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Automatic differentiation - can it help with GSTH inversions?

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The solution of an inverse problem is often casted as an optimization problem which can be solves by deterministic, i.e., Gradient- or Hessian-based methods. In these cases the necessary calculation of the derivatives of the objective function involves the derivatives of the forward problem. For forward problems with more complicated physics which are becoming more popular also in GSTH inversion, the calculation of these accurate derivatives is not straightforward, and error-prone.

Automatic differentiation (AD) is a set of techniques which can be used to automatically calculate the derivative of the forward problem given in the form of a code written in a programming language like Fortran, MATLAB, or C. These techniques to transform a computer program rely on a systematic application of the chain rule to the elementary operations of the code. This can be done in forward mode, following the control flow of the original code, but also in reverse mode, producing a discrete analog of the adjoint. Unlike calculation of derivatives by divided differences, AD does not introduce additional numerical truncation error into the Jacobian.

At RWTH Aachen university a freely available AD tool called ADiMat is being developed to transform MATLAB codes by automatic differentiation. We will demonstrate the use of ADiMat on an FD-based simulator including phase change effects. We investigate how its use improves the performance of the inverse solver. Additionally, further uses of the Jacobian for model appraisal will be shown.