such a heat-transfer coefficient evolves according to the boundary constraint.

The figure presents results of application of the method to a two-dimensional annular region. This example illustrates the clustering of grid points near the inner boundary of the annulus. It also illustrates how the grid evolves automatically with one or more time-varying boundary condition(s) — in this case, rotation of the inner boundary relative to the outer boundary or vice versa. In a case involving time-varying boundary conditions, the solution at each time step serves as a starting point for the solution at the next time step.

This work was done by Upender K. Kaul of Ames Research Center.

Inquiries concerning rights for the commercial use of this invention should be addressed to the Technology Partnerships Division, Ames Research Center, (650) 604-2954. Refer to ARC-14710-1

Automated Knowledge Discovery From Simulators

Active learning process efficiently explores simulator input space.

NASA's Jet Propulsion Laboratory, Pasadena, California

A computational method, SimLearn, has been devised to facilitate efficient knowledge discovery from simulators. Simulators are complex computer programs used in science and engineering to model diverse phenomena such as fluid flow, gravitational interactions, coupled mechanical systems, and nuclear, chemical, and biological processes. SimLearn uses active-learning techniques to efficiently address the "landscape characterization problem." In particular, SimLearn tries to determine which regions in "input space" lead to a given output from the simulator, where "input space" refers to an abstraction of all the variables going into the simulator, e.g., initial conditions, parameters, and interaction equations. Landscape characterization can be viewed as an attempt to invert the forward mapping of the simulator and recover the inputs that produce a particular output.

Given that a single simulation run can take days or weeks to complete even on a large computing cluster, Sim-Learn attempts to reduce costs by reducing the number of simulations needed to effect discoveries. Unlike conventional data-mining methods that are applied to static predefined datasets, SimLearn involves an iterative process in which a "most informative" dataset is constructed dynamically by using the simulator as an oracle. On each iteration, the algorithm models the knowledge it has gained through previous simulation trials and then chooses which simulation trials to run next. Running these trials through the simulator produces new data in the form of input-output pairs.

The overall process is embodied in an algorithm that combines support vector machines (SVMs) with active learning. SVMs use learning from examples (the examples are the input-output pairs generated by running the simulator) and a principle called maximum margin to derive predictors that generalize well to new inputs. In SimLearn, the SVM plays the role of modeling the knowledge that has been gained through previous simulation trials. Active learning is used to determine which new input points would be most informative if their output were known. The selected input points are run through the simulator to generate new information that can be used to refine the SVM. The process is then repeated. SimLearn carefully balances exploration (semi-randomly searching around the input space) versus exploitation (using the current state of knowledge to conduct a tightly focused search).

During each iteration, SimLearn uses not one, but an ensemble of SVMs. Each SVM in the ensemble is characterized by different hyperparameters that control various aspects of the learned predictor - for example, whether the predictor is constrained to be very smooth (nearby points in input space lead to similar output predictions) or whether the predictor is allowed to be "bumpy." The various SVMs will have different preferences about which input points they would like to run through the simulator next. Sim-Learn includes a formal mechanism for balancing the ensemble SVM preferences so that a single choice can be made for the next set of trials.

Initial tests with two real-world scien-

tific simulators have shown that Sim-Learn is effective in reducing the number of trials needed to accurately identify the regions of input space leading to particular output behaviors. In the first application involving simulations of collisions between asteroids and the gravitational interactions between the resulting fragments, parameters of the two colliding asteroids that lead to binary pairs (gravitationally bound fragments in orbit around a common center of mass) were identified using only half the simulation trials needed to obtain equivalent knowledge from a grid-based sampling approach. In the second application involving simulations of the Earth's magnetosphere, there was a corresponding reduction by a factor of six in the number of simulation trials required.

This work was performed by Michael Burl, Dennis DeCoste, Dominic Mazzoni, and Lucas Scharenbroich of Caltech and Brian Enke and William Merline of the Southwest Research Institute for NASA's Jet Propulsion Laboratory. Further information is contained in a TSP (see page 1).

The software used in this innovation is available for commercial licensing. Please contact Karina Edmonds of the California Institute of Technology at (626) 395-2322. Refer to NPO-43399.

Electro-Optical Modulator Bias Control Using Bipolar Pulses

Bias is automatically adjusted to maintain maximum extinction during "off" periods.

NASA's Jet Propulsion Laboratory, Pasadena, California

An improved method has been devised for controlling the DC bias applied to an electro-optical crystal that is part of a Mach-Zehnder modulator that generates low-duty-cycle optical pulses for a pulse-position modulation (PPM) optical data-communication system. In such a system, it is desirable to minimize the transmission of light during the intervals between pulses, and for this purpose, it is necessary to maximize the extinction ratio of the modulator (the ratio between the power transmitted during an "on" period and the power transmitted during an "off" period). The present method is related to prior dither error feedback methods, but unlike in those methods, there is no need for an auxiliary modulation subsystem to generate a dithering signal. Instead, as described below, dither is effected through alternation of the polarity of the modulation signal.



Figure 1. A **Mach-Zehnder Modulator** is a Mach-Zehnder interferometer that includes an electro-optical crystal for varying the difference between the lengths of its two optical paths. If V_{bias} is set at the optimum value, then the output optical power varies as a symmetrical function of V_{RF} .