Data Assimilation in Atmospheric CTMs: I. Computational Tools

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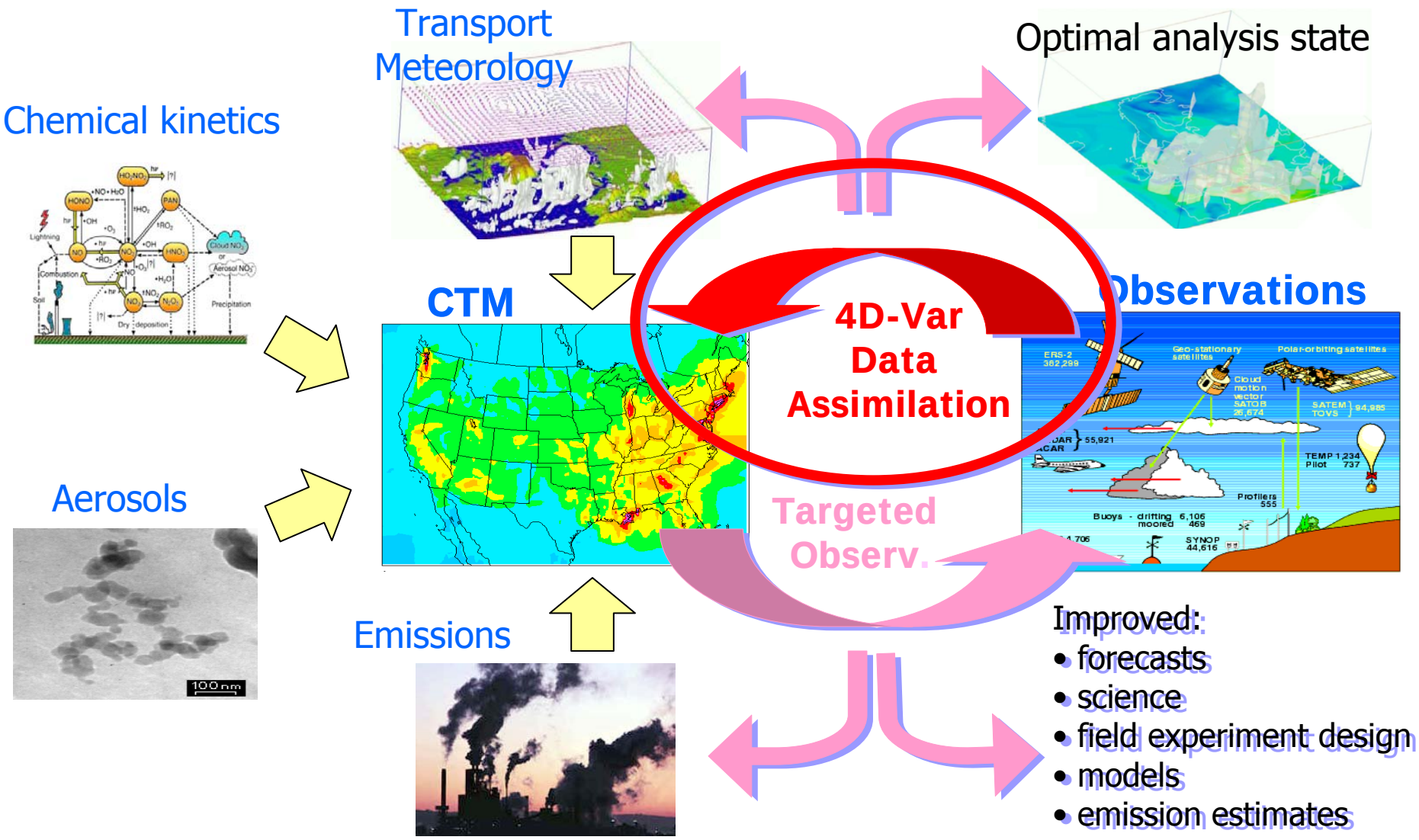
J.H. Seinfeld et al. (Caltech)

NSF ITR AP&IM 0205198

Virginia Tech

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



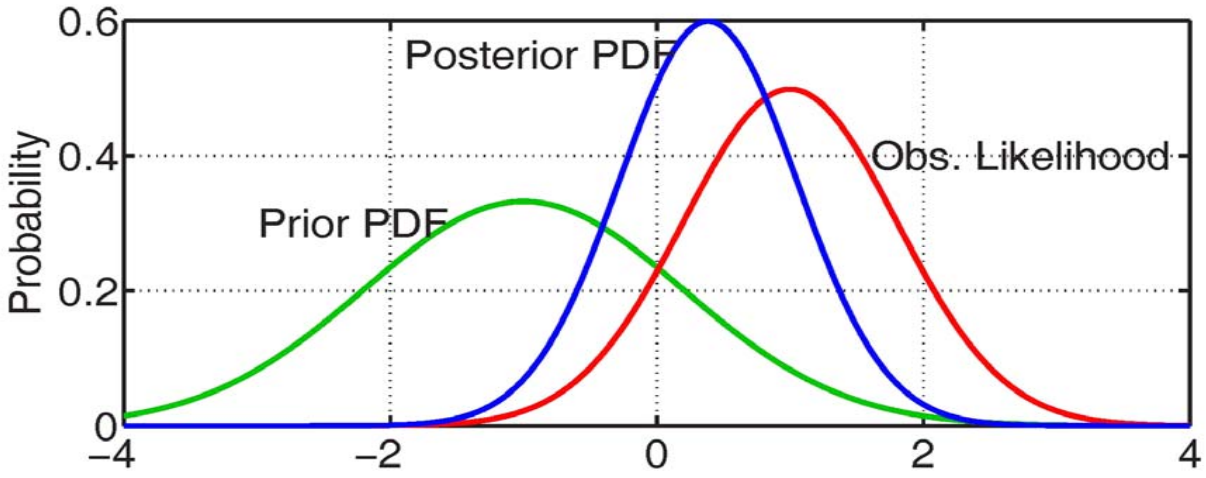
Best estimate of the state/parameters is obtained by combining multiple sources of information

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: $$P\left[y^k \,\middle|\, z^k_{\text{obs}} \dots z^0_{\text{obs}} \right] = \frac{P[z^k_{\text{obs}} | y^k] \cdot P[y^k \,|\, z^{k-1}_{\text{obs}} \dots z^0_{\text{obs}}]}{\int P[z^k_{\text{obs}} | y] \cdot P[y | z^{k-1}_{\text{obs}} \dots z^0_{\text{obs}}]\, dy} = \frac{P_R[\varepsilon^k_{\text{obs}}] \cdot P_B[y^k]}{\dots}$$



Methods:

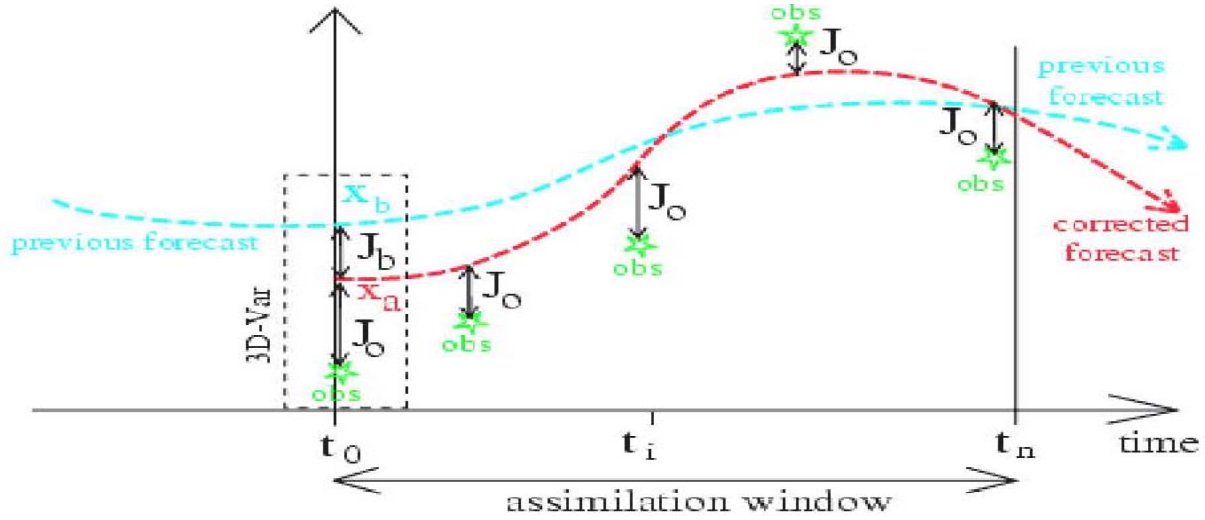
4D-Var, EnKF

[Picture from J.L. Anderson]

In the 4D-Var approach D.A. is formulated as a PDE-constrained optimization problem (gradient-based)

$$\min_{\mathbf{y}^0} \psi\left(\mathbf{y}^0\right)=\frac{1}{2}\left(\mathbf{y}^0-\mathbf{y}^b\right)^{\mathrm{T}}\mathbf{B}^{-1}\left(\mathbf{y}^0-\mathbf{y}^b\right)+\frac{1}{2}\sum_{k=1}^{N}\left(\mathbf{H}^k\mathbf{y}^k-\mathbf{z}^k\right)^{\mathrm{T}}\mathbf{R}_k^{-1}\left(\mathbf{H}^k\mathbf{y}^k-\mathbf{z}^k\right)$$

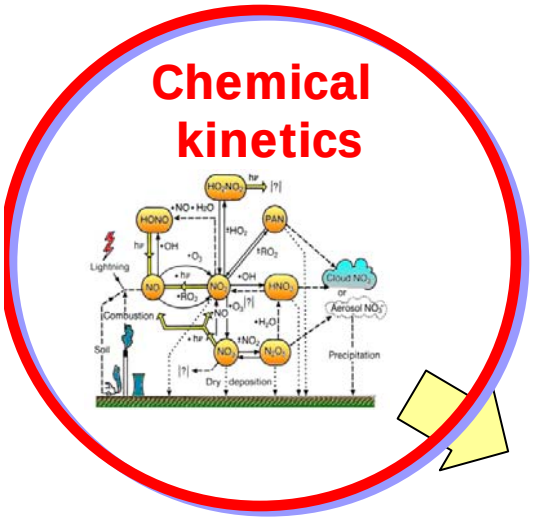
subject to $\mathbf{y}^k = M\left(t^{k-1},\mathbf{y}^{k-1},\mathbf{p}\right), \quad k=1,2,\ldots$



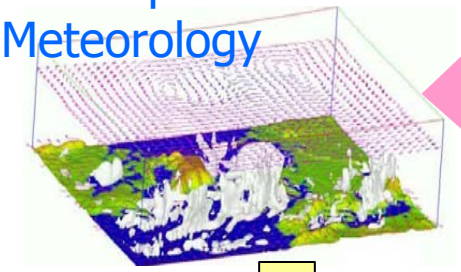
[Picture from F. Bouttier, P. Courtier]

Gradient: $$\boldsymbol{\lambda}=\nabla_{\mathbf{y}^0}\psi=\left(\frac{\partial\psi}{\partial\mathbf{y}^0}\right)^{T}=\mathbf{B}^{-1}\left(\mathbf{y}^0-\mathbf{y}^b\right)+\sum_{k=1}^{N}\left(\frac{\partial\mathbf{y}^k}{\partial\mathbf{y}^0}\right)^{\mathrm{T}}\left(\mathbf{H}^k\right)^{\mathrm{T}}\mathbf{R}_k^{-1}\left(\mathbf{H}^k\mathbf{y}^k-\mathbf{z}^k\right)$$

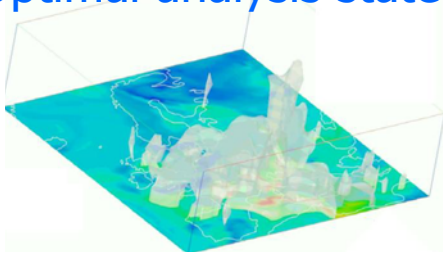
Adjoints of stiff chemical kinetics: formulation, challenges, and automatic implementation



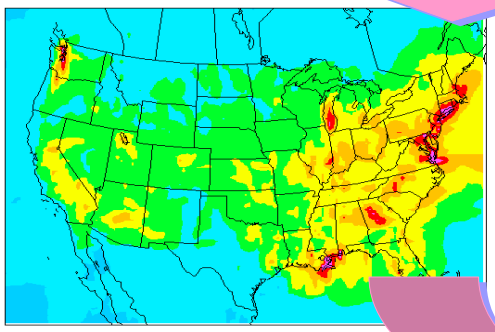
Transport Meteorology



Optimal analysis state

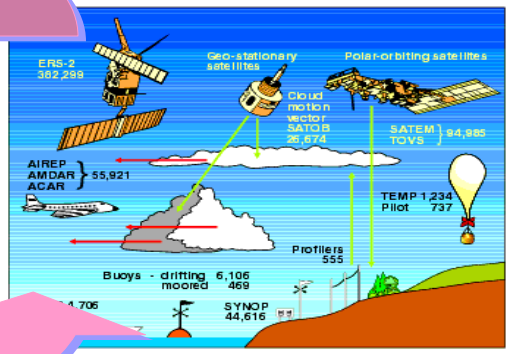


CTM

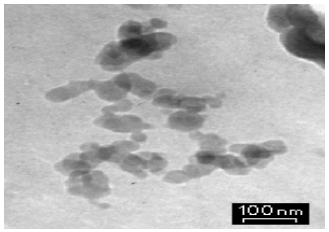


Data Assimilation

Observations



Aerosols



Targeted Observ.

Emissions

Improved:
- forecasts
- science
- field experiment design
- models
- emission estimates

KPP automatically generates simulation and direct/adjoint sensitivity code for chemistry

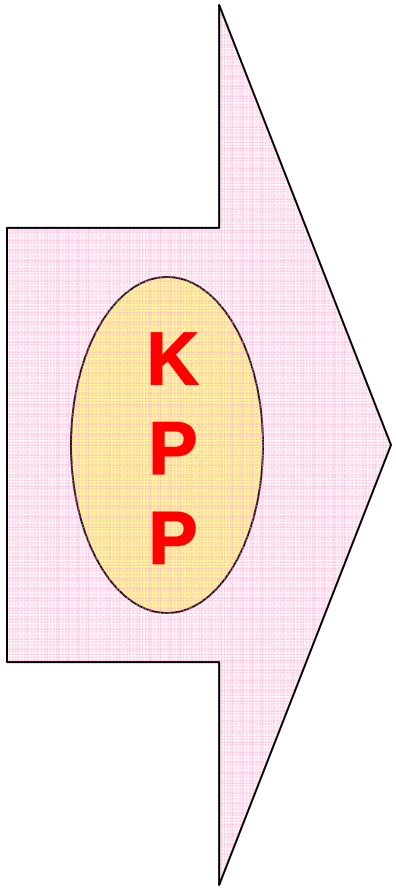
Chemical mechanism

```
#INCLUDE atoms

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

#DEFFIX
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  + M  = O   + M      :  7.1E-11;
O1D  + O3 = 2O2          :  1.2E-10;
NO   + O3 = NO2 + O2 :  6.0E-15;
NO2  + O  = NO  + O2     :  1.0E-11;
NO2  + hv = NO  + O      :  1.2E-02*S;
```



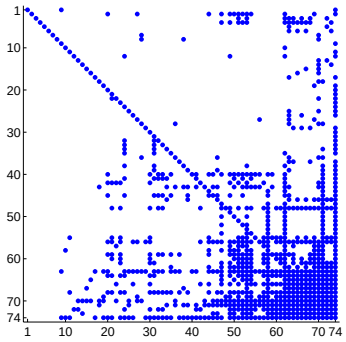
Simulation code

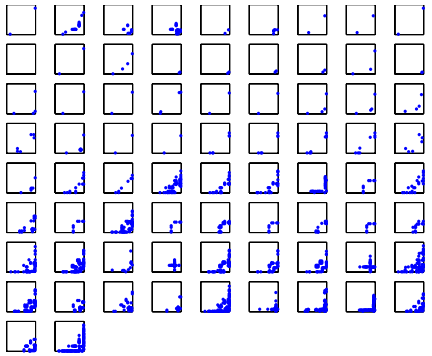
```
SUBROUTINE FunVar ( V,  F, RCT, DV )
   INCLUDE 'small.h'
    REAL*8 V(NVAR), F(NFIX)
    REAL*8 RCT(NREACT), DV(NVAR)
C A - rate for each equation
    REAL*8 A(NREACT)
C Computation of equation rates
    A(1) = RCT(1)*F(2)
    A(2) = RCT(2)*V(2)*F(2)
    A(3) = RCT(3)*V(3)
    A(4) = RCT(4)*V(2)*V(3)
    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_{fwd})

$$\begin{cases} \mathbf{y^{n+1}} = \mathbf{y^n} + \sum_{j=1}^{s} m_j \mathbf{k_j}, \quad \mathbf{Y^i} = \mathbf{y^n} + \sum_{j=1}^{i-1} a_{i,j} \mathbf{k_j} \\ \left[\frac{1}{h\gamma}\mathbf{I} - \mathbf{J^n}\right] \cdot \mathbf{k_i} = \mathbf{f}\left(\mathbf{Y^i}\right) + \sum_{j=1}^{i-1} \frac{1}{h} c_{i,j} \mathbf{k_j}, \quad 1 \le i \le s \end{cases}$$

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

$$\begin{cases} \left[\frac{1}{h\gamma}\mathbf{I} - \left(\mathbf{J^n}\right)^{\mathbf{T}}\right] \cdot \mathbf{u}_i = m_i \boldsymbol{\lambda}^{\mathbf{n+1}} + \sum_{j=i+1}^{s} \left(a_{j,i}\mathbf{v_j} + \frac{1}{h} c_{j,i} \mathbf{u_j}\right), \quad \mathbf{v_i} = \mathbf{J}^{\mathbf{T}}\left(\mathbf{Y^i}\right) \cdot \mathbf{u}_i \\ \boldsymbol{\lambda}^{\mathbf{n}} = \boldsymbol{\lambda}^{\mathbf{n+1}} + \sum_{\mathbf{i=1}}^{\mathbf{s}} \left(\mathbf{H^n} \times \mathbf{k_i}\right)^{\mathbf{T}} \cdot \mathbf{u_i} + \sum_{\mathbf{i=1}}^{\mathbf{s}} \mathbf{v_i} \end{cases}$$

[Sandu et.al., 2002]

Runge-Kutta methods and their adjoints are well suited for inverse chemical kinetic problems

RK Method

$$\mathbf{y}^{\mathbf{n+1}} = \mathbf{y}^{\mathbf{n}} + h\sum_{i=1}^{s} b_i \mathbf{f}\left(\mathbf{Y}^{\mathbf{i}}\right), \quad \mathbf{Y}^{\mathbf{i}} = \mathbf{y}^{\mathbf{n}} + h\sum_{i=1}^{s} a_{i,j} \mathbf{f}\left(\mathbf{Y}^{\mathbf{j}}\right)$$

Continuous Adjoint

$$\boldsymbol{\lambda}^{\mathbf{n}} = \boldsymbol{\lambda}^{\mathbf{n+1}} + h\sum_{i=1}^{s} b_i \mathbf{J}^{\mathbf{T}}\left(\mathbf{y}^{\mathbf{n+1-c_i h}}\right)\cdot \boldsymbol{\Lambda}^{\mathbf{i}}, \quad \boldsymbol{\Lambda}^{\mathbf{i}} = \boldsymbol{\lambda}^{\mathbf{n+1}} + h\sum_{j=1}^{s} a_{i,j} \mathbf{J}^{\mathbf{T}}\left(\mathbf{y}^{\mathbf{n+1-c_i h}}\right)\cdot \boldsymbol{\Lambda}^{\mathbf{j}}$$

Discrete Adjoint

[Hager, 2000]

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

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).

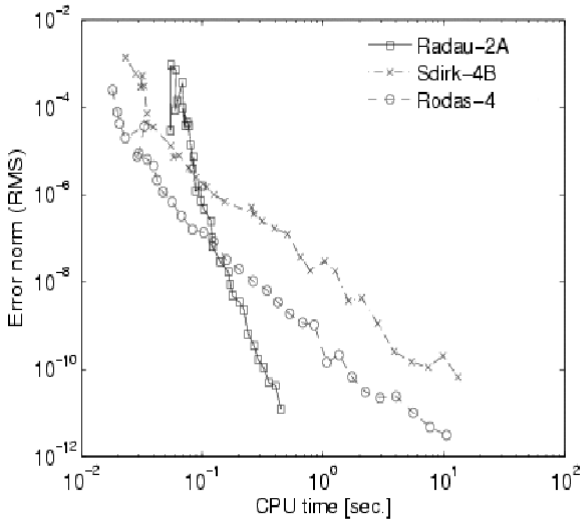
Stiff behavior. For SPP apply RK with invertible coefficient matrix A and R(∞) = 0. If the cost function depends only on the non-stiff variable y then $\lambda_z = 0$ and λ_y are solved with the same accuracy as the original method, within $O(\varepsilon)$.

[Sandu et al., 2005]

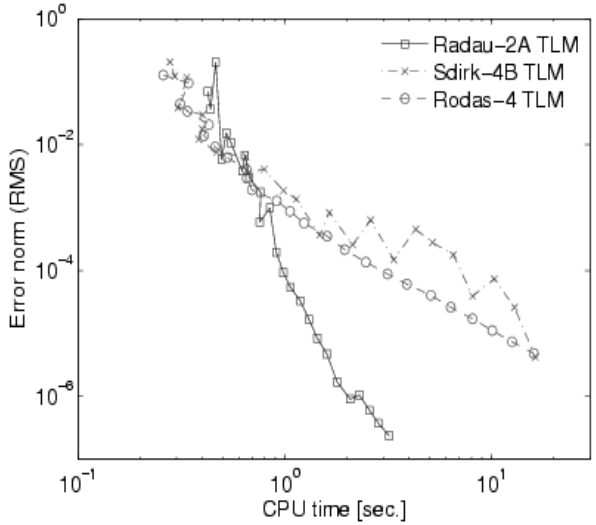
Methods available in the KPP numerical library

- 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.

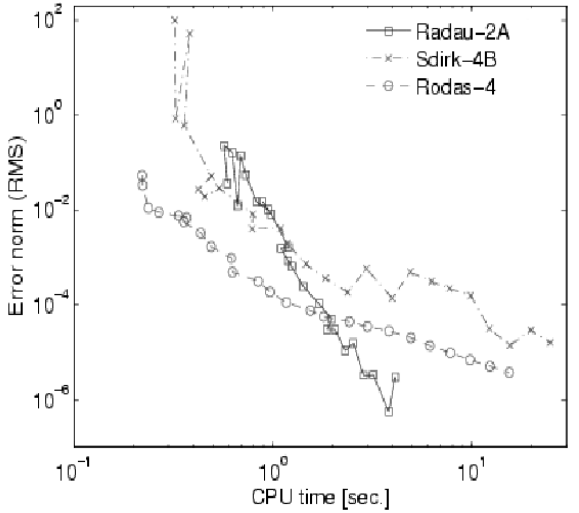
Forward



TLM (DDM)

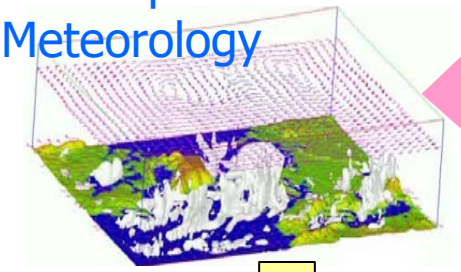


Discrete ADJ

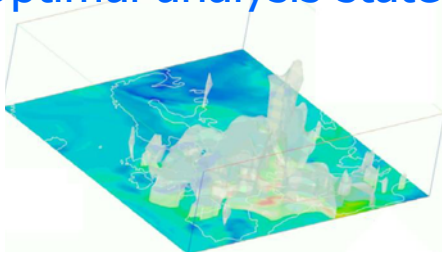


Adjoints for Integral-PDE aerosol dynamic equations: formulation and challenges

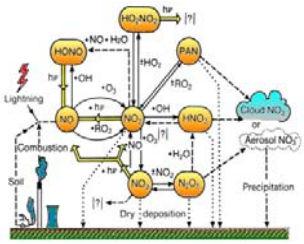
Transport
Meteorology



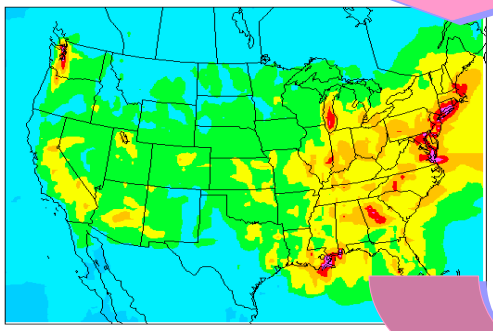
Optimal analysis state



Chemical kinetics

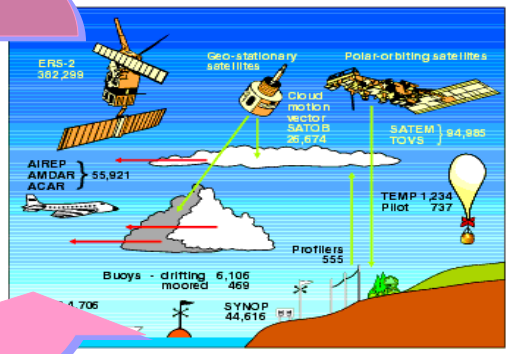


CTM

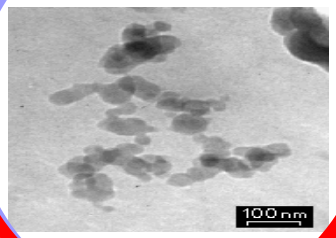


Data
Assimilation

Observations



Aerosols

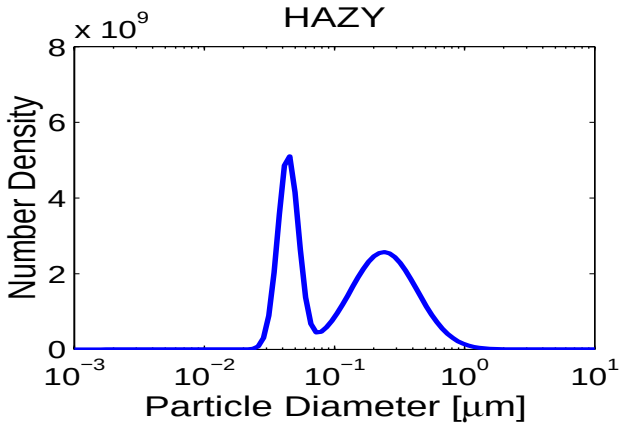


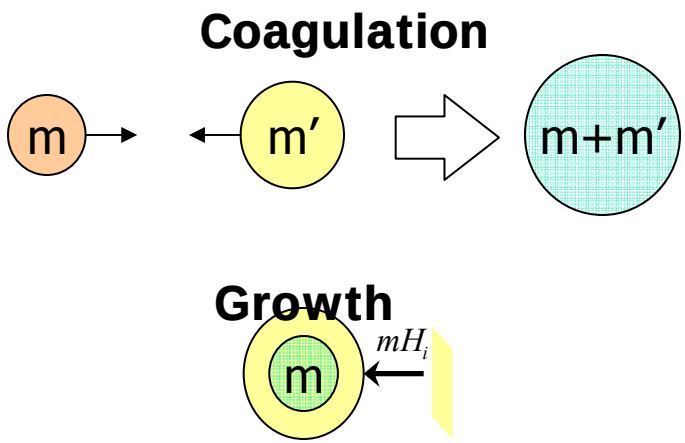
Targeted
Observ.

Emissions

Improved:
- forecasts
- science
- field experiment design
- models
- emission estimates

Populations of aerosols (particles in the atmosphere) are described by their mass density





Aerosol dynamic equation - IPDE

$$\frac{\partial q_i}{\partial t} = \int_0^m \beta(m', m-m')\, q_i(m', t)\, \frac{q(m-m', t)}{m-m'}\, dm'$$

$$- q_i \int_0^\infty \beta(m, m')\, \frac{q(m', t)}{m'}\, dm'$$

$$+ H_i q - \frac{\partial}{\partial m}\left(mHq_i\right) + m_i S - Lq_i + R_i(q)$$

$$q_i\left(m, t = t^0\right) = q_i^0(m), \qquad 1 \le i \le n,$$

$$q_i(m = 0, t) = 0, \quad q_i(m = \infty, t) = 0\ .$$

Adjoint aerosol dynamic models are needed to solve inverse problems

$$\frac{\partial \lambda_i}{\partial t} = -\int_0^\infty \beta(m,m')(m')^{-1}\left[\lambda_i(m+m',t)-\lambda_i(m,t)\right]q(m',t)\,dm' + L\lambda_i \qquad t_+^{k-1} \le t \le t_-^k$$

Continuous adjoint equation

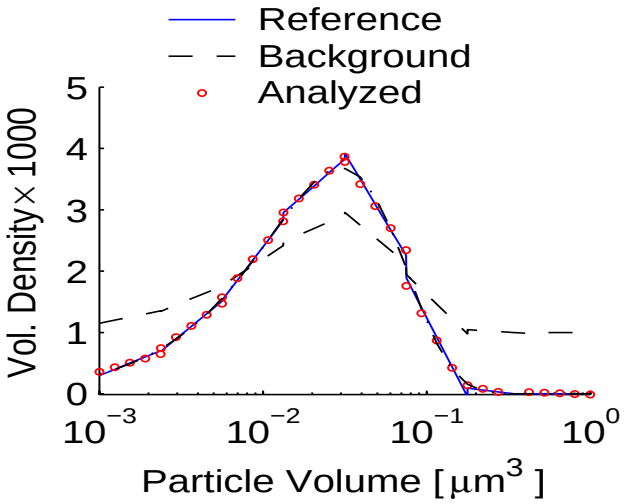
$$-\int_0^\infty \beta(m',m)\,m^{-1}\sum_{j=1}^{n}\left[\lambda_j(m+m',t)-\lambda_j(m,t)\right]q_j(m',t)\;dm' - \sum_{j=1}^{n} H_j\lambda_j - mH\frac{\partial \lambda_i}{\partial m}$$

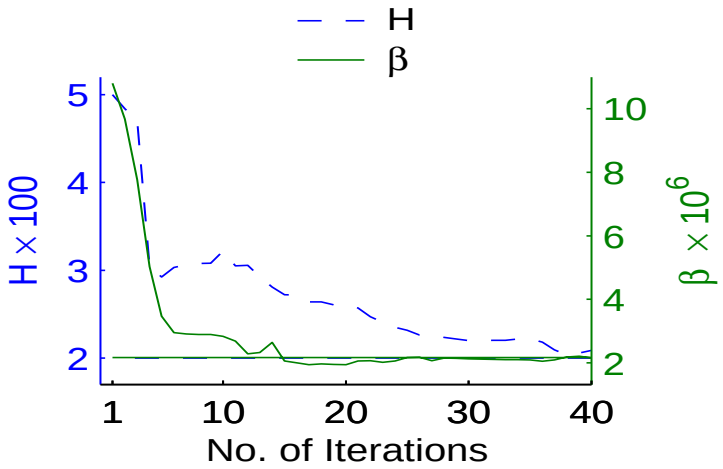
$$\lambda_i\left(m,t^N\right)=0, \quad \lambda_i(m,t_-^k)=\lambda_i(m,t_+^k)+h_{q_i}^T R_k^{-1}\left(y^k-h(q^k)\right)$$

$$\lambda_i\left(m,t^0\right)=\lambda_i\left(m,t_+^0\right)+p_{q_i}^T B^{-1}\left(p-p^B\right), \quad \lambda_i(0,t)=0\,.$$

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

[Sandu et. al., 2005; Henze et. al., 2004]



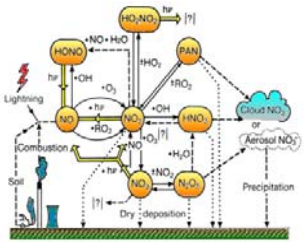


Discrete adjoint models for numerical advection: formulation and challenges

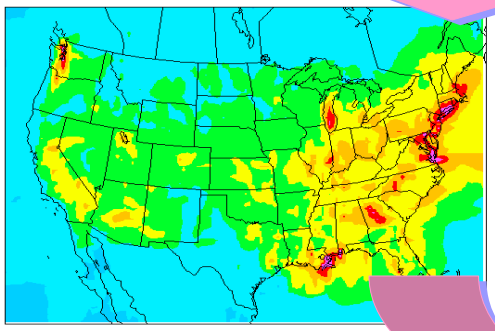
Transport
Meteorology

Optimal analysis state

Chemical kinetics

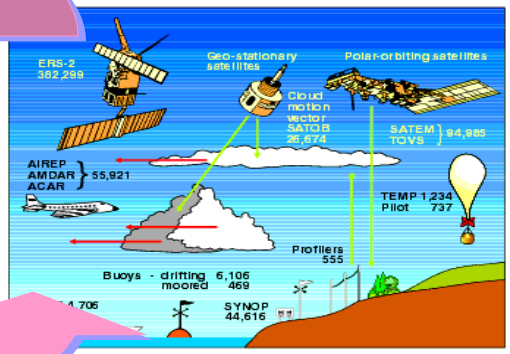


CTM

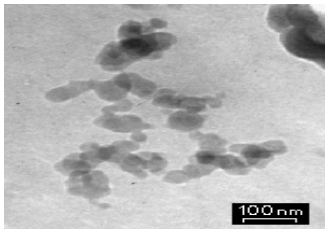


Data
Assimilation

Observations



Aerosols

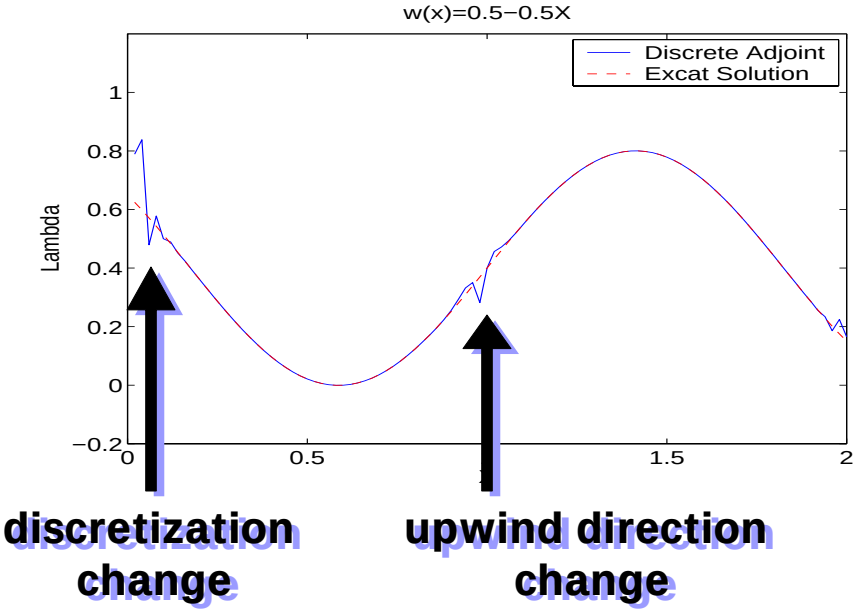


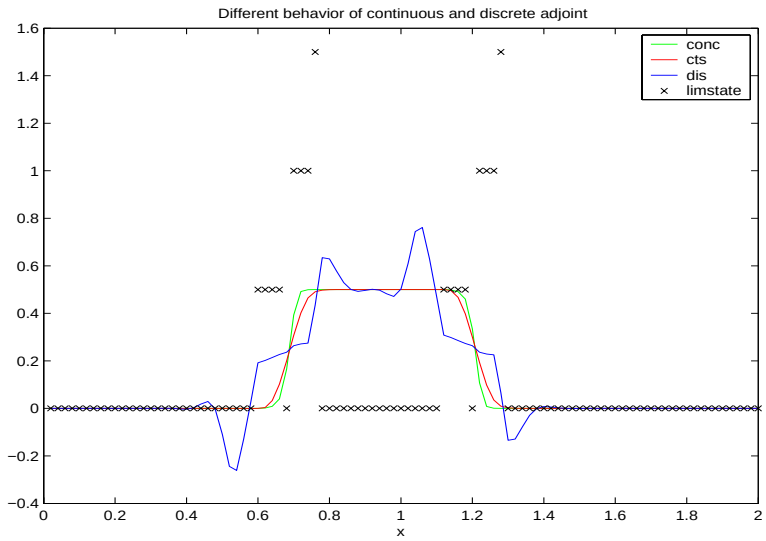
Targeted
Observ.

Emissions

Improved:
- forecasts
- science
- field experiment design
- models
- emission estimates

Discrete adjoints of advection numerical schemes can become pointwise inconsistent with the adjoint PDE





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

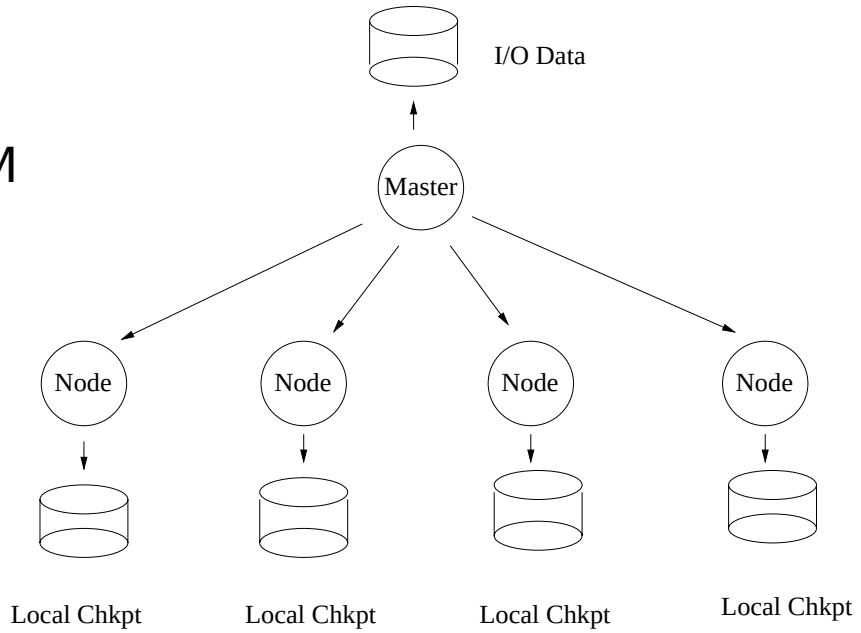
Chemistry: KPP
- Forward: sparse Rosenbrock, RK, LMM
- DDM sensitivity (Rosenbrock, LMM)
- Discrete adjoints: Rosenbrock
- Continuous adjoints: Rosenbrock, RK, LMM

Aerosols: 0-D, not yet 3-D

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

Parallelization: with PAQMSG

Distributed, 2-level checkpointing scheme



[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)