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Algorithmic Differentiation of Numerical Methods: Second-Order Tangent and Adjoint Solvers for Systems of Parametrized Nonlinear Equations

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Abstract. Forward and reverse modes of algorithmic differentiation (AD) transform implementations of multivariate vector functions $F : I\!R^n \rightarrow I\!R^m$ as computer programs into tangent and adjoint code, respectively. The reapplication of the same ideas yields higher derivative code. In particular, second derivatives play an important role in nonlinear programming. Second-order methods based on Newton's algorithm promise faster convergence in the neighbourhood of the minimum by taking into account second derivative information. The adjoint mode is of particular interest in large-scale gradient-based nonlinear optimization due to the independence of its computational cost on the number of free variables. Solvers for parametrized systems of n equations embedded into the evaluation of the objective function for a (without loss of generality) unconstrained nonlinear optimization problem require the Hessian of the objective with respect to the free variables implying the need for second derivatives of the nonlinear solver. The local computational overhead as well as the additional memory requirement for the computation of second-order tangents or second-order adjoints of the solution vector with respect to parameters by a fully algorithmic method (derived by AD) can quickly become prohibitive for large values of n. Both can be reduced significantly by the second-order symbolic approach to differentiation of the underlying numerical method to be discussed in this paper.

1 Introduction and Summary of the Results

This paper builds on [NLLT12], in which the first-order algorithmic differentiation (AD) [GW08,Nau12] of solvers for systems of nonlinear equations is discussed. In this paper we consider two alternative approaches for evaluating the second derivatives of numerical simulation programs which contain calls to solvers for parameterized systems of n nonlinear equations. The first approach is the *algorithmic version* (derived by AD) of computing second derivatives in which the local computational overhead as well as the additional memory requirement for the computation of second-order tangents or second-order adjoints of the solution vector with respect to the parameters can quickly become prohibitive for large values of n. The second approach is differentiation of the underlying mathematical formulation (*symbolic version*) which computes the derivatives of the solution under the assumption that the exact solution has been reached. Therefore the accuracy of the calculated derivatives depends on the accuracy of the solution, but it reduces the computational complexity by orders of magnitude.

With forward and reverse modes of AD as the two fundamental approaches to the computation of truncation-free first derivatives, there are 4 combinations yielding second derivatives, namely forward over forward (FoF), forward over reverse (FoR), reverse over forward (RoF) and reverse over reverse (RoR) [GW08,Nau12]. In this paper we focus on FoF and FoR for reasons laid out later in this work.

The run time and memory overhead for algorithmic and symbolic approaches to the differentiation of an iterative (e.g. Newton-type) method for the solution of nonlinear systems is shown in Table 1.

	Symbolic		Algorithmic	
	FoF	FoR	FoF	FoR
Memory	$O(n^2)$	$O(n^2)$	$O(n^2)$	$\nu \cdot O(n^3)$
Run Time	$O(n^3)$	$O(n^3)$	$\nu \cdot O(n^3)$	$\nu \cdot O(n^3)$

Table 1. Computational complexity and memory requirement of one projection with second-order algorithmic and symbolic tangent and adjoint modes of differentiation for ν (e.g. Newton) iterations applied to systems of n nonlinear equations.

Computing the second derivatives by a fully algorithmic method corresponds to a straight application of AD without taking into account any mathematical properties of the numerical method. It turns out to be the worst approach in terms of computational efficiency. The performance of the different approaches depends on the number of the iterations ν performed by the nonlinear solver (e.g. Newton steps) and on the problem size n. Any nonlinear solver with a direct linear solver called in each step, which approaches to solution of the nonlinear system, will do the same (e.g. SIMPLE). We do not really rely on Newton as the nonlinear solver. In this paper we refer to Newton's algorithm for parameterized systems of nonlinear equations as an example to show the complexities in algorithmic mode (see Sections 4.1 and 5.1).

2 Foundations

In this section we recall some aspects from [NLLT12]. We consider the computation of second-order tangents (directional derivatives) $\mathbf{x}^{(1,2)} \in I\!R^n$ as well as second-order adjoints $\boldsymbol{\lambda}_{(1)}^{(2)} \in I\!R^m$ for solvers of parametrized systems of nonlinear equations described by the residual

$$\mathbf{r} = F(\mathbf{x}, \boldsymbol{\lambda}) : I\!R^n \times I\!R^m \rightarrow I\!R^n. \tag{1}$$

For a given $\boldsymbol{\lambda} \in I\!R^m$, a vector $\mathbf{x} \in I\!R^n$ is sought such that $F(\mathbf{x}, \boldsymbol{\lambda}) = 0$.

Without loss of generality, the nonlinear solver is assumed to be embedded into the unconstrained convex nonlinear programming problem (NLP)

$$\min_{\mathbf{z} \in I\!R^q} f(\mathbf{z})$$

for a given objective function $f : I\!R^q \rightarrow I\!R$. In the context of second-order derivative-based methods (e.g. Newton) the gradient and the Hessian of $y =$

$f(\mathbf{z}) \in I\!R$ with respect to $\mathbf{z} \in I\!R^q$ need to be computed, which involves the second derivative of the nonlinear solver itself.

As in [NLLT12], f is decomposed as

$$y = f(\mathbf{z}) = p(S(\mathbf{x}^0, P(\mathbf{z}))), \tag{2}$$

where $P : I\!R^q \to I\!R^m$ denotes the part of the computation that precedes the nonlinear solver $S : I\!R^n \times I\!R^m \to I\!R^n$ and where $p : I\!R^n \to I\!R$ maps the result $\mathbf{x}$ onto the scalar objective y.

Most of our arguments will be based on the following algorithmic description of Equation (2)

$$\boldsymbol{\lambda} = P(\mathbf{z}) \tag{3}$$
$$\tilde{\mathbf{x}} = S(\mathbf{x}^0, \boldsymbol{\lambda}) \tag{4}$$
$$y = p(\tilde{\mathbf{x}}). \tag{5}$$

The parameters $\boldsymbol{\lambda} \in I\!R^m$ are computed as functions of $\mathbf{z} \in I\!R^q$ by the given implementation of P. They enter the nonlinear solver S as arguments as well as the given initial estimate $\mathbf{x}^0 \in I\!R^n$ of the solution $\mathbf{x} \in I\!R^n$. Finally, the computed approximation $\tilde{\mathbf{x}}$ of the solution $\mathbf{x}$ is reduced to a scalar objective value $y \in I\!R$ by the given implementation of p. In this paper, P is called the preprocessor, S is called the nonlinear solver and p is called the postprocessor.

As an example for a nonlinear solver we consider Newton's method. A basic version of Newton's algorithm for parameterized systems of nonlinear equations $F(\mathbf{x}, \boldsymbol{\lambda}) = 0$ yields

```
for $i = 0, \ldots, \nu$
    $A := F'(\mathbf{x}^i, \boldsymbol{\lambda}) \equiv \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}^i, \boldsymbol{\lambda})$        (6)
    $\mathbf{b} := -F(\mathbf{x}^i, \boldsymbol{\lambda})$
    $\mathbf{s} := \mathbf{L}(A, \mathbf{b}) \quad (\Rightarrow A \cdot \mathbf{s} = \mathbf{b})$        (7)
    $\mathbf{x}^{i+1} := \mathbf{x}^i + \mathbf{s}.$        (8)
```

While the symbolic approach does not rely on a specific method for the solution of the nonlinear system, the algorithmic version requires insight into the individual algorithmic steps performed by the nonlinear solver.

3 First- and Higher-Order Algorithmic Differentiation

We mention some significant elements of AD described in further detail in [GW08,Nau12]. Without loss of generality, the following discussion will be based on the residual function in Equation (1). In the following we use the notation from [Nau12] which is partially inspired by the notation used in [GW08]. Let therefore be

$$\mathbf{u} \equiv \begin{pmatrix} \mathbf{x} \\ \boldsymbol{\lambda} \end{pmatrix} \in I\!R^h$$

and $h = n + m$. AD yields semantical transformations of the given implementation of $F : I\!R^h \rightarrow I\!R^n$ as a computer program into first and potentially also higher (k-th order) derivative code. For this purpose F is assumed to be k times symbolically differentiable for $k = 1, 2, \ldots$.

For AD to become applicable, the given implementation of F is assumed to decompose into a *single assignment code* (SAC) as follows

$$\begin{aligned} &\text{for } j = h, \ldots, h + q + n - 1 \\ &\quad v_j = \varphi_j(v_i)_{i \prec j}, \end{aligned}$$

where $i \prec j$ denotes a direct dependence of v_j on v_i. The result of each *intrinsic function*[1] φ_j is assigned to a unique auxiliary variable v_j. The h *independent inputs* $u_i = v_i$, for $i = 0, \ldots, h - 1$, are mapped onto n *dependent outputs* $r_j = v_{h+q+j}$, for $j = 0, \ldots, n - 1$. The values of q *intermediate variables* v_k are computed for $k = h, \ldots, h + q - 1$.

The SAC induces a directed acyclic graph (DAG) $G = (V, E)$ with integer vertices $V = \{0, \ldots, h + q + n - 1\}$ and edges $E = \{(i, j) | i \prec j\}$. The vertices are sorted topologically with respect to variable dependence inducing a partial order according to $\forall i, j \in V : (i, j) \in E \Rightarrow i < j$.

The intrinsic functions φ_j are assumed to posses jointly symbolic partial derivatives with respect to their arguments. Association of the local partial derivatives with their corresponding edges in the DAG yields a *linearized DAG*. The linearized DAG of our reference objective is shown in Fig. 1 (a) with (high-level) intrinsic functions P, S, and p.

By the chain rule of differential calculus, the entries of the Jacobian $A = (a_{i,j}) \equiv \nabla F(\mathbf{u})$ can be computed as

$$a_{i,j} = \sum_{\pi \in [i \rightarrow h+q+j]} \prod_{(k,l) \in \pi} c_{l,k}, \tag{9}$$

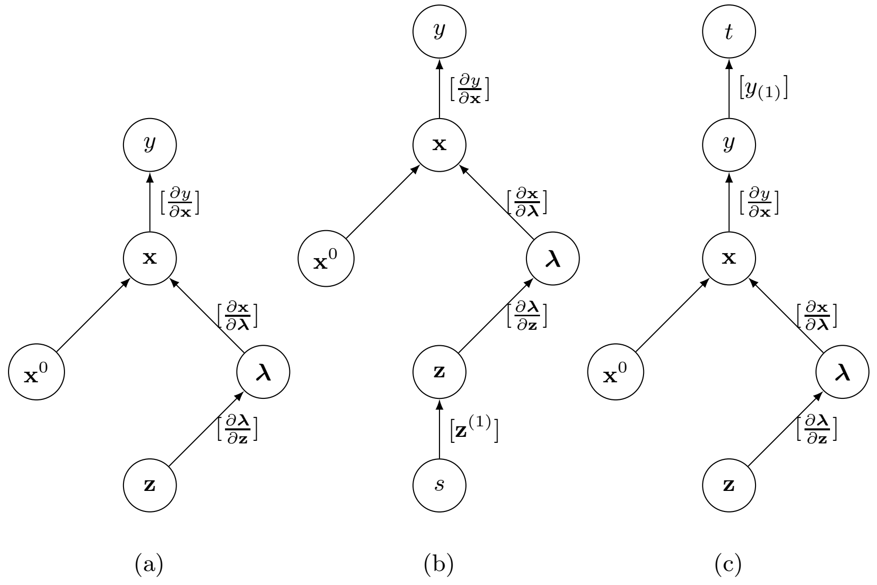
where

$$c_{l,k} \equiv \frac{\partial \varphi_l}{\partial v_k}(v_w)_{w \prec l}$$

and where $[i \rightarrow h+q+j]$ denotes the set of all paths that connect the independent vertex i with the dependent vertex $h + q + j$ [Bau74]. For example, according to Fig. 1 (a)

$$\frac{\partial f}{\partial \mathbf{z}} \equiv \frac{\partial y}{\partial \mathbf{z}} = \frac{\partial p}{\partial \mathbf{x}} \cdot \frac{\partial S}{\partial \boldsymbol{\lambda}} \cdot \frac{\partial P}{\partial \mathbf{z}} = \frac{\partial y}{\partial \mathbf{x}} \cdot \frac{\partial \mathbf{x}}{\partial \boldsymbol{\lambda}} \cdot \frac{\partial \boldsymbol{\lambda}}{\partial \mathbf{z}}.$$

[1] Intrinsic functions can range from fundamental arithmetic operations $(+, *, \ldots)$ and built-in (into the used programming language) functions $(\sin, \exp, \ldots)$ to potentially highly complex numerical algorithms such as routines for interpolation, numerical integration, or the solution of systems of linear or nonlinear equations. In its basic form, AD is defined for the arithmetic operators and built-in functions. A formal extension of this concept to higher-level intrinsics turns out to be reasonably straight forward. For a complex algorithm to become an intrinsic function all we require is the existence of and knowledge about the partial derivatives of its results with respect to its arguments.



y
$[\frac{\partial y}{\partial \mathbf{x}}]$
$\mathbf{x}$
$[\frac{\partial \mathbf{x}}{\partial \boldsymbol{\lambda}}]$
$\mathbf{x}^0$
$\boldsymbol{\lambda}$
$[\frac{\partial \boldsymbol{\lambda}}{\partial \mathbf{z}}]$
$\mathbf{z}$
(a)
y
$[\frac{\partial y}{\partial \mathbf{x}}]$
$\mathbf{x}$
$\mathbf{x}^0$
$[\frac{\partial \mathbf{x}}{\partial \boldsymbol{\lambda}}]$
$\boldsymbol{\lambda}$
$[\frac{\partial \boldsymbol{\lambda}}{\partial \mathbf{z}}]$
$\mathbf{z}$
$[\mathbf{z}^{(1)}]$
s
(b)
t
$[y_{(1)}]$
y
$[\frac{\partial y}{\partial \mathbf{x}}]$
$\mathbf{x}$
$[\frac{\partial \mathbf{x}}{\partial \boldsymbol{\lambda}}]$
$\mathbf{x}^0$
$\boldsymbol{\lambda}$
$[\frac{\partial \boldsymbol{\lambda}}{\partial \mathbf{z}}]$
$\mathbf{z}$
(c)

Fig. 1. Reference Problem: (a) Linearized DAG; (b) Tangent Extension; (c) Adjoint Extension

3.1 First-Order Tangent Model

The Jacobian $\nabla F = \nabla F(\mathbf{u})$ of a multivariate vector function $\mathbf{r} = F(\mathbf{u})$, $F : I\!R^h \to I\!R^n$, induces a linear mapping $I\!R^h \to I\!R^n$, where $h = n + m$, defined by

$$\mathbf{u}^{(1)} \mapsto < \nabla F, \mathbf{u}^{(1)} > \equiv \nabla F(\mathbf{u}) \cdot \mathbf{u}^{(1)} \quad .$$

A first-order tangent projection of ∇F in direction $\mathbf{u}^{(1)} \in I\!R^h$ is defined as the usual matrix-vector product $\nabla F(\mathbf{u}) \cdot \mathbf{u}^{(1)}$. Alternatively, we use the inner product notation $< \nabla F, \mathbf{u}^{(1)} >$ as introduced in [Nau12].

The function $F^{(1)} : I\!R^h \times I\!R^h \to I\!R^n$, defined as

$$\mathbf{r}^{(1)} = F^{(1)}(\mathbf{u}, \mathbf{u}^{(1)}) = < \nabla F, \mathbf{u}^{(1)} > \tag{10}$$

is referred to as the *tangent model* of F. Let $[\nabla F]_{k,j} = \frac{\partial [\mathbf{r}]_k}{\partial [\mathbf{u}]_j} \in I\!R^{n \times h}$ with $k = 0, ..., n-1$ and $j = 0, ..., h-1$ be a 2-tensor (a matrix). Hence, Equation (10) yields

$$[\mathbf{r}^{(1)}]_k = < [\nabla F]_{k,*}, \mathbf{u}^{(1)} > \equiv \sum_{j=0}^{h-1} [\nabla F]_{k,j} \cdot [\mathbf{u}^{(1)}]_j \quad ,$$

for $k = 0, ..., n-1$. The kth row of ∇F is denoted by $[\nabla F]_{k,*}$. The expression $< [\nabla F_{k,*}], \mathbf{u}^{(1)} >$ denotes the usual scalar product of two vectors in $I\!R^h$. This tensor notation will be required for the discussion of higher derivative models in Section 3.3 and the following.

The directional derivatives $\mathbf{r}^{(1)}$ can be regarded as the partial derivative of $\mathbf{r}$ with respect to an auxiliary scalar variable s, where initially

$$\mathbf{u}^{(1)} \equiv \frac{\partial \mathbf{u}}{\partial s} \quad .$$

Interpretation of chain rule on the corresponding linearized DAG (the tangent extension of the original linearized DAG) yields

$$\mathbf{r}^{(1)} \equiv \frac{\partial \mathbf{r}}{\partial s} = \frac{\partial \mathbf{r}}{\partial \mathbf{u}} \cdot \frac{\partial \mathbf{u}}{\partial s} =< \nabla F, \mathbf{u}^{(1)} > .$$

For example, in Figure 1(b) the tangent extension of the linearized DAG of our reference objective is shown. Equation (9) yields $y^{(1)} = \frac{\partial y}{\partial \mathbf{z}} \cdot \mathbf{z}^{(1)} =< \frac{\partial y}{\partial \mathbf{z}}, \mathbf{z}^{(1)} >$. Note that $\frac{\partial y}{\partial \mathbf{z}} \in I\!R^{1\times q}$.

Tangent (also: forward) mode software tools for AD transform a given implementation

```
F(u, r)
```

of Equation $\mathbf{r} = F(\mathbf{u})$ with input u$\hat{=}\mathbf{u}$ and output r $\hat{=}\mathbf{r}$ into the (algorithmic) tangent subroutine

```
t1_F(u, t1_u, r, t1_r)
```

where t1_u $\hat{=}\mathbf{u}^{(1)}$ and t1_r $\hat{=}\mathbf{r}^{(1)}$. A prefix *t*1_ marks 1st-order tangent mode. The Jacobian of the residual with respect to **u** can be accumulated by letting t1_u range over the Cartesian basis vectors in $I\!R^h$. The individual columns of the Jacobian are returned in t1_r while r contains the value of the residual. The complexity of this model for evaluating the whole Jacobian is $O(h) \cdot Cost(F)$.

3.2 First-Order Adjoint Model

The adjoint of a linear operator is its transpose [DS88], since

$$< \mathbf{u}^{(1)}, \mathbf{u}_{(1)} >=< \mathbf{u}^{(1)}, \nabla F^T(\mathbf{u}) \cdot \mathbf{r}_{(1)} >=< \mathbf{r}^{(1)}, \mathbf{r}_{(1)} >=< \nabla F(\mathbf{u}) \cdot \mathbf{u}^{(1)}, \mathbf{r}_{(1)} > .$$

Consequently, the transposed Jacobian $\nabla F^T = \nabla F(\mathbf{u})^T$ of a multivariate vector function $\mathbf{r} = F(\mathbf{u})$, $F : I\!R^h \to I\!R^n$, induces a linear mapping $I\!R^n \to I\!R^h$ defined by

$$\mathbf{r}_{(1)} \mapsto < \mathbf{r}_{(1)}, \nabla F(\mathbf{u}) > \equiv \nabla F(\mathbf{u})^T \cdot \mathbf{r}_{(1)} \quad .$$

A first-order adjoint projection of ∇F in direction $\mathbf{r}_{(1)}$ is defined as the usual matrix-vector product $\nabla F(\mathbf{u})^T \cdot \mathbf{r}_{(1)}$. Alternatively, we use the inner product notation $< \mathbf{r}_{(1)}, \nabla F(\mathbf{u}) >$ as introduced in [Nau12].

The function $F_{(1)} : I\!R^h \times I\!R^n \to I\!R^h$, defined as

$$\mathbf{u}_{(1)} = F_{(1)}(\mathbf{u}, \mathbf{r}_{(1)}) =< \mathbf{r}_{(1)}, \nabla F(\mathbf{u}) > \tag{11}$$

is referred to as the *adjoint model* of F. Let $\nabla F = [\nabla F]_{k,j} = \frac{\partial [\mathbf{r}]_k}{\partial [\mathbf{u}]_j} \in I\!R^{n\times h}$ with $k = 0, ..., n-1$ and $j = 0, ..., h-1$ be a 2-tensor (a matrix). Hence, Equation (11) yields

$$[\mathbf{u}_{(1)}]_j =< \mathbf{r}_{(1)}, [\nabla F]_{*,j} > \equiv \sum_{k=0}^{n-1} [\nabla F]_{k,j} \cdot [\mathbf{r}_{(1)}]_k \quad ,$$

for $j = 0, ..., h-1$. The jth column of ∇F is denoted by $[\nabla F]_{*,j}$. The expression $< \mathbf{r}_{(1)}, [\nabla F]_{*,j} >$ denotes the usual scalar product of two vectors in $I\!R^n$.

Adjoints can be regarded as partial derivatives of an auxiliary scalar variable t with respect to $\mathbf{r}$ and $\mathbf{u}$, where

$$\mathbf{r}_{(1)} \equiv \left(\frac{\partial t}{\partial \mathbf{r}}\right)^T \quad \text{and} \quad \mathbf{u}_{(1)} \equiv \left(\frac{\partial t}{\partial \mathbf{u}}\right)^T .$$

By the chain rule, we get

$$\mathbf{u}_{(1)} \equiv \left(\frac{\partial t}{\partial \mathbf{u}}\right)^T = \left(\frac{\partial \mathbf{r}}{\partial \mathbf{u}}\right)^T \cdot \left(\frac{\partial t}{\partial \mathbf{r}}\right)^T = \nabla F^T \cdot \mathbf{r}_{(1)} \quad .$$

For example, in Figure 1(c) the adjoint extension of the linearized DAG of our reference objective is shown. Equation (9) yields $\mathbf{z}_{(1)} = \frac{\partial y}{\partial \mathbf{z}}^T \cdot y_{(1)} =< y_{(1)}, \frac{\partial y}{\partial \mathbf{z}} >$.

Adjoint (also: reverse) mode software tools for AD transform a given implementation

```
F(u, r)
```

of Equation $\mathbf{r} = F(\mathbf{u})$ with u$\hat{=}\mathbf{u}$ and r $\hat{=}\mathbf{r}$ into the (algorithmic) adjoint subroutine

```
a1_F(u, a1_u, r, a1_r)
```

where a1_u $\hat{=}\mathbf{u}_{(1)}$ and a1_r $\hat{=}\mathbf{r}_{(1)}$. A prefix a1_ marks 1st-order adjoint mode. The Jacobian of the residual with respect to $\mathbf{u}$ can be accumulated by letting a1_r range over the Cartesian basis vectors in $I\!R^n$ while setting a1_u=0. The individual rows of the Jacobian are returned in a1_u. The output argument r contains the value of the residual. The complexity of this model for evaluating the whole Jacobian is $O(n) \cdot Cost(F)$.

3.3 Second-Order Tangent Model

The Hessian $\nabla^2 F = \nabla^2 F(\mathbf{u})$ of a multivariate vector function $\mathbf{r} = F(\mathbf{u})$, $F : I\!R^h \rightarrow I\!R^n$, induces a bilinear mapping $I\!R^h \times I\!R^h \rightarrow I\!R^n$ defined by

$$(\mathbf{u}^{(1)}, \mathbf{u}^{(2)}) \mapsto < \nabla^2 F, \mathbf{u}^{(1)}, \mathbf{u}^{(2)} > = << \nabla^2 F, \mathbf{u}^{(1)} >, \mathbf{u}^{(2)} > .$$

A second-order tangent projection $< \nabla^2 F, \mathbf{u}^{(1)}, \mathbf{u}^{(2)} >$ of a symmetric 3-tensor $\nabla^2 F$, where

$$\nabla^2 F = [\nabla^2 F]_{k,i,j} = \frac{\partial [r]_k}{\partial [\mathbf{u}]_i \partial [\mathbf{u}]_j}$$

for $k = 0, ..., n-1$ and $i, j = 0, ..., h-1$ with $[\nabla^2 F]_{k,i,j} = [\nabla^2 F]_{k,j,i}$ for $i, j = 0, ..., h-1$, in directions $\mathbf{u}^{(1)}, \mathbf{u}^{(2)} \in I\!R^h$ is a first-order tangent projection in direction $\mathbf{u}^{(2)}$ of the first-order tangent projection of $\nabla^2 F$ in direction $\mathbf{u}^{(1)}$, which is $<< \nabla^2 F, \mathbf{u}^{(1)} >, \mathbf{u}^{(2)} >$.

The function $F^{(1,2)} : I\!R^h \times I\!R^h \times I\!R^h \rightarrow I\!R^n$, which is defined as

$$\mathbf{r}^{(1,2)} = F^{(1,2)}(\mathbf{u}, \mathbf{u}^{(1)}, \mathbf{u}^{(2)}) \equiv < \nabla^2 F, \mathbf{u}^{(1)}, \mathbf{u}^{(2)} > \quad (12)$$

is referred to as the *second-order tangent model* of F. The Hessian tensor $(\nabla^2 F)$ is projected along its two domain dimensions (of size h) in directions $\mathbf{u}^{(1)}$ and $\mathbf{u}^{(2)}$.

Let $\nabla^2 F$ be a symmetric 3-tensor as defined above and

$$B =< \nabla^2 F, \mathbf{u}^{(1)} >\in I\!R^{n\times h} \quad ,$$
$$\mathbf{r}^{(1,2)} =< B, \mathbf{u}^{(2)} >=< \nabla^2 F, \mathbf{u}^{(1)}, \mathbf{u}^{(2)} >\in I\!R^{n} \quad .$$

Then,

$$b_{k,j} = \sum_{i=0}^{h-1} [\nabla^2 F]_{k,j,i} \cdot [\mathbf{u}^{(1)}]_i$$

for $j = 0, ..., h-1$ and $k = 0, ..., n-1$. Hence, Equation (12) yields

$$[\mathbf{r}^{(1,2)}]_k = \sum_{j=0}^{h-1} b_{k,j} \cdot [\mathbf{u}^{(2)}]_j = \sum_{j=0}^{h-1}\sum_{i=0}^{h-1} [\nabla^2 F]_{k,j,i} \cdot [\mathbf{u}^{(1)}]_i \cdot [\mathbf{u}^{(2)}]_j \quad ,$$

for $k = 0, ..., n-1$.

Application of tangent mode to the tangent model

$$\mathbf{r}^{(1)} = F^{(1)}(\mathbf{u}, \mathbf{u}^{(1)}) \equiv< \nabla^2 F, \mathbf{u}^{(1)} >$$

yields

$$\mathbf{r}^{(1,2)} =< \nabla F, \mathbf{u}^{(1,2)} > + < \nabla^2 F, \mathbf{u}^{(1)}, \mathbf{u}^{(2)} > \quad ,$$

where $\mathbf{u}^{(2)} \equiv \frac{\partial \mathbf{u}}{\partial s}$ and $\mathbf{u}^{(1,2)} \equiv \frac{\partial \mathbf{u}^{(1)}}{\partial s}$. Thus, for $\mathbf{u}^{(1,2)} = 0$, Equation (12) follows.

Second-order tangent (also: forward-over-forward) mode software tools for AD transform a given implementation

```
F(u, r)
```

of Equation $\mathbf{r} = F(\mathbf{u})$ with u $\hat{=}\mathbf{u}$ and r $\hat{=}\mathbf{r}$ into the (algorithmic) second-order tangent subroutine

```
t2_t1_F (u, t2_u, t1_u, t2_t_1_u, r, t2_r, t1_r, t2_t1_r)
```

where additionally t1_u $\hat{=}\mathbf{u}^{(1)}$, t2_u $\hat{=}\mathbf{u}^{(2)}$, t2_t1_u $\hat{=}\mathbf{u}^{(1,2)}$, t1_r $\hat{=}\mathbf{r}^{(1)}$, t2_r $\hat{=}\mathbf{r}^{(2)}$, and t2_t1_r $\hat{=}\mathbf{r}^{(1,2)}$. The prefix tm_ marks tangent versions of program variables (and of F itself) generated by the mth application of forward mode AD. The Hessian at point $\mathbf{u}$ can be accumulated by setting $\mathbf{u}^{(1,2)} = 0$ initially and by letting $\mathbf{u}^{(1)}$ and $\mathbf{u}^{(2)}$ range independently over Cartesian basis vectors in $I\!R^h$. The individual columns of the Hessian are returned in t2_t1_r while t1_r and t2_r contain the individual columns of the Jacobian and r contains the value of the residual. This model yields a computational complexity of $O(h^2) \cdot Cost(F)$ for the accumulation of the whole Hessian.

3.4 Second-Order Adjoint Model

With tangent and adjoint as the two basic modes of AD there are three combinations remaining, each of them involving at least one application of adjoint mode. In [Nau12] we show the mathematical equivalence of the various incarnations of second-order adjoint mode (that is, forward-over-reverse, reverse-over-forward, and reverse-over-reverse) due to symmetry within the Hessian of twice symbolically differentiable multivariate vector functions. All three variants compute projections of the Hessian tensor in the image dimension (of size n) and the domain dimension (of size h) with potentially varying computational costs due to implementation issues; see [Nau12]. In the following forward-over-reverse mode AD is explained.

The Hessian $\nabla^2 F = \nabla^2 F(\mathbf{u})$ of a multivariate vector function $\mathbf{r} = F(\mathbf{u})$, $F : I\!R^h \to I\!R^n$, induces a bilinear mapping $I\!R^n \times I\!R^h \to I\!R^h$ defined by

$$(\mathbf{r}_{(1)}, \mathbf{u}^{(2)}) \mapsto < \mathbf{r}_{(1)}, \nabla^2 F, \mathbf{u}^{(2)} > = << \mathbf{r}_{(1)}, \nabla^2 F >, \mathbf{u}^{(2)} > \quad .$$

A second-order adjoint projection $< \mathbf{r}_{(1)}, \nabla^2 F, \mathbf{u}^{(2)} >$ of a symmetric 3-tensor $\nabla^2 F$, where

$$\nabla^2 F = [\nabla^2 F]_{k,i,j} = \tfrac{\partial [r]_k}{\partial [\mathbf{u}]_i \partial [\mathbf{u}]_j}$$

for $k = 0, ..., n-1$ and $i, j = 0, ..., h-1$ with $[\nabla^2 F]_{k,i,j} = [\nabla^2 F]_{k,j,i}$ for $i, j = 0, ..., h-1$, in directions $\mathbf{r}_{(1)} \in I\!R^n$ and $\mathbf{u}^{(2)} \in I\!R^h$ is a first-order tangent projection in direction $\mathbf{u}^{(2)}$ of the first-order adjoint projection of $\nabla^2 F$ in direction $\mathbf{r}_{(1)}$, which is $<< \mathbf{r}_{(1)}, \nabla^2 F >, \mathbf{u}^{(2)} >$.

The function $F_{(1)}^{(2)} : I\!R^h \times I\!R^n \times I\!R^h \to I\!R^h$, which is

$$\mathbf{u}_{(1)}^{(2)} = F_{(1)}^{(2)}(\mathbf{u}, \mathbf{r}_{(1)}, \mathbf{u}^{(2)}) \equiv < \mathbf{r}_{(1)}, \nabla^2 F(\mathbf{x}), \mathbf{u}^{(2)} > \qquad (13)$$

is referred to as the *second-order adjoint model* of F. The Hessian tensor $(\nabla^2 F)$ is projected in directions $\mathbf{r}_{(1)} \in I\!R^n$ and $\mathbf{u}^{(2)} \in I\!R^h$.

Let $\nabla^2 F$ be a symmetric 3-tensor as defined above and

$$\begin{aligned} B &= < \mathbf{r}_{(1)}, \nabla^2 F > \in I\!R^{h \times h} \quad , \\ \mathbf{u}_{(1)}^{(2)} &= < B, \mathbf{u}^{(2)} > = < \mathbf{r}_{(1)}, \nabla^2 F, \mathbf{u}^{(2)} > \in I\!R^h \quad . \end{aligned}$$

Then,

$$b_{i,j} = \textstyle\sum_{k=0}^{n-1} [\mathbf{r}_{(1)}]_k \cdot [\nabla^2 F]_{k,i,j}$$

for $i, j = 0, ..., h-1$. Hence, Equation (13) yields

$$[\mathbf{u}_{(1)}^{(2)}]_i = \sum_{j=0}^{h-1} b_{i,j} \cdot [\mathbf{u}^{(2)}]_j = \sum_{j=0}^{h-1} \sum_{k=0}^{n-1} [\mathbf{r}_{(1)}]_k \cdot [\nabla^2 F]_{k,i,j} \cdot [\mathbf{u}^{(2)}]_j \quad ,$$

for $i = 0, ..., h-1$.

Application of tangent mode to the adjoint model

$$\mathbf{u}_{(1)} = F_{(1)}(\mathbf{u}, \mathbf{r}_{(1)}) =< \mathbf{r}_{(1)}, \nabla F(\mathbf{u}) >$$

yields

$$\mathbf{u}_{(1)}^{(2)} =< \mathbf{r}_{(1)}^{(2)}, \nabla F(\mathbf{x}) > + < \mathbf{r}_{(1)}, \nabla^2 F(\mathbf{x}), \mathbf{u}^{(2)} > \quad ,$$

where $\mathbf{u}^{(2)} \equiv \frac{\partial \mathbf{u}}{\partial s}$ and $\mathbf{r}_{(1)}^{(2)} \equiv \frac{\partial \mathbf{r}_{(1)}}{\partial s}$. Thus, for $\mathbf{r}_{(1)}^{(2)} = 0$ Equation (13).

Second-order adjoint (also: forward-over-reverse) mode software tools for AD transform a given implementation

```
F(u, r)
```

of Equation $\mathbf{r} = F(\mathbf{u})$ with u $\hat{=}\mathbf{u}$ and r $\hat{=}\mathbf{r}$ into the (algorithmic) second-order adjoint subroutine

```
t2_a1_F (u, t2_u, a1_u, t2_a1_u, r, t2_r, a1_r, t2_a1_r)
```

Subscripts of second-order adjoint subroutine and variable names are replaced with the prefixes a1_ and t2_; for example, a1_u $\hat{=}\mathbf{u}_{(1)}$, t2_u $\hat{=}\mathbf{u}^{(2)}$, t2_a1_u $\hat{=}\mathbf{u}_{(1)}^{(2)}$, a1_r $\hat{=}\mathbf{r}_{(1)}$, t2_r $\hat{=}\mathbf{r}^{(2)}$, and t2_a1_r $\hat{=}\mathbf{r}_{(1)}^{(2)}$. The computation of a projection of the Hessian in directions $\mathbf{u}^{(2)}$ and $\mathbf{r}_{(1)}$ requires $\mathbf{r}_{(1)}^{(2)} = 0$ initially. The entire Hessian can be accumulated by letting $\mathbf{u}^{(2)}$ and $\mathbf{r}_{(1)}$ range over Cartesian basis vectors in $I\!R^h$ and $I\!R^n$ respectively. The individual rows of the Hessian are returned in t2_a1_u while a1_u contains the individual rows of the Jacobian and r contains the value of the residual. This model yields the computational complexity of $O(h \cdot n) \cdot Cost(F)$ for the accumulation of the whole Hessian.

3.5 Third-Order Tangent Model

The third derivative tensor $\nabla^3 F = \nabla^3 F(\mathbf{u}) \in I\!R^n \times I\!R^h \times I\!R^h \times I\!R^h$ of a multivariate vector function $\mathbf{r} = F(\mathbf{u}), F : I\!R^h \mapsto I\!R^n$ induces a trilinear mapping $I\!R^h \times I\!R^h \times I\!R^h \rightarrow I\!R^n$ defined by

$$(\mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \mathbf{u}^{(3)}) \rightarrow < \nabla^3 F, \mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \mathbf{u}^{(3)} > = <<< \nabla^3 F, \mathbf{u}^{(1)} >, \mathbf{u}^{(2)} >, \mathbf{u}^{(3)} > \quad .$$

A third-order tangent projection $< \nabla^3 F, \mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \mathbf{u}^{(3)} >$ of a symmetric 4-tensor $\nabla^3 F$, where

$$\nabla^3 F = [\nabla^3 F]_{k,i,j,l} = \frac{\partial [\mathbf{r}]_k}{[\partial \mathbf{u}]_i [\partial \mathbf{u}]_j [\partial \mathbf{u}]_l}$$

for $k = 0, ..., n-1$ and $i, j, l = 0, ..., h-1$ with $[\nabla^3 F]_{k,i,j,l} = [\nabla^3 F]_{k,\pi(i,j,l)}$ for any permutation π of i, j, l, in directions $\mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \mathbf{u}^{(3)} \in I\!R^h$ is a first-order tangent projection in direction $\mathbf{u}^{(3)}$ of a second-order tangent projection of $\nabla^3 F$ in directions $\mathbf{u}^{(1)}$ and $\mathbf{u}^{(2)}$, which is $<< \nabla^3 F, \mathbf{u}^{(1)}, \mathbf{u}^{(2)} >, \mathbf{u}^{(3)} >$. It is a first-order tangent projection in direction $\mathbf{u}^{(3)}$ of a first-order tangent projection in direction $\mathbf{u}^{(2)}$ of a first-order tangent projection of $\nabla^3 F$ in direction $\mathbf{u}^{(1)}$, i.e. $<<< \nabla^3 F, \mathbf{u}^{(1)} >, \mathbf{u}^{(2)} >, \mathbf{u}^{(3)} >$.

The function $F^{(1,2,3)} : I\!R^h \times I\!R^h \times I\!R^h \times I\!R^h \rightarrow I\!R^n$, defined as

$$\mathbf{r}^{(1,2,3)} = F^{(1,2,3)}(\mathbf{u}, \mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \mathbf{u}^{(3)}) \equiv < \nabla^3 F(\mathbf{u}), \mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \mathbf{u}^{(3)} > \qquad (14)$$

is referred to as the *third-order tangent model* of F. The 4-tensor $\nabla^3 F$ is projected along its three domain dimensions (of size h) in directions $\mathbf{u}^{(1)}, \mathbf{u}^{(2)}$ and $\mathbf{u}^{(3)}$.

Let $\nabla^3 F$ be a symmetric 4-tensor as defined above and

$$B =< \nabla^3 F, \mathbf{u}^{(1)} >\in I\!R^n \times I\!R^h \times I\!R^h \quad , \text{ that is}$$
$$b_{k,i,j} = \sum_{l=0}^{h-1} [\nabla^3 F]_{k,i,j,l} \cdot [\mathbf{u}^{(1)}]_l \quad ,$$

for $k = 0, ..., n-1$ and $i, j = 0, ..., h-1$. Moreover,

$$C =< B, \mathbf{u}^{(2)} >=<< \nabla^3 F, \mathbf{u}^{(1)} >, \mathbf{u}^{(2)} >\in I\!R^n \times I\!R^h \quad , \text{ that is}$$
$$c_{k,i} = \sum_{j=0}^{h-1} b_{k,i,j} \cdot [\mathbf{u}^{(2)}]_j = \sum_{j=0}^{h-1}\sum_{l=0}^{h-1} [\nabla^3 F]_{k,i,j,l} \cdot [\mathbf{u}^{(1)}]_l \cdot [\mathbf{u}^{(2)}]_j \quad ,$$

for $k = 0, ..., n-1$ and $i = 0, ..., h-1$. Then we have

$$\mathbf{r}^{(1,2,3)} =< C, \mathbf{u}^{(3)} >=<<< \nabla^3 F, \mathbf{u}^{(1)} >, \mathbf{u}^{(2)} >, \mathbf{u}^{(3)} >\in I\!R^n \quad , \text{ that is}$$
$$[\mathbf{r}^{(1,2,3)}]_k = \sum_{i=0}^{h-1} c_{k,i} \cdot [\mathbf{u}^{(3)}]_i = \sum_{i=0}^{h-1}\sum_{j=0}^{h-1}\sum_{l=0}^{h-1} [\nabla^3 F]_{k,i,j,l} \cdot [\mathbf{u}^{(1)}]_l \cdot [\mathbf{u}^{(2)}]_j \cdot [\mathbf{u}^{(3)}]_i \quad ,$$

for $k = 0, ..., n-1$.

Application of tangent mode to the second-order tangent model

$$\mathbf{r}^{(1,2)} =< \nabla^2 F, \mathbf{u}^{(1)}, \mathbf{u}^{(2)} >$$

yields

$$\mathbf{r}^{(1,2,3)} =< \nabla^2 F(\mathbf{u}), \mathbf{u}^{(1,3)}, \mathbf{u}^{(2)} > + < \nabla^2 F(\mathbf{u}), \mathbf{u}^{(1)}, \mathbf{u}^{(2,3)} > + < \nabla^3 F(\mathbf{u}), \mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \mathbf{u}^{(3)} >,$$

where $\frac{\partial \mathbf{u}}{\partial s} = \mathbf{u}^{(3)}$, $\frac{\partial \mathbf{u}^{(1)}}{\partial s} = \mathbf{u}^{(1,3)}$ and $\frac{\partial \mathbf{u}^{(2)}}{\partial s} = \mathbf{u}^{(2,3)}$. Thus, for $\mathbf{u}^{(1,3)} = \mathbf{u}^{(2,3)} = 0$, Equation (14) follows.

Third-order tangent (also: forward-over-forward-over-forward) mode software tools for AD transform a given implementation

```
F(u, r)
```

of Equation $\mathbf{r} = F(\mathbf{u})$ with u $\hat{=}\mathbf{u}$ and r $\hat{=}\mathbf{r}$ into the (algorithmic) second-order tangent subroutine

```
t3_t2_t1_F(u, t3_u, t2_u, t3_t2_u, t1_u, t3_t1_u, t2_t1_u, t3_t2_t1_u,
           r, t3_r, t2_r, t3_t2_r, t1_r, t3_t1_r, t2_t1_r, t3_t2_t1_r)
```

where t1_u $\hat{=}\mathbf{u}^{(1)}$, t2_u $\hat{=}\mathbf{u}^{(2)}$,t3_u $\hat{=}\mathbf{u}^{(3)}$, t2_t1_u $\hat{=}\mathbf{u}^{(1,2)}$, t3_t1_u $\hat{=}\mathbf{u}^{(1,3)}$, t3_t2_u $\hat{=}\mathbf{u}^{(2,3)}$, t3_t2_t1_u $\hat{=}\mathbf{u}^{(1,2,3)}$, t1_r $\hat{=}\mathbf{r}^{(1)}$,t2_r $\hat{=}\mathbf{r}^{(2)}$,t3_r $\hat{=}\mathbf{r}^{(3)}$, t2_t1_r $\hat{=}\mathbf{r}^{(1,2)}$, t3_t1_r $\hat{=}\mathbf{r}^{(1,3)}$, t3_t2_r $\hat{=}\mathbf{r}^{(2,3)}$ and t3_t2_t1_r $\hat{=}\mathbf{r}^{(1,2,3)}$. First-order projection of $\nabla^3 F$ in directions $\mathbf{u}^{(1)}, \mathbf{u}^{(2)}$ and $\mathbf{u}^{(3)}$ are returned in t1_r, t2_r and t3_r by letting $\mathbf{u}^{(1)}, \mathbf{u}^{(2)}$ and $\mathbf{u}^{(3)}$ range independently over Cartesian basis vector in $I\!R^h$. Corresponding second-order projections are returned in t2_t1_r, t3_t2_r and t3_t1_r. The third derivatives are returned in t3_t2_t1_r. This model yields the computational complexity of $O(h^3) \cdot Cost(F)$ for evaluating the whole third derivative tensor.

3.6 Third-Order Adjoint Model

Due to issues in implementation, the preferred approach to the computation of higher derivatives of multivariate scalar functions is the repeated application of forward mode AD to the first-order adjoint code.

The third derivative tensor $\nabla^3 F = \nabla^3 F(\mathbf{u}) \in I\!R^n \times I\!R^h \times I\!R^h \times I\!R^h$ of a multivariate vector function $\mathbf{r} = F(\mathbf{u}), F : I\!R^h \mapsto I\!R^n$ induces a trilinear mapping $I\!R^n \times I\!R^h \times I\!R^h \to I\!R^h$ defined by

$$(\mathbf{r}_{(1)}, \mathbf{u}^{(2)}, \mathbf{u}^{(3)}) \to < \mathbf{r}_{(1)}, \nabla^3 F, \mathbf{u}^{(2)}, \mathbf{u}^{(3)} > = <<< \mathbf{r}_{(1)}, \nabla^3 F >, \mathbf{u}^{(2)} >, \mathbf{u}^{(3)} > \quad .$$

A third-order adjoint projection $< \mathbf{r}_{(1)}, \nabla^3 F, \mathbf{u}^{(2)}, \mathbf{u}^{(3)} >$ of a symmetric 4-tensor $\nabla^3 F$, where

$$\nabla^3 F = [\nabla^3 F]_{k,i,j,l} = \frac{\partial [\mathbf{r}]_k}{[\partial \mathbf{u}]_i [\partial \mathbf{u}]_j [\partial \mathbf{u}]_l}$$

for $k = 0, ..., n-1$ and $i, j, l = 0, ..., h-1$ with $[\nabla^3 F]_{k,i,j,l} = [\nabla^3 F]_{k,\pi(i,j,l)}$ for any permutation π of i, j, l, in directions $\mathbf{r}_{(1)} \in I\!R^n$ and $\mathbf{u}^{(2)}, \mathbf{u}^{(3)} \in I\!R^h$ is a first-order tangent projection in direction $\mathbf{u}^{(3)}$ of the second-order adjoint projection of $\nabla^3 F$ in directions $\mathbf{r}_{(1)}$ and $\mathbf{u}^{(2)}$, that is $<< \mathbf{r}_{(1)}, \nabla^3 F, \mathbf{u}^{(2)} >, \mathbf{u}^{(3)} >$. It is a first-order tangent projection in direction $\mathbf{u}^{(3)}$ of the first-order tangent projection in direction $\mathbf{u}^{(2)}$ of the first-order adjoint projection of $\nabla^3 F$ in direction $\mathbf{r}_{(1)}$, i.e. $<< \mathbf{r}_{(1)}, \nabla^3 F >, \mathbf{u}^{(2)} >, \mathbf{u}^{(3)} >$.

The function $F_{(1)}^{(2,3)} : I\!R^h \times I\!R^n \times I\!R^h \times I\!R^h \to I\!R^h$, defined as

$$\mathbf{u}_{(1)}^{(2,3)} = F_{(1)}^{(2,3)}(\mathbf{u}, \mathbf{r}_{(1)}, \mathbf{u}^{(2)}, \mathbf{u}^{(3)}) \equiv < \mathbf{r}_{(1)}, \nabla^3 F(\mathbf{u}), \mathbf{u}^{(2)}, \mathbf{u}^{(3)} > \qquad (15)$$

is referred to as the *third-order adjoint model* of F. The 4-tensor $\nabla^3 F$ is projected in directions $\mathbf{r}_{(1)} \in I\!R^n$ and $\mathbf{u}^{(2)}, \mathbf{u}^{(3)} \in I\!R^h$.

Let $\nabla^3 F$ be a symmetric 4-tensor as defined above and

$$B = < \mathbf{r}_{(1)}, \nabla^3 F > \in I\!R^h \times I\!R^h \times I\!R^h \quad , \text{ that is}$$

$$b_{i,j,l} = \sum_{k=0}^{n-1} [\mathbf{r}_{(1)}]_k \cdot [\nabla^3 F]_{k,i,j,l} \quad ,$$

for $i, j, l = 0, ..., h-1$. Moreover,

$$C =< B, \mathbf{u}^{(2)} >=<< \mathbf{r}_{(1)}, \nabla^3 F >, \mathbf{u}^{(2)} >\in I\!R^h \times I\!R^h \quad \text{, that is}$$

$$c_{i,j} = \sum_{l=0}^{h-1} b_{i,j,l} \cdot [\mathbf{u}^{(2)}]_l = \sum_{l=0}^{h-1} \sum_{k=0}^{n-1} [\mathbf{r}_{(1)}]_k \cdot [\nabla^3 F]_{k,i,j,l} \cdot [\mathbf{u}^{(2)}]_l \quad ,$$

for $i, j = 0, ..., h-1$. Then we have

$$\mathbf{u}_{(1)}^{(2,3)} =< C, \mathbf{u}^{(3)} >=<<< \mathbf{r}_{(1)}, \nabla^3 F >, \mathbf{u}^{(2)} >, \mathbf{u}^{(3)} >\in I\!R^h \quad \text{, that is}$$

$$[\mathbf{u}_{(1)}^{(2,3)}]_i = \sum_{j=0}^{h-1} c_{i,j} \cdot [\mathbf{u}^{(3)}]_j = \sum_{j=0}^{h-1} \sum_{l=0}^{h-1} \sum_{k=0}^{n-1} [\mathbf{r}_{(1)}]_k \cdot [\nabla^3 F]_{k,i,j,l} \cdot [\mathbf{u}^{(2)}]_l \cdot [\mathbf{u}^{(3)}]_j \quad ,$$

for $i = 0, ..., h-1$.

Application of tangent mode to the second-order adjoint model

$$\mathbf{u}_{(1)}^{(2)} =< \mathbf{r}_{(1)}, \nabla^2 F(\mathbf{u}), \mathbf{u}^{(2)} >$$

yields

$$\mathbf{u}_{(1)}^{(2,3)} =< \mathbf{r}_{(1)}^{(3)}, \nabla^2 F(\mathbf{u}), \mathbf{u}^{(2)} >< \mathbf{r}_{(1)}, \nabla^2 F(\mathbf{u}), \mathbf{u}^{(2,3)} > + < \mathbf{r}_{(1)}, \nabla^3 F(\mathbf{u}), \mathbf{u}^{(2)}, \mathbf{u}^{(3)} >,$$

where $\frac{\partial \mathbf{u}}{\partial s} = \mathbf{u}^{(3)}$, $\frac{\partial \mathbf{r}_{(1)}}{\partial s} = \mathbf{r}_{(1)}^{(3)}$ and $\frac{\partial \mathbf{u}^{(2)}}{\partial s} = \mathbf{u}^{(2,3)}$. Thus, for $\mathbf{r}_{(1)}^{(3)} = \mathbf{u}^{(2,3)} = 0$, Equation (15) follows.

Third-order adjoint (also: forward-over-forward-over-reverse) mode software tools for AD transform a given implementation

```
F(u, r)
```

of Equation $\mathbf{r} = F(\mathbf{u})$ with u $\hat{=}\mathbf{u}$ and r $\hat{=}\mathbf{r}$ into the (algorithmic) second-order tangent subroutine

```
t3_t2_a1_F(u, t3_u, t2_u, t3_t2_u, a1_u, t3_a1_u, t2_a1_u, t3_t2_a1_u,
           r, t3_r, t2_r, t3_t2_r, a1_r, t3_a1_r, t2_a1_r, t3_t2_a1_r)
```

where a1_u $\hat{=}\mathbf{u}_{(1)}$, t2_u $\hat{=}\mathbf{u}^{(2)}$, t3_u $\hat{=}\mathbf{u}^{(3)}$, t2_a1_u $\hat{=}\mathbf{u}_{(1)}^{(2)}$, t3_a1_u $\hat{=}\mathbf{u}_{(1)}^{(3)}$,t3_t2_u $\hat{=}\mathbf{u}^{(2,3)}$, t3_t2_t1_u $\hat{=}\mathbf{u}_{(1)}^{(2,3)}$, a1_r $\hat{=}\mathbf{r}_{(1)}$, t2_r $\hat{=}\mathbf{r}^{(2)}$, t3_r $\hat{=}\mathbf{r}^{(3)}$, t2_a1_r $\hat{=}\mathbf{r}_{(1)}^{(2)}$, t3_a1_r $\hat{=}\mathbf{r}_{(1)}^{(3)}$, t3_t2_r $\hat{=}\mathbf{r}^{(2,3)}$ and t3_t2_a1_r $\hat{=}\mathbf{r}_{(1)}^{(2,3)}$. The computation of the projection of tensor $\nabla^3 F$ in directions $\mathbf{u}^{(2)}, \mathbf{u}^{(3)}$ and $\mathbf{r}_{(1)}$ requires $\mathbf{u}^{(2,3)} = 0$ and $\mathbf{r}_{(1)}^{(3)} = 0$ initially. The entire tensor can be accumulated by letting $\mathbf{u}^{(2)}, \mathbf{u}^{(3)}$ and $\mathbf{r}_{(1)}$ range over Cartesian basis vectors in $I\!R^h, I\!R^h$ and $I\!R^n$ respectively. The third partial derivatives are returned in t3_t2_a1_u. This model yields the computational complexity of $O(n \cdot h^2) \cdot Cost(F)$ for evaluating the whole third derivative tensor.

The application of forward or reverse mode AD to any of the third derivative models yields fourth derivative information and so forth.

The derivative code that is generated by AD can compute projections of derivative tensors of arbitrary order, for example, (transposed) Jacobian-vector products in the first-order case, Hessian-vector products in the scalar second-order case, and so forth. Sums of the projections of tensors of various orders are returned by higher derivative code. AD users need to understand the effects of choosing certain directions for these projections (the *seeding* of the derivative code) in order to be able to retrieve (*harvest*) the desired results. For more information refer to [GW08,Nau12].

4 Second-Order Tangent Nonlinear Solver

We distinguish between two alternative approaches to the generation of second-order tangent solvers for systems of nonlinear equations. A *algorithmic* second-order tangent version of the solver computes second-order directional derivatives of the approximation of the solution, which is actually computed by the algorithm. Second-order AD is applied to the individual statements of the given implementation yielding an increase of roughly four in memory requirement as well as operations count.

A second-order *symbolic* tangent version of the solver computes the second directional derivatives of the solution under the assumption that the exact solution $\mathbf{x}^*$ has been reached. The nonlinear system $F(\mathbf{x}, \boldsymbol{\lambda}) = 0$ can be differentiated symbolically in this case. In symbolic tangent mode, the computation of second-order directional derivatives amounts to the solution of a linear system based on the Jacobian of F with respect to $\mathbf{x}^*$, which results in a significant reduction of the computational overhead in comparison with the algorithmic tangent version. The discrepancies in the results computed by second-order algorithmic and symbolic tangent nonlinear solvers depend on the accuracy of the approximation of the *primal* solution.

4.1 Algorithmic Mode

As an example for a nonlinear solver we solve the nonlinear system in Equation (1) with Newton's algorithm. The latter uses the Jacobian of the nonlinear system $(\nabla F(\mathbf{x}^i))$ at the current iterate $\mathbf{x}^i$ to determine the next Newton step.

A first-order tangent version of Newton's algorithm requires second directional derivatives of the residual. Consequently, second-order tangent version of the Newton's algorithm requires third directional derivatives of the given implementation of F.

As shown in [NLLT12], the first-order algorithmic tangent version of the given objective with Newton's algorithm used for the solution of the embedded parametrized system of nonlinear equations results from the straight application of tangent mode AD to Equations (6)–(8) as follows

For $i = 0, \ldots, \nu$:

$$A = \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}^i, \boldsymbol{\lambda}) \tag{16}$$

$$
\begin{aligned}
A^{(1)} &= < \frac{\partial^2 F}{\partial \mathbf{x} \partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda}), \begin{pmatrix} \mathbf{x}^{i\ (1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} > \\
\mathbf{b} &= -F(\mathbf{x}^i,\boldsymbol{\lambda}) \\
\mathbf{b}^{(1)} &= - < \frac{\partial F}{\partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda}), \begin{pmatrix} \mathbf{x}^{i\ (1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} > \\
\mathbf{s} &= \mathbf{L}(A,\mathbf{b}) \\
\mathbf{s}^{(1)} &= < \frac{\partial \mathbf{L}}{\partial(A,\mathbf{b})}(A,\mathbf{b}), \begin{pmatrix} A^{(1)} \\ \mathbf{b}^{(1)} \end{pmatrix} > \\
\mathbf{x}^{i+1} &= \mathbf{x}^i + \mathbf{s} \\
\mathbf{x}^{i+1\ (1)} &= \mathbf{x}^{i\ (1)} + \mathbf{s}^{(1)}
\end{aligned} \tag{17}
$$

The linear solver ($\mathbf{L}$) is augmented at the statement-level with local tangent models, thus roughly duplicating the required memory as well as the number of operations performed.

Reapplication of tangent AD to Equations (16)–(17) yields

for $i = 0, \ldots, \nu$:

$$
\begin{aligned}
A &= \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}^i,\boldsymbol{\lambda}) = < \frac{\partial F}{\partial \mathbf{x}}, I_n > = < \frac{\partial F}{\partial(\mathbf{x},\boldsymbol{\lambda})}, \overset{(\in \mathbb{R}^{(n+m)\times n})}{\begin{pmatrix} I_n \\ \mathbf{0}_m \end{pmatrix}} > \qquad (18) \\
A^{(2)} &= < \frac{\partial^2 F}{\partial \mathbf{x} \partial(\mathbf{x},\boldsymbol{\lambda})}, \begin{pmatrix} \mathbf{x}^{i\ (2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > = < \frac{\partial^2 F}{\partial(\mathbf{x},\boldsymbol{\lambda})^2}, \begin{pmatrix} I_n \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{i\ (2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \\
A^{(1)} &= < \frac{\partial^2 F}{\partial \mathbf{x} \partial(\mathbf{x},\boldsymbol{\lambda})}, \begin{pmatrix} \mathbf{x}^{i\ (1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} > = < \frac{\partial^2 F}{\partial(\mathbf{x},\boldsymbol{\lambda})^2}, \begin{pmatrix} I_n \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{i\ (1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} > \\
A^{(1,2)} &= < \frac{\partial^2 F}{\partial \mathbf{x} \partial(\mathbf{x},\boldsymbol{\lambda})}, \begin{pmatrix} \mathbf{x}^{i\ (1,2)} \\ \boldsymbol{\lambda}^{(1,2)} \end{pmatrix} > + < \frac{\partial^3 F}{\partial \mathbf{x} \partial(\mathbf{x},\boldsymbol{\lambda})^2}, \begin{pmatrix} \mathbf{x}^{i\ (1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{i\ (2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \\
&= < \frac{\partial^2 F}{\partial \mathbf{x} \partial(\mathbf{x},\boldsymbol{\lambda})}, I_n, \begin{pmatrix} \mathbf{x}^{i\ (1,2)} \\ \boldsymbol{\lambda}^{(1,2)} \end{pmatrix} > + < \frac{\partial^3 F}{\partial \mathbf{x} \partial(\mathbf{x},\boldsymbol{\lambda})^2}, I_n, \begin{pmatrix} \mathbf{x}^{i\ (1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{i\ (2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \\
&= < \frac{\partial^2 F}{\partial(\mathbf{x},\boldsymbol{\lambda})^2}, \begin{pmatrix} I_n \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{i\ (1,2)} \\ \boldsymbol{\lambda}^{(1,2)} \end{pmatrix} > + < \frac{\partial^3 F}{\partial(\mathbf{x},\boldsymbol{\lambda})^3}, \begin{pmatrix} I_n \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{i\ (1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{i\ (2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \\
\mathbf{b} &= -F(\mathbf{x}^i,\boldsymbol{\lambda}) \\
\mathbf{b}^{(2)} &= - < \frac{\partial F}{\partial(\mathbf{x},\boldsymbol{\lambda})}, \begin{pmatrix} \mathbf{x}^{i\ (2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \\
\mathbf{b}^{(1)} &= - < \frac{\partial F}{\partial(\mathbf{x},\boldsymbol{\lambda})}, \begin{pmatrix} \mathbf{x}^{i\ (1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} > \\
\mathbf{b}^{(1,2)} &= - < \frac{\partial F}{\partial(\mathbf{x},\boldsymbol{\lambda})}, \begin{pmatrix} \mathbf{x}^{i\ (1,2)} \\ \boldsymbol{\lambda}^{(1,2)} \end{pmatrix} > - < \frac{\partial^2 F}{\partial(\mathbf{x},\boldsymbol{\lambda})^2}, \begin{pmatrix} \mathbf{x}^{i\ (1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{i\ (2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \\
\mathbf{s} &= \mathbf{L}(A,\mathbf{b}) \\
\mathbf{s}^{(2)} &= < \frac{\partial \mathbf{L}}{\partial(A,\mathbf{b})}(A,\mathbf{b}), \begin{pmatrix} A^{(2)} \\ \mathbf{b}^{(2)} \end{pmatrix} >
\end{aligned}
$$

$$\mathbf{s}^{(1)} =< \frac{\partial \mathbf{L}}{\partial (A,\mathbf{b})}(A,\mathbf{b}), \begin{pmatrix} A^{(1)} \\ \mathbf{b}^{(1)} \end{pmatrix} >$$
$$\mathbf{s}^{(1,2)} =< \frac{\partial \mathbf{L}}{\partial (A,\mathbf{b})}(A,\mathbf{b}), \begin{pmatrix} A^{(1,2)} \\ \mathbf{b}^{(1,2)} \end{pmatrix} > + < \frac{\partial^2 \mathbf{L}}{\partial (A,\mathbf{b})^2}(A,\mathbf{b}), \begin{pmatrix} A^{(1)} \\ \mathbf{b}^{(1)} \end{pmatrix}, \begin{pmatrix} A^{(2)} \\ \mathbf{b}^{(2)} \end{pmatrix} >$$

$$\begin{aligned} \mathbf{x}^{i+1} &= \mathbf{x}^i + \mathbf{s} \\ \mathbf{x}^{i+1\ (2)} &= \mathbf{x}^{i\ (2)} + \mathbf{s}^{(2)} \\ \mathbf{x}^{i+1\ (1)} &= \mathbf{x}^{i\ (1)} + \mathbf{s}^{(1)} \\ \mathbf{x}^{i+1\ (1,2)} &= \mathbf{x}^{i\ (1,2)} + \mathbf{s}^{(1,2)} \quad , \end{aligned}$$

where all derivatives of F, e.g. $\frac{\partial F}{\partial (\mathbf{x},\boldsymbol{\lambda})}$ are evaluated at point $(\mathbf{x}^i, \boldsymbol{\lambda})$.

In Equation (18), $I_n \in I\!R^{n\times n}$ is the identity matrix, filled with m zero rows yielding $\begin{pmatrix} I_n \\ \mathbf{0}_m \end{pmatrix} \in I\!R^{(n+m)\times n}$. Furthermore, the differentiation of $\mathbf{L}(A,\mathbf{b}) \in I\!R^n$ with respect to $(A,\mathbf{b})$ is done through serialization of $(A,\mathbf{b})$, meaning that $A \in I\!R^{n\times n}$ and $\mathbf{b} \in I\!R^n$, $(A,\mathbf{b})$ is considered as a vector of size n^2+n. Consequently, $\frac{\partial \mathbf{L}}{\partial (A,\mathbf{b})}(A,\mathbf{b}) \in I\!R^{n\times(n^2+n)}$ and $\frac{\partial^2 \mathbf{L}}{\partial (A,b)^2}(A,b) \in I\!R^{n\times(n^2+n)\times(n^2+n)}$. Similarly we get $\begin{pmatrix} A^k \\ \mathbf{b}^k \end{pmatrix} \in I\!R^{n^2+n}$ for $k = (1), (2)$ or $(1,2)$.

In the above equations, first, second and third derivatives of F with respect to $(\mathbf{x}^i, \boldsymbol{\lambda})$ are required when computing third-order tangents of F with respect to $(\mathbf{x}^i, \boldsymbol{\lambda})$ using AD software tools, the function value as well as derivatives up to third order are evaluated.

In this case, the required memory is four times the memory (MEM) required by the nonlinear solver itself, i.e. $MEM(\mathbf{L}) \sim O(n^2)$ and the number of operations is four times the operations (OPS) performed by the nonlinear solver itself, i.e., $OPS(\mathbf{L}) \sim \nu \cdot O(n^3)$.

4.2 Symbolic Mode

Lemma 1 (Differentiation of a Matrix-Vector Product).
Let $\mathbf{G}(\mathbf{c}) =< \mathbf{A}(\mathbf{c}), \mathbf{b}(\mathbf{c}) >$ *be a symbolic bilinear map in which* $A(\mathbf{c}) \in \mathbf{R^{m\times n}}, \mathbf{b}(\mathbf{c}) \in \mathbf{R^n}$ *and* $\mathbf{G} : \mathbf{R^{m\times n}} \times \mathbf{R^n} \to \mathbf{R^m}$ *are differentiable functions. Differentiation of* $\mathbf{G}$ *with respect to* $\mathbf{c}$ *yields*

$$\mathbf{G^{(1)}}(\mathbf{c}) =< \mathbf{A^{(1)}}(\mathbf{c}), \mathbf{b}(\mathbf{c}) > + < \mathbf{A}(\mathbf{c}), \mathbf{b^{(1)}}(\mathbf{c}) > \quad .$$

Proof. Let $\mathbf{G^{(1)}} = \frac{\partial}{\partial \mathbf{c}} \mathbf{G}(\mathbf{c})$ and $\mathbf{G^{(1)}} \in \mathbf{R^m}$. Then we have

$$\begin{aligned}
\mathbf{G}^{(1)} &= \frac{\partial}{\partial \mathbf{c}} < A(\mathbf{c}), \mathbf{b}(\mathbf{c}) > \\
\mathbf{g}_i^{(1)} &= \frac{\partial}{\partial \mathbf{c}} \left(\sum_{j=1}^{n} a_{i,j}(\mathbf{c}) \cdot \mathbf{b}_j(\mathbf{c}) \right) = \sum_{j=1}^{n} \frac{\partial}{\partial \mathbf{c}} (a_{i,j}(\mathbf{c}) \cdot \mathbf{b}_j(\mathbf{c})) \\
&= \sum_{j=1}^{n} (\frac{\partial a_{i,j}(\mathbf{c})}{\partial \mathbf{c}} \cdot \mathbf{b}_j(\mathbf{c}) + a_{i,j}(\mathbf{c}) \cdot \frac{\partial \mathbf{b}_j(\mathbf{c})}{\partial \mathbf{c}}) \\
&= \sum_{j=1}^{n} \frac{\partial a_{i,j}(\mathbf{c})}{\partial \mathbf{c}} \cdot \mathbf{b}_j(\mathbf{c}) + \sum_{j=1}^{n} a_{i,j}(\mathbf{c}) \cdot \frac{\partial \mathbf{b}_j(\mathbf{c})}{\partial \mathbf{c}}) \quad ,
\end{aligned}$$

for $i = 1, \ldots, m$. Consequently,

$$\mathbf{G}^{(1)} = \frac{\partial A(\mathbf{c})}{\partial \mathbf{c}} \cdot \mathbf{b}(\mathbf{c}) + A(\mathbf{c}) \cdot \frac{\partial \mathbf{b}(\mathbf{c})}{\partial \mathbf{c}} =< A^{(1)}(\mathbf{c}), \mathbf{b}(\mathbf{c}) > + < A(\mathbf{c}), \mathbf{b}^{(1)}(\mathbf{c}) > \quad .$$

For further information refer to [Gil08].

Lemma 2. *Let* $T \in I\!R^{n \times (n+m) \times (n+m)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)} \in I\!R^n$ *and* $\boldsymbol{\lambda}^{(1)}, \boldsymbol{\lambda}^{(2)} \in I\!R^m$. *Then we have*

$$\begin{aligned}
< T, \begin{pmatrix} \mathbf{x}^{(1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} >= < T, \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > + < T, \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > \\
+ < T, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > + < T, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} >
\end{aligned}$$

Proof. Let $\mathbf{a} = \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix}, \mathbf{b} = \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix}, \mathbf{c} = \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \mathbf{d} = \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} \in \mathbf{R^{n+m}}$. Therefore, we have

$$
\begin{aligned}
&< T, \begin{pmatrix}\mathbf{x}^{(1)}\\ \mathbf{0}_m\end{pmatrix}, \begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} > + < T, \begin{pmatrix}\mathbf{x}^{(1)}\\ \mathbf{0}_m\end{pmatrix}, \begin{pmatrix}\mathbf{x}^{(2)}\\ \mathbf{0}_m\end{pmatrix} > \\
&+ < T, \begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(1)}\end{pmatrix}, \begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} > + < T, \begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(1)}\end{pmatrix}, \begin{pmatrix}\mathbf{x}^{(2)}\\ \mathbf{0}_m\end{pmatrix} > \\
&= \sum_{j=0}^{n+m}\sum_{k=0}^{n+m} T_{ijk}\cdot a_k \cdot d_j + \sum_{j=0}^{n+m}\sum_{k=0}^{n+m} T_{ijk}\cdot a_k \cdot b_j \\
&+ \sum_{j=0}^{n+m}\sum_{k=0}^{n+m} T_{ijk}\cdot c_k \cdot d_j + \sum_{j=0}^{n+m}\sum_{k=0}^{n+m} T_{ijk}\cdot c_k \cdot b_j \\
&= \sum_{j=0}^{n+m}\sum_{k=0}^{n+m} T_{ijk}\cdot (\begin{pmatrix}\mathbf{x}^{(1)}\\ \mathbf{0}_m\end{pmatrix}\cdot \begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} + \begin{pmatrix}\mathbf{x}^{(1)}\\ \mathbf{0}_m\end{pmatrix}\cdot \begin{pmatrix}\mathbf{x}^{(2)}\\ \mathbf{0}_m\end{pmatrix} \\
&+ \begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(1)}\end{pmatrix}\cdot \begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} + \begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(1)}\end{pmatrix}\cdot \begin{pmatrix}\mathbf{x}^{(2)}\\ \mathbf{0}_m\end{pmatrix}) \\
&= \sum_{j=0}^{n+m}\sum_{k=0}^{n+m} T_{ijk}\cdot (\begin{pmatrix}\mathbf{x}^{(1)}\\ \mathbf{0}_m\end{pmatrix}\cdot \left(\begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} + \begin{pmatrix}\mathbf{x}^{(2)}\\ \mathbf{0}_m\end{pmatrix}\right) + \begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(1)}\end{pmatrix}\cdot \left(\begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} + \begin{pmatrix}\mathbf{x}^{(2)}\\ \mathbf{0}_m\end{pmatrix}\right)) \\
&= \sum_{j=0}^{n+m}\sum_{k=0}^{n+m} T_{ijk}\cdot (\begin{pmatrix}\mathbf{x}^{(1)}\\ \mathbf{0}_m\end{pmatrix}\cdot \left(\begin{pmatrix}\mathbf{x}^{(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix}\right) + \begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(1)}\end{pmatrix}\cdot \left(\begin{pmatrix}\mathbf{x}^{(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix}\right)) \\
&= \sum_{j=0}^{n+m}\sum_{k=0}^{n+m} T_{ijk}\cdot (\begin{pmatrix}\mathbf{x}^{(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix}\cdot \left(\begin{pmatrix}\mathbf{x}^{(1)}\\ \mathbf{0}_m\end{pmatrix} + \begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(1)}\end{pmatrix}\right)) \\
&= \sum_{j=0}^{n+m}\sum_{k=0}^{n+m} T_{ijk}\cdot (\begin{pmatrix}\mathbf{x}^{(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix}\cdot \left(\begin{pmatrix}\mathbf{x}^{(1)}\\ \mathbf{0}_m\end{pmatrix} + \begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(1)}\end{pmatrix}\right)) \\
&= \sum_{j=0}^{n+m}\sum_{k=0}^{n+m} T_{ijk}\cdot \begin{pmatrix}\mathbf{x}^{(1)}\\ \boldsymbol{\lambda}^{(1)}\end{pmatrix}\cdot \begin{pmatrix}\mathbf{x}^{(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} \quad \text{for} \quad i = 0, ..., n \\
&= < T, \begin{pmatrix}\mathbf{x}^{(1)}\\ \boldsymbol{\lambda}^{(1)}\end{pmatrix}, \begin{pmatrix}\mathbf{x}^{(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} >
\end{aligned}
$$

Theorem 1. Symbolic Second-Order Tangent Solvers of Nonlinear Equation: *Let $\mathbf{r} = F(\mathbf{x}(\boldsymbol{\lambda}), \boldsymbol{\lambda}) : I\!R^n \times I\!R^m \rightarrow I\!R^n$ for a given $\boldsymbol{\lambda} \in I\!R^m$, a vector $\mathbf{x} \in R^n$ is sought such that $F(\mathbf{x}(\boldsymbol{\lambda}), \boldsymbol{\lambda}) = 0$. Second-order tangent differentiation of $F(\mathbf{x}, \boldsymbol{\lambda}) = 0$ at the solution $\mathbf{x} = \mathbf{x}^*$ with respect to $\boldsymbol{\lambda}$, i.e., computation of $\mathbf{x}^{(1,2)} \in I\!R^n$, amounts to the solution of the linear system*

$$
\frac{\partial F}{\partial \mathbf{x}} \cdot \mathbf{x}^{(1,2)} =< \frac{\partial F}{\partial \mathbf{x}}, \mathbf{x}^{(1,2)} >= - < \nabla^2 F, \begin{pmatrix}\mathbf{x}^{(1)}\\ \boldsymbol{\lambda}^{(1)}\end{pmatrix}, \begin{pmatrix}\mathbf{x}^{(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} > \quad . \qquad (19)
$$

Proof (Version 1).

As shown in [NLLT12], first-order symbolic tangent differentiation of $F(\mathbf{x}(\boldsymbol{\lambda}), \boldsymbol{\lambda}) = 0$ at the solution $\mathbf{x} = \mathbf{x}^*$ with respect to $\boldsymbol{\lambda}$, i.e., computation of $\mathbf{x}^{(1)}$, yields

$$\frac{\partial F}{\partial \mathbf{x}}(\mathbf{x},\boldsymbol{\lambda})\cdot \mathbf{x}^{(1)} = -\frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x},\boldsymbol{\lambda})\cdot \boldsymbol{\lambda}^{(1)} \tag{20}$$

which is a linear system and $\frac{\partial F}{\partial \mathbf{x}}$ is the Jacobian matrix. This equation can be written as

$$\frac{\partial F}{\partial \mathbf{x}}(\mathbf{x},\boldsymbol{\lambda})\cdot \mathbf{x}^{(1)} + \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x},\boldsymbol{\lambda})\cdot \boldsymbol{\lambda}^{(1)} =< \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x},\boldsymbol{\lambda}), \mathbf{x}^{(1)} > + < \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x},\boldsymbol{\lambda}), \boldsymbol{\lambda}^{(1)} > . \tag{21}$$

An alternative for evaluating the second directional derivatives of the solution $\mathbf{x} = \mathbf{x}^*$ with respect to $\boldsymbol{\lambda}$ in $F(\mathbf{x},\boldsymbol{\lambda}) = 0$ is to differentiate Equation (21) with respect to $\boldsymbol{\lambda}$

$$\begin{aligned} &\frac{d}{d\boldsymbol{\lambda}}\left(< \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x},\boldsymbol{\lambda}), \mathbf{x}^{(1)} > + < \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x},\boldsymbol{\lambda}), \boldsymbol{\lambda}^{(1)} >\right)\cdot \boldsymbol{\lambda}^{(2)} \\ &= < \frac{d < \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x},\boldsymbol{\lambda}), \mathbf{x}^{(1)} >}{d\boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > + < \frac{d < \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x},\boldsymbol{\lambda}), \boldsymbol{\lambda}^{(1)} >}{d\boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > \quad , \end{aligned} \tag{22}$$

where $< \frac{d< \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x},\boldsymbol{\lambda}),\mathbf{x}^{(1)}>}{d\boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >$ and $< \frac{d< \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x},\boldsymbol{\lambda}),\boldsymbol{\lambda}^{(1)}>}{d\boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >$ are the total derivatives of $g_1 =< \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x},\boldsymbol{\lambda}), \mathbf{x}^{(1)} >$ and $g_2 =< \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x},\boldsymbol{\lambda}), \boldsymbol{\lambda}^{(1)} >$ with respect to $\boldsymbol{\lambda}$ respectively. Because g_1 and g_2 depend on $\mathbf{x}$ as well as $\boldsymbol{\lambda}$, we have

$$\begin{aligned} < \frac{dg_1}{d\boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > &=< \frac{\partial g_1}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > + < \frac{\partial g_1}{\partial \mathbf{x}}, \underbrace{< \frac{\partial \mathbf{x}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >}_{=\mathbf{x}^{(2)}} > \\ &=< \frac{\partial < \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x},\boldsymbol{\lambda}), \mathbf{x}^{(1)} >}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > + < \frac{\partial < \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x},\boldsymbol{\lambda}), \mathbf{x}^{(1)} >}{\partial \mathbf{x}}, \mathbf{x}^{(2)} > \quad , \end{aligned} \tag{23}$$

$$\begin{aligned} < \frac{dg_2}{d\boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > &=< \frac{\partial g_2}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > + < \frac{\partial g_2}{\partial \mathbf{x}}, \underbrace{< \frac{\partial \mathbf{x}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >}_{=\mathbf{x}^{(2)}} > \\ &=< \frac{\partial < \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x},\boldsymbol{\lambda}), \boldsymbol{\lambda}^{(1)} >}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > + < \frac{\partial < \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x},\boldsymbol{\lambda}), \boldsymbol{\lambda}^{(1)} >}{\partial \mathbf{x}}, \mathbf{x}^{(2)} > . \end{aligned} \tag{24}$$

According to Theorem 1, the first term on the right hand side of Equation (23) yields

$$\begin{aligned} < \frac{\partial < \frac{\partial F}{\partial \mathbf{x}}, \mathbf{x}^{(1)} >}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > &= < \frac{\partial^2 F}{\partial \mathbf{x}\partial \boldsymbol{\lambda}}, \mathbf{x}^{(1)}, \boldsymbol{\lambda}^{(2)} > + < \frac{\partial F}{\partial \mathbf{x}}, < \frac{\partial \mathbf{x}^{(1)}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >> \\ &= < \frac{\partial^2 F}{\partial (\mathbf{x},\boldsymbol{\lambda})^2}, \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \\ &\quad + < \frac{\partial F}{\partial \mathbf{x}}, < \frac{\partial \mathbf{x}^{(1)}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >> \\ &= < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > + < \frac{\partial F}{\partial \mathbf{x}}, \mathbf{x}^{(1,2)} > . \end{aligned}$$

Similarly, the second term on the right hand side of Equation (23) becomes

$$\begin{aligned} < \frac{\partial < \frac{\partial F}{\partial \mathbf{x}}, \mathbf{x}^{(1)} >}{\partial \mathbf{x}}, \mathbf{x}^{(2)} > &=< \frac{\partial^2 F}{\partial \mathbf{x}^2}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)} > + < \frac{\partial F}{\partial \mathbf{x}}, < \underbrace{\frac{\partial \mathbf{x}^{(1)}}{\partial \mathbf{x}}}_{0}, \mathbf{x}^{(2)} >> \\ &=< \underbrace{\frac{\partial^2 F}{\partial (\mathbf{x}, \boldsymbol{\lambda})^2}}_{\nabla^2 F}, \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > . \end{aligned}$$

Applying Theorem 1, the first term on the right hand side of Equation (24) yields

$$\begin{aligned} < \frac{\partial < \frac{\partial F}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(1)} >}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > &=< \frac{\partial^2 F}{\partial \boldsymbol{\lambda}^2}, \boldsymbol{\lambda}^{(1)}, \boldsymbol{\lambda}^{(2)} > + < \frac{\partial F}{\partial \boldsymbol{\lambda}}, < \underbrace{\frac{\partial \boldsymbol{\lambda}^{(1)}}{\partial \boldsymbol{\lambda}}}_{0}, \boldsymbol{\lambda}^{(2)} >> \\ &=< \underbrace{\frac{\partial^2 F}{\partial (\mathbf{x}, \boldsymbol{\lambda})^2}}_{\nabla^2 F}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > . \end{aligned}$$

Similarly, the second term on the right hand side of Equation (24) becomes

$$\begin{aligned} < \frac{\partial < \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x}, \boldsymbol{\lambda}), \boldsymbol{\lambda}^{(1)} >}{\partial \mathbf{x}}, \mathbf{x}^{(2)} > &=< \frac{\partial^2 F}{\partial \boldsymbol{\lambda} \partial \mathbf{x}}, \boldsymbol{\lambda}^{(1)}, \mathbf{x}^{(2)} > + < \frac{\partial F}{\partial \boldsymbol{\lambda}}, < \underbrace{\frac{\partial \boldsymbol{\lambda}^{(1)}}{\partial \mathbf{x}}}_{0}, \mathbf{x}^{(2)} >> \\ &=< \underbrace{\frac{\partial^2 F}{\partial (\mathbf{x}, \boldsymbol{\lambda})^2}}_{\nabla^2 F}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > . \end{aligned}$$

Consequently, Equation (22) yields

$$\begin{aligned} &< \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > + < \frac{\partial F}{\partial \mathbf{x}}, \mathbf{x}^{(1,2)} > + < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > \\ &+ < \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > + < \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > = 0 \end{aligned}$$

$$\begin{aligned} < \frac{\partial F}{\partial \mathbf{x}}, \mathbf{x}^{(1,2)} > &= - < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > - < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > \\ &- < \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > - < \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > \end{aligned}$$

Therefore, according to Theorem 2,

$$< \frac{\partial F}{\partial \mathbf{x}}, \mathbf{x}^{(1,2)} > = \frac{\partial F}{\partial \mathbf{x}} \cdot \mathbf{x}^{(1,2)} = - < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \quad .$$

In the above equation, the right hand side can be calculated by second-order tangent AD. Computing the right hand side and the Jacobian matrix $\frac{\partial F}{\partial \mathbf{x}}$ with AD, this system can be solved by using the same linear solver as applied for computation of the first-order symbolic tangent $\mathbf{x}^{(1)}$ in Equation (21), e.g. Gauss.

Proof (Version 2).

As shown in [NLLT12], the first-order symbolic tangent differentiation of $F(\mathbf{x}(\boldsymbol{\lambda}), \boldsymbol{\lambda}) = 0$ at the solution $\mathbf{x} = \mathbf{x}^*$ with respect to $\boldsymbol{\lambda}$, i.e., the computation of $\mathbf{x}^{(1)}$, yields

$$\begin{aligned}
\frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}, \boldsymbol{\lambda}) \cdot \mathbf{x}^{(1)} &= -\frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x}, \boldsymbol{\lambda}) \cdot \boldsymbol{\lambda}^{(1)} && (25)\\
\frac{\partial F}{\partial \mathbf{x}} \cdot \mathbf{x}^{(1)} &= - < \frac{\partial F}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(1)} > \\
\frac{\partial F}{\partial \mathbf{x} \partial \boldsymbol{\lambda}} \cdot \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix} &= - < \frac{\partial F}{\partial \mathbf{x} \partial \boldsymbol{\lambda}}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} > \\
\nabla F \cdot \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix} &= - < \nabla F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} > \quad , && (26)
\end{aligned}$$

which is a linear system of type $A\mathbf{c} = \mathbf{b}$, where $A = \nabla F$, $\mathbf{c} = \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix}$ and $\mathbf{b} = - < \nabla F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} >$.

An option to evaluate the second-order directional derivatives of the solution $\mathbf{x} = \mathbf{x}^*$ with respect to $\boldsymbol{\lambda}$ in $F(\mathbf{x}, \boldsymbol{\lambda}) = 0$ is to apply the symbolic first-order tangent version for linear solvers to Equation (26) .

As shown in [Gil08], for the linear system $A\mathbf{c} = \mathbf{b}$ we have

$$\begin{aligned}
\mathbf{c} &= \mathbf{L}(A, \mathbf{b}) \quad , \\
\mathbf{c}^{(1)} &= \mathbf{L}^{(1)}(A, A^{(1)}, \mathbf{b}, \mathbf{b}^{(1)}) =< \frac{\partial \mathbf{c}}{\partial A}, A^{(1)} > + < \frac{\partial \mathbf{c}}{\partial \mathbf{b}}, \mathbf{b}^{(1)} > \quad , && (27)
\end{aligned}$$

where

$$\begin{aligned}
A \cdot < \frac{\partial \mathbf{c}}{\partial A}, A^{(1)} > &= -A^{(1)} \cdot \mathbf{c} \quad , && (28)\\
A \cdot < \frac{\partial \mathbf{c}}{\partial \mathbf{b}}, \mathbf{b}^{(1)} > &= \mathbf{b}^{(1)} \quad . && (29)
\end{aligned}$$

For the computation of Equation (27) the matrices $A, A^{(1)} \in I\!R^{n \times (n+m)}$ are assumed to be serialized. Therefore, differentiation of $\mathbf{c} \in I\!R^{n+m}$ with respect to $A \in I\!R^{n^2+n\cdot m}$, gives a matrix $\frac{\partial \mathbf{c}}{\partial A} \in I\!R^{(n+m)\times(n^2+n\cdot m)}$. Projecting this matrix in direction $A^{(1)} \in I\!R^{n^2+n\cdot m}$ yields $< \frac{\partial \mathbf{c}}{\partial A}, A^{(1)} > \in I\!R^{n+m}$.

Computing $A^{(1)}$, $\mathbf{b}^{(1)}$ and $\mathbf{c}^{(1)}$ in Equation (26) yields

$$
\begin{aligned}
A &= \nabla F \quad , \\
A^{(1)} &=< \frac{d\,(\nabla F)}{d\boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > \\
&=< \frac{\partial(\nabla F)}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > + < \frac{\partial(\nabla F)}{\partial \mathbf{x}}, \underbrace{< \frac{\partial \mathbf{x}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >}_{=\mathbf{x}^{(2)}} > \\
&=< \frac{\partial(\nabla F)}{\partial \mathbf{x} \partial \boldsymbol{\lambda}}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > + < \frac{\partial(\nabla F)}{\partial \mathbf{x} \partial \boldsymbol{\lambda}}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > \\
&=< \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > + < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > \\
&=< \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \quad ,
\end{aligned}
$$

where $A, A^{(1)} \in I\!R^{n \times (n+m)}$. Moreover,

$$
\begin{aligned}
\mathbf{b} &= - < \nabla F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} > \quad , \\
\mathbf{b}^{(1)} &= \frac{d}{d\boldsymbol{\lambda}} \left(- < \nabla F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} > \right) \cdot \boldsymbol{\lambda}^{(2)} \\
&= - < \frac{\partial < \nabla F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} >}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > - < \frac{\partial < \nabla F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} >}{\partial \mathbf{x}}, \overbrace{< \frac{\partial \mathbf{x}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >}^{=\mathbf{x}^{(2)}} > \\
&= - < \frac{\partial < \nabla F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} >}{\partial \mathbf{x} \partial \boldsymbol{\lambda}}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > - < \frac{\partial < \nabla F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix} >}{\partial \mathbf{x} \partial \boldsymbol{\lambda}}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > \\
&= - < \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > - < \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > \\
&= - < \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \quad ,
\end{aligned}
$$

and

$$
\begin{aligned}
\mathbf{c} &= \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix} \quad , \\
\mathbf{c}^{(1)} &= \frac{d}{d\boldsymbol{\lambda}} \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix} \cdot \boldsymbol{\lambda}^{(2)} = \frac{\partial \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix}}{\partial \boldsymbol{\lambda}} \cdot \boldsymbol{\lambda}^{(2)} \\
&= \begin{pmatrix} \frac{\partial \mathbf{x}^{(1)}}{\partial \boldsymbol{\lambda}} \cdot \boldsymbol{\lambda}^{(2)} \\ \mathbf{0}_m \end{pmatrix} = \begin{pmatrix} \mathbf{x}^{(1,2)} \\ \mathbf{0}_m \end{pmatrix} \quad .
\end{aligned}
$$

Now applying Equations (28)-(29) to the linear system in Equation (26) we have

$$\begin{aligned}
\nabla F \cdot < \frac{\partial \mathbf{c}}{\partial A}, A^{(1)} > &= - < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \cdot \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix} \\
&= - < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix} > \quad , \\
\nabla F \cdot < \frac{\partial \mathbf{c}}{\partial \mathbf{b}}, \mathbf{b}^{(1)} > &= - < \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \quad .
\end{aligned}$$

Consequently, Equation (27) yields

$$\begin{aligned}
\begin{pmatrix} \mathbf{x}^{(1,2)} \\ \mathbf{0}_m \end{pmatrix} &= - (\nabla F)^{-1} \cdot < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix} > \\
&\quad - (\nabla F)^{-1} \cdot < \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \\
\nabla F \cdot \begin{pmatrix} \mathbf{x}^{(1,2)} \\ \mathbf{0}_m \end{pmatrix} &= - < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{0}_m \end{pmatrix} > - < \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \\
\nabla F \cdot \begin{pmatrix} \mathbf{x}^{(1,2)} \\ \mathbf{0}_m \end{pmatrix} &= - < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \\
\frac{\partial F}{\partial \mathbf{x}} \cdot \mathbf{x}^{(1,2)} &= - < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \quad .
\end{aligned}$$

Both $\frac{\partial F}{\partial \mathbf{x}}$ and the right hand side can be computed automatically by AD.

The required memory for evaluating the symbolic second-order tangent nonlinear solver is the memory required by the nonlinear solver itself (e.g. Equation (7) in Newton's algorithm), i.e. $MEM(\mathbf{L}) \sim O(n^2)$. In Equation (19) the complexity of evaluating the right hand side is $O(1) \cdot Cost(F)$. The decomposition of the Jacobian ($\frac{\partial F}{\partial \mathbf{x}}$) which is done in the evaluation of the first-order partial derivatives with symbolic tangent (Equation (20) or Equation (25)) at the cost of $O(n^3)$ can also be used in evaluating the second-order directional derivatives. Solving the linear system (Equation (19)) e.g. with forward/backward substitution at the cost of $O(n^2)$, the overall complexity of evaluating the symbolic second-order tangent directional derivatives $\mathbf{x}^{(1,2)}$ is proportional to $O(n^3)$.

5 Second-Order Adjoint Nonlinear Solver

As in Section 4 we distinguish between second-order algorithmic and symbolic modes when deriving adjoint solvers for systems of nonlinear equations. Similar remarks regarding numerical consistency between the primal and the adjoint solvers apply.

5.1 Algorithmic Mode

As mentioned in the previous section, solving the nonlinear system (Equation (1)) with e.g. Newton, the nonlinear solver uses the Jacobian of the nonlinear system

($\nabla F(\mathbf{x}^i)$) at the current iterate $\mathbf{x}^i$ to determine the next Newton step. First-order adjoint version of Newton's algorithm requires second directional derivatives of the residual. Consequently, second-order adjoint version of the Newton's algorithm requires the third directional derivatives of the given implementation of F.

It should be considered that the memory requirement for the algorithmic adjoint nonlinear solver becomes proportional to the number of operations performed by the nonlinear solver. Data required within the reverse section is recorded in the forward section. The resulting memory requirement is likely to exceed the available resources for most real-world applications. Checkpointing techniques can help keeping the required memory feasible at the expense of additional function evaluations, See [GW08,Nau12] for details.

As it is shown in [NLLT12], the first-order algorithmic adjoint version of the given objective with Newton ' s algorithm which is used for the solution of the embedded parametrized systems of nonlinear equations results from the straight application of adjoint mode AD to Equations (6)–(8). The application of (incremental) adjoint mode AD to Equations (6)–(8) (without checkpointing) yields

for $i = 0, \ldots, \nu$

$$\begin{aligned}
(A, \tau) &:= \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}^i, \boldsymbol{\lambda}) && (30)\\
(\mathbf{b}, \tau) &:= -F(\mathbf{x}^i, \boldsymbol{\lambda}) \\
(\mathbf{s}, \tau) &:= \mathbf{L}(A, \mathbf{b}) && (31)\\
\mathbf{x}^{i+1} &:= \mathbf{x}^i + \mathbf{s} && (32)
\end{aligned}$$

for $i = \nu, \ldots, 0$

$$\begin{aligned}
\mathbf{x}^i_{(1)} &:= \mathbf{s}_{(1)} := \mathbf{x}^{i+1}_{(1)} \\
\begin{pmatrix} A_{(1)} \\ \mathbf{b}_{(1)} \end{pmatrix} &:= \mathbf{L}_{(1)}(\mathbf{s}_{(1)}, \tau) \\
\begin{pmatrix} \mathbf{x}^i_{(1)} \\ \boldsymbol{\lambda}_{(1)} \end{pmatrix} &:= \begin{pmatrix} \mathbf{x}^i_{(1)} \\ \boldsymbol{\lambda}_{(1)} \end{pmatrix} + < \mathbf{b}_{(1)}, \frac{\partial F}{\partial(\mathbf{x}, \lambda)}(\mathbf{x}^i, \boldsymbol{\lambda}) > (\tau) && (33)\\
&\quad + < A_{(1)}, \frac{\partial^2 F}{\partial \mathbf{x} \partial(\mathbf{x}, \boldsymbol{\lambda})}(\mathbf{x}^i, \boldsymbol{\lambda}) > (\tau).
\end{aligned}$$

Data required within the reverse section is recorded on a data structure [2] τ in the augmented forward section (Equations (30)–(32)). The input value of $\boldsymbol{\lambda}_{(1)}$ depends on the context in which the nonlinear solver is called. In the specific scenario given by Equations (3)–(5) it is initially equal to zero as adjoints of intermediate (neither input nor output) variables should be; see, for example,

[2] Using AD overloading tool, e.g. dco (Derivative Code by Overloading), datas required within the reverse section will be recorded on tape, whereas by using AD source transformation tool, e.g. dcc (Derivative Code Compiler), datas required within the reverse section will be recorded on stack.

[GW08]. In Equation (33) the projections of $\frac{\partial F}{\partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda})$ and $\frac{\partial^2 F}{\partial\mathbf{x}\partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda})$ in directions $\mathbf{b}_{(1)}$ and $A_{(1)}$ respectively depend on τ, i.e., the projections on the reverse section are dependent on the datas recorded on tape during the forward section.

Both the Jacobian accumulation in Equation (30) and the linear solver in Equation (31) are treated straightforwardly with an application of AD software.

As mensioned above, datas in the forward section are recorded on tape to be used in the calculations on the reverse section. In the following for simplicity and better readability we omit the τ.

Applying second-order algorithmic adjoint of AD to Equations (6)–(8) yields

for $i = 0, \ldots, \nu$

$$\begin{aligned}
A &:= \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}^i,\boldsymbol{\lambda}) \\
A^{(2)} &:=< \frac{\partial^2 F}{\partial\mathbf{x}\partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda}), \begin{pmatrix} \mathbf{x}^{i\ (2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \\
\mathbf{b} &:= -F(\mathbf{x}^i,\boldsymbol{\lambda}) \\
\mathbf{b}^{(2)} &:= - < \frac{\partial F}{\partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda}), \begin{pmatrix} \mathbf{x}^{i\ (2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \\
\mathbf{s} &:= \mathbf{L}(A,\mathbf{b}) \\
\mathbf{s}^{(2)} &:=< \frac{\partial \mathbf{L}}{\partial(A,\mathbf{b})}(A,\mathbf{b}), \begin{pmatrix} A^{(2)} \\ \mathbf{b}^{(2)} \end{pmatrix} > \\
\mathbf{x}^{i+1} &:= \mathbf{x}^i + \mathbf{s} \\
\mathbf{x}^{i+1\ (2)} &:= \mathbf{x}^{i\ (2)} + \mathbf{s}^{(2)} \quad ,
\end{aligned}$$

followed by

for $i = \nu, \ldots, 0$

$$\begin{aligned}
\mathbf{x}^i_{(1)} &:= \mathbf{s}_{(1)} := \mathbf{x}^{i+1}_{(1)} \\
\mathbf{s}^{(2)}_{(1)} &:= \mathbf{s}^{(2)}_{(1)} + \mathbf{x}^{i+1(2)}_{(1)} \\
\mathbf{x}^{(2)}_{(1)} &:= \mathbf{x}^{(2)}_{(1)} + \mathbf{x}^{i+1(2)}_{(1)} \\
\begin{pmatrix} A_{(1)} \\ \mathbf{b}_{(1)} \end{pmatrix} &:=< \mathbf{s}_{(1)}, \frac{\partial \mathbf{L}}{\partial(A,\mathbf{b})}(A,\mathbf{b}) > \\
\begin{pmatrix} A^{(2)}_{(1)} \\ \mathbf{b}^{(2)}_{(1)} \end{pmatrix} &:= \begin{pmatrix} A^{(2)}_{(1)} \\ \mathbf{b}^{(2)}_{(1)} \end{pmatrix} + < \mathbf{s}^{(2)}_{(1)}, \frac{\partial \mathbf{L}}{\partial(A,\mathbf{b})}(A,\mathbf{b}) > \\
&\qquad + < \mathbf{s}_{(1)}, \frac{\partial^2 \mathbf{L}}{\partial(A,\mathbf{b})^2}(A,\mathbf{b}), \begin{pmatrix} A^{(2)} \\ \mathbf{b}^{(2)} \end{pmatrix} >
\end{aligned}$$

$$\begin{pmatrix}\mathbf{x}^i_{(1)}\\ \boldsymbol{\lambda}_{(1)}\end{pmatrix} := \begin{pmatrix}\mathbf{x}^i_{(1)}\\ \boldsymbol{\lambda}_{(1)}\end{pmatrix} + < A_{(1)}, \frac{\partial^2 F}{\partial \mathbf{x}\partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda}) > \\ - < \mathbf{b}_{(1)}, \frac{\partial F}{\partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda}) > \tag{34}$$

$$\begin{pmatrix}\mathbf{x}^{i(2)}_{(1)}\\ \boldsymbol{\lambda}^{(2)}_{(1)}\end{pmatrix} := \begin{pmatrix}\mathbf{x}^{i(2)}_{(1)}\\ \boldsymbol{\lambda}^{(2)}_{(1)}\end{pmatrix} + < A^{(2)}_{(1)}, \frac{\partial^2 F}{\partial \mathbf{x}\partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda}) > \\ - < \mathbf{b}^{(2)}_{(1)}, \frac{\partial F}{\partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda}) > \\ + < A_{(1)}, \frac{\partial^3 F}{\partial \mathbf{x}\partial(\mathbf{x},\boldsymbol{\lambda})^2}(\mathbf{x}^i,\boldsymbol{\lambda}), \begin{pmatrix}\mathbf{x}^{i(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} > \\ - < \mathbf{b}_{(1)}, \frac{\partial^2 F}{\partial(\mathbf{x},\boldsymbol{\lambda})^2}(\mathbf{x}^i,\boldsymbol{\lambda}), \begin{pmatrix}\mathbf{x}^{i(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} > \tag{35}$$

where all the derivatives of F, e.g. $\frac{\partial F}{\partial(\mathbf{x},\boldsymbol{\lambda})}$ are evaluated at point $(\mathbf{x}^i,\boldsymbol{\lambda})$. The same as previous section, the differentiation of $\mathbf{L}(A,\mathbf{b}) \in I\!R^n$ with respect to $(A,\mathbf{b})$ is done through serialization of $(A,\mathbf{b})$, meaning that $A \in I\!R^{n\times n}$ and $\mathbf{b} \in I\!R^n$, $(A,\mathbf{b})$ is considered as a vector of size n^2+n. Consequently, $\frac{\partial \mathbf{L}}{\partial(A,\mathbf{b})}(A,\mathbf{b}) \in I\!R^{n\times(n^2+n)}$ and $\frac{\partial^2 \mathbf{L}}{\partial(A,\mathbf{b})^2}(A,\mathbf{b}) \in I\!R^{n\times(n^2+n)\times(n^2+n)}$. The serialization is also applied for $\begin{pmatrix}A_{(1)}\\ \mathbf{b}_{(1)}\end{pmatrix}$, $\begin{pmatrix}A^{(2)}\\ \mathbf{b}^{(2)}\end{pmatrix}$ and $\begin{pmatrix}A^{(2)}_{(1)}\\ \mathbf{b}^{(2)}_{(1)}\end{pmatrix} \in I\!R^{n^2+n}$. Furthermore, the expressions $< A_{(1)}, \frac{\partial^2 F}{\partial \mathbf{x}\partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda}) >$ in Equation (34) and $< A^{(2)}_{(1)}, \frac{\partial^2 F}{\partial \mathbf{x}\partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda}) >$ in Equation (35) denote a projection image dimension of length $n^2(\Leftarrow n\times n)$ of the first derivative of the Jacobian $\frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}^i,\boldsymbol{\lambda})$ with respect to $\mathbf{x}$ and $\boldsymbol{\lambda}$ (the Hessian $\frac{\partial^2 F}{\partial \mathbf{x}\partial(\mathbf{x},\boldsymbol{\lambda})}(\mathbf{x}^i,\boldsymbol{\lambda})$) in the direction obtained by a corresponding serialization of $A_{(1)}$ and $A^{(2)}_{(1)}$ respectively. The expression $< A_{(1)}, \frac{\partial^3 F}{\partial \mathbf{x}\partial(\mathbf{x},\boldsymbol{\lambda})^2}(\mathbf{x}^i,\boldsymbol{\lambda}), \begin{pmatrix}\mathbf{x}^{i(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} >$ in Equation (35) denotes a projection image dimension of length $n^2(\Leftarrow n\times n)$ of the second derivative of the Jacobian $\frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}^i,\boldsymbol{\lambda})$ with respect to $\mathbf{x}$ and $\boldsymbol{\lambda}$ (the 4-tensor $\frac{\partial^3 F}{\partial \mathbf{x}\partial(\mathbf{x},\boldsymbol{\lambda})^2}(\mathbf{x}^i,\boldsymbol{\lambda})$) in the direction obtained by a corresponding serialization of $A_{(1)}$ and in direction $\begin{pmatrix}\mathbf{x}^{i(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix}$.

In the above equations, first, second and third derivatives of F with respect to $(\mathbf{x}^i,\boldsymbol{\lambda})$ are required when computing third-order adjoints of F with respect to $(\mathbf{x}^i,\boldsymbol{\lambda})$ using AD software tools, the function value as well as derivatives up to third-order are evaluated.

In this case, the number of operations is four times the operations (OPS) performed by the nonlinear solver itself, i.e., $\nu\cdot O(n^3)$. The required memory in this case is proportional to the number of operations, i.e., $\nu\cdot O(n^3)$. All these computations can be done automatically using AD software tools.

5.2 Symbolic Mode

Theorem 2. Symbolic Second-Order Adjoint Solvers of Nonlinear Equation: *Let* $\mathbf{r} = F(\mathbf{x}(\boldsymbol{\lambda}),\boldsymbol{\lambda}) : I\!R^n \times I\!R^m \to I\!R^n$ *for a given* $\boldsymbol{\lambda} \in I\!R^m$*, a vector* $\mathbf{x} \in R^n$ *is sought such that* $F(\mathbf{x}(\boldsymbol{\lambda}),\boldsymbol{\lambda}) = 0$*. Let* $\mathbf{z} \in I\!R^n$ *and*

$$\frac{\partial F}{\partial \mathbf{x}}^T(\mathbf{x},\boldsymbol{\lambda})\cdot \mathbf{z} = -\mathbf{x}_{(1)} \quad . \tag{36}$$

Furthermore, let $\mathbf{z}^{(2)} =< \frac{\partial \mathbf{z}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >$ *,* $\mathbf{z}^{(2)} \in I\!R^n$ *and*

$$\frac{\partial F}{\partial \mathbf{x}}^T \cdot \mathbf{z}^{(2)} = -< \mathbf{z}, \nabla^2 F, \begin{pmatrix}\mathbf{x}^{(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} > -\mathbf{x}^{(2)}_{(1)} \quad .$$

Second-order adjoint differentiation of $F(\mathbf{x},\boldsymbol{\lambda}) = 0$ *at the solution* $\mathbf{x} = \mathbf{x}^*$ *with respect to* $\boldsymbol{\lambda}$*, i.e., computation of* $\boldsymbol{\lambda}^{(2)}_{(1)} \in I\!R^m$*, yields*

$$\begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(2)}_{(1)}\end{pmatrix} + =< \mathbf{z}, \nabla^2 F, \begin{pmatrix}\mathbf{x}^{(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} > + < \mathbf{z}^{(2)}, \nabla F > \quad . \tag{37}$$

Proof (Version 1). As shown in [NLLT12], first-order symbolic adjoint differentiation of $F(\mathbf{x}(\boldsymbol{\lambda}),\boldsymbol{\lambda}) = 0$ at the solution $\mathbf{x} = \mathbf{x}^*$ with respect to $\boldsymbol{\lambda}$, i.e., computation of $\boldsymbol{\lambda}_{(1)}$, yields

$$< \mathbf{z}, \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x},\boldsymbol{\lambda}) >= -\mathbf{x}_{(1)} \quad , \tag{38}$$

$$\boldsymbol{\lambda}_{(1)} + =< \mathbf{z}, \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x},\boldsymbol{\lambda}) > \quad , \tag{39}$$

where Equation (38) is a linear system based on transposed Jacobian of F with respect to $\mathbf{x}$, followed by Equation (39) for computing $\boldsymbol{\lambda}_{(1)}$.

An alternative for evaluating the second directional derivatives of the solution $\mathbf{x} = \mathbf{x}^*$ with respect to $\boldsymbol{\lambda}$ in $F(\mathbf{x},\boldsymbol{\lambda}) = 0$ is to differentiate Equations (38)–(39) with respect to $\boldsymbol{\lambda}$. Differentiating Equation (38) yields

$$\frac{d}{d\boldsymbol{\lambda}} < \mathbf{z}, \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x},\boldsymbol{\lambda}) > \cdot \boldsymbol{\lambda}^{(2)} = \frac{d}{d\boldsymbol{\lambda}}(-\mathbf{x}_{(1)}) \cdot \boldsymbol{\lambda}^{(2)} \quad .$$

Applying Theorem 1 to the above equation yields

$$< \frac{d}{d\boldsymbol{\lambda}}(\mathbf{z}) \cdot \boldsymbol{\lambda}^{(2)}, \frac{\partial F}{\partial \mathbf{x}} > + < \mathbf{z}, \frac{d}{d\boldsymbol{\lambda}}(\frac{\partial F}{\partial \mathbf{x}}) \cdot \boldsymbol{\lambda}^{(2)} >= -\frac{\partial \mathbf{x}_{(1)}}{\partial \boldsymbol{\lambda}} \cdot \boldsymbol{\lambda}^{(2)}$$

$$<< \frac{\partial \mathbf{z}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >, \frac{\partial F}{\partial \mathbf{x}} > + < \mathbf{z}, \frac{\partial^2 F}{\partial \mathbf{x} \partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > + < \mathbf{z}, \frac{\partial^2 F}{\partial \mathbf{x}^2}, < \frac{\partial \mathbf{x}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >> \\ = - < \frac{\partial \mathbf{x}_{(1)}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >$$

$$< \mathbf{z}^{(2)}, \frac{\partial F}{\partial \mathbf{x}} > + < \mathbf{z}, \frac{\partial^2 F}{\partial \mathbf{x} \partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > + < \mathbf{z}, \frac{\partial^2 F}{\partial \mathbf{x}^2}, \mathbf{x}^{(2)} >= -\mathbf{x}^{(2)}_{(1)}$$

and hence

$$\frac{\partial F}{\partial \mathbf{x}}^T \cdot \mathbf{z}^{(2)} = - < \mathbf{z}, \frac{\partial^2 F}{\partial \mathbf{x} \partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > - < \mathbf{z}, \frac{\partial^2 F}{\partial \mathbf{x}^2}, \mathbf{x}^{(2)} > -\mathbf{x}^{(2)}_{(1)} \tag{40}$$

$$\begin{aligned}\nabla^T F \cdot \mathbf{z}^{(2)} &= - < \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > - < \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > - \begin{pmatrix} \mathbf{x}_{(1)}^{(2)} \\ \mathbf{0}_m \end{pmatrix} \\ &= - < \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > - \begin{pmatrix} \mathbf{x}_{(1)}^{(2)} \\ \mathbf{0}_m \end{pmatrix} \quad , \end{aligned} \tag{41}$$

which is a linear system that can be solved by using a linear solver in order to evaluate $\mathbf{z}^{(2)} \in I\!R^n$. The right hand side can be evaluated in AD by projection of the Hessian ($\nabla^2 F$) in directions $\mathbf{z}$ and $\begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix}$. Furthermore, $\mathbf{x}_{(1)}^{(2)}$ can also be calculated in AD.

Differentiation of Equation (39) with respect to $\boldsymbol{\lambda}$ yields

$$\begin{aligned} \frac{d}{d\boldsymbol{\lambda}}(\boldsymbol{\lambda}_{(1)}) \cdot \boldsymbol{\lambda}^{(2)} + &= \frac{d}{d\boldsymbol{\lambda}} < \mathbf{z}, \frac{\partial F}{\partial \boldsymbol{\lambda}} > \cdot \boldsymbol{\lambda}^{(2)} \\ \frac{d\boldsymbol{\lambda}_{(1)}}{d\boldsymbol{\lambda}} \cdot \boldsymbol{\lambda}^{(2)} + &= < \frac{d}{d\boldsymbol{\lambda}}(\mathbf{z}) \cdot \boldsymbol{\lambda}^{(2)}, \frac{\partial F}{\partial \boldsymbol{\lambda}} > + < \mathbf{z}, \frac{d}{d\boldsymbol{\lambda}}(\frac{\partial F}{\partial \boldsymbol{\lambda}}) \cdot \boldsymbol{\lambda}^{(2)} > \\ < \frac{\partial \boldsymbol{\lambda}_{(1)}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > + &= << \frac{\partial \mathbf{z}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >, \frac{\partial F}{\partial \boldsymbol{\lambda}} > + < \mathbf{z}, < \frac{\partial^2 F}{\partial \boldsymbol{\lambda}^2}, \boldsymbol{\lambda}^{(2)} >> \\ &\quad + < \mathbf{z}, \frac{\partial^2 F}{\partial \boldsymbol{\lambda} \partial \mathbf{x}}, < \frac{\partial \mathbf{x}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >> \\ \boldsymbol{\lambda}_{(1)}^{(2)} + &= < \mathbf{z}^{(2)}, \frac{\partial F}{\partial \boldsymbol{\lambda}} > + < \mathbf{z}, \frac{\partial^2 F}{\partial \boldsymbol{\lambda}^2}, \boldsymbol{\lambda}^{(2)} > + < \mathbf{z}, \frac{\partial^2 F}{\partial \boldsymbol{\lambda} \partial \mathbf{x}}, \mathbf{x}^{(2)} > \\ \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}_{(1)}^{(2)} \end{pmatrix} + &= < \mathbf{z}^{(2)}, \frac{\partial F}{\partial (\mathbf{x}, \boldsymbol{\lambda})} > + < \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > + < \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > \end{aligned} \tag{42}$$

$$\begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}_{(1)}^{(2)} \end{pmatrix} + = < \mathbf{z}^{(2)}, \nabla F > + < \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \quad . \tag{43}$$

Evaluation of the above equation can also be done in AD by projection of the Jacobian (∇F) in direction $\mathbf{z}^{(2)}$. The $< \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} >$ projection is already computed in Equation (41).

Proof (Version 2).
As shown in [NLLT12], first-order symbolic adjoint differentiation of $F(\mathbf{x}(\boldsymbol{\lambda}), \boldsymbol{\lambda}) = 0$ at the solution $\mathbf{x} = \mathbf{x}^*$ with respect to $\boldsymbol{\lambda}$, i.e., the computation of $\boldsymbol{\lambda}_{(1)}$, yields

$$< \mathbf{z}, \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}, \boldsymbol{\lambda}) >= -\mathbf{x}_{(1)} \quad , \tag{44}$$

$$\boldsymbol{\lambda}_{(1)} + =< \mathbf{z}, \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x}, \boldsymbol{\lambda}) > \quad . \tag{45}$$

Equation (44) becomes

$$\frac{\partial F}{\partial \mathbf{x}}^T (\mathbf{x}, \boldsymbol{\lambda}) \cdot \mathbf{z} = -\mathbf{x}_{(1)}$$

$$\frac{\partial F}{\partial \mathbf{x} \partial \boldsymbol{\lambda}}^T \cdot \mathbf{z} = -\begin{pmatrix} \mathbf{x}_{(1)} \\ \mathbf{0}_m \end{pmatrix}$$

$$\nabla F^T \cdot \mathbf{z} = -\begin{pmatrix} \mathbf{x}_{(1)} \\ \mathbf{0}_m \end{pmatrix} \quad , \tag{46}$$

which is a linear system of type $A\mathbf{c} = \mathbf{b}$, with $A = \nabla F^T$, $\mathbf{c} = \mathbf{z}$ and $\mathbf{b} = -\begin{pmatrix} \mathbf{x}_{(1)} \\ \mathbf{0}_m \end{pmatrix}$.

An option to evaluate the second derivative of the solution $\mathbf{x} = \mathbf{x}^*$ with respect to $\boldsymbol{\lambda}$ in $F(\mathbf{x}, \boldsymbol{\lambda}) = 0$ is to apply the first-order tangent symbolic version for linear solvers to Equation (44) (or Equation (46)) and then differentiate the Equation (45) with respect to $\boldsymbol{\lambda}$.

As shown in [NL12], for the linear system $A\mathbf{c} = \mathbf{b}$ we have

$$\mathbf{c} = \mathbf{L}(A, \mathbf{b}) \quad ,$$

$$\mathbf{c}^{(1)} = \mathbf{L}^{(1)}(A, A^{(1)}, \mathbf{b}, \mathbf{b}^{(1)}) = < \frac{\partial \mathbf{c}}{\partial A}, A^{(1)} > + < \frac{\partial \mathbf{c}}{\partial \mathbf{b}}, \mathbf{b}^{(1)} > \quad , \tag{47}$$

where

$$A \cdot < \frac{\partial \mathbf{c}}{\partial A}, A^{(1)} > = -A^{(1)} \cdot \mathbf{c} \quad , \tag{48}$$

$$A \cdot < \frac{\partial \mathbf{c}}{\partial \mathbf{b}}, \mathbf{b}^{(1)} > = \mathbf{b}^{(1)} \quad . \tag{49}$$

The same as before, for the computation of Equation (47) the matrices $A, A^{(1)} \in I\!R^{n \times (n+m)}$ are assumed to be serialized. Therefore, differentiation of $\mathbf{c} \in I\!R^{n+m}$ with respect to $A \in I\!R^{n^2 + n \cdot m}$, gives a matrix $\frac{\partial \mathbf{c}}{\partial A} \in I\!R^{(n+m) \times (n^2 + n \cdot m)}$. Projecting this matrix in direction $A^{(1)} \in I\!R^{n^2 + n \cdot m}$ yields $< \frac{\partial \mathbf{c}}{\partial A}, A^{(1)} > \in I\!R^{n+m}$.

In this case $A = \nabla F^T$ and $\mathbf{c} = \mathbf{z}$, therefore $A^{(1)} \cdot \mathbf{c}$ yields

$$\begin{aligned} A^{(1)} \cdot \mathbf{c} &= (\frac{d}{d\boldsymbol{\lambda}}(\nabla F^T) \cdot \boldsymbol{\lambda}^{(2)}) \cdot \mathbf{z} \\ &= < \mathbf{z}, \frac{\partial(\nabla F^T)}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} > + < \mathbf{z}, \frac{\partial(\nabla F^T)}{\partial \mathbf{x}}, \overbrace{< \frac{\partial \mathbf{x}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >}^{=\mathbf{x}^{(2)}} > \\ &= < \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > + < \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \mathbf{0}_m \end{pmatrix} > \\ &= < \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \quad . \end{aligned}$$

Hence, Equation (48) yields

$$\nabla F^T \cdot < \frac{\partial \mathbf{c}}{\partial A}, A^{(1)} > = - < \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \quad .$$

In this case $\mathbf{b} = -\begin{pmatrix} \mathbf{x}_{(1)} \\ \mathbf{0}_m \end{pmatrix}$, therefore $\mathbf{b}^{(1)}$ yields

$$\mathbf{b}^{(1)} = \frac{d}{d\boldsymbol{\lambda}}(-\begin{pmatrix}\mathbf{x}_{(1)}\\ \mathbf{0}_m\end{pmatrix}) \cdot \boldsymbol{\lambda}^{(2)} = -\begin{pmatrix}\frac{\partial \mathbf{x}_{(1)}}{\partial \boldsymbol{\lambda}} \cdot \boldsymbol{\lambda}^{(2)}\\ \mathbf{0}_m\end{pmatrix} = -\begin{pmatrix}\mathbf{x}^{(2)}_{(1)}\\ \mathbf{0}_m\end{pmatrix} \quad .$$

Consequently, Equation (49) yields

$$\nabla F^T \cdot < \frac{\partial \mathbf{c}}{\partial \mathbf{b}}, \mathbf{b}^{(1)} >= -\begin{pmatrix}\mathbf{x}^{(2)}_{(1)}\\ \mathbf{0}_m\end{pmatrix} \quad .$$

In this case $\mathbf{c} = \mathbf{z}$, therefore $\mathbf{c}^{(1)}$ yields

$$\mathbf{c}^{(1)} = \frac{d}{d\boldsymbol{\lambda}}(\mathbf{z}) \cdot \boldsymbol{\lambda}^{(2)} = \frac{\partial \mathbf{z}}{\partial \boldsymbol{\lambda}} \cdot \boldsymbol{\lambda}^{(2)} =< \frac{\partial \mathbf{z}}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >= \mathbf{z}^{(2)} \quad .$$

Consequently, Equation (47) becomes

$$\mathbf{z}^{(2)} = (\nabla F)^{-T} \cdot \left(- < \mathbf{z}, \nabla^2 F, \begin{pmatrix}\mathbf{x}^{(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} >\right) - (\nabla F)^{-T} \cdot \begin{pmatrix}\mathbf{x}^{(2)}_{(1)}\\ \mathbf{0}_m\end{pmatrix}$$

$$\nabla F^T \cdot \mathbf{z}^{(2)} = - < \mathbf{z}, \nabla^2 F, \begin{pmatrix}\mathbf{x}^{(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} > - \begin{pmatrix}\mathbf{x}^{(2)}_{(1)}\\ \mathbf{0}_m\end{pmatrix} \quad . \tag{50}$$

Both $\frac{\partial F}{\partial \mathbf{x}}$ and the right hand side can be computed automatically by AD. The linear system can be solved by using a linear solver in order to evaluate $\mathbf{z}^{(2)}$.

The differentiation of Equation (45) with respect to $\boldsymbol{\lambda}$ is similar to *proof 1* Equations (42)–(43). As a result we have

$$\begin{pmatrix}\mathbf{0}_n\\ \boldsymbol{\lambda}^{(2)}_{(1)}\end{pmatrix} + =< \mathbf{z}^{(2)}, \nabla F > + < \mathbf{z}, \nabla^2 F, \begin{pmatrix}\mathbf{x}^{(2)}\\ \boldsymbol{\lambda}^{(2)}\end{pmatrix} > \quad .$$

The required memory for evaluating the symbolic second-order adjoint nonlinear solver is the memory required by the nonlinear solver itself (e.g. Equation (7) in Newton's algorithm), i.e. $MEM(\mathbf{L}) \sim O(n^2)$. In Equation (37), the complexity of evaluating the right hand side is $O(1) \cdot Cost(F)$. The decomposition of the Jacobian which is done in Equation (36) for the evaluation of $\mathbf{z}$ at the cost of $O(n^3)$ can also be used in evaluating the second-order directional derivatives. Solving the linear system Equation (41) (or Equation (50)) e.g. with forward/backward substitution at the cost of $O(n^2)$, the overall complexity of evaluating the symbolic second-order adjoint directional derivatives $\boldsymbol{\lambda}^{(2)}_{(1)}$ is proportional to $O(n^3)$.

6 IMPLEMENTATION

One can differentiate a system of numerical simulation by applying AD tools. If the simulation system contains a nonlinear solver, the preferable way is to differentiate the nonlinear system symbolically, for example, in our system (Equations (3)–(5)), differentiating Equation (3) and Equation (5) with algorithmic mode

(AD tools) and evaluating the derivatives of Equation (4) theoretically. This means that the theoretical results should be integrated into the existing software, which is not straightforward. For this purpose, we define an initiative generic API [3], which facilitates the exploitation of mathematical and structural knowledge inside of often highly complex tangent and adjoint numerical simulations.

Similar to [NLLT12], as a representative case study for the implementation of higher-level (user-defined) intrinsics in the context of overloading AD tools we consider the solver {S(n,x,lbd)} for systems of n nonlinear equations with inputs x=x^0 and {lbd}=$\boldsymbol{\lambda}$ and output x=x^*. More generically, the proposed approach allows users of AD tools to treat arbitrary parts of the primal code as *external functions*. The latter yield *gaps* in the tape due to their passive evaluation within the forward section of the adjoint code. These gaps need to be filled by corresponding user-defined adjoint functions to be called by the tape interpreter within the reverse section of the adjoint code. This concept is part of the overloading AD tool `dco` [NLL14].

In the following we focus on the external function interface of `dco/c++` in the context of second-order tangent and adjoint modes. The preferred method of implementation of second-order tangent external functions is through replacement of the overloaded primal function with a user-defined version. One should not expect to be presented with *the* method for filling gaps in the data flow of second-order tangent or adjoint numerical simulations. There are always several alternatives that implement mathematically equivalent functions. The particular choice made for `dco/c++` is meant to be both intuitive and easy to maintain. The overloading AD tool ADOL-C [GJU96] features a similar, but less generic external function concept.

Our simulation system (Equations (3)–(5)) yields

```
template <typename TYPE>
inline TYPE costfunction(int n, std::vector<TYPE> &z) {
    std::vector<TYPE> lambda(n), x(n, 0), residual(n);
    int iter = 0;
    preprocessor(n, z, lambda);
    if (Alg)
        iter = Alg_S(n, x, lambda);
    else
        iter = Symb_S(n, x, lambda);
    std::vector<double> x_a(n);
    generate_measurements(n, x_a);
    TYPE J = postprocessor(n, x, x_a);
    return J;
}
```

In the above implementation, λ is initialized by calling preprocessor function. After initializing λ the nonlinear solver is called, in which λ is input and $\mathbf{x}$ is input as well as output. There are two alternative implementations for the nonlinear solver. If the differentiation is done algorithmically, Alg_S function should be called, otherwise, if the differentiation is done symbolically, Symb_S function should be called. At last, the optimization function (postprocessor) is called, which optimizes the inputs (λ) with respect to the real measurements (x_a).

[3] Application Programming Interface

6.1 Algorithmic Approach

The primal nonlinear solver function S is made generic with respect to the floating-point data type {FT} yielding

```
template <class FT>
void S(int n, std::vector<FT> &x, std::vector<FT> &lbd);
```

Thus it can be instantiated with the `dco/c++` data type {dco::t2s_t1s::type} and `dco/c++` data type {dco::t2s_a1s::type} , which implement second-order tangent and adjoint modes respectively.

```
template <class T>
int Alg_S(int n, std::vector<T> &x, std::vector<T> &lambda)
{   return S(n, x, lambda); }
```

In adjoint mode, a tape of the entire computation is generated and interpreted as discussed in Section 5.1. Therefore, there is no gap in tape.

6.2 Symbolic Approach

In the following, we focus on the symbolic second-order tangent and adjoint modes for nonlinear solvers discussed in Sections 4.2 and 5.2 respectively.

Based on Fig.2 in [NLLT12], Fig. 2 in the following is the linearized DAG for second-order tangent mode of our simulation system.

In Listing 1.1, the computation of both first- and second-order tangent mode of the nonlinear solver is shown. As mentioned in Section 4.2, the first-order symbolic tangent differentiation of a nonlinear system $F(\mathbf{x}(\boldsymbol{\lambda}), \boldsymbol{\lambda}) = 0$ at the solution $\mathbf{x} = \mathbf{x}^*$ with respect to $\boldsymbol{\lambda}$, i.e., computation of $\mathbf{x}^{(1)}$, yields

$$\frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}, \boldsymbol{\lambda}) \cdot \mathbf{x}^{(1)} = - < \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x}, \boldsymbol{\lambda}), \boldsymbol{\lambda}^{(1)} > \quad . \tag{51}$$

Differentiating the first-order tangent mode of the nonlinear solver results the second-order tangent mode of it, i.e.

$$\frac{\partial F}{\partial \mathbf{x}} \cdot \mathbf{x}^{(1,2)} = - < \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(1)} \\ \boldsymbol{\lambda}^{(1)} \end{pmatrix}, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > \quad . \tag{52}$$

The computation of $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(1,2)}$ amount to the solution of linear systems which are based on the Jacobian matrix $\frac{\partial F}{\partial \mathbf{x}}$.

A specialization of the generic primal solver `S` for `dco`'s scalar second-order tangent type {dco::t2s_t1s::type} is shown in Listing 1.1.

```
int Symb_S(int n, std::vector<dco::t2s_t1s::type> &x, std::vector<
    dco::t2s_t1s::type> &lambda)
{
    std::vector<dco::t2s_t1s::type> residual(n);
    std::vector<double> px(n), plambda(n), presidual(n), t1lambda(n)
        , t2lambda(n), tu1(n), tu2(n), b1(n), b2(n), out1(n), rhs(n),
        t2s_t1s_u(n);
    std::vector<std::vector<double> > J_dr_dx(n, vector<double>(n));
    int** P;
```

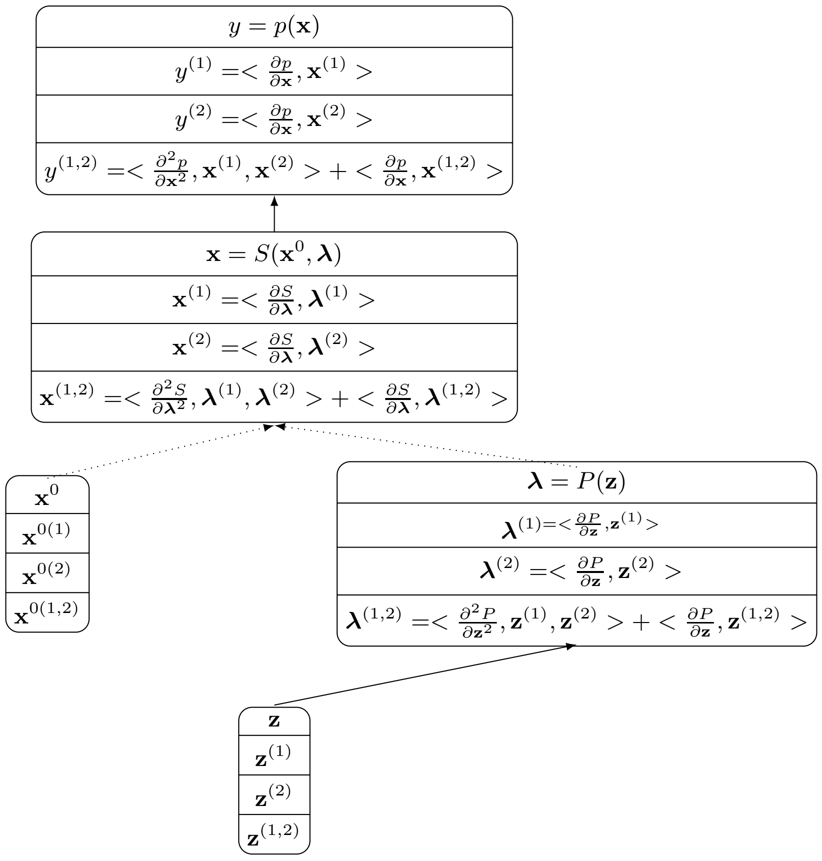

$y = p(\mathbf{x})$
$y^{(1)} =< \frac{\partial p}{\partial \mathbf{x}}, \mathbf{x}^{(1)} >$
$y^{(2)} =< \frac{\partial p}{\partial \mathbf{x}}, \mathbf{x}^{(2)} >$
$y^{(1,2)} =< \frac{\partial^2 p}{\partial \mathbf{x}^2}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)} > + < \frac{\partial p}{\partial \mathbf{x}}, \mathbf{x}^{(1,2)} >$
$\mathbf{x} = S(\mathbf{x}^0, \boldsymbol{\lambda})$
$\mathbf{x}^{(1)} =< \frac{\partial S}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(1)} >$
$\mathbf{x}^{(2)} =< \frac{\partial S}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >$
$\mathbf{x}^{(1,2)} =< \frac{\partial^2 S}{\partial \boldsymbol{\lambda}^2}, \boldsymbol{\lambda}^{(1)}, \boldsymbol{\lambda}^{(2)} > + < \frac{\partial S}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(1,2)} >$
$\mathbf{x}^0$
$\mathbf{x}^{0(1)}$
$\mathbf{x}^{0(2)}$
$\mathbf{x}^{0(1,2)}$
$\boldsymbol{\lambda} = P(\mathbf{z})$
$\boldsymbol{\lambda}^{(1)} =< \frac{\partial P}{\partial \mathbf{z}}, \mathbf{z}^{(1)} >$
$\boldsymbol{\lambda}^{(2)} =< \frac{\partial P}{\partial \mathbf{z}}, \mathbf{z}^{(2)} >$
$\boldsymbol{\lambda}^{(1,2)} =< \frac{\partial^2 P}{\partial \mathbf{z}^2}, \mathbf{z}^{(1)}, \mathbf{z}^{(2)} > + < \frac{\partial P}{\partial \mathbf{z}}, \mathbf{z}^{(1,2)} >$
$\mathbf{z}$
$\mathbf{z}^{(1)}$
$\mathbf{z}^{(2)}$
$\mathbf{z}^{(1,2)}$

Fig. 2. Implementation of second-order tangent mode NLS: Solid lines represent the computation of derivatives in algorithmic mode. Dotted lines denote the computation of derivatives in symbolic mode. In the given example, we have $\mathbf{x}^{0(1)} = \mathbf{x}^{0(2)} = \mathbf{x}^{0(1,2)} = 0$, therefore they are not mentioned in the proceeding computations.

```
    dco::t2s_t1s::get(x, px);
    dco::t2s_t1s::get(lambda, plambda);
    int iter = S(n, px, plambda);
    dco::t2s_t1s::get(lambda, t1lambda, 1);
    dco::t2s_t1s::get(lambda, t2lambda, 0, 2);
    dco::t2s_t1s::set(lambda, plambda);
    for (int i=0; i<n; i++)
        x[i] = px[i];
    F(n, x, lambda, residual);
    dco::t2s_t1s::get(residual, b1, 1);
    dco::t2s_t1s::get(residual, b2, 2);
    for (int ii = 0; ii < n; ii++) {
        b1[ii] *= -1;
        b2[ii] *= -1;
    }
    dr_dx_tgl(n, px, plambda, presidual, J_dr_dx);
    P = LUDecomp(n, J_dr_dx);
    FBsolve(n, P, J_dr_dx, b1, tu1);
    FBsolve(n, P, J_dr_dx, b2, tu2);
    dco::t2s_t1s::set(x, tu1, 1);
    dco::t2s_t1s::set(x, tu2, 2);
    dco::t2s_t1s::set(lambda, plambda);
    dco::t2s_t1s::set(x, px);
```

```
30      F(n, x, lambda, residual);
31      dco::t2s_t1s::get(residual, out1, 1, 2);
32      for(int i=0; i<n; i++)
33          rhs[i]= (-1)*out1[i];
34      FBsolve(n, P, J_dr_dx, rhs, t2s_t1s_u);
35      dco::t2s_t1s::set(x, t2s_t1s_u, 1, 2);
36      return iter;
37  }
```

Listing 1.1. External function for symbolic second-order tangent mode of S

In Listing 1.1, $\lambda^{(\mathbf{1})}$ and $\lambda^{(\mathbf{2})}$ are evaluated in lines 10 and 11 respectively. The function F is the nonlinear problem. Having $\lambda^{(\mathbf{1})}$ and $\lambda^{(\mathbf{2})}$, b1=$< \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x}, \boldsymbol{\lambda}), \boldsymbol{\lambda}^{(1)} >$ and b2=$< \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x}, \boldsymbol{\lambda}), \boldsymbol{\lambda}^{(2)} >$ are evaluated in lines 16 and 17 respectively. The Jacobian matrix(J_dr_dx) is computed using the algorithmic tangent mode in line 22 and in line 23 it is decomposed. In lines 24 and 25 the linear systems for $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ in Equation (51) are solved respectively. In line 26, tu1 is set to $\mathbf{x}^{(1)}$ and in line 27, tu2 is set to $\mathbf{x}^{(2)}$. Up to this point, the first-order tangent derivatives are evaluated. The right hand side of Equation (52) is computed in line 33. The linear system in Equation (52) is solved in line 34 using the already decomposed Jacobian matrix. Finally, t2s_t1s_u is set to $\mathbf{x}^{(1,2)}$ in line 35.

Based on Fig.2 in [NLLT12], Fig. 3 in the following is the linearized DAG for second-order adjoint mode of our simulation system.

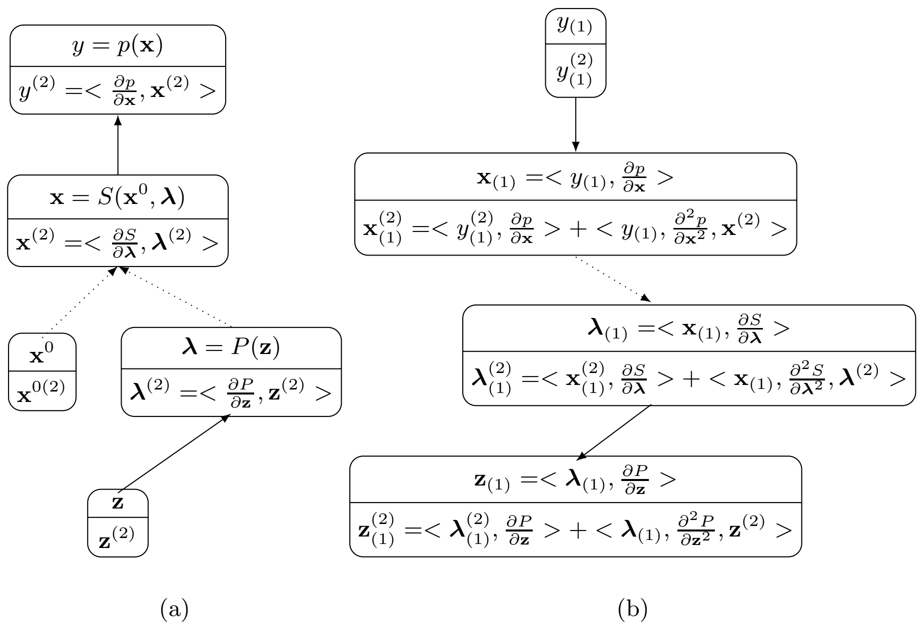

$y = p(\mathbf{x})$
$y^{(2)} =< \frac{\partial p}{\partial \mathbf{x}}, \mathbf{x}^{(2)} >$
$\mathbf{x} = S(\mathbf{x}^0, \boldsymbol{\lambda})$
$\mathbf{x}^{(2)} =< \frac{\partial S}{\partial \boldsymbol{\lambda}}, \boldsymbol{\lambda}^{(2)} >$
$\mathbf{x}^0$
$\mathbf{x}^{0(2)}$
$\boldsymbol{\lambda} = P(\mathbf{z})$
$\boldsymbol{\lambda}^{(2)} =< \frac{\partial P}{\partial \mathbf{z}}, \mathbf{z}^{(2)} >$
$\mathbf{z}$
$\mathbf{z}^{(2)}$
$y_{(1)}$
$y_{(1)}^{(2)}$
$\mathbf{x}_{(1)} =< y_{(1)}, \frac{\partial p}{\partial \mathbf{x}} >$
$\mathbf{x}_{(1)}^{(2)} =< y_{(1)}^{(2)}, \frac{\partial p}{\partial \mathbf{x}} > + < y_{(1)}, \frac{\partial^2 p}{\partial \mathbf{x}^2}, \mathbf{x}^{(2)} >$
$\boldsymbol{\lambda}_{(1)} =< \mathbf{x}_{(1)}, \frac{\partial S}{\partial \boldsymbol{\lambda}} >$
$\boldsymbol{\lambda}_{(1)}^{(2)} =< \mathbf{x}_{(1)}^{(2)}, \frac{\partial S}{\partial \boldsymbol{\lambda}} > + < \mathbf{x}_{(1)}, \frac{\partial^2 S}{\partial \boldsymbol{\lambda}^2}, \boldsymbol{\lambda}^{(2)} >$
$\mathbf{z}_{(1)} =< \boldsymbol{\lambda}_{(1)}, \frac{\partial P}{\partial \mathbf{z}} >$
$\mathbf{z}_{(1)}^{(2)} =< \boldsymbol{\lambda}_{(1)}^{(2)}, \frac{\partial P}{\partial \mathbf{z}} > + < \boldsymbol{\lambda}_{(1)}, \frac{\partial^2 P}{\partial \mathbf{z}^2}, \mathbf{z}^{(2)} >$
(a)
(b)

Fig. 3. *Mind the gap* in the tape – Implementation of second-order adjoint symbolic NLS mode: Solid lines represent the generation (in the forward section of the tangent and adjoint code shown in (a)) and interpretation (in the reverse section of the first- and second-order adjoint code shown in (b)) of the tape. Dotted lines denote gaps in the tape to be filled by a corresponding user-defined adjoint function. In the given example, we have $\mathbf{x}^{0(2)} = 0$, therefore $\mathbf{x}^{0(2)}$ is not mentioned in the proceeding computations.

In the following implementations, the computation of both first- and second-order adjoint mode of the nonlinear solver is shown. As mentioned in Section 5.2, the first-order symbolic adjoint differentiation of a nonlinear system $F(\mathbf{x}(\lambda), \lambda) = 0$ at the solution $\mathbf{x} = \mathbf{x}^*$ with respect to λ, i.e., computation of $\lambda_{(\mathbf{1})}$, yields:

$$\boldsymbol{\lambda}_{(1)} + =< \mathbf{z}, \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x}, \boldsymbol{\lambda}) >, \quad \text{where} \quad \frac{\partial F}{\partial \mathbf{x}}(\mathbf{x}, \boldsymbol{\lambda})^T \cdot \mathbf{z} = -\mathbf{x}_{(1)} \ . \tag{53}$$

Differentiating the first-order adjoint mode of the nonlinear solver results the second-order adjoint mode of it, i.e., computation of $\boldsymbol{\lambda}_{(1)}^{(2)}$, which yields

$$\begin{pmatrix} \mathbf{0}_n \\ \boldsymbol{\lambda}_{(1)}^{(2)} \end{pmatrix} + =< \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > + < \mathbf{z}^{(2)}, \nabla F > \quad , \tag{54}$$

where,

$$\frac{\partial F}{\partial \mathbf{x}}^T \cdot \mathbf{z}^{(2)} = - < \mathbf{z}, \nabla^2 F, \begin{pmatrix} \mathbf{x}^{(2)} \\ \boldsymbol{\lambda}^{(2)} \end{pmatrix} > - \mathbf{x}_{(1)}^{(2)} \quad . \tag{55}$$

A specialization of the generic primal solver S for dco's scalar second-order adjoint type {dco::t2s_a1s::type} marks the gap in the tape, records data that is required for filling the gap during interpretation, and runs the primal solver passively (without taping); see Listing 1.2.

```
typedef dco::t2s_a1s::type::VALUE_TYPE base_type;
typedef base_type::VALUE_TYPE base_base_type;
typedef dco::t2s_a1s::external_function_data ext_data_S;
void t2s_a1s_S(dco::t2s_a1s::external_function_data* data);

int Symb_S(int n, std::vector<dco::t2s_a1s::type> &x, std::vector<
    dco::t2s_a1s::type> &lambda)
{
    ext_data_S *data= dco::t2s_a1s::global_tape->create_ext_fcn_data
        <ext_data_S >(t2s_a1s_S);
    std::vector<base_type> plambda(n), px(n);
    std::vector<base_base_type> pplambda(n), ppx(n), b2(n),
        presidual(n), dxdl_tgl(n), t2lambda(n);
    std::vector<std::vector< base_base_type> > J_dr_dx(n, vector<
        base_base_type> (n));
    std::vector<dco::t2s_a1s::type> residual(n);
    data->register_input(lambda, plambda);
    dco::t2s_a1s::get(x, ppx);
    dco::t2s_a1s::get(lambda, pplambda);
    int its = S(n, ppx, pplambda);
    dco::t2s_a1s::get(lambda, t2lambda, 0, 2);
    dco::t1s::set(plambda, pplambda);
    for (int i=0; i<n; i++)
        x[i] = ppx[i];
    F(n, x, lambda, residual);
    dco::t2s_a1s::get(residual, b2, 0, 2);
    for (int i = 0; i < n; i++) b2[i] *= -1;
    dr_dx_tgl(n, ppx, pplambda, presidual, J_dr_dx);
    int **P = LUDecomp(n, J_dr_dx);
    FBsolve(n, P, J_dr_dx, b2, dxdl_tgl);
    for (int i=0; i<n; i++){
        px[i] = ppx[i];
29            plambda[i] = pplambda[i]; }
30        dco::t1s::set(px, dxdl_tgl, 1);
31        dco::t1s::set(plambda, t2lambda, 1);
32        data->write_to_checkpoint(n);
33        data->write_to_checkpoint(plambda);
34        data->write_to_checkpoint(px);
35        data->register_output(px, x);
36        return its;
37    }
```

Listing 1.2. External function for symbolic second-order adjoint mode of S

In Listing 1.2, data type base_type is used for overloaded first-order solution and data type base_base_type is used for explicit second-order solution. The passive evaluation of primal and tangent mode of the solver augmented with recording of data required by t2_a1_S. There is a forward declaration of t2_a1_S in line 4. In function Symb_S, the first-order tangent mode of the primal nonlinear solver (S) is computed (see Equation (51)). For this purpose, the evaluation of the Jacobian matrix is required, which is done by algorithmic tangent mode in line 24 and is decomposed in line 25. The evaluation of b1=$< \frac{\partial F}{\partial \boldsymbol{\lambda}}(\mathbf{x}, \boldsymbol{\lambda}), \boldsymbol{\lambda}^{(1)} >$ is done in line 22. The linear system in Equation (51) is solved in line 26. In lines 30 and 31, dxdl_tgl is set to $\mathbf{x}^{(1)}$ and t2lambda is set to $\boldsymbol{\lambda}^{(1)}$ respectively. At the end, the required datas for backward interpretation are written to checkpoint.

The tape interpreter fills the gap between the tapes of P and p by calling the function {t2s_a1s_S} which implements the $\boldsymbol{\lambda}_{(1)}$ and $\boldsymbol{\lambda}_{(1)}^{(2)}$ symbolically, see Listing 1.3. Refer to Fig. 3 for graphical illustration.

```
39    void t2s_a1s_S(dco::t2s_a1s::external_function_data* data)
40    {
41        int n;
42        data->read_from_checkpoint(n);
43        std::vector<double> lambda(n), x(n), a1_x(n), min_a1_x(n),
              t2lambda(n), z(n), r(n), dz_dl(n), t2_a1_x(n), dxdl(n,0),
              a1s_l(n,0), a1s_x(n,0), dxdl_tgl(n),  rhs1(n), res1(n),
              dfdl_mult_dzdl(n, 0);
44        std::vector<base_type> xb(n);
45        std::vector<dco::t2s_a1s::type> alambda(n), alambda_1(n), ax(n),
               ax_1(n), ares(n), ares_1(n);
46        int **P;
47        std::vector<std::vector<double> > J_dr_dx(n, vector<double>(n));
48        data->get_output_adjoint(xb);
49        dco::t1s::get(xb, a1_x);
50        dco::t1s::get(xb, t2_a1_x, 1);
51        std::vector<base_type> plambda(n), px(n), output(n);
52        data->read_from_checkpoint(plambda);
53        data->read_from_checkpoint(px);
54        dco::t1s::get(px, dxdl_tgl, 1);
55        dco::t1s::get(plambda, t2lambda, 1);
56        dco::t1s::get(px, x);
57        dco::t1s::get(plambda, lambda);
58        dr_dx_adj(n, x, lambda, r, J_dr_dx);
59        P = LUDecomp(n, J_dr_dx);
60        for (int i=0; i<n; i++) min_a1_x[i]=(-1)*a1_x[i];
61        FBsolveT(n, P, J_dr_dx, min_a1_x, z);
62        dco::t2s_a1s::tape::iterator pos1 = dco::t2s_a1s::global_tape->
              get_position();
63      for (int i=0; i<n; i++) {
64          alambda[i] = lambda[i];
65          ax[i] = x[i];}
66      dco::t2s_a1s::set(alambda, t2lambda , 0, 2);
67      dco::t2s_a1s::global_tape->register_variable(alambda);
68      dco::t2s_a1s::set(ax, dxdl_tgl , 0, 2);
69      dco::t2s_a1s::global_tape->register_variable(ax);
70      dco::t2s_a1s::tape::iterator pos2 = dco::t2s_a1s::global_tape->
            get_position();
71      F(n, ax, alambda, ares);
72      dco::t2s_a1s::set(ares, z, -1);
73      dco::t2s_a1s::global_tape->interpret_adjoint_to(pos2);
74      dco::t2s_a1s::get(alambda, dxdl, -1);
75      dco::t1s::set(output, dxdl);
76      dco::t2s_a1s::get(alambda, a1s_l, -1, 2);
77      dco::t2s_a1s::get(ax, a1s_x, -1, 2);
78      dco::t2s_a1s::global_tape->reset_to(pos1);
79      for (int i=0; i<n; i++)
80          rhs1[i] = (-1)*(a1s_x[i]+t2_a1_x[i]);
81      FBsolveT(n, P, J_dr_dx, rhs1, dz_dl);
82      for (int i=0; i<n; i++) {
83          alambda_1[i] = lambda[i];
84          ax_1[i] = x[i];}
85      dco::t2s_a1s::global_tape->register_variable(alambda_1);
86      dco::t2s_a1s::tape::iterator pos3 = dco::t2s_a1s::global_tape->
            get_position();
87      F(n, ax_1, alambda_1, ares_1);
88      dco::t2s_a1s::set(ares_1, dz_dl, -1);
89      dco::t2s_a1s::global_tape->interpret_adjoint_to(pos3);
90      dco::t2s_a1s::get(alambda_1, dfdl_mult_dzdl, -1);
91      dco::t2s_a1s::global_tape->reset_to(pos1);
92      for (int i=0; i<n; i++) {
93          res1[i] = a1s_l[i] + dfdl_mult_dzdl[i];
94          dco::t1s::set(output[i], res1[i], 1);
95          data->increment_input_adjoint(output[i]);
96      }
97  }
```

Listing 1.3. Adjoint function t2s_a1s_S

In Listing 1.3, the datas that were written to checkpoint will be read. In line 48 the adjoint of the output, i.e. $\mathbf{x}_{(1)}$, is evaluated and it is set to a1_x in the next line. In line 50, $\mathbf{x}_{(1)}^{(2)}$ is set to t2_a1_x. The evaluations of the $\mathbf{x}^{(1)}$ and $\boldsymbol{\lambda}^{(1)}$ that were done in Listing 1.2 in lines 30 and 31 will be read here in lines 54 and 55 respectively. The Jacobian matrix is computed with algorithmic adjoint mode in line 58 and is decomposed in the next line. In line 61 the linear system in Equation (53) is solved for computing $\mathbf{z}$ with transposed Jacobian matrix. In line 74, the first-order symbolic adjoint dxdl=$\boldsymbol{\lambda}_{(1)}$ in Equation (53) is evaluated. The right hand side of Equation (55) is computed in line 80 and the linear system for $\mathbf{z}^{(2)}$ with transposed Jacobian is solved in the next line. The right hand side of Equation (54) is computed in line 93. The variable output was set in line 75 to $\boldsymbol{\lambda}_{(1)}$, therefore, in line 94 output$^{(1)}$ = $\boldsymbol{\lambda}_{(1)}^{(2)}$ =res1. At the end, the output is incremented in line 95.

The benefit of this approach is two-fold. First, taping of the nonlinear solver is avoided yielding a substantial reduction in memory requirement of the overloading based adjoint. Second, the actual adjoint mappings can be implemented in t2s_a1s_S more efficiently than by interpretation of a corresponding tape. As a general approach the external function feature can/should be applied whenever a similar reduction in memory requirement / computational cost can be expected. Users of `dco/c++` are encouraged to extend the run time library with user-defined intrinsics for (domain-specific) numerical kernels such as, for example, turbulence models in computational fluid dynamics or pay off functions in mathematical finance.

The external function interface of `dco/c++` facilitates a hybrid overloading / source transformation approach to AD. Currently, none of the available source transformation tools covers the entire latest C++ or Fortran standards. Moreover, these tools can be expected to struggle keeping up with the evolution of the programming languages for the foreseeable future. Mature source transformation AD tools such as Tapenade [HP13] can handle (considerable subsets of) C and/or Fortran 95. They can (and should) be applied to suitable selected parts of the given C++XX or Fortran 20XX code. Integration into an enclosing overloading AD solution via the external function interface is typically rather straight forward. The hybrid approach to AD promises further improvements in terms of robustness and computational efficiency.

7 Case Studies

In this section we consider a case study for one dimensional and another case study for two dimensional nonlinear system. We optimize the case studies using a second-order derivative-based method, in which the derivatives are computed with both symbolic and algorithmic tangent and adjoint modes. Furthermore, the run-time overhead as well as the memory requirement of various methods of evaluating second-order directional derivatives are compared.

7.1 One Dimensional Eliptic PDE

As a case study we solve the one dimensional nonlinear differential equation

$$\begin{aligned} \nabla^2(z \cdot u^*) + u^* \cdot \nabla(z \cdot u^*) = 0 \quad &\text{on} \quad \Omega = (0,1) \\ u^* = 10 \ \text{ and } \ z = 1 \quad &\text{for} \ \ x = 0 \\ u^* = 20 \ \text{ and } \ z = 1 \quad &\text{for} \ \ x = 1 \end{aligned}$$

with parameters $z(x)$. For given measurements $u^m(x)$ we state the following parameter fitting problem for z

$$z^* = \arg \min_{z \in I\!R} J(z)$$

with

$$J(z) = \|u(x,z) - u^m(x)\|_2^2 \ . \tag{59}$$

The measurements $u^m(x)$ are generated by a given set of parameters (the "real" parameter distribution $z^*(x)$)[4]. With an equidistant central finite difference discretization we get for a given $\mathbf{u}$ (discretized and, hence, vector-valued variables

[4] Here we do not have the real datas, so we apply a small perturbation to our results and suppose that these are the real ones.

are written as bold letters) the residual function

$$[\mathbf{r}]_i = \frac{1}{h^2} \cdot ([\mathbf{z}]_{i-1}[\mathbf{u}]_{i-1} - 2[\mathbf{z}]_i[\mathbf{u}]_i + [\mathbf{z}]_{i+1}[\mathbf{u}]_{i+1}) \\ +[\mathbf{u}]_i \cdot \frac{1}{2h} \cdot ([\mathbf{z}]_{i+1}[\mathbf{u}]_{i+1} - [\mathbf{z}]_{i-1}[\mathbf{u}]_{i-1})$$

with $h = 1/n$ and n the number of discretization points yielding a system of n nonlinear equations

$$\mathbf{r}(\mathbf{u}, \mathbf{z}) = 0 \quad , \quad \mathbf{u} \in I\!R^n, \mathbf{z} \in I\!R^n \ , \tag{62}$$

which is solved by Newton's method yielding in the i-th Newton iteration the linear system

$$\nabla \mathbf{r}|_{\mathbf{u}=\mathbf{u}_i} \cdot \Delta\mathbf{u} = -\mathbf{r}|_{\mathbf{u}=\mathbf{u}^i} \ .$$

The vector $\mathbf{u}^i$ is updated with the Newton step

$$\mathbf{u}^{i+1} = \mathbf{u}^i + \Delta\mathbf{u} \ .$$

In order to solve the parameter fitting problem, we apply a Newton's method in optimization algorithm which includes a small step size $\alpha > 0$ to the algorithmic objective $J(\mathbf{z})$

$$\mathbf{z}^{k+1} = \mathbf{z}^k - \alpha \cdot \nabla^2 J(\mathbf{z}^k)^{-1} \cdot \nabla J(\mathbf{z}^k) \quad ,$$

where the computation of the Jacobian and Hessian of J at the current iterate $\mathbf{z}^k$ includes the differentiation of the nonlinear solver for $\mathbf{u}^*$, i.e., differentiation of the solver for Equation (62).

According to the Equations (3)–(5), the preprocessor $\boldsymbol{\lambda} = P(\mathbf{z})$ is the identity, while the nonlinear problem is the one dimensional nonlinear function (Equation (60)–(61)) which is solved by a nonlinear solver (e.g. Newton's algorithm) and the postprocessor $p(\mathbf{u})$ computes the cost functional $J(\mathbf{z})$ (Equation (59)).

The goal is to apply Newton's method in optimization algorithm (Equation (63)) in order to minimize the postprocessor J and optimize the initial values $\mathbf{z}_i$ (the inputs) in the preprocessor. For this purpose the computation of the Jacobian and Hessian of J at the current iterate $\mathbf{z}^k$ is required, this includes the evaluation of the Jacobian and Hessian of the postprocessor, nonlinear solver and preprocessor.

In the following the algorithmic FoF (forward over forward) is the evaluation of the first- and second-order directional derivatives with the first- and second-order tangent mode of AD (Section 3.1 and Section 3.3) respectively. The algorithmic FoR (forward over reverse) is the evaluation of the first- and second-order directional derivatives with the first- and second-order adjoint mode of AD (Section 3.2 and Section 3.4) respectively. The symbolic FoF is the evaluation of first- and second-order directional derivatives with symbolic first- and second-order tangent mode as Equation (20) and Equation (19) respectively. The symbolic FoR is the evaluation of first- and second-order directional derivatives with symbolic first- and second-order adjoint mode as Equation (39) and Equation (37) respectively.

A straightforward approach for approximating derivatives involves the use of finite differences. Finite difference approximation (FD) for the derivatives are derived by truncating the Taylor series expansion of the function $g = f(x)$ about a point x. The accuracy of the approximations critically depends on the step size h. More specifically, finite difference approximations for the derivatives can be inaccurate because of truncation or condition errors.

The evaluation of the second-order directional derivatives with finite difference in several variables yields

$$\frac{\partial^2 f}{\partial x \partial y} \approx \frac{f(x+h_1,y+h_2)-f(x+h_1,y-h_2)-f(x-h_1,y+h_2)+f(x-h_1,y-h_2)}{4h_1h_2}.$$

The discrepancy of evaluating the second-order directional derivatives of the postprocessor J with respect to the initial values in preprocessor $\mathbf{z}_i$ with finite difference (Equation 7.1) and algorithmic FoF in the first iteration of the optimization yields

$$Discrepancy = \| \frac{\partial^2 J}{\partial z^2}_{FD} - \frac{\partial^2 J}{\partial z^2}_{Algorithmic} \| \quad .$$

Setting $n = 10$ and the accuracy of the nonlinear solver $\delta = 10^{-6}$, the discrepancy for different step sizes of finite difference $h = h_1 = h_2$ is shown in Table 2.

h	Discrepancy
10^{-1}	16.67
10^{-2}	0.15
10^{-3}	0.001
10^{-4}	0.0001
10^{-5}	0.019
10^{-6}	1.92

Table 2. Discrepancy of the evaluation of second-order directional derivatives with finite difference and algorithmic for different step sizes of finite difference.

The discrepancy of the results will be very small by setting $h = h_1 = h_2 = 10^{-4}$, however this step size is not the smallest one. Therefore finding a suitable step size in finite difference approximation is very crucial.

One should also notice that for the same conditions, i.e., $n = 10$ and $\delta = 10^{-6}$, the discrepancy of the second-order directional derivatives computed by algorithmic and symbolic is proportional to zero (see Figure 6).

The fully algorithmic part of the derivative computation is done by the software tool `dco/c++` [LLN11], implementing AD by overloading in C++. The implementation of symbolic tangent over tangent and tangent over adjoint methods is supported by a custom user interface (see Section 6). For the symbolic part of the derivative computation, the evaluation of the directional derivatives of the preprocessor and the postprocessor will be done by algorithmic mode and only the first- and second-order directional derivatives of the nonlinear solver will be evaluated symbolically.

In the following we compare run time of the optimization of postprocessor (J) with respect to the preprocessor (initial values $\mathbf{z}_i$) by Equation (63) for various differentiated versions of the nonlinear solver. In this paper we set ϵ as the accuracy of the postprocessor ($J(\mathbf{z}) < \epsilon$), which computes the costfunctional (Equation (59)) and δ would be the accuracy of our nonlinear solver ($\mathbf{r}(\mathbf{u}, \mathbf{z}) < \delta$).

	Symbolic		Algorithmic		Finite
n	FoF	FoR	FoF	FoR	Diff.
10	0.1	0.05	0.47	0.09	0.3
20	0.99	0.1	4.25	0.35	2.54
30	4.59	0.28	21.92	1.27	16.18
40	14.58	0.6	73.23	3.4	41.17
50	36.99	1.16	186.87	7.4	-
80	277.55	4.84	1475.36	41.26	-
100	813.47	10.88	-	106.39	-
150	-	44.0	-	560.11	-
200	-	127.69	-	1726.65	-
250	-	307.53	-	-	-

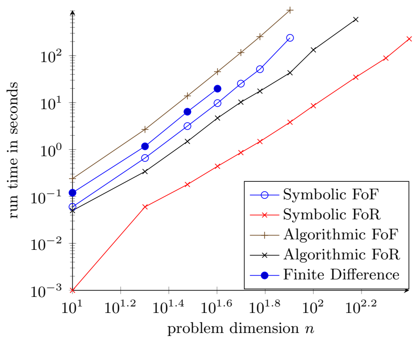


Fig. 4. Run time (in seconds) overhead comparison of optimizing our 1D sample problem with different differentiation methods. The (-) sign implies no convergence after 2000 seconds.

In Fig. 4 we observe the expected behaviour for the computational overhead induced by the various differentiation methods for optimizing the postprocessor J with respect to the initial values in preprocessor $\mathbf{z}$. In this example the accuracy of the nonlinear solver (Newton) for solving the nonlinear system (Equation (62)) is set to $\delta = 1e-6$ and the accuracy of the optimization in postprocessor is set to $\epsilon = 1e-6$. We observe that in both cases of symbolic and algorithmic, the complexity is less if the derivatives be calculated by the adjoint mode. Optimization using symbolic first- and second-order adjoint mode for calculation of the directional derivatives requires less duration, however, the optimization spends the most time by applying algorithmic first- and second-order tangent for evaluating the derivatives. Optimization using finite difference with $h_1 = h_2 = 10^{-5}$ spends less time than algorithmic second-order tangent, but for ($n >= 50$) it does not converge and it is not as accurate as other differentiation methods introduced in this paper.

In our test case, for second-order algorithmic adjoint, the first- and second-order directional derivatives of preprocessing, nonlinear solver and postprocessing are calculated with adjoint AD, this means the storage of some variables in tape and then use the stored variables in tape for backward propagation of derivative values. In this case the checkpoints are not needed. However, for second-order symbolic adjoint, the directional derivatives of preprocessing and postprocessing are calculated by algorithmic adjoint, in which some variables are also stored in tape in order to be used for backward propagation of derivative values. But the directional derivatives of nonlinear solver are computed with symbolic first- and second-order adjoint, in which the required variables for computing the directional derivatives will not be stored in tape, but in checkpoints. The memory requirement of second-order algorithmic adjoint contains the memory occupied by tape, however for symbolic version the memory requirement is the memory occupied by tape and checkpoint.

Memory Requirement ($\nu = 5$)		
n	Symbolic FoR	Algorithmic FoR
10	0.006	0.92
20	0.01	4.38
30	0.02	11.46
40	0.02	23.21
50	0.03	40.71
60	0.03	65.02
80	0.04	138.37
100	0.05	251.8
150	0.08	766.79
200	0.11	1719.2
300	0.16	5470.3
500	0.27	24096.1

Table 3. Memory Requirement for evaluating the second-order adjoint mode of the nonlinear solver (Newton) for our 1D sample problem in MB for different Problem-Dimensions.

Table 3 illustrates the memory requirement for evaluating the second-order symbolic and algorithmic adjoint mode of the nonlinear solver (Newton) for our 1D sample problem with constant number of nonlinear solver's (Newton) iterations ($\nu = 5$) and different problem sizes (n). It shows that, the memory requirement in second-order algorithmic adjoint mode is considerably higher than in the symbolic one, but for both cases it is proportional to the size of the problem.

Table 4 illustrates the memory requirement for evaluating the second-order symbolic and algorithmic adjoint mode of the nonlinear solver (Newton) for our 1D sample problem with constant problem dimension $n = 40$ and different nonlinear solver's (Newton) iterations (ν). In the symbolic mode the differentiation is done symbolically after the computation of the exact solution of the nonlinear system. It means that the memory is just needed to register the solutions of the nonlinear solver (here $\tilde{\mathbf{x}}$) and not the intermediate values of the nonlinear solver's algorithm. Therefore by setting the problem size (n) constant, it remains unchanged by varying the number of nonlinear solver's iterations (ν). However, in the algorithmic mode for calculation of the derivatives we should go through the algorithm (line-by-line differentiation) ν times, so the memory requirement is proportional to the number of iterations.

Memory Requirement ($n = 40$)		
ν	Symbolic FoR	Algorithmic FoR
1	0.02	4.49
2	0.02	9.02
3	0.02	13.75
4	0.02	18.48
5	0.02	23.21
6	0.02	27.94
10	0.02	46.85
15	0.02	70.49
20	0.02	94.14
30	0.02	141.42
50	0.02	236.0
100	0.02	472.43
300	0.02	1418.16
500	0.02	2363.88
1000	0.02	4728.2
2000	0.02	9456.84

Table 4. Memory Requirement for evaluating the second-order adjoint mode of the nonlinear solver (Newton) for our 1D sample problem in MB for different number of Newton's iterations.

7.2 Two Dimensional Eliptic PDE

As a two dimensional case study, we consider the two-dimensional Solid Fuel Ignition problem (also known as the Bratu problem) from the MINPACK-2 test problem collection [ACM91] which is given by the elliptic partial differential equation

$$\Delta x - z \cdot e^x = 0 \quad , \tag{64}$$

where $x = x(q_0, q_1)$ is computed over some bounded domain $\Omega \subsetneq I\!R^2$ with boundary $\Gamma \subsetneq I\!R^2$ and Dirichlet boundary conditions $x(q_0, q_1) = g(q_0, q_1)$ for $(q_0, q_1) \in \Gamma$. For simplicity, we focus on the unit square $\Omega = [0, 1]^2$ and we set

$$g(q_0, q_1) = \begin{cases} 1 & \text{if } q_0 = 1 \\ 0 & \text{otherwise} \end{cases} \quad .$$

We use finite differences as a basic discretization method. Its aim is to replace the differential

$$\Delta x \equiv \frac{\partial^2}{\partial q_0^2} + \frac{\partial^2}{\partial q_1^2}$$

with a set of algebraic equations, thus transforming Equation (64) into a system of nonlinear equations that can be solved by nonlinear solvers.

According to [Nau12] the system of nonlinear equations to be solved is

$$-4 \cdot \mathbf{x}_{i,j} + \mathbf{x}_{i+1,j} + \mathbf{x}_{i-1,j} + \mathbf{x}_{i,j+1} + \mathbf{x}_{i,j-1} = h^2 \cdot \mathbf{z}_{i,j} \cdot e^{\mathbf{x}_{i,j}} \quad , \tag{65}$$

for $i, j = 1, \ldots, n-1$. Discretization of the boundary conditions yields $\mathbf{x}_{n,j} = 1$ and $\mathbf{x}_{i,0} = \mathbf{x}_{0,j} = \mathbf{x}_{i,n} = 0$ for $i, j = 1, \ldots, n-1$.

According to the Equations (3)–(5), the preprocessor is the identity $\boldsymbol{\lambda}_{i,j} = \mathbf{z}_{i,j}$, the solution process is the two dimensional nonlinear function (Equation (65)) which is solved by a nonlinear solvers (e.g. Newton's algorithm). Considering $\mathbf{x}^m_{i,j}$ as real datas[5] the postprocessor computes the cost functional which is

$$J(\mathbf{z}) = \|\mathbf{x}^*(z) - \mathbf{x}^m\|_2^2 \, . \tag{66}$$

The goal is to apply Newton's method in optimization algorithm (Equation (63)) in order to minimize the postprocessor J and optimize the initial values (the inputs) $\mathbf{z}_{i,j}$ in the preprocessor. For this purpose the computation of the Jacobian and Hessian of J at the current iterate $\mathbf{z}^k$ is required, this includes the evaluation of the Jacobian and Hessian of the postprocessor, nonlinear solver and preprocessor.

The fully algorithmic part of the derivative computation is done by the software tool `dco/c++` [LLN11], implementing AD by overloading in C++. The implementation of symbolic tangent over tangent and tangent over adjoint methods is supported by a custom user interface. For the symbolic part of the derivative computation, the evaluation of the directional derivatives of the preprocessor and the postprocessor will be done by algorithmic mode and only the first- and second-order directional derivatives of the nonlinear solver will be evaluated symbolically.

In the following, we set ϵ as the accuracy of the postprocessor ($J(\mathbf{z}) < \epsilon$), which computes the costfunctional (see Equation (66)) and δ would be the accuracy of our nonlinear solver (Newton) to solve the nonlinear system Equation (65).

In this section we compare run time of the optimization of postprocessor (J) with respect to the preprocessor (initial values $\mathbf{z}_{i,j}$) by Equation (63) for various differentiated versions of the nonlinear solver.

In Fig. 5 we observe the expected behaviour for the computational overhead induced by the various differentiation methods for optimizing the postprocessor J with respect to the initial values in preprocessor $\mathbf{z}$. In this example the accuracy of the nonlinear solver for solving the nonlinear problem (e.g. with Newton) is set to $\delta = 1e - 12$ and the accuracy of the optimization is set to $\epsilon = 1e - 2$. It shows that in both cases of symbolic and algorithmic, the complexity is less if the derivatives be calculated by the adjoint mode. Optimization using symbolic first- and second-order adjoint mode for calculation of directional derivatives requires less duration, however, the optimization spends the most time by applying algorithmic first- and second-order tangent for evaluating the derivatives.

[5] Here again we do not have the real datas, so we apply a small perturbation to our results and suppose that these are the real ones.

n	Symbolic		Algorithmic	
	FoF	FoR	FoF	FoR
4 × 4	0.05	0.01	0.17	0.03
6 × 6	0.84	0.05	3.92	0.29
8 × 8	11.32	0.35	64.67	2.54
10 × 10	89.59	1.39	573.51	14.67
11 × 11	218.59	2.62	1454.23	31.95
12 × 12	495.53	4.83	-	74.17
15 × 15	-	25.46	-	485.43
20 × 20	-	277.36	-	-

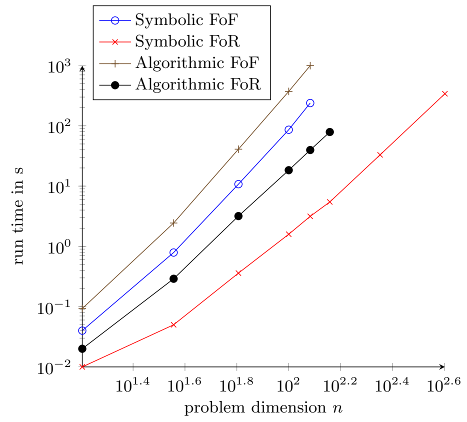


Fig. 5. Run time (in seconds) overhead comparison of optimizing our 2D sample problem with different differentiation methods. The (-) sign implies no convergence after 2000 seconds.

One should also consider that, as mentioned before, the memory requirement of second-order algorithmic contains the memory occupied by tape, however for symbolic version the memory requirement is the memory occupied by tape and checkpoint.

Memory Requirement ($\nu = 8$)		
n	Symbolic FoR	Algorithmic FoR
3 × 3	0.003	0.15
4× 4	0.005	0.83
5× 5	0.007	3.1
6× 6	0.01	9.16
10× 10	0.03	201.21
15× 15	0.06	2438.57
20 × 20	0.11	14401.5
25 × 25	0.17	56988.3
30 × 30	0.24	-

Table 5. Memory Requirement for evaluating the second-order adjoint mode of the nonlinear solver (Newton) for our 2D sample problem in MB for different Problem-Dimensions. The (-) sign implies that the memory is full on a machine with 128 GB RAM.

Table 5 illustrates the memory requirement for evaluating the second-order symbolic and algorithmic adjoint mode of the nonlinear solver (Newton) for our 2D sample problem with constant number of nonlinear solver's (Newton) iterations ($\nu = 8$) and different problem sizes (n) of nonlinear system for adjoint second-order algorithmic and symbolic. It shows that the memory requirement of algorithmic adjoint mode is considerably higher than the symbolic one, but the memory requirement is proportional to the size of the problem for both cases. In the algorithmic mode, the memory was full for $n >= (30 \times 30)$ on a machine (Heisenberg) with 128 GB RAM.

Table 6 illustrates the memory requirement for evaluating the second-order symbolic and algorithmic adjoint mode of the nonlinear solver (Newton) for our

Memory Requirement ($n = 10 \times 10$)		
ν	Symbolic FoR	Algorithmic FoR
1	0.03	22.94
2	0.03	48.41
3	0.03	73.88
4	0.03	99.34
5	0.03	124.81
6	0.03	150.28
8	0.03	201.21
10	0.03	252.14
15	0.03	379.47
20	0.03	506.8
30	0.03	761.47
50	0.03	1270.79
100	0.03	2544.1
200	0.03	5090.73
500	0.03	12730.6
1000	0.03	25463.8

Table 6. Memory Requirement for evaluating the second-order adjoint mode of the nonlinear solver (Newton) for our 2D sample problem in MB for different number of Newton's iterations.

1D sample problem with constant problem dimension $n = 10 \times 10$ and different number of nonlinear solver's (Newton) iterations (ν). In the symbolic mode the differentiation is done symbolically after the computation of the exact solution of the nonlinear system. It means that the memory is just needed to register the solutions of the nonlinear solver (here $\tilde{\mathbf{x}}$) and not the intermediate values of the nonlinear solver's algorithm. Therefore by setting the problem size (n) constant, it remains unchanged by varying the number of nonlinear solver's iterations (ν). However, in the algorithmic mode for calculation of the derivatives we should go through the algorithm (line-by-line differentiation) ν times, so the memory requirement is proportional to the number of iterations.

In the solution process the directional derivatives of the solution are computed by a *symbolic* version of the solver under the assumption that the exact solution $\mathbf{x}^*$ has been reached. $F(\mathbf{x}, \mathbf{z}) = 0$ can be differentiated symbolically in this case. However, for computing the derivatives with algorithmic modes of AD, the whole algorithm would be differentiated. For example, suppose $F(\mathbf{x}, \mathbf{z}) < \delta$. The discrepancies in the results computed by second-order algorithmic and symbolic nonlinear solvers depend on the accuracy (δ) of the approximation of the *primal* solution process. In the following we compare the directional derivatives of the postprocessor J (Equation 66) with respect to the initial values in preprocessor $\mathbf{z}_{i,j}$ computed with symbolic FoF and algorithmic FoF for different nonlinear solver accuracies (δ) in the first iteration of the optimization's algorithm

$$Q = \| \frac{\partial^2 J}{\partial \mathbf{z}^2}_{Symbolic} - \frac{\partial^2 J}{\partial \mathbf{z}^2}_{Algorithmic} \|.$$

As it is shown in the Fig. 6, for $n = (6 \times 6)$ in our 2D test case, by increasing the δ in Newton algorithm (our nonlinear solver) the discrepancies in the results

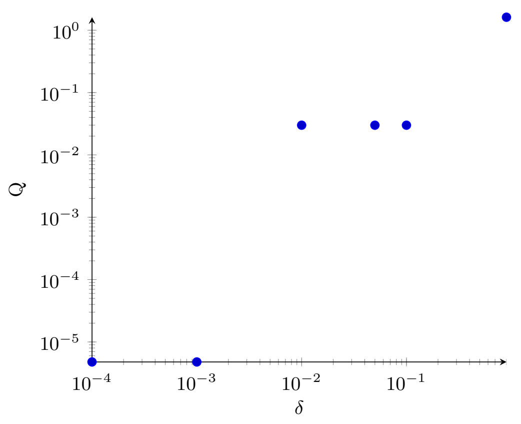


Fig. 6. The Discrepancies in the Derivatives Computed by Second-Order Algorithmic and Symbolic for different Nonlinear Solver Accuracies (δ).

computed by second-order algorithmic and symbolic will be larger. Therefore, in order to have a more exact derivative evaluation in symbolic computation of the derivatives of nonlinear systems, the accuracy of the nonlinear solver (δ) should tend to zero.

8 Conclusion

In this paper we discussed second-order algorithmic and symbolic direct solvers for systems of nonlinear equations. Mathematical insight yields a reduction of the computational overhead for evaluating second-order directional derivatives. Computing derivatives by a fully algorithmic method corresponding to a straight application of AD without taking into account any mathematical or structural properties of the numerical method turns out to be the worst approach in terms of computational efficiency. The performance of the different approaches depends on the number of (Newton) iterations ν and on the problem size n. As an alternative we considered the symbolic second-order differentiation of numerical simulation programs which contain calls to solvers for parameterized systems of n nonlinear equations and compared them with the algorithmic version (AD) of computing second derivatives. In Fig. 4 for 1D- and in Fig. 5 for 2D-eliptic partial differential equation (PDE) we observe that in both cases of second-order symbolic and algorithmic, the complexity of the optimization is less if the derivatives be calculated by the adjoint mode. Optimization using symbolic first- and second-order adjoint mode for evaluation of the directional derivatives requires less time, however, applying algorithmic first- and second-order tangent for the evaluation of the directional derivatives spends the most time.

Directional derivatives of the solution are computed by a symbolic tangent and adjoint version of the solver under the assumption that the exact solution $\mathbf{x}^*$ has been reached. $F(\mathbf{x}, \boldsymbol{\lambda}) = 0$ can be differentiated symbolically in this case, however algorithmic tangent and adjoint versions of the solver compute directional derivatives of the approximation of the solution which are actually computed by the algorithm. This yields the discrepancies in the results computed by algorithmic and symbolic tangent and adjoint. In Fig. 6 it is shown that by increasing the accuracy of the nonlinear solver (δ) the discrepancies in the results computed by second-order algorithmic and symbolic will be larger.

Furthermore, the memory requirement of adjoint second-order symbolic is the memory which is used by tape and checkpoint and it depends on the size of the problem (refer to Table 3 and Table 5 for 1D- and 2D-eliptic PDE respectively), whereas in algorithmic version it is the memory which is used by tape and it depends on the size of the problem and on the number of iterations performed by the nonlinear solver's algorithm (refer to Table 4 and Table 6 for 1D- and 2D-eliptic PDE respectively).

1D Case Study

In the following, the implementation of our 1-dim nonlinear problem, i.e. 1-dim case study in Section 7.1, as well as the nonlinear solver (here, Newton's algorithm) are presented. The complete codes of the second-order symbolic and algorithmic tangent and adjoint modes of the nonlinear solver are illustrated in Section 6. At the end, the implementation of the *main* functions for second-order tangent, adjoint and finite difference of the nonlinear solver are exposed.

Nonlinear Problem

```
/******************** Function.hpp ********************/
template <typename TYPE>
inline void preprocessor(int n, std::vector<TYPE> &z, std::vector<
    TYPE> &lambda)
{
     for(int i=0; i<n; i++)
          lambda[i] = z[i];
}

template <typename TYPE2>
inline TYPE2 F(int n, std::vector<TYPE2> &x, std::vector<TYPE2> &
    lambda, std::vector<TYPE2> &residual) {
     TYPE2 delta = (TYPE2)(1.0 / n);
     TYPE2 norm_res = (TYPE2)(0);
     TYPE2 left, right;

     for (int i = 0; i < n; i++) {
          if (i == 0)
               left = 10;
          else
               left = (TYPE2)lambda[i-1]*x[i-1];
          if (i == n-1)
               right = 20;
          else
               right = (TYPE2)lambda[i+1]*x[i+1];
          residual[i] = (right + left - 2*(TYPE2)lambda[i]*x[i]) /
                         (delta*delta) + x[i]*(right-left)/(2*delta);
          norm_res += pow(residual[i], 2);
     }
     norm_res = sqrt(norm_res);
     return norm_res;
}

template <typename TYPE>
inline TYPE postprocessor(int n, std::vector<TYPE> &x, std::vector<
    double> &x_a) {

     TYPE J = (TYPE)0.;
     for (int i=0; i<n; i++)
          J += pow(x_a[i] - x[i], 2); // x_a are real measurements.
     J /= (TYPE)(n);
     return J;
}
```

Newton's Solver for Nonlinear Equations

```
/******************** Newton.hpp ********************/
```

```
template <class T>
int S(int n, std::vector<T> &x, std::vector<T> &lambda)
{
    std::vector<T> dx(n), r(n), x_orig(n);
    std::vector<T> residual(n), rph(n), rmh(n), xph(n), xmh(n);

    // compute Jacobian of F with respect to x
    vector<vector<T> > Jacobian(n, vector<T>(n));
    T norm_residual;
    int nr_iterations;
    int iter=0;

    for (nr_iterations=0;; nr_iterations++) {
        // compute Jacobian and residual using finite difference
        for (int i=0; i<n; i++)
            x_orig[i]=x[i];
        double hh=1e-8;
        for (int i=0; i<n; i++) {
         for (int j=0; j<n; j++) {
            x[j] = (T)x_orig[j];
            xph[j] = (T)x_orig[j];
            xmh[j] = (T)x_orig[j];}
            F(n,x,lambda,r);
            xph[i] = xph[i] + hh;
            F(n,xph,lambda,rph);
            xmh[i] = xmh[i] - hh;
            F(n,xmh,lambda,rmh);
            for (int j=0; j<n; j++) {
                T deriv = (rph[j]-rmh[j])/(2*hh);
                T derivative = (T) 0.;
                derivative = deriv;
                residual[j]=r[j];
                Jacobian[j][i] = derivative;
            } // j
        } // i
        // solve Newton system by LU-decomposition of Jacobian
        // negate residual
        for(int i=0; i<n; i++)
            residual[i] = -residual[i];
        int **P = LUDecomp(n, Jacobian);
        FBsolve(n, P, Jacobian, residual, dx);
        // update x and evaluate new residual
        for (int i=0; i<n; i++) x[i]+=dx[i];
        norm_residual=F(n,x,lambda,r);
        for (int j=0; j<n; j++) residual[j] = r[j];
        iter++;
        if (norm_residual<=newton_eps) break;
    }
    return iter;
}
```

main Functions:
Second-Order Tangent Mode

```
/******************** main_t2s_t1s.cpp ********************/
#include <iostream>
#include <stdlib.h>
#include <fenv.h>
#include <vector>

```

```
bool Disc;
bool Cont;
const double newton_eps = 1e-6;
const double eps = 1e-6;

#include "dco.hpp"
DCO_DEFINE_GLOBAL_TAPE_POINTER

#include "Function.hpp"
#include "Newton.hpp"

using namespace std;

int main(int argc, char *argv[]) {
    Disc = false;
    Cont = true;
    int n=10;
    if (argc >= 2)
        n = atoi(argv[1]);
    if (argc >= 3)
        Disc = true;
    std::vector<double> xv(n), z(n,1.1), dJ_dz(n,0);
    std::vector<std::vector<double> > H_dJ_dz(n, std::vector<double
        >(n));
    std::vector<dco::t2s_t1s::type> az(n);
    for (int i=0; i<n; i++)
        for (int j=0; j<n; j++)
            H_dJ_dz[i][j] = 0.;
    // Newton Optimization
    int iter = 0;
    double norm_dJ = 10;
    double J;
    double sum = 0;
    while(norm_dJ > eps) {
        ++iter;
        for (int ii=0; ii<n; ii++) {
            for(int jj=0; jj<n; jj++) {
                for (int i = 0; i < n; i++)  az[i] = z[i];
                dco::t2s_t1s::set(az[ii], 1.0, 0, 2);
                dco::t2s_t1s::set(az[jj], 1.0, 1);
                dco::t2s_t1s::type aJ = costfunction(n, az);
                dco::t2s_t1s::get(aJ, J);
                dco::t2s_t1s::get(aJ,dJ_dz[jj], 1);
                dco::t2s_t1s::get(aJ, H_dJ_dz[ii][jj], 1, 2);
                sum += H_dJ_dz[ii][jj]*H_dJ_dz[ii][jj];
            }  // jj

        }  // ii

        Gauss(n, H_dJ_dz, dJ_dz, xv);
        double alpha = 1.;
        double tJ = J+1;
        while (tJ > J) {
            for (int i=0; i<n; i++) {
                double val;
                dco::t2s_t1s::get(az[i], val);
                z[i] = val - alpha*xv[i];
            }
            tJ = costfunction(n, z);
            alpha /= 2.0;
        }   // while (tJ > J)
        J = tJ;
        norm_dJ = 0;
        for (int i=0; i<n; i++) {
            norm_dJ += dJ_dz[i]*dJ_dz[i];
        }
        norm_dJ = sqrt(norm_dJ);
    }  // while(norm_J > eps)

    cout << "--------------------------------------" << endl;
    cout << "J=  " << J << endl;
    cout << "Norm of second derivative is:  " << sqrt(sum) << endl;
    return 0;
}
```

Second-Order Adjoint Mode

```
/******************* main_t2s_a1s.cpp *******************/
#include <iostream>
#include <stdlib.h>
#include <fenv.h>
#include <vector>

bool Disc;
bool Cont;
const double newton_eps = 1e-6;
const double eps = 1e-6;

#include "dco.hpp"
DCO_DEFINE_GLOBAL_TAPE_POINTER

#include "Function.hpp"
#include "Newton.hpp"

using namespace std;

int main(int argc, char *argv[]) {
    Disc = false;
    Cont = true;
    int n=10;
    if (argc >= 2)
        n = atoi(argv[1]);
    if (argc >= 3)
        Disc = true;
    std::vector<double> xv(n), z(n, 1.1), dJ_dz(n, 0);
    std::vector<std::vector<double> > H_dJ_dz(n, std::vector<double>
         (n));
    std::vector<dco::t2s_a1s::type> az(n);
    for (int i=0; i<n; i++)
        for (int j=0; j<n; j++)
            H_dJ_dz[i][j] = 0.;
     // take chunk tape
    dco::t2s_a1s::global_tape = dco::t2s_a1s::tape::create();

    // Newton Optimization
    int iter = 0;
    double norm_dJ = 10;
    double J;
    double sum = 0;
    while(norm_dJ > eps) {
        ++iter;
        for (int ii=0; ii<n; ii++) {
            for (int i=0; i<n; i++)  az[i] = z[i];
            dco::t2s_a1s::set(az[ii], 1.0, 0, 2);
            for (int i=0; i<n; i++)
                dco::t2s_a1s::global_tape->register_variable(az[i]);
            dco::t2s_a1s::tape::iterator position = dco::t2s_a1s::
                global_tape->get_position();
            dco::t2s_a1s::global_tape->zero_adjoints();
            for (int i=0; i<n; i++) dco::t2s_a1s::set(az[i], z[i]);
            dco::t2s_a1s::type aJ = costfunction(n, az);
            double mem_tape = dco::t2s_a1s::global_tape->
                get_tape_memory_size();
            double mem_checkpoint = dco::t2s_a1s::global_tape->
                get_checkpoint_memory_size();
            cout << "mem_tape:␣␣" << mem_tape << endl;
            cout << "mem_checkpoint:␣␣" << mem_checkpoint << endl;
            dco::t2s_a1s::set(aJ, 1., -1);
            dco::t2s_a1s::get(aJ, J);
            dco::t2s_a1s::global_tape->
                interpret_and_reset_adjoint_to(position);
            for (int i=0; i<n; i++) {
                dco::t2s_a1s::get(az[i], dJ_dz[i], -1);
                dco::t2s_a1s::get(az[i], H_dJ_dz[i][ii], -1, 2);
                sum += H_dJ_dz[i][ii]*H_dJ_dz[i][ii];
            }

        } //ii

        Gauss(n, H_dJ_dz, dJ_dz, xv);
        double alpha = 1.;
        double tJ = J+1;
        while (tJ > J) {
            for (int i=0; i<n; i++) {
                double val;
                dco::t2s_a1s::get(az[i], val);
                z[i] = val - alpha*xv[i];
            }
            tJ = costfunction(n, z);
            alpha /= 2.0;
        }   // while (tJ > J)
        J = tJ;
        norm_dJ = 0;
        for (int i=0; i<n; i++) {
            norm_dJ += dJ_dz[i]*dJ_dz[i];
        }
        norm_dJ = sqrt(norm_dJ);
    }  // while(norm_J > eps)
    cout << "------------------------------------------" << endl;
    cout << "J=␣␣" << J << endl;
    cout << "Norm␣of␣second␣derivative␣is:␣␣" << sqrt(sum) << endl;
    return 0;
}
```

Second-Order Finite Difference

```
/******************** main_fd.cpp ************************/
#include <iostream>
#include <stdlib.h>
```

```
#include <fenv.h>
#include <vector>

double passive_time;
double forward_time;

const double newton_eps = 1e-6;
const double eps = 1e-6;

#include "dco.hpp"

#include "Function_FD.hpp"
#include "Newton.hpp"

using namespace std;

int main(int argc, char *argv[]) {

    int n=10;
    if (argc >= 2)
        n = atoi(argv[1]);

    std::vector<double> xv(n), z(n, 1.1), z_fd(n), dJ_dz(n, 0);
    std::vector<std::vector<double> > H_dJ_dz(n, std::vector<double>
         (n));
    for (int i=0; i<n; i++)
        for (int j=0; j<n; j++)
            H_dJ_dz[i][j] = 0.;

    // Newton Optimization
    int iter = 0;
    double norm_dJ = 10;
    double J;
    double sum = 0;

    double h1 = 1e-05;
    double h2 = 1e-05;

    while(norm_dJ > eps) {

        // computing the Jacobian with Finite Difference
        for (int ii=0; ii<n; ii++) {
            for (int i = 0; i < n; i++)
                z_fd[i] = z[i];
            z_fd[ii] += h1;
            double Jph = costfunction(n, z_fd);
            z_fd[ii] -= 2*h1;
            double Jmh = costfunction(n, z_fd);
            dJ_dz[ii] = (Jph-Jmh) / (2*h1);
        }
        // computing the Hessian with Finite Difference
        for (int ii=0; ii<n; ii++) {
            for(int jj=0; jj<n; jj++) {
                for (int i = 0; i < n; i++)
                    z_fd[i] = z[i];
                z_fd[ii] += h1;
                z_fd[jj] += h2;
                double J_1 = costfunction(n, z_fd);
                z_fd[jj] -= 2*h2;
                double J_2 = costfunction(n, z_fd);
                z_fd[ii] -= 2*h1;
                double J_4 = costfunction(n, z_fd);
                z_fd[jj] += 2*h2;
                double J_3 = costfunction(n, z_fd);
                H_dJ_dz[ii][jj] = (J_1 - J_2 - J_3 + J_4) / (4*h1*h2
                    );
                sum += H_dJ_dz[ii][jj]*H_dJ_dz[ii][jj];
            }  // jj
        }  // ii

        J = costfunction(n, z);
        Gauss(n, H_dJ_dz, dJ_dz, xv);
        double alpha = 1.;
        double tJ = J+1;
        while (tJ > J) {
            for (int i=0; i<n; i++) {
                double val = z[i];
                z[i] = val - alpha*xv[i];
            }
            tJ = costfunction(n, z);
            alpha /= 2.0;
        }   // while (tJ > J)

        J = tJ;
        norm_dJ = 0;
        for (int i=0; i<n; i++)
            norm_dJ += dJ_dz[i]*dJ_dz[i];
        norm_dJ = sqrt(norm_dJ);

    }  // while(norm_J > eps)
    cout << "----------------------------------------" << endl;
    cout << "J=  " << J << endl;
    cout << "Norm of second derivative is:  " << sqrt(sum) << endl;
    return 0;
}
```

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