Algorithmic Differentiation as Sensitivity Analysis in Cloud Microphysics

M. Hieronymus[1], M. Baumgartner[1], A. Miltenberger[1] & A. Brinkmann[1]

1) Johannes Gutenberg University Mainz

Abstract

The formation of clouds, precipitation, and radiative forcing depends on cloud microphysics. However, cloud microphysical processes act on scales too small to be resolved directly. Parameterizations of these processes are a well-known source of uncertainties in weather and climate models. The goal of a sensitivity analysis is to quantify and attribute the uncertainty of a cloud microphysical model to different parameters. Typically, a sensitivity analysis considers only a few model parameters and requires multiple simulations with varying perturbations of model parameters.

We apply algorithmic differentiation to identify parameters with a large impact and assess the point in time at which they affect the simulation by calculating hundreds of gradients during the simulation. This method avoids the need for multiple simulations by running only a single simulation at the cost of roughly one third more compute time.

Sensitivity Analysis With a Single Simulation

Using Algorithmic Differentiation (AD), we can

- efficiently evaluate the Jacobian of any implemented model,
- identify parameters of interest via the magnitude of their gradients,
- and identify time steps with distinct process activations.

How do we get there?

- Implement Seifert-Beheng two-moment cloud scheme similar to COSMO and ICON in C++
- Simulate microphysics along given trajectories and analyze the sensitivities
- Validate sensitivities by comparing to perturbed parameter ensembles
- Identify parameters of interest via the magnitude of their gradients
- Identify time steps with different sensitivity patterns

Gathering Sensitivities

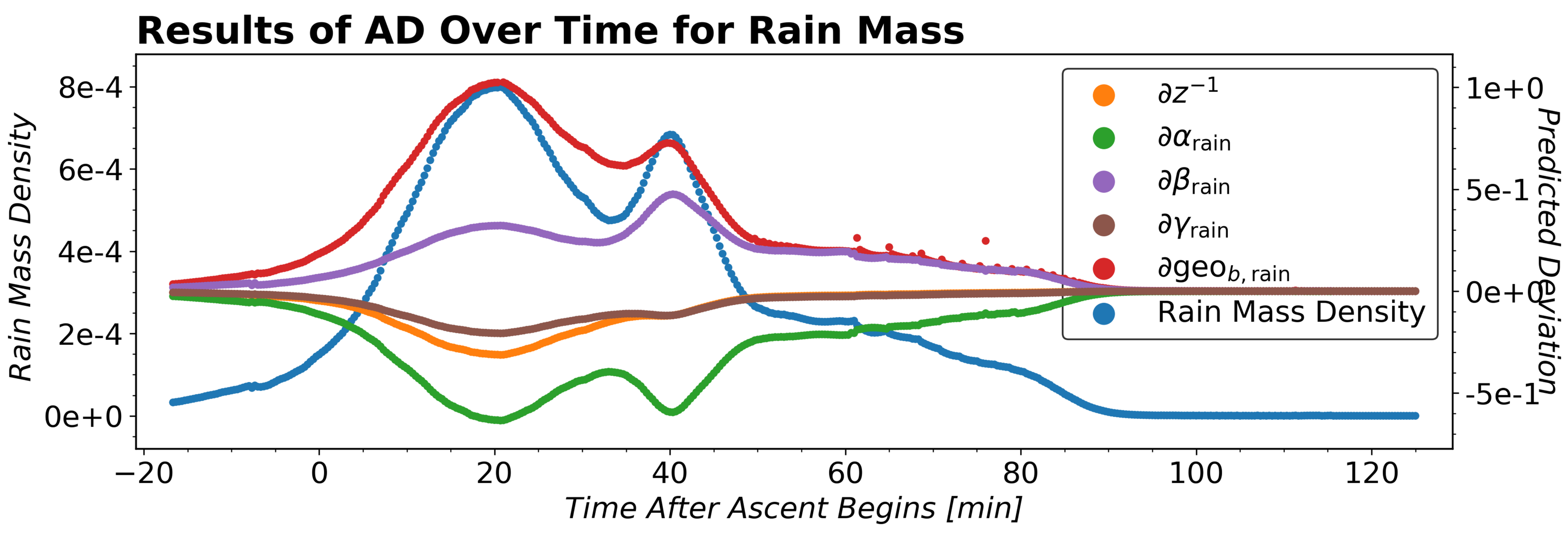


Fig. 1: An example for sensitivities for rain mass density and its five most influential parameters in this time period.

- Sensitivity: How large is the impact if we perturb a parameter by 10%?
- Simulate microphysics along given trajectories and gather gradients
- AD: Predict impact of model parameters at every time step using the gradients

Validating Sensitivities with Ensembles

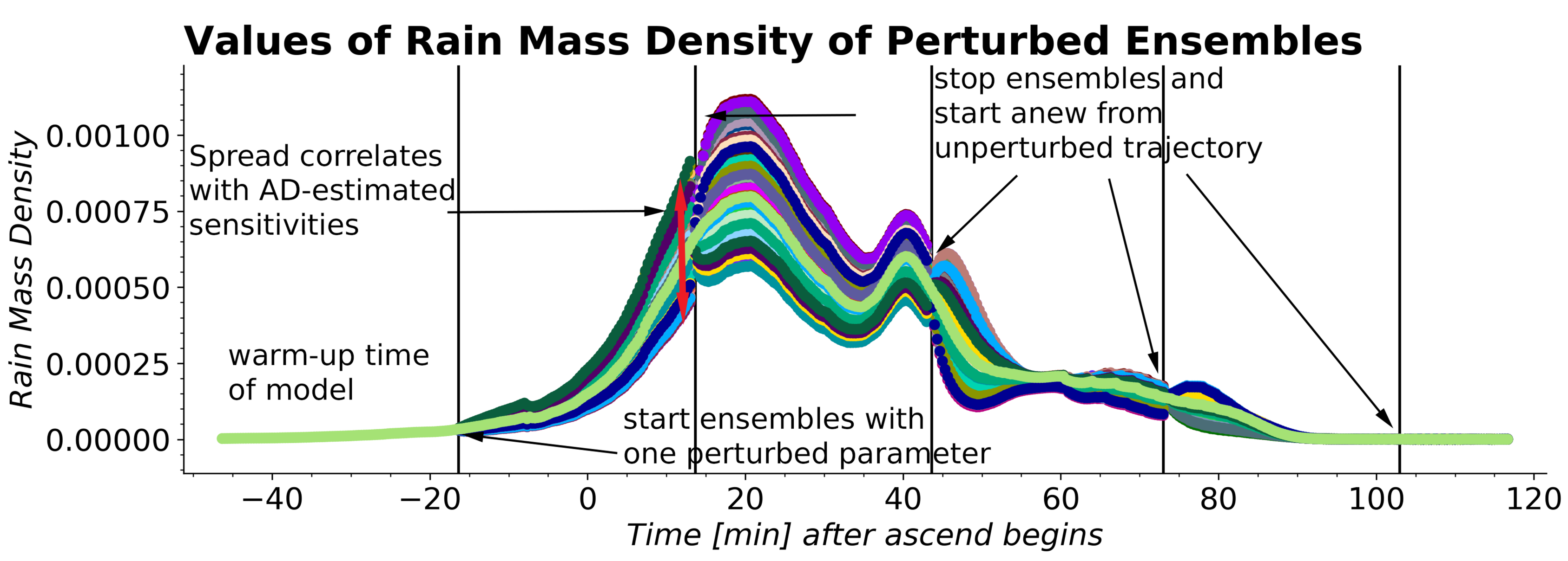


Fig. 2: An example for sensitivities for rain mass density and its five most influential parameters in this time period.

- Run ensembles every 30 min along the unperturbed trajectory for 30 min
- Each member has one randomly perturbed model parameter drawn from a uniform distribution
- Compare AD-estimated and ensemble-estimated deviation for validation

Gradients and Ensemble Spread

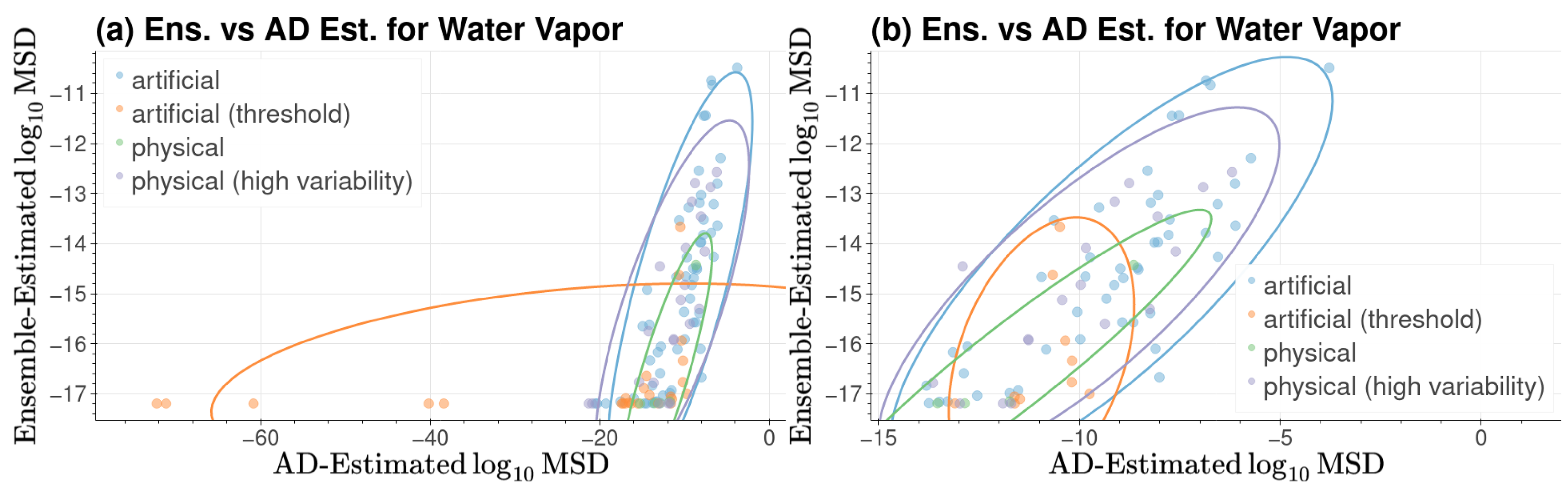


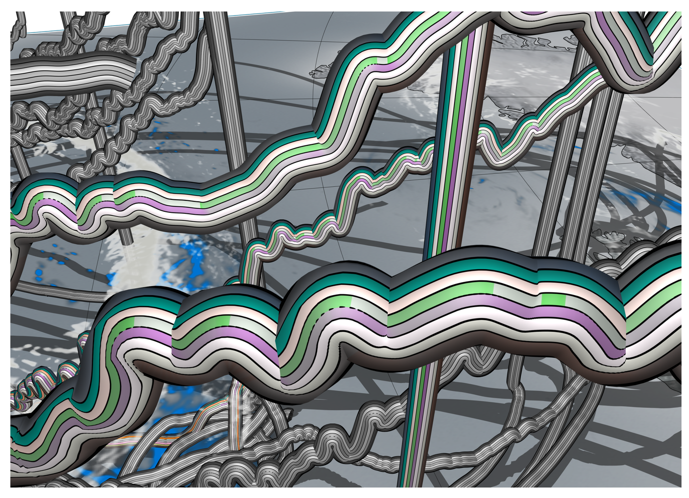
Fig. 3: Comparison of ensemble-estimated vs AD-estimated deviation for water vapor, where (b) is zoomed in at the top right of (a). Each symbol indicates one model parameter. The ellipses are 90% confidence ellipses.

- As guidance: Grouping parameters into different categories
- Parameters with large gradients show higher correlations to ensemble-estimated deviation
- The correlation is not linear, i.e., the AD-estimated deviation can overestimate the ensemble-estimated deviation by up to eight magnitudes

Identifying Patterns

With Met3D, we can investigate gradients of different trajectories.

- Gradient w.r.t. parameter for CCN activation (green) vs gradient w.r.t. parameter for cloud droplet collision (purple)
- Alternating gradients and therefore processes only for slantwise ascending trajectories



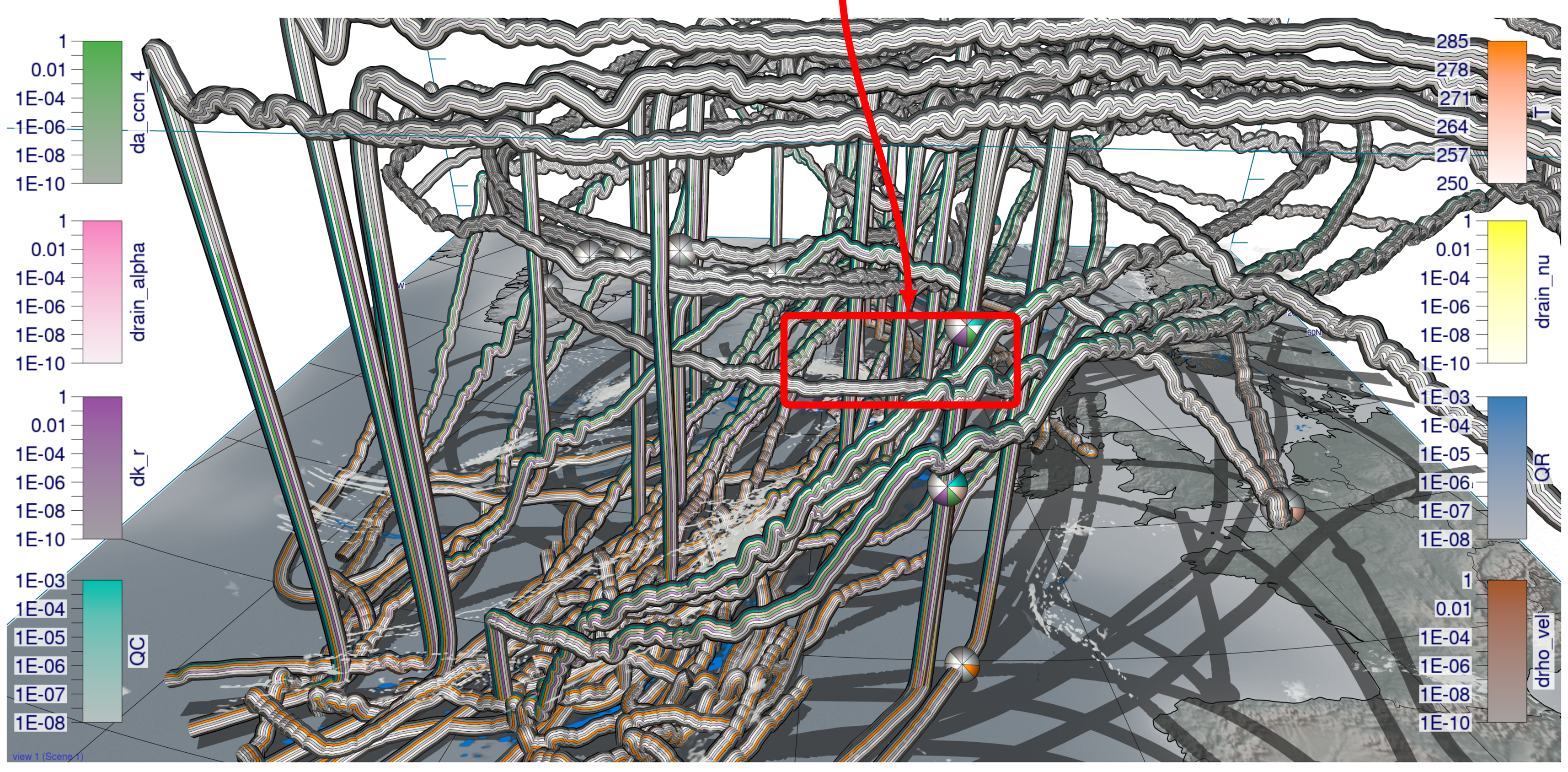


Fig. 4: A subset of trajectories related to Vladiana. Labels starting with 'd' are gradients w.r.t. different parameters.

Discussion and Outlook

- Algorithmic Differentiation can be used to gather sensitivities at every time step for **hundreds of parameters at once**
- The most influential parameters for the immediate further **evolution** of the cloud **can be determined with AD** by applying ranked correlation
- Gradients at every time step are **relevant for more extended simulation periods** (at least 30 minutes; see 90% confidence ellipses depicting a high rank correlation between AD- and ensemble-estimation)
- The most important process representations involving uncertain parameters for our WCB trajectories are the **mass-diameter and fall velocity-diameter relationships, the CCN activation, and heterogeneous freezing**

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contact: mhieronymus@uni-mainz.de