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Niloofar Safiran and Uwe Naumann

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Toward Adjoint OpenFOAM

Niloofar Safiran and Uwe Naumann

LuFG Informatik 12 - STCE, RWTH Aachen University, Germany
{safiran, naumann}@stce.rwth-aachen.de

Abstract. OpenFOAM is a package which simplifies the implementation of physical models by mimicking the form of partial differential equations in software. Use of OpenFOAM is rapidly expanding in the research community and among industrial users, covering a wide range of continuum models. AD provides accurate derivative values and better runtime performance of the adjoint model compared with finite differences. This paper presents a transformation of the OpenFOAM code that can be used for calculating derivatives with adjoint mode of AD. An example based on ODE is considered here.

1 Introduction

The OpenFOAM (Open Field Operation and Manipulation) CFD Toolbox is a free, open source CFD software package produced by OpenCFD Ltd. It has a large user base across most areas of engineering and science, from both commercial and academic organisations. OpenFOAM has an extensive range of features to solve anything from complex fluid flows involving chemical reactions, turbulence and heat transfer, to solid dynamics and electromagnetics. It includes tools for meshing, a parallelised mesher for pre- and post-processing.

The aim of this paper is **Applying Algorithmic Differentiation (AD) in OpenFOAM** and as result **Adjoint OpenFOAM** , i.e., calculating the derivative with adjoint mode of algorithmic differentiation by operator overloading (DCO/C++).

Here it is shown how to relate DCO/C++ with OpenFOAM and use it to calculate the derivatives of one simple ODE with tangent-linear and adjoint mode AD in OpenFOAM. Calculating the derivatives accurately and efficiently (which AD does) plays a very important role in sensitivity analysis and optimization.

2 ODE in OpenFOAM

The main part of ODE solver in OpenFOAM can be found in:

$FOAM_SRC/ODE

For the initial value ODE problem, there are three different kinds of methods in OpenFOAM:

RK: Runge-Kutta
KRR4: Kaps-Rentrop

SIBS: Semi-Implicit Bulirsh-Stoer

which can be found in $FOAM_SRC/ODE/ODESolvers/:

RK/ , KRR4/ , SIBS/ respectively.

In this description, I consider only the KRR4 method. For the system

$$y' = f(y) \tag{1}$$

implicit differencing gives

$$y_{n+1} = y_n + hf(y_{n+1}) \tag{2}$$

In general this is some nasty set of nonlinear equations that has to be solved iteratively at each step. If we try linearizing the equations as in Newton's method we will have

$$y_{n+1} = y_n + h\left[f(y_n) + \left.\frac{\partial f}{\partial y}\right|_{y_n} .(y_{n+1} - y_n)\right] \tag{3}$$

Here $\partial f/\partial y$ is the matrix of the partial derivatives of the right hand side (the Jacobian matrix). Rearrange equation (3) into the form

$$y_{n+1} = y_n + h\left[1 - h\frac{\partial f}{\partial y}\right]^{-1} .f(y_n) \tag{4}$$

If h is not too big, only one iteration of Newton's method may be accurate enough to solve equation (2) using equation (4). In other words at each step we have to invert the matrix

$$1 - h\frac{\partial f}{\partial y} \tag{5}$$

to find y_{n+1}.

A Rosenbrock (Kaps-Rentrop) method seeks the solution of the form

$$y(x_0 + h) = y_0 + \sum_{i=1}^{s} c_i k_i \tag{6}$$

where the corrections k_i are found by solving s linear equations that generalize the structure in (4):

$$(1-\gamma h f').k_i = hf\left(y_0 + \sum_{j=1}^{i-1} \alpha_{ij} k_j\right) + hf'.\sum_{j=1}^{i-1} \gamma_{ij} k_j, \quad i = 1, ..., s \tag{7}$$

Here we denote the Jacobian matrix by f'. The coefficients γ, c_i, α_{ij} and γ_{ij} are fixed constants independent of the problem. If $\gamma = \gamma_{ij} = 0$, this is simply a Runge-Kutta scheme. Equation (7) can be solved successively for $k_1, k_2, ...$.

Crucial to the success of a stiff integration scheme is an automatic stepsize adjustment which here will be done in "ODESolver.C".

To minimize the matrix-vector multiplications on the right hand side of the (7), we rewrite the equation in terms of quantities

$$g_i = \sum_{j=1}^{i-1} \gamma_{ij} k_j + \gamma k_i \tag{8}$$

The equation then takes the form

$$\begin{aligned}
(1/\gamma h - f').g_1 &= f(y_0) \\
(1/\gamma h - f').g_2 &= f(y_0 + a_{21} g_1) + c_{21} g_1/h \\
(1/\gamma h - f').g_3 &= f(y_0 + a_{31} g_1 + a_{32} g_2) + (c_{31} g_1 + c_{32} g_2)/h \\
(1/\gamma h - f').g_4 &= f(y_0 + a_{41} g_1 + a_{42} g_2 + a_{43} g_3) + (c_{41} g_1 + c_{42} g_2 + c_{43} g_3)/h
\end{aligned} \tag{9}$$

In the implementation of Kaps-Rentrop algorithm, OpenFOAM provides a routine in the ODE class (in file "ODE.H") called *derivatives* that returns f (called $dydx$) as a function of x and y. It also supplies a routine *jacobian* that returns f' (called $dfdy$) and $\partial f/\partial x$ (called $dfdx$) as a function of x and y .

3 Simple ODE

Given initial value ODE:

$y' = \cos(\alpha x), y(0) = 0$

We want to solve our own ODE with OpenFOAM, we will write it in
$FOAM_APP/ test/ ODETest.

At the begining of the code we firstly define the dimension of our ODE:

```
label nEqns() const
{
```

```
  return 1;

}
```

Because in our case the order of the ordinary differential equation is '1'. Then change our ODE to the first order ODE.

$y' = dydx[0] = \cos(\alpha x)$

```
    void derivatives
    (
        const scalar x,
        const scalarField& y,
        scalarField& dydx
    ) const
    {
    scalar alpha = 1.0;
        dydx[0] = cos(alpha*x);

    }
```

Then we calculate the Jacobian for both x and y:

Suppose $f = \cos(\alpha x)$

The Jacobian for x in our case : $\frac{\partial f}{\partial x} = -\alpha \sin(\alpha x)$

The Jacobian for y in our case : $\frac{\partial f}{\partial y} = 0$

```
    void jacobian
    (
        const scalar x,
        const scalarField& y,
        scalarField& dfdx,
        scalarSquareMatrix& dfdy
    ) const
    {
    scalar alpha = 1.0;
        dfdx[0] = (-1)*alpha*sin(alpha*x);

        dfdy[0][0] = 0.0;

    }
```

Finally we define the method of solver and add the initial values in our case and solve our ODE in the main function:

```
int main(int argc, char *argv[])
{
    word ODESolverName("KRR4");

    testODE ode;
    autoPtr<ODESolver> odeSolver =
                    ODESolver::New(ODESolverName, ode);

    scalar xStart = 0.0;          \\ starting time
    scalarField yStart(ode.nEqns());
    yStart[0] = 0.0;              \\ y(0) = 0

    scalarField dyStart(ode.nEqns());
    ode.derivatives(xStart, yStart, dyStart);

    scalar x = xStart;
    scalar xEnd = x + 1.0;        \\ end time
    scalarField y = yStart;

    scalar hEst = 0.001;          \\ the time step

    odeSolver->solve(ode, x, xEnd, y, 1e-4, hEst);

    Info <<  nl << "y = " << y << endl;
    Info << "\nEnd\n" << endl;

    return 0;
}
```

Then we need to compile the file so that we can run it in OpenFOAM using the linux command *"wmake"*. We get:

```
Selecting ODE solver KRR4

y = 0.841471

End
```

If we solve our ODE analytically we can see that:

$$y' = \cos(\alpha x) \Rightarrow \int y' = \int \cos(\alpha x)$$

$\Rightarrow y = \int \cos(\alpha x) = \frac{1}{\alpha} \sin(\alpha x)$

for $\alpha = 1.0$ and $x : 0 \rightarrow 1$:

$y = \sin(1) - \sin(0) = 0.841470985$

which is the same as the result we obtained above.

4 Algorithmic Differentiation

Algorithmic Differentiation (AD), sometimes alternatively called automatic differentiation, is a method for computing derivatives of output of numerical programs with respect to its inputs both accurately (with machine precision) and efficiently. The two basic modes of AD – forward and reverse – and combinations thereof yield products of a vector with Jacobian, its transposed, or Hessian respectively.

Numerical simulation programs map potentially very large number of input parameters (let there be n) onto often much fewer outputs (say m of them, also refer to as objectives). The classical numerical approach to quantifying the sensitivities of those objectives with respect to the parameters through Finite Difference quotients increase the computational complexity by a factor of $O(n)$. The number of parameters may reach values of the order of $n = 10^9$. Hence forward sensitivity analysis would require n runs of the simulation, which is simply not feasible. Reverse (or Adjoint) methods and corresponding program transformation techniques have been developed to replace the dependence on n with that on the number of objectives m. Often the number of objectives is equal to 1. In this case adjoint programs deliver the sensitivities of the objective with respect to all input parameters with an increase in the computational complexity of $O(1)$.

Methods of implementation of AD:

- Overloading $\rightarrow$ STCE tool : dco
- Source transforming $\rightarrow$ STCE tool : dcc

In this paper I will only consider dco.

5 Derivative Code by Overloading

Derivative Code by Overloading (DCO/C++) is a developement of the institute *Software and Tools for Computational Engineering* (LuFG Infomatik 12, RWTH Aachen) implementing AD. The range of capabilities covered by DCO/C++ is deriven by different application research subjects. This paper discusses the application of DCO/C++ in OpenFOAM.

The objective is to provide an efficient and robust tool for the computation of the projection of derivatives of arbitrary order of the a function given as an implementation in C/C++. Additionally the capability of coupling the robust overloading technique with optimized computer generated or hand-written external computations of adjoint projection is provided.

The main idea of DCO/C++ is to use the so-called *active variable* concept. DCO/C++ provides data types for tangent-linear and adjoint projection. Thereby adjoint projections require an additional data structure for saving data during the forward sweep. This is covered by a *tape*. The tape can be thought of as directed acyclic graph holding all necessary information for reverse sweep.

All data types and tapes are C++-objects inside the namespace *dco*. Additionally every data type has its own namespace:

namespace	**classes**	**description**
dco::t1s	type	tangent-linear 1st-order floating point type
dco::a1s	type static_tape	adjoint 1st-order floating point type data structure for propagating adjoints
dco::t2s_a1s	type static_tape	tangent-linear over adjoint 2nd-order floating point type data structure for propagating 2nd-order adjoints

Every data type holds not only a floating point value but also the derivative information, e.g. the tangent-linear type for a variable $\boldsymbol{x}$ must hold the value and also $\boldsymbol{x}^{(1)}$, the adjoint type for a variable $\boldsymbol{x}$ must hold the value and also $\boldsymbol{x}_{(1)}$, etc.. To access those additional components there are *set* and *get* routines. Those functions are globally defined in the appropriate namespace.

In DCO/C++ the mathematical operators like $+, -, *, /$ and standard features such as *sin, cos, pow,* etc. with their own operators or functions are overwritten. These are desiged so that for each calculation with an *active variable* the derivative will also be computed.

6 Applying DCO/C++ in OpenFOAM

The purpose of this section is to compute the derivative of our ODE (see section 3) with respect to α in OpenFOAM with DCO/C++, i.e.,

$$\underbrace{\frac{\partial}{\partial\alpha}\underbrace{\{y' = \cos(\alpha x)\}}_{ODESolver:KRR4}}_{DCO/C++}$$

The very first task is to change the data types of the *active variables* into $dco :: t1s :: type$ (or $dco :: a1s :: type$) for $tangent - linear$ (or $adjoint$). Here the *active variables* are:

α : which is independent and has *scalar* type,
y : which is dependent and has $scalarField$ type.

In OpenFOAM nearly all of the data types are based on *scalar* type which is defined on two basic types *double* and $float$, in which *double* type is preput.

First of all the definition of the basic type *double* in OpenFOAM must be found. This definition is in "*doubleScalar.H*" in $\$FOAM\_SRC/OpenFOAM/primitives/Scalar/doubleScalar$ which has the form:

typedef double doubleScalar;

A list of changes that should be done to OpenFOAM are:

1) Add *"dco.hpp"* and the related files to *$FOAM_SRC/OpenFOAM/lnInclude*.

2) In *$FOAM_SRC/OpenFOAM/primitives/Scalar/doubleScalar.H* :

- Include the header file *"dco.hpp"* , i.e., *#include"dco.hpp"*.
- Change the *" typedef double doubleScalar "* to *" typedef dco::t1s::type doubleScalar "*.
- Delete the inline functions for *hypot, atan2, etc* , because all of them are defined in *"dco.hpp"* for dco type.
- Add a function to return the double value of the dco type, later we will see the usage of this function.

```
inline double value (Scalar s)
{
    return dco::t1s::value(s);
}
```

  which the *dco::t1s::value* function is defined in *tlm_type.hpp* and returns the value of the dco type.

3) In *$FOAM_SRC/OpenFOAM/primitives/Scalar/doubleFloat.H* :

- Include the header file *"dco.hpp"* , i.e., *#include"dco.hpp"*.
- Change all *double* types to *dco::t1s::type*.

4) In *$FOAM_SRC/OpenFOAM/primitives/Scalar/Scalar.H* :

- Delete all standard C++ transcendental functions because they are defined in the dco file for dco type.

5) In *$FOAM_SRC/OpenFOAM/db/IOstreams/IOstreams/IOstreams.H* the cast to *integer* is needed. So we use the function *"value"* to change *dco::t1s::type* to *double* and then cast it to *int* :

- Code:
  return int (10*num + SMALL);
  Solution:
  return int (10* value(num) + value(SMALL));
- Code:
  return int (versionNumber_);
  Solution:
  return int (value(versionNumber_));

- Code:
  return int (10.0 * (versionNumber_ - majorVersion());
  Solution:
  return int (10.0 * (value(versionNumber_) - majorVersion());

6) Eliminating

- UNARY_FUNCTIONS ,
- BINARY_TYPE_OPERATOR and
- BesselFunction

from all files containing them e.g. from
$\$FOAM\_SRC/OpenFOAM/fields/Fields/scalarField/scalarField.H$,
because all of the unary functions and binary operators are defined in dco files for dco type.

Furthermore, delete the "::" at the begining of the functions like abs(), sqrt(), etc, for example:
Code: return ::abs(s);
Solution: return abs(s);

7) In $\$FOAM\_SRC/OpenFOAM/db/IOstream/token/token.H$ one union is used. DCO/C++ does not support any unoin. Deleting the union will not cause error in the program.

8) In $\$FOAM\_SRC/OpenFOAM/db/IOstream/token/tokenI.H$ delete all functions and variables related to union.

9) In some cases a cast to dco type is needed. For example in
$\$FOAM\_SRC/lagrangian/basic/Particle/ParticleI.H$:

Code :

$scalar\ l1 = -0.5 * (ap - :: sqrt(cp));$
$scalar\ l2 = -0.5 * (ap + :: sqrt(cp));$

Solution:

$scalar\ l1 = scalar(-0.5) * (ap - sqrt(cp));$
$scalar\ l2 = scalar(-0.5) * (ap + sqrt(cp));$

10) For simplicity, we comment all of the ODESolvers in $\$FOAM\_SRC/ODE/Make/files$ out except for the Runge-Kutta and KRR4 .

11) The goal is to compute $\frac{\partial y}{\partial \alpha}$, so the changes of α should be observed. Therefore, add α to the signature of the *"solve"* function.

As it is shown in section 3, the dependency of α and y is written in functions *derivatives* and *jacobian*, changing also the signature of those functions we will have:

```
    void derivatives
    (
        const scalar x,
        const scalarField& y,
        scalarField& dydx,
        scalar& alpha
    ) const
    {

        dydx[0] = cos(alpha*x);
    }
```

```
    void jacobian
    (
        const scalar x,
        const scalarField& y,
        scalarField& dfdx,
        scalarSquareMatrix& dfdy,
        scalar& alpha
    ) const
    {
        dfdx[0] = (-1)*alpha*sin(alpha*x);

        dfdy[0][0] = 0.0;

    }
};
```

In the jacobian function $\partial f/\partial x$ and also $\partial f/\partial y$ are calculated. Another alternative is to use DCO/C++ locally to compute them. This is especially efficient for more comlex equation(s) which the derivatives are not easy to calculate.

The process of applying the adjoint mode of the DCO/C++ is the same as the tangent-linear mode, the only difference is that instead of *"dco::t1s::type"* use *"dco::a1s::type"*.

For tangent-linear mode the definitions of the *set* and *get* routines in the main function are:

```
int main(int argc, char *argv[])
{
    word ODESolverName("KRR4");

    testODE ode;
    autoPtr<ODESolver> odeSolver = ODESolver::New(ODESolverName, ode);

    scalar xStart = 0.0;
```

```
    scalar alpha = 1.0;
    scalarField yStart(ode.nEqns());
    yStart[0] = 0.0;

    scalarField dyStart(ode.nEqns());
    ode.derivatives(xStart, yStart, dyStart, alpha);

    scalar x = xStart;
    scalar xEnd = x + 1.0;
    scalarField y = yStart;

    scalar hEst = 0.001;

    double derivative = 0;

    dco::t1s::set(alpha, 1.0, 1);

    odeSolver->solve(ode, x, xEnd, y, 1e-4, hEst, alpha);

    dco::t1s::get(y[0], derivative, 1);

    std::cout << nl << "y = " << y[0].v << std::endl;
    std::cout << nl << "Derivative:  y = " << derivative << std::endl;

    Info << "\nEnd\n" << endl;

    return 0;
}
```

For adjoint mode the definitions of the *set* and *get* routines in the main function are:

```
int main(int argc, char *argv[])
{
    word ODESolverName("KRR4");

    testODE ode;
    autoPtr<ODESolver> odeSolver = ODESolver::New(ODESolverName, ode);

    scalar xStart = 0.0;
    scalar alpha = 1.0;
    scalarField yStart(ode.nEqns());
    yStart[0] = 0.0;

    dco::a1s::static_tape tape(1e05);
    tape.register_variable(alpha);
```

```
    scalarField dyStart(ode.nEqns());
    ode.derivatives(xStart, yStart, dyStart, alpha);

    scalar x = xStart;
    scalar xEnd = x + 1.0;
    scalarField y = yStart;

    scalar hEst = 0.001;

    double derivative = 0;

    odeSolver->solve(ode, x, xEnd, y, 1e-4, hEst, alpha);

    dco::a1s::set(y[0], 1.0, -1);
    tape.interpret_reverse();

    dco::a1s::get(alpha, derivative, -1);


    std::cout << nl << "y = " << y[0].v << std::endl;
    std::cout << nl << "Derivative:  y = " << derivative << std::endl;

    Info << "\nEnd\n" << endl;

    return 0;
}
```

12) Running the ODE Library *"wmake libso ODE"* in $FOAM_SRC.

13) Running our ODETest with *"wmake"*. We get:

```
Selecting ODE solver KRR4

y = 0.841471

Derivative:  y = -0.301169

End
```

In Section 3 the analytical solution of our ODE is shown:

$$y' = cos(\alpha x) \rightarrow y = \frac{1}{\alpha}\sin(\alpha x)$$

The derivative with respect to α will be:

$\frac{\partial y}{\partial \alpha} = \frac{\partial}{\partial \alpha}\{\frac{1}{\alpha}\sin(\alpha x)\} = -\frac{1}{\alpha^2}\sin(\alpha x) + \frac{x}{\alpha}\cos(\alpha x)$

for $\alpha = 1.0$ and $x : 0 \rightarrow 1$:

$\{-\sin(1) + \cos(1)\} - \{-\sin(0) + 0\} = -0.301168679$

which is the same as the result we obtained above.

7 Future Work

The aim of this paper was computing $\frac{\partial y}{\partial \alpha}$ where y is given as solution of ODE to be solved by one of the methods of OpenFOAM ' s ODESolver.

An interesting area of future work is expanding the application of DCO/C++ in all examples and *"solve"* functions of OpenFOAM. KRR4 solver requires Jacobian matrix and also $\partial f/\partial x$ that both can be computed by DCO/C++ locally instead of calculating it manually, because sometimes the functions are so complicated that manual calculation will not be easy. Another opportunity to make the computations more efficiet is that only the data types of active variables are dco types not all of the variables. In this paper actually we define the *"scalar"* to be the dco type, although we just needed the dco type for y and α. For this purpose the appropriate unary function and binary operators should also be defined in OpenFOAM. It means that it should differentiate between e.g. $\cos(scalar\ a)$ and $\cos(active\_type\ a)$.

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