Automatic Linearization using Functional Programming for Scientific Computing

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Our approach is to ease the specification of differential equations for numerical computation. During the implementation of any physical model the most error prone as well as time consuming part is the linearization required to obtain the elements of the Jacobian matrix.

We overcome these problems by implementing only the linear functional dependence of equations on variables around $\mathbf{x}$. We introduce a computer assisted programming framework within the C++ programming language where derivatives are implicitly available and do not have to be specified explicitly. This is one of the major advantages, we specify equations with different dependent variables. The amount of implementation effort is reduced to the specification of the equations, the explicit specification of derivatives is performed by the computer.

The elements of the framework are truncated Taylor series of the following form $f_0 + \sum_i c_i \cdot \Delta x_i$. We then introduce a framework of basic operations on Taylor series, which can handle truncated polynomial expansions by applying the operations and linearization.

Our method results in the same equations as conventional methods, however, it imposes a minimum of external specification effort. In general, all discretization schemes which use line-wise assembly based on finite differences as well as finite volumina can be handled using the described formalism.

In the final paper we will also describe the application of functional programming approach coupled with topological traversal algorithms.