

## 5.005 Replacing the integrator: modelling atmospheric chemistry with machine learning .

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Abstract:

Atmospheric chemistry is a high-dimensionality, large-data problem and so may be suited to machine-learning algorithms. One application would be to replace the integration of the simultaneous ordinary differential equations that represent atmospheric chemistry with a machine learning representation. To explore this, the GEOS-Chem model is run for a year archiving the concentration of the transported tracers before and after each chemical time-step together with information about the physical state for each gridbox. For each tracer, a machine learning algorithm (regression forest) is created to predict the concentration of the tracer in the next time-step based on the training data. Running the model forward for a different year using the machine learning rather than the differential equations shows that the machine learning approach has significant skill compared to the standard differential equation methodology. Replacing the integration methodology with a machine learning one, allows a number of new options for solving atmospheric chemistry which have a range of advantages and disadvantages for air quality forecasting and for the exploitation of new computer hardware. These will be discussed and suggestions for future developments made.