1. Introduction

Data assimilation is a statistical technique to modify the state of a running model in response to data, based on sequential Bayesian estimation. The EnKF accesses the model only as a black box. It is suitable for a wide range of problems and relatively easy to combine with existing modeling software. However, the ensemble size needed can be large, and the amount of computation required in EnKF can be significant when the EnKF is modified to suppress spurious long-range correlations. We propose a new variant of EnKF that can overcome these difficulties by the use of FFT. The new method is applied to the morphing EnKF, which is needed for the fire application, but the FFT EnKF can be used with or without morphing.

2. Data Assimilation

We first briefly describe the EnKF for reference. The EnKF advances in time an ensemble of simulations $u_1, \ldots, u_N$, which approximates the probability distribution of the model state $u$. The simulations are then advanced in
time until the analysis time, when new data \( d \) arrives. It is assumed that the data error is known, \( d - Hu \sim N(0, R) \) given \( u \), where \( H \) is the observation operator and \( R \) is the data error covariance matrix. The ensemble, now called the forecast ensemble, is combined with the data to give the analysis ensemble by the EnKF formulas\(^4\)

\[
u_{a_k} = u_k + C_N H^T (HC_N H^T + R)^{-1} \left( d + e_k - Hu_k \right),
\]

where \( C_N \) is an estimate of the covariance of the model state, and \( e_k \) is a random perturbation \( e_k \sim N(0, R) \). The analysis ensemble \( u_{a_1}, \ldots, u_{a_N} \) is then used as the initial condition for a new simulation, advanced to a new analysis time, and the analysis cycle repeats.

In the standard EnKF,\(^4\) \( C_N \) is the sample covariance computed from the ensemble. Under suitable assumptions, it can be proved that the ensemble converges for large \( N \) to a sample from the Kalman filtering distribution and \( C_N \) converges to the true covariance.\(^5\)

2.1. FFT EnKF and Covariance Estimation by FFT

The EnKF formulation (1) relies on linear algebra only and it is oblivious to any structure of the model state. Large ensembles (30-100 and more) are often needed.\(^2\) We are interested in obtaining a reasonable approximation of the covariance matrix from a very small sample. For this, we take advantage of the fact that the simulation state \( u \) is a block vector, where the blocks are values of the modelled physical fields on grids of points in a spatial domain \( \Omega \), which are (discrete versions of) smooth random functions, i.e., realizations of random fields. The covariance of a random field drops off quickly with distance, and it is often the case in geostatistics that random fields are stationary, that is, the covariance between two points depends on their distance vector only.\(^6\) But for a small sample, the ensemble covariance is a matrix of low rank with large off-diagonal elements even at a great distance. Therefore, localization techniques are used, such as tapering, which consists of multiplication of the terms of the sample covariance by a fixed function to force the dropoff of the covariance away from the diagonal, resulting in a more accurate approximation of covariance for small samples.\(^7\) However, solving a system with the resulting approximate covariance matrix is expensive, because efficient dense linear algebra, which relies on the representation of the sample covariance matrix as the product of two rectangular matrices,\(^8\) can no longer be used.

For simplicity, we explain the FFT EnKF in the 1D case. Higher-dimensional cases work exactly the same. Also, we consider first the case
when the model state consists of one block only.

The basic operation in the EnKF (1) is the multiplication $v = C_N u$ of a vector $u$ by an approximate covariance matrix $C_N$. Denote by $u(x_i)$ the entry of vector $u$, corresponding to node $x_i$ and suppose for the moment that the random field is stationary, that is, its covariance matrix satisfies $C(x_i, x_j) = c(x_i - x_j)$ for some covariance function $c$. Then $v$ is the convolution

$$v(x_i) = \sum_j C(x_i, x_j) u(x_j) = \sum_j u(x_j) c(x_i - x_j).$$

The discrete Fourier transform changes convolution to multiplication entry by entry. Hence, if the random field is stationary, multiplication by its covariance matrix becomes multiplication by a diagonal matrix in the frequency domain.

The proposed method of covariance estimation consists of computing the sample covariance of the ensemble in the frequency domain, and neglecting all of its off-diagonal terms. This is justified by the assumption that the covariance depends mainly on the distance.

(1) Given ensemble $[u_k]$, apply a FFT operator $F$ to each member to obtain the member $\hat{u}_k = Fu_k$ in the frequency domain.

(2) Compute the approximate forecast covariance matrix $\hat{C}_N$ in the frequency domain as the diagonal matrix with the diagonal entries $\hat{c}_i$ equal to the diagonal entries of the sample covariance of the ensemble $[\hat{u}_k]$,

$$\hat{c}_i = \frac{1}{N-1} \sum_{k=1}^{N} |\hat{u}_{ik} - \bar{u}_i|^2, \quad \bar{u}_i = \frac{1}{N} \sum_{k=1}^{N} \hat{u}_{ik}. \quad (2)$$

Multiplication by the approximate covariance matrix $C_N$ then becomes in the frequency domain

$$u = C_N v \iff \hat{u} = F u, \quad \hat{v} = \hat{c} \bullet \hat{u}, \quad v = F^{-1} \hat{v},$$

where $\bullet$ is entry-by-entry multiplication, $(\hat{c} \bullet \hat{u})_i = \hat{c}_i \hat{u}_i$. In the important case $H = I$ and $R = rI$ (the whole state is observed and the data errors are uncorrelated and the same at every point), considered here, the EnKF (1) in the frequency domain reduces to entry-by-entry operations,

$$\hat{u}^2_k = \hat{u}_k + \hat{c} \bullet (\hat{c} + r)^{-1} \bullet (\hat{d} + \hat{c}_k - \hat{u}^f_k). \quad (3)$$
In an application, the state has multiple variables. The state vector, its covariance, and the observation matrix then have the block form

\[
\begin{align*}
\mathbf{u} &= \begin{bmatrix} u^{(1)} \\ \vdots \\ u^{(n)} \end{bmatrix}, \\
\mathbf{C} &= \begin{bmatrix} C^{(11)} & \cdots & C^{(1M)} \\ \vdots & \ddots & \vdots \\ C^{(M1)} & \cdots & C^{(MM)} \end{bmatrix}, \\
\mathbf{H} &= \begin{bmatrix} H^{(1)} & \cdots & H^{(M)} \end{bmatrix}.
\end{align*}
\] (4)

Assume that the first variable is observed, then

\[
H^{(1)} = I, \quad H^{(2)} = 0, \ldots, \quad H^{(M)} = 0.
\]

The EnKF (1) then simplifies to

\[
u_k^{(j), a} = \mathbf{u}_k^{(j)} + C^{(j1)}_N \left( C^{(11)}_N + \mathbf{R} \right)^{-1} \left( \mathbf{d} + \mathbf{e}_k - \mathbf{u}_k^{(1)} \right), \quad j = 1, \ldots, M, \quad (5)
\]

which becomes in the frequency domain

\[
\tilde{\nu}_k^{(j), a} = \tilde{\mathbf{u}}_k^{(j)} + \tilde{C}^{(j1)}_N \left( \tilde{C}^{(11)}_N + \tilde{\mathbf{R}} \right)^{-1} \left( \tilde{\mathbf{d}} + \tilde{\mathbf{e}}_k - \tilde{\mathbf{u}}_k^{(1)} \right),
\] (6)

where the spectral cross-covariance between field \( j \) and field 1 is approximated from

\[
\tilde{c}^{(j1)}_i = \frac{1}{N-1} \sum_{k=1}^{N} \left( \tilde{u}_{ik}^{(j)} - \tilde{\mathbf{u}}_i^{(j)} \right) \left( \tilde{u}_{ik}^{(1)} - \tilde{\mathbf{u}}_i^{(1)} \right), \quad \tilde{\mathbf{u}}_i^{(j)} = \frac{1}{N} \sum_{k=1}^{N} \tilde{u}_{ik}^{(j)}. \quad (7)
\]

### 2.2. Morphing EnKF

To treat position errors in addition to amplitude errors, FFT EnKF is combined with the morphing EnKF.\(^3\)\(^8\) The method uses an additional ensemble member \( u_{N+1} \), called the reference member. Given an initial state \( u \), the initial ensemble is given by \( u_{N+1} = u \) and

\[
u_k^{(i)} = \left( u_{N+1}^{(i)} + r_k^{(i)} \right) \circ (I + T_k), \quad k = 1, \ldots, N, \quad (8)
\]

where \( r_k^{(i)} \) are random smooth functions on \( \Omega \), \( T_k \) are random smooth mappings \( T_k : \Omega \to \Omega \), and \( \circ \) denotes composition. Thus, the initial ensemble has both amplitude and position variability, and the position change is the same for all blocks. Random smooth functions and mappings are generated by FFT as a Fourier series with random coefficients that decay quickly with frequency.

The data \( \mathbf{d} \) is an observation of \( u^{(1)} \), and it is expected that it differs from the model in addition as well as in the position of significant features, such as firelines. The first blocks of \( u_1, \ldots, u_N \) and \( \mathbf{d} \) are then registered against the first block of the reference member \( u_{N+1} \). We find registration mappings \( T_k : \Omega \to \Omega, \quad k = 0, \ldots, N \) such that

\[
u_k^{(1)} \approx u_{N+1}^{(1)} \circ (I + T_k), \quad T_k \approx 0, \quad \nabla T_k \approx 0, \quad k = 0, \ldots, N,
\]
where $d = u_0^{(1)}$. Define the registration residuals $r_k^{(j)} = u_k^{(j)} (I + T_k)^{-1} - u_{N+1}^{(j)}$, $k = 0, \ldots, N$. The morphing transform maps each ensemble member $u_k$ into the extended state vector

$$u_k \mapsto \tilde{u}_k = M_{u_{N+1}}(u_k) = (T_k, r_k^{(1)}, \ldots, r_k^{(M)}).$$

Similarily, the data becomes the extended data vector $d \mapsto \tilde{d} = (T_0, r_0^{(1)})$. The FFT EnKF method (6) is applied to the transformed ensemble $\tilde{u}_1, \ldots, \tilde{u}_N$ with the observation operator given by $(T, r^{(1)}, \ldots, r^{(M)}) \mapsto (T, r^{(1)})$. The cross-covariances between $x$ and $y$ components of $T$ and $r^{(1)}$ are neglected, so the covariance $C^{(11)}$ in (5) consists of three diagonal matrices, and (6) applies. The new transformed reference member is obtained as

$$u_k^{a,(i)} = M_{u_{N+1}}^{-1}(\tilde{u}_k^{a}) = (u_{N+1}^{(i)} + r_k^{a,(i)}) \circ (I + T_k^a), \quad k = 1, \ldots, N+1.$$

3. The Wildland Fire Model

We only summarize the model very briefly. See Ref. 8 for further details, references, and acknowledgements.

The fire model runs on a 2D rectangular grid on the Earth surface, called the fire grid. The model postulates fire line propagation speed as a function of wind and terrain slope, and an exponential decay of fuel by combustion after the ignition. The fire area is represented by a level set function as the set of points where the level set function is negative. The level set function satisfies a partial differential equation, which is solved numerically on the fire grid by explicit time stepping. Ignition is achieved by setting the value of the level set function so that it is negative in the ignition region. The state of the fire model consists of the level set function and the ignition time at the fire grid nodes. Other derived quantities included in the state vector are the fuel fraction burned and the heat flux from the combustion.

The fire model is coupled with the Weather Research Forecasting (WRF) atmospheric model, which runs on a much coarser 3D grid. In every time step, the fire model inputs the horizontal wind velocity, and the heat and vapor fluxes output from the fire model are inserted into the atmospheric model. The fire model is distributed as WRF-Fire with WRF, and the latest development version is also available from the authors.
4. Computational Results
We have used the optimization method from Ref. 3 for registration. We have used the real sin FFT, which forces zero change on the boundary. We have used a standard ideal problem distributed with WRF-Fire. The model has a $420 \times 420$ fire mesh and a $42 \times 42 \times 41$ atmospheric mesh. The fuel was the same on the whole domain. The model was initialized with the wind blowing diagonally across the grid, and two line ignitions and one circle ignition occur within the first 4 seconds of simulation time. After one minute of simulation time, when the fire was established and one of the line fires has merged with the circular fire, the simulation was stopped and an initial ensemble was generated by random smooth perturbation both in position and in amplitude. Artificial data was created by a similar perturbation. The forecast was taken the same as the initial ensemble. The described data assimilation algorithm was then applied with 5 members, with the results shown in Fig. 1 for the morphing EnKF and Fig. 2 for the morphing FFT EnKF. We see that the EnKF was not able to approach that data at all with such a small ensemble, while the FFT EnKF delivered an ensemble around the correct data shape.

5. Conclusion
We have shown that the morphing FFT EnKF is capable of data assimilation in a wildfire simulation, which exhibits sharp boundaries and coherent features. We have shown that the FFT EnKF can deliver acceptable results with a very small ensemble (5 members), unlike the standard EnKF, which is known to work with morphing for this application, but only with a much larger ensemble. Further development, involving multiple variables and multiple analysis cycles, will be presented elsewhere.

6. Acknowledgements
This work was supported by NSF grants CNS-0719641 and ATM-0835579.

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Fig. 1. The morphing EnKF with 5 ensemble members, applied to the ground heat flux from the WRF-Fire model. The ensemble size is not sufficient, the correct analysis is not even approximately in the span of the forecast, and the EnKF cannot reach it.

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Fig. 2. The morphing FFT EnKF with 5 ensemble members, applied to the ground heat flux from the WRF-Fire model. The analysis ensemble moved towards the data.