



July 28, 2026

Introducing CREDIT-chem: A Hybrid Physics–Machine Learning Framework for Modeling Atmospheric Aerosol Chemistry

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A Collaboration Between NCAR CISL-MILES and NCAR ACOM



Why Model Atmospheric Chemistry?

Regional Air Quality Forecasts

- Atmospheric aerosols, such as Black Carbon, greatly impact public health

Global Climate Forcings

- Atmospheric aerosols play a very important role in our climate, influencing factors such as radiative balance, cloud microphysics, and precipitation patterns



What Wrong With Current Models?

Why Do We Need New Frameworks?

Explicit Physical Models (ex: GECKO)



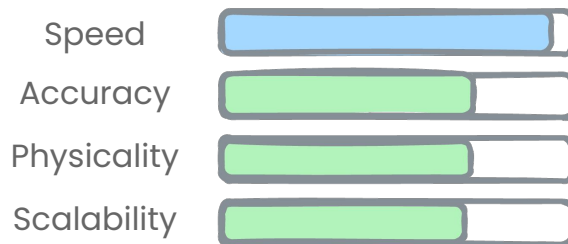
Paramaritized Physical Models (ex: CAM6-chem)



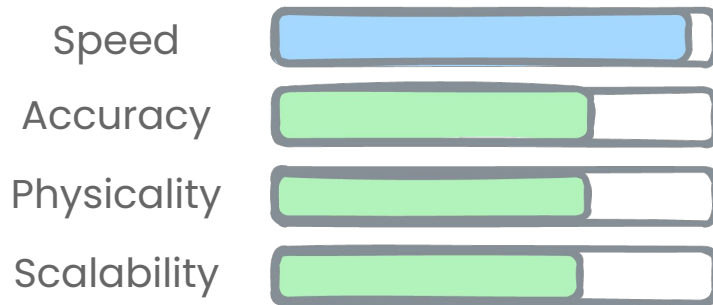
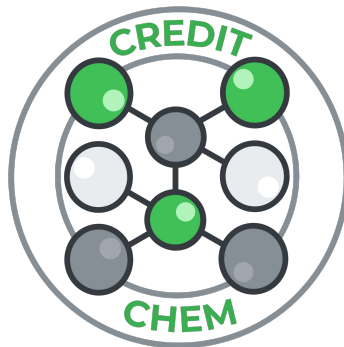
Traditional ML Models (ex: Microsoft-Aurora)



???



Introducing, CREDIT-chem



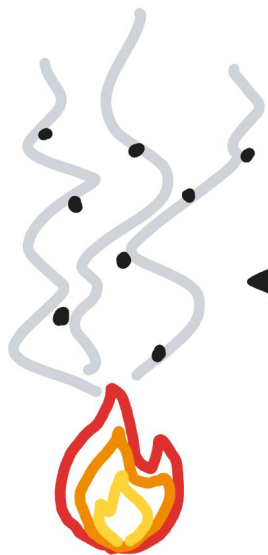
What are we specifically modeling?

Emphasis on Black Carbon (BC)

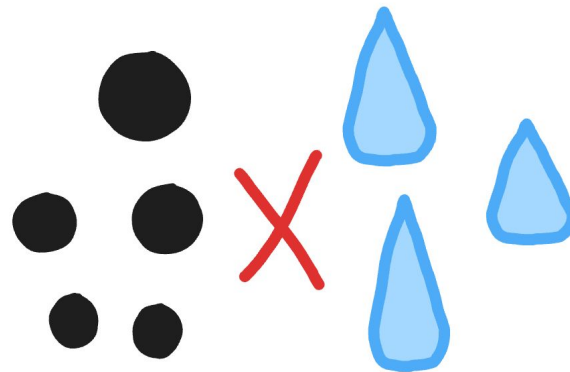
Simulating primary organic matter (POM), secondary organic aerosols (SOA), and sulfates as well

Background into Black Carbon

Black Carbon Background



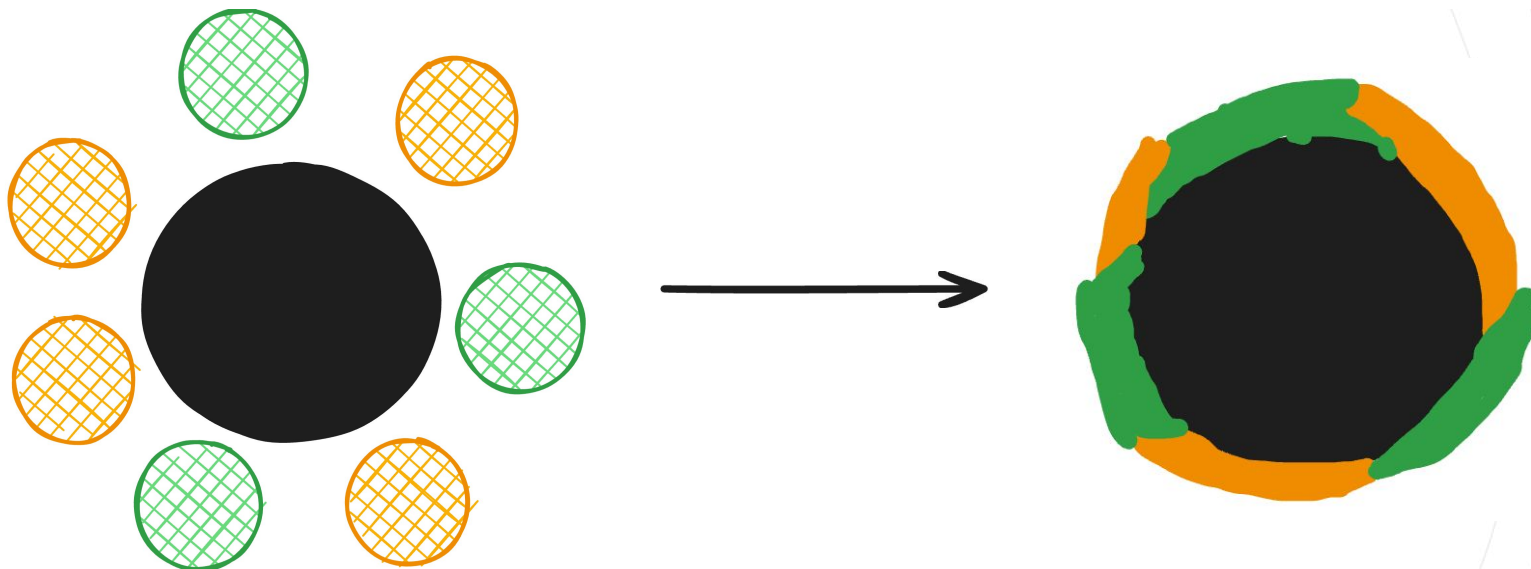
Black Carbon (BC) comes from incomplete combustion of carbon-based fuels, like wood or diesel



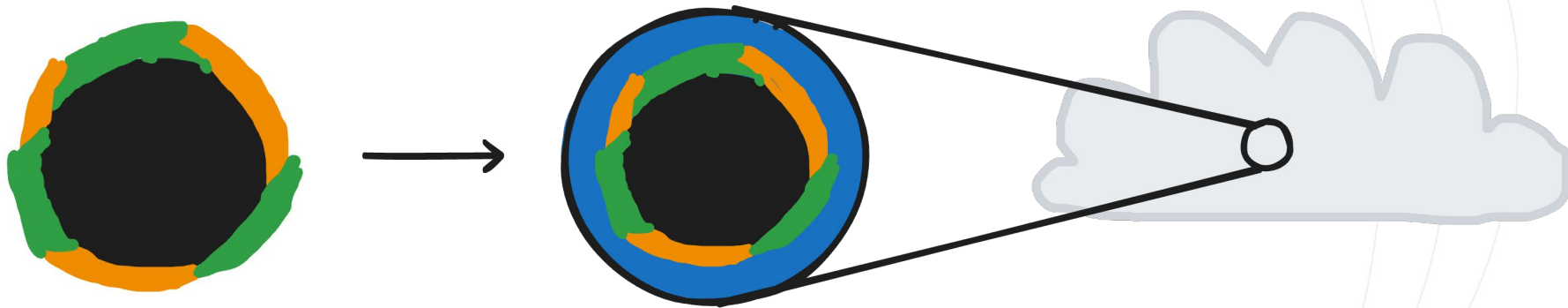
BC in its “young”, freshly emitted state is very hydrophobic and cannot act as a cloud condensation nuclei (CCN)

Black Carbon Background

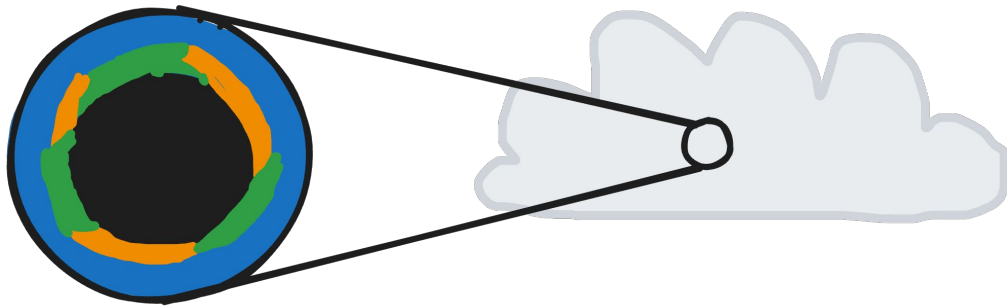
Sulfates and Secondary Organic Aerosols (SOAs) throughout time condensate onto the “young” BC. After the BC particle has been coated enough, it becomes “aged”, in which it is much more hydrophilic and a much better cloud condensation nuclei



Water will then condensate onto the
“aged” BC, and it is then classified as
“cloud-borne” BC



When “cloud-borne” BC precipitates out of its cloud, the BC falls to the surface and “deposes”, ending the BC’s journey



Back to CREDIT-chem, how is CREDIT-chem's framework different from other models?

Explicit Physical Models (ex: GECKO)



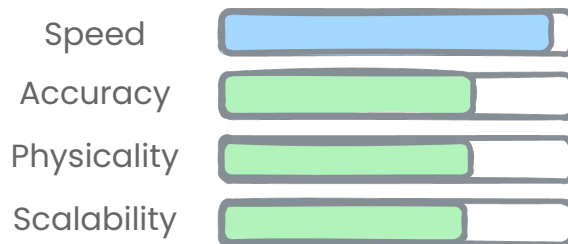
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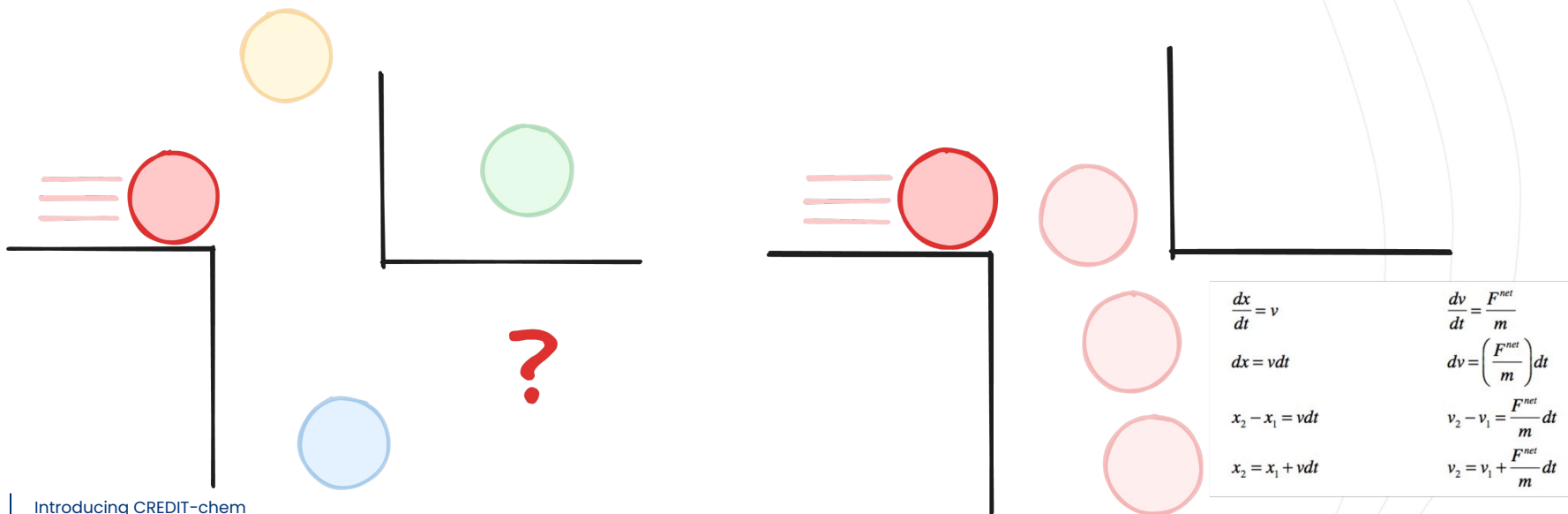
Traditional ML Models (ex: Microsoft-Aurora)



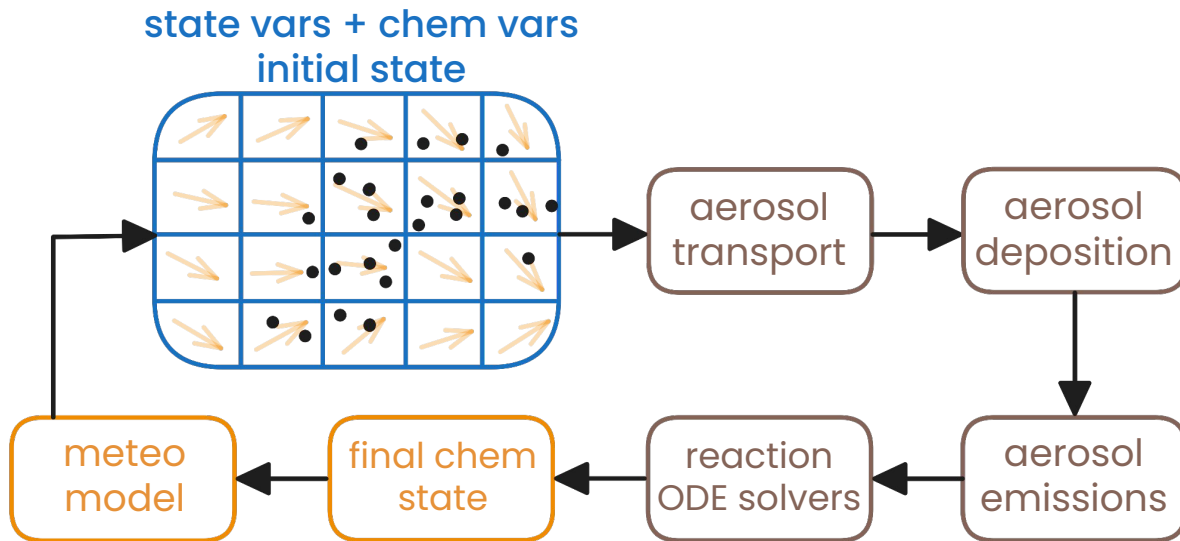
CREDIT-chem (in theory)



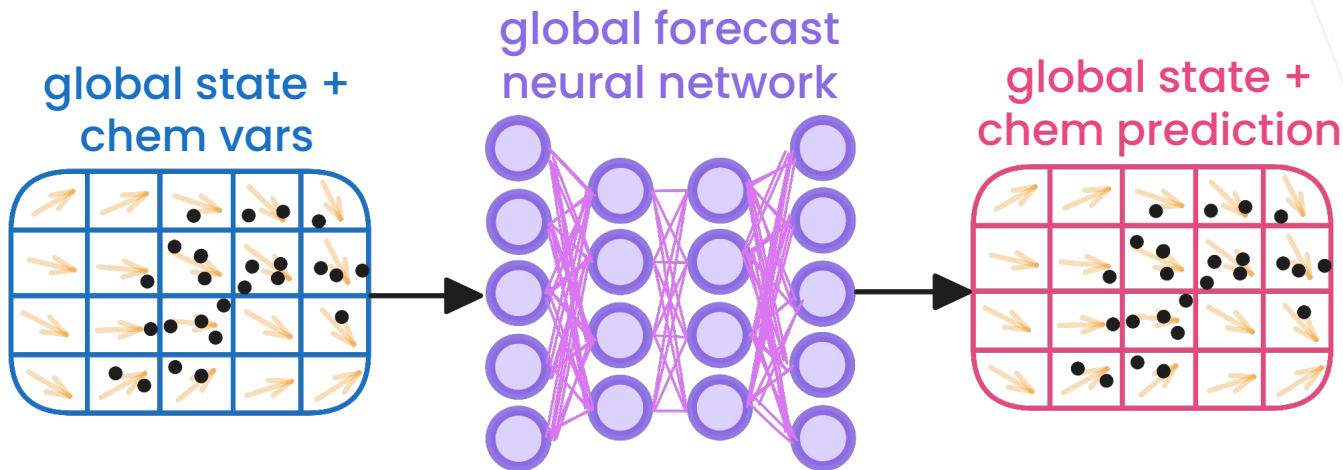
A Machine Learning (ML) model learns through statistical pattern recognition, rather than explicit physical processes



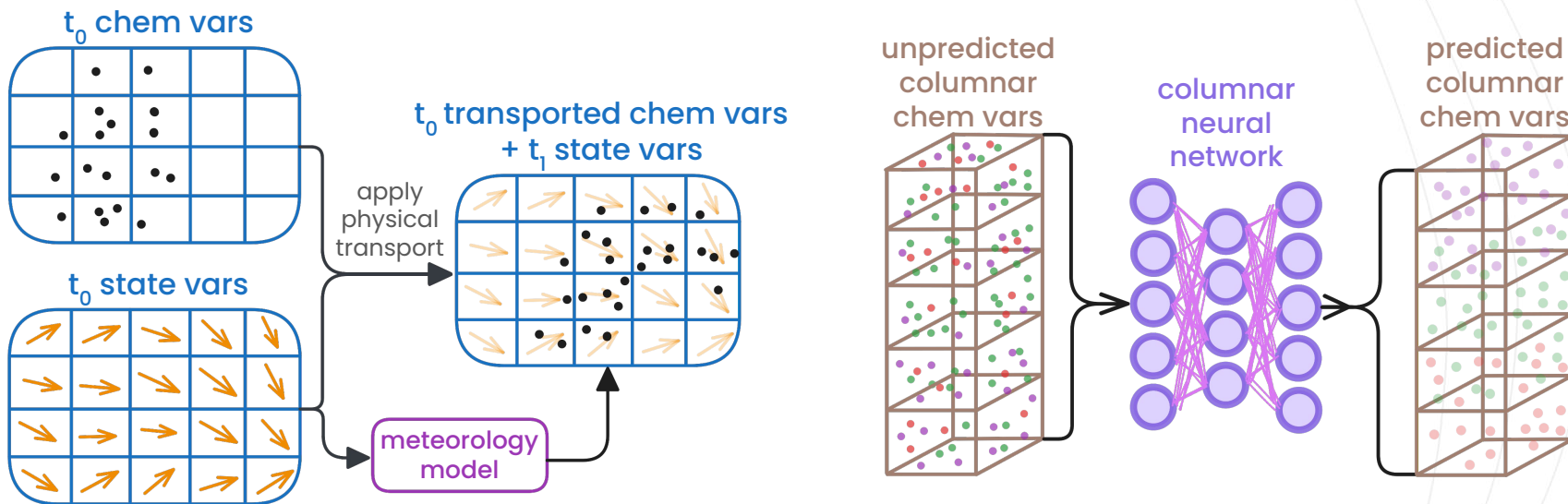
Workflow for a Physics-Based Model



Workflow for a Full Machine Learning Model



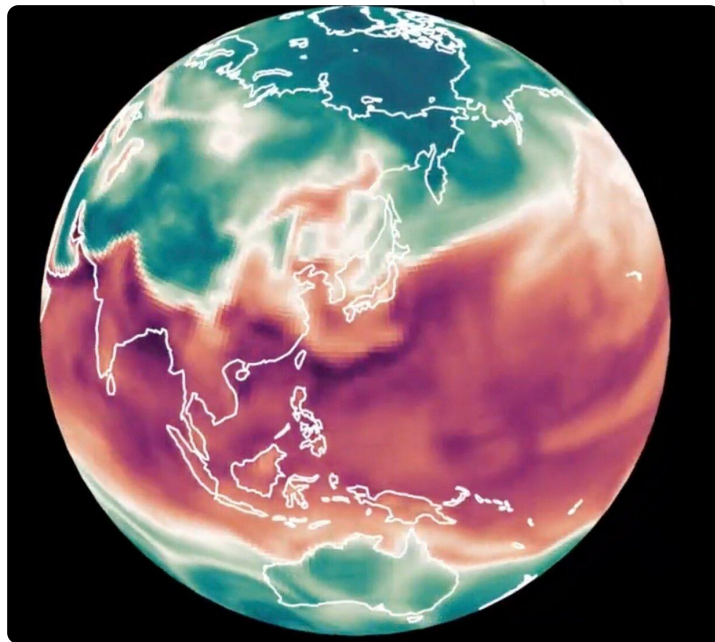
Hybrid Workflow for CREDIT-chem



NOTE: Physical transport
is NOT ML based

Input/Training Data

- Our specific test case is trained on CAM6-chem model outputs
 - ~1° resolution, 32 vertical levels, 1-hour time step
- Forecasts Black Carbon (BC), Primary Organic Matter (POM), Secondary Organic Aerosols (SOAs), and Sulfates
 - Meteorological inputs are given, they not forecasted as a part of CREDIT-chem
- *Note that CREDIT-chem can train on any chemistry model data, not just the ones listed*

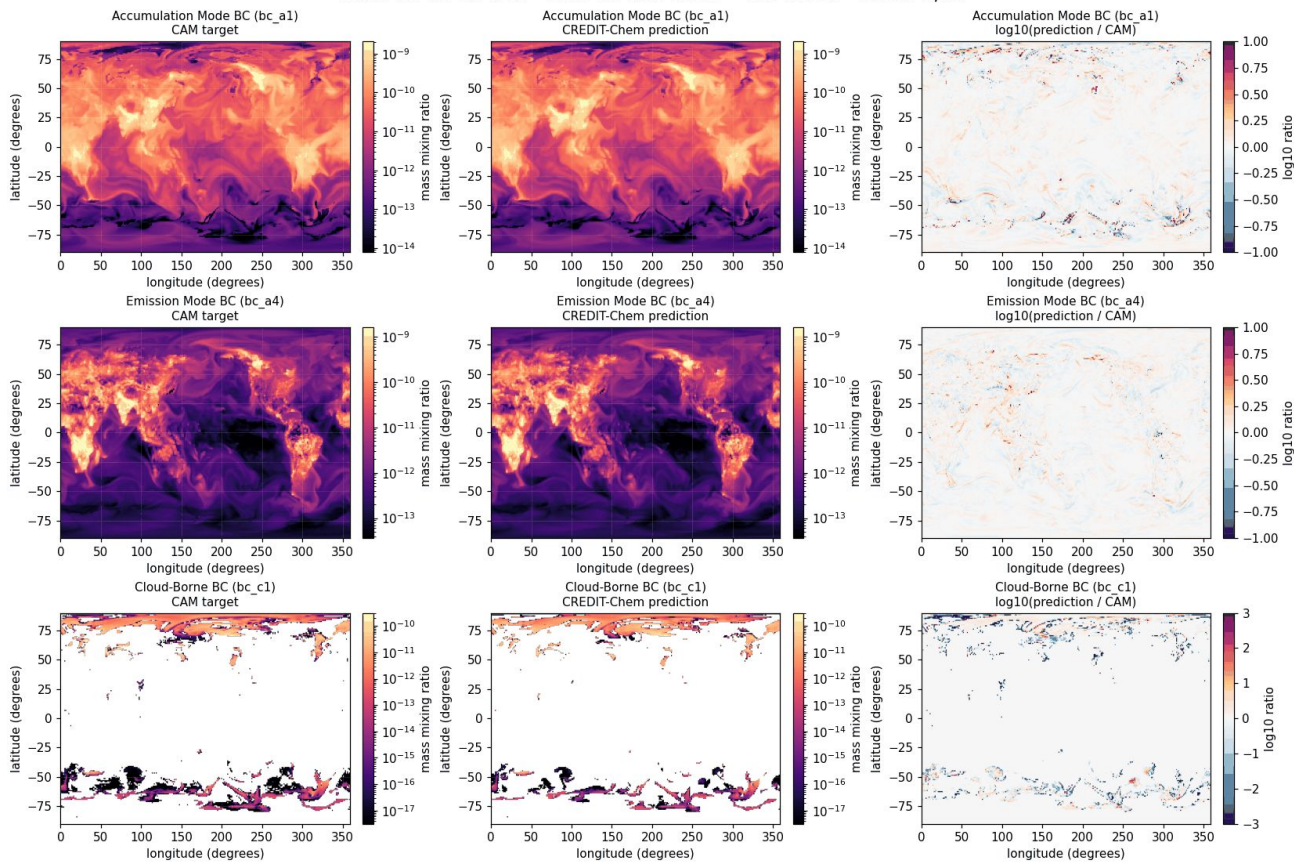


How well does CREDIT-chem actually perform?

CREDIT-chem Results

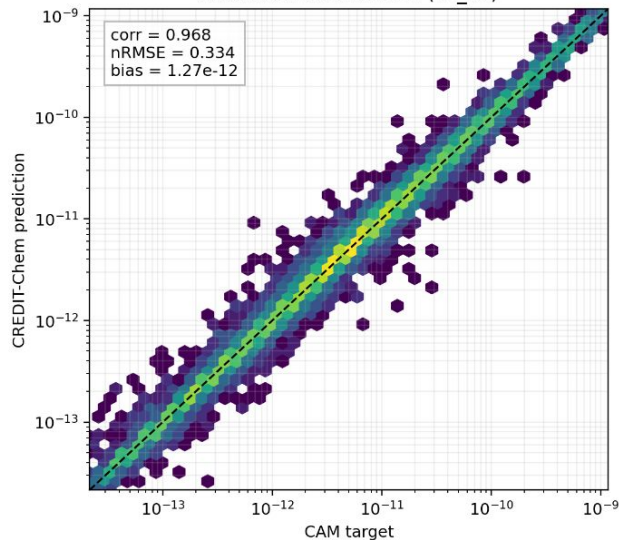


Held-out CAM comparison: BC target, CREDIT-Chem prediction, and error
2023-09-01 02 UTC · near-surface level = 957.6 hPa · frame 1/23

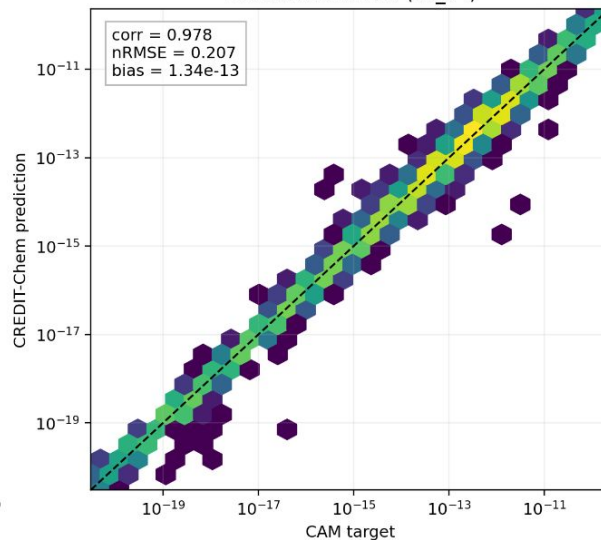


CREDIT-Chem prediction versus CAM target in physical space

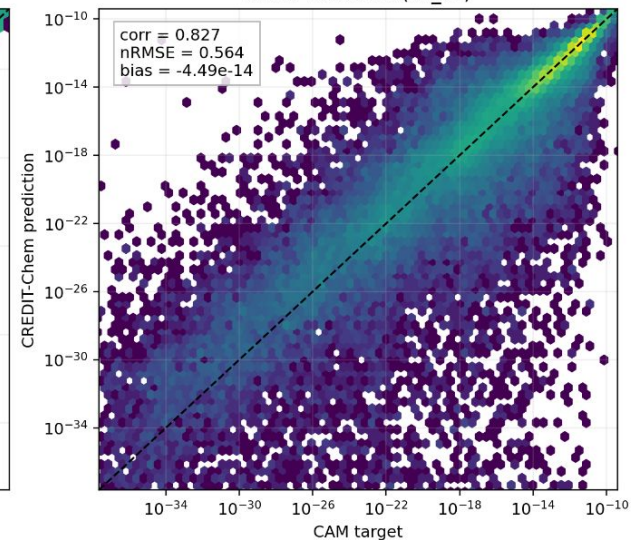
Accumulation Mode BC (bc_a1)



Emission Mode BC (bc_a4)



Cloud-Borne BC (bc_c1)



High Accuracy & Speed

CREDIT-chem matches CAM6-chem outputs with high correlation while accelerating inference time by multiple orders of magnitude.

Long-Term Stability

Preliminary multi-step rollouts demonstrate strong stability over extended time horizons, validating CREDIT-chem's use for both short-term forecasting and long-term climate runs.

Comparative Performance

Fully end-to-end ML models can still outperform the hybrid setup under specific conditions, though they remain severely bound by spatial resolution scaling constraints..

High-Resolution Testing

While CREDIT-chem's design is theoretically built to scale, testing accuracy and performance at sub-degree global resolutions remains ongoing work.

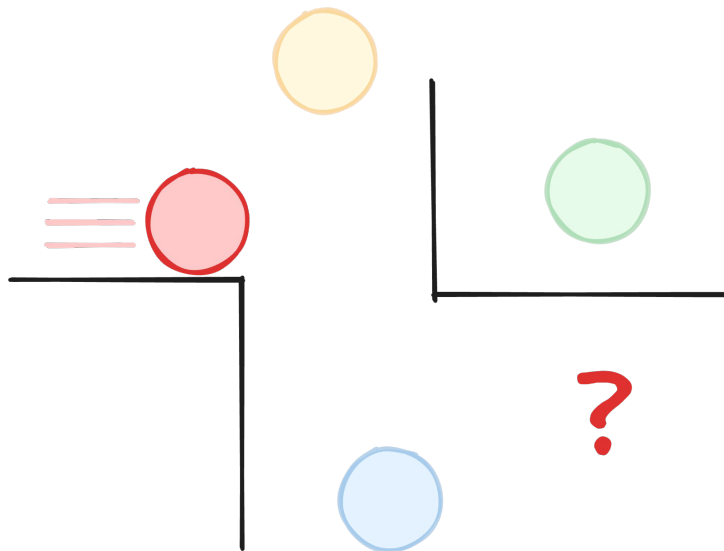
Thank you!

A special thanks again to my mentors: DJ, Charlie, Alma, Ben, and John, as well as many other interns and staff here at NCAR/UCAR for their guidance and support on this project. In addition, I'd like to thank NCAR and the SIParCS program for giving me the opportunity and resources to complete this work.

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Background into Machine Learning

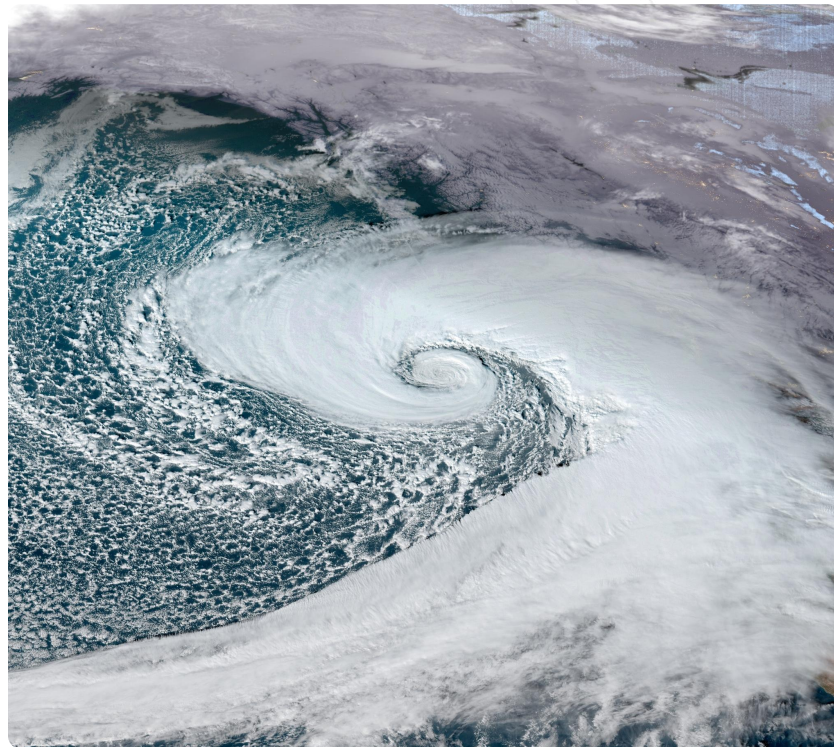
A Machine Learning (ML) learns through pattern recognition, rather than explicit physical processes



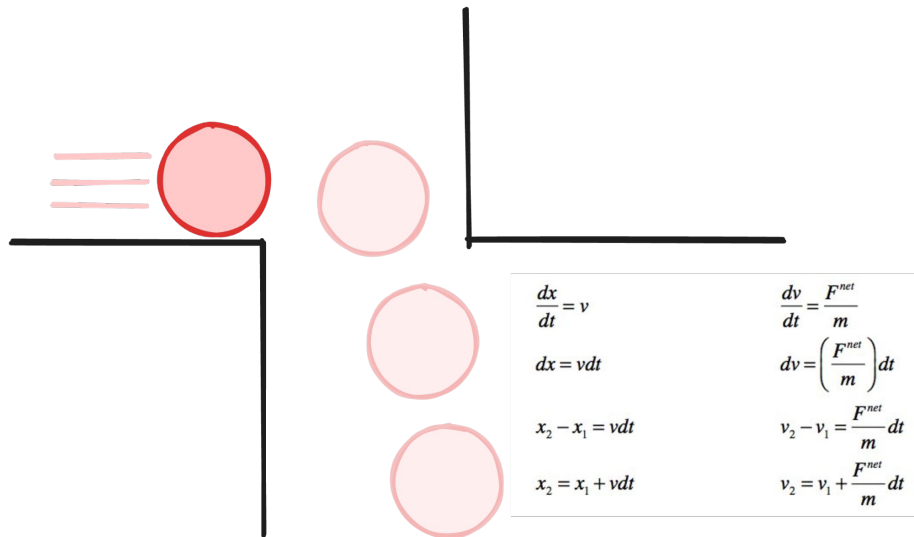
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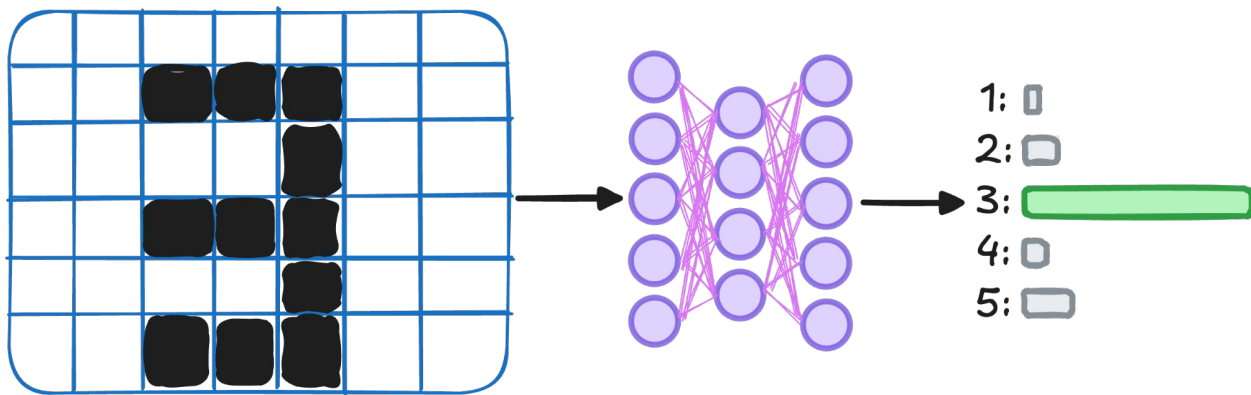
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A Machine Learning (ML) learns through pattern recognition, rather than explicit physical processes

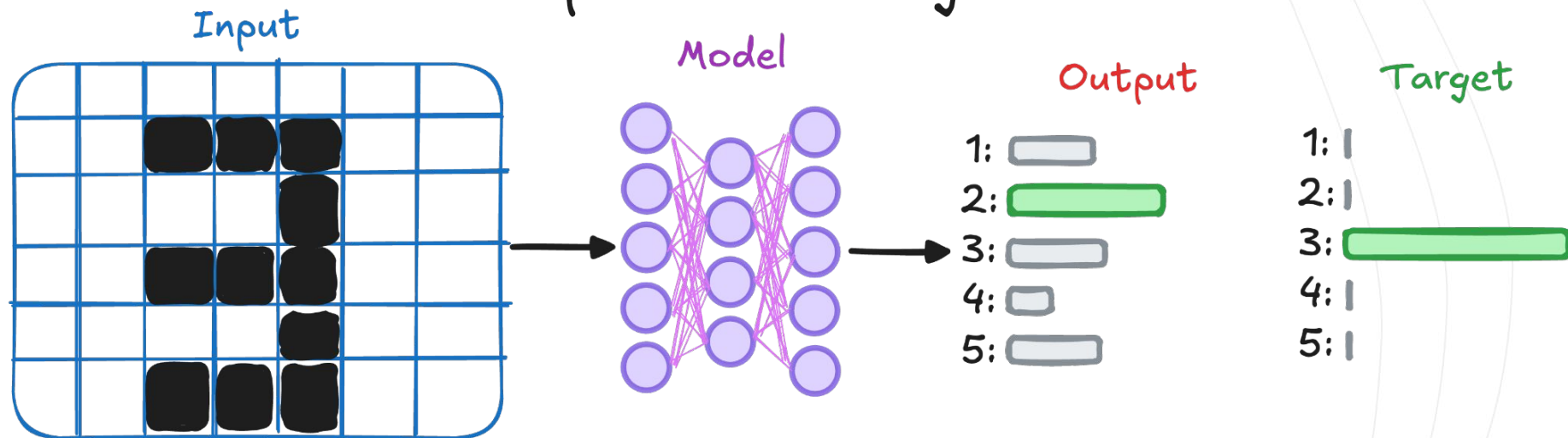


How does the model "learn"
this pattern recognition?



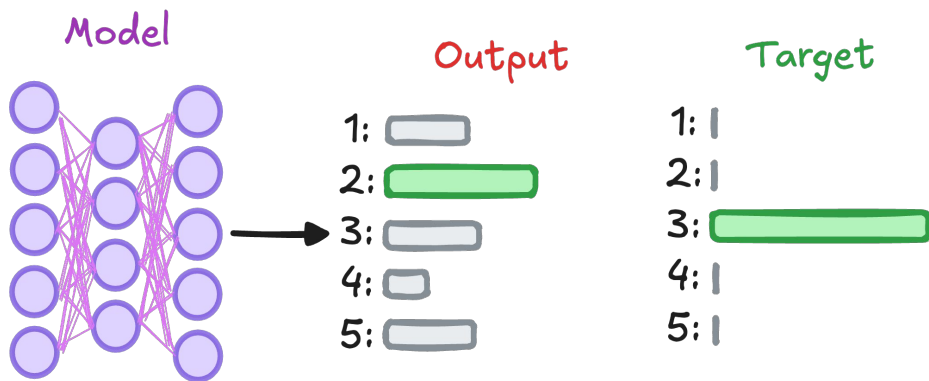
From a big picture standpoint, ML models
try to learn weights and biases to produce
an output that matches some "target"

How does the model "learn"
this pattern recognition?

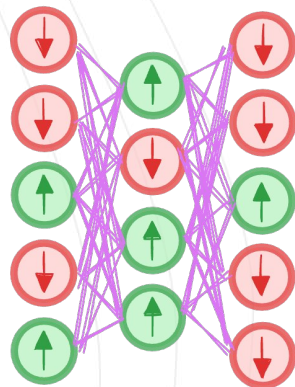
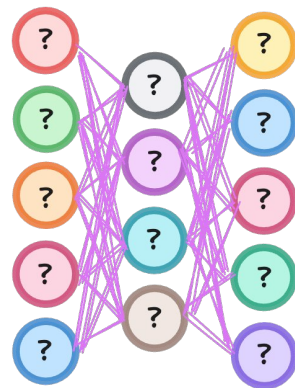


This is the general schema of how a ML model is trained

How does the model "learn"
this pattern recognition?



You want to make your model's
output be closer to the target

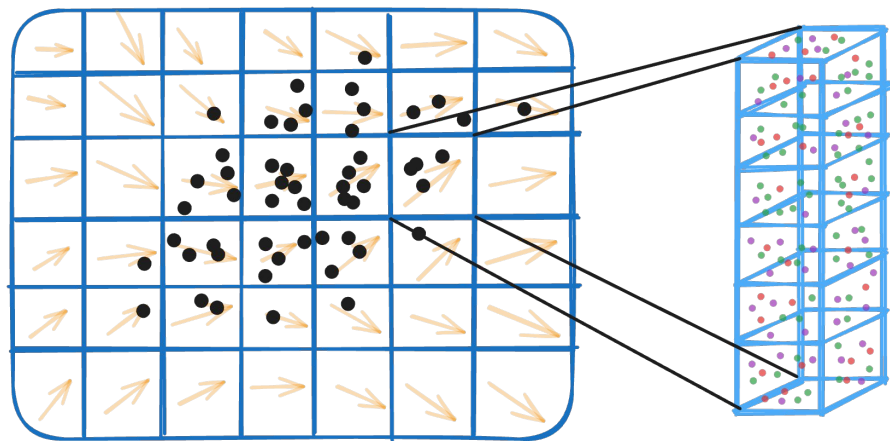


You "randomly" tweak each weight
of the model, until you find a direction
that takes you closer to the target

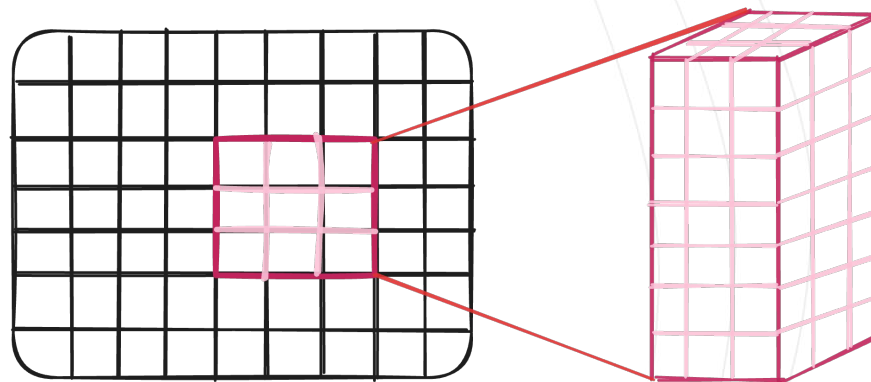
How CREDIT-chem works

How CREDIT-chem works

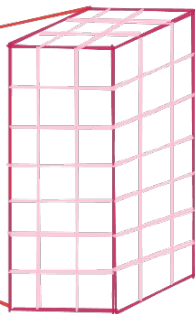
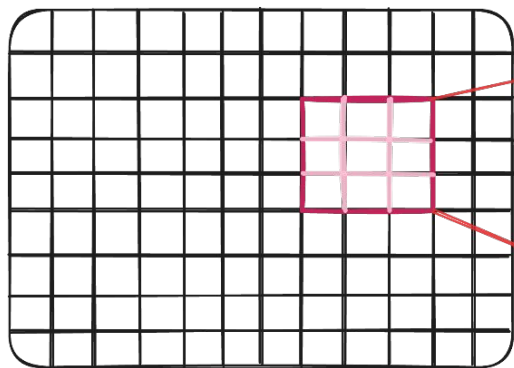
chem-columnar



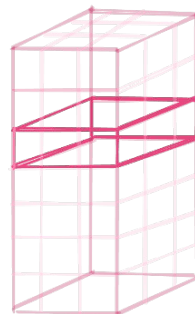
chem-cubed



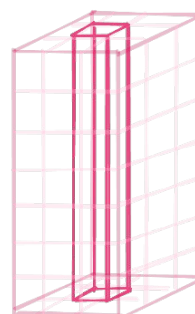
Full ML Model (chem-cubed)



Grab an $n \times n$ cube,
centered
at the col of
interest



The model will then
send information
only horizontally
between *all* layers



The model then does
chemistry vertically
only in the center
column



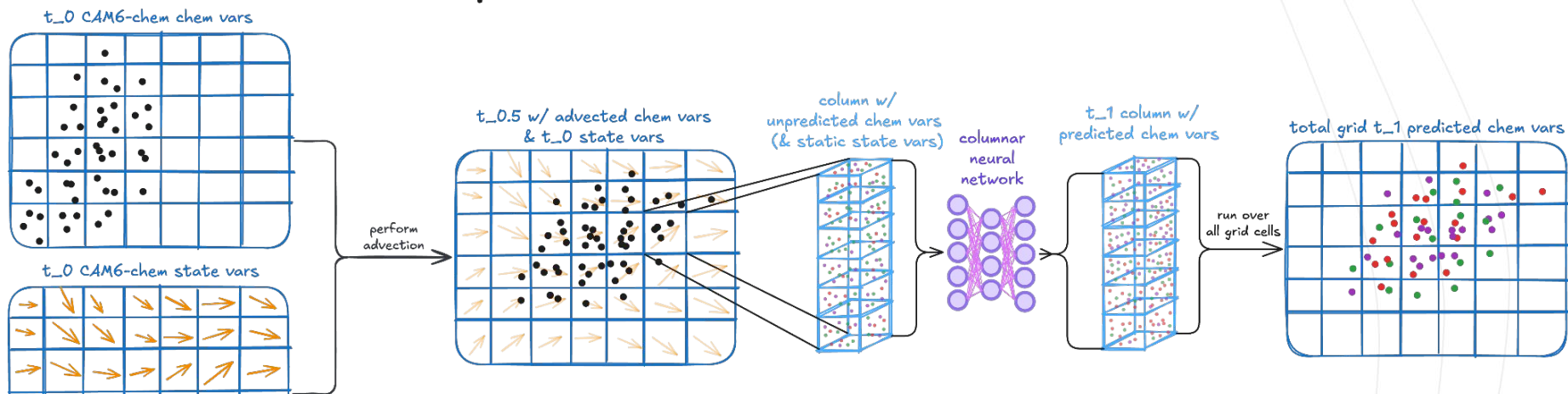
That center column
is then your model
output

IMPORTANT NOTE: There is no physical advection/
transport in this model, it will all be implicitly learned
by the ML model

More technical breakdown...

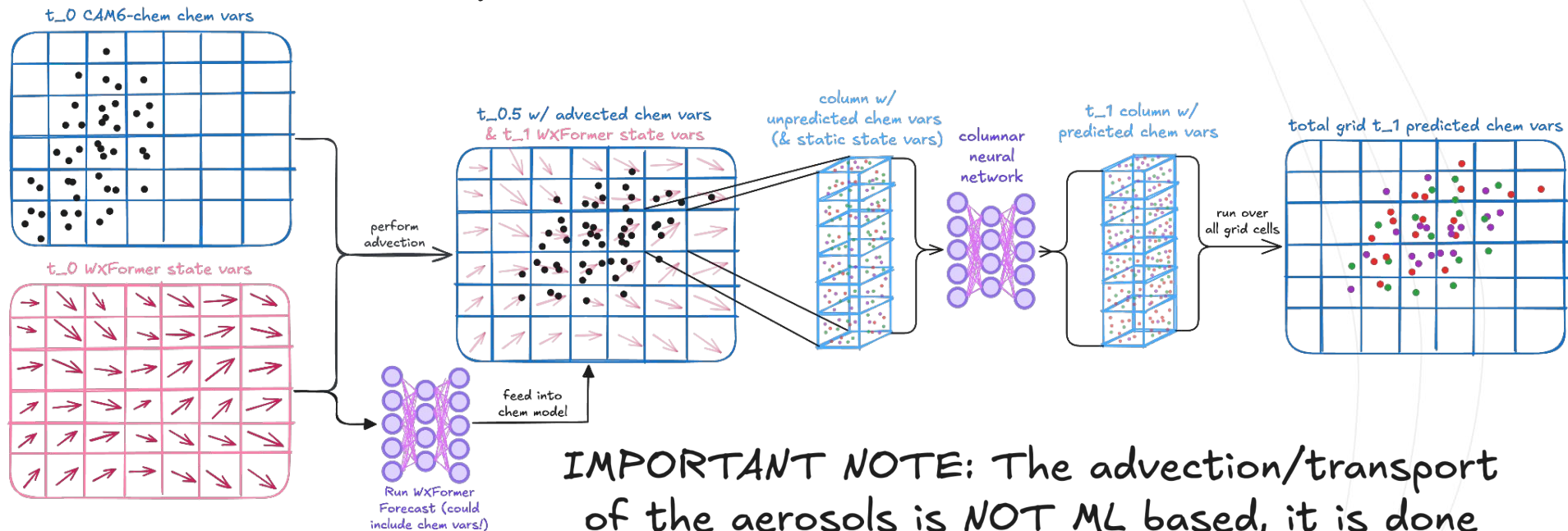
- Tensor “cubing” is all VMapped
- “Microbatches” of cubes are used, since entire time slice is way to expensive
- All preblocks and postblocks (quantile transform, cube packing, cube shuffling) are done on GPU
- 9 Months of Hourly Data, ~1 deg resolution, 32 pressure levels + 1 surface level
- Black Carbon concentrations are prognostic, Black Carbon deposition is diagnostic, Black Carbon emissions and state vars are dynamic forcings
 - ~90–175 total vars, depending on how much you are simulating

Hybrid Model (chem-columnar)



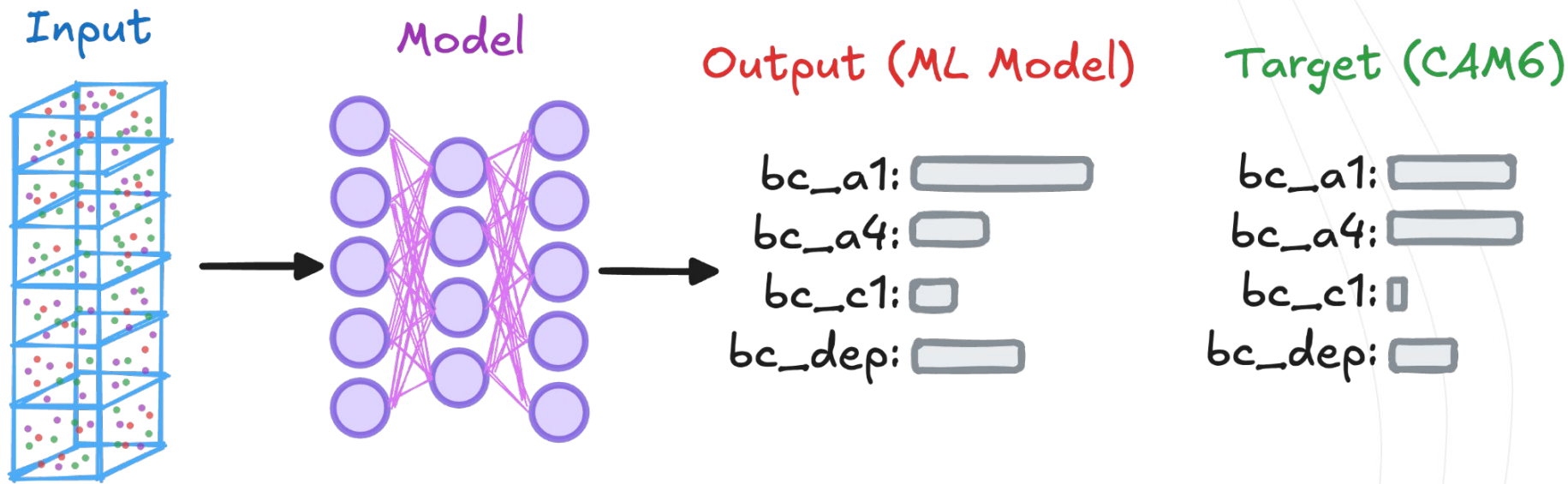
IMPORTANT NOTE: The advection/transport of the aerosols is *NOT* ML based, it is done using a physics-based semi-lagrangian scheme

Hybrid Model (chem-columnar)



IMPORTANT NOTE: The advection/transport of the aerosols is *NOT* ML based, it is done using a physics-based semi-lagrangian scheme

How CREDIT-chem works



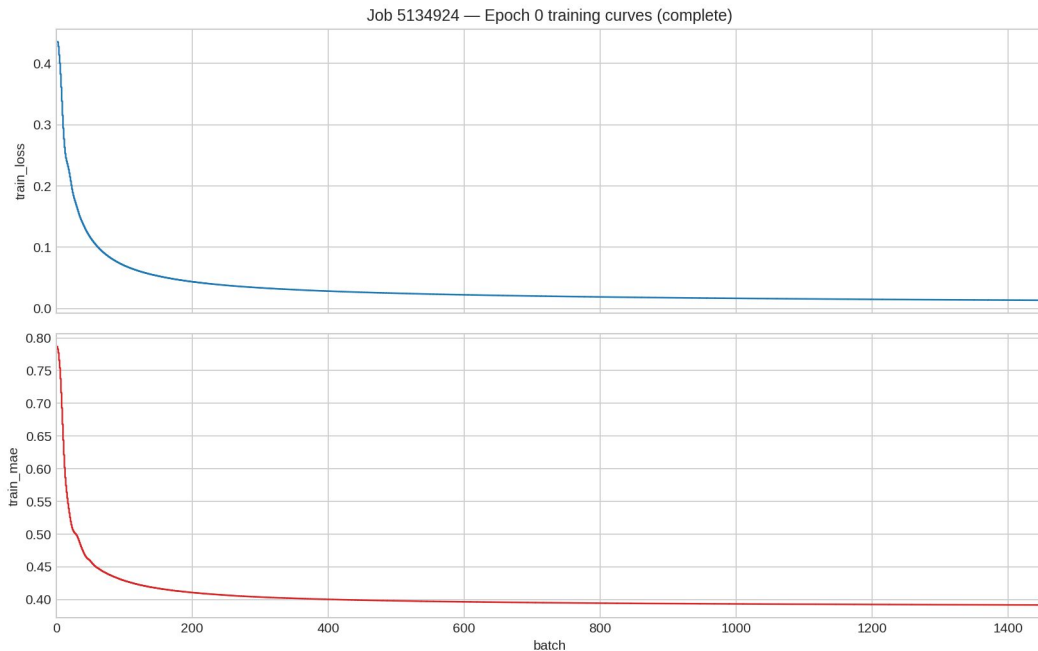
IMPORTANT NOTE: The ML model can only be as good as the data it is trained on (in this case, CAM6-chem)

(Very) Preliminary Results

Preliminary Results (chem-cubed)



Our training loss and
MAE both converge
very well after 1 epoch!
(~300mil training
examples)



Preliminary Results (chem-cubed)

GPU Usage is at ~100% for most of the training!
Drops every ~15 mins,
look into that...



Thank You!

GUIDANCE & INSTRUCTIONS:

COVER PAGES

- **The wave graphics and photo** are set up and can be accessed in the Master Slide pages. Click: View/Master/Slide Master to access.
- **To change the photo** right-click on the image in Slide Master view and select change picture and navigate to your desired image.
- Please try to leave the wave graphics and logo in the same position they appear at in the Master Slides.
- **Cover title text boxes** are not part of the Slide Master pages. Please use the title text boxes that appear on the example pages in Normal view. Take note of the different sized and formatted text elements (e.g. Date, title, subhead, presenters, etc...)
- **The Orange Accent Bar** should extend to the top and bottom of cover text content (e.g. Date & Presenter Credits). This needs to be adjusted manually – depending on the total length/height of your content. Notes set in small text at the bottom, should not be included for extending the accent bar.
- **The Light Blue accent divider** should appear between the title/subhead and the presenters. Try to keep 10pt spacing above and below it. That setting can be accessed by clicking Format/Paragraph.
- **Turning on Guides** can help with establishing clean layouts. To see the guides click View/Grids & Guides/Guides. Do the same to turn off.

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SEPTEMBER 15, 2025

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UCAR**

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GUIDANCE & INSTRUCTIONS:

INTERIOR PAGES – 1

- **Page titles** have an auto expanding side bar and a bottom rule divider. This title component is not part of the Slide Master pages. For new pages, please copy and paste the title component from another example page. Or you can duplicate an entire example page that already has that component.
- **Bullet indent styling** is set up in the Slide Master pages for 5 levels. If you create a new text box that is not apart of the Slide Master pages, the Master bullet styling will be lost and you will have to adjust bullet color and indentation manually if you want to match to the Master.
- **Creating new text boxes** that are not apart of the Slide Master pages will default to the appropriate font and color as long as you paste in new copy without formatting. Ctrl+Shift+V (Windows) or Cmd+Option+Shift+V (Mac)
- **Turning on Guides** can help with establishing clean layouts. To see the guides click View/Grids & Guides/Guides. Do the same to turn off.
- **Large photos** placed in the layouts should have slightly rounded corners. After inserting and sizing your photo appropriately, double click the image which takes you to the Picture Format tab. With the photo selected click the dropdown arrow on the Crop button and go to Crop to Shape. Select the rounded corner shape. Manually drag the small yellow square on the top left of the photo to make the corners have subtle rounding.

GUIDANCE & INSTRUCTIONS:

INTERIOR PAGES – 2

- **Body copy font size** is generally set to 12pts for one and two column layouts. Font size for three and four column layouts are set to 10pts to allow for more content. Adjust either of those to be smaller if need be.
 - **Smaller subheads** within body copy need to be formatted manually, if required. See below for how to size/style two levels of subheads.
-

SUBHEAD 1

Poppins Bold, 15pt

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SUBHEAD 2

Poppins Bold, 12pt –
OR same size as body text

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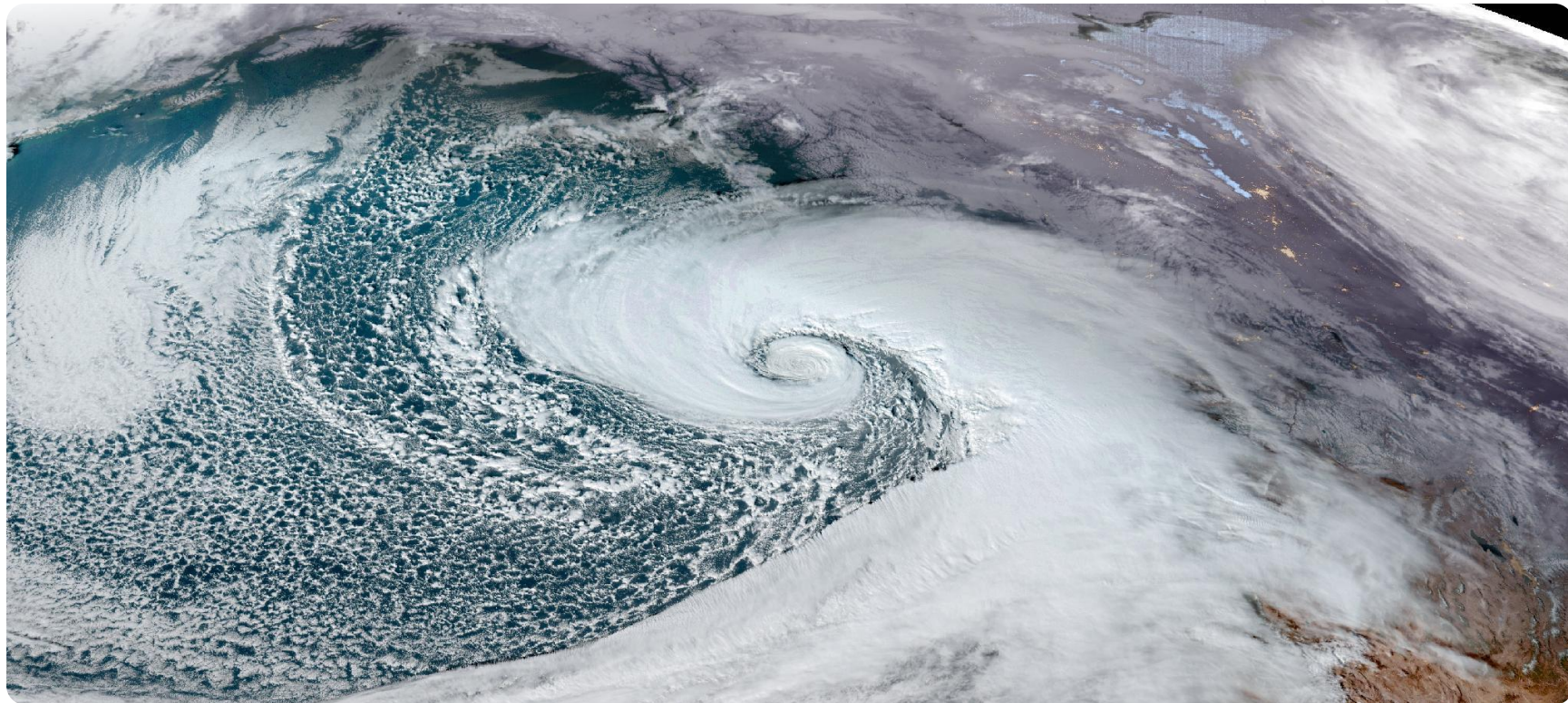


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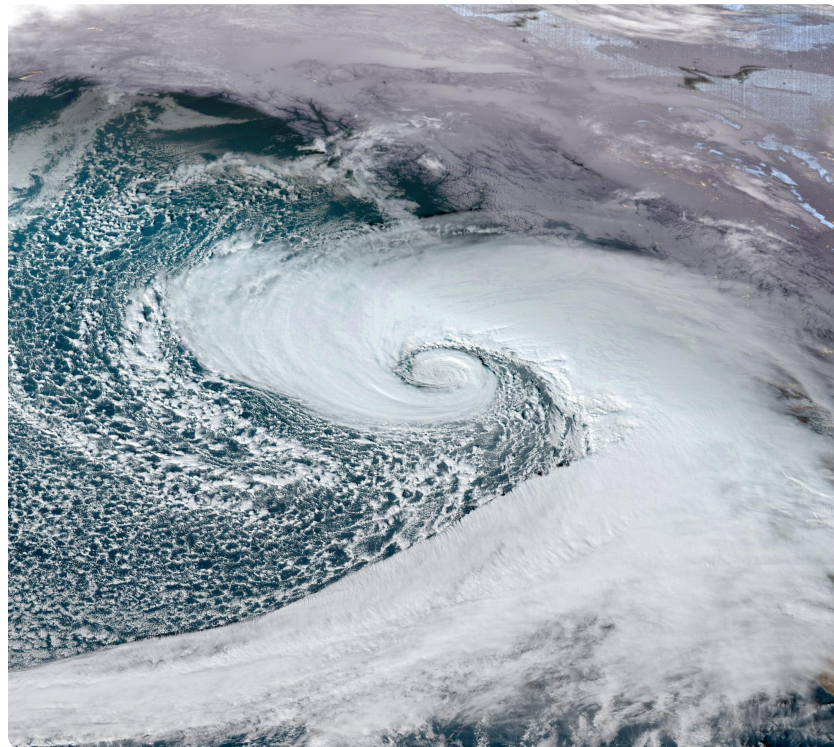
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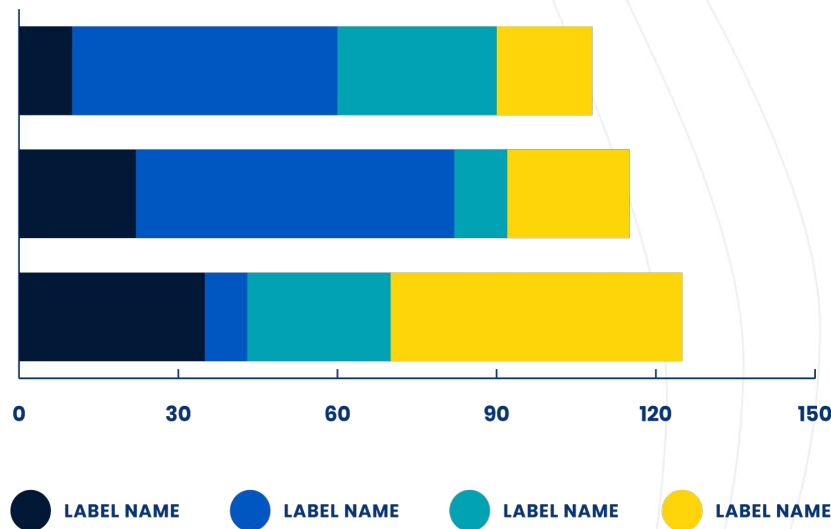
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Sed neque quam morbi	Duis rhoncus facilisis enim sit venenatis diam ornare	Sed neque quam morbi lorem vel vehicula	Duis rhoncus facilisis enim sit venenatis diam