

we have demonstrated the versatility and robustness of MoL based on SiC and TR-BDF2 in solving a challenging class of pseudo-parabolic equations.

Evaluation of Serial and Parallel Shared-Memory Distance-1 Graph Coloring Algorithms

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Among the many application areas of graphs is modeling of irregular data structures in various problems occurring in linear algebra, preconditioners, community detection, scheduling, and mesh adaptation. Within the scope of computational science and engineering, the standard graph coloring problem, the distance-1 coloring, is typically used to select independent sets on which subsequent parallel computations can be performed. As graph coloring is an active field of research, numerous algorithms are available, each offering different advantages and disadvantages. Due to the broad availability of modern many- and multi-core systems a lot of research has recently been conducted on shared-memory parallel graph coloring algorithms, culminating in new approaches for coloring and, in particular, balancing graphs, i.e., balancing the resulting population of the different color classes.

We compare several serial as well as shared-memory parallel graph coloring algorithms for the standard graph coloring problem based on specific reference graphs. Our reference graphs cover a wide range of different graph types and applications and are of varying difficulty for the algorithms, due to their different structure. Our investigation deals with well established as well as recently published algorithms and particularly investigates balancing capabilities, as unbalanced graph coloring potentially limits the parallel scalability of a target application. An overview on speedup and scalability, used number of colors, and their color balancing for the different reference graphs is provided. It is shown that, aside from being faster, the parallel approaches produce similar results as the serial methods, but for specific cases the serial algorithms still constitute a good option, when certain properties, e.g., balancing, are of major importance. Finally, we provide guidelines, based on the relative performance of the different algorithms, for picking the optimal algorithm for a specific use case.

Calculation of Potential for Multi-Atomic Systems with Varied Electron Density

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We propose a high precision method of finding of potential for multi-atomic quantum-mechanical tasks in real space. The method is based on dividing of electron density and potential of a multi-atomic system into two parts. The first part of density is found as a sum of spherical atomic densities; the second part is a variation of density generated by interatomic interaction. The first part of potential is formed by the first part of density and may be calculated correctly using simple integrals. The second part of potential is found through a Poisson equation from the second part of density. To provide a high precision we divided a work space into Voronoy's polyhedrons and