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A targeted {AD} approach is presented to calculate directional second order derivatives of ODE/DAE embedded functionals accurately and efficiently.

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Wan, Hong Yao  
(Submitted on 20 Nov  
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programming has  
emerged as a key  
programming  
paradigm empowering

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rapid developments of deep learning while its applications to important computational methods such as Monte Carlo remain largely unexplored.

## **Automatic Differentiable Monte Carlo: Theory and Application**

Automatic differentiation is distinct from symbolic differentiation and



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numerical differentiation (the method of finite differences). Symbolic differentiation can lead to inefficient code and faces the difficulty of converting a computer program into a single expression, while numerical differentiation can introduce round-off errors in the discretization process and cancellation.

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Automatic differentiation (AD, also called "algorithmic" or "computational differentiation") is a set of techniques to calculate exact derivatives of functions or programs in an automatic way. It is neither symbolic differentiation, nor something like finite

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Automatic

Differentiation (AD) is a  
collection of

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techniques to obtain analytical derivatives of differentiable functions, in the case where these functions are provided in the form of a computer program.

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differentiation techniques and strategies for the implementation of robust and powerful tools. Computational scientists and engineers will benefit from the discussion of applications, which provide insight into effective strategies for using automatic differentiation for design optimization, sensitivity analysis, and uncertainty

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algorithms : theory**

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Automatic differentiation (AD) can be applied straightforwardly to obtain all necessary partial derivatives (usually first and, possibly, second derivatives) regardless of a code s complexity. However, the space and time efficiency of AD can be dramatically



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improved - sometimes transforming a problem from intractable to highly feasible - if inherent problem structure is used to apply AD in a judicious manner.

## **Automatic Differentiation in MATLAB Using ADMAT with ...**

differentiation (AD) is a powerful tool that allows calculating derivatives of

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implemented algorithms with respect to all of their parameters up to machine precision, without the need to explicitly add any additional functions. Thus, AD has great potential in quantum

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Quantum Chemistry  
with ...**

Adjoint algorithmic  
differentiation (AAD)

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enables automated computation of gradients of such cost functions implemented as computer programs. To backpropagate adjoint derivatives, excessive memory is potentially required to store the intermediate partial derivatives on a dedicated data structure, referred to as the “tape”.

## **GPU-Accelerated Adjoint Algorithmic**

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