Data Assimilation in Atmospheric CTMs: I. Computational Tools

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Information feedback loops between CTMs and observations: data assimilation and targeted meas.

Chemical kinetics  
Transport  
Meteorology  
CTM  
Optimal analysis state  
Observations  

Improve:  
- forecasts  
- science  
- field experiment design  
- models  
- emission estimates
Best estimate of the state/parameters is obtained by combining multiple sources of information

**Model** (encapsulating knowledge on the physics, chemistry, thermodynamics, etc)

**Background** (encapsulating best a-priori knowledge of the state)

**Observations** (encapsulating new information about reality)

**Bayes:**

\[
P[y^k | z_0^{k-1} \cdots z_0^{0}] = \frac{P[z_0^{k} | y^k] \cdot P[y^k | z_0^{k-1} \cdots z_0^{0}]}{\int P[z_0^{k} | y] \cdot P[y | z_0^{k-1} \cdots z_0^{0}] dy} = P_R[e_0^{k}] \cdot P_B[y^k] \]

**Methods:**

4D-Var, EnKF

[Picture from J.L. Anderson]
In the 4D-Var approach D.A. is formulated as a PDE-constrained optimization problem (gradient-based)

\[
\min_{y^0} \psi(y^0) = \frac{1}{2}(y^0 - y^b)^T B^{-1} (y^0 - y^b) + \frac{1}{2} \sum_{k=1}^{N} (H^k y^k - z^k)^T R^{-1}_k (H^k y^k - z^k)
\]

subject to \( y^k = M(t^{k-1}, y^{k-1}, p), \quad k = 1, 2, \ldots \)

Gradient: \( \lambda = \nabla_{y^0} \psi = \left(\frac{\partial \psi}{\partial y^0}\right)^T = B^{-1}(y^0 - y^b) + \sum_{k=1}^{N} \left(\frac{\partial y^k}{\partial y^0}\right)^T (H^k)^T R^{-1}_k (H^k y^k - z^k) \)
Adjoint of stiff chemical kinetics: formulation, challenges, and automatic implementation.
KPP automatically generates simulation and direct/adjoint sensitivity code for chemistry

Chemical mechanism

```plaintext
#INCLUDE atoms

#DEFVAR
O = O; O1D = O;
O3 = O + O + O;
NO = N + O;
NO2 = N + O + O;

#DEFIX
O2 = O + O; M = ignore;

#EQUATIONS { Small Stratospheric }
O2 + hv = 2O               : 2.6E-10*S;
O    + O2 = O3              : 8.0E-17;
O3  + hv = O   + O2      : 6.1E-04*S;
O    + O3 = 2O2            : 1.5E-15;
O3  + hv = O1D + O2    : 1.0E-03*S;
O1D  + O3 = 2O2           : 7.1E-11;
NO   + O3 = NO2 + O2       : 1.2E-02*S;
```

Simulation code

```plaintext
SUBROUTINE FunVar ( V, F, RCT, DV )
   INCLUDE 'small.h'
   REAL*8 V(NVAR), F(NFIX)
   REAL*8 RCT(NREACT), DV(NVAR)
   C A - rate for each equation
   REAL*8 A(NREACT)
   C Computation of equation rates
   A(1) = RCT(1)*F(2)
   A(2) = RCT(2)*V(2)*F(2)
   A(3) = RCT(3)*V(3)
   A(4) = RCT(4)*V(2)*V(3)
   A(5) = RCT(5)*V(3)
   A(6) = RCT(6)*V(1)*F(1)
   A(7) = RCT(7)*V(1)*V(3)
   A(8) = RCT(8)*V(3)*V(4)
   A(9) = RCT(9)*V(2)*V(5)
   A(10) = RCT(10)*V(5)
   C Aggregate function
   DV(1) = A(5)-A(6)-A(7)
   DV(2) = 2*A(1)-A(2)+A(3)-A(4)+A(6)-&A(9)+A(10)
   DV(3) = A(2)-A(3)-A(4)-A(5)-A(7)-A(8)
   DV(4) = -A(8)+A(9)+A(10)
   DV(5) = A(8)-A(9)-A(10)
END
```

[Damian et.al., 1996; Sandu et.al., 2002]
Rosenbrock, Runge-Kutta, Sdirk methods and their adjoints are efficiently implemented by KPP

**SAPRC-99**
Sparse Jacobian and Hessian

**Rosenbrock Method**
\( T_{\text{fwd}} \)

\[
\begin{align*}
\mathbf{y}^{n+1} &= \mathbf{y}^n + \sum_{j=1}^{s} m_j \mathbf{k}_j, \\
\mathbf{Y}^i &= \mathbf{y}^n + \sum_{j=1}^{i-1} a_{i,j} \mathbf{k}_j \\
\left[ \frac{1}{h^\gamma} \mathbf{I} - \mathbf{J}^n \right] \cdot \mathbf{k}_i &= \mathbf{f}(\mathbf{Y}^i) + \sum_{j=1}^{i-1} \frac{1}{h} c_{i,j} \mathbf{k}_j, \quad 1 \leq i \leq s
\end{align*}
\]

**Discrete Adjoint**
\( T \approx 2.3 T_{\text{fwd}} \)

\[
\begin{align*}
\left[ \frac{1}{h^\gamma} \mathbf{I} - (\mathbf{J}^n)^T \right] \cdot \mathbf{u}_i &= m_i \lambda^{n+1} + \sum_{j=i+1}^{s} \left( a_{j,i} \mathbf{v}_j + \frac{1}{h} c_{j,i} \mathbf{u}_j \right), \quad \mathbf{v}_i = (\mathbf{J}^T(\mathbf{Y}^i)) \cdot \mathbf{u}_i \\
\lambda^n &= \lambda^{n+1} + \sum_{i=1}^{s} \left( \mathbf{H}^n \times \mathbf{k}_i \right)^T \cdot \mathbf{u}_i + \sum_{i=1}^{s} \mathbf{v}_i
\end{align*}
\]

[Sandu et al., 2002]
Runge-Kutta methods and their adjoints are well suited for inverse chemical kinetic problems

RK Method

\[ y^{n+1} = y^n + h \sum_{i=1}^{s} b_i f(Y^i), \quad Y^i = y^n + h \sum_{i=1}^{s} a_{i,j} f(Y^j) \]

Continuous Adjoint

\[ \lambda^n = \lambda^{n+1} + h \sum_{i=1}^{s} b_i J^T(y^{n+1-c_i h}) \cdot \Lambda^i, \quad \Lambda^i = \lambda^{n+1} + h \sum_{j=1}^{s} a_{i,j} J^T(y^{n+1-c_i h}) \cdot \Lambda^j \]

Discrete Adjoint

\[ \lambda^n = \lambda^{n+1} + \sum_{i=1}^{s} \theta^i, \quad \theta^i = h J^T(Y^i) \cdot \left[ b_i \lambda^{n+1} + \sum_{j=1}^{s} a_{j,i} \theta^j \right] \]

**Consistency:** The discrete adjoint of RK method of order \( p \) is an order \( p \) discretization of the adjoint equation. (Proof using elementary differentials of transfer functions).

**Stiff behavior.** For SPP apply RK with invertible coefficient matrix \( A \) and \( R(\infty) = 0 \). If the cost function depends only on the non-stiff variable \( y \) then \( \lambda_z = 0 \) and \( \lambda_y \) are solved with the same accuracy as the original method, within \( O(\varepsilon) \).

[Sandu et al., 2005]
Methods available in the KPP numerical library

- **FIRK** 3-stage: Radau-2A (ord.5), Radau-1A (ord.5), Lobatto-3C (ord.4), Gauss (ord.6)
- **SDIRK**: 2a, 2b (2s, ord.2), 3a (3s, ord.2), 4a, 4b (5s, ord.4)
- **Rosenbrock**: Ros2, Ros3, Ros4, Rodas3, Rodas4.

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**Forward**

**TLM (DDM)**

**Discrete ADJ**
Adjoint for Integral-PDE aerosol dynamic equations: formulation and challenges

- Chemical kinetics
- Aerosols
- Transport
- Meteorology
- Optimal analysis state
- Data Assimilation
- Targeted Observ.
- Observations
- Improved:
  - forecasts
  - science
  - field experiment design
  - models
  - emission estimates

Emissions

CTM

DDDAS@ICCS 2007
Beijing, May 29, 2007
Populations of aerosols (particles in the atmosphere) are described by their mass density.

Aerosol dynamic equation - IPDE

\[
\frac{\partial q_i}{\partial t} = \int_0^m \beta(m',m-m')q_i(m',t) \frac{q(m-m',t)}{m-m'} \, dm' \\
- q_i \int_0^\infty \beta(m,m') \frac{q(m',t)}{m'} \, dm' \\
+ H_i q - \frac{\partial}{\partial m} (m H q_i) + m_i S - L q_i + R_i(q)
\]

\[
q_i(m,t = t^0) = q_i^0(m), \quad 1 \leq i \leq n, \\
q_i(m = 0,t) = 0, \quad q_i(m = \infty, t) = 0.
\]
Adjoint aerosol dynamic models are needed to solve inverse problems

\[
\frac{\partial \lambda_i}{\partial t} = -\int_{0}^{\infty} \beta(m, m') (m')^{-1} [\lambda_i(m + m', t) - \lambda_i(m, t)] q(m', t) \, dm' + L \lambda_i \quad t_{k-1} \leq t \leq t_k
\]

Continuous adjoint equation

\[
\begin{align*}
-\int_{0}^{\infty} \beta(m, m') m^{-1} & \sum_{j=1}^{n} [\lambda_j(m + m', t) - \lambda_j(m, t)] q_j(m', t) \, dm' - \sum_{j=1}^{n} H_j \lambda_j - m H \frac{\partial \lambda_i}{\partial m} \\
\lambda_i(m, t_N) &= 0, \quad \lambda_i(m, t_k^+) = \lambda_i(m, t_k^-) + h_i T R_k^{-1} (y_k - h(q_k)) \\
\lambda_i(m, t_0) &= \lambda_i(m, t_+^0) + p_i T B^{-1} (p - p^B), \quad \lambda_i(0, t) = 0.
\end{align*}
\]

Observations of density in each bin allow the recovery of initial distribution and of parameters

[Sandu et. al., 2005; Henze et. al., 2004]
Discrete adjoint models for numerical advection: formulation and challenges

Chemical kinetics

Aerosols

CTM

Data Assimilation

Targeted Observ.

Optimal analysis state

Emissions

Improved:
• forecasts
• science
• field experiment design
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• emission estimates

Observations

Improved:

Meteorology

Beijing, May 29, 2007
Discrete adjoints of advection numerical schemes can become pointwise inconsistent with the adjoint PDE.

\[ w(x) = 0.5 - 0.5X \]

Change of forward scheme pattern:
- Change of upwinding
- Sources/sinks
- Inflow boundaries scheme
Example: 3rd order upwind FD

Active forward limiters act as pseudo-sources in adjoint
Example: minmod

[Liu and Sandu, 2005]
The 4D-Var tools have been implemented in parallel adjoint STEM and are being applied to real data.

**Chemistry:** KPP
- Forward: sparse Rosenbrock, RK, LMM
- DDM sensitivity (Rosenbrock, LMM)
- Discrete adjoints: Rosenbrock
- Continuous adjoints: Rosenbrock, RK, LMM

**Aerosols:** 0-D, not yet 3-D

**Transport:**
- Forward: upwind FV, FD, FE
- Adjoints for linear upwind FD

**Parallelization:** with PAQMSG

[Sandu et.al., 2003, 2004; Carmichael et. al., 2003, 2004]
Dynamic integration of chemical data and atmospheric models is an important, growing field

- **Current state of the art:**
  - the tools needed for 4d-Var chemical data assimilation are in place:
    - (adjoints for stiff systems, aerosols, transport; singular vectors, parallelization and multi-level checkpointing schemes, models of background errors)
  - their strengths demonstrated using real (field campaign) data; ambitious science projects are ongoing
  - ensemble-based chemical data assimilation is new, but promising

- **Computational tools are being widely adopted:**
  - EPA (CMAQ), JPL (GEOS–Chem), NCAR and NOAA (WRF-Chem), Canadian Meteorological Centre, Max Planck Institute Germany (MESSY), University of Koeln (EURAD - EURopean Air Pollution Dispersion)