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A time-parallel approach to strong-constraint four-dimensional variational data assimilation

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ABSTRACT

A parallel-in-time algorithm based on an augmented Lagrangian approach is proposed to solve four-dimensional variational (4D-Var) data assimilation problems. The assimilation window is divided into multiple sub-intervals that allows parallelization of cost function and gradient computations. The solutions to the continuity equations across interval boundaries are added as constraints. The augmented Lagrangian approach leads to a different formulation of the variational data assimilation problem than the weakly constrained 4D-Var. A combination of serial and parallel 4D-Vars to increase performance is also explored. The methodology is illustrated on data assimilation problems involving the Lorenz-96 and the shallow water models.

1. Introduction

Predicting the behavior of complex dynamical systems, such as the atmosphere, requires using information from observations to decrease the uncertainty in the forecast. Data assimilation combines information from a numerical model, prior knowledge, and observations (all with associated errors) in order to obtain an improved estimate of the true state of the system. Data assimilation is an important application of data-driven application systems (DDDAS [4], or InfoSymbiotic systems) where measurements of the physical system are used to constrain simulation results. Two approaches to data assimilation have gained widespread popularity: variational and ensemble-based methods. The ensemble-based methods are rooted in statistical theory, whereas the variational approach is derived from optimal control theory. The variational approach formulates data assimilation as a nonlinear optimization problem constrained by a numerical model. The initial conditions (as well as boundary conditions, forcing, or model parameters) are adjusted to minimize the discrepancy between the model trajectory and a set of time-distributed observations. In real-time operational settings the data assimilation process is performed in cycles: observations within an assimilation window are used to obtain an optimal trajectory, which provides the initial condition for the next time window, and the process is repeated in the subsequent cycles. The variational methodology is widely adopted by national and international numerical weather forecast centers to provide the initial state for their forecast models [5].

The process of solving the nonlinear optimization to obtain the initial conditions of a 4D-Var is highly sequential since the minimization procedure consists of sequential iterations, each iteration requires at least one forward model integration followed by an integration of the adjoint model, and each integration performs a sequence of timesteps over the entire analysis window [18]. Parallel 4D-Var simulations currently rely on spatial decomposition. Trémolet and Le Dimet have shown

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how variational data assimilation can be used to couple models and to perform it in parallel in the spatial direction [37]. In [27], the author considers different data distribution strategies to perform parallel variational data assimilation in the spatial direction. An implementation of 4D-Var by exploiting spatial parallelism for chemical data assimilation has been described in [17]. A scalable approach for variational data assimilation is presented in [15]. The authors achieve parallelism by dividing the 3D-Var into multiple local 3D-Var sub-problems. Multiple copies of the modified 3D-Var problem, which ensures feasibility at the boundaries of the sub-domains, are solved across processors and the global 3D-Var minimum is obtained by collecting the local minima.

The current generation of computers are becoming more parallel, while the individual processor speed is increasing slowly. As our understanding of the physics improves, the computer models become more complex. Space parallelism alone is likely to be insufficient to run 4D-Var efficiently on the new computer architectures. Unless advanced and scalable parallel algorithms to solve the 4D-Var are developed, determining initial state to forecast using 4D-Var might become infeasible in the foreseeable future.

Fisher [18] achieves time parallelism in the context of incremental weak-constraint 4D-Var. Weak-constraint 4D-Var removes the model constraints which are replaced by penalties in the cost function. The incremental approach solves a linearized optimization problem in the inner loop. This linearized problem is equivalent to solving a saddlepoint system, and this solution can be efficiently time-parallelized [18]. Ulbrich [38] proposes an SQP approach where the time dimension is parallelized using a "parareal" approach. A different approach is to formulate the discrete optimality system and to solve it using parallel linear algebra: Biros and Ghattas use Krylov space schemes [8], while Borzi uses space–time multigrid schemes [10]. Navon et al. have used the augmented Lagrangian approach to perform data assimilation in [20,26]. However, to the best of our knowledge this is the first work that uses the augmented Lagrangian framework to propose a time-parallel implementation of strong-constraint 4D-Var. A conference version of the current paper was presented at ICCS 2015 [31].

The focus of this work is on developing a scalable time-parallel algorithm to solve the strong-constraint 4D-Var problem. The algorithm evaluates the important components of 4D-Var namely, cost function and gradient computations in parallel. This work addresses an important challenge associated with computing the solutions to 4D-Var problem: scalability in the temporal direction. The solution presented here is based on the augmented Lagrangian framework. The paper is organized as follows: Section 2 gives a brief description about data assimilation and 4D-Var. In Section 3 we show how the 4D-Var can be reformulated using augmented Lagrangian technique so that the gradient and cost function evaluations can be parallelized. The most important contribution of this work is that it achieves parallelism in temporal direction. This work can be easily extended to achieve parallelism in spatio-temporal directions. Section 4 gives a detailed description of the parallel algorithm. Section 5 shows the numerical experiments with a small but chaotic Lorenz-96 model and a relatively large shallow water model on a sphere and Section 6 gives concluding remarks and future directions.

2. Four-dimensional variational data assimilation

Data assimilation (DA) is the fusion of information from priors, imperfect model predictions, and noisy data, to obtain a consistent description of the true state $\mathbf{x}^{\rm true}$ of a physical system [9,14,21,33,34]. The estimate that fuses all these sources of information is called the analysis $\mathbf{x}^{\rm a}$, which under certain statistical assumptions of the model and errors is provably the best estimate of the true state.

The prior information encapsulates our current knowledge of the system. Usually the prior information is contained in a background estimate of the state $\mathbf{x}^{\rm b}$ and the corresponding background error covariance matrix $\mathbf{B}$.

The model captures our knowledge about the physical laws that govern the evolution of the system. The model evolves an initial state $\mathbf{x}_0 \in \mathbb{R}^n$ at the initial time t_0 to future states $\mathbf{x}_{\rm k} \in \mathbb{R}^n$ at future times $t_{\rm k}$. A general model equation is represented as follows:

$$\mathbf{x}_{\rm k} = \mathcal{M}_{t_0 \to t_{\rm k}} (\mathbf{x}_0) \, . \tag{1}$$

Observations are noisy snapshots of reality available at discrete time instances. Specifically, measurements $\mathbf{y}_{\rm k} \in \mathbb{R}^m$ of the physical state $\mathbf{x}^{\rm true}(t_{\rm k})$ are taken at times $t_{\rm k}$, $\rm k = 1, \cdots, \mathit{N}$. The model state is related to observations by the following relation:

$$\begin{aligned} \mathbf{y}_{\rm k} &= \mathcal{H}(\mathbf{x}_{\rm k}) - \varepsilon_{\rm k}^{\rm obs}, \quad {\rm k} = 1, \cdots, N, \\ \varepsilon_{\rm k}^{\rm obs} &= \varepsilon_{\rm k}^{\rm representativeness} + \varepsilon_{\rm k}^{\rm measurement} \, . \end{aligned} \tag{2}$$

The observation operator $\mathcal{H}$ maps the model state space onto the observation space. The observation error term $\left(\varepsilon_{\rm k}^{\rm obs}\right)$ accounts for both measurement and representativeness errors. Measurement errors are due to imperfect sensors. The representativeness errors are due to the inaccuracies of the mathematical and numerical approximations inherent to the model.

Variational methods solve the data assimilation problem in an optimal control framework, where one finds the control variable which minimizes the mismatch between the model forecasts and the observations. Strong-constraint 4D-Var assumes that the model (1) is perfect [33,34]. The control parameters are the initial conditions $\mathbf{x}_0$, which uniquely determine the state of the system at all future times via the model equation (1). The background state is the prior best estimate of the initial conditions $\mathbf{x}_0^{\rm b}$, and has an associated initial background error covariance matrix $\mathbf{B}_0$. Observations $\mathbf{y}_{\rm k}$ at $t_{\rm k}$ have the