Scalable Parallel-in-Time Simulation of Extreme-Scale Chaotic Systems

Re: Call for Position Papers: DOE Applied Mathematics Research for Exascale Computing

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1. Need for space-time parallelism in extreme-scale computing

Many DOE applications involve simulation of multiscale nonlinear dynamical systems that exhibit chaos. Examples include weather and climate, turbulent combustion, nuclear reactor physics, plasma dynamics in fusion, and multi-body problems in molecular dynamics. The quantities that are to be predicted often require simulations of long times. With significantly more time steps than the number of grid points in any single spatial dimension, these simulations often suffer from poor strong scaling. This is because current unsteady simulations are typically parallel only in space, and data is transferred at subdomain boundaries at each time step. Parallel efficiency of this approach quickly deteriorates as the number of grid points per core decreases below a few thousand. Lack of parallelism in the time domain can become a bottleneck, particularly in an extreme-scale computing environment.

An enabling mathematical framework for next-generation extreme-scale computing should enable space-time parallel simulations. These simulations subdivide the 4-dimensional space-time computational domain. Each computing core handles a contiguous subdomain of the simulation space-time. Compared to subdivision only in the 3-dimensional space, space-time parallel simulations can achieve significantly higher level of concurrency, and reduce the ratio of inter-core communication to floating point operations. Each core computes the solution over a fraction of the entire simulation time window (Fig 1), reducing the simulation turnaround time.

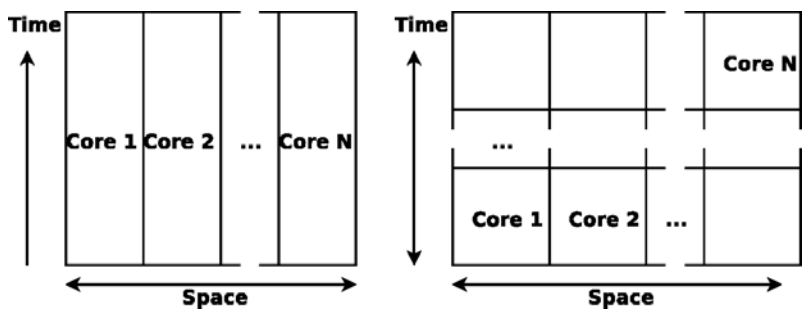

Fig 1. Illustration of spatial parallelism (left) and space-time parallelism (right).

Space-time parallel simulations can significantly reduce the ratio of data movement to floating point operations, thus achieving high parallel efficiency on extreme scale parallel machines. Combined with next generation computing hardware, this could reduce time-to-solution of extreme scale simulations from days to minutes. The reduced turnaround time could enable many applications such as design optimization, real-time inference and decision making based on high-fidelity simulations.

2. Scalability bottleneck of space-time parallel method based on initial value problems

Time domain parallel methods have a long history. Most time domain parallel methods divide the simulation time interval into small time chunks. They start with an initial estimate obtained by a coarse solver. Iterations are then performed over the entire solution history, aiming to converge to the solution of the initial value problem. In particular, the Parareal method has been demonstrated to converge for large scale turbulent plasma simulations. However, many time parallel methods suffer from a common scalability barrier in the presence of chaotic dynamics. The number of iterations for reaching a given tolerance is often proportional to the length of the time domain. As a result, the overall computation cost scales with the square of the time domain length.

The cause of this poor scalability is the ill-conditioning of initial value problems of chaotic systems. A small perturbation to a chaotic dynamical system can cause a large change in the state of the system at a later time. This sensitivity causes a significant barrier to fast convergence of time domain parallel methods. In the Parareal method, for example, a small correction made in the earlier time chunks can result in a large update in later time chunks. As a result, the later time chunks can only converge after the earlier time chunks converge, leading to increased number of required iterations as the length of the time domain increases. This poor scalability is particularly severe for extreme scale systems with a wide range of chaotic timescales [1].

3. Scalable space-time parallel method based on the least squares formulation

Efficient time domain parallelism can only be achieved through reformulating a chaotic simulation into a well-conditioned problem. This can be achieved by replacing the initial value problem with a least squares problem [1], whose solution satisfies the governing equations and is well-conditioned. Such an approach is appropriate when the long-time behavior is more important than the early transients.

Stability of the least squares problem is demonstrated by Fig 2. Because it does not suffer from ill-conditioning found in chaotic initial value problems, it overcomes a fundamental barrier to efficient time-parallelism. The least squares problem can be solved efficiently using parallel cyclic reduction for small systems and parallel multigrid for large systems [1]. Fig 3 demonstrates the parallel efficiency of the parallel multigrid solver when applied to the chaotic Lorenz system.

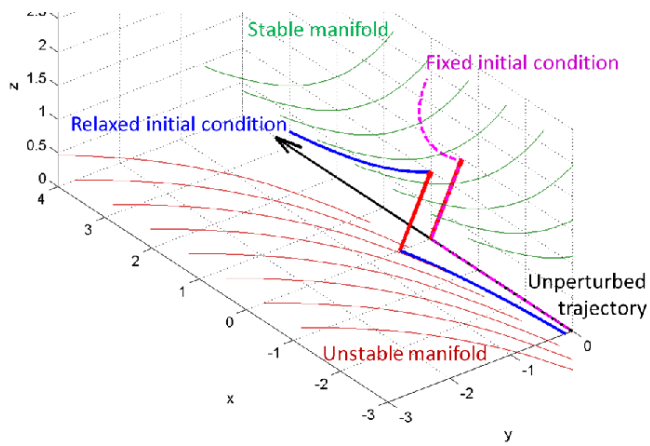

Fig 2. Geometric illustration of the response of a chaotic dynamical system to an impulse perturbation. The black arrow represents an unperturbed trajectory running along the z-axis. The red arrows represent the perturbation. The magenta dashed line represents the perturbed trajectory with fixed initial condition. The blue line represents a perturbed trajectory with relaxed initial condition.

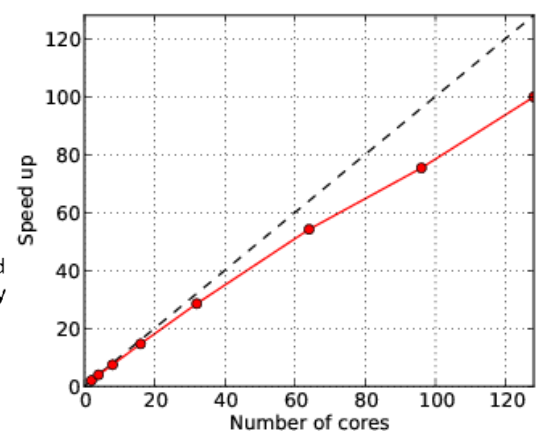

Fig 3. Speed up of time-parallel solution of the least squares problem for the Lorenz attractor. 4096 time steps are allocated per core. The same convergence criterion is used.

4. Summarize of the primary advantages of the least squares formulation

1. **Parallel in time.** The proposed formulation enables a new paradigm of space-time parallel computational simulations that effectively use next generation extreme-scale computers.
2. **Superior conditioning.** The proposed formulation can be proved to have low condition numbers, making methods for optimization, uncertainty quantification and inference easy to apply.

Reference

[1] Q. Wang, S. Gomez and P. Blonigan. Towards Scalable Parallel-in-Time Turbulent Flow Simulations. Submitted to Physics of Fluids. ArXiv:1211.2437