An Efficient Graph Coloring Algorithm for Stencil-based Jacobian Computations

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Numerical methods for the solution of partial differential equations constitute an important class of techniques in scientific computing. Often, the discretization is based on approximating the partial derivatives by finite differences on a regular Cartesian grid. The resulting computations are structured in the sense of updating a large, multidimensional array by a stencil operation. A stencil defines the update of the value at a grid point based on values at neighboring grid points.

We consider the problem of computing the Jacobian matrix of some functions that is given in the form of a computer program involving stencil operations on a regular Cartesian grid. Due to the stencil operations this Jacobian matrix is sparse. The exploitation of the stencil-type to compute this sparse Jacobian matrix using automatic differentiation with minimal computational effort can be modeled as a graph coloring problem [1]. By definition, exact solutions of this combinatorial optimization problem use the minimal number of colors. Exact solutions in terms of explicit formuæ are known for various stencil types [2, 4, 5]. However, a formula for the exact solution is not readily available for an arbitrary stencil type. So, by ignoring any structure implied by a given stencil, it is not uncommon to use coloring heuristics for general graphs. These heuristics try to approximate the exact solution and will, most likely, not attain the minimal number of colors. Recently, Lülfesmann and Kawarabayashi [3] introduced a graph coloring algorithm for an arbitrary stencil on a regular multidimensional Cartesian grid that computes the exact solution. This algorithm eliminates the need for deriving an explicit formula for the exact solution. It is based on a divide-and-conquer approach that establishes a hierarchy of vertex separators that recursively decomposes the grid into smaller and smaller subgrids. The main advantage of this algorithm is that it always computes a coloring with the minimal number of colors. However, the disadvantage of this algorithm is its high computational complexity. In fact, there are problem instances reported in [3] where, compared to the running time of a traditional graph coloring heuristic, the running time of this algorithm is larger than a factor of more than 800.

So, there is urgent need to look for alternative ways to compute exact solutions of this structured graph coloring problem while reducing the resulting running time. In this extended abstract we propose a novel graph coloring algorithm for stencil-based Jacobian computations on a regular Cartesian grid whose running time is independent of the grid size. The main advantage of this new approach is twofold: First, it computes a coloring with a minimal number of colors. Second, its computational complexity is low. The disadvantage is that we currently can not prove that this algorithm computes a solution for every given stencil type. It is currently open whether or not there is any stencil type where the algorithm terminates without computing a solution. However, we carried out extensive numerical experiments

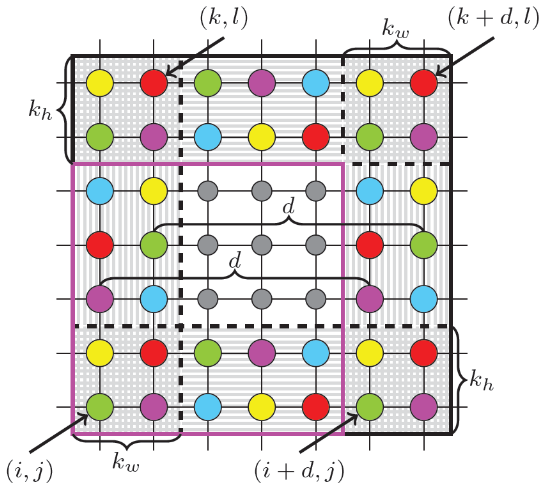

Figure 1: A 7×7 colored tile with a minimal coloring for the five-point stencil.

varying stencil types and observed that the new algorithm successfully computed a solution for all considered stencil types.

The main idea of the new algorithm is to color a small subgrid whose coloring allows to color a larger grid of arbitrary size. We call such a subgrid a *colored tile*. For the sake of simplicity, the following discussion is restricted to grids in two dimensions. However, the algorithm also generalizes to multidimensional Cartesian grids. A colored tile consists of two pairs of rectangular regions with the following property. A pair of two rectangular regions is called *consistent* if and only if the two rectangular regions have the same number of grid points in each grid dimension and all corresponding grid points are colored identically. In Figure 1, the pair of the two 2×7 rectangular regions on the left and right border of the 7×7 colored tile are consistent, because the color of a grid point (i, j) is identical to the color of the grid point $(i + d, j)$. Similarly, the top and bottom 7×2 rectangular regions are also consistent. Therefore, the 5×5 region indicated by the box with the purple frame in the bottom left corner can be used to color a larger grid by repeatedly placing this region next to each other in horizontal and vertical direction. To ensure a valid coloring, the width k_w and height k_h of the consistent rectangular regions are important and depend on the given stencil type. These values are chosen by taking into account grid points which we call *structurally non-orthogonal*.

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