Parallel Space-time Methods for Time Dependent Optimization Problems

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Traditional parallel algorithms solve time dependent problems time step by time step, i.e., the simulation of the later time step is based on the fully accurate solution of one or several earlier time steps. The parallelism is restricted to each time step, and the algorithms are purely sequential in the time dimension. The sequential-in-time nature of the algorithms has not been a major concern in the past because the parallelism in space is usually enough to fill up most of the machines. However, in the upcoming generations of supercomputers, the number of processors is expected to be much larger, and it makes sense to consider to extract some level of parallelism in the time dimension.

Generally speaking, "time" is a sequential concept, the solution $u(x;t^{k+1})$ cannot be computed without knowing the solution $u(x;t^k)$ at the previous time step. However, since both $u(x;t^{k+1})$ and $u(x;t^k)$ are computed iteratively, their *approximate* solutions do not necessarily have the sequential dependency and can be obtained simultaneously. Based on this observation, several classes of algorithms have been developed. Waveform relaxation is one of the time-parallel methods to solve systems of ordinary differential equations with initial condition. In this method, the matrix from the discretized system is separated into lower, diagonal and upper components. The decoupling of the matrix allows independent solving of each uncoupled system in parallel. For parabolic PDEs, a semi-discretization is applied to transform PDEs into ODEs, then the resulting systems can be solved by the waveform relaxation method. In order to accelerate the convergence, several variants of waveform relaxation are developed, for example, multigrid waveform relaxation method or Schwarz waveform relaxation method. The space-time multigrid method for parabolic PDEs considers time as an additional dimension beside the spacial dimensions. It applies the multigrid operators of smoothing coarsening, restriction and prolongation on the whole grid combining both temporal and spacial domains. The parareal algorithm proposed by Lions, Maday and Turinici is an iterative method to solve evolution problems in a time-parallel manner. The advantage of this algorithm is that it successfully approximates the solutions later in time before accurately approximating the solutions at earlier times. This algorithm has received great attention since it was proposed, and several variants are presented in different frameworks, for example, PITA (parallel implicit time integrator), space-time multigrid and multiple shooting method.

Initial success of these time parallel algorithms has been observed for some classes of problems, in this position paper, we propose to further study some of the approaches for certain much more difficult, time critical problems including time-dependent inverse problems, and time dependent flow control problems. Both problems belong to the family of unsteady optimization problems constrained by partial differential equations. Traditional approaches for solving these optimization problems require to solve repeatedly a forward-in-time system of PDEs, an adjoint backward-in-time system of PDEs and a system with respect to the objective functions. The three subsystems have to be solved one after another. These sequential steps are not desirable for large scale parallel computing. In addition, within each of the PDEs subsystem solves, the problems are solved one time step at a time. As one can see clearly that there are LOTS of sequential steps in these methods, especially when the application requires the solution in a long period of time.

For example, in the pollution source identification problem for monitoring air or underground water resource qualities, a time dependent inverse problem needs to be solved, and the solution is the location and pollution intensity at point $x(t)$, for $x \in \Omega$ and $t \in (0, T)$. Current technologies introduce parallelism by partitioning Ω, but are purely sequential in the time dimension. Because of the noise in the measurement data, the number of spatial points is often not too large and therefore the available parallelism is limited, which is often acceptable on a small machine, but will be a painful issue for the upcoming generation of machines with a very large number of processors. The same problem appears in other time dependent optimization problems, such as real time control of unsteady fluid flows.

To solve the coupled space-time problems efficiently on large scale machines, many applied mathematics and computational science issues have to be carefully studied, such as, new discretization methods (adaptive space-time discritization, implicit across many time levels, ...), new stability theory, multilevel solvers (space-time coarsing, restrication and interpolation), space-time domain decomposition methods, uncertainity in both space and time, etc.

Of course, one of the main concerns of the space-time approach is the large memory requirement when the solution at many time levels are simultaneously saved in memory. It is important to investigate the trade off between the extra memory demand and the extra degree of parallelism, which implies shorter total compute time.

Most existing adaptive mesh methods and software don't allow adaptivity in time and therefore new meshing algorithms and software will be needed. Moreover, most existing software packages for solving PDEs and optimization problems assume the time and space problems are solved separately. To accommodate new space-time methods, new software platforms will likely to be necessary.