



SOX

**OSSE - based
Mission and Instrument
Concept Exploration**

**Meemong Lee, PhD
Richard Weidner, PhD
Kevin Bowman, PhD**

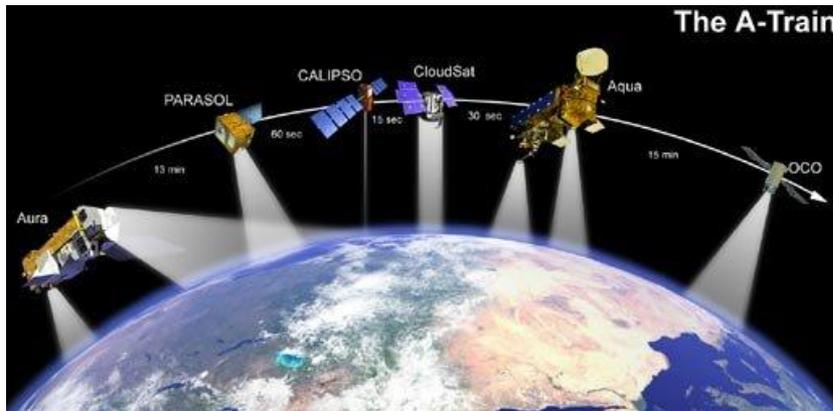
Jet Propulsion Laboratory
California Institute of Technology

SOX



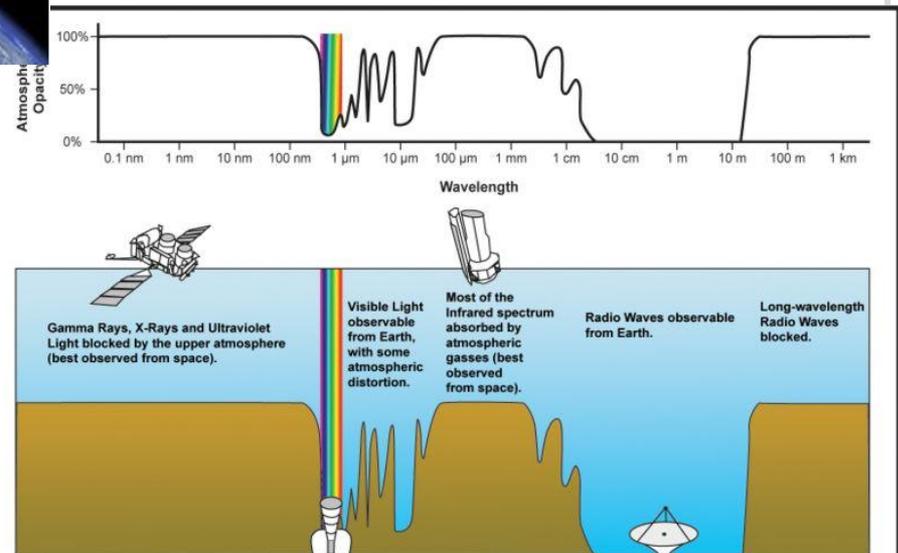
❖ Background

Atmospheric sounding



An **atmospheric sounding** is a measurement of vertical distribution of physical properties of the atmospheric column such as pressure, temperature, wind direction, liquid water content, ozone concentration, pollution, and other properties.

Spectral lines are highly atom-specific, and can be used to identify the chemical composition of any medium capable of letting light pass through it.





Measurement Physics

Satellite instruments (active and passive) simply measure the RADIANCE L that reaches the top of the atmosphere at given frequency ν . The measured radiance is related to geophysical atmospheric variables (T, Q, O_3) by the radiative transfer equation

$$L(\nu) = \int_0^\infty B(\nu, T(z)) \left[\frac{d\tau(\nu)}{dz} \right] dz + \begin{array}{l} \text{Surface} \\ \text{emission} \end{array} + \begin{array}{l} \text{Surface} \\ \text{reflection/} \\ \text{scattering} \end{array} + \begin{array}{l} \text{Cloud/rain} \\ \text{contribution} \end{array} + \dots$$

$$L(\nu) \approx \int_0^\infty B(\nu, T(z)) \left[\frac{dTR(\nu)}{dz} \right] dz$$

B : Planck function
 TR : transmittance
 $T(z)$: temperature
 Z : altitude



Atmospheric state modeling

GEOSChem

Emissions

Aircraft emissions
 Anthropogenic emissions
 Biofuel emissions
 Biogenic emissions
 Biomass burning emissions
 Lightning NOx emissions
 Ship emissions
 Soil NOx emissions
 Volcanic emissions

Aerosols

Sulfate aerosols
 Sea salt aerosols
 Mineral dust aerosols
 Carbonaceous aerosols
 Aerosol optical properties
 Aerosol microphysics

Deposition

Dry deposition
 Wet deposition

MET fields

GMAO GEOS-4
 GMAO GEOS-5
 GMAO MERRA

Chemistry

Nox-Ox-hydrocarbon-aerosol
 KPP chemical solver
 Linoz stratospheric ozone chemistry
 FAST-J photolysis mechanism
 Dicarbonyls simulation
 Bromine chemistry mechanism
 CMAQ interface

Dynamics

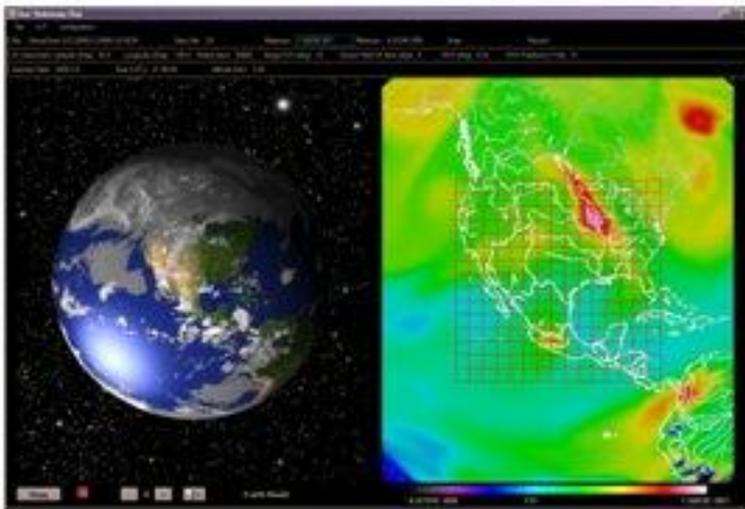
Advection (TPCORE).
 Boundary layer mixing
 Cloud convection,
 Dynamic tropopause



Emerging paradigm

Data assimilation
Model evaluation

Earth system models



Observing systems



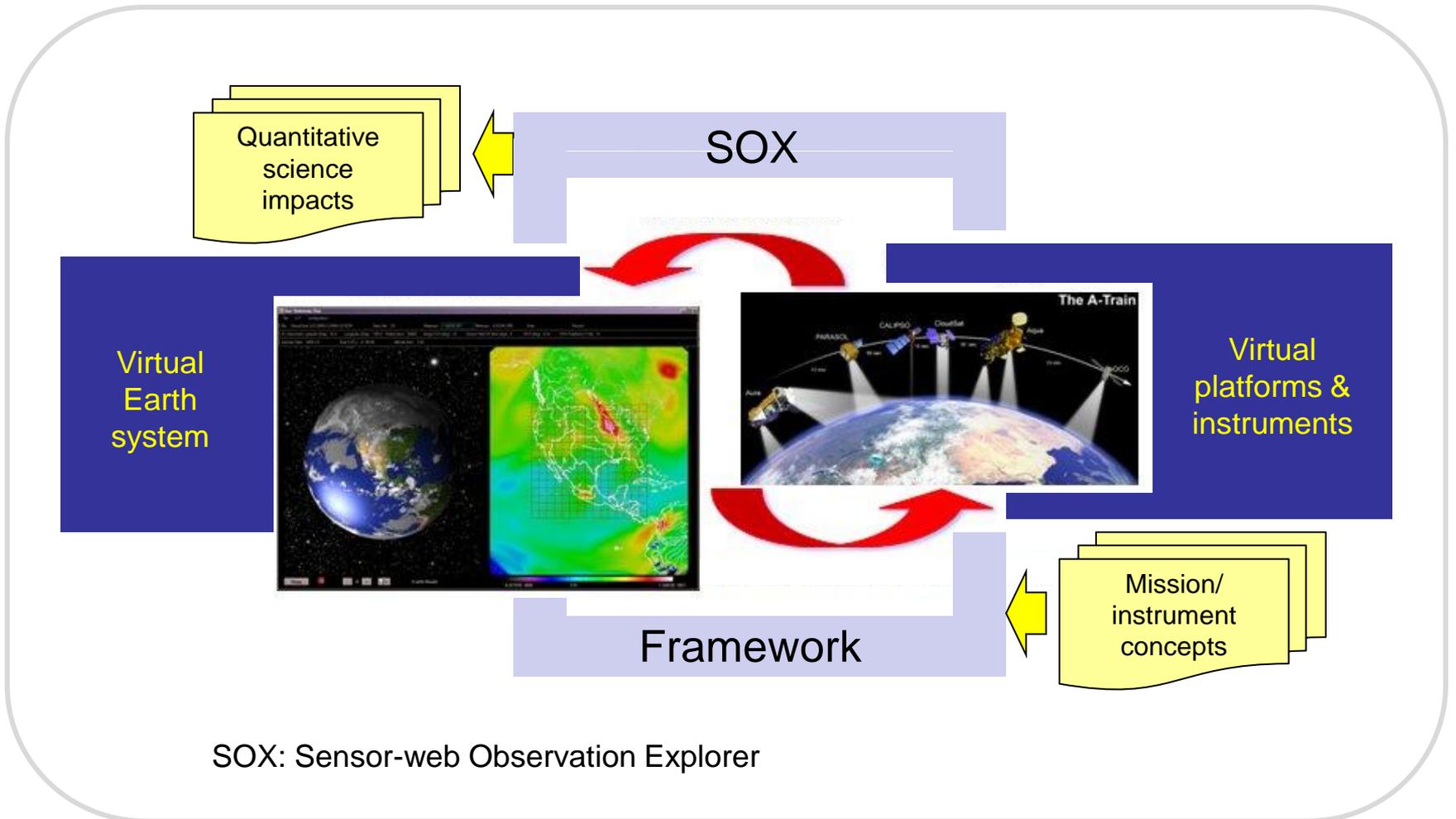
Mission planning
Data acquisition



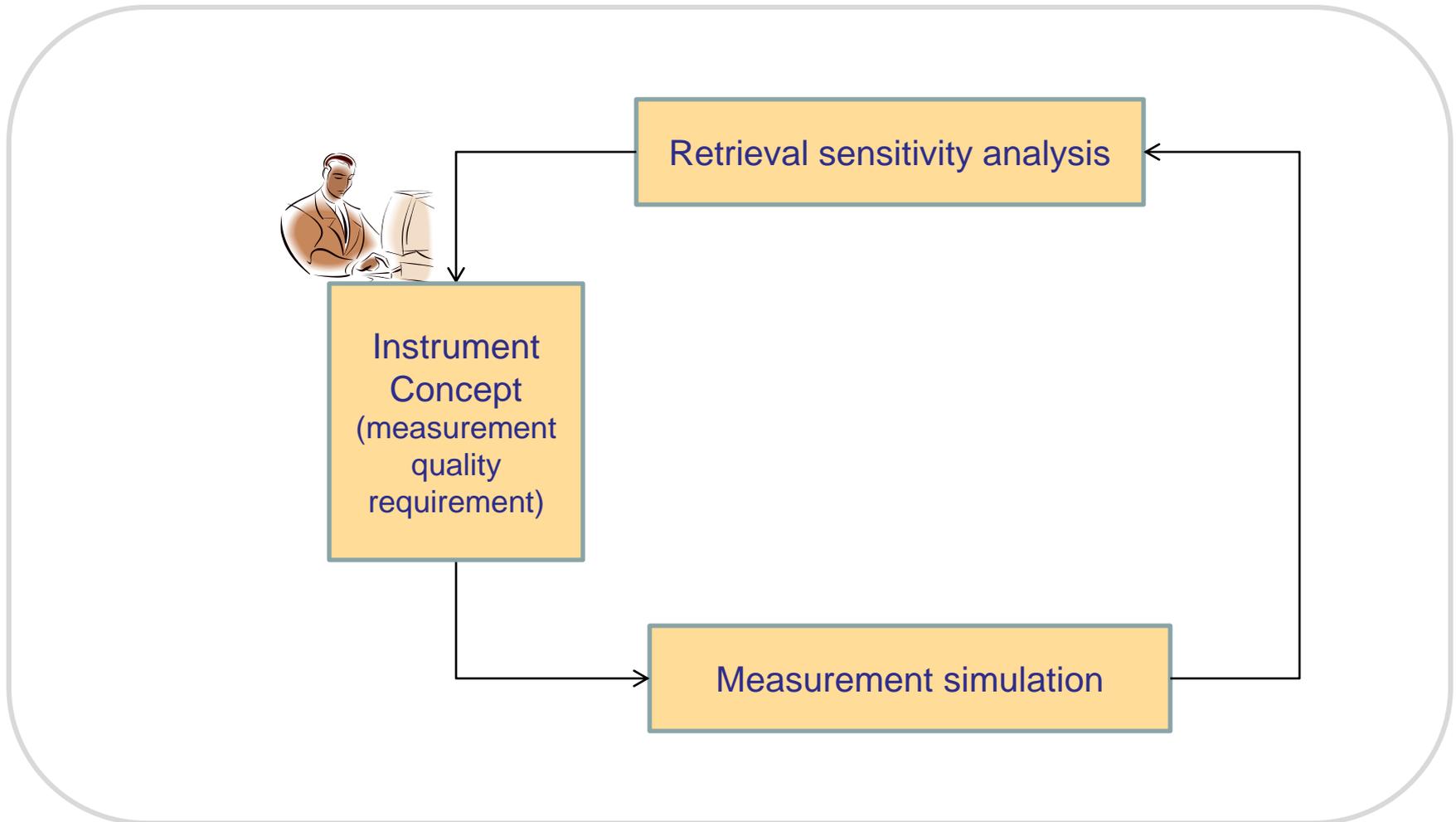
❖ SOX framework



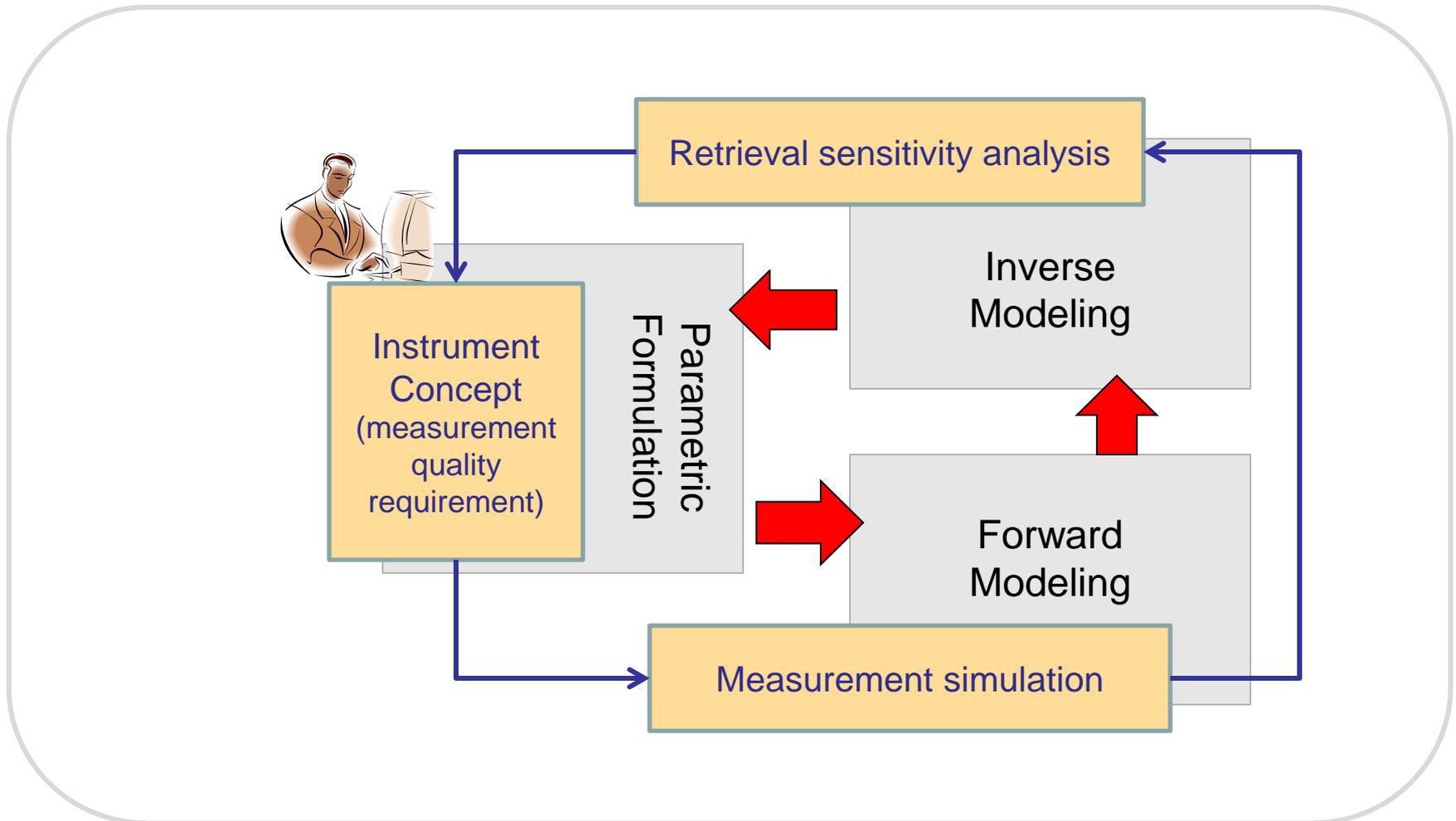
Observing system simulation experiment (OSSE)



Instrument concept exploration



Instrument concept exploration





Parametric Formulation

What to measure?

Spectral coverage (IR, UV, IR+UV)

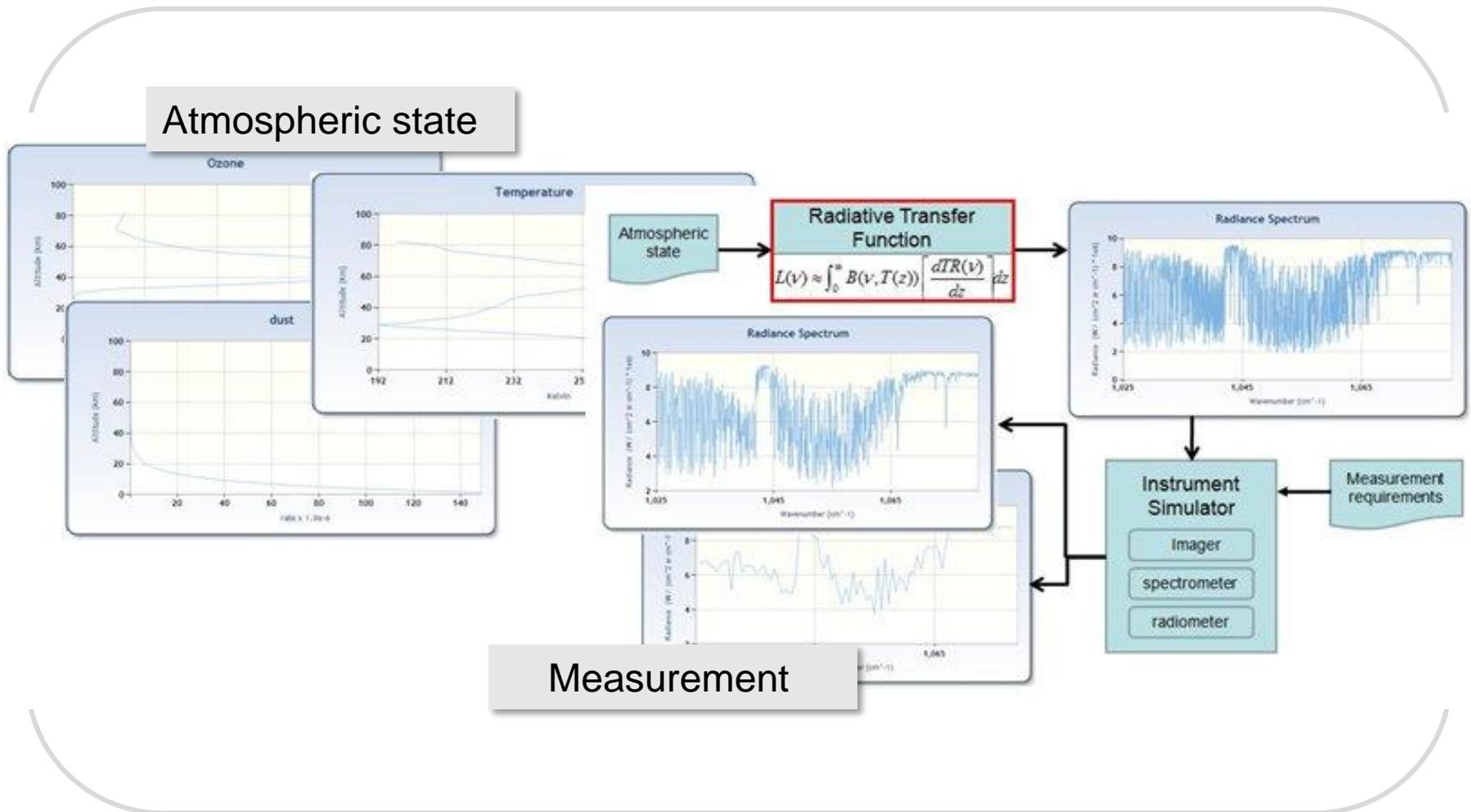
How precisely?

Spatial & spectral resolution

How accurately?

SNR/ NESR, channel linearity

Forward Modeling

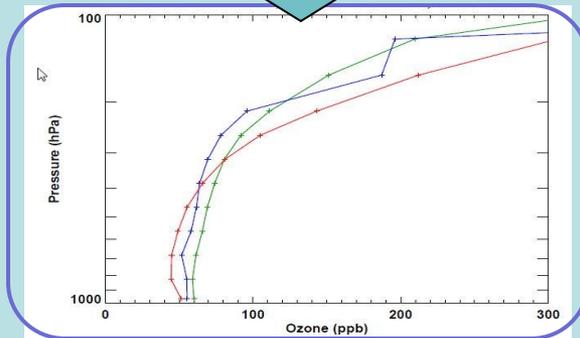
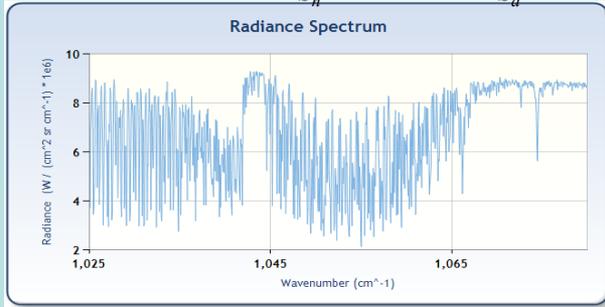




Inverse Modeling

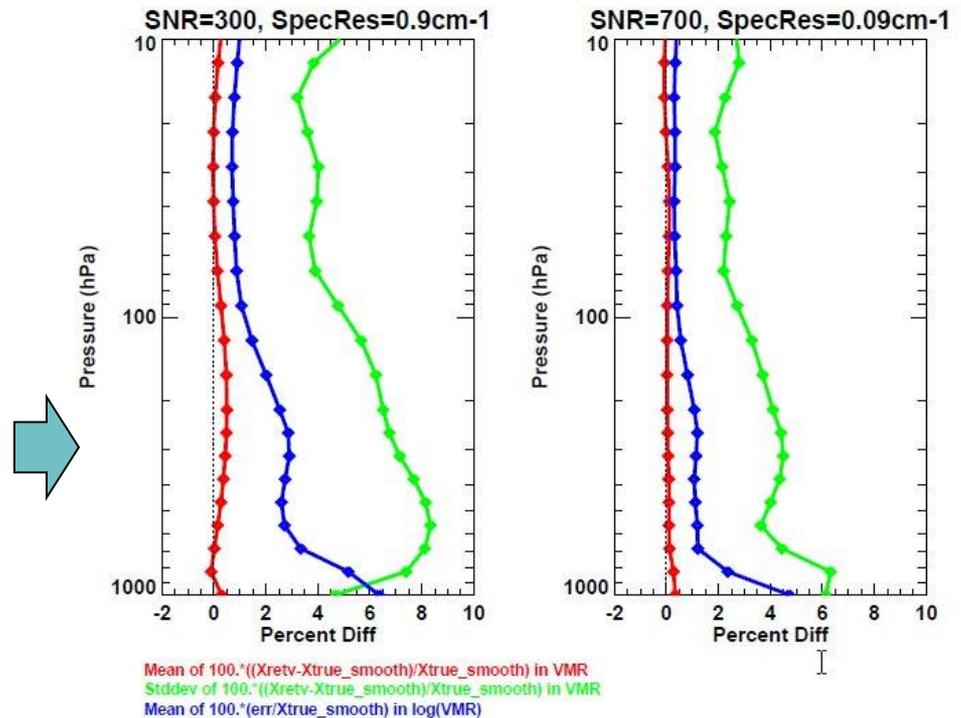
Retrieval analysis

$$\|y - F(x_a)\|_{S_n^{-1}}^2 + \|x - x_a\|_{S_a^{-1}}^2$$

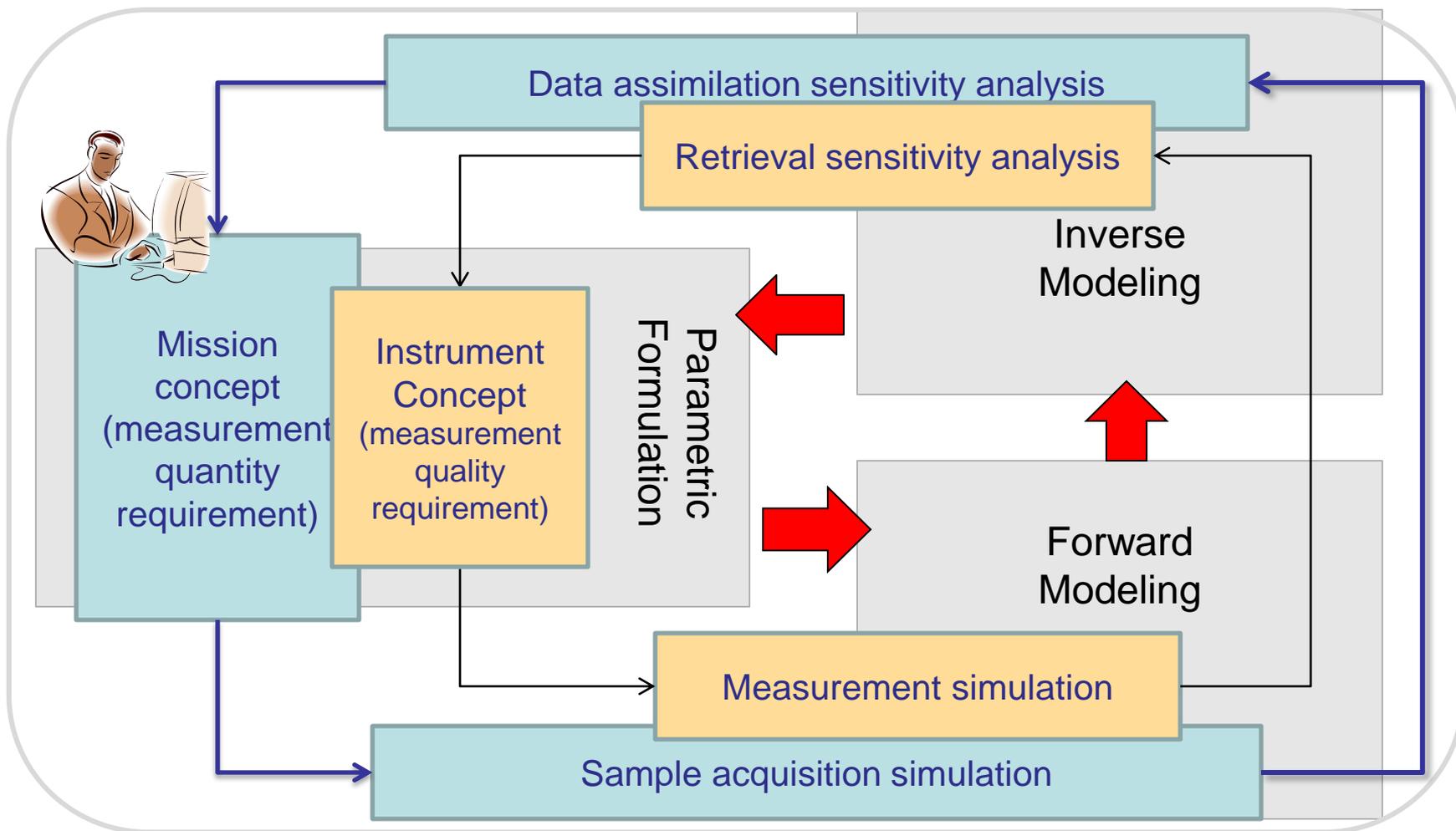


$$\hat{x} = x_a + A(x - x_a) + Gn$$

O₃ retrieval performance sensitivity



Mission concept exploration





Parametric Formulation

What to measure?

O₃, CO, CO₂

Where?

Land, Ocean, Coast, Globe, N. America

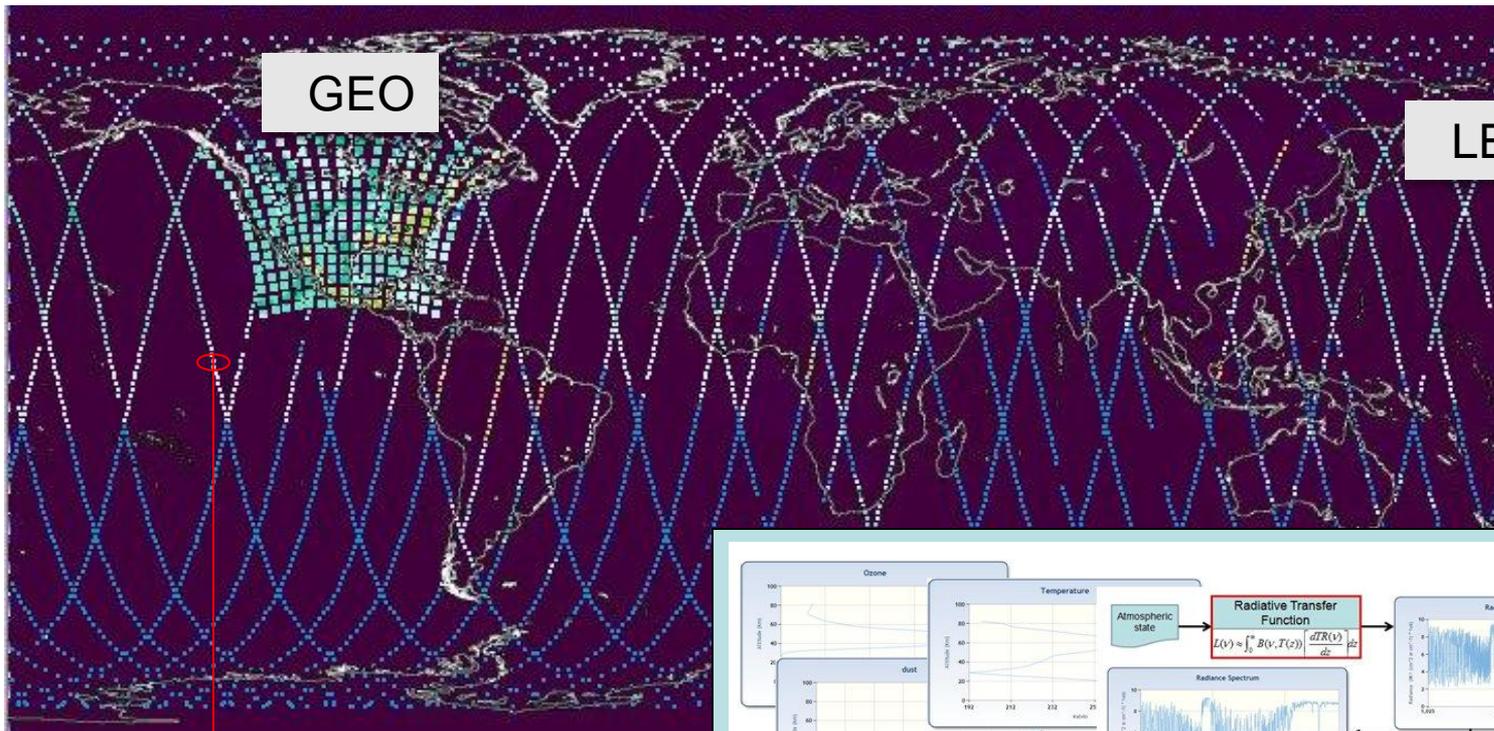
When?

Day, Night, anytime

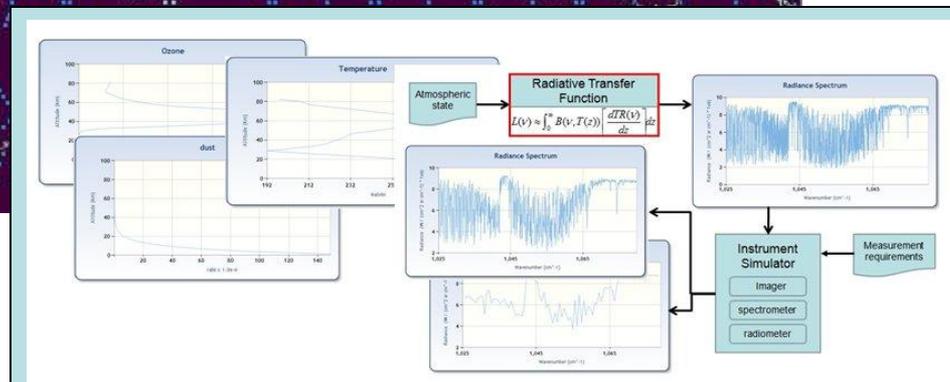
How often?

hourly, daily, monthly

Forward Modeling



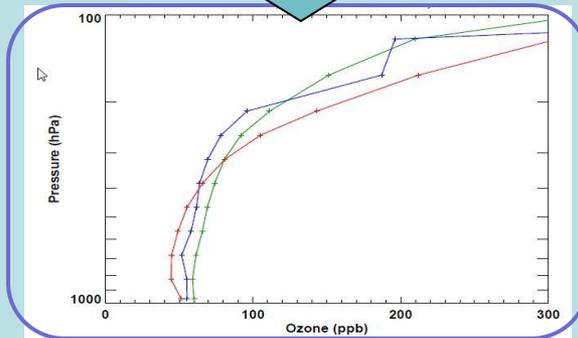
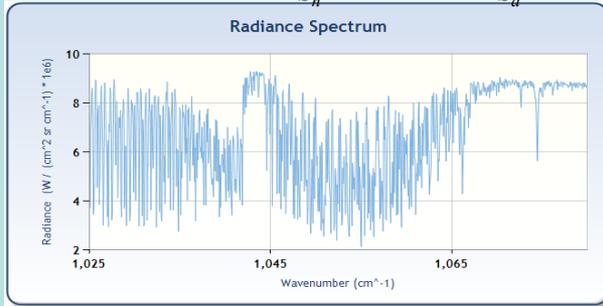
Per sample →



Inverse Modeling

Retrieval analysis

$$\|y - F(x_a)\|_{S_n^{-1}}^2 + \|x - x_a\|_{S_a^{-1}}^2$$

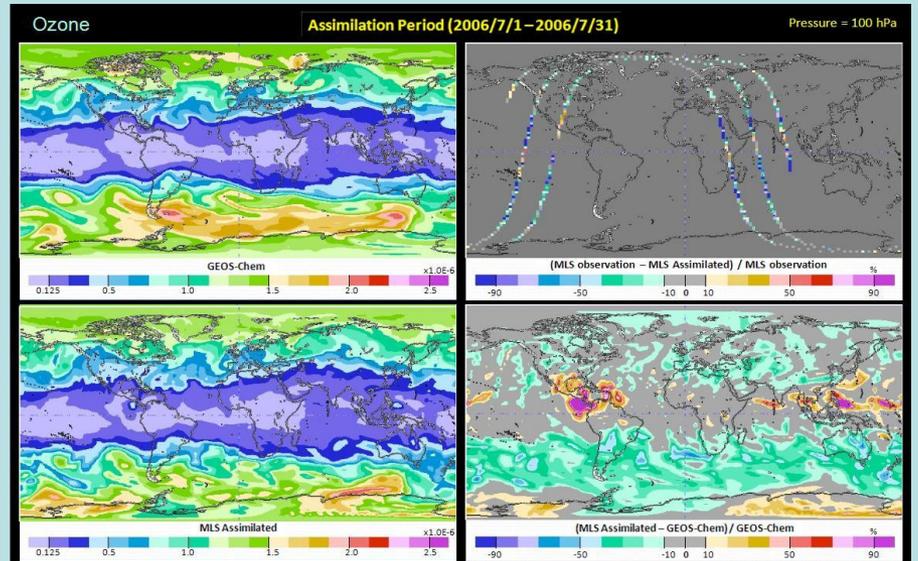


$$\hat{x} = x_a + A(x - x_a) + Gn$$

Assimilation analysis

$$H_i(\bullet) = x_a + A_i(\bullet - x_a)$$

$$\sum_i \|\hat{x}_i - H_i(x)\|_{(G_i S_i G_i^T)^{-1}}^2 + \|x_0 - x_B\|_{B^{-1}}^2$$

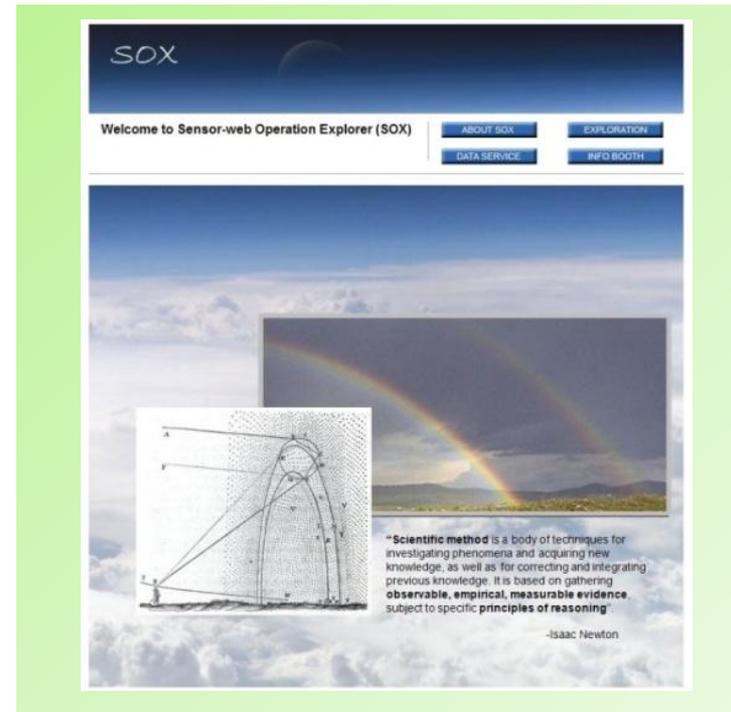




❖ OSSE PROCESS

Service-oriented process

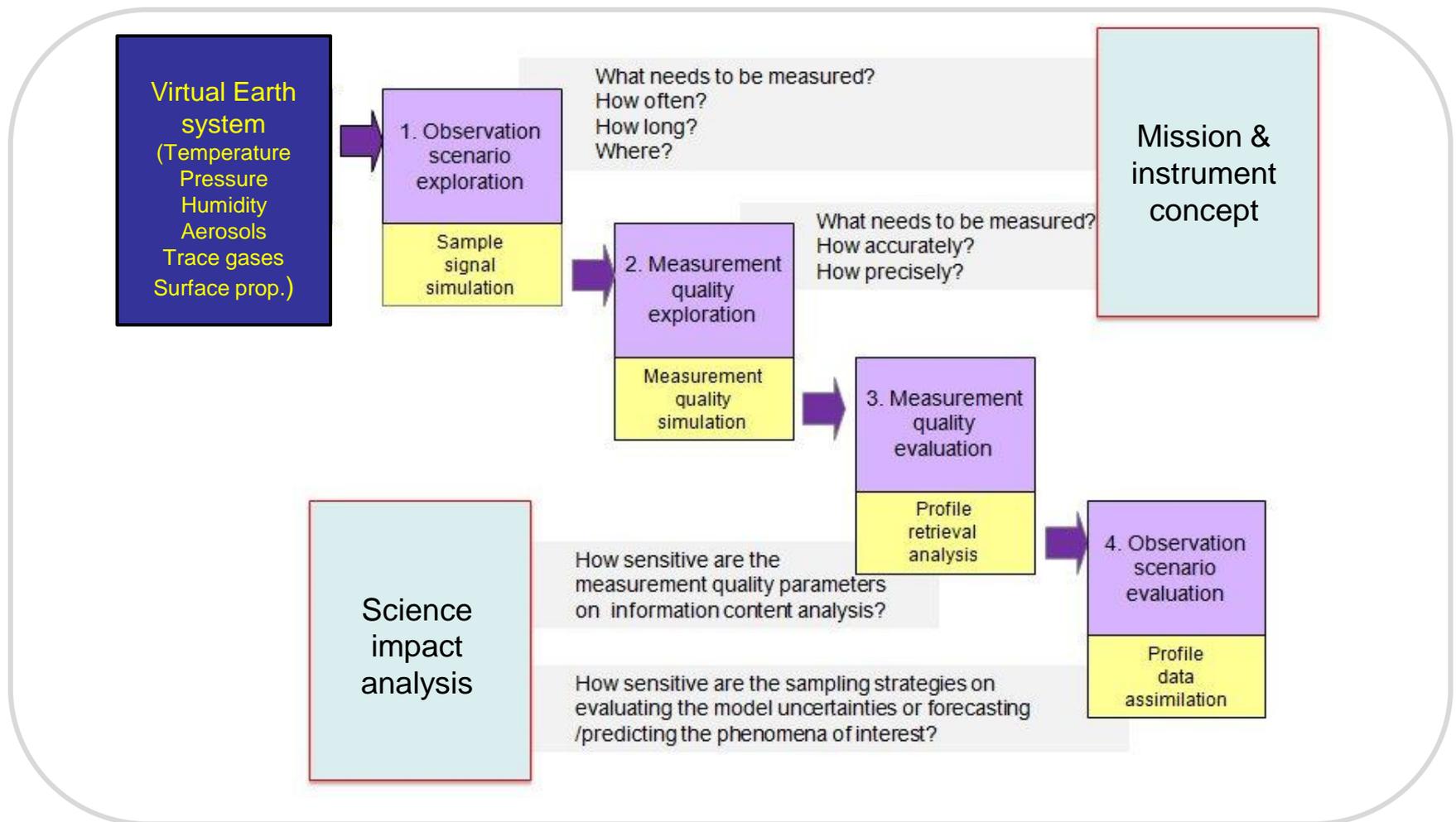
- ❖ **Linear**
designed as a series of steps
- ❖ **Chronological**
steps executed in time-sequence
- ❖ **Cumulative**
adding value at each step
- ❖ **Synchronous**
each step dependent and waiting upon the previous steps.



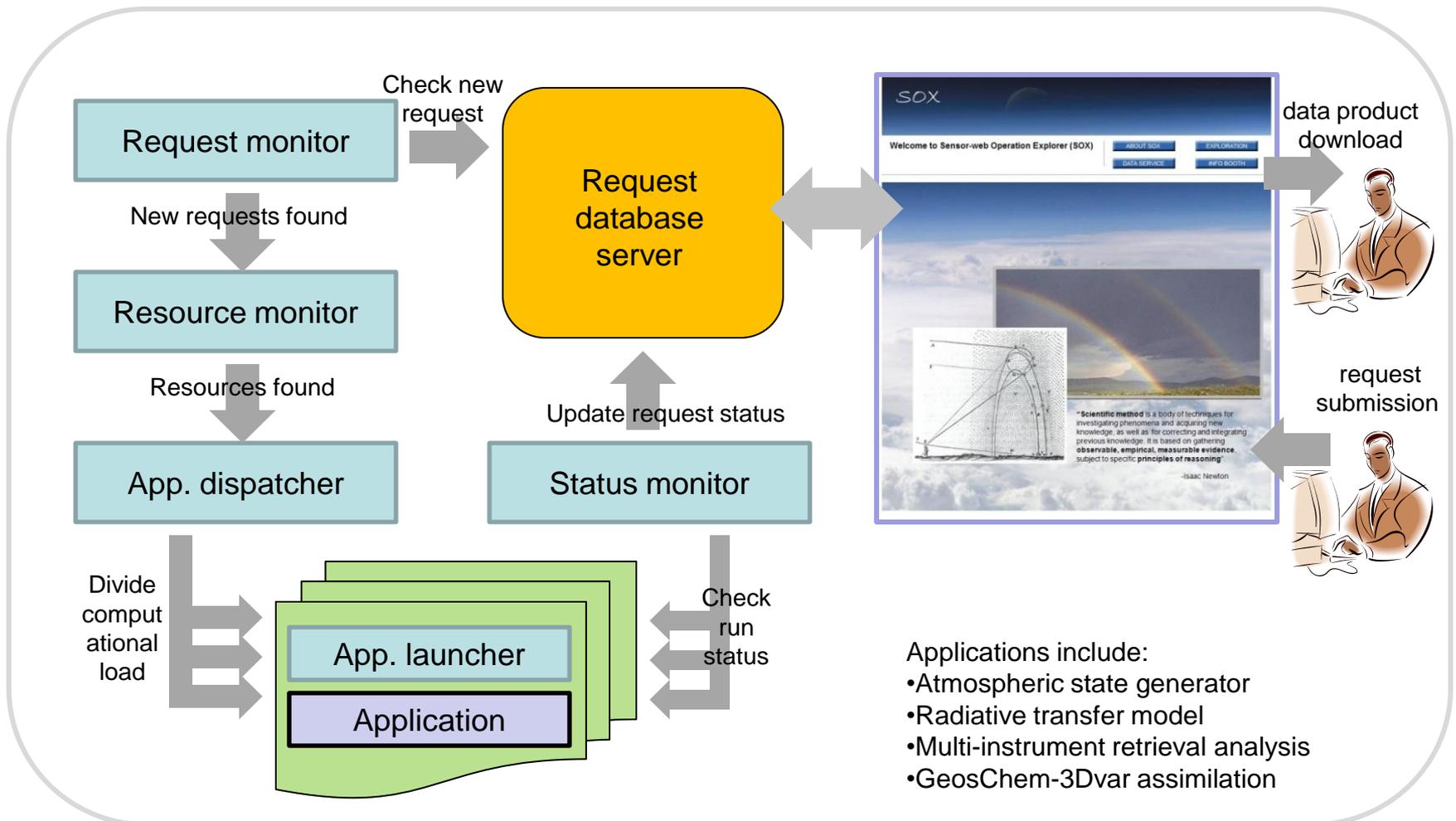
- Henry Ford



OSSE process flow



Process flow





❖ **Technology infusion**



GEOCAPE - OSSE

Annamarie Eldering (JPL)

Susan Kalaweik (JPL)

Ming Luo (JPL)

Meemong Lee (JPL)

Zheng Qu (Raytheon)



Technology Infusion

GEOCAPE mission study team led by Dr. Annmarie Eldering utilized the SOX framework for validating instrument concepts and exploring alternative observation scenarios.

Instrument concept →

	coverage (wn)	resolution (wn)	SNR
IR (6)	970-1080	0.6, 0.06	300,500,700
UV (3)	29000-37200	82	300,500,700
IR+UV (18)	All combinations of the above		

wn: wave number (1/wave length in cm)

Observation scenario →

Orbit : GEO stationary
 Target area: O₃ over North America
 Footprint coverage : 16 x 16 (~2deg x 2 deg)
 Sampling frequency : 3 hours
 No. of instruments: IR only, UV only, and IR+UV
 Experiment duration : July/1 – July/7

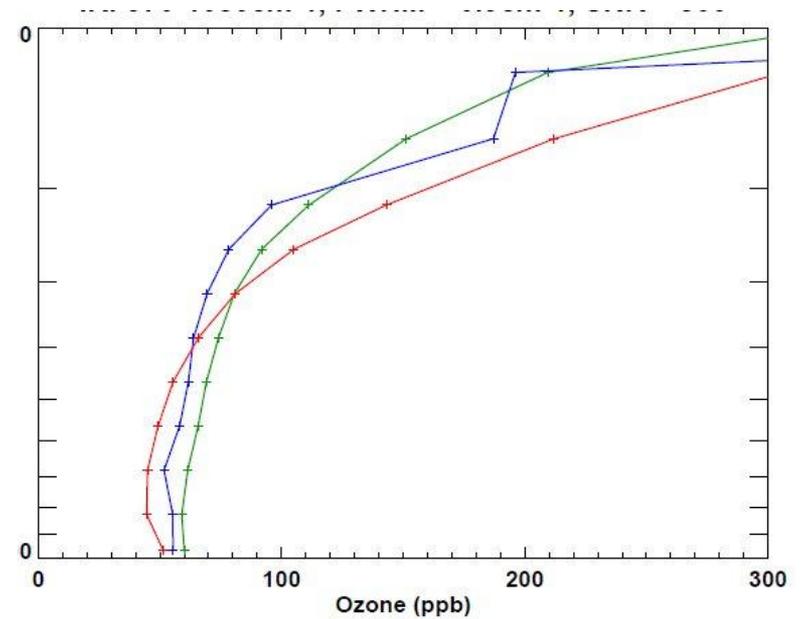
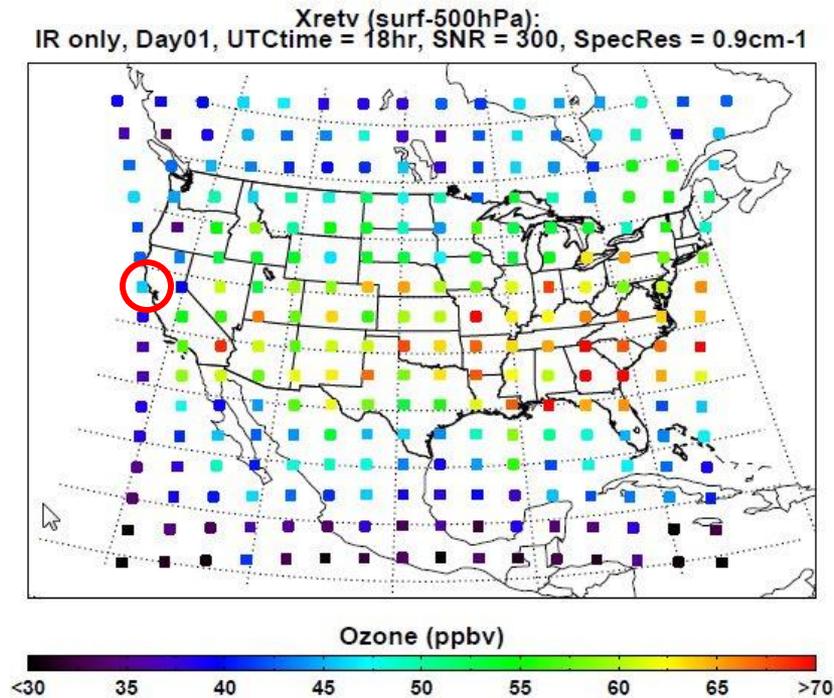
RTMs →

IR : LBLRTM (Line by line radiative transfer model)
 UV: LIDORT (linearized discrete ordinate radiative transfer model)

Daily samples: 16x16x8 = 2048

Daily measurements: 2048*(6+3+18) = 55296

GEOCAPE-OSSE

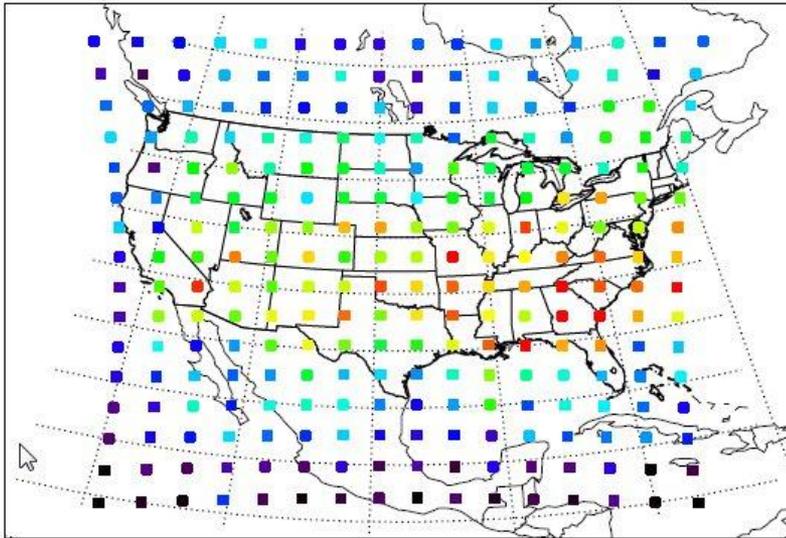
IR: 970-1080 cm⁻¹, FWHM = 0.9 cm⁻¹, SNR = 300

retrieved, a priori, truth



GEOCAPE-OSSE

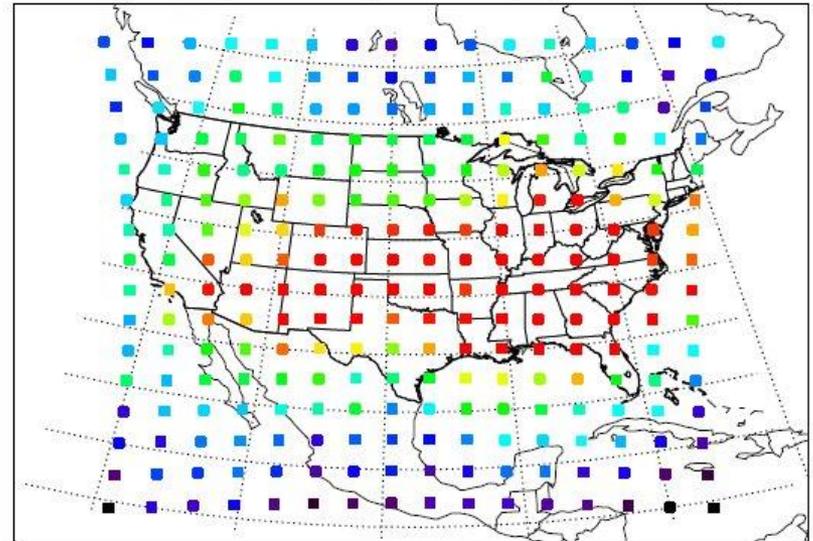
Xrtv (surf-500hPa):
IR only, Day01, UTCtime = 18hr, SNR = 300, SpecRes = 0.9cm⁻¹



Ozone (ppbv)

<30 35 40 45 50 55 60 65 >70

Xrtv (surf-500hPa):
IR only, Day01, UTC = 18hr, SNR = 700, SpecRes = 0.09cm⁻¹



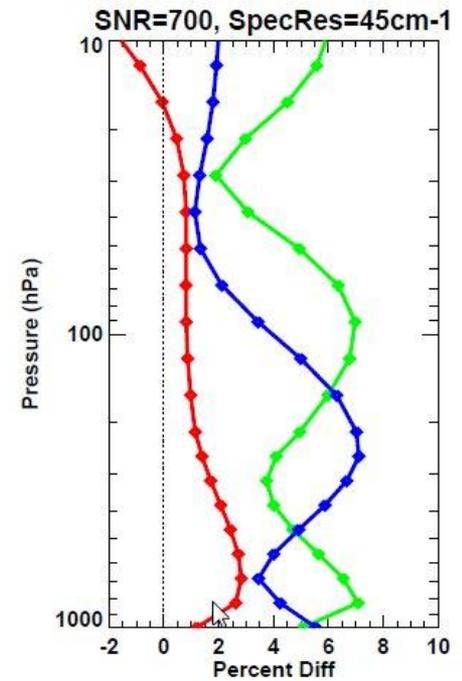
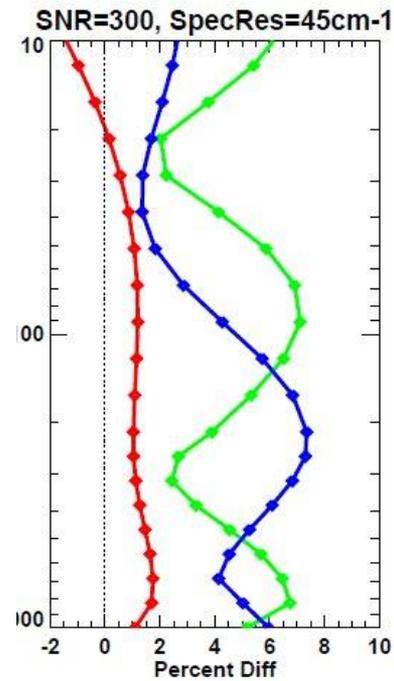
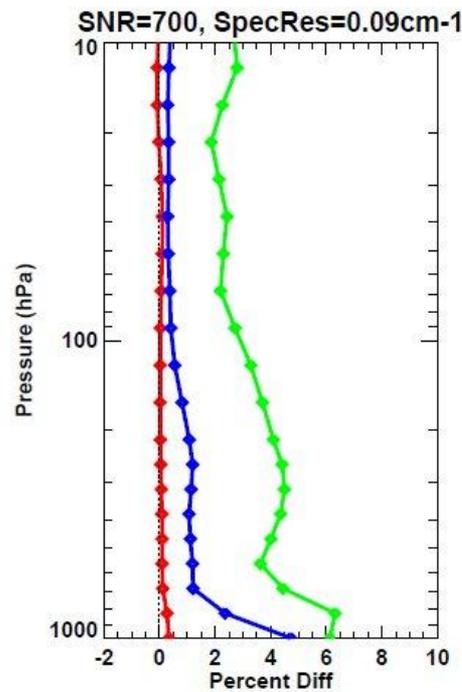
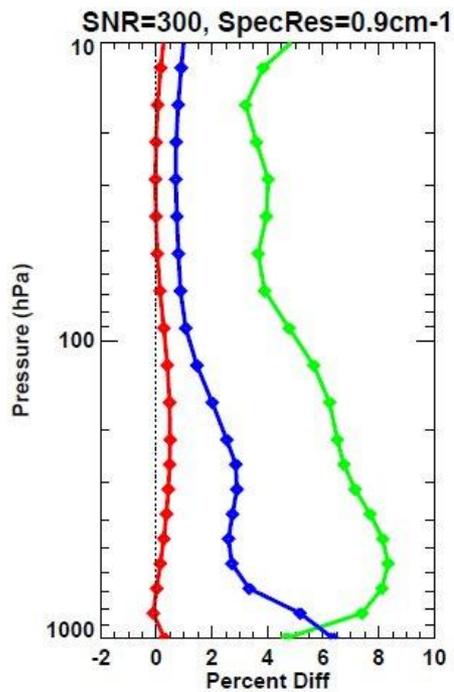
Ozone (ppbv)

<30 35 40 45 50 55 60 65 >70

GEOCAPE-OSSE

IR: 970-1080 cm⁻¹

UV: 29000-37200 cm⁻¹



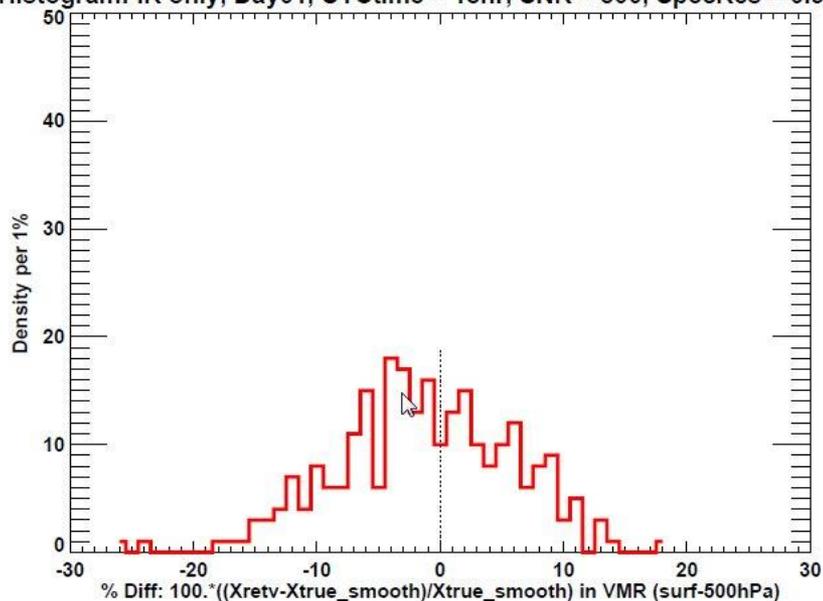
Mean of $100 \cdot ((X_{\text{retv}} - X_{\text{true_smooth}}) / X_{\text{true_smooth}})$ in VMR
 Stddev of $100 \cdot ((X_{\text{retv}} - X_{\text{true_smooth}}) / X_{\text{true_smooth}})$ in VMR
 Mean of $100 \cdot (\text{err} / X_{\text{true_smooth}})$ in log(VMR)

Mean of $100 \cdot ((X_{\text{retv}} - X_{\text{true_smooth}}) / X_{\text{true_smooth}})$ in VMR
 Stddev of $100 \cdot ((X_{\text{retv}} - X_{\text{true_smooth}}) / X_{\text{true_smooth}})$ in VMR
 Mean of $100 \cdot (\text{err} / X_{\text{true_smooth}})$ in log(VMR)

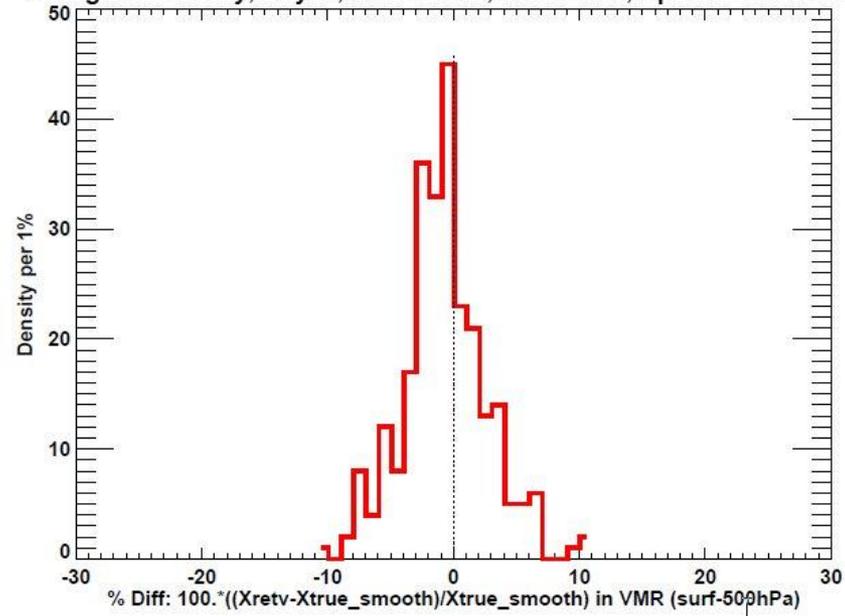


GEOCAPE-OSSE

Histogram: IR only, Day01, UTCtime = 18hr, SNR = 300, SpecRes = 0.9cm-1



Histogram: IR only, Day01, UTC = 18hr, SNR = 700, SpecRes = 0.09cm-1





Technology Infusion

MLS – OSE/OSSE

Nathaniel Livesey (JPL)

Meemong Lee (JPL)

Michelle Santee (JPL)

Jessica Neu (JPL)

Kevin Bowman (JPL)



Technology Infusion

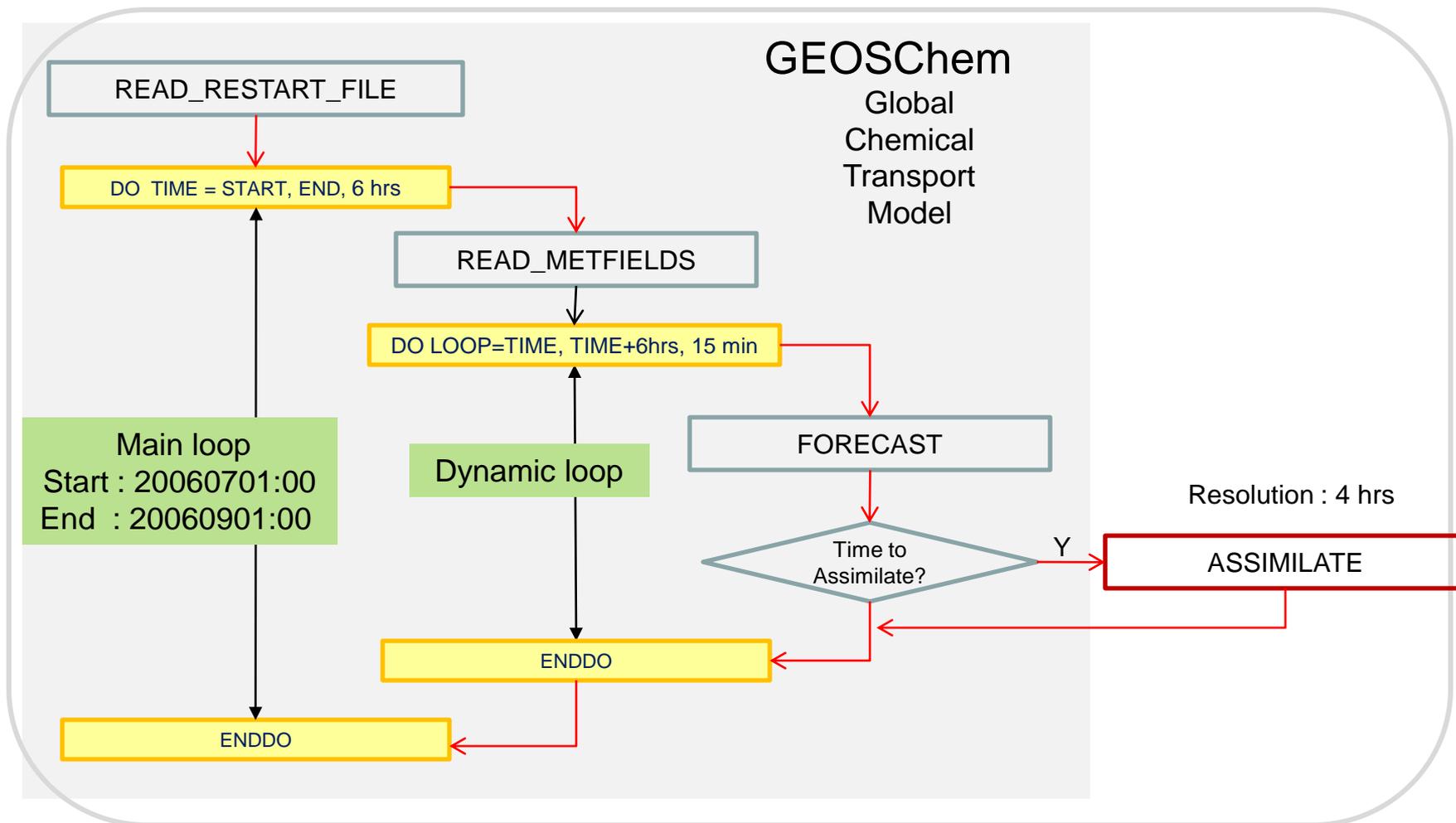
Microwave limb sounder (MLS) project led by Dr. Nathaniel Livesey utilized the SOX framework for assimilating MLS ozone observations (level 2 product) to evaluate the science impact of MLS observation in studying the process controlling the upper tropospheric composition.

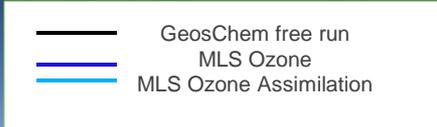
Product name	Useful range	Significant averaging needed ^g	Quality threshold ^f	Convergence threshold ^f	Differences needed ^f
BrO	10–3.2 hPa	yes	1.2	1.5	yes
CH ₃ CN ^e	Unclear	N/A	N/A	N/A	N/A
ClO	100–1.0 hPa	no	0.8	1.5	see text
CO	215–0.0046 hPa	no	0.2 ^f	1.8	no
GP ^{gh}	316–0.001 hPa	no	0.6	1.2	no
H ₂ O ^h	316–0.002 hPa	no	0.9	N/A	no
HCl	100–0.15 hPa	no	1.0	1.5	no
HCN	10–0.1 hPa	no	0.2	2.0	no
HNO ₃	215–3.2 hPa	no	0.4	1.8	no
HO ₂	22–0.032 hPa	yes	N/A	1.1	yes
HOCl	10–2.2 hPa	yes	1.4	1.5	no
IWC ^{hi}	261–68 hPa	no	N/A	N/A	no
IWP ^j	N/A	no	N/A	N/A	no
N ₂ O	100–1.0 hPa	no	0.5	1.55	no
O ₃ ^k	215–0.022 hPa	no	0.4 ^f	1.8	no
OH	32–0.0032 hPa	no	N/A	1.1	no
RH ^{hl}	316–0.002 hPa	no	0.9	N/A	no
SO ₂ ^{em}	215–10 hPa	no	0.4	1.8	no
Temperature ^{hn}	316–0.001 hPa	no	0.6	1.2	no



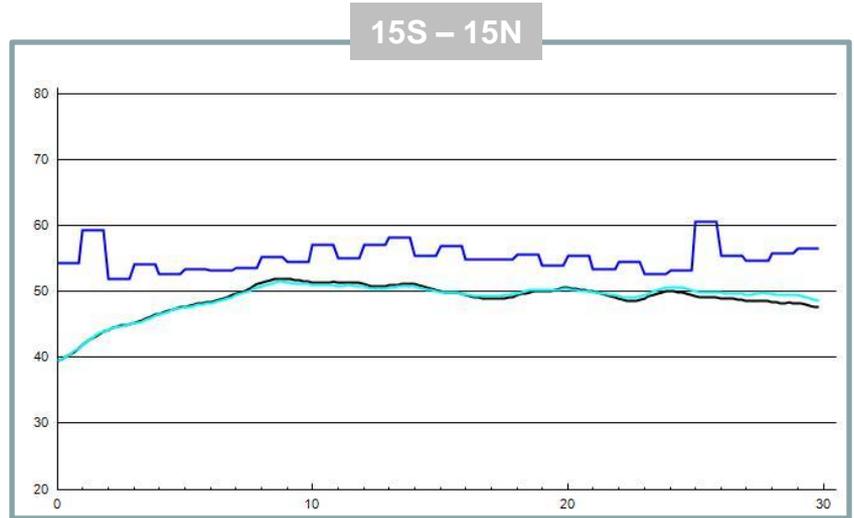
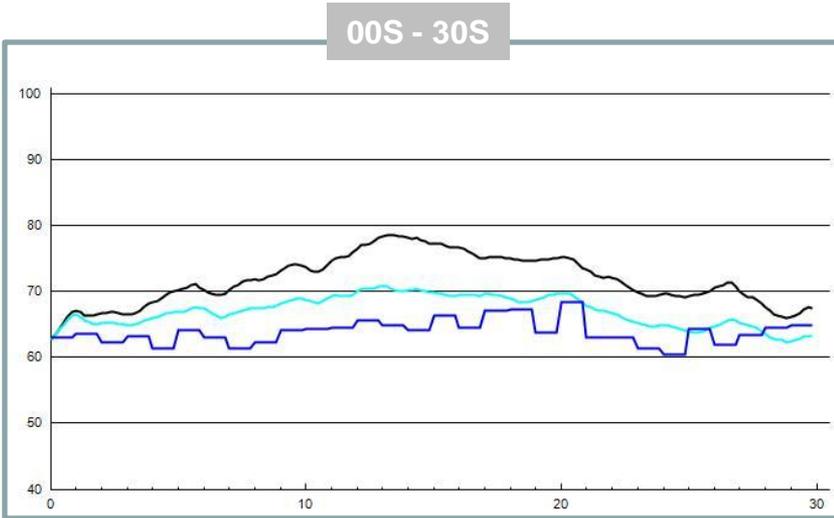
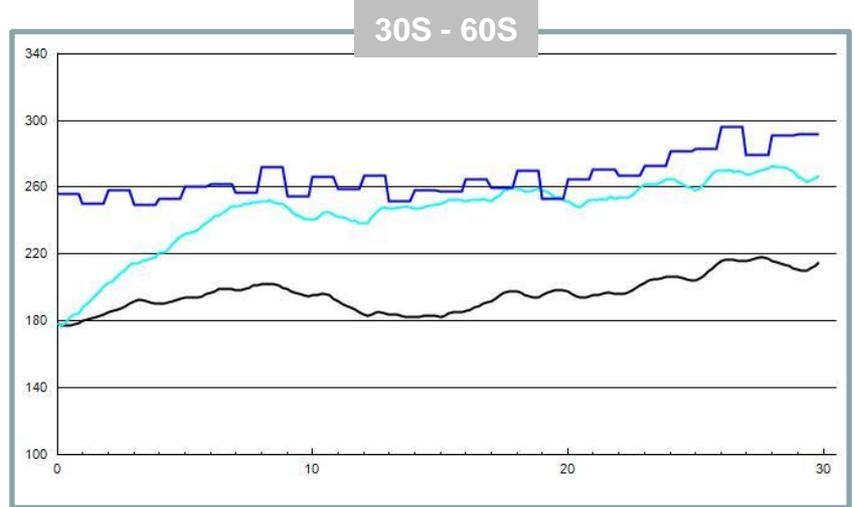
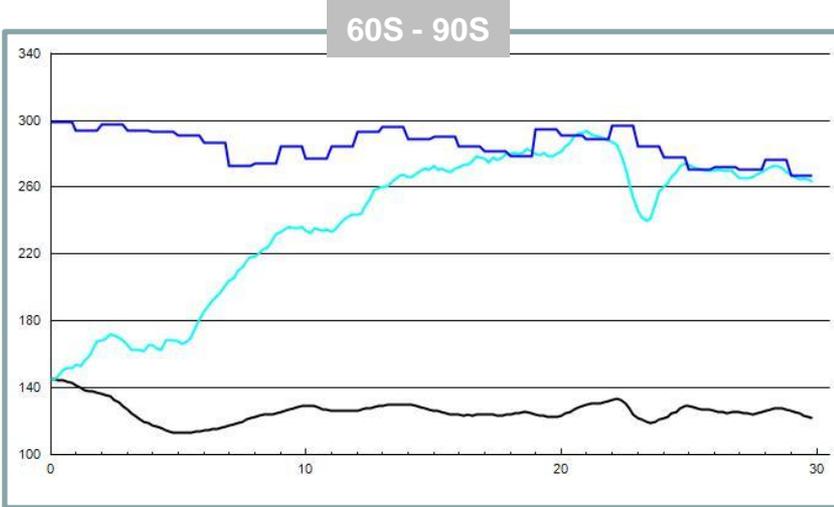
MLS-OSE/OSSE

GEOSChem

Global
Chemical
Transport
Model



P=200 hPa

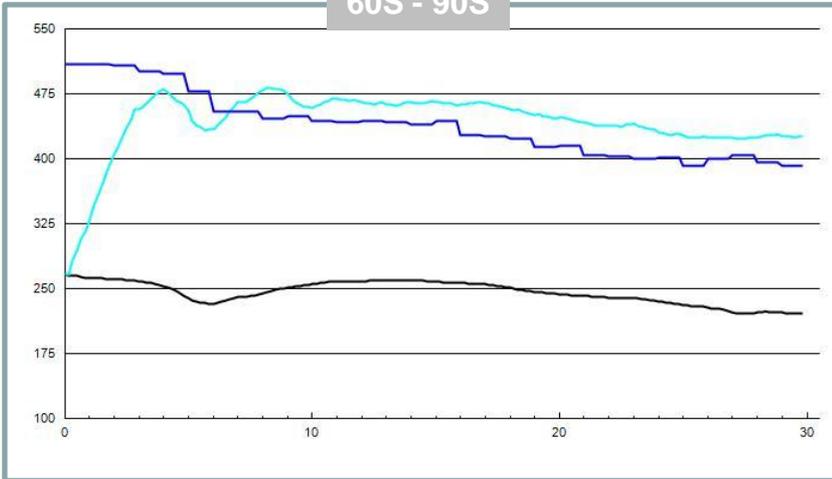




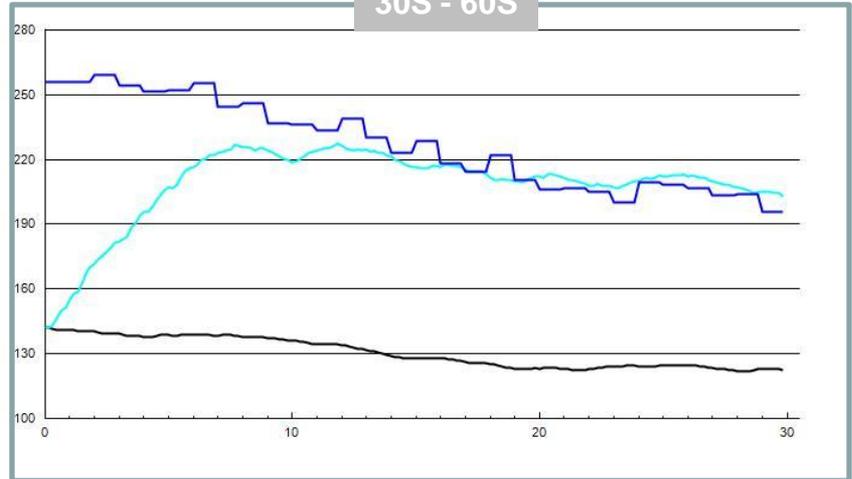
— GeosChem free run
— MLS Ozone
— MLS Ozone Assimilation

P=200 hPa

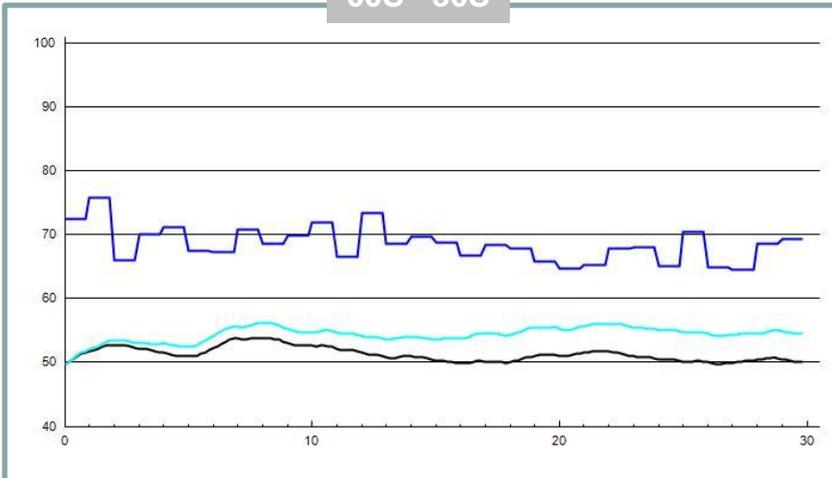
60S - 90S



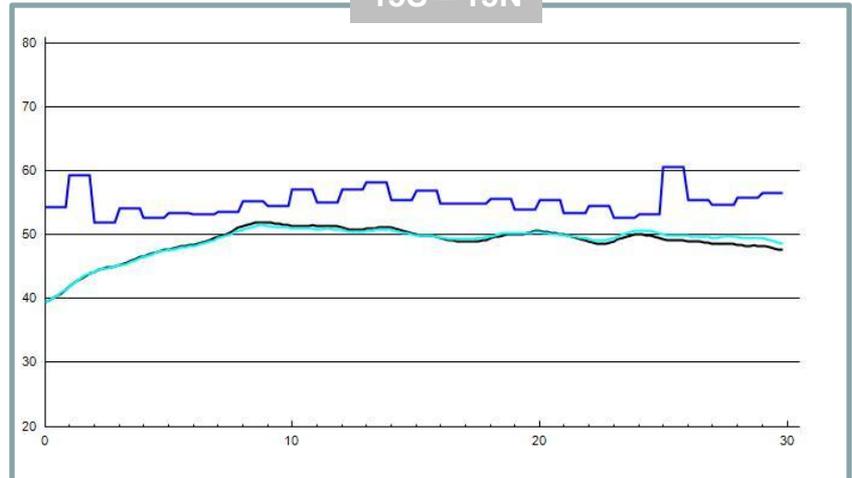
30S - 60S



00S - 30S



15S - 15N

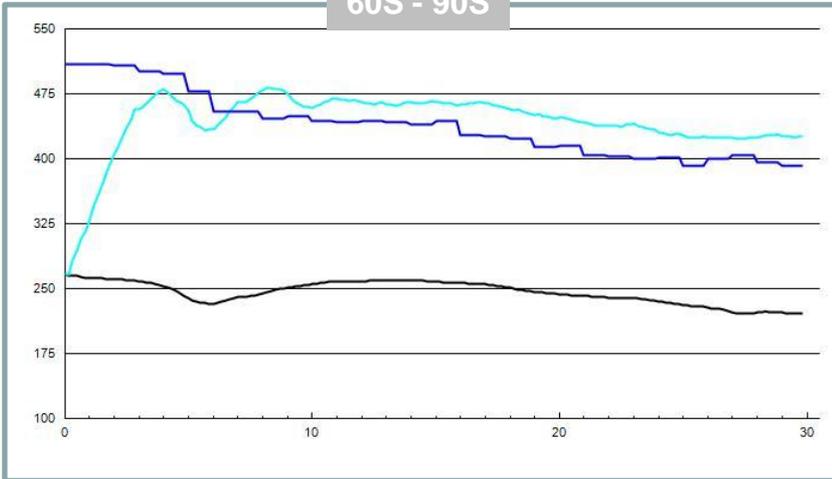




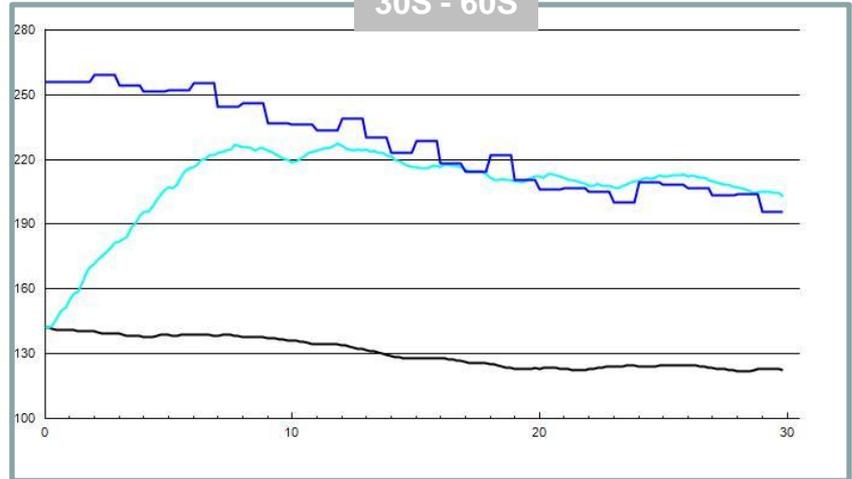
— GeosChem free run
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P=200 hPa

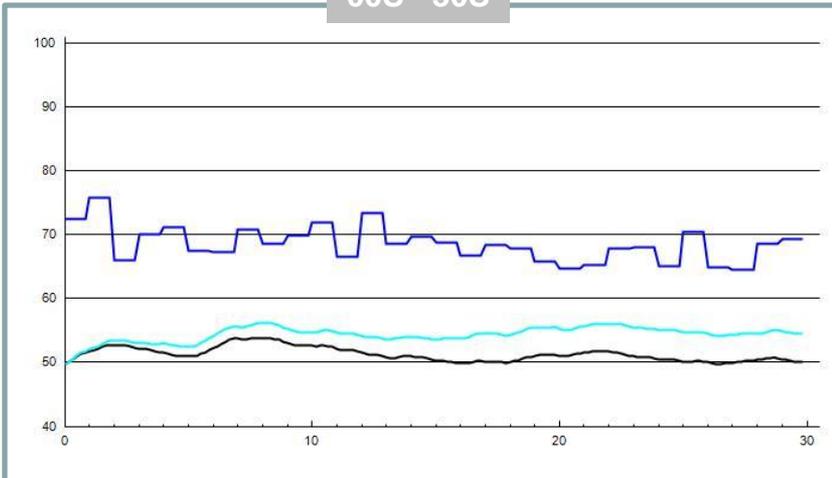
60S - 90S



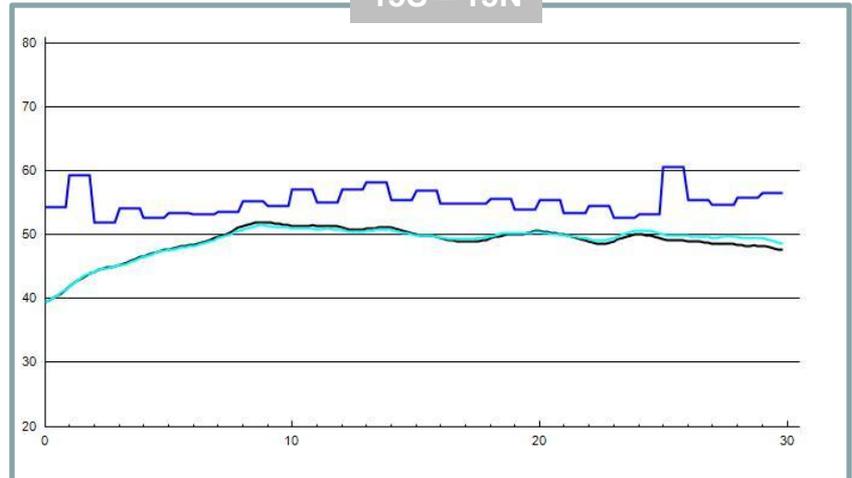
30S - 60S



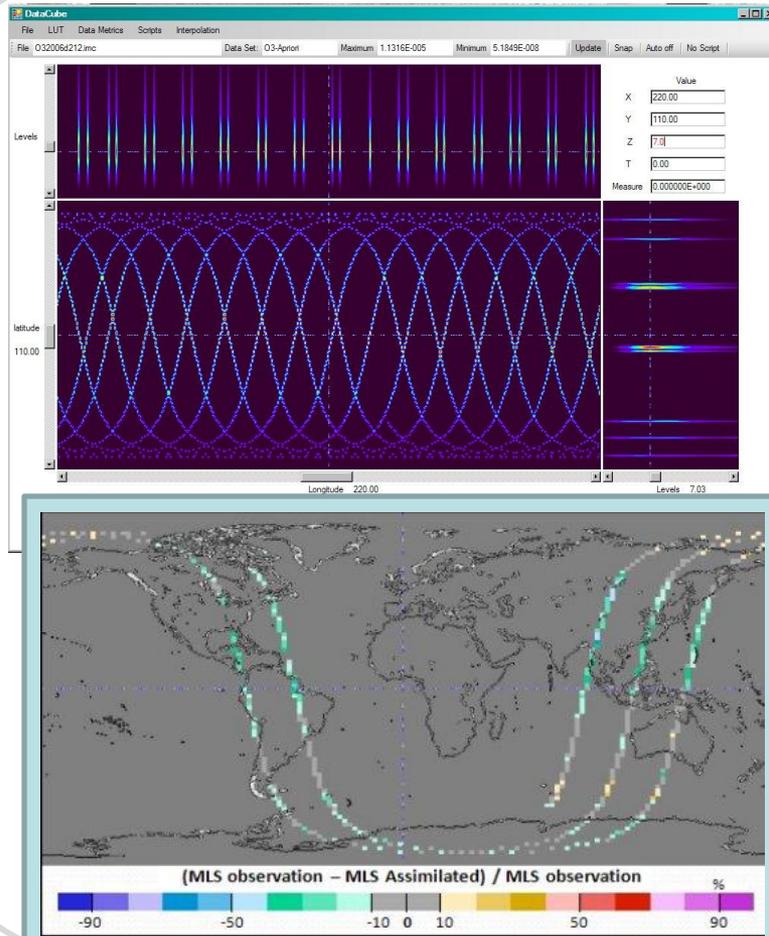
00S - 30S



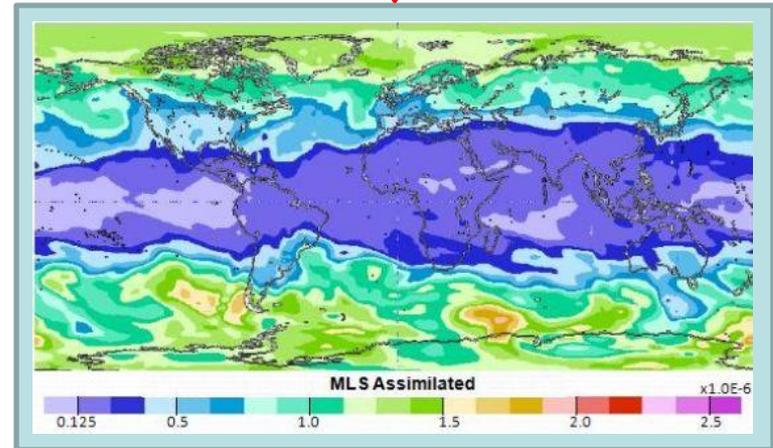
15S - 15N



MLS-OSE/OSSE

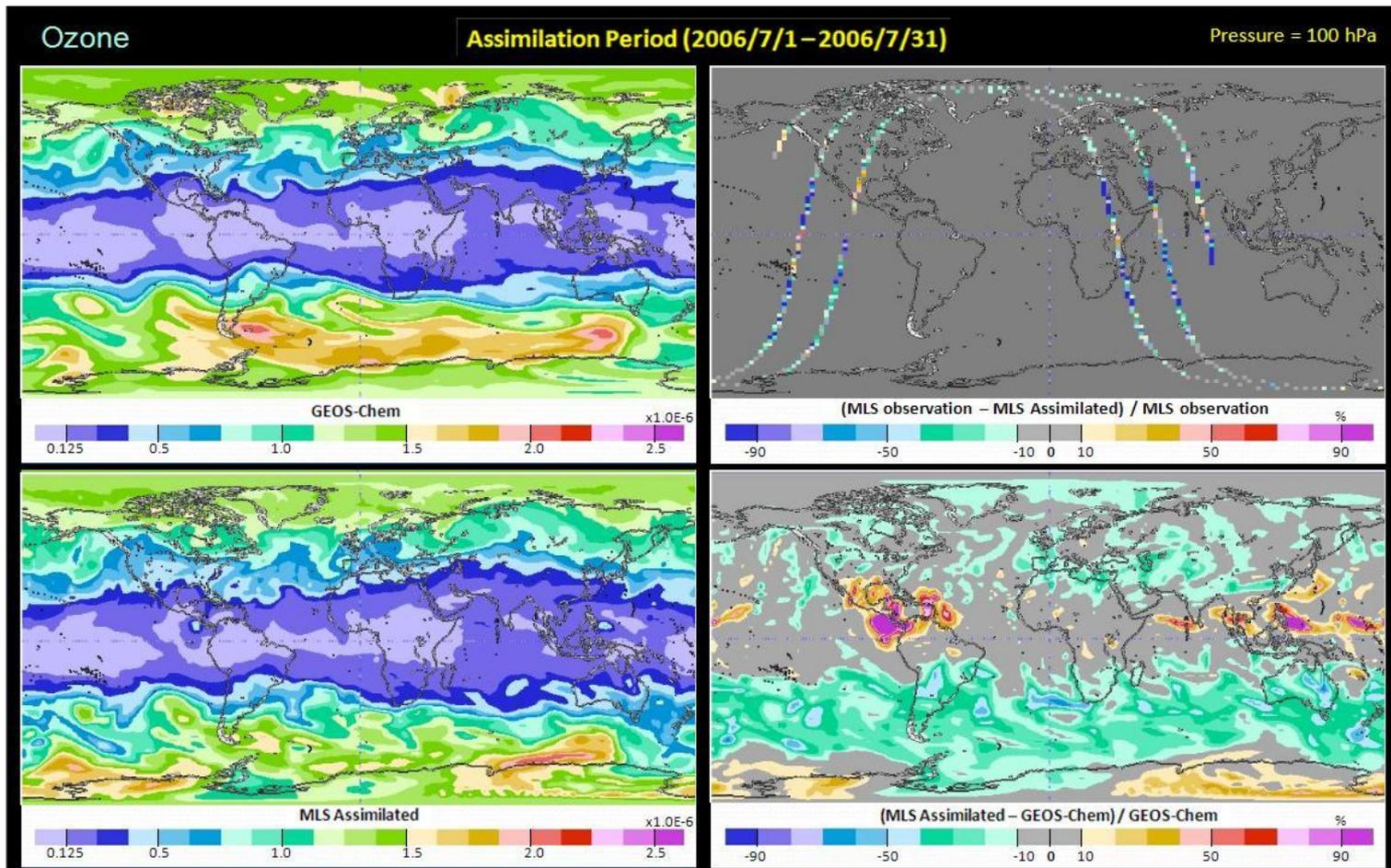


O3 observation
assimilation



Observation -
assimilated

MLS-OSE/OSSE





GHGIS - OSSE

Kevin Bowman (JPL)

Meemong Lee (JPL)

Richard Weidner (JPL)

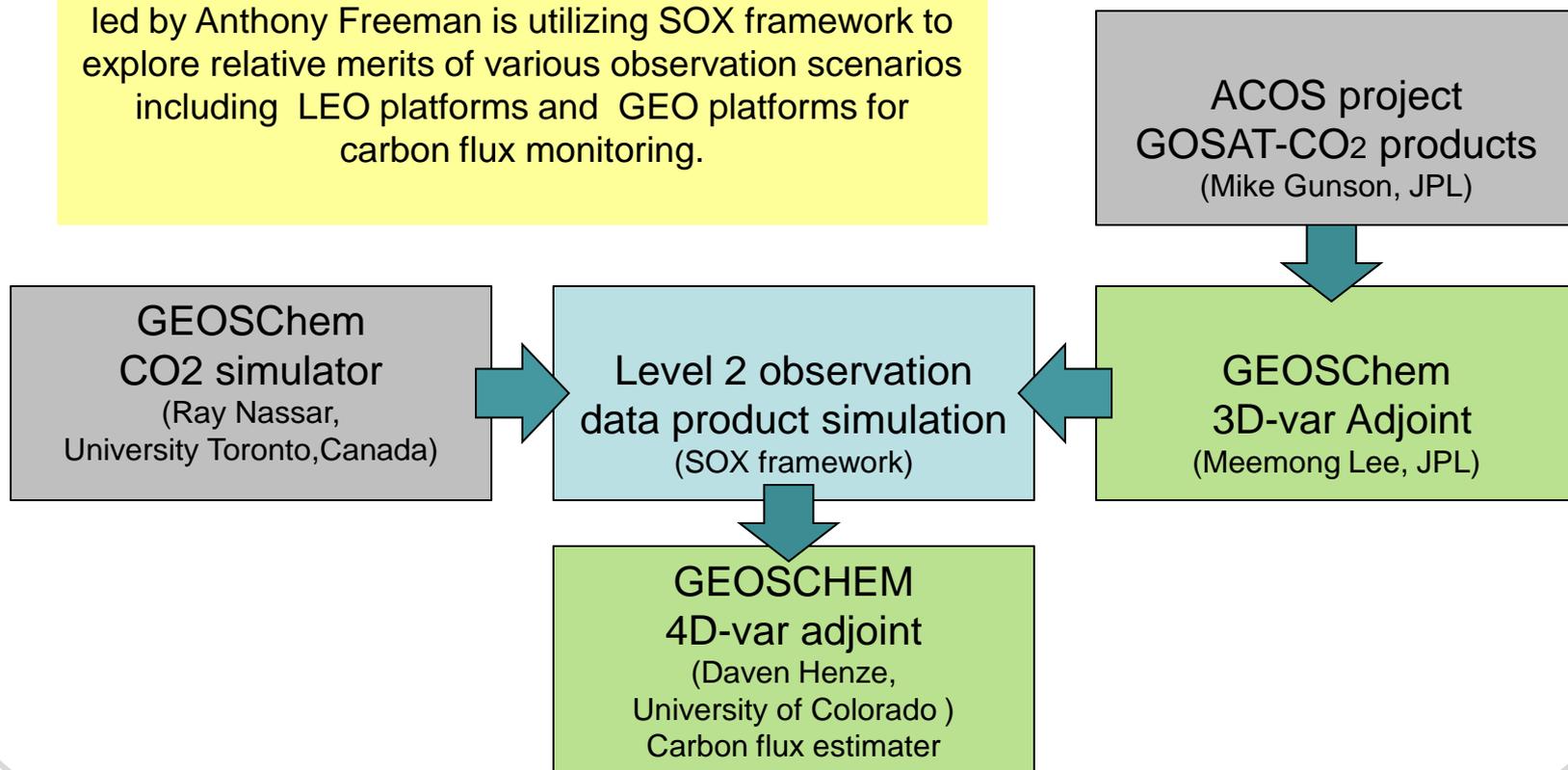
John Worden (JPL)

Anthony Freeman (JPL)



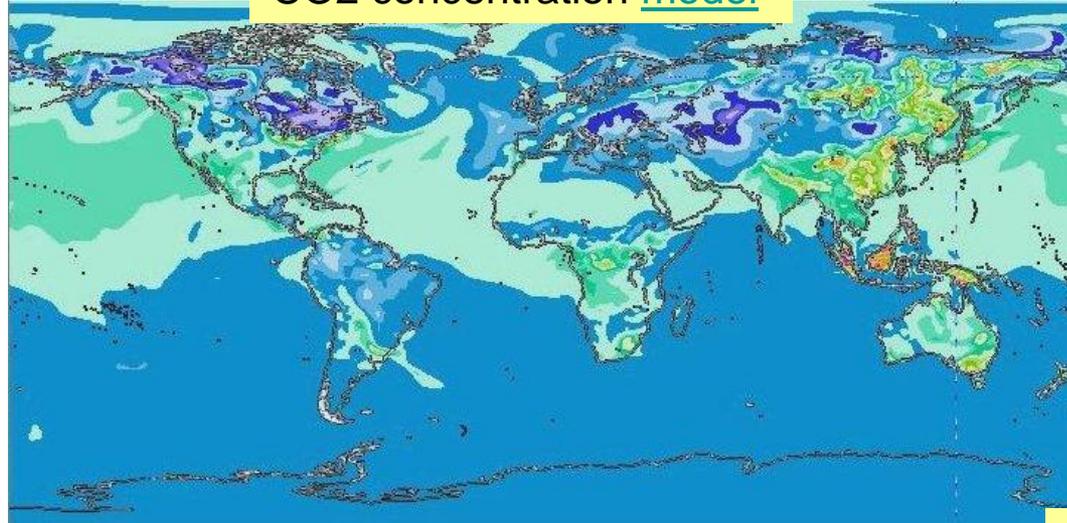
GHGIS-OSSE

Green house gas information system (GHGIS) project led by Anthony Freeman is utilizing SOX framework to explore relative merits of various observation scenarios including LEO platforms and GEO platforms for carbon flux monitoring.

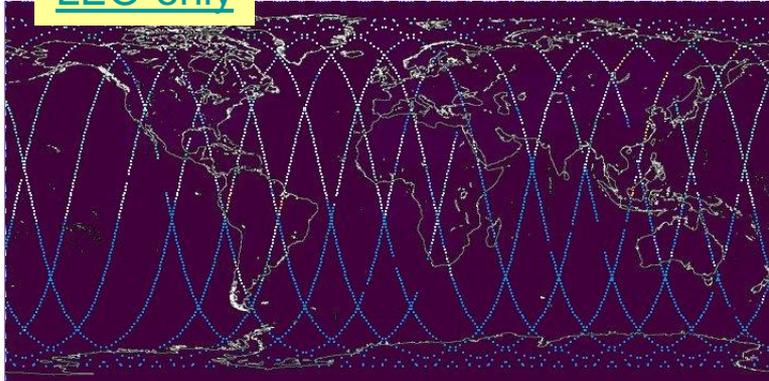


GHGIS-OSSE

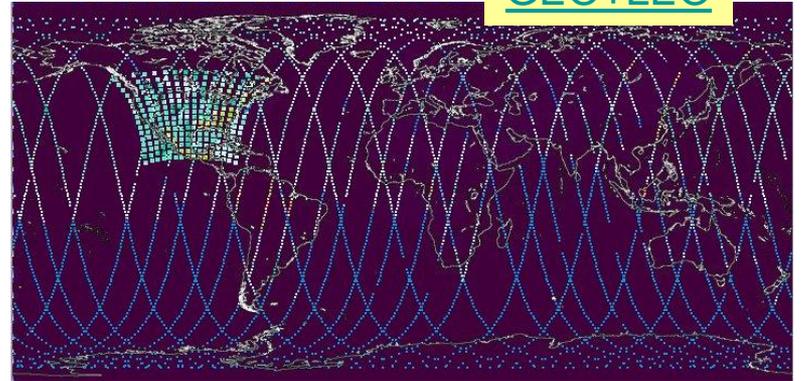
CO2 concentration model



LEO-only



GEO+LEO





SOX

**OSSE - based
Mission and Instrument
Concept Exploration**

**Meemong Lee, PhD
Richard Weidner, PhD
Kevin Bowman, PhD**

Jet Propulsion Laboratory
California Institute of Technology