3D and 4D Visualization of Atmospheric Chemistry

Presented to:
Rocky Mountain EHS Peer Group
Denver, Colorado

Carl Drews,
Software Engineer, NCAR / ACOM

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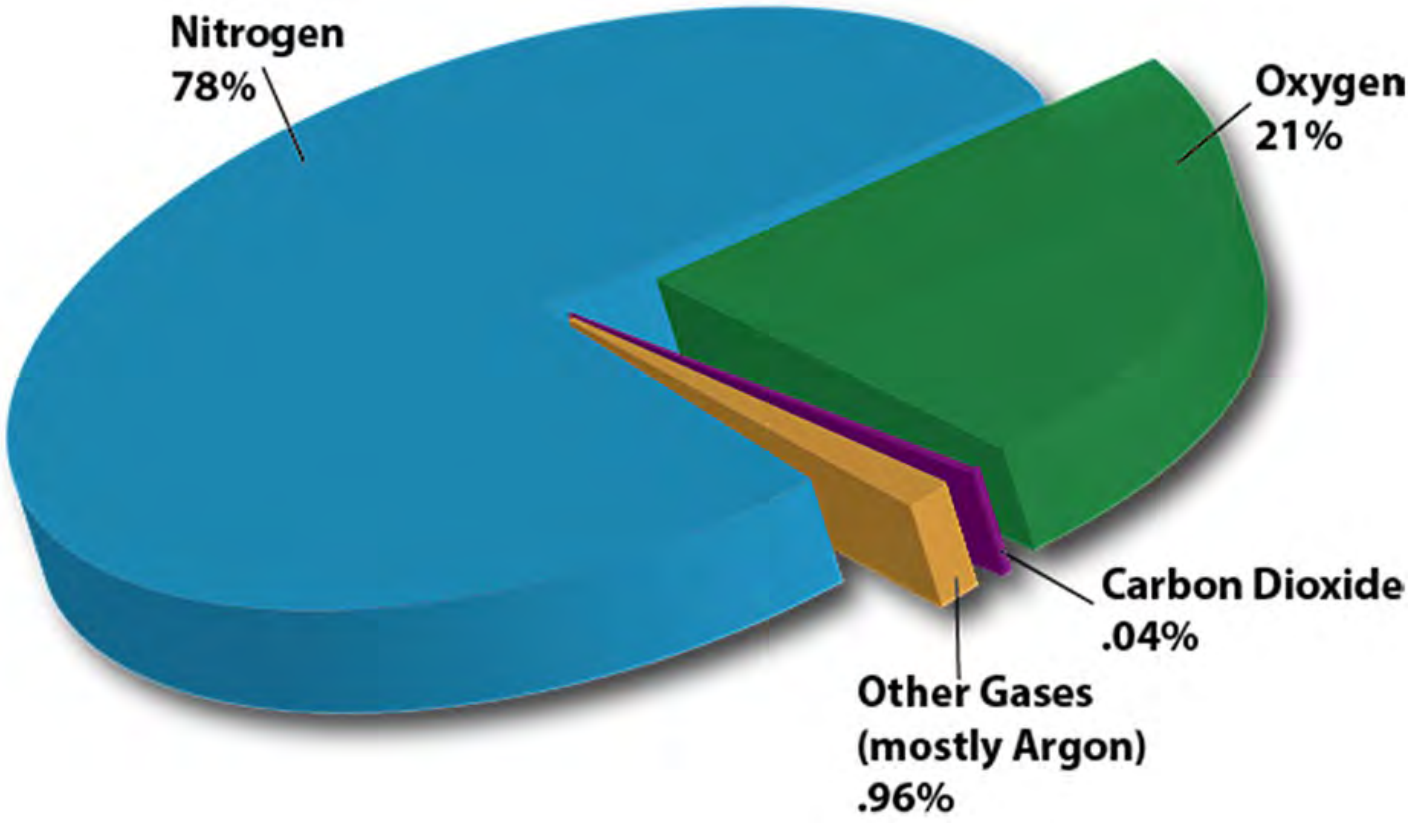
Who I am and what I do

- Carl Drews, Software Engineer at Atmospheric Chemistry Observations & Modeling laboratory (ACOM), National Center for Atmospheric Research (NCAR), Boulder, Colorado.
  - **drews@ucar.edu**
- NCAR is a Federally Funded Research & Development Corporation.
- We create research products and make them freely available.
- Part of my job is to disseminate this information to all of you.

Atmospheric Chemistry



Gases in Earth's Atmosphere (UCAR)
https://scied.ucar.edu/image/gases-earths-atmosphere

Observations

- Satellites:
  - MOPITT, TROPOMI, MODIS, GOES, VIIRS
- TOLNet lidars:
  - TOPAZ, AMOLITE, CCNY, EAARL, Hampton, LMOL, RO3QET
- Ground:
  - PANDORA, NDACC, Thule (Greenland), Mauna Loa, Manitou Experimental Forest
- Aircraft:
  - NASA DC-8 and WB-57, NSF/NCAR GV HIAPER, C-130;
  - TOGA, CAFS, LIF NOx, Picarro, Aerodyne CS-108.

Trace Organic Gas Analyzer (TOGA)

Requestable instrument. Measures all these chemical species:
https://www2.acom.ucar.edu/voc-measurements/voc-measurements

NMHCs	LLOD; ppt
Alkanes	
Propane	5
Isobutane	1
n-Butane	1
Isopentane	1
n-Pentane	1
2-Methylpentane	0.5
3-Methylpentane	0.5
n-Hexane	0.5
n-Heptane	1
2,2,4-Trimethylpentane	0.5
n-Octane	0.5
Alkenes	
Propene	5
1-Butene/Isobutene	1
cis-2-Butene	1
trans-2-Butene	1
Isoprene	1
α-Pinene	1
β-Pinene/Myrcene	1
Camphene	1
Limonene/3-Carene	1
Tricyclene	1
Aromatics	
Benzene	0.3
Toluene	0.3
Ethylbenzene	0.2
p-/m-Xylene	0.2
o-Xylene	0.2
Styrene	0.1
Ethynylbenzene	TBD

OVOCs	LLOD; ppt
Aldehydes	
Formaldehyde (HCHO)	20
Acetaldehyde (CH_3CHO)	5
Propanal	2
Isobutanal	TBD
Butanal	1
Acrolein (CH_2CHCHO)	1
Methacrolein	1
2-Butenal (Crotonaldehyde)	2
Furfural	TBD
3-Furaldehyde	TBD
Ketones	
Acetone	5
MEK	0.5
MVK	0.5
2,3-Butanedione	TBD
Alcohols	
Methanol (CH_3OH)	5
Ethanol (C_2H_5OH)	2
2-Propanol	4
Ethenol	TBD
MBO (2-Methyl-3-Buten-2-ol)	1
Esters	
Methyl Formate	TBD
Methyl Acetate	TBD
Methyl Propionate	TBD
Ethyl Acetate	TBD
Ethers/Furans	
MTBE (Methyl t-Butyl Ether)	0.3
Furan	1
THF (Tetrahydrofuran)	TBD

OVOCs	LLOD; ppt
Ethers/Furans (cont'd)	
2-Methylfuran	0.5
3-Methylfuran	0.5
2,3-Dimethylfuran	TBD
2,4-Dimethylfuran	TBD
2,5-Dimethylfuran	TBD
2-Ethylfuran	TBD
3-Ethylfuran	TBD
2-Vinylfuran	TBD
3-Vinylfuran	TBD
1,3-Dioxolane	TBD

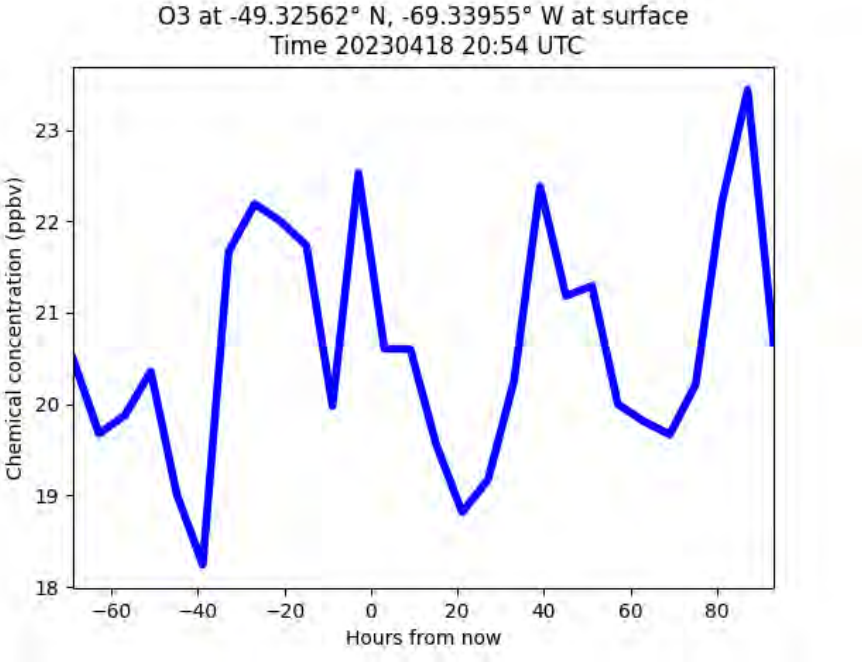
Nitrogen-containing VOCs	LLOD; ppt
Nitriles	
HCN (Hydrogen Cyanide)	5
Acetonitrile (CH_3CN)	1
Propanenitrile	1
Acrylonitrile	1
Methylacrylonitrile	2
Nitrates	
Methyl Nitrate	TBD
Ethyl Nitrate	TBD
Isopropyl Nitrate	2
n-Propyl Nitrate	2
t-Butyl Nitrate	2
2-Butyl Nitrate/Isobutyl Nitrate	2
n-Butyl Nitrate	2
Other	
Pyrrole	TBD
Nitromethane (CH_3NO_2)	TBD

Halogenated VOCs	LLOD; ppt
CH_3Cl	1
CH_2Cl_2	1
$CHCl_3$	1
CCl_4	1
C_2Cl_4	0.1
1,2-Dichloroethane	0.5
CH_3CCl_3	0.5
CH_3Br	1
CH_2Br_2	0.03
$CHBr_3$	0.1
CH_3I	0.03
CH_2I_2	0.05
C_2H_5I	0.5
CH_2ICl	0.05
$CHBrCl_2$	0.05
$CHBr_2Cl$	0.03
CFC-11	5
CFC-12	1
CFC-113	1
CFC-114	1
HCFC-22	1
HCFC-141a	1
HCFC-142b	TBD
HFC-134a	1

Sulfur-containing VOCs	LLOD; ppt
OCS	1
CS_2 (Carbon Disulfide)	0.2
CH_3SH (Methanethiol)	TBD
DMS (Dimethyl Sulfide)	1
C_3O_2 (Carbon Suboxide)	TBD

Computer Models

- Models are my favorite, because they provided gridded output.
- WACCM, WRF-Chem, CAM-Chem.
  - Download models and output.
- Use data assimilation from all those measurements.
- Example: Ozone time series over Kerguelen Islands.



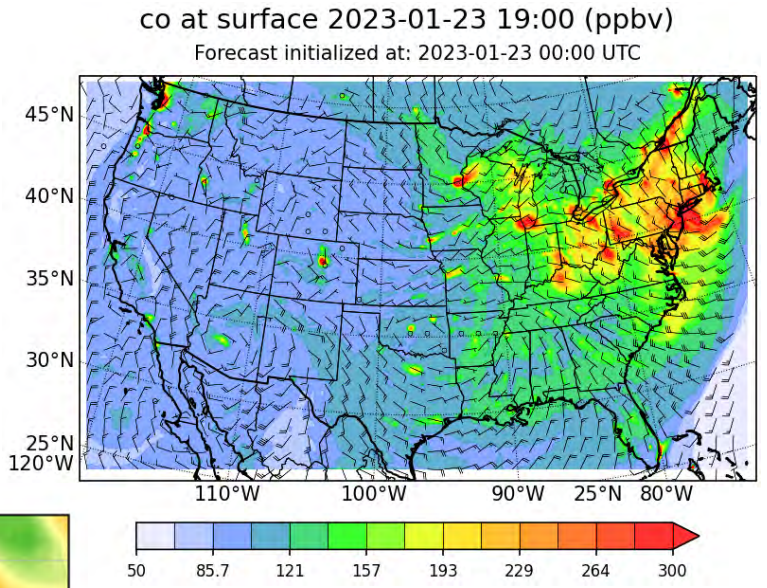
The Four Dimensions

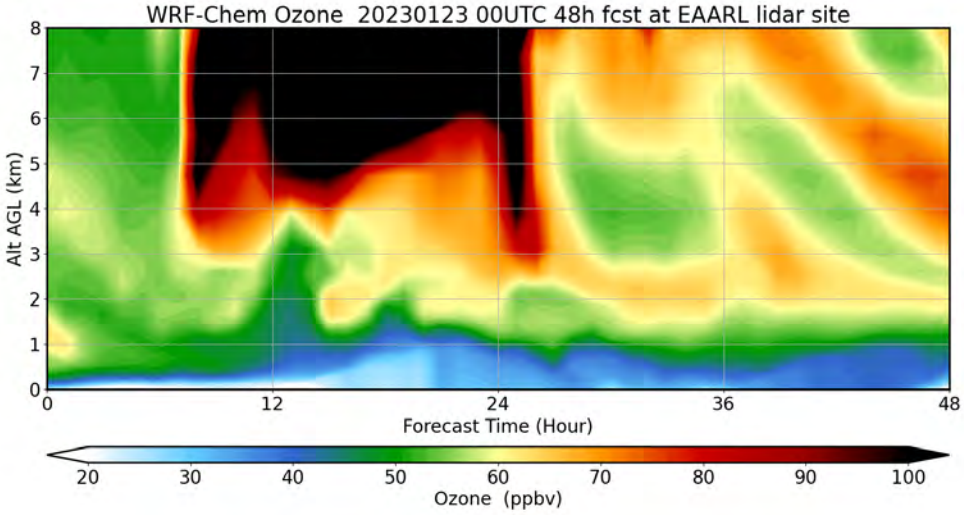
- float CO01(time, lev, lat, lon) ; WACCM
- float o3(Time, bottom_top, south_north, west_east) ; WRF-Chem
- float NOx(t, z, y, x) Cartesian

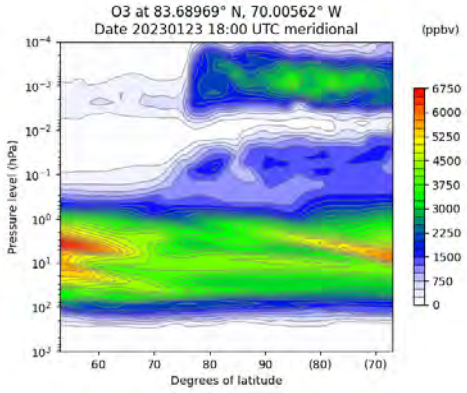
2D Plots are Common at ACOM

Clockwise:

- WRF-Chem lon-lat
- WACCM lat-level
- WRF-Chem time-lev







TOLNet plots by Bo Wang and Carl Drews.

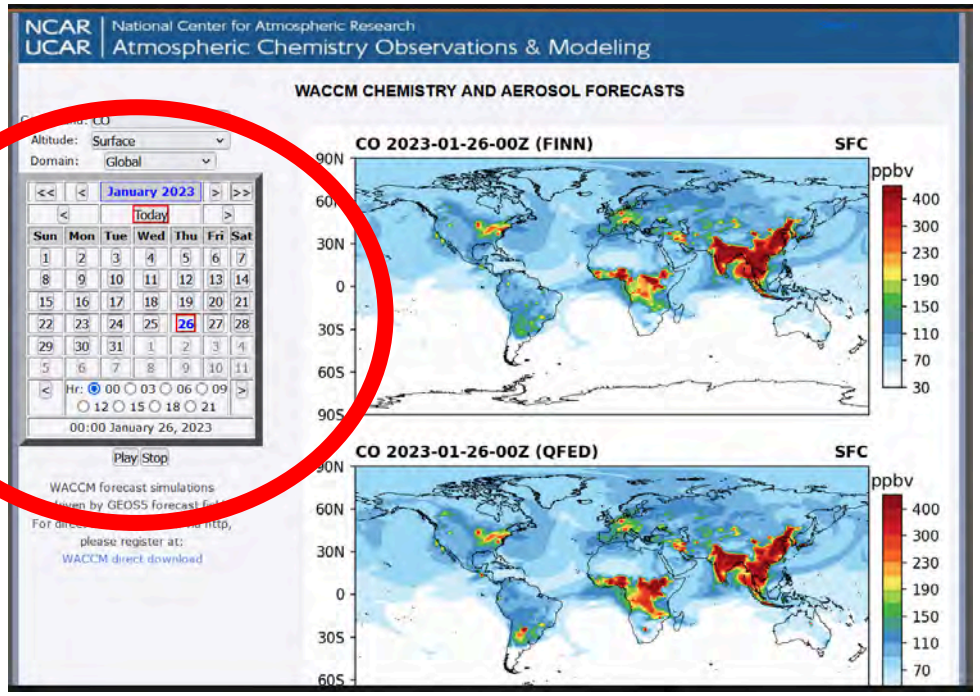
Computer Screen

Good with x-y dimensions, and **also with time**.
Your screen refreshes at 60 Hertz. The hard part is pushing images into that frame buffer fast enough.

Animation at ACOM

- X-y and time dimensions; 3D.
- Harder than *Seinfeld*, but we do it.
- Calendar control or MP4 animations.

Calendar control



WACCM plots by Shawn Honomichl.

Three Spatial Dimensions

I have to convince you that your computer screen is a window into a 3D world, even though we all know it's just a 2D array of RGB pixels, indexed by x and y (row and column).

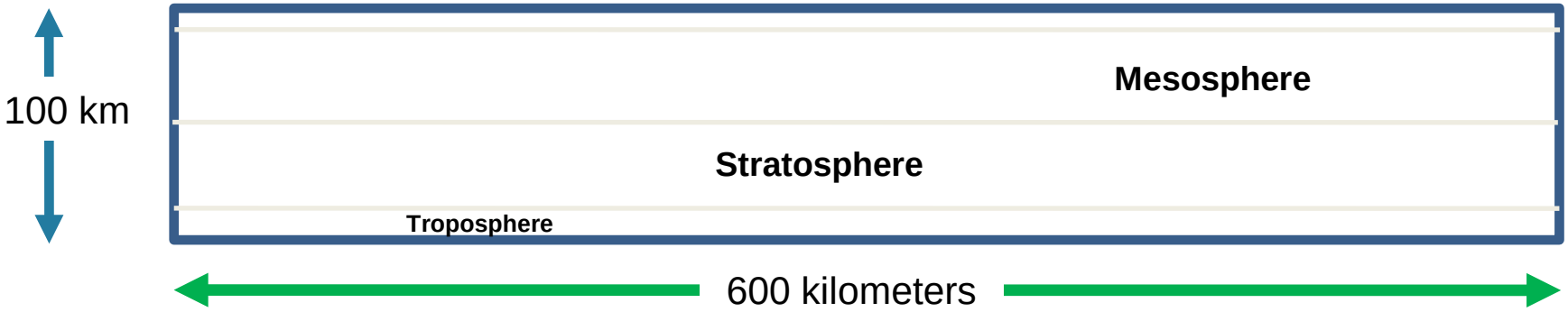
https://commons.wikimedia.org/wiki/File:SMPTE_Color_Bars.svg

https://commons.wikimedia.org/wiki/File:Television_reporter_doing_standup_close_report.jpg

What can go wrong?

- Scale is disturbed.
  - Outstretched hand “touching” Pyramid of Khafre.
  - Sand in foreground gives no scale.

Earth's atmosphere is rather thin



Scale cross-section of the atmosphere over Colorado.

Most of the action happens in the troposphere . . . so . . .

Vertical exaggeration: 3x – 300x

Clouds

- Amorphous and ill-defined blobs up in the sky.
  - No obvious sense of scale.
  - But very beautiful! https://cloudappreciationsociety.org/

https://commons.wikimedia.org/wiki/File:Cumulus_cloud.jpg

https://commons.wikimedia.org/wiki/File:Smoke_plume_(6089086736).jpg

Thunderheads – how high are these?

https://commons.wikimedia.org/wiki/File:Thunderhead_(nicholas_t).jpg

https://scied.ucar.edu/image/kelvin-helmholtz-clouds

Vertical structure (altitude) may be very important for aircraft; safety and chemical measurements.

Techniques for 3D on a 2D screen

- Axes (back and side walls are rulers).
- Shading (sunlight from a certain angle).
- Perspective (lines vanish into the distance).
- Motion (allow viewpoint to rotate, using t-dimension).
- Haze (objects in distance are obscured).
- Transparency (see-through film).
  - The A of RGBA (Alpha channel).

I want to convince your eyes to *lift the figures off the page*.

Shading

Brightness of the surface color is adjusted according to the angle of the surface with the light source (sun).

Perspective

- Parallel lines converge in the distance.
- Objects get smaller as they become farther away from the viewer.

https://commons.wikimedia.org/wiki/File:Moving_Freight_Train_(2952122815).jpg

Haze

- Objects farther away are obscured by the atmosphere (haze, smoke, fog, pollution).

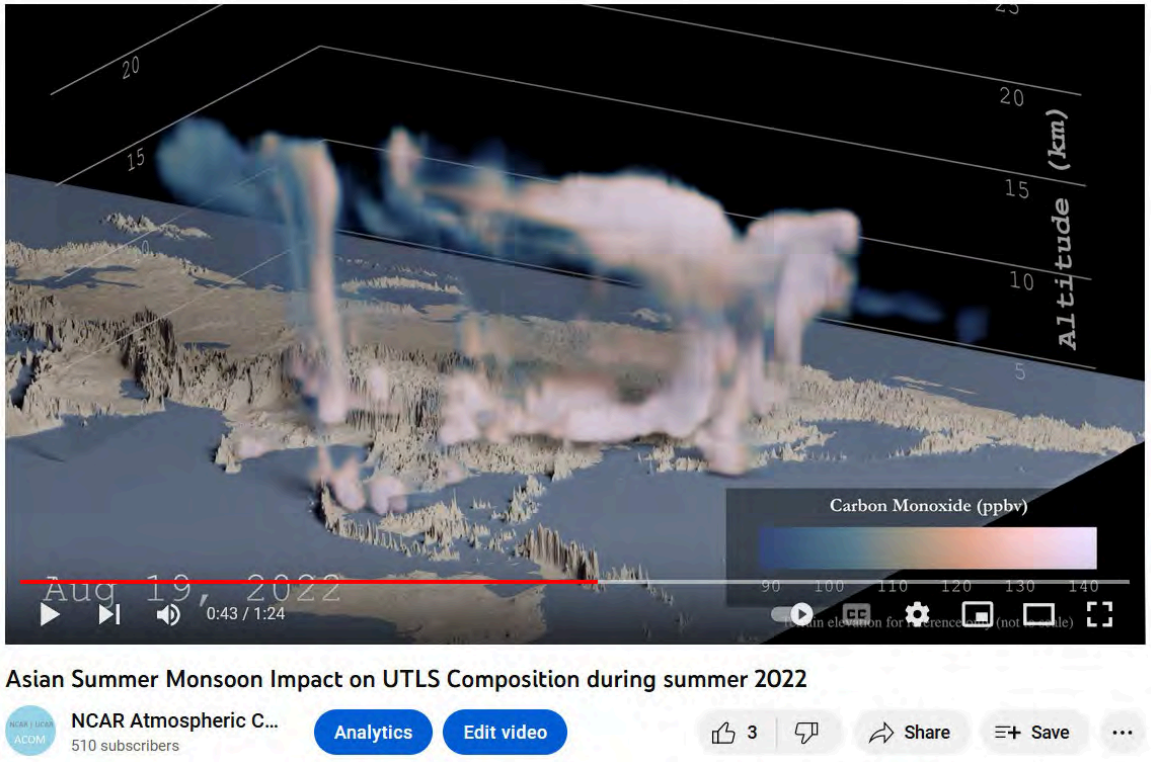
https://commons.wikimedia.org/wiki/File:Blue_Ridge_Mountains_view.jpg

NCAR VAPOR: Point Cloud Model

- ACCLIP animation by Ren Smith and Matt Rehme (VAST, VisLab).
- https://www.youtube.com/watch?v=LzBBcmG4sYs

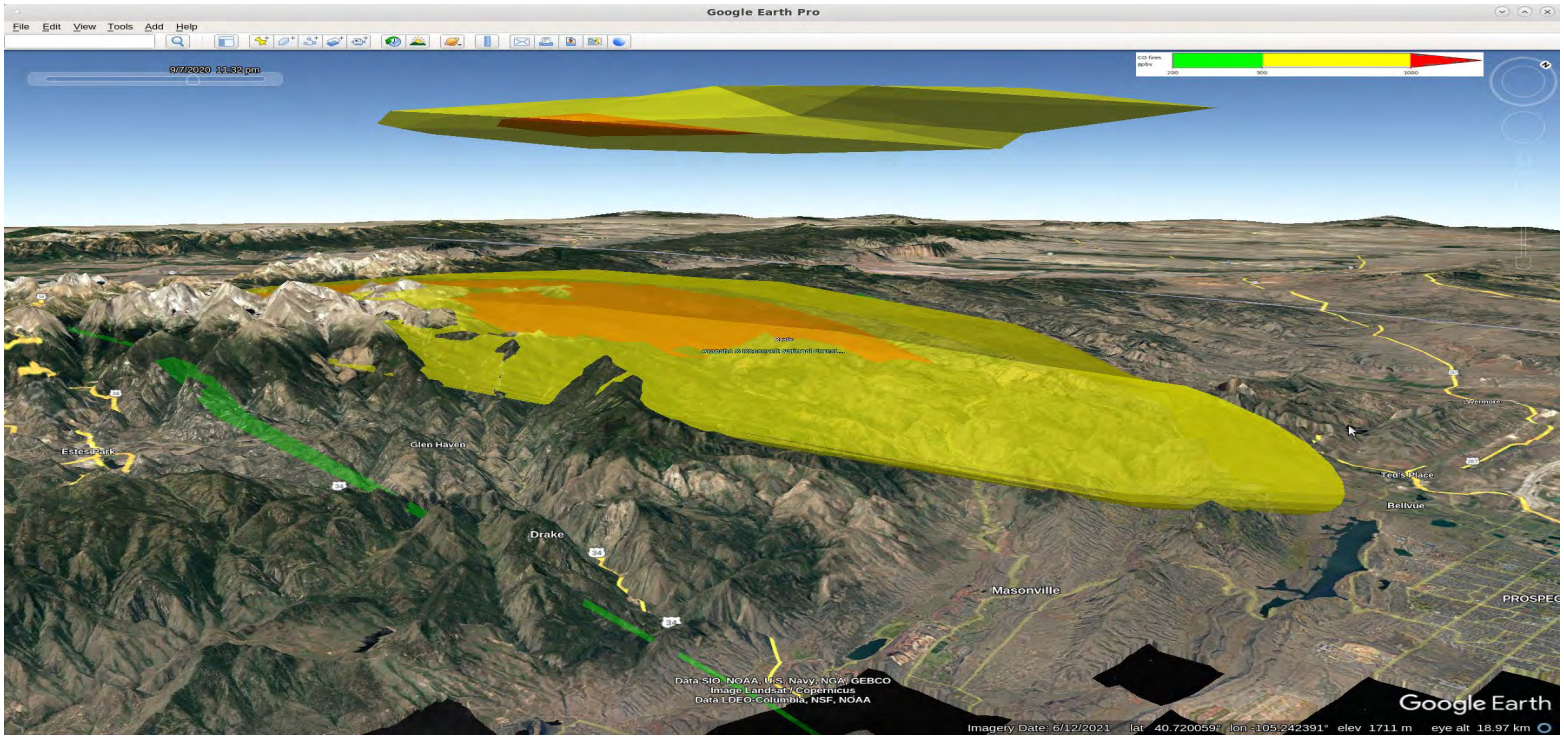
How do you represent an amorphous blob of semi-transparent gas/aerosols hanging up there in space?

- Vertical exaggeration = **300x**.
- Axes on the back walls.

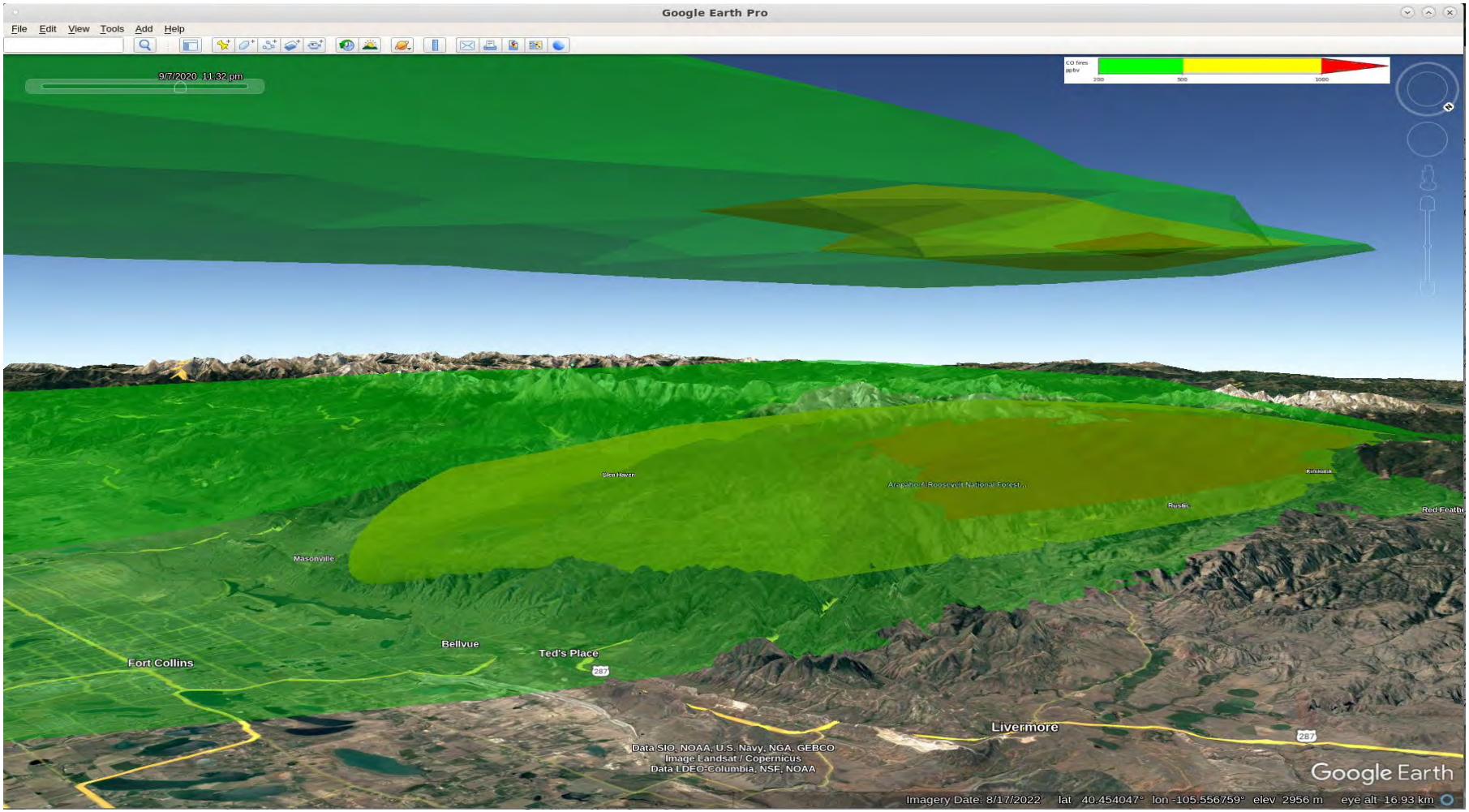


Isosurface Model

- 3D contour plot of CO (not filled, these are shells).
- Nested surfaces of increasing transparency.
  - Green = 200 ppbv, yellow = 500 ppbv, red = 1000 ppbv.
- Google Earth is the viewing platform.



Cameron Peak Fire - Sept 7, 2020 5:32 MT

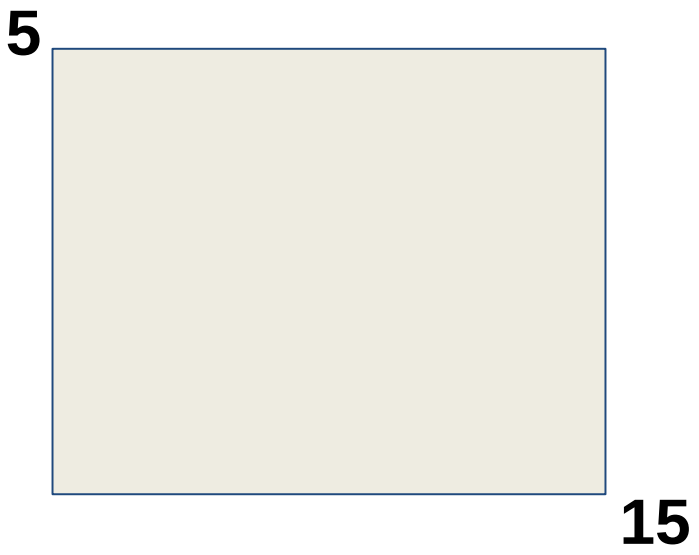


Marching Cubes

- The algorithm that generates the isosurface.
  - “Crawling” implementation in Python at NCAR/ACOM by Carl Drews.
  - https://github.com/NCAR/Marching-Cubes

Marching Squares: If at least one vertex is below the isovalue and at least one is above, then that square is part of the 2D isoline.

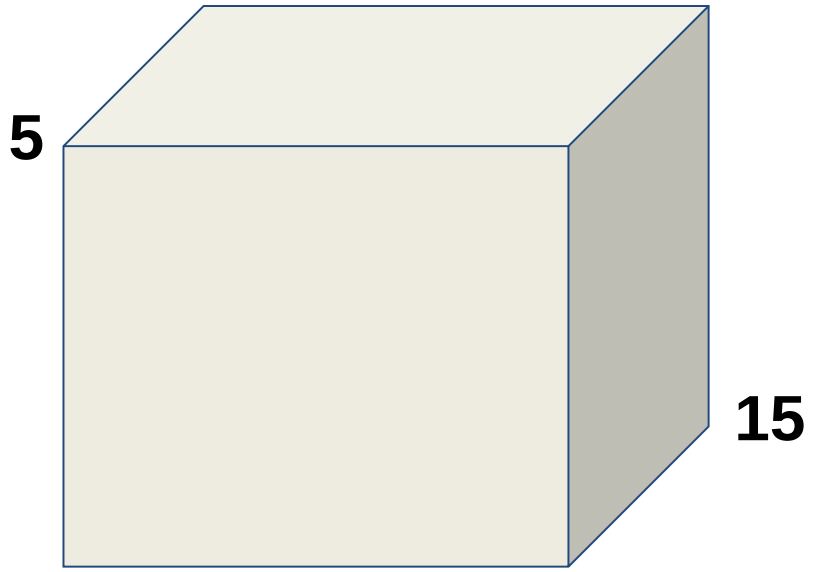
Consider isovalue = **10**.



…extended to Marching Cubes

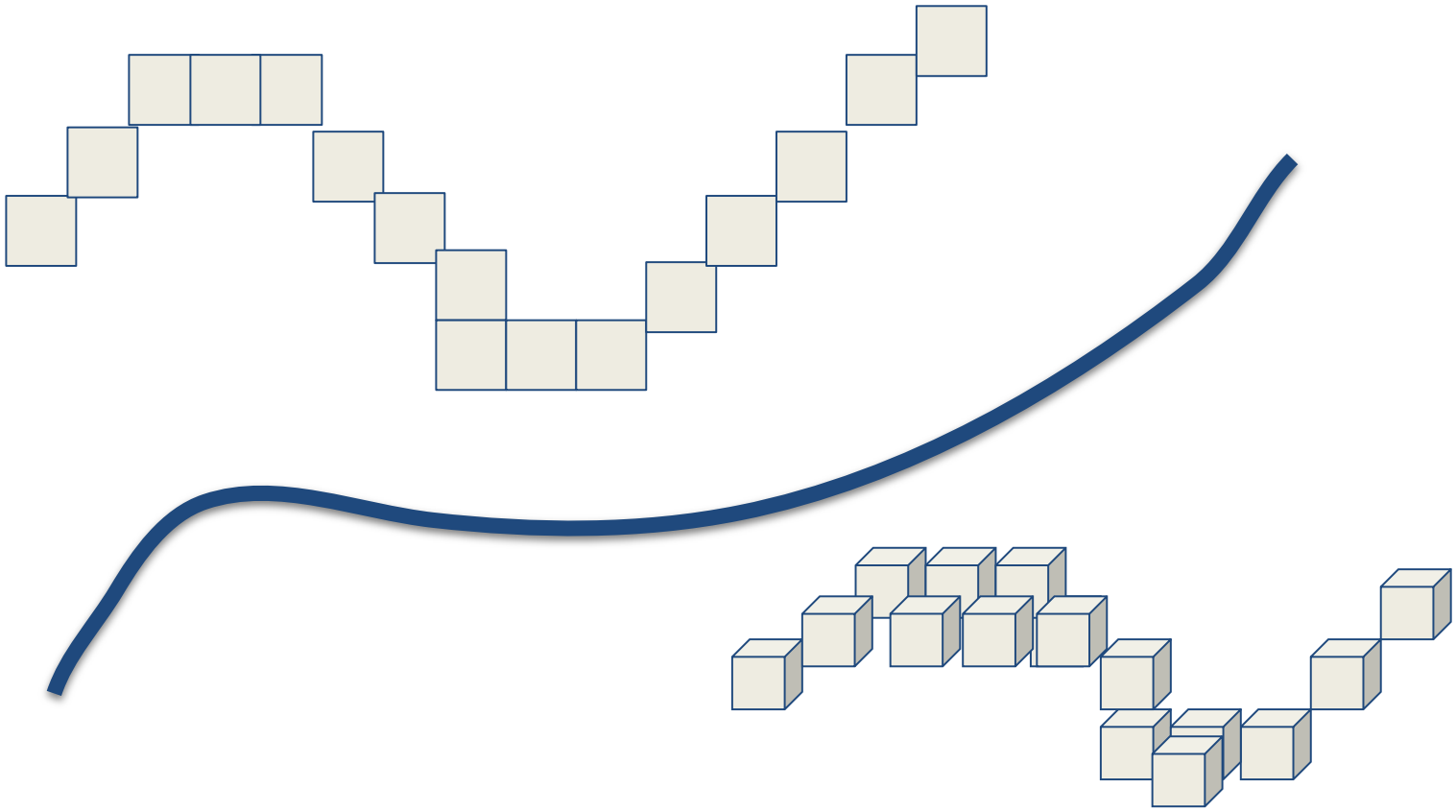
If at least one vertex is below the isovalue and at least one is above, then that cube is part of the 3D isosurface.

Consider isovalue = **10**.



Grid resolution

If we had very high grid resolution, we would be done.

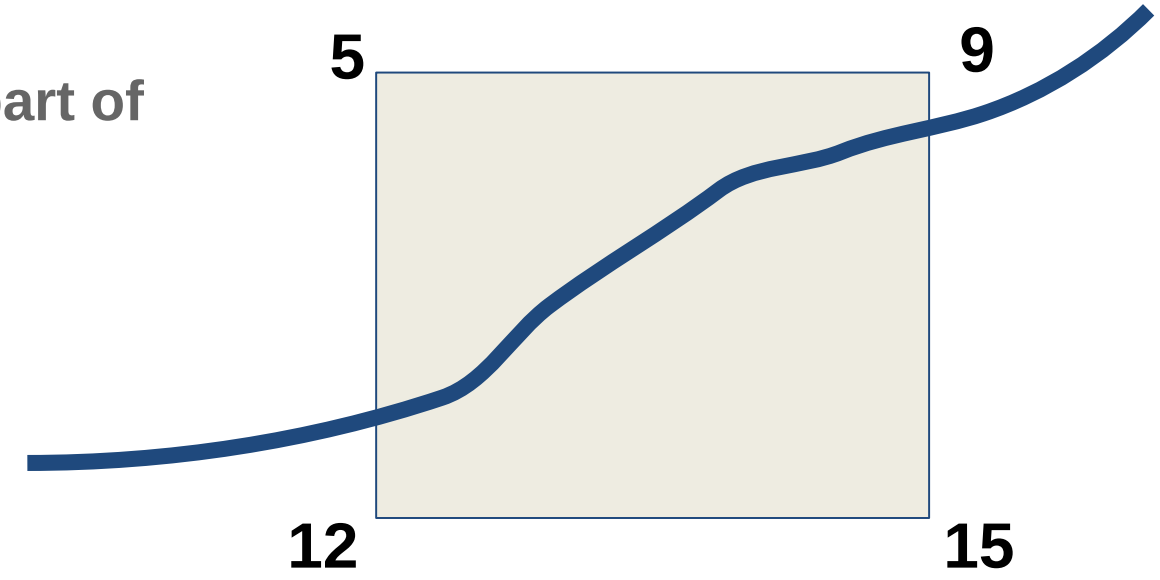


Inside a Single Cell

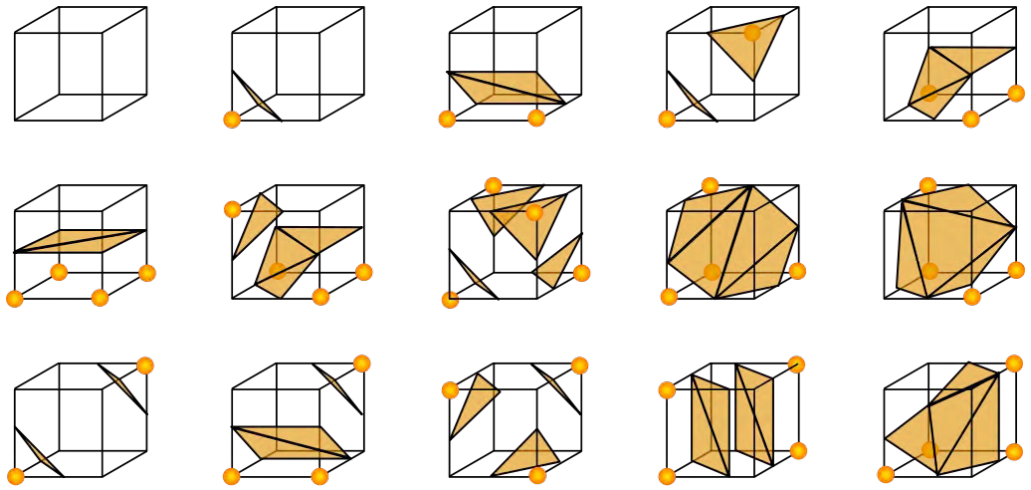
Usually grid resolution is too coarse, and we want to see the isosurface within a single cell. 2D contour plots are more than just squares, and this approach makes better use of data.

Consider isovalue = **10**.

This is the hard part of Marching Cubes.



Lookup Table of Cases for Triangulation



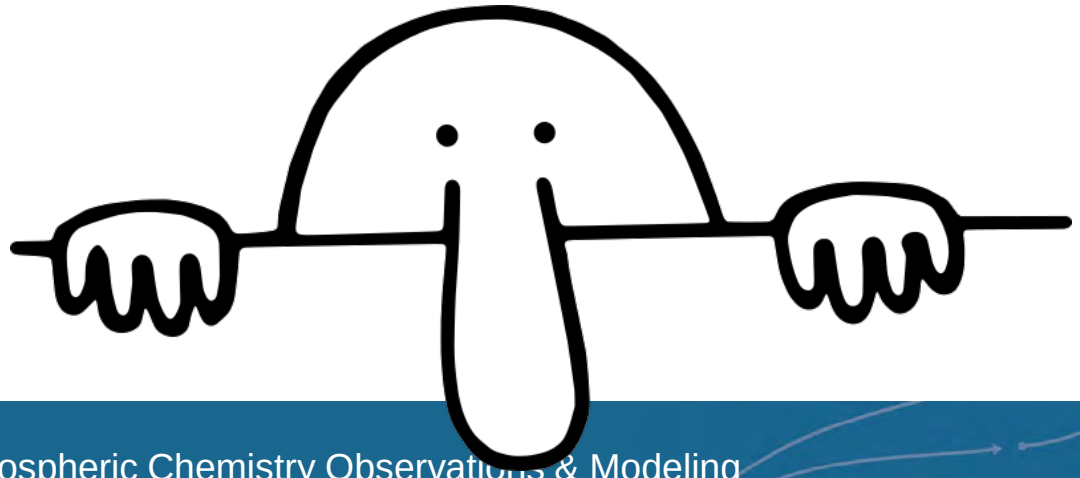
https://commons.wikimedia.org/wiki/File:MarchingCubes.svg GNU Public License.

8 cube vertices, and each vertex can be in two states: inside or outside the isosurface.
Total cases = 2^8 = **256**.
Reduce by symmetry and reflection to **15**, or **33**.
730 sub-cases in Lewiner 2003 implementation.

Drews 2022: Crawl instead

Drews, C. (2022). **Marching cubes without lookup cases: Crawl the edge crossings instead**. In *Improving Scientific Software Conference 2022*. National Science Foundation (NSF).

- Crawl along the faces of cube, from edge crossing to edge crossing.
- Make decisions at the ambiguities.
- Crawl over the next edge crossing like “Kilroy was here”.
- Keep track of your path, and accumulate 3D polygons.

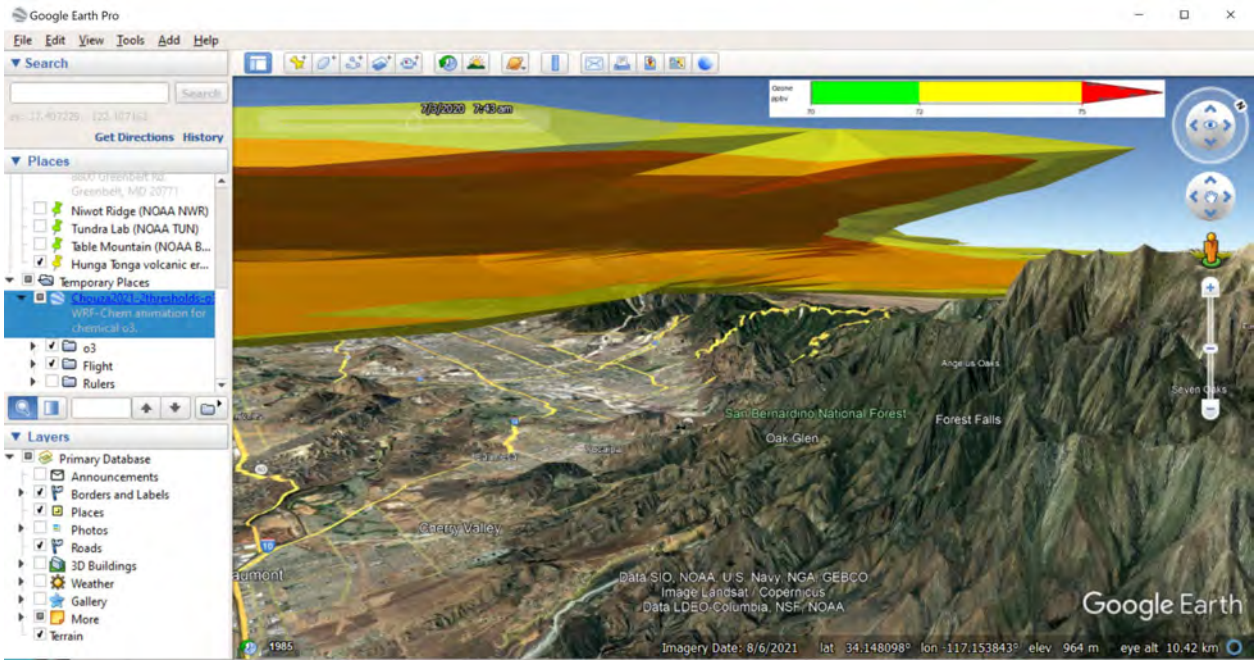


Triangles!

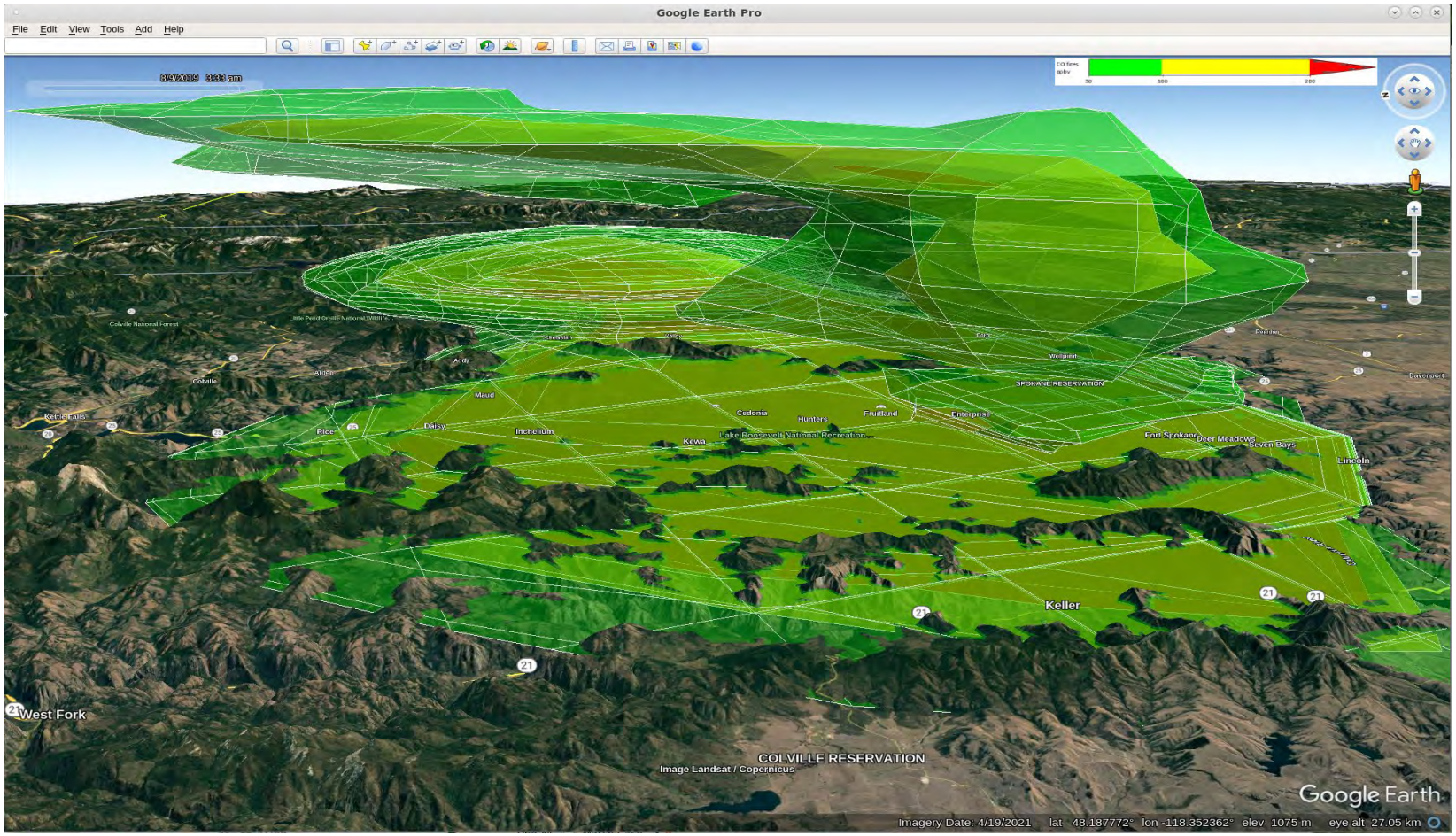
The edge crawler collects triangles and higher-order polygons.
Any rectangles are almost certainly **twisted** in 3D space (saddle).

Tens of Thousands of Triangles!!!

- Generate many triangles.
- Multiple time steps in WRF-Chem or WACCM.
- Encapsulate into KMZ archive.
- Display with Google Earth (rendering engine).

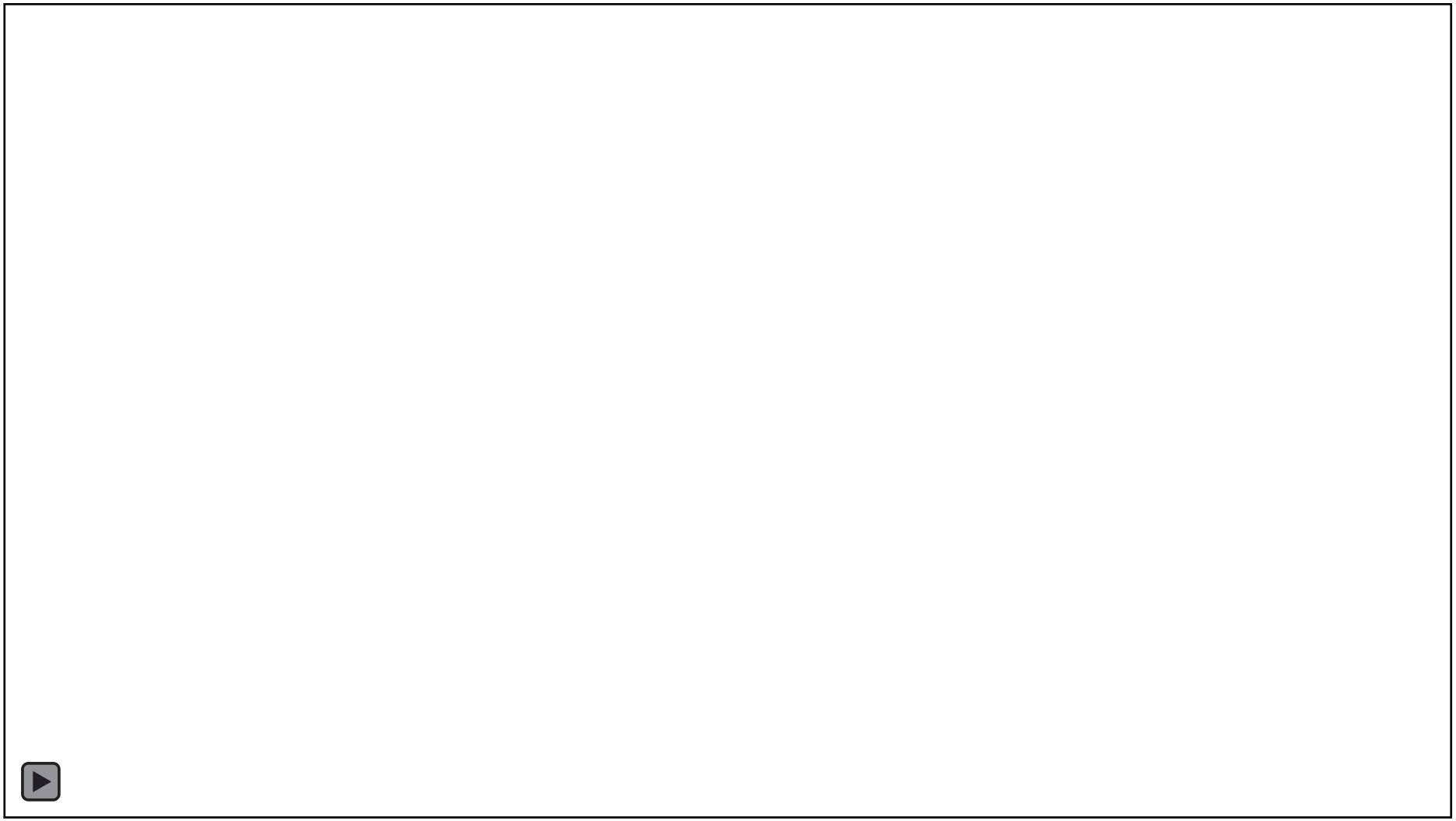


Grid lines for scale and perspective

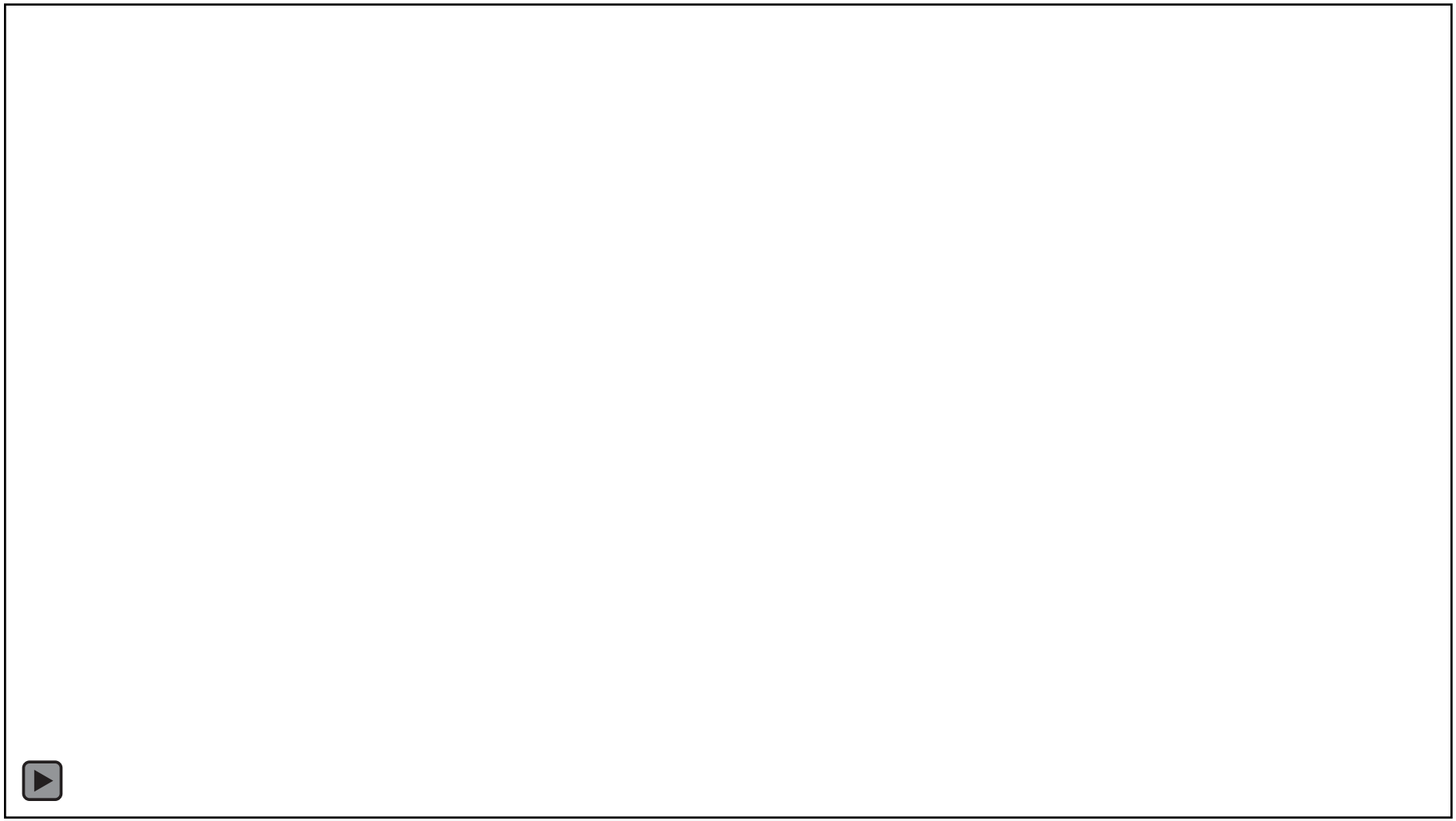


Pyrocumulus clouds at Williams Flats Fire - August 8, 2019 at 9:33 PM Mountain.

Williams Flats Fire and Flight – August 8, 2019

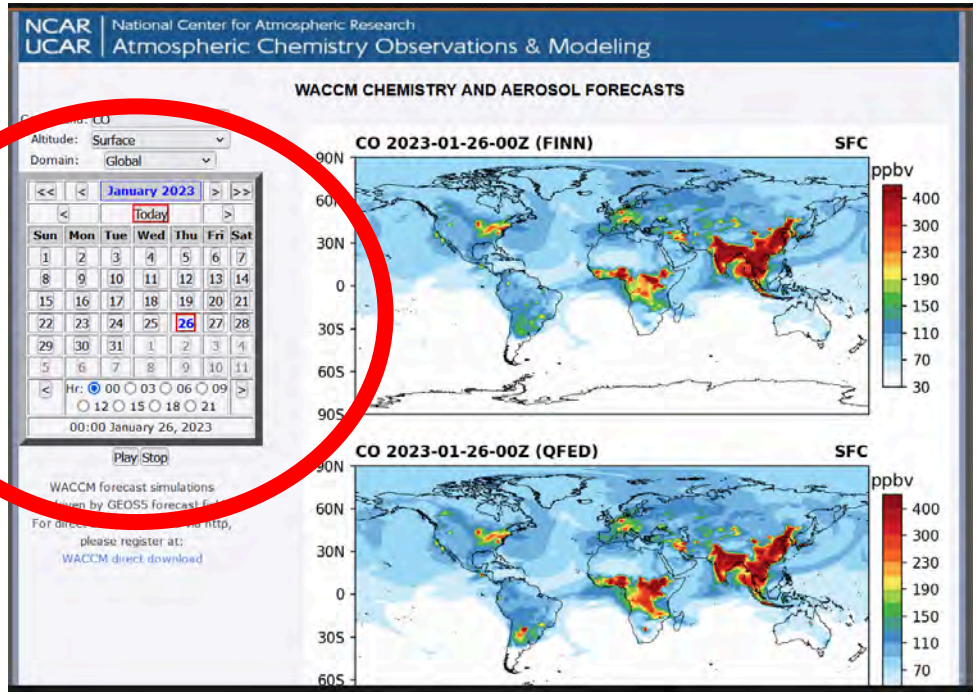


Motion alone – Northern California - 20210817



Animation complications: Javascript

Calendar control

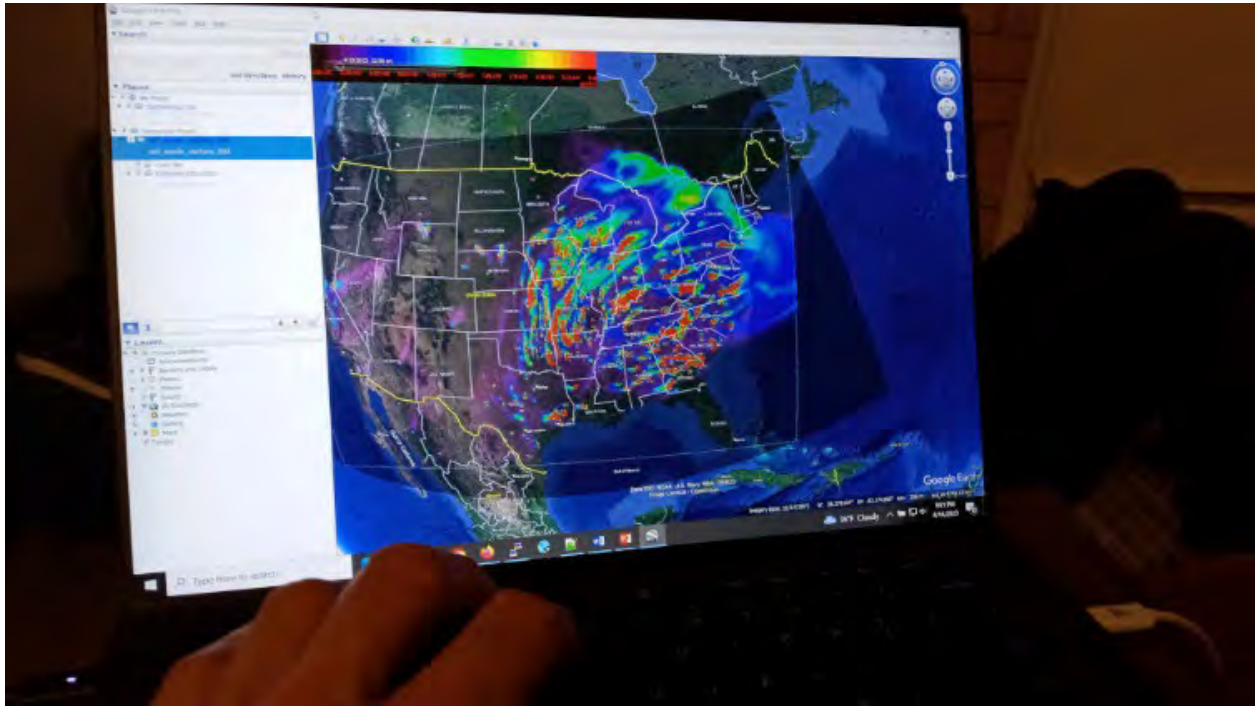


Need many images indexed by date-time.

WACCM plots by Shawn Honomichl.

Internet connection may not be able to keep up with Javascript requests to re-load the image for the next time frame.

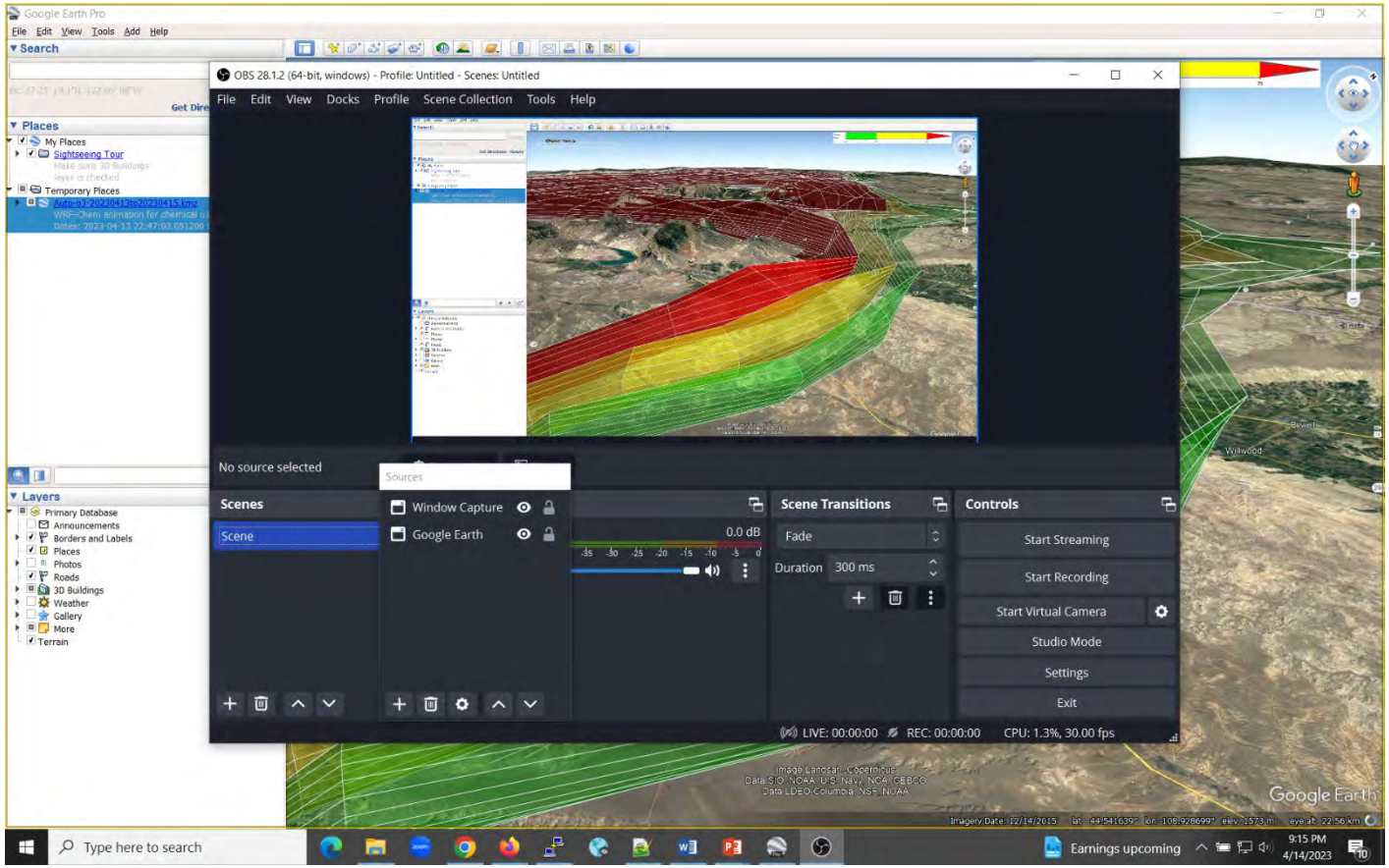
Animation complications: Live demo



CO Fire KMZ overlays by Gabriele Pfister.

When I run Google Earth with 4D, I can hear the cooling fans turn on. My GPU (Graphics Processing Unit) is loaded. Several times my laptop dropped the connection during a Zoom call. Very awkward!

Animation complications: Recording an MP4 video file



OBS Studio works better than built-in Google Earth recording. MP4 files are large; 10 – 20 MB each for this presentation.

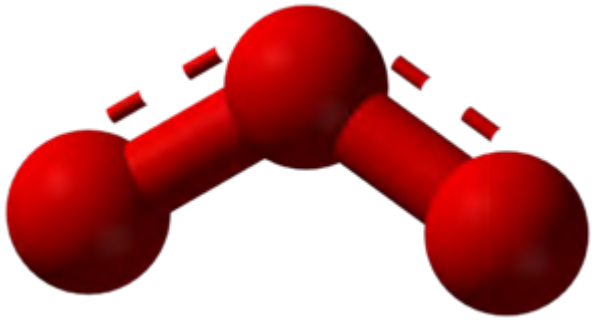
The challenges and rewards of ozone

Challenges:

- Higher concentration above 15km (tropopause). Much higher!
- Sources of O3 are above 15km and at surface.

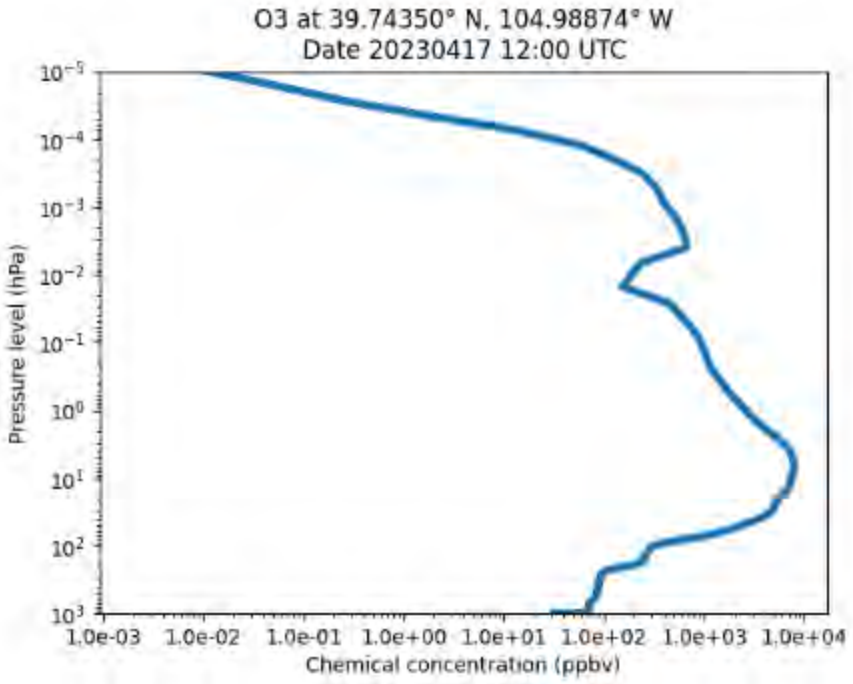
Rewards:

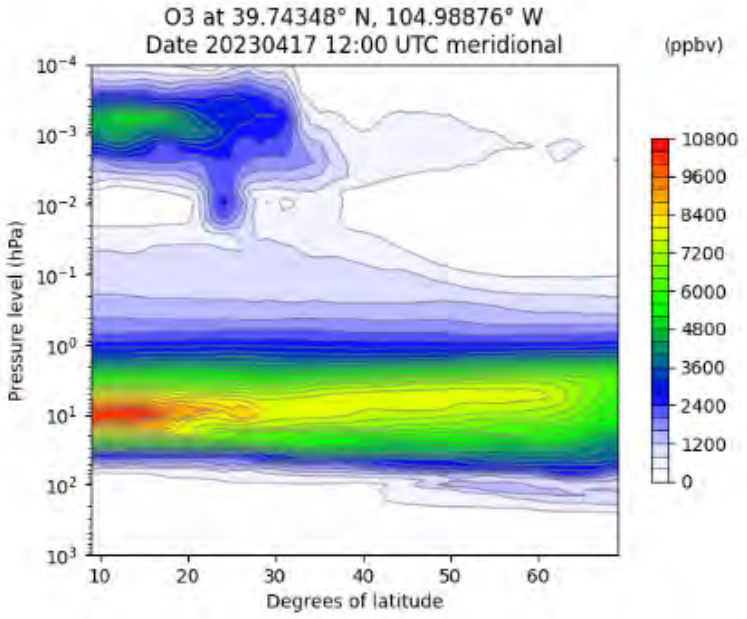
- Invisible -> visualization is needed!
- Regulatory trouble if ozone exceeds 70 ppbv for 8 hours.



https://commons.wikimedia.org/wiki/File:Ozone-CRC-MW-3D-balls.png

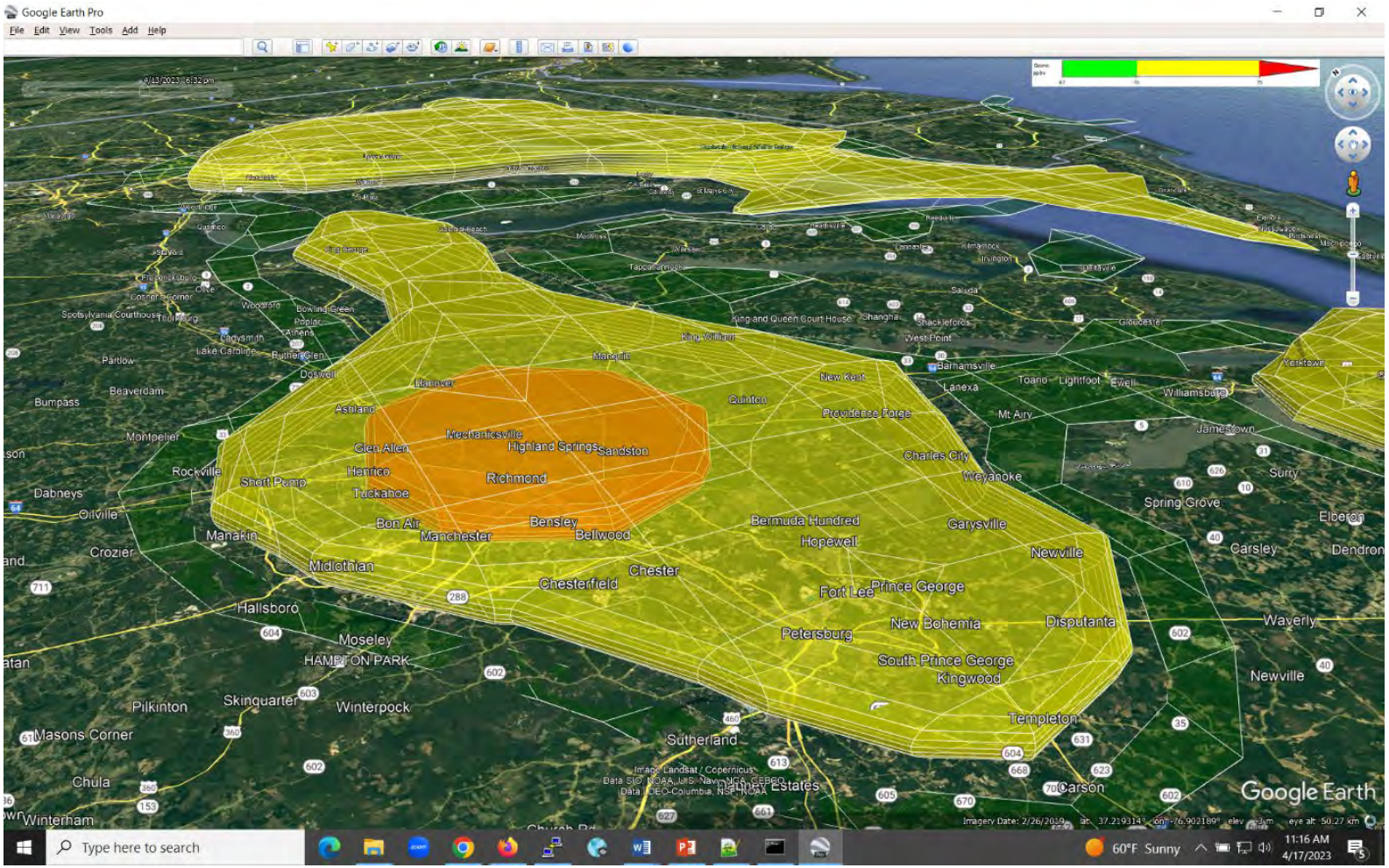
Ozone concentration with altitude



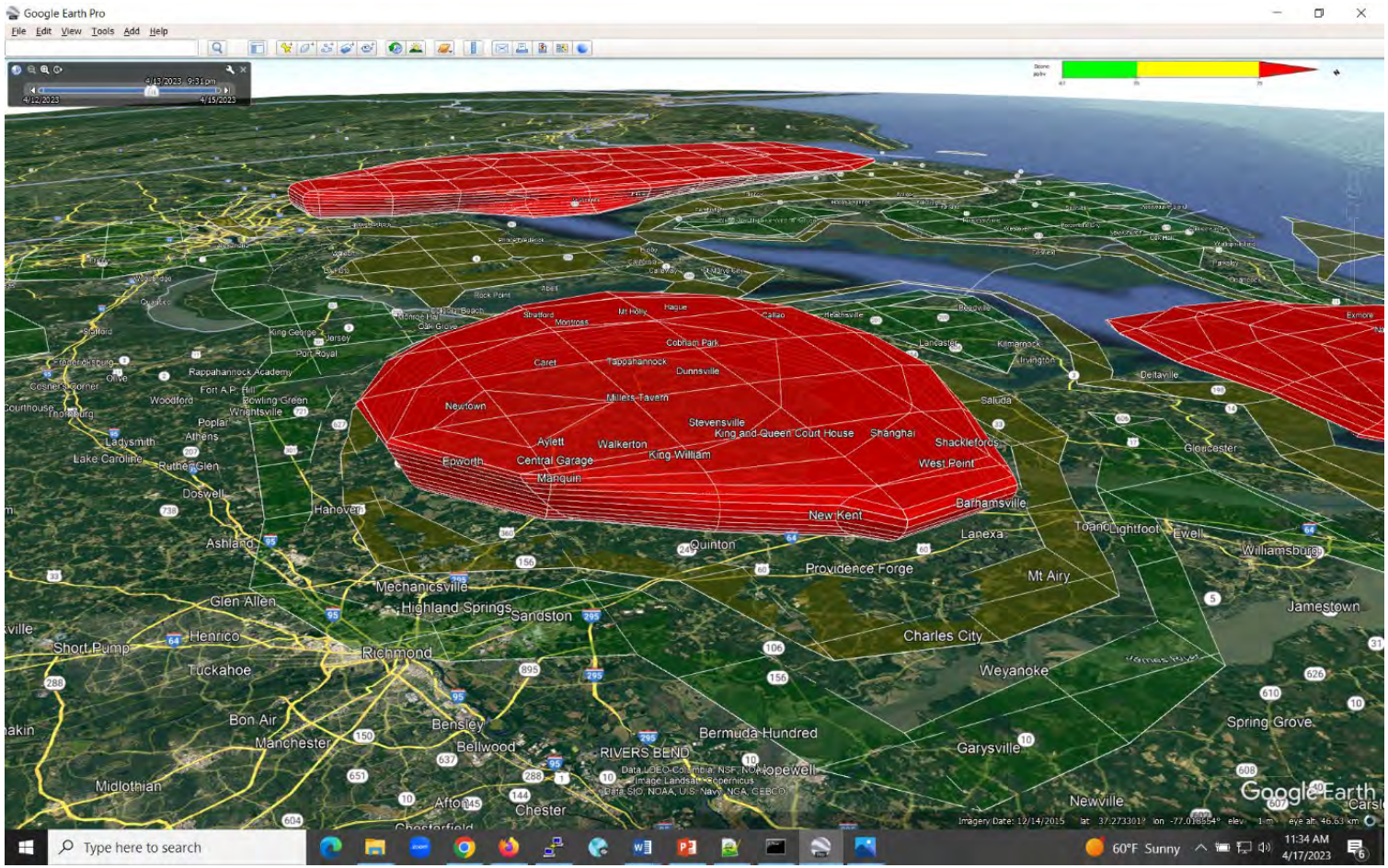


Ozone sounding and meridional section at 370 17th Street, Denver, CO 80202; Monday, April 17, 2023.

High ozone over Richmond, VA
April 13, 2023 at 12:32 pm

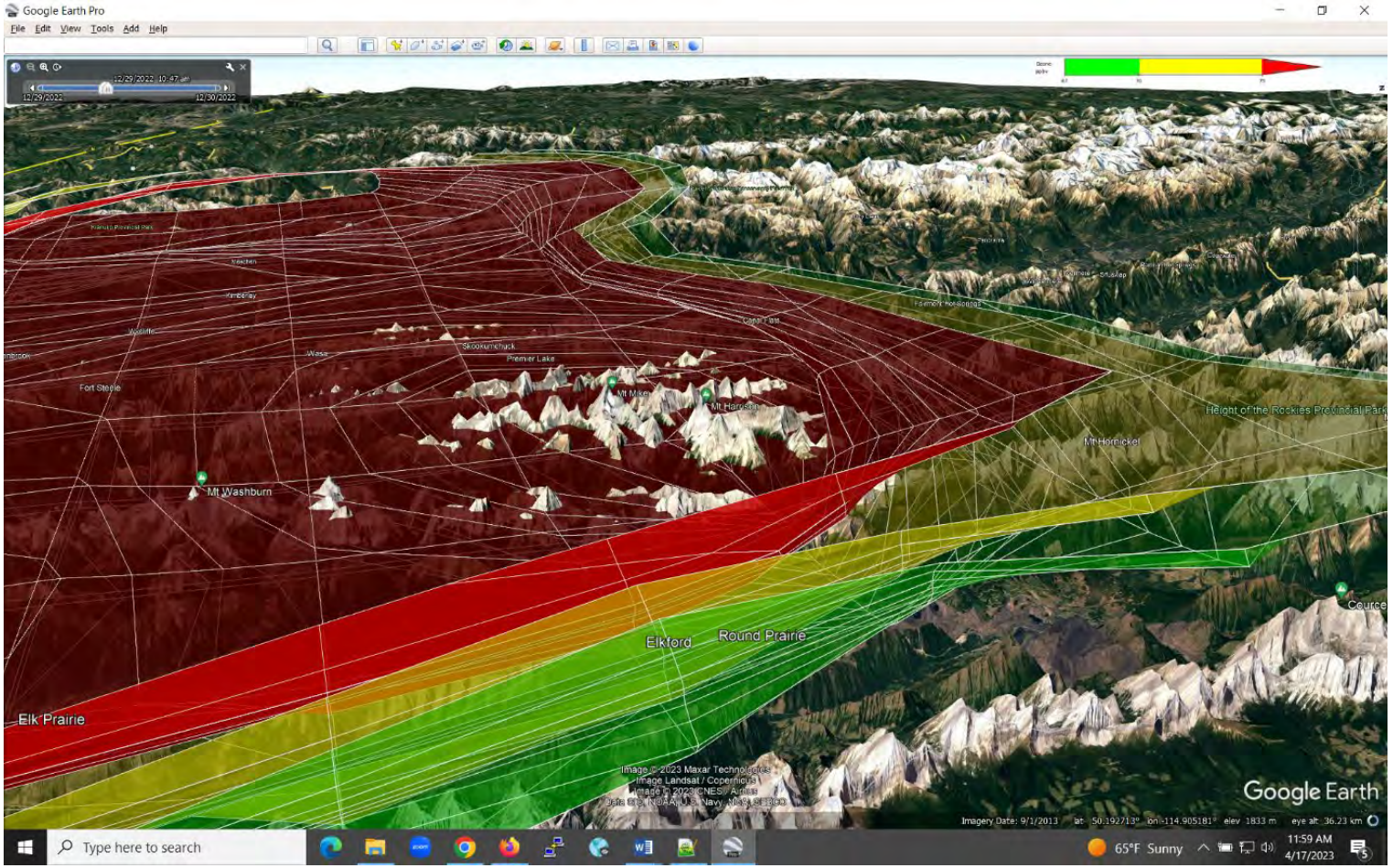


High ozone east of Richmond, VA
April 13, 2023 at 3:31 pm



What happens in Richmond does not stay in Richmond . . .

High ozone over Mt. Harrison, British Columbia
December 29, 2022 at 10:47 UTC



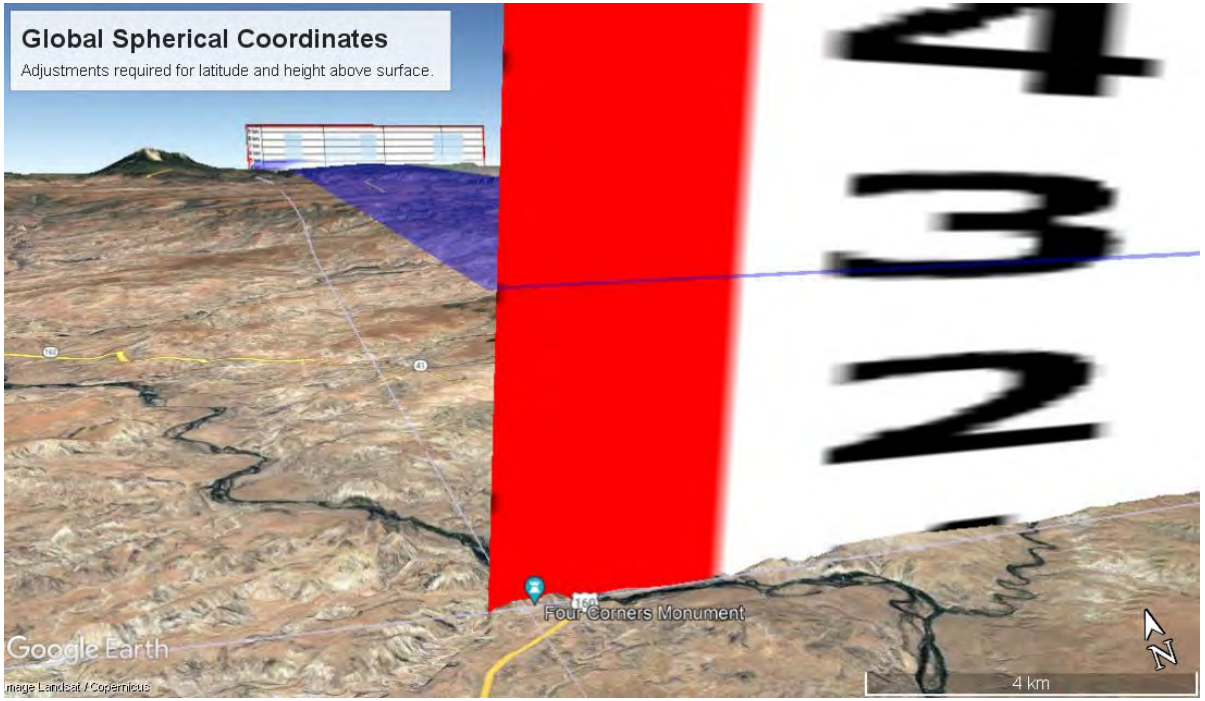
Well . . . It's ***not*** a bubble. Summit = 11,020 feet. Cutoff altitude = 4 km.

Stratospheric Intrusion

- Under certain meteorological conditions, the stratosphere dips down into the troposphere.
- Ozone comes down with it.
- Highest terrain is most likely to be affected.

Citation:
Homeyer, C. R., Bowman, K. P., Pan, L., Zondlo, M. A., & Bresch, J. F. (2011). Convective injection into stratospheric intrusions. Journal Of Geophysical Research-Atmospheres, 116, D23304. doi:10.1029/2011JD016724
See especially Figure 14.

How high is that cloud?

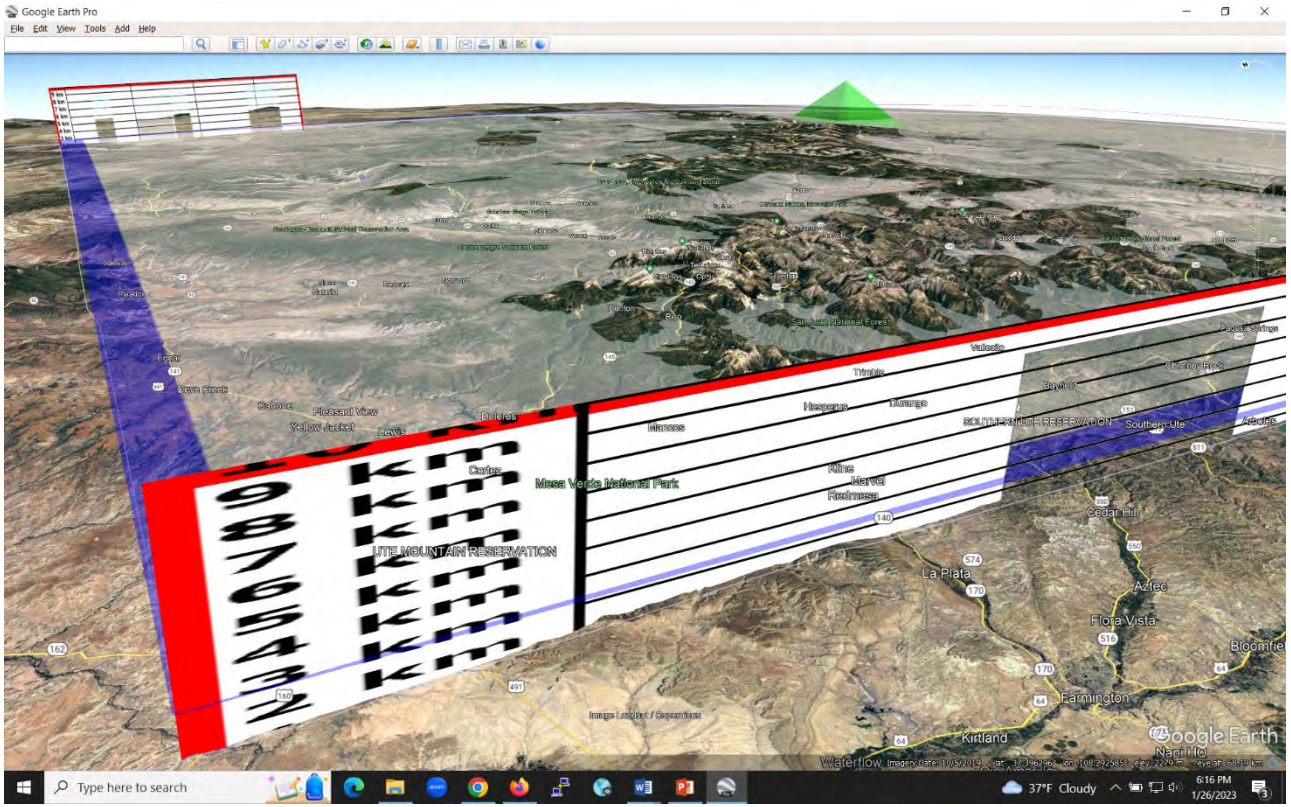


The earth is curved. Very difficult to sight accurately to a distant ruler.

The adjustment from center of Colorado - New Mexico border (State Line Peak) to Four Corners is **5.7 km** north and **7.6 km** down. Otherwise wall flies away from the earth's surface.

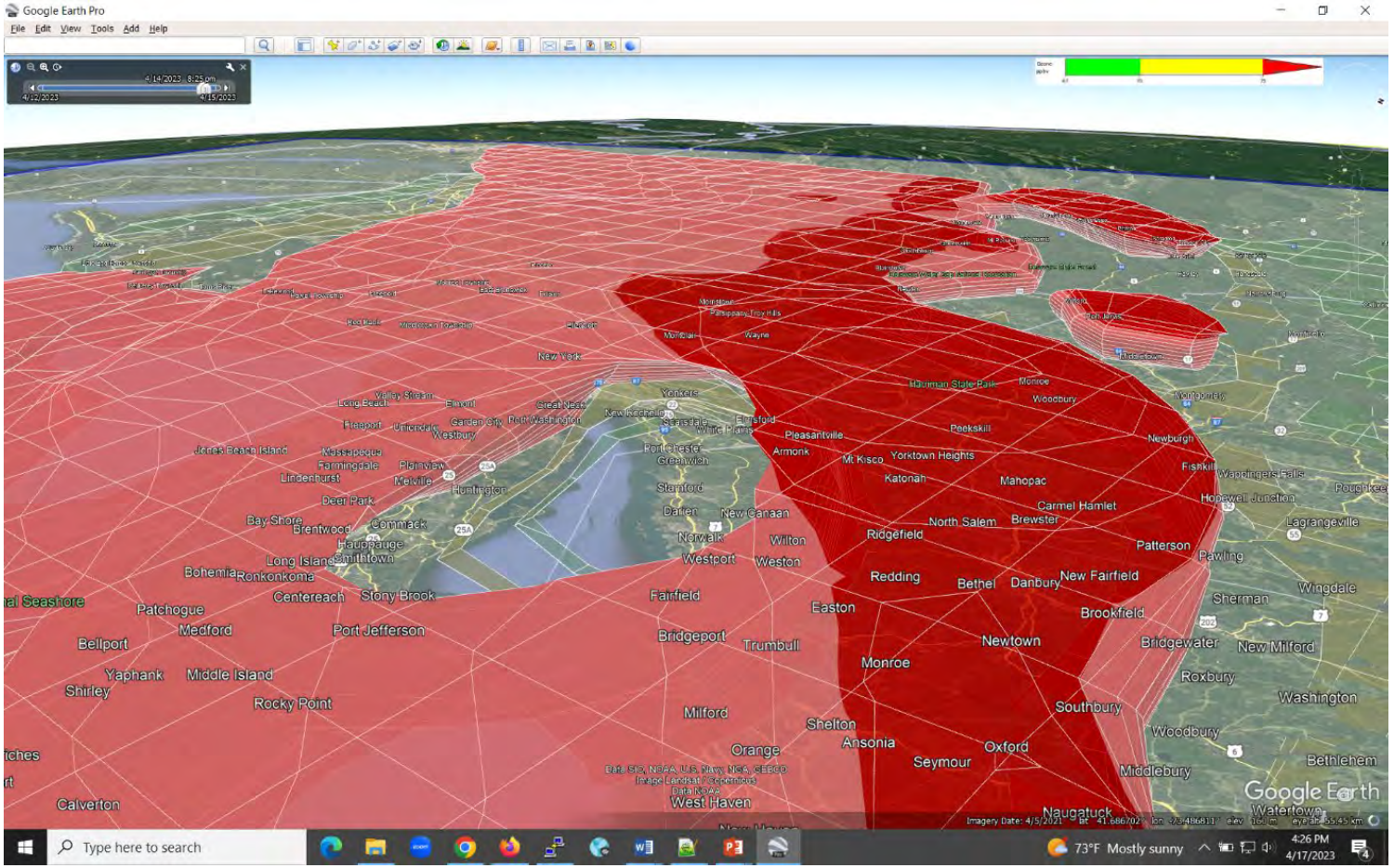
Accurate height

Use horizontal surface to measure altitude.



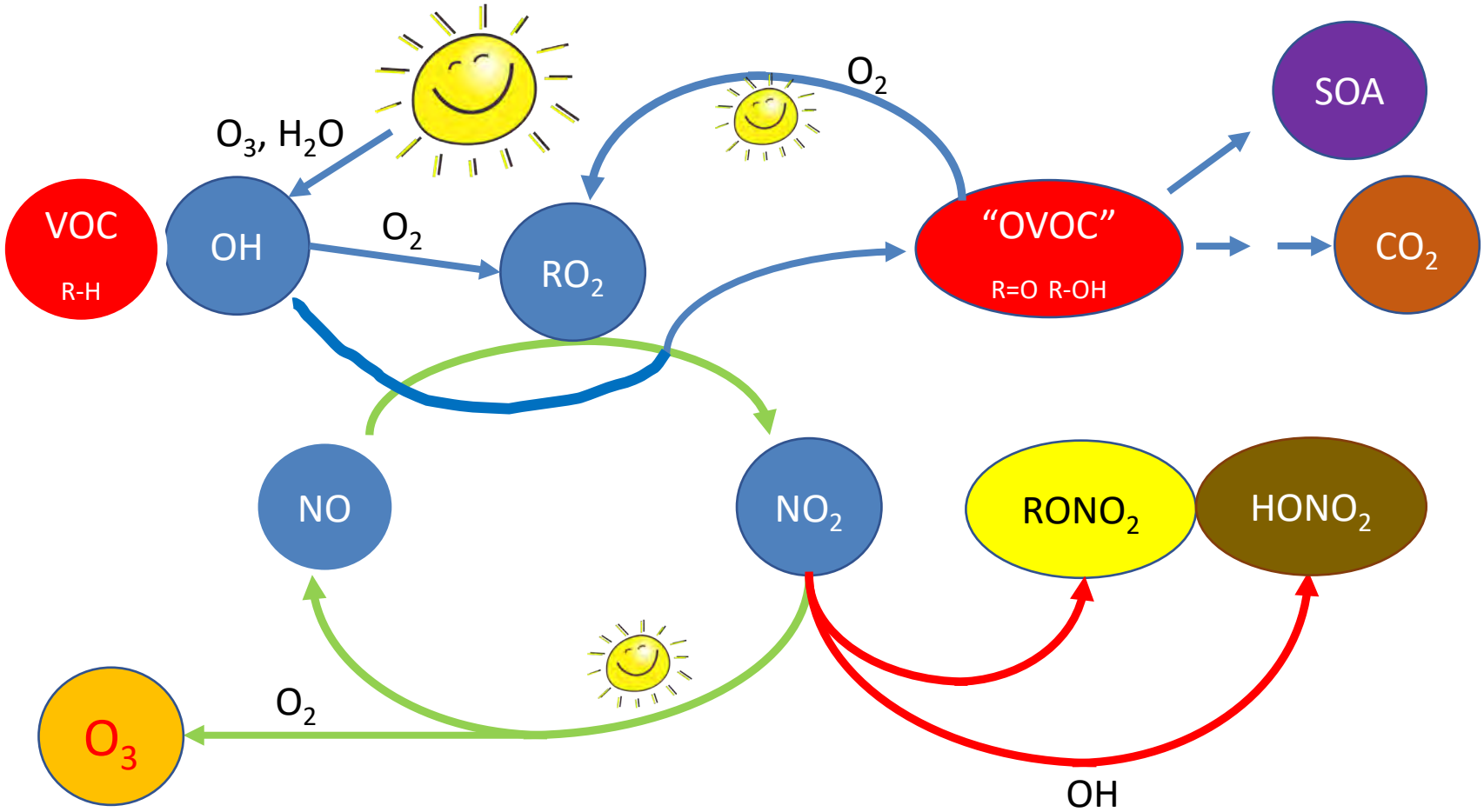
3000 meters = 9,842 feet

Ozone height over New York City
April 14, 2023 at 2025 UTC



Transparent surface at 2,100 meters = 6,890 feet.

Ozone hole over New York City? Probably NOx.



NOx-Ozone cycle by Frank Flocke.

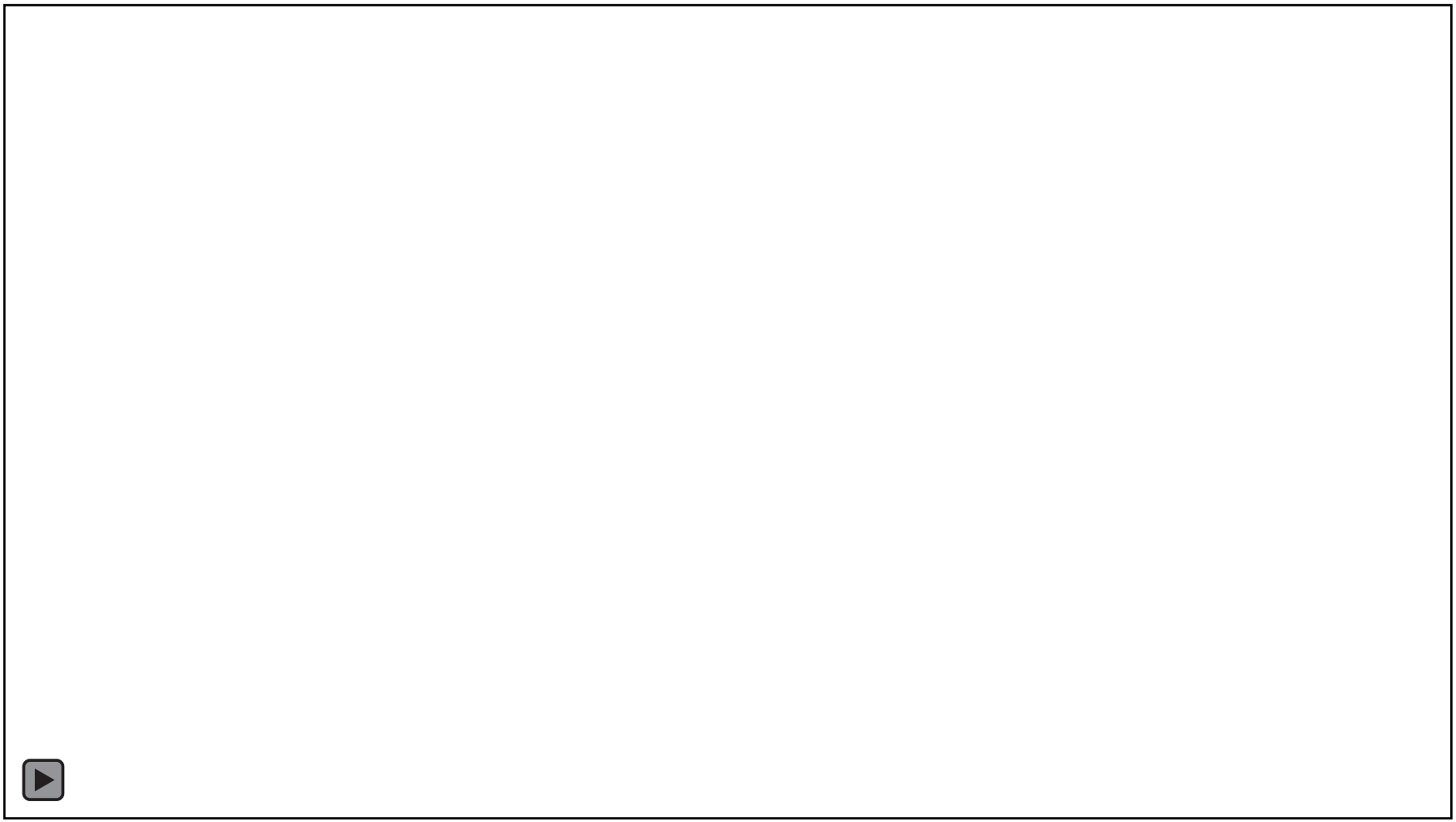
Airplanes and flight tracks

- Use KML elements:
  - Placemark, gx:Track, when, gx:coord, Model
- Smoother animation than re-creating shape in new position.
- Multiple airplanes.

NSF/NCAR Gulfstream V
(photo: Sam Hall)

NASA WB-57

ACCLIP Research Flight, South Korea; August 19, 2022



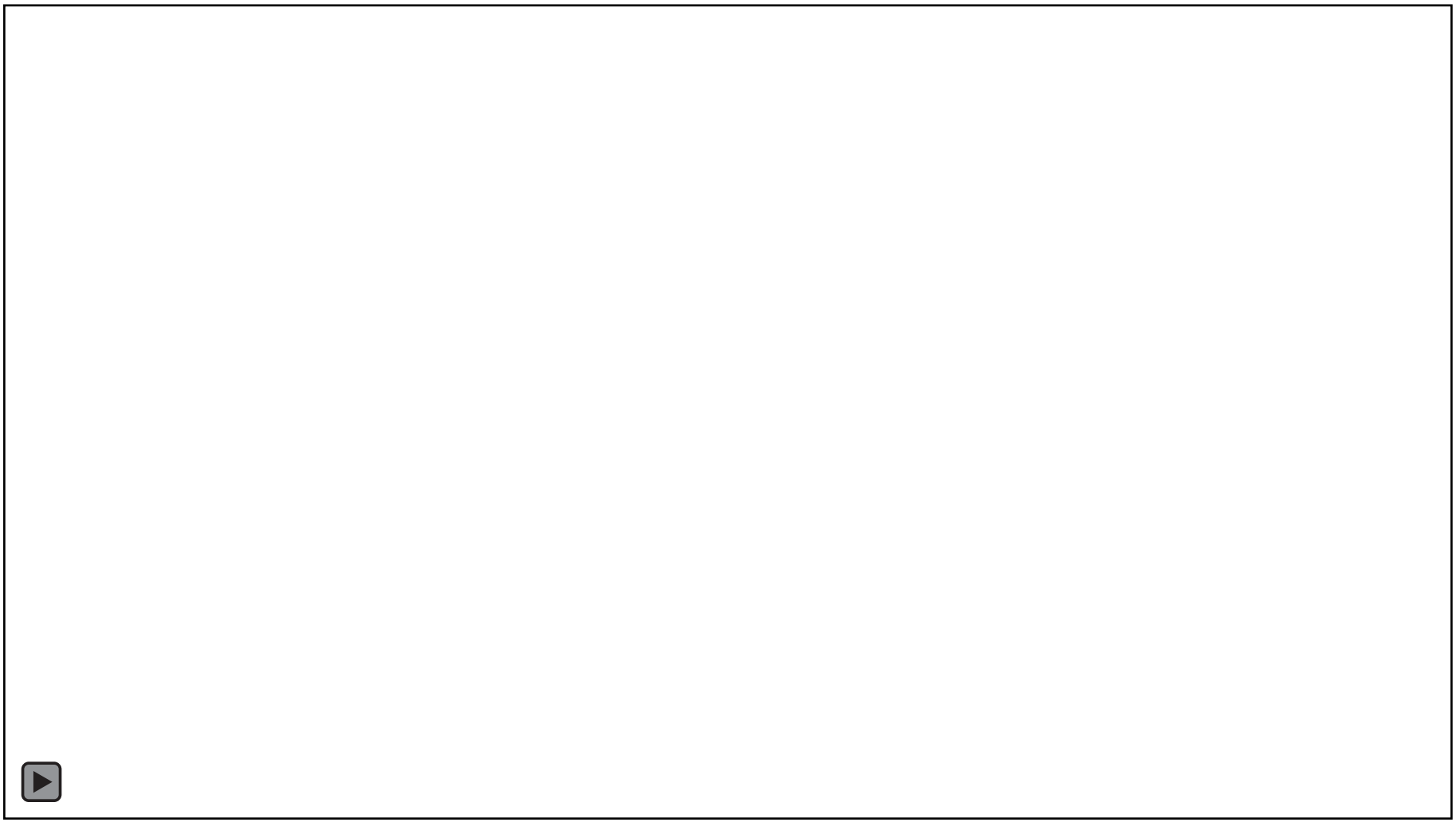
https://www.acom.ucar.edu/About_us/web-tv.shtml
https://www.acom.ucar.edu/About_us/Videos/ACCLIP-WB57-RF10-August19-2022.mp4

Back-trajectories of air parcels

Our research aircraft just sampled some chemical. Where did that chemical come from? What is the source of that air parcel?

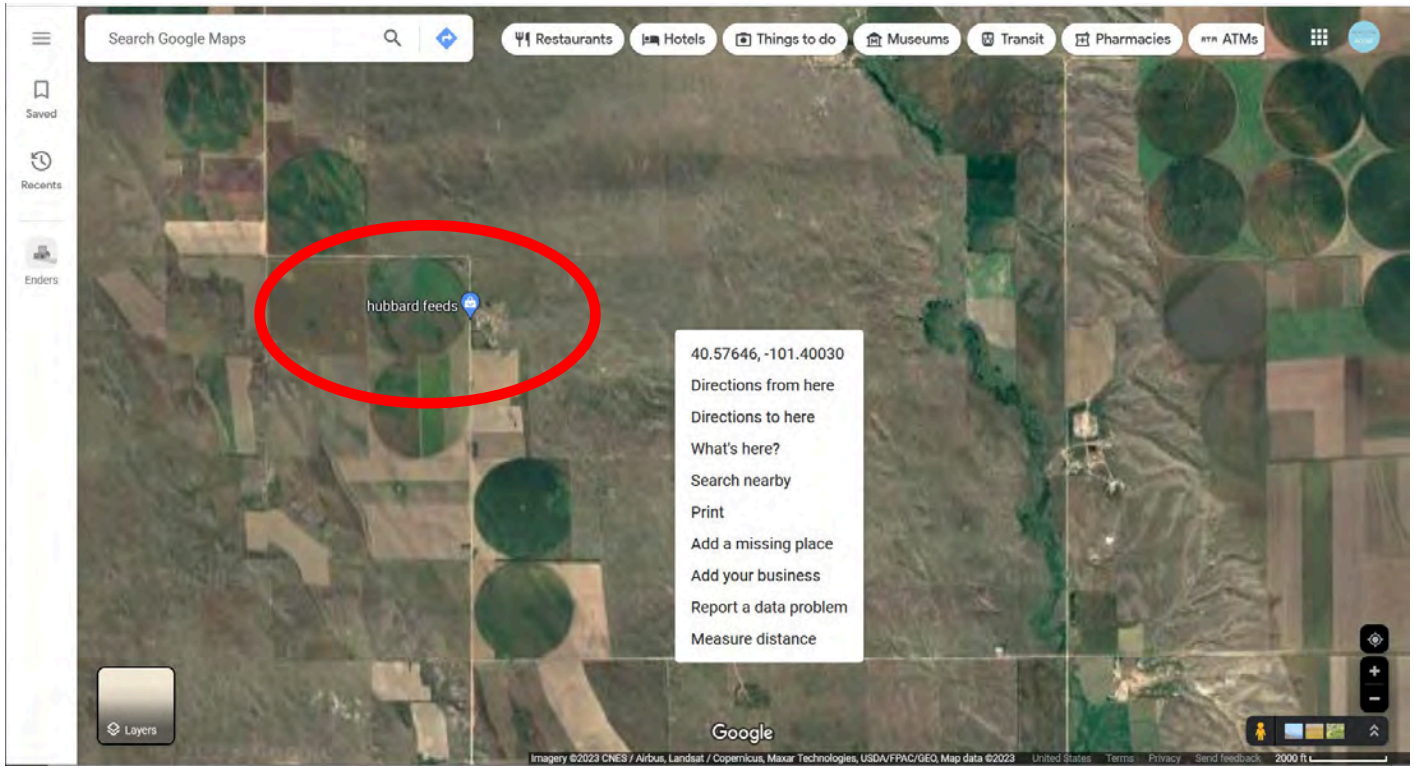
NASA DC-8 instrumented for FIREX-AQ campaign during July-August 2019.

Air parcel trajectories over the Western Pacific

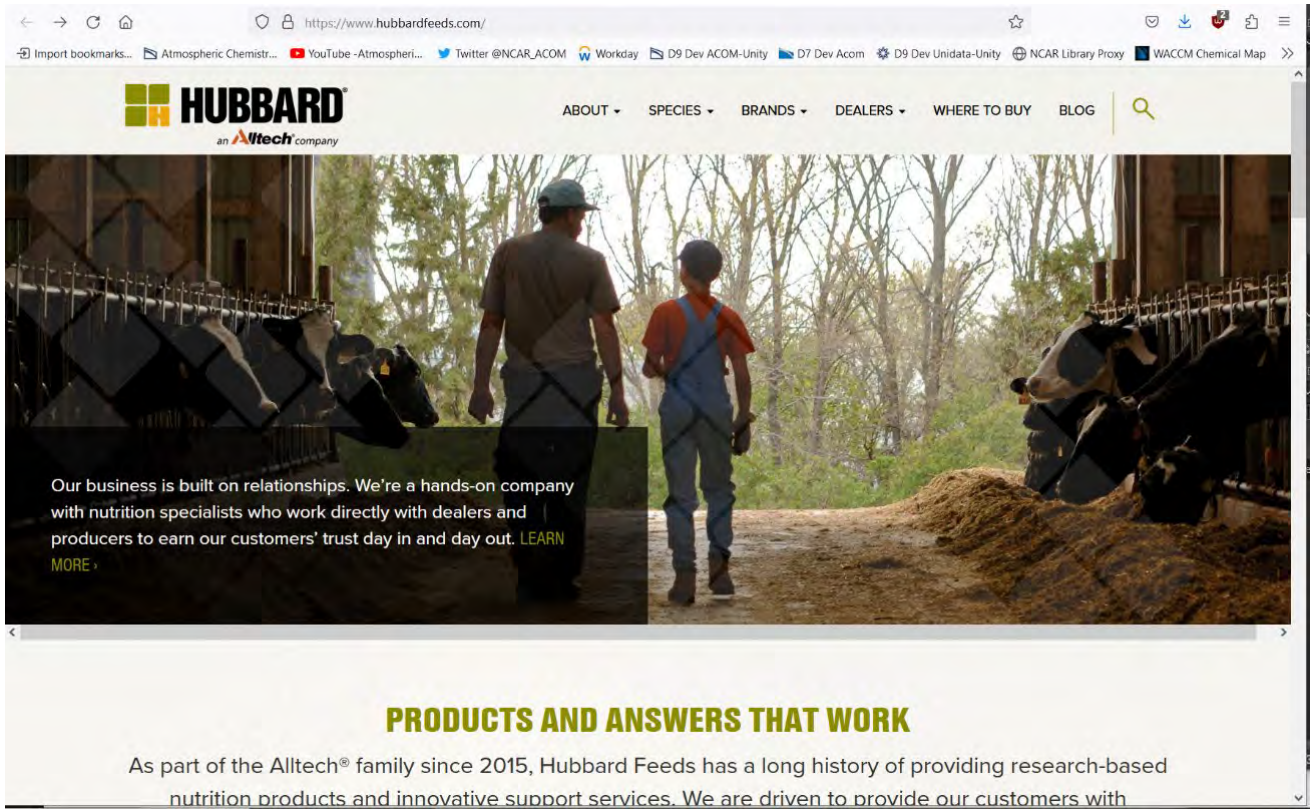


Example: Ozone exceedance over Enders, Nebraska

Maximum surface value of [ozone] 0.07396125048398972 ppmv occurred at 40.57630920410156 N, -101.39999389648438 W on 2022-12-13 14:00:00

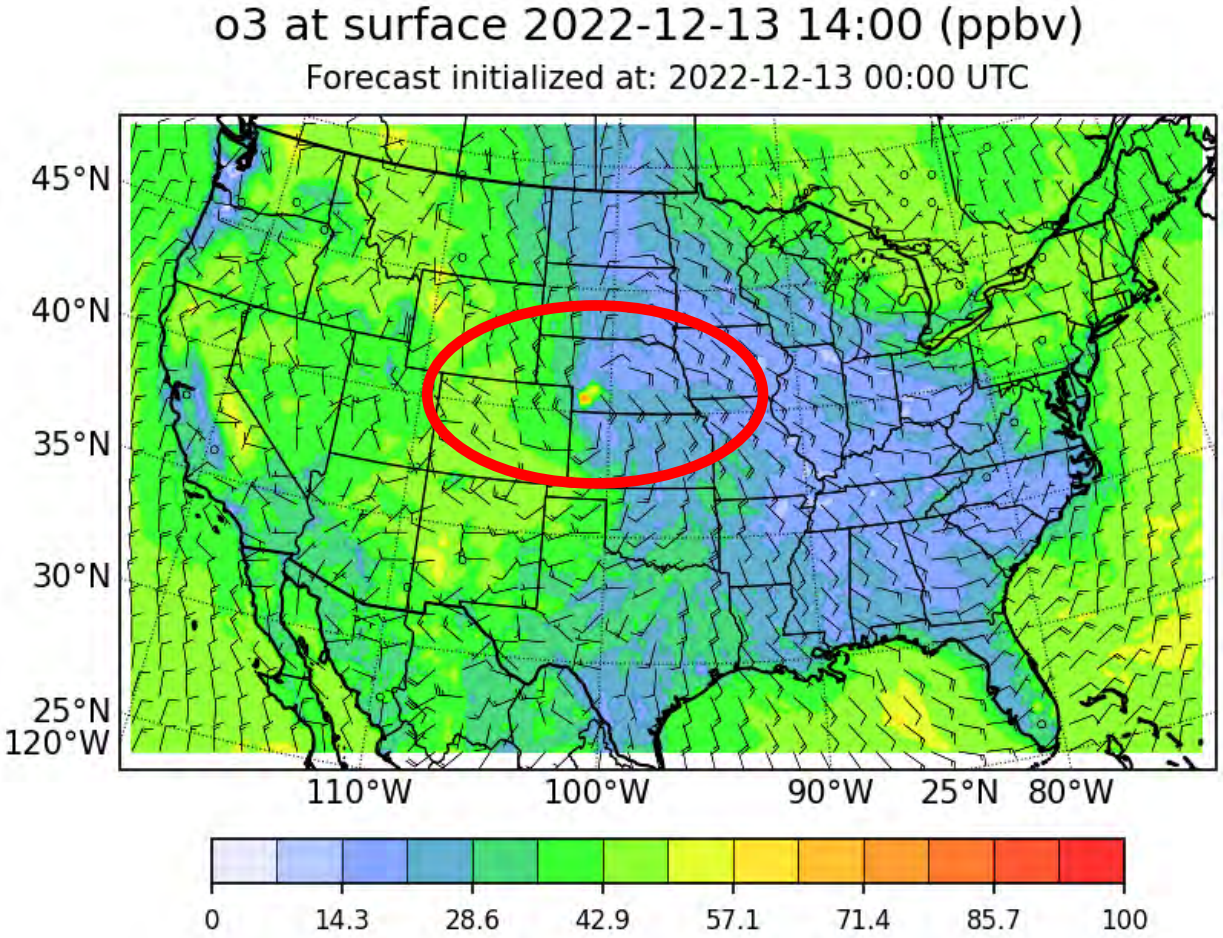


What's going on there?



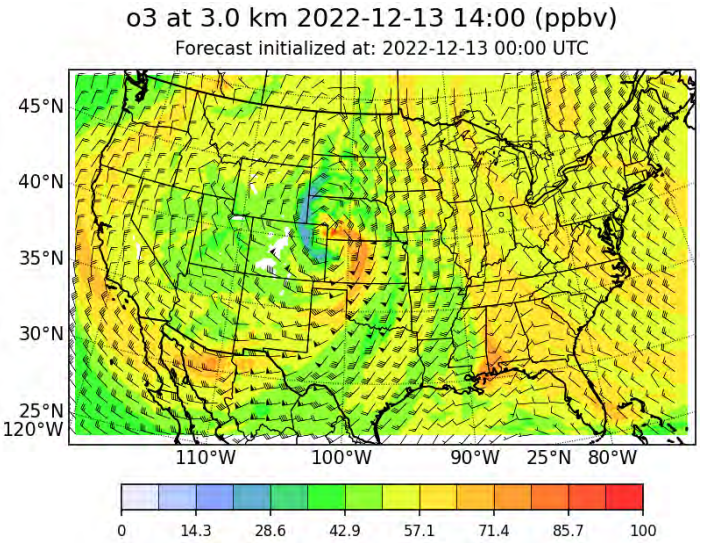
Enders, Nebraska is 3 hours and 40 minutes away from Denver by car. But . . . something doesn't seem right.

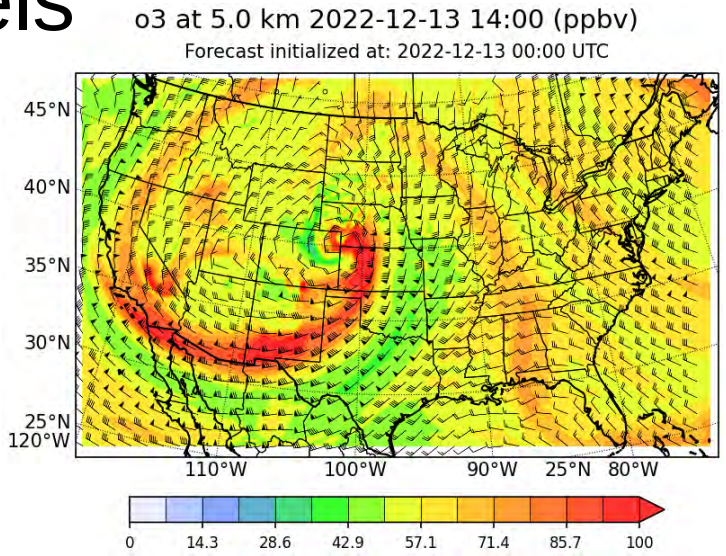
Look at the WRF-Chem output

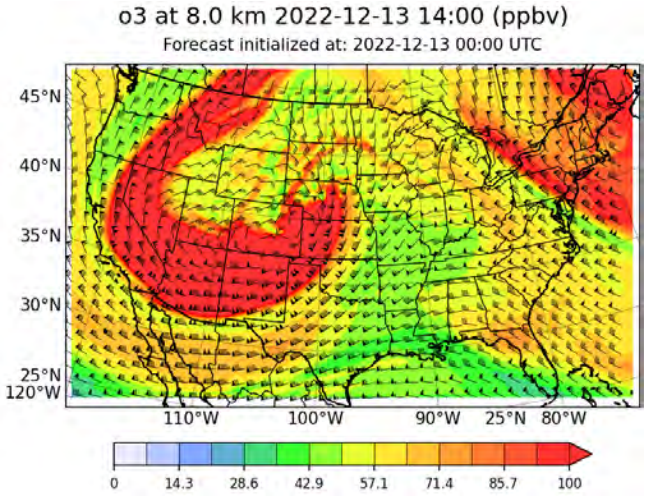


The wind field . . . !

Look at the higher levels



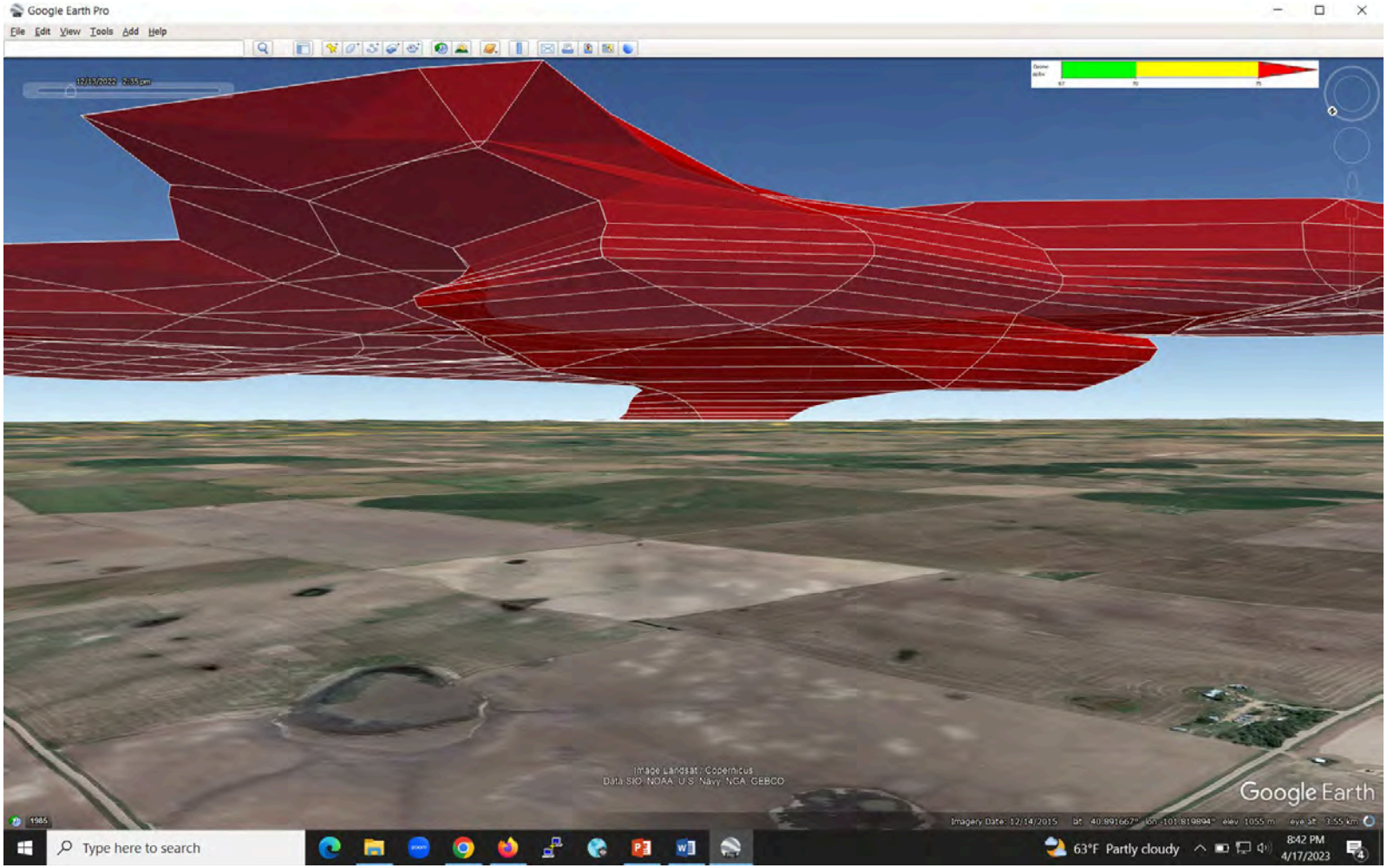




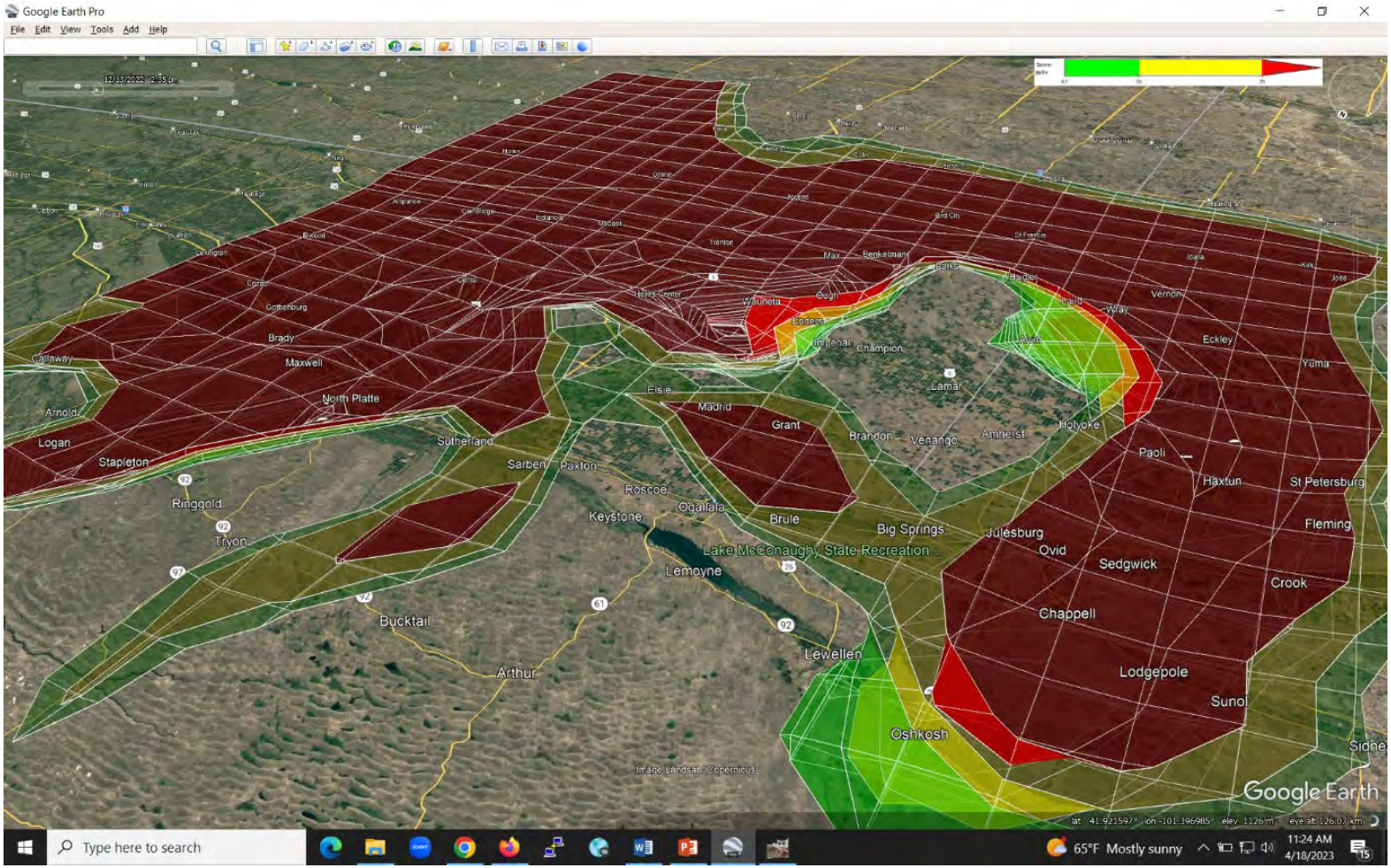
A cyclonic storm is bringing ozone from the stratosphere down to the surface – in a farmer's field near Enders, Nebraska!

A **Stratospheric Intrusion Event**.

Stratospheric intrusion in 3D



Stratospheric Intrusion from above



Visualization is for insight

For the general public, colleagues, and you.

Chouza, Fernando, Thierry Leblanc, Mark Brewer, Patrick Wang, Sabina Piazzolla, Gabriele Pfister, Rajesh Kumar, Carl Drews, Simone Tilmes, Louisa Emmons, Matthew Johnson, 2021: **The impact of Los Angeles Basin pollution and stratospheric intrusions on the surrounding San Gabriel Mountains as seen by surface measurements, lidar, and numerical models**. *Atmospheric Chemistry and Physics*, OpenSky.

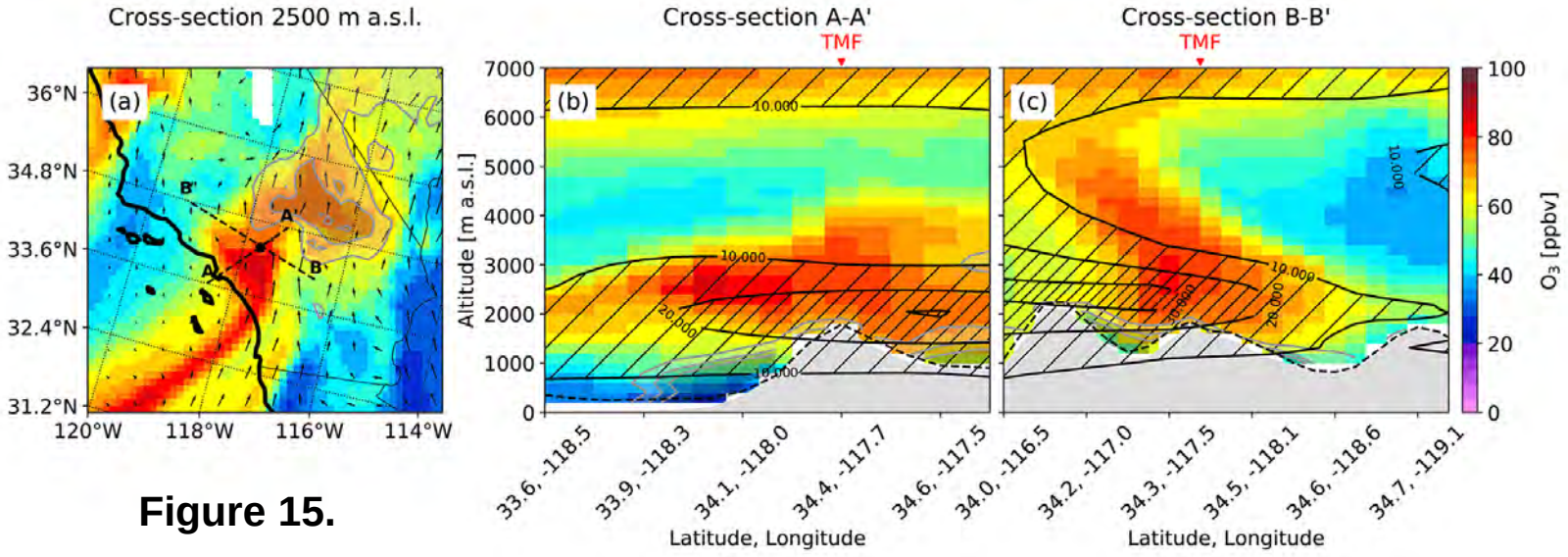
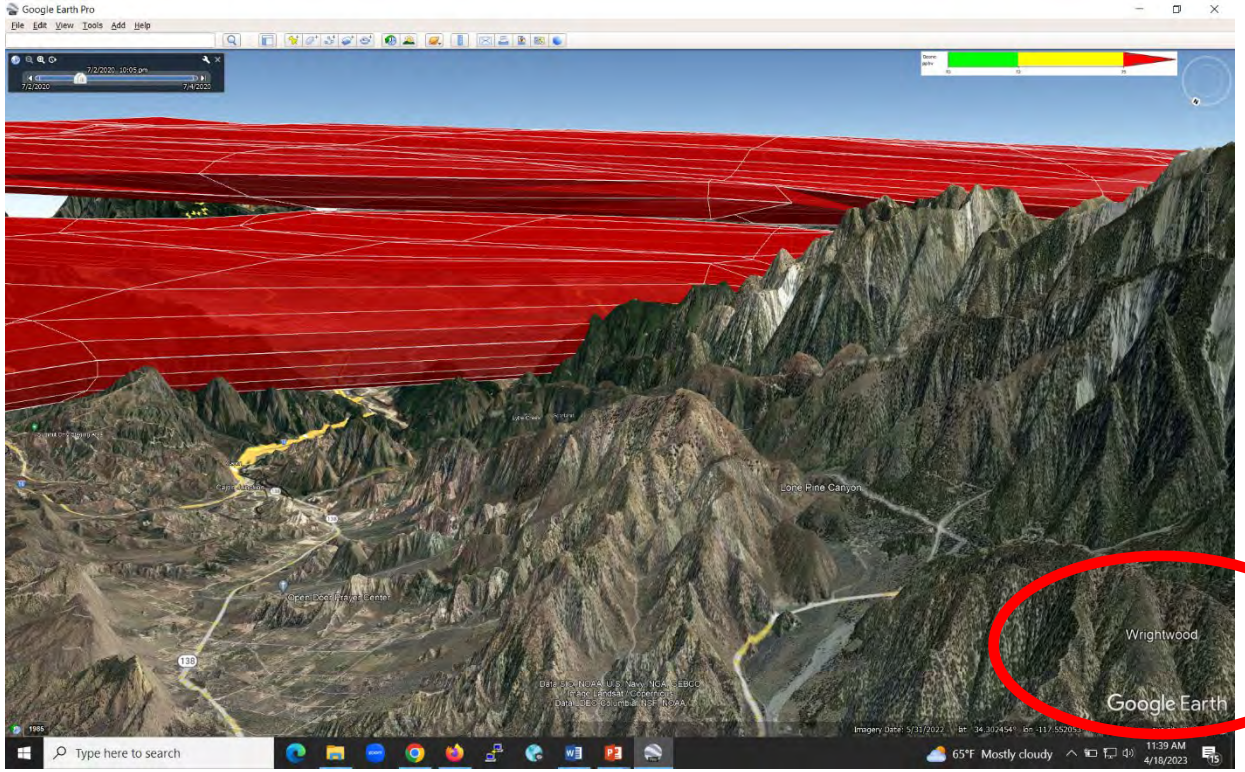


Figure 15.

Ozone at Cajon Junction, Los Angeles July 2, 2020 at 22:05 UTC

Chouza 2021 shows **two** combined ozone events: stratospheric intrusion **and** urban ozone.



NASA JPL Table Mountain Facility

Archives of KMZ files for WRF-Chem evaluation

- Generated for CO_fire and O3 every day.
- https://www.acom.ucar.edu/firex-aq/FIREX-AQ/Evaluation/KMZ/
- Also animations of CO_fire over CONUS (Gabriele Pfister).
- Download. Review. Repeat . . .

Questions?

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National Center for Atmospheric Research (NCAR)
Boulder, Colorado USA

Urban smoke plumes

- Scale too small for WRF-Chem (regional).
- Suitable for LES (Large Eddy Simulation).
- Or Flexpart (Lagrangian model).

CNN.com; April 12, 2023