Compiler-based Differentiation of Higher-Order Numerical Simulation Codes using Interprocedural Checkpointing

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***Abstract*—Based on algorithmic differentiation, we present a derivative code compiler capable of transforming implementations of multivariate vector functions into a program for computing derivatives. Its unique reapplication feature allows the generation of code of an arbitrary order of differentiation, where resulting values are still accurate up to machine precision compared to the common numerical approximation by finite differences. The high memory load resulting from the adjoint model of Algorithmic Differentiation is circumvented using semi-automatic interprocedural checkpointing enabled by the joint reversal scheme implemented in our compiler. The entire process is illustrated by a one dimensional implementation of Burgers' equation in a generic optimization setting using for example Newton's method. In this implementation, finite differences are replaced by the computation of adjoints, thus saving an order of magnitude in terms of computational complexity.**

***Keywords*-Algorithmic Differentiation; Source Transformation; Optimization; Numerical Simulation; Checkpointing**

I. Introduction

A typical problem in fluid dynamics is given by the continuous Burgers equation [2]

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} \quad , \tag{1}$$

describing shock waves moving through gases. u denotes the velocity field of the fluid with viscosity ν. Similar governing equations represent the core of many numerical simulations. Such simulations are often subject to various optimization techniques involving derivatives. Thus, Burgers' equation will serve as a case study for a compiler-based approach to the accumulation of the required derivatives.

Suppose we solve the differential equation in (1) by discretization using finite differences on an equidistant one-dimensional grid with n_x points. For given initial conditions $u_{i,0}$ with $0 < i \leq n_x$ we simulate a physical process by integrating over n_t time steps according to the leapfrog/DuFort-Frankel scheme presented in [3]. At time step j we compute $u_{i,j+1}$ for time step $j+1$ according to

$$\begin{aligned} u_{i,j+1} = u_{i,j-1} &- \frac{\Delta t}{\Delta x}\left(u_{i,j}\left(u_{i+1,j} - u_{i-1,j}\right)\right) \\ &+ \frac{2\Delta t}{\Delta x^2}\left(u_{i+1,j} - \left(u_{i,j+1} + u_{i,j-1}\right) + u_{i-1,j}\right), \end{aligned} \tag{2}$$

where Δt is the time interval and Δx is the distance between two grid points. In general, if the initial conditions $u_{i,0}$ cannot be accurately measured, they are essentially replaced by approximated values. To improve their accuracy additional observed values $u^{ob} \in \mathbb{R}^{n_x \times n_t}$ are taken into account. The discrepancy between observed values $u^{ob}_{i,j}$ and simulated values $u_{i,j}$ are evaluated by the cost function

$$y = \frac{1}{2}\sum_{i=1}^{n_x}\sum_{j=1}^{n_t}(u_{i,j} - u^{ob}_{i,j})^2 \quad , \tag{3}$$

which allows us to obtain improved estimations for the initial conditions by applying, for example, Newton's method [4] to solve the data assimilation problem with Burgers' equation as constraints [5]. The single Newton steps are repeated until the residual cost y undercuts a certain threshold.

In Section II, we introduce Algorithmic Differentiation (AD) as implemented by our derivative code compiler `dcc` covering both the tangent-linear as well as the adjoint model. Section III provides a user's perspective on the application of `dcc`. Higher-order differentiation models are discussed in Section IV. Finally, the results of our case study are discussed in Section VII.

II. Algorithmic Differentiation

The minimization of the residual is implemented by resorting to Newton's second-order method for minimization. In general, Newton's method may be applied to arbitrary differentiable multivariate vector functions $\mathbf{y} = F(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}^m$. This algorithm heavily depends on the accurate and fast computation of Jacobian and Hessian values, since one iterative step $\mathbf{x}_i \to \mathbf{x}_{i+1}$ is computed by

$$\mathbf{x}_{i+1} = \mathbf{x}_i - \nabla^2 F(\mathbf{x}_i)^{-1} \cdot \nabla F(\mathbf{x}_i) \quad . \tag{4}$$

The easiest method of approximating partial derivatives $\nabla_{x_i} F$ uses the finite difference quotient

$$\nabla_{x_i} F(\mathbf{x}) \approx \frac{F(\mathbf{x} + h \cdot \mathbf{e_i}) - F(\mathbf{x})}{h} \quad , \tag{5}$$

for the Cartesian basis vector $\mathbf{e_i} \in \mathbb{R}^n$ and with $\mathbf{x} \in \mathbb{R}^n$, $h \to 0$. In order to accumulate the Jacobian of a multivariate function the method is rerun n times to perturb each component of the input vector $\mathbf{x}$. The main advantage of this method resides in its straightforward implementation; no additional changes to the code of the function F are necessary. However, the derivatives accumulated through finite differences are only approximations. This represents a major drawback for codes that simulate highly nonlinear systems, resulting in truncation and cancellation errors or simply providing wrong results. In particular by applying the Taylor expansion to the second-order centered difference quotient we derive a machine precision induced approximation error of $\frac{\epsilon}{h^2}$, with ϵ being the rounding error.

AD [6] solves this problem analytically, changing the underlying code to compute derivatives by applying symbolic differentiation rules to individual assignments and using the chain rule to propagate derivatives along the flow of control. The achieved accuracy only depends on the machine's precision ϵ. There exist two distinct derivative models, differing in the order of application of the associative chain rule. Let ∇F be the Jacobian of F. The *tangent-linear* code

$$\begin{aligned} & F\big(\overset{\downarrow}{\mathbf{x}}, \underset{\downarrow}{\mathbf{y}}\big) \xrightarrow{\texttt{dcc}} \dot{F}\big(\overset{\downarrow}{\mathbf{x}}, \overset{\downarrow}{\dot{\mathbf{x}}}, \underset{\downarrow}{\mathbf{y}}, \underset{\downarrow}{\dot{\mathbf{y}}}\big) \quad , \\ & \text{where} \\ & \qquad \dot{\mathbf{y}} = \nabla F(\mathbf{x}) \cdot \dot{\mathbf{x}} \\ & \text{and} \quad \mathbf{y} = F(\mathbf{x}) \quad , \end{aligned} \tag{6}$$

of F computes the directional derivative $\dot{\mathbf{y}}$ of the outputs $\mathbf{y}$ with respect to the inputs $\mathbf{x}$ for a given direction $\dot{\mathbf{x}} \in \mathbb{R}^n$, while arrows designate inputs and outputs. By iteratively setting $\dot{\mathbf{x}}$ equal to each of the n Cartesian basis vectors in $\mathbb{R}^n$, we accumulate the entire Jacobian. This leads to a runtime complexity identical to finite differences of $\mathcal{O}(n) \cdot cost(F)$, where $cost(F)$ denotes the computational cost of a single function evaluation.

By exploiting the associativity of the chain rule, the *adjoint* code

$$\begin{aligned} & F\big(\overset{\downarrow}{\mathbf{x}}, \underset{\downarrow}{\mathbf{y}}\big) \xrightarrow{\texttt{dcc}} \bar{F}\big(\overset{\downarrow}{\mathbf{x}}, \overset{\downarrow}{\bar{\mathbf{x}}}, \underset{\downarrow}{\mathbf{y}}, \underset{\downarrow}{\bar{\mathbf{y}}}\big) \quad , \\ & \text{where} \\ & \qquad \mathbf{y} = F(\mathbf{x}) \\ & \text{and} \quad \bar{\mathbf{x}} = \bar{\mathbf{x}} + \nabla F(\mathbf{x})^{\mathsf{T}} \cdot \bar{\mathbf{y}} \quad , \end{aligned} \tag{7}$$

of F computes *adjoints* $\bar{\mathbf{x}} \in \mathbb{R}^n$ of the inputs $\mathbf{x}$ for given adjoints $\bar{\mathbf{y}} \in \mathbb{R}^m$ of the outputs. To accumulate the entire Jacobian we have to iteratively set $\bar{\mathbf{y}}$ equal to each Cartesian basis vector of $\mathbb{R}^m$ yielding a runtime complexity of $\mathcal{O}(m) \cdot cost(F)$. Note that for scalar functions with $m = 1$ the accumulation of the Jacobian amounts to the computation of one gradient yielding a runtime cost of $\mathcal{O}(1) \cdot cost(F)$ for the adjoint model compared to $\mathcal{O}(n) \cdot cost(F)$ for the tangent-linear model. In this particular case, we are able to compute gradients at a small constant multiple of the cost of a single function evaluation. The reduction of this factor down toward the theoretical minimum of three [6] is one of the major challenges addressed by ongoing research and development in the field of AD [7], [8].

The core idea of this paper is to develop a source transformation tool or compiler that transforms a given C code into its differentiated version. In general, this increases the differentiation order from d to $d + 1$. I.e., by taking as an input a handwritten first-order code we end up with a second-order code. Taking this insight a step further we want that our tool accepts its output as an input. Thus, starting from a given code, we are able to iteratively generate an arbitrary order of differentiation code. This unique feature is being presented in Section IV.

Furthermore our derivative code compiler is able to use checkpointing techniques for the adjoint mode, by using joint reversal as opposed to split reversal as a reveral technique. This will be explained in Section V.

III. dcc - A Derivative Code Compiler

Numerical optimization problems are commonly implemented as multivariate scalar functions $y = F(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$, describing some residual y of a numerical model. We assume that the goal is to minimize a norm of this residual y by adapting the inputs $\mathbf{x}$. Therefore, for better readability and without the loss of generality, in this paper, we will only cover multivariate scalar functions.

The main link between dcc and the mathematical models of AD is the ability to decompose each function implementation into single assignment code (SAC) as follows:

$$\begin{aligned} & \text{for } j = n, \ldots, n+p \\ & \qquad v_j = \varphi_j(v_i)_{i \prec j} \quad . \end{aligned} \tag{8}$$

The entire program is regarded as a sequence of $p + 1$ elemental statements. In each statement an elemental function φ_j is applied to a set of variables $(v_i)_{i \prec j}$ yielding the unique *intermediate* variable v_j with $i \prec j$ denoting a dependence of v_j on v_i. The *independent* inputs are given by $v_i = x_i$ for $i = 0, \ldots, n-1$ while the *dependent* output of F is the final value $y = v_{n+p}$. When dcc applies the tangent-linear model to each of the $p + 1$ assignments, we obtain

$$\begin{aligned} & \text{for } j = n, \ldots, n+p \\ & \qquad \dot{v}_j = \sum_{i \prec j} \frac{\partial \varphi_j}{\partial v_i} \cdot \dot{v}_i \\ & \qquad v_j = \varphi_j(v_i)_{i \prec j} \quad . \end{aligned} \tag{9}$$

Considering the j-th assignment in (9), the local k-th entry of the gradient $(\frac{\partial \varphi_j}{\partial v_k})_{k \prec j}$ is provided in $\dot{v}_j$ by setting $\dot{v}_k$

to one and all $(\dot{v}_i)_{k \neq i \prec j}$ to zero. The gradient component $(\frac{\partial y}{\partial x_k})_{k \in \{0,\ldots,n-1\}}$ is obtained by evaluating (9) and setting $\dot{x}_k$ to one and all other $(\dot{x}_i)_{k \neq i \in \{0,\ldots,n-1\}}$ to zero. To get the whole gradient we have to evaluate (9) n times letting $\dot{\mathbf{x}}$ range over the Cartesian basis vectors in $\mathbb{R}^n$. The adjoint model is acquired by transforming (8) into:

$$\begin{aligned} &\text{for } j = n, \ldots, n+p \\ &\quad v_j = \varphi_j(v_i)_{i \prec j} \\ &\text{for } i \prec j \text{ and } j = n+p, \ldots, n \\ &\quad \bar{v}_i = \bar{v}_i + \frac{\partial \varphi_j}{\partial v_i}(v_k)_{k \prec j} \cdot \bar{v}_j \quad . \end{aligned} \tag{10}$$

The first part consists of the original assignments $j = n, \ldots, n+p$ and is called *forward section*. The *reverse section* follows with the computation of the adjoint variables in the order $j = n+p, \ldots, n$. Note the reversed order of the assignments as well as the changed data flow of the left and right-hand sides compared with the original assignments. To compute the local gradient $(\frac{\partial \varphi_j}{\partial v_k})_{k \prec j}$ we have to initialize $(\bar{v}_i)_{i \prec j}$ with zero and $\bar{v}_j$ with one. The initialization with zero is mandatory because $(\bar{v}_i)_{i \prec j}$ occurs in (10) on both sides of the adjoint assignment. According to (7), the adjoint variable $\bar{v}_j$ is an input variable. Therefore it is initialized with the Cartesian basis vector in $\mathbb{R}$.

The important advantage of the adjoint model is that by evaluating (10) only once we obtain the full gradient $\frac{\partial y}{\partial \mathbf{x}}$ in $\bar{x}_i = \bar{v}_i$ for $i = 0, \ldots, n-1$. To achieve this we have to initialize $(\bar{x}_i)_{i=0,\ldots,n-1}$ with zero and $\bar{y}$ with one. As mentioned above $\bar{\mathbf{x}}$ must be zero because it occurs not only on the left-hand side in (7) and y is initialized with the value of the Cartesian basis vector in $\mathbb{R}$.

In (8), we assumed that the input code is given as a SAC. This is an oversimplification in terms of real codes. The adjoint code has to deal with the fact that real code variables are overwritten frequently. One way to simulate the predicate of unique intermediate variables is to store certain left-hand side variables on a stack during the augmented forward section. Candidates for storing on the stack are those variables that are being overwritten and are required for later use during the computation of the local gradients and associated adjoints. Before evaluating the corresponding adjoint assignment in the reverse section the values are restored from the stack.

For illustration purposes we consider Listing 1 showing an implementation of the non-linear reduction $y(\mathbf{x}) = \prod_{i=0}^{n-1} \sin(x_i)$. `dcc` parses only functions with **void** as a return type (line 1). All inputs and return values are passed through the arguments, which in turn only consist of arrays (called by pointers) and scalar values (called by reference). Additionally we may pass an arbitrary number of integer arguments by value or by reference. We assume that all differentiable functions are implemented using values of type **double**. Therefore, only variables of type **double** are directly affected by the differentiation process.

```
1  void t1_f(int n, double* x, double* t1_x
2                 , double& y, double& t1_y)
3  {
4    ...
5    for(int i=0;i<n;i++) {
6      y=y*sin(x[i]);
7      t1_y=t1_y*sin(x[i])+y*cos(x[i])*t1_x[i];
8    }
9    ...
10 }
```

Listing 2: Tangent-linear version of `f` as generated by `dcc`

```
1  for(int i=0; i<n;i++) {
2    t1_x[i]=1;
3    t1_f(n, x, t1_x, y, t1_y);
4    gradient[i]=t1_y;
5    t1_x[i]=0;
6  }
```

Listing 3: Driver for `t1_f`

```
1  void f(int n, double *x, double &y)
2  {
3    int i=0;
4    y=0;
5    for(i=0;i<n;i++) {
6      y=y*sin(x[i]);
7    }
8  }
```

Listing 1: dcc input code.

Using the command line `dcc f.c -t`, we instruct the compiler to use the tangent-linear (`-t`) mode in order to generate the function `t1_f` (**t**angent-linear, **1**st-order version of `f`) presented in Listing 2. The original function arguments `x` and `y` are augmented with their associated tangent-linear variables `t1_x` and `t1_y`. Inside a driver program this code has to be rerun n times letting the input vector `t1_x` range over the Cartesian basis vectors in $\mathbb{R}^n$ to accumulate the entire gradient. Listing 3 shows how to use the generated code of Listing 2 in a driver program. Lines 2 and 5 let input variable `t1_x` range over the Cartesian basis vectors. By setting `t1_x[i]` to 1 the function `t1_f` (line 3) computes the partial derivative of `y` with respect to `x[i]`.

The command line `dcc f.c -a` tells `dcc` to apply the adjoint mode (`-a`) to `f.c`. The result is the function `a1_f` (**a**djoint, **1**st-order version of `f`) shown in Listing 4. As in the tangent-linear case each function argument is augmented by an associated adjoint component, here `a1_x` and `a1_y`. As mentioned above we need a stack in the adjoint code for storing data during the forward section. The *augmented forward section* uses stacks to store values that are being overwritten and to store the control flow. The actual implementation of the stack is not under consideration here; therefore we replaced the calls to the stacks with macro definitions for better readability. By default, `dcc` generates

code that uses static arrays, which ensures high runtime performance. There are three different stacks used in the adjoint code. The stack called CS is for storing the control flow, FDS takes floating point values and IDS keeps integer values. The unique identifier of the two basic blocks [9] in the forward section are stored in lines 6 and 9. For example, after evaluating the augmented forward section of Listing 4, the stack CS contains the following sequence

$$0, \underbrace{1, \ldots, 1}_{\text{n times}} \tag{11}$$

In line 10, variable y is stored onto the stack because it is overwritten in each iteration although needed in line 21. Hence, we restore the value of y in line 20. For the same reason we store and restore the value of i in line 11 and 19. The reverse section consist of a loop that processes the control flow stack CS. The basic block identifiers are restored from the stack and depending on the value, the corresponding adjoint basic block is executed. For example, the sequence given in (11) as content in the CS stack leads to a n-times evaluation of the adjoint basic block one and afterward one evaluation of the adjoint basic block zero. The basic block one in line 9 to 11 has the corresponding adjoint basic block in line 19 to 22. In contrast to (7), in line 22 the adjoint a1_y is not incremented but assigned. This is due to the fact that y is on both hand sides of the original assignment in line 10. This brings an aliasing effect into play. This effect can be avoided with help of intermediate variables; making this code difficult to read. For that reason we show the adjoint assignment without intermediate variables. dcc generates adjoint assignments with intermediate variables and incrementation of the left-hand side as shown in (7). The dcc-generated code and the one shown here are semantically equivalent. To accumulate the gradient using the function a1_f, we again have to write a driver, presented in Listing 5. It is sufficient to initialize the adjoint variable a1_y and call the adjoint function a1_f only once to get the whole gradient (line 2), illustrating the reduced runtime complexity of the adjoint mode.

```
1  a1_y=1;
2  a1_f(n, x, a1_x, y, a1_y);
3  for(int j=0; j<n;j++)
4     gradient[j]=a1_x[j];
```

Listing 5: Driver for a1_f

IV. Higher Order Differentiation

Numerical optimization algorithms often involve higher-order derivative models. Thus, the need for Hessians is imminent. With this in mind, dcc was designed to generate higher-order derivative codes effortlessly using its *reapplication feature*. dcc is able to generate jth-order derivative code by reading $(j-1)$th-order derivative code as the input. In this section we will focus on second-order models.

```
1  void a1_f(int n, double* x, double* a1_x,
2                   double& y, double& a1_y)
3  {
4    int i=0;
5    // augmented forward section
6    CS_PUSH(0);
7    y=0;
8    for ( i=0; i<n; i++) {
9           CS_PUSH(1);
10          FDS_PUSH(y); y=y*sin(x[i]);
11          IDS_PUSH(i);
12   }
13   // reverse section
14   while (CS_NON_EMPTY) {
15          if (CS_TOP==0) {
16            a1_y=0;
17          }
18          if (CS_TOP==1) {
19            IDS_POP(i);
20            FDS_POP(y);
21            a1_x[i]+=y*cos(x[i])*a1_y;
22            a1_y=sin(x[i])*a1_y;
23          }
24          CS_POP;
25   }
26 }
```

Listing 4: Adjoint dcc output

The tangent-linear mode reapplied to the first-order tangent-linear code (6) with $m = 1$ for scalar functions yields the second-order tangent-linear code

$$\dot{F}\big(\overset{\downarrow}{\mathbf{x}}, \overset{\downarrow}{\dot{\mathbf{x}}}, y, \dot{y}\big) \xrightarrow{\texttt{dcc}} \tilde{\dot{F}}\big(\overset{\downarrow}{\mathbf{x}}, \overset{\downarrow}{\tilde{\mathbf{x}}}, \overset{\downarrow}{\dot{\mathbf{x}}}, \overset{\downarrow}{\dot{\tilde{\mathbf{x}}}}, y, \tilde{y}, \dot{y}, \dot{\tilde{y}}\big) \quad ,$$

where

$$\begin{aligned} \dot{\tilde{y}} &= \left(\nabla^2 F(\mathbf{x}) \cdot \dot{\mathbf{x}}\right)^{\intercal} \cdot \tilde{\mathbf{x}} + \nabla F(\mathbf{x}) \cdot \dot{\tilde{\mathbf{x}}} \quad , \\ \dot{y} &= \nabla F(\mathbf{x}) \cdot \dot{\mathbf{x}} \quad , \\ \tilde{y} &= \nabla F(\mathbf{x}) \cdot \tilde{\mathbf{x}} \quad \text{and} \\ y &= F(\mathbf{x}) \quad . \end{aligned} \tag{12}$$

Again, dcc generates exactly the implementation of the mathematical model. As we see in (12), the term $\nabla F(\mathbf{x}) \cdot \dot{\tilde{\mathbf{x}}}$ must be equal to 0 in order to accumulate the entries of the Hessian $\nabla^2 F$. As a consequence, $\dot{\tilde{\mathbf{x}}}$ must be set to 0 on input. The product $\left(\nabla^2 F(\mathbf{x}) \cdot \dot{\mathbf{x}}\right)^{\intercal} \cdot \tilde{\mathbf{x}}$ represents a projection of the Hessian, determined by the vectors $\dot{\mathbf{x}}$ and $\tilde{\mathbf{x}}$. In our case with $m = 1$ the Hessian $\nabla^2 F \in \mathbb{R}^{n \times n}$ has n^2 entries.

To compute the entry $\nabla F_{i,j}$ of the Hessian the vectors $\tilde{\mathbf{x}}$ and $\dot{\mathbf{x}}$ have to be set to the i-th and j-th Cartesian basis vectors, respectively. In order to accumulate the whole Hessian this step has to be repeated for each entry, yielding a computational complexity of $\mathcal{O}\big(n^2\big) \cdot cost(F)$. Taking either adjoint or tangent-linear first-order input code, we reapply dcc by invoking dcc -t -d 2 t1_foo.cpp. This tells dcc to generate second-order (-d 2) tangent-linear (-t) derivative code while avoiding internal namespace clashes.

Looking at the possible combinations of the two differentiation models, there exist another three second-order

models. We may either apply the adjoint model to the tangent-linear code or apply the adjoint mode to the adjoint code. We will focus on the model where tangent-linear mode is applied to the adjoint code, called *tangent-linear over adjoint* mode.

This time the adjoint code (7) is taken as the input for the reapplication of the tangent-linear mode, obtaining

$$\bar{F}\big(\overset{\downarrow}{\mathbf{x}}, \underset{\downarrow}{\overset{\downarrow}{\bar{\mathbf{x}}}}, y, \underset{\downarrow}{\overset{\downarrow}{\bar{y}}}\big) \xrightarrow{\texttt{dcc}} \dot{\bar{F}}\big(\overset{\downarrow}{\mathbf{x}}, \underset{\downarrow}{\overset{\downarrow}{\dot{\mathbf{x}}}}, \underset{\downarrow}{\overset{\downarrow}{\bar{\mathbf{x}}}}, \underset{\downarrow}{\dot{\bar{\mathbf{x}}}}, y, \underset{\downarrow}{\dot{y}}, \underset{\downarrow}{\overset{\downarrow}{\bar{y}}}, \underset{\downarrow}{\dot{\bar{y}}}\big) \quad ,$$

where

$$\begin{aligned} \dot{y} &= \nabla F(\mathbf{x}) \cdot \dot{\mathbf{x}} \quad , \\ y &= F(\mathbf{x}) \quad , \\ \dot{\bar{\mathbf{x}}} &= \dot{\bar{\mathbf{x}}} + \dot{\mathbf{x}}^{\intercal} \cdot \nabla^2 F(\mathbf{x}) \cdot \bar{y} + \nabla F(\mathbf{x})^{\intercal} \cdot \dot{\bar{y}} \quad \text{and} \\ \bar{\mathbf{x}} &= \bar{\mathbf{x}} + \nabla F(\mathbf{x})^{\intercal} \cdot \bar{y} \quad . \end{aligned} \tag{13}$$

The generated implementation computes the term $\dot{\mathbf{x}}^{\intercal} \cdot \nabla^2 F(\mathbf{x}) \cdot \bar{y}$. This time we do not end up with one single entry, but we are able to harvest one complete row $\nabla^2 F_i$ of the Hessian in $\dot{\bar{\mathbf{x}}}$. To achieve this, the term $\nabla F(\mathbf{x})^{\intercal} \cdot \dot{\bar{y}}$ and thus $\dot{\bar{y}}$ must be set to 0 on input. The scalar $\bar{y}$ must be set to 1. Finally to compute a row of the Hessian $\nabla^2 F_i$, $\dot{x}$ must be set to the i-th Cartesian basis vector. As such, we have to rerun this model n times in order to accumulate the whole Hessian, yielding only a linear increase in runtime complexity of $\mathcal{O}(n) \cdot cost(F)$.

The desired `dcc` command is `dcc -a -d 2 t1_foo.cpp` resulting in the file `a2_t1_foo.cpp`. The option `-a` instructs `dcc` to generate adjoint code.

V. Reversal Strategies - Checkpointing

One inherent disadvantage of the adjoint AD model over the tangent-linear model is its high memory consumption. In the reverse section of an adjoint code, each adjoint computation of a non-linear operation is dependent on a value computed during the forward run. As we have seen in Section III this value is stored on a data stack if it happens to be overwritten. In real world programs this process is not the exception but the rule. Memory locations are rewritten and reused as often as possible so that the program is as memory efficient as possible. For the adjoint AD model this results in one consumed memory location for nearly every statement. For example, updating a thousand times a variable of type double precision (e.g., $x = x + y^2$) results at least in an additional memory usage of eight thousand bytes. For each execution of this statement we have one value pushed on the stack by $FDS\_PUSH(x)$.

There are several strategies to address this issue. We will present checkpointing, the core method of every AD tool to reduce memory consumption. In particular we will focus on how `dcc` deals with checkpointing and how the memory footprint may be influenced by the user.

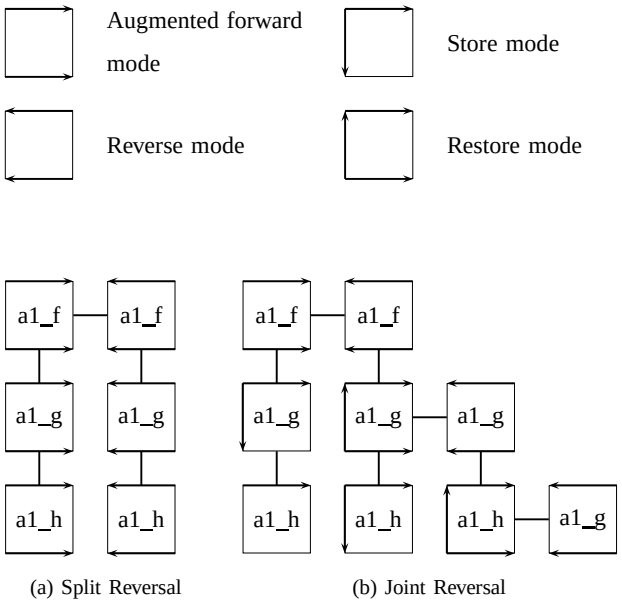


Figure 1: Reversal models

First we look at the reversal strategy of `dcc`. In general the adjoint model consists of a forward section and a reverse section. What happens in the case of interprocedural code where a function calls an arbitrary number of functions. There are two distinct ways of adjoining interprocedural code, namely *split reversal* and *joint reversal*.

Split reversal, presented in Figure 1a is the straightforward way of adjoining code. It strictly sticks to the adjoint model. The original code is executed in an augmented forward run. The augmentation essentially amounts to the additional stack operations introduced in Section III. These stacks are global data structures in `dcc`.

The augmented forward section is visualized by a square with two right arrows  . One arrow stands for the values that are pushed on the stack. The other arrow represents the original function evaluation. The augmented forward section of f calls the augmented forward section of g, which itself calls the augmented forward section of h. Each function pushes its computed values on the floating point data stack (FDS).

After the augmented forward section of f the reverse section of f starts, marked by a square with two left arrows  . This corresponds to the reverse adjoint computation with the needed function values being popped from the stack. Through the reverse section of f the reverse sections of g and h are eventually called.

In the end, there are two ways of calling a function in split reversal: in augmented forward mode and reverse mode. Memory consumption of split reversal is always directly related to the sum of pushes in the forward section.

Joint reversal, as shown in Figure 1b exploits the interprocedural structure of the program by introducing checkpoint-

ing at each function call. Each function needs to be able to store and restore its arguments.

We first start by calling f in augmented forward mode $\vec{\square}$. If a function runs in augmented forward mode it will make subcalls in *store mode* $\downarrow\square$. Store mode results in g storing its arguments (down arrow) and running the original code of g (right arrow), which itself calls the original code of h (right arrow).

The reverse mode of f calls g in restore mode $\overleftarrow{\square}$. g restores its arguments and runs in augmented forward mode leading to h called in store mode. In joint reversal the forward section is immediately followed by the reverse section. So g starts its reverse section resulting in h called in restore mode. h restores its arguments and starts its forward section followed by the reverse section. After h has returned, g finished its reverse section, which eventually leads to f finalizing its reverse section.

By joining the forward and reverse section, the values that are pushed on the stack in the forward section are being popped from the stack in the following reverse section. This has two benefits. For one, memory access is structurally more local leading to a more efficient exploitation of cache memory. Additionally, memory consumption is significantly reduced since interprocedural code consumes far less memory than the sum of all the push operations. In split reversal we had two ways of calling a function whereas in joint reversal we have three; store, restore+augmented forward and reverse mode. We now compare the two reversal schemes along the call graph presented in Figure 1.

For the sake of simplicity, we assume that the original function evaluation, the forward section and the reverse section of f,g and h have each a computational cost of 1. Additionally, we assume that all the pushes of a function's forward section have a memory consumption of 1. Finally, we assume that storing the arguments of a function has no additionally memory footprint. Taking all of this into account we now compare the two reversal schemes on the call graph presented in Figure 1.

Split reversal runs all three functions in their forward and reverse section. So we end up with a computational cost of six. All the forward sections are called after each other, therefore the memory consumption is three.

In joint reversal after f has finished its forward section we have a memory consumption of 1. Only the values of f have been pushed on the stack. We assume that g is called in the middle of f. So half of the values were popped from the stack at the moment when g is called in restore mode (memory=0.5). When g ends its forward section, memory consumption is at 1.5. Assuming that h is called in the middle of g we end up with a peak memory consumption of 2 after the forward section of h. The computational cost amounts to the number of squares in the picture, which is equal to 9.

In general, joint reversal is a trade off between memory consumption and computational cost. Memory consumption is reduced by a third from 3 to 2 whereas the computation cost has risen by fifty percent from 6 to 9. There has been more investigations into the mixing of these two strategies. [10] shows that the optimal reversal strategy is NP-complete. dcc uses joint reversal as its sole reversal scheme putting the emphasis on memory efficient code. In the next chapter we will demonstrate how we exploit this feature to achieve a more efficient memory footprint for our Burgers simulation.

VI. Burgers Implementation

As has been described in Section I we compute the velocity field according to (2). We use dynamic programming by introducing a data array u[i][j] storing the velocity for a grid point i in time step j. The function h implementing the computation of the velocity field has the following signature:

```
1  void h(int& nx, // number of grid points
2         int t0, // first time step to start
               with
3         int n, // number of time steps to
               compute
4         double& cost, // cost function
5         double** uob, // observations
6         double** ub, // basic states
7         double** u, // model solutions
8         double* ui, // initial conditions
9         double& dx, // space increment
10        double& dt, // time increment
11        double& r, // Reynolds number
12        double& dtdx,
13        double& c0,
14        double& c1
15 )
```

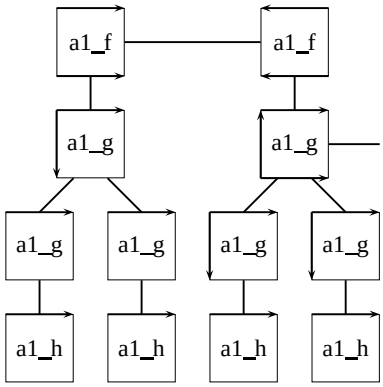
Listing 6: Function h

This function computes u[i][j] and updates cost for all grid points $x_i,\ 0 \leq i < nx$ and for all time steps $t_0 \leq j < n$. Supposing that for each time step we need do $c \cdot n_x$ pushes on the stack, we end up with approximately $c \cdot n_x \cdot n$ pushes for the entire simulation. This is also the memory consumption for calling the adjoint code a1_h.

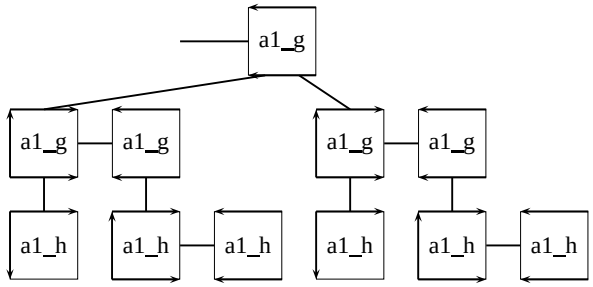
The code will now be restructured according to a recursive checkpointing scheme by relying on the interprocedural joint reversal mode present in dcc.

```
1  void h(...) {
2    ...
3    half=n-t0/2;
4    t1=t0+half; n0=t1; n1=n;
5    if(diff > 2) {
6        g(nx,t0,n0,cost,uob,ub,u,ui,dx,dt,r,
             dtdx,c0,c1);
7        g(nx,t1,n1,cost,uob,ub,u,ui,dx,dt,r,
             dtdx,c0,c1);
8    }
9    else
10       h(nx,t0,n,cost,uob,ub,u,ui,dx,dt,r,
             dtdx,c0,c1);
11 }
```

Listing 7: Function h



(a) Call graph of a1_f



(b) Call graph of a1_f (cont.)

Figure 2: Burgers recursive call tree joint reversal

g has the same signature as h. Its task is to decompose the interval of time steps, calling h on a subinterval of $[t_0, n]$.

The resulting call tree as well as its joint reversed counterpart is illustrated in Figure 2.

We assume that the h has a computational cost of 1 over the entire interval from t_0 to n. If we call h in over the entire interval we end up with a forward and a reverse section adding up to a computational cost of 2. In our new structure we assume that f and g have no computational cost and no memory consumption. In our example h has a cost of $\frac{1}{2}$ since it only runs over half the interval of t_0 to n. We call h 10 times. Thus the computational cost of this call tree is 5. Note that this is independent from the depth of our recursive call tree. The memory consumption though is halved at every increase of the recursive call three depth. Ultimately memory consumption can be reduced to the number of pushes in one single time step.

VII. Case Study

A. Differentiation of the original code

As discussed in Section I, we run a test case on an inverse problem based on Burgers' equation (1). As a start we take the code presented in [3] implementing the original function with the signature of

Table I: Time and memory requirements for gradient computation

n	250	500	1000	2000
f (s)	0.03	0.08	0.15	0.32
TLM (s)	33	109	457	1615
ADJ (s)	0.21	0.43	0.85	1.82
TLM-ADJ (s)	150	587	2286	8559
IDS size	7500502	15001002	30002002	60004002
FDS size	5000002	10000002	20000002	40000002
CS size	7500503	15001003	30002003	60004003

```
1 void f(int n, int nt, double& cost, double**
      u, double* ui...)
2 {
3 ...
4 }
```

Listing 8: Signature of Burgers' function

Taking n grid points of ui as the initial conditions we integrate over nt timesteps. The values are saved in the two dimensional array u for each grid point i and time step j.

To solve the inverse problem we need the derivatives of cost with respect to the initial conditions ui.

The results in Table I represent the runtime of one full gradient accumulation as well as the memory requirements in adjoint and tangent-linear mode. Additionally one Hessian accumulation is performed using the tangent-linear over adjoint model (13). Different problem sizes are simulated with varying n. We also mention the different stack size shown in Section III.

If we assume four bytes per integer and control stack element plus eight bytes for a floating data stack element we end up with a memory requirement of $\approx$ 610 MB for the Hessian accumulation. The tests were running on a GenuineIntel computer with Intel(R) Core(TM)2 Duo CPU and with 2000.000 MHz CPU.

The execution time of the tangent-linear gradient computation is growing proportionally to the problem size nx and the execution time of f:

$$FM : \frac{cost(F')}{cost(F)} \sim \mathcal{O}(n). \tag{14}$$

The single executon of *t1_f* takes approximately twice as long as the execution of *f*.

The execution time of the adjoint gradient computation is growing only proportional to the execution time of f:

$$AM : \frac{cost(F')}{cost(F)} \sim \mathcal{O}(1). \tag{15}$$

Finally we accumulate the Hessian using tangent-linear over adjoint mode. Here, the runtime is growing linearly with respect to n as well as f since the dimension of the dependent cost is equal to 1.

$$FM - AM : \frac{cost(F'')}{cost(F)} \sim \mathcal{O}(n). \tag{16}$$

Table II: Recursive checkpointing with $n = 100000$. Interval size of 100000 amounts to no recursion.

Interval size	FDS size	Runtime(s)
100000	29999610	69,3
10000	2062706	74,9
1000	433242	76,5
100	229410	79,1
10	202292	88,3

For scalar functions in particular, the runtime complexity for accumulating the Hessian using AD is the same as the runtime complexity of the gradient accumulation using finite difference. This enables developers to implement a second-order model where a first-order model has been used so far.

B. Differentiation using recursive checkpointing

Based on the recursive checkpointing scheme presented in Section V and its implementation in Section VI we conducted benchmarks varying the interval size threshold for `diff` where the recursion of `g` will stop by eventually calling `h`. The first order adjoint model was applied to compute a single gradient accumulation. The benchmarks were run on a cluster node consisting of a single thread on a Sun Enterprise T5120 cluster.

At an interval size of 100 we see major memory savings of around 98% whereas the runtime is only marginally increased by around 15% from 69,3s to 79,1s. This illustrates that checkpointing is crucial to reduce a computational problem in memory space while keeping the runtime complexity at a feasible level.

VIII. Conclusion & Future Work

We have presented a source transformation compiler for a restricted subset of C/C++. As such, `dcc` runs on any system with a valid C/C++ compiler making it a very portable tool. Its unique reapplication feature allows code to be transformed up to an arbitrary order of differentiation. While relying to the adjoint model for the higher-order differentiation, we save one order of magnitude of computational cost compared to a tangent-linear only or finite difference code. However, the adjoint model poses a high memory load, making an efficient checkpointing scheme crucial. Otherwise, a computation for large scale codes is even unfeasible. This is solved by resorting to interprocedural checkpointing, enabled by the joint reversal structure of the generated adjoint code. We illustrated the entire development process along a case study based on a one-dimensional implementation of the Burgers equation.

Not mentioned in this paper are several extensions not directly linked to the derivative code compiler presented here. As large simulation codes run on cluster systems, they mostly rely on parallelization techniques. The most widely used parallelization method is MPI. Hence, while applying the adjoint mode all the MPI calls need to be reversed too [11]. This feature has been integrated into `dcc` using an adjoint MPI library [12]. Additionally there are attempts to achieve the same goal with OpenMP [13]. For the sake of brevity we also did not mention the program analysis `dcc` performs like for example *activity* and *TBR* analyses [14].

The compiler is open-source software (Eclipse Public License) and available upon request. This paper should serve as first guideline on how to differentiate C code using this tool.

Finally, the development of `dcc` is largely application driven, especially with regard to its ability in parsing the entire C/C++ language.

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