DOCTORAL THESIS

Computational methods in air quality data

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Abstract

In this thesis, we have investigated several computational methods on data assimilation for air quality prediction, especially on the characteristic of sparse matrix and the underlying information of gradient in the concentration of pollutant species.

In the first part, we have studied the ensemble Kalman filter (EnKF) for chemical species simulation in air quality forecast data assimilation. The main contribution of this paper is to study the sparse data observations and make use of the matrix structure of the Kalman filter updated equations to design an algorithm to compute the analysis of chemical species in the air quality forecast system efficiently. The proposed method can also handle the combined observations from multiple species together. We have applied the proposed method and tested its performance for real air quality data assimilation. Numerical examples have demonstrated the efficiency of the proposed computational method for Kalman filter update, and the effectiveness of the proposed method for NO_2, NO, CO, SO_2, O_3, PM2.5 and PM10 in air quality data assimilation.

For the second part, we have proposed and developed an optimization approach for data assimilation by using the gradients of the forecast of state variables. We have studied an objective function consisting of two data-fitting terms. The first term is based on the difference between the gradients of the forecast and the analysis of the state variables while the second term is based on the difference between the observations and the projected analysis of state variables. Here the existence and uniqueness of the analysis solution of the proposed objective function are shown. The solution can be calculated by using the conjugate gradient method iteratively. Experimental results based on the Community Multi-scale Air Quality (CMAQ) are presented. We then showed that the prediction performance of the proposed method is better than that of other testing methods in air quality and weather data assimilation.

Within the third part, we have set up an automatic workflow to connect the management system of the chemical transport model - CMAQ with our proposed data assimilation methods. The setup has successfully integrated the data assimilation into the management system and shown that the accuracy of the prediction has risen

to a new level. This technique has transformed the system into a real-time and high-precision system. When the new observations are available, the predictions can then be estimated almost instantaneously. Then the agencies are able to make the decisions and respond to the situations immediately. In this way, citizens are able to protect themselves effectively. Meanwhile, it allows the mathematical algorithm to be industrialized implying that the improvements on data assimilation have directly positive effects on the developments of the environment, the human health and the society. Therefore, this has become an inspiring indication to encourage us to study, achieve and even devote more research into this promising method.

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