Simulation, Analysis, and Validation of Computational Models

— Case Studies III: Weather and Climate —

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Overview

- Modelling weather
- Modelling climate

Weather vs. climate

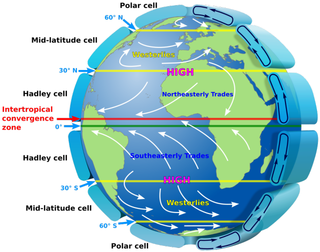
- Weather is the state of the atmosphere (troposphere <20km) and depends on
  - Atmospheric circulation (wind, jet stream)
  - Fluctuations of oceanic currents (El niño, el niña)
  - Dust particles (Pinatubo volcano (1991) -0.4 deg)
- Climate is the average weather over many years and depends on the state of the surface of the earth (air, water, ice, carbon, methane, biosphere, atmosphere <500km)
  - Geographic features
  - Solar irradiance (and space weather)
- Special cases:
  - Micro climate (walled garden, cave, afforestation)
  - Long-term weather prediction: Reoccurring patterns

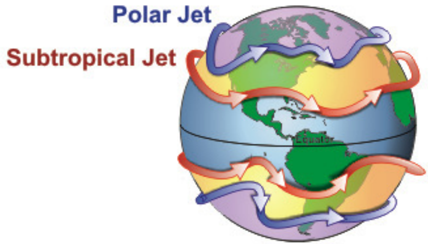
The story of the butterfly effect

- Digital computer (Royal McBee LGP-30) to simulate temperature, wind speed etc. by modeling 12 variables (1961)
- Re-started simulation in the middle of its run by re-entering data from a printout.
- Surprisingly, the prediction was now completely different from the previous calculation, because of rounding a decimal number from 6-digit precision to 3-digits.
- The consensus at the time would have been that it should have no practical effect. However, Lorenz discovered that small changes in initial conditions produced large changes in long-term results.
- "Two states differing by imperceptible amounts may eventually evolve into two considerably different states ..." Edward Lorenz (who coined the notion of the butterfly effect).

https://en.wikipedia.org/wiki/Edward_Norton_Lorenz

Atmospheric circulation





Frokor (Commons)

Classical weather prediction

- Over various ranges, precise predictions limited to 7 - 14 days
  - chaotic dynamics + noise
  - measurement precision
  - surface grid density
  - height resolution (atmospheric layering)
  - cost, capacity, subgrid parametrisation, knowledge representation
- Exceptional events are less likely to be predicted correctly both for analytical and statistical methods
  - Power-law event distribution
  - Less frequent in historical data so far
  - Extreme weather warnings on short time scales
  - Risk estmation is an important research topic

Numerical weather prediction

- Linear combinations of predictors X_i to estimate predicant $\hat{Y}$ (random variables)

$$\hat{Y} = a_0 + a_1 X_1 + \cdots + a_k X_k$$

determine a_i by minimising RMSE of a set of predicted values and respective observations

$$\frac{1}{N} \sum_{j=1}^{N} (y_j - \hat{y}_j)$$

- Calculation over surface grid
- *Model output statistics* based on multiple linear regression as an ensemble method as proxy for probability (requires post-processing to remove biases)

Glahn & Lowry (1972) The use of model output statistics (MOS) in objective weather forecasting. *J. Appl. Meteorol.* 11, 1203-1211.

Classical weather prediction

- Global models on 10 km – 50 km grid cells
- Limited area model with 1 – 15 km grid cells
- 6h interval (Global Forecast System, GFS)
- E.g. Unified Model (UM) Met Office (UK):
  - 36-hour forecasts from the operational 1.5 km resolution
  - 48-hour forecasts from 12 km grid (North Atlantic)
  - 144-hour forecasts from 25 km grid (global)
- Uncertainly is evaluated by ensemble algorithms with 50 - 1000 instances (at different resolutions and with noisy initialisation): long term prognosis possible at agreement.
- Tools: Navier-Stokes equation, ideal gas law ($p \cdot V = \text{const}$), first law of thermodynamics ($\Delta U = Q - P\ \Delta V$), continuity equations, radiative transfer, statistical postprocessing

Mathematical background

- Navier Stokes equation describes the momentum balance

$$\rho\left(\frac{\partial \mathrm{v}}{\partial t}+(\mathrm{v}\cdot\nabla)\mathrm{v}\right)=-\nabla p+\mu\Delta\mathrm{v}+(\lambda+\mu)\nabla(\nabla\cdot\mathrm{v})+\mathrm{f}.$$

v flow velocity, p pressure, ρ density, λ volume viscosity , μ dynamic viscosity , f gravity and Coriolis force per volume

- Stokes equation (creeping flow, friction > inertia)

$$0=-\nabla p+\mu\,\Delta\mathrm{v}+\mathrm{f}$$

- Euler equation (no viscosity: $\lambda=\mu=0$, no vertices)

$$\rho\frac{\partial \mathrm{v}}{\partial t}+\rho\underbrace{(\mathrm{v}\cdot\nabla)\mathrm{v}}_{\text{convection}}=-\nabla p+\mathrm{f}$$

Derivatives in 3D

- ∇ nabla (scalar to vector)

$$\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$$

- Δ Laplace (scalar (to vector) to scalar)

$$\Delta = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$$

  or as a (formal) scalar product $\nabla \cdot \nabla = \Delta$

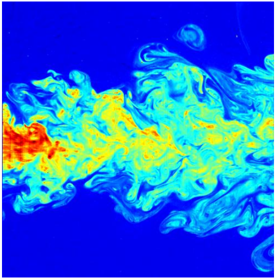
- $\nabla \cdot \mathrm{v} = \left(\frac{\partial}{\partial x} v_x + \frac{\partial}{\partial y} v_y + \frac{\partial}{\partial z} v_z \right)$ (vector to scalar)
- $\nabla \times \mathrm{v}$ (vector to vector), Hessian: $\nabla\nabla v$ (scalar to matrix)

Interpretation of the Navier Stokes equation

- Parabolic equation differential equation
- Applicable to Newtonian fluids where viscous stresses are proportional to the rate of change of the fluid's velocity vector.
- Arise from applying Isaac Newton's second law to fluid motion (momentum, force, friction)
- Explain transition from laminar flow to turbulence and formation of boundary layers

Find a proof or a counter-example that in 3D plus time, given an initial velocity field, there exists a vector velocity and a scalar pressure field, which are both smooth and globally defined, that solve the Navier–Stokes equations.

(Clay Math. Inst.)



Long-range weather forecast

- medium range (up to 15 days ahead);
- extended range (up to 46 days ahead)
- long range (up to one year ahead).

Forecasts and predictability in the long range, e.g. based on pattern recognition:

- Cyclic sea surface temperature change, every "few" years in the central-east equatorial Pacific (El Niño: +0.5 deg, La Niña -0.5 deg)

European Centre for Medium Range Weather Forecasts

Machine learning approaches

- Machine learning approaches may be suboptimal
- System behavior dominated by spatial or temporal context
- Amending machine learning or focus on contextual cues for seasonal forecasting and modeling of long-range spatial connections across multiple time-scales?
- Hybrid approach coupling physical processes with deep learning.
  - Testing ML against complex physical models based on surrogate data from physics models
  - Testing theoretical assumptions (parametrisation or interaction strengths) by ML
  - Critical evaluation of data acquisition

Reichstein e.a. (2019) Deep learning and process understanding for data-driven Earth system science. *Nature* **566**, 195-204.

GraphCast

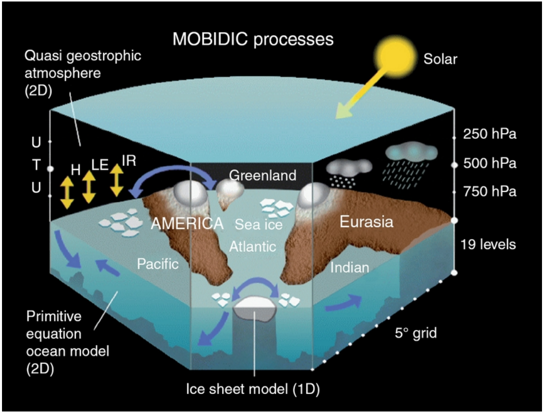
- 10-day forecasts in $<$ 1min on a TPUv4
- 36.7 M parameters in GNN (better scalable than transformers)
- 1M grid points ($0.25^\circ \times 0.25^\circ$) as compared to ($0.1^\circ \times 0.1^\circ$) of alternative approaches
- Pre-training: 4 weeks on 32 TPUv4's using 39 years (1979–2017) of historical data from ECMWF (European Centre for Medium-Range Weather Forecasts), open source
- Autoregressive training regime: model predicted step used as input for predicting this step.
- Severe event forecasting improveable; outperforming ECMWF
- Trained using atmospheric data. Also possible to use agricultural data to predict harvests; ecology data to predict deforestation and biodiversity etc.
- Deterministic forecasts: Less suited to manage uncertainty

Rémi Lam e.a. (2022) GraphCast: Learning skillful medium-range global weather forecasting. arXiv:2212.12794.

Numerical climate models

- Similar to weather forecast models
  - Discretisation
  - Several ranges
  - Regional or global
- Different
  - Time scales
  - Short-range changes (weather) is averaged-out
  - Less dependent on current data, but several other features are incorporated (such as ice sheet data, vegetation, human activity)
- Some models are used for both weather and climate predictions

What is a climate model?



H. Goosse (2015) Climate system dynamics and modeling. Cambridge U Press.

Energy balance models

- Solar irradiation (latitude, altitude, weather, air quality)
- Diffusion to space (albedo, latitude, altitude, weather, air quality)
- Lateral energy transport (latitude, distance to sea currents)
- Storage (vegetation, agriculture)
- Energy sources (urbanisation, transport, air traffic)
- Interaction of multiple factors

Zero-dimensional models

$$(1-a)S = 4\epsilon\sigma T^4$$

S incoming solar radiation per unit area

a Earth's average albedo,

T Earth's average surface temperature

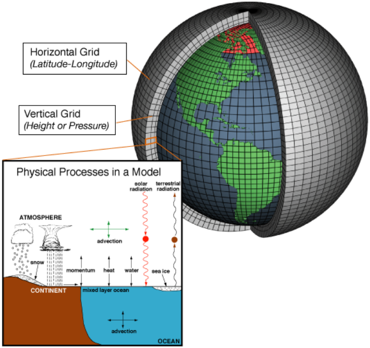
ϵ effective emissivity of Earth's

σ Stefan–Boltzmann constant

Mechanisms: Increase albedo to decrease temperature?

Complex climate models

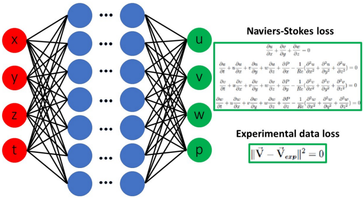
- General agreement on some features of future climate, divergence on many details
- Scenarios rather than prognosis
- Models can be correct now, but fail in the past
- Sudden changes (ice core data) are problematic
- Complexity



Physics-informed neural networks

Physics-informed ML

- Efficient machine learning
- Physics-informed reinforcement learning, active learning
- Physics-informed regularisation



Understanding system physics

- Qualitative modelling by identification of underlying regularities
- Learning to simulate complex phenomena from sparse data based on physics priors (PDE).
- Closed loop systems to perform process optimization

see e.g. https://www.youtube.com/watch?v=ISp-hq6AH3Q

Conclusion

- Weather prediction started with modest tools, but gained fundamental insights early on
- Weather forecast and modeling of climate changes seem to be similar, but the learning problem is different
- Combination of physics models and machine learning is essential

Next topics

- Testing
- Validation
- Verification
- Confidence