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ANALYSIS OF AN OPERATOR SPLITTING METHOD IN 4D-VAR

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Abstract. In this paper, we present a framework of 4D variational data assimilation (4D-Var) in Hilbert spaces and discuss Marchuk-Strang operator splitting methods for 4D-Var. Convergence analysis of the operator splitting methods is made.

1. **Introduction.** Variational data assimilation has important applications in atmosphere models and chemical transport models [1, 9, 13]. Data assimilation systems utilize two sources of data: observations and a recent forecast valid at a known time. For many practical problems, observation sets are distributed in 3D space plus time, corresponding to 4D data assimilation (4D-Var). 4D-Var is a method of estimating a set of parameters by optimizing the fit between the solution of a model and a set of observations which the model is meant to predict. The unknown model parameters may be the model's initial conditions. Determining the model parameters is very important and complex and has become a science in itself. 4D-Var is a process where a state forecast and observations are combined to produce a best (optimal) estimate or an analysis of the state [9].

4D-Var is typically an optimal control problem and the parameters are often constrained by evolution differential operators. In the paper, we will restrict a parameter in the 4D-Var to representing the initial condition of a nonlinear evolution differential operator. Hence the 4D-Var problem reads as follows: "what initial condition will fit the model to best predict the given observations?" To solve the 4D-Var, one often needs to compute the gradient and even Hessian of a functional which relates the parameter and the model solution. For this purpose, a first order adjoint model and a second order adjoint model are needed to solve.

In many 4D-Var problems, the differential operators in forward model , adjoint model and tangent linear model, have complicated structures and consist of different parts (e.g., advection operators, diffusion operators and reaction operators), and the different parts may be solved by different numerical schemes. Splitting methods are often used in solving these complicated models. The basic idea behind operator splitting is to break a complicated problem into smaller or simpler subproblems such that different parts can be solved efficiently with appropriate numerical schemes.

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In this paper, we present a 4D-Var in functional setting and discuss the symmetric operator splitting methods in the 4D-Var problem.

The paper is organized as follows. In Section 2, we present a framework for functional 4D-Var in in Hilbert spaces. In section 3, we apply the Marchuk-Strang multicomponent operator splitting to the 4D-Var and make convergence analysis for the splitting method. In Section 4, we draw some conclusions.

2. 4D Variational Data Assimilation in Hilbert Spaces.

2.1. A functional 4D-Var. In this subsection, we present a framework for 4D-Var in a nonlinear functional on Hilbert spaces.

Let V be Hilbert space with inner product $(\cdot,\cdot)_V$ and $U = \{\phi : [t_0, T] \longrightarrow V\}$ be a Hilbert space. Let $u^B \in V$ be the background of the initial value, i.e., the initial guess in the assimilation procedure. Let $B^{-1} : V \to V$ be a covariance operator of the estimated background error, which is linear and symmetric. Let $H(t)$ be an observation operator which depends on time t. We simply write $H = H(t)$ when no confusion occurs. Typically, H maps space U onto a proper subspace U_o of U. Let u_{obs} be the real observations depending on time t. Let $R^{-1} : U_o \to U_o$ be a linear symmetric covariance operator accounting for observations and representativeness errors. We define an optimization functional (or cost functional) as following:

$$\mathcal{J}(u^0, u) = \frac{1}{2}(u^0 - u^B, B^{-1}(u^0 - u^B)) + \frac{1}{2}(Hu - u_{obs}, R^{-1}(Hu - u_{obs}))_{U_0}, \quad (1)$$

where $u \in U$, $u^0 \in V$ and

$$(\cdot,\cdot)_{U_0} = \int_{t_0}^{T} (\cdot,\cdot)(s)ds.$$

Here $(\cdot,\cdot)$ inside the integral represents the inner product of the space $U_o(s)$ (for fixed time s). In this paper, we will use $(\cdot,\cdot)$ to represent generic inner products to avoid using many notations. Different spaces may have different definitions for the $(\cdot,\cdot)$ (e.g., observations in U_o and the corresponding inner product $(\cdot,\cdot)$ means $(\cdot,\cdot)_{U_o}$), but they can be easily made out in the context. The optimization functional $\mathcal{J}$ measures the difference between the model output u and the observation u_{obs} and the deviation of the solution from the background state u^B.

In practical situations, the observation u_{obs} is evaluated at a set of discrete moments $\{t_k\}_{k=0}^N$ in the time interval $[t_0, T]$. For these cases, the optimization functional is rewritten as

$$\mathcal{J}(u^0, u) = \frac{1}{2}(u^0 - u^B, B^{-1}(u^0 - u^B)) + \frac{1}{2}\sum_{k=0}^{N}(H_k u^k - u^k_{obs}, R_k^{-1}(H_k u^k - u^k_{obs})). \quad (2)$$

Let $S(t)$ be a nonlinear operator to represent a predefined forecast model. Ten 4D-Var reads as the minimization problem,

$$\hat{u^0} = \arg\min\{\mathcal{J}(u^0, u) : u(t) = S(t)u^0\},$$

where the model state $u(t)$ is subject to the forward model equation,

$$u(t) = S(t)u^0. \quad (3)$$

Let $\bar{S}(t)$ be the linearization of $S(t)$. We define a tangent linear model corresponding to (3) as following:

$$\delta u(t) = \bar{S}(t)\delta u^0, \quad (4)$$

where $\delta u(t)$ is the perturbation of $u(t)$ and δu^0 is the perturbation of u^0. Equation (4) demonstrates the relation between the two perturbations through the linearlization $\bar{S}(t)$ of the forecast model $S(t)$. Let $\bar{S}^*(t)$ be the adjoint of $\bar{S}(t)$, $\bar{H}^*(t)$ the adjoint of $\bar{H}(t)$, and $\bar{H}(t)$ a linearization of $H(t)$. Let ∇_{u^0} be the Fréchet derivative operator (or gradient operator) with respect to u^0 in the space U and $\nabla^2_{u^0}$ the second derivative operator with respect to u^0. By the equation $u(t) = S(t)u^0$, it follows that

$$\nabla_{u^0}\mathcal{J}(u^0, u) = B^{-1}(u^0 - u^B) + \int_{t_0}^{T} \bar{S}^*\bar{H}^*R^{-1}(Hu - u_{obs})(s)ds \tag{5}$$

and

$$\nabla^2_{u^0}\mathcal{J}(u^0, u) = B^{-1} + \int_{t_0}^{T} \bar{S}^*\bar{H}^*R^{-1}\bar{H}\bar{S}ds. \tag{6}$$

To numerically approximate (1), one needs to discretize time. Because the optimization functional is the same as in (2) in most practical problems and the time discretization of (1) is similar to (2), we focus on discussing the optimization functional defined in (2) instead of the time discretization of (1).

In the rest of the paper, we will use the optimization functional in (1) to discuss the continuous time 4D-Var and use the functional in (2) to discuss the numerical 4D-Var, i.e., time is discretized.

The 4D-Var defined previously is a nonlinear constrained optimization problem and it is often hard to solve in general. Here we make two assumptions to simplify the problem and clarify the numerical process.

Assumption 1: *The forecast model $S(t)$ can be represented as the product of intermediate forecast steps. Let $S_{[t,t+\tau]}$ be the forecast step from t to $t+\tau$. Then $u(t+\tau) = S_{[t,t+\tau]}u(t)$. and for $t_k = t_0 + k\tau$,*

$$u(t_k) = S_{[t_{k-1},t_k]} \cdots S_{[t_1,t_2]}S_{[t_0,t_1]}u^0.$$

Assumption 1 means that the forward model is an integration of a numerical prediction model starting with u^0 as the initial value. The assumption implies the idea of an operator splitting method.

Assumption 2: *At any time, HSu^0 admits a first order Taylor expansion around u^B*

$$HSu^0 = HSu^B + \bar{H}\bar{S}(u^0 - u^B),$$

where $\bar{H} = \bar{H}(t)$ is the linearization of the observation operator $H(t)$ and $\bar{S} = \bar{S}(t)$ is the tangent linear model of $S(t)$.

Assumption 2 is a tangent linear hypothesis and implies that $\nabla_{u^0}HS(u^0) = \bar{H}\bar{S}$. Let $\bar{S}_{[t_{k-1},t_k]} = \nabla_u S_{[t_{k-1},t_k]}u|_{t=t_{k-1}}$, $\bar{S}_{[t_0,t_k]} = \Pi_{i=1}^{k}\bar{S}_{[t_{i-1},t_i]}$, and $\bar{H}_k = \nabla_u Hu|_{t=t_k}$. Consequently, it can be verified [5, 4] that

$$\nabla_{u^0}\mathcal{J}(u^0, u) = \nabla_{u^0}\mathcal{J} = B^{-1}(u^0 - u^B) + \sum_{k=0}^{N} \bar{S}^*_{[t_k,t_0]}\bar{H}^*_k R_k^{-1}(H_k u^k - u^k_{obs}) \tag{7}$$

and

$$\nabla^2_{u^0}\mathcal{J}(u^0, u) = B^{-1} + \sum_{k=0}^{N} \bar{S}^*_{[t_k,t_0]}\bar{H}^*_k R_k^{-1}\bar{H}_K\bar{S}_{[t_0,t_k]}. \tag{8}$$

2.2. **4D-Var Constraint Specified by A Differential Operator.** For simplicity of discussion, we restrict ourself to the case that the constraint $u(t) = S(t)u^0$ is defined by a nonlinear evolution operator A on a Hilbert space U. Then the 4D-Var problem can be formulated as following: seek the solution $\phi \in U$ of

$$\left\{ \begin{array}{rcl} D_t\phi &=& A(\phi) \\ \phi(t=t_0) &=& u^0 \\ \hat{u^0} &=& \arg\inf_{u^0} \mathcal{J}(u^0,\phi), \end{array} \right. \tag{9}$$

where $\mathcal{J}(u^0,\phi)$ is defined in (1). Here we assume that the nonlinear evolution equation in (9) has a unique solution.

By applying variational calculus techniques, we can show that the optimal control problem (9) is equivalent to the optimal system as form [4] stated by

$$\left\{ \begin{array}{rcl} D_t\phi &=& A(\phi) \\ \phi(t=t_0) &=& u^0 \\ -D_t\phi^* &=& (\nabla A(\phi))^*\phi^* - \bar{H}^* R^{-1}(H\phi - \phi_{obs}) \\ \phi^*(t=T) &=& 0 \\ \phi^*(t=t_0) &=& B^{-1}(u^0 - u^B), \end{array} \right. \tag{10}$$

where $\phi \in U$ and $\phi^* \in U$.

Remark 1. Let $S^A(t)$ denote an operator semigroup with generator A. By the notation of a semigroup,

$$\phi(t) = S^A(t)u^0.$$

Hereafter we adopt similar notations for semigroups. If A is a maximal dissipative operator on V, the exponential formula of the nonlinear semigroup [2] is

$$S^A(t)u^0 = \lim_{n\to\infty}(1 - \frac{t}{n}A)^{-n}u^0,$$

where the limit is taken in strong topology sense. Further,

$$\phi^*(t) = -\int_t^T S^{-(\nabla A(\phi))^*}(t-s)(\bar{H}^*R^{-1}(H\phi - \phi_{obs}))(s)ds, \tag{11}$$

where $S^{-(\nabla A(\phi))^*}(t) = e^{-(\nabla A(\phi))^* t}$ because the generator $-(\nabla A(\phi))^*$ is a bounded linear operator.

We consider the forward problem from (9)

$$\left\{ \begin{array}{rcl} D_t\phi &=& A(\phi) \\ \phi(t=t_0) &=& u^0 \end{array} \right. \tag{12}$$

Define the tangent linear (perturbation) problem of (12) by the form

$$\left\{ \begin{array}{rcl} D_t\delta\phi - (\nabla A(\phi))\delta\phi &=& 0 \\ \phi_0(t=t_0) &=& \delta u^0 \end{array} \right. \tag{13}$$

and the adjoint problem by the form

$$\left\{ \begin{array}{rcl} -D_t\phi^* &=& (\nabla A(\phi))^*\phi^* - \bar{H}^*R^{-1}(H\phi - \phi_{obs}) \\ \phi^*(t=T) &=& 0. \end{array} \right. \tag{14}$$

We want to know how sensitive the functional $\mathcal{J}$ is to the perturbation $\delta\phi$. Let $\delta_\phi\mathcal{J}$ be the perturbation of $\mathcal{J}(u^0,\phi)$ when $\delta\phi$ is nonzero. Then

$$\delta_\phi\mathcal{J} = -(\delta u^0, \phi^*(t=t_0)). \tag{15}$$

The proof can be found in [4]. Equation (15) demonstrates the sensitivity of the functional $\mathcal{J}(u^0, \phi)$ related to initial value u^0. From the above, we see that the solution ϕ^* of the adjoint problem (14) accounts for the sensitivity of the functional $\mathcal{J}$ to the initial value.

Let ϕ^{**} be the solution of the second order adjoint problem by

$$\left\{\begin{array}{rcl} -D_t\phi^{**} & = & (\nabla A(\phi))^*\phi^{**} + (\nabla^2 A(\phi)\delta\phi)^*\phi^* - \partial^2_\phi \mathcal{J}(\phi^0, \phi)\delta\phi \\ \phi^{**}(t=T) & = & 0, \end{array}\right. \tag{16}$$

where ϕ^* is the solution of the first order adjoint equation (14) and $\nabla^2 A(\phi)$ is the second derivative (Hessian) of A. Second order adjoint information is often used in data assimilation while applying numerical optimization algorithms [5]. Particularly, Hessian vector products are used in the computation of Hessian singular vectors in data assimilation [12].

3. **Marchuk-Strang Operator Splitting Method in 4D-Var.** This section is devoted to realizing *Assumption 1* by operator splitting techniques.

When $A(\phi)$ in (9) consists of different parts, one can use splitting methods to solve (12) [6]. The idea of operator splitting is to break a complex problem into some simpler subproblems such that each subproblem can be solved efficiently by different numerical schemes. There are many operator splitting methods, here we will discuss the 4D-Var by the most popular operator splitting method: Marchuk-Strang symmetrical multi-component splitting [8, 11].

For any $v \in U$ and any operator g on U, we define a Lie operator [6] $\mathcal{A}$ associated with A by

$$\mathcal{A}g(v) = g'(v)A(v).$$

By the definition, Lie operator $\mathcal{A}$ is a linear operator on the space of operators acting on the solution space U. Let $A(\phi) = \sum_{j=1}^M A_j(\phi)$. Then we have

$$\mathcal{A} = \sum_j^M \mathcal{A}_j,$$

where $\mathcal{A}_j$ is the Lie operator associated with each operator A_j. So for the solution $\phi(t)$ of (12),

$$\mathcal{A}g(\phi(t)) = g'(\phi(t))A(\phi(t)) = \frac{\partial}{\partial t} g(\phi(t)).$$

Let I be identity operator. Lie-Taylor series [3] implies that

$$\phi(t+\tau) = (e^{\tau\mathcal{A}}I)\phi(t).$$

Because $A(\phi) = \sum_{j=1}^M A_j(\phi)$, the problem (12) is split into M subproblems, i.e., $D_t\phi_j = A_j(\phi_j)$, $j = 1, \cdots, M$. By applying the Marchuk-Strang multi-component splitting over the intervals $[t_k, t_{k+1}]$, where $t_{k+1} = t_k + \tau$ with time step τ, we have

$$\left\{\begin{array}{rcl} D_t\phi_1 & = & A_1(\phi_1), \quad \phi_1(t_k) = \phi_1'(t_k), \quad t \in [t_k, t_k + \frac{\tau}{2}] \\ & \cdots & \\ D_t\phi_{M-1} & = & A_{M-1}(\phi_{M-1}), \quad \phi_{M-1}(t_k) = \phi_{M-2}(t_k + \frac{\tau}{2}), \\ & & t \in [t_k, t_k + \frac{\tau}{2}] \\ D_t\phi_M & = & A_M(\phi_M), \quad \phi_M(t_k) = \phi_{M-1}(t_k + \frac{\tau}{2}), \quad t \in [t_k, t_k + \tau] \\ D_t\phi'_{M-1} & = & A_{M-1}(\phi'_{M-1}), \quad \phi'_{M-1}(t_k + \frac{\tau}{2}) = \phi_M(t_{k+1}), \\ & & t \in [t_k + \frac{\tau}{2}, t_{k+1}] \\ & \cdots & \\ D_t\phi'_1 & = & A_1(\phi'_1), \quad \phi_1(t_k + \frac{\tau}{2}) = \phi'_2(t_{k+1}), \quad t \in [t_k + \frac{\tau}{2}, t_{k+1}]. \end{array}\right. \tag{17}$$

Let $\mathcal{S}_{j,\frac{1}{2}\tau} = e^{\frac{1}{2}\tau\mathcal{A}_j}$, $\mathcal{S}_{M,\tau} = e^{\tau\mathcal{A}_M}$, and ϕ_k be approximations of $\phi(t_k)$, $k = 1, \cdots, N$. By Baker-Campbell-Hausdorf formula of Lie operator [6], it follows that

$$\phi(t_{k+1}) = \mathcal{S}_{1,\frac{1}{2}\tau} \cdots \mathcal{S}_{M-1,\frac{1}{2}\tau}\mathcal{S}_{M,\tau}\mathcal{S}_{M-1,\frac{1}{2}\tau} \cdots \mathcal{S}_{1,\frac{1}{2}\tau} I\phi(t_k) + O(\tau^3) \tag{18}$$

and that

$$\phi_{k+1} = \mathcal{S}_{1,\frac{1}{2}\tau} \cdots \mathcal{S}_{M-1,\frac{1}{2}\tau}\mathcal{S}_{M,\tau}\mathcal{S}_{M-1,\frac{1}{2}\tau} \cdots \mathcal{S}_{1,\frac{1}{2}\tau} I\phi_k. \tag{19}$$

Let $\mathcal{S}_{[t_k,t_{k+1}]} = \mathcal{S}_{1,\frac{1}{2}\tau} \cdots \mathcal{S}_{M-1,\frac{1}{2}\tau}\mathcal{S}_{M,\tau}\mathcal{S}_{M-1,\frac{1}{2}\tau} \cdots \mathcal{S}_{1,\frac{1}{2}\tau}$ be the splitting procedure over the time interval $[t_k, t_{k+1}]$. Then

$$\phi_N = \Pi_{k=0}^{N-1}\mathcal{S}_{[t_k,t_{k+1}]} I\phi_0. \tag{20}$$

Remark 2. By the Lie operator formalism, a nonlinear splitting is transformed into the compositions of linear operators and hence *Assumption 1* is realized.

Remark 3. The term $O(\tau^3)$ in (18) represents the leading term of the local splitting error. The symmetrical operator splitting scheme has second order consistency in time because $\tau^{-1}\|\phi(t_{k+1}) - \phi(t_k)\| = O(\tau^2)$. If $A_j(\phi)$ and $A_l(\phi)$ commute each other, i.e., for any $j \neq l$, $A_j'A_l = A_jA_l'$, where A_j' is the derivative with regard to ϕ, then splitting error is vanished [6].

Remark 4. In fact, (20) produces a general Strang's product formula

$$\lim_{n\to\infty}[e^{\frac{t}{2n}\mathcal{A}_1} \cdots e^{\frac{t}{2n}\mathcal{A}_{M-1}} e^{\frac{t}{n}\mathcal{A}_M} e^{\frac{t}{2n}\mathcal{A}_{M-1}} \cdots e^{\frac{t}{2n}\mathcal{A}_1}]^n Iu^0 = e^{t\mathcal{A}}Iu^0.$$

Remark 5. If all A_j's are linear on ϕ, then we can represent the numerical solution of (12) by linear operator semi-groups,

$$\phi_{k+1} = S^{A_1}(\frac{1}{2}\tau) \cdots S^{A_{M-1}}(\frac{1}{2}\tau)S^{A_M}(\tau)S^{A_{M-1}}(\frac{1}{2}\tau) \cdots S^{A_1}(\frac{1}{2}\tau)\phi_k,$$

where $S^{A_i}(\frac{1}{2}\tau)$ $(i = 1, \cdots, M)$ denotes the operator semigroup and A_i are the corresponding generators. Here it only requires that A_i, $i = 1, \cdots, M$, are closed, densely defined linear operators, but can be unbounded. By the exponential formula of linear semigroups [2],

$$S^{A_i}(\frac{1}{2}\tau) = \lim_{n\to\infty} e^{A_i(I-\frac{A_i}{n})^{-1}\frac{1}{2}\tau}, \quad i = 1, \cdots M-1,$$

and the limit is taken in strong topology sense. Similarly we can find the exponential formula for $S^{A_M}(t)$.

The operator splitting method is also applied to the perturbation equation (13) such that

$$\delta\phi_{k+1} = \bar{\mathcal{S}}_{1,\frac{1}{2}\tau} \cdots \bar{\mathcal{S}}_{M-1,\frac{1}{2}\tau}\bar{\mathcal{S}}_{M,\tau}\bar{\mathcal{S}}_{M-1,\frac{1}{2}\tau} \cdots \bar{\mathcal{S}}_{1,\frac{1}{2}\tau}\delta\phi_k := \bar{\mathcal{S}}_{[t_k,t_{k+1}]}\delta\phi_k$$

and

$$\delta\phi_N = \Pi_{k=0}^{N-1}\bar{\mathcal{S}}_{[t_k,t_{k+1}]}\delta\phi_0,$$

where $\bar{\mathcal{S}}_{j,\frac{1}{2}\tau} = S^{\nabla A_j(\phi)}(\frac{1}{2}\tau) = e^{\frac{1}{2}\tau\nabla A_j(\phi)}$, $j = 1, \cdots, M-1$, and $\bar{\mathcal{S}}_{M,\tau} = S^{\nabla A_M(\phi)}(\tau)$ $= e^{\tau\nabla A_M(\phi)}$.

Similarly, the adjoint model (14) is split into M subproblems, i.e., $-D_t\phi_j^* = (\nabla A_j(\phi))^*\phi_j^*$, $j = 1, \cdots, M$. By the Marchuk-Strang symmetrical multi-component splitting over $[t_{k+1}, t_k]$, it follows

$$\left\{\begin{array}{rcl} -D_t\phi_1^* &=& (\nabla A_1(\phi))^*\phi_1^*, \quad \phi_1^*(t_{k+1}) = \phi_1^{*'}(t_{k+1}), \quad t\in[t_{k+1}, t_k+\frac{\tau}{2}] \\ & \cdots & \\ -D_t\phi_{M-1}^* &=& (\nabla A_{M-1}(\phi))^*\phi_{M-1}^*, \quad \phi_{M-1}^*(t_{k+1}) = \phi_{M-2}^*(t_{k+1}-\frac{\tau}{2}), \\ && t\in[t_{k+1}, t_k+\frac{\tau}{2}] \\ -D_t\phi_M^* &=& (\nabla A_M(\phi))^*\phi_M^*, \quad \phi_M(t_{k+1})^* = \phi_{M-1}^*(t_{k+1}-\frac{\tau}{2}), \\ && t\in[t_{k+1}, t_k] \\ -D_t\phi_{M-1}^{*'} &=& (\nabla A_{M-1}(\phi))\phi_{M-1}^{*'}, \quad \phi_{M-1}^{*'}(t_k+\frac{\tau}{2}) = \phi_M^*(t_k), \\ && t\in[t_k+\frac{\tau}{2}, t_k] \\ & \cdots & \\ -D_t\phi_1^{*'} &=& (\nabla A_1(\phi))^*\phi^{*'}, \quad \phi_1^{*'}(t_k+\frac{\tau}{2}) = \phi_2^{*'}(t_k), \\ && t\in[t_k+\frac{\tau}{2}, t_k]. \end{array}\right. \tag{21}$$

Consequently, we have

$$\bar{\mathcal{S}}_{j,\frac{1}{2}\tau}^* = e^{-\frac{1}{2}\tau(\nabla A_j(\phi))^*}, \quad (j=1,\cdots,M-1), \quad \bar{\mathcal{S}}_{M,\tau}^* = e^{-\tau(\nabla A_M(\phi))^*} \tag{22}$$

and

$$\left\{\begin{array}{rcl} \phi_k^* &=& \bar{\mathcal{S}}_{[t_{k+1},t_k]}^*\phi_{k+1}^* + \partial_{\phi_k}\mathcal{J}(u^0,\phi) \\ &=& \bar{\mathcal{S}}_{1,-\frac{1}{2}\tau}^*\cdots\bar{\mathcal{S}}_{M-1,-\frac{1}{2}\tau}^*\bar{\mathcal{S}}_{M,-\tau}^*\bar{\mathcal{S}}_{M-1,-\frac{1}{2}\tau}^*\cdots\bar{\mathcal{S}}_{1,-\frac{1}{2}\tau}^*\phi_{k+1}^* \\ && +\partial_{\phi_k}\mathcal{J}(u^0,\phi) \\ \phi_N^* &=& 0, \end{array}\right. \tag{23}$$

where $\partial_{\phi_k}\mathcal{J}(u^0,\phi)$ be the partial differential of $\mathcal{J}(u^0,\phi)$ with respect to ϕ_k for a fixed first argument u^0 and $\phi=\{\phi_0,\cdots,\phi_N\}$.

Finally, we use the Marchuk-Strang symmetric splitting for the second order adjoint problem (16), we can obtain that

$$\left\{\begin{array}{rcl} \phi_k^{**} &=& \bar{\mathcal{S}}_{[t_{k+1},t_k]}^*\phi_{k+1}^{**} + (\bar{\bar{\mathcal{S}}}_{[t_k,t_{k+1}]}\delta\phi_k)^*\phi_{k+1}^* + \partial_{\phi_k}^2\mathcal{J}(u^0,\phi)\delta\phi_k \\ \phi_N^{**} &=& 0, \end{array}\right. \tag{24}$$

where $\bar{\bar{\mathcal{S}}}_{[t_k,t_{k+1}]} = \bar{\bar{\mathcal{S}}}_{1,\frac{1}{2}\tau}\cdots\bar{\bar{\mathcal{S}}}_{M-1,\frac{1}{2}\tau}\bar{\bar{\mathcal{S}}}_{M,\tau}\bar{\bar{\mathcal{S}}}_{M-1,\frac{1}{2}\tau}\cdots\bar{\bar{\mathcal{S}}}_{1,\frac{1}{2}\tau}$ and $\bar{\bar{\mathcal{S}}}_{j,\frac{1}{2}\tau} = e^{\frac{1}{2}\tau\nabla^2A_j(\phi)}$, $j=1,\cdots,M-1$, $\bar{\bar{\mathcal{S}}}_{M,\tau} = e^{\tau\nabla^2A_M(\phi)}$.

Let $\nabla_{u^0}^\tau\mathcal{J}(u^0,\phi(u^0))$ be the numerical approximation of $\nabla_{u^0}\mathcal{J}(u^0,\phi(u^0))$ by the operator splitting method and $\nabla_{u^0}^{2,\tau}\mathcal{J}(u^0,\phi(u^0))$ the numerical approximation of $\nabla_{u^0}^2\mathcal{J}(u^0,\phi(u^0))$. Then one gets the following theorem.

Theorem 3.1. *Let ϕ^* be defined in (23) and ϕ^{**} be defined in (24). Then Marchuk-Strang operator splitting gives rise to*

$$\begin{aligned} \nabla_{u^0}^\tau\mathcal{J}(u^0,\phi(u^0)) &= \phi_0^* + B^{-1}(u^0-u^B) \\ \nabla_{u^0}^{2,\tau}\mathcal{J}(u^0,\phi(u^0))\delta u^0 &= \phi_0^{**} + B^{-1}\delta u^0, \end{aligned} \tag{25}$$

where ϕ_0^* is the operator splitting solution at t_0 defined in (23) and ϕ_0^{**} is the operator splitting solution at t_0 defined in (24).

Proof. Since $\partial_{\phi_k}\mathcal{J} = \bar{H}_k^* R_k^{-1}(H_k\phi_k - \phi_k^{obs})$, it follows from (7) that

$$\begin{aligned}\nabla_{u^0}^{\tau}\mathcal{J} =& B^{-1}(u^0 - u^B) + \sum_{k=0}^{N} \bar{\mathcal{S}}^*_{[t_k,t_0]}\partial_{\phi_k}\mathcal{J} \\ =& B^{-1}(u^0 - u^B) + \sum_{k=0}^{N} \bar{\mathcal{S}}^*_{[t_1,t_0]}\cdots\bar{\mathcal{S}}^*_{[t_k,t_{k-1}]}\partial_{\phi_k}\mathcal{J} \\ =& B^{-1}(u^0 - u^B) + I\partial_{u^0}\mathcal{J} + \bar{\mathcal{S}}^*_{[t_1,t_0]}(\partial_{\phi_1}\mathcal{J} \\ &+ \bar{\mathcal{S}}^*_{[t_2,t_1]}(\partial_{\phi_2}\mathcal{J} + \cdots + \bar{\mathcal{S}}^*_{[t_{N-1},t_{N-2}]}(\partial_{\phi_{N-1}}\mathcal{J} + \bar{\mathcal{S}}^*_{[t_N,t_{N-1}]}\partial_{\phi_N}\mathcal{J}))).\end{aligned} \tag{26}$$

By the recurrence definition of ϕ_k^* in (23), it follows that

$$\nabla_{u^0}^{\tau}\mathcal{J} = \phi_0^* + B^{-1}(u^0 - u^B).$$

This verifies the first equation in (25). The proof of the second equation in (25) is similar to the proof of first equation in (25). This completes the proof. □

Remark 6. By Theorem 3.1, we use the solutions of the first order adjoint equation (23) to evaluate the gradient of the cost functional and the second order adjoint (24) to compute Hessian vector products.

Here we give a brief discussion for stability of the operator splitting scheme. If for the subproblems, the following is satisfied:

$$\|e^{\frac{1}{2}\tau\mathcal{A}_j}\| \le e^{\frac{1}{2}\tau\omega_j}, \quad j = 1, \cdots, j-1, \quad \text{and} \quad \|e^{\tau\mathcal{A}_M}\| \le e^{\tau\omega_M}, \tag{27}$$

then $\|\phi_{k+1}\| \le e^{\tau\omega}\|\phi_k\|$, where $\omega = \sum_{j=1}^{M}\omega_j$. Consequently, the stability holds on any finite time interval $[t_0, T]$ if $\omega > 0$. It also holds for an arbitrary large time interval when $\omega \le 0$. In practice the operator splitting scheme is stable if each sub-step is stable. By Lax's equivalence theorem [7], consistency and stability together imply convergence, and higher order consistency yields faster convergence. In particular, the following theorem specifies the global splitting error:

Theorem 3.2. *Let* $\mu(\nabla A(\phi)) := \lim_{h\to 0+}\frac{\|I + h\nabla A(\phi)\| - 1}{h} \le \lambda$*, then*

$$\|\phi(t_n) - \phi_n\| \le C\tau^3(e^{n\lambda\tau} - 1)(e^{\lambda\tau} - 1)^{-1},$$

where C *is a positive number independent of* τ*.*

Proof. One can find the proof in [4]. For completeness, we present the proof.
If the perturbation of the initial condition of (12) is δu^0, then by the perturbation equation (13) and using a semigroup expression, we have

$$\delta\phi(t) = e^{t\nabla A(\phi)}\delta u^0.$$

Consequently,

$$\|\delta\phi(t)\| \le \|e^{t\nabla A(\phi)}\|\|\delta u^0\| \le e^{\mu(\nabla A(\phi))}\|\delta u^0\| \le e^{\lambda t}\|\delta u^0\|, \tag{28}$$

where we have used Proposition 2.1 in [10] in the second step. By (18), the local splitting errors do not exceed $C\tau^3$ for some constant C. In computing ϕ_2 there is an error of $C\tau^3$ in the initial condition, and by (28), the effect of this error at t_2 is $C\tau^3 e^{\lambda\tau}$. Thus, the global splitting error at t_2 is $C\tau^3 + C\tau^3 e^{\lambda\tau}$. Similarly the global splitting error at t_3 is

$$C\tau^3 + (C\tau^3 + C\tau^3 e^{\lambda\tau})e^{\lambda\tau}.$$

Repeating the procedure in the same way we find that the global splitting error at t_n is

$$\sum_{k=1}^{n} C\tau^3 e^{(n-k)\lambda\tau} = C\tau^3 \sum_{k=0}^{n-1} e^{k\lambda\tau} = C\tau^3(e^{n\lambda\tau}-1)(e^{\lambda\tau}-1)^{-1}.$$

□

Proposition 1. *The global Marchuk-Strang splitting error in the 4D-Var is second order for time step of length* τ*.*

Proof. By the equality $e^z - 1 = O(z)$, a straightforward calculation implies that

$$(e^{n\lambda\tau}-1)(e^{\lambda\tau}-1)^{-1} = O(\frac{1}{\tau}).$$

By Theorem 3.2, $\|\phi(t_n) - \phi_n\| = O(\tau^2)$. The proof is completed. □

By utilizing Theorem 3.2 and Proposition 1, the following proposition follows immediately.

Proposition 2. [4] *Let* $\nabla^{\tau}_{u^0}\mathcal{J}(u^0, \phi(u^0))$ *be the approximation of* $\nabla_{u^0}\mathcal{J}(u^0, \phi(u^0))$ *by the Marchuk-Strang operator splitting method. If* $\mu(\nabla A(\phi))$ *and* $\mu((\nabla A(\phi))^*)$ *are bounded, then*

$$\|\nabla_{u^0}\mathcal{J}(u^0, \phi(u^0)) - \nabla^{\tau}_{u^0}\mathcal{J}(u^0, \phi(u^0))\| \le C\tau^2,$$

where C *is a positive number independent of* τ*.*

Similarly we can estimate the local and global splitting error for $\|\nabla^2_{u^0}\mathcal{J}(u^0, \phi(u^0)) v - \nabla^{2,\tau}_{u^0}\mathcal{J}(u^0, \phi(u^0))v\|$ for any user-defined element v.

We remark that [13] used the operator splitting method for a chemical transport model and obtained some interesting numerical results.

4. **Conclusions.**

In this paper, we presented a framework for 4D-Var and discuss the Marchuk-Strang symmetrical operator splitting methods in the functional 4D-Var.

Constructing and solving adjoint models give rise to an efficient approach to evaluate the gradient and Hessian of the optimization functional with respect to an unknown parameter. When the forward model and adjoint models have complicated structures and consist of different parts, one can use the operator splitting method. The Marchuk-Strang symmetrical multi-component splitting method in the 4D-Var gives rise to a second order splitting error for time step.

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REFERENCES

[1] V. Akcelik, G. Biros, A. Draganescu, O. Ghattas, J. Hill, and B. v. BloemenWaanders, *Inversion of airborne contaminants in a regional model*, in "Lecture Notes in Computer Science series", **3993** (2006), 481–488.
[2] V. Barbu, "Nonlinear Semigroups and Differential Equations in Banach Spaces," Editura Academiei, Bucuresti, 1976.
[3] W. Hundsdorfer and J. G. Verwer, "Numerical Solutions of Time-Dependent Advection-Diffusion-Reaction Equations," Springer-Verlag, New York, 2003.
[4] L. Jiang and C. C. Douglas, *An analysis of 4D variational data assimilation and its application*, Computing, **84** (2009), 97–120.
[5] F.X. Le Dimet, I.M. Navon, and D. Daescu, *Second order information in data assimilation*, Monthly Weather Review, **130** (2002), 629–648.

[6] D. Lanser and J. G. Verwer, *Analysis of operator splitting for advection-diffusion-reaction problems from air pollution modelling*, J. Comput. Appl. Math. **111** (1999), 201–216.
[7] P. Lax, " Functional Analysis," Wiley Interscience, New York, 2002.
[8] G. Marchuk, " Adjoint Equations and Analysis of Complex System," Springer-Verlag, New York, 1995.
[9] F. A. Rihan and C. G. Collier, "Four-Dimensional Data Assimilation and Numerical Weather Prediction," CERS Data Assimilation Technical Report No. 1 (2003), University of Salford, UK.
[10] G. Söderlind, *The logarithmic norm. history and modern theory*, Bit., Vol. **46** (2006), 631–652.
[11] G. Strang, *On the construction and comparison of difference schemes*, SIAM J. Numer. Anal. **5** (1968), 506–517.
[12] Z. Wang, K. Droegemeier, and L. White, *The adjoint newton algorithm for large-scale unconstrained optimization in meteorology applications*, Comput. Optim. Appl., **10** (1998), 283–320.
[13] L. Zhang and A. Sandu, *Data assimilation in multiscale chemical transport models*, in "Lecture Notes in Computer Science series", **4487** (2007), 1026–1033, Springer-Verlag, Heidelberg.

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