CoDiPack 2.0: Lessons learned and new ideas

M. Sagebaum, J. Blühdorn

AG Scientific Computing
TU Kaiserslautern

23rd European Workshop on Automatic Differentiation
Overview

- History
- Lessons learned
- New ideas
- Programming performance mistakes
- Current performance values
History of CoDiPack

- **19.06.2015**: Initial release v1.0
  - Jacobian taping approach with linear index management
  - External function support

- **23.12.2015**: Release v1.1
  - Jacobian taping approach with reuse index management
  - Preaccumulation support
  - Template files for binary and unary operators

- **07.04.2016**: Release v1.2
  - ReferenceActiveReal
  - Reuse index management with assign optimization
  - Full vector support
  - Module based implementation of tapes

- **14.09.2016**: Release v1.3
  - Primal value taping approach

- **16.02.2017**: Release v1.4
  - Higher order derivative helper
  - Read/write tapes from files
  - Management of multiple tapes

- **18.12.2017**: Release v1.5
  - Custom adjoint vector support
  - TapeVectorHelper
  - ExternalFunctionHelper
  - PreaccumulationHelper
  - StatementPushHelper

- **15.03.2018**: Release v1.6
  - Forward evaluation of tapes (basic support)
  - Generalized function for stack evaluation

- **30.10.2018**: Release v1.7
  - Forward evaluation of tapes (full support)
  - Primal evaluation of tapes

- **07.01.2019**: Release v1.8
  - Automatic Jacobian combination for statements
  - Dropped tape modules approach, switched to inheritance of structures

- **10.10.2019**: Release v1.9
  - EvaluationHelper
  - TapeHelper
  - Expression logic definition rework
History of CoDiPack

- **19.06.2015: Initial release v1.0**
  - Jacobian taping approach with linear index management
  - External function support
- **23.12.2015: Release v1.1**
  - Jacobian taping approach with reuse index management
  - Preaccumulation support
  - Template files for binary and unary operators
- **07.04.2016: Release v1.2**
  - ReferenceActiveReal
  - Reuse index management with assign optimization
  - Full vector support
  - Module based implementation of tapes
- **14.09.2016: Release v1.3**
  - Primal value taping approach
- **16.02.2017: Release v1.4**
  - Higher order derivative helper
  - Read/write tapes from files
  - Management of multiple tapes
- **18.12.2017: Release v1.5**
  - Custom adjoint vector support
  - TapeVectorHelper
  - ExternalFunctionHelper
  - PreaccumulationHelper
  - StatementPushHelper
- **15.03.2018: Release v1.6**
  - Forward evaluation of tapes (basic support)
  - Generalized function for stack evaluation
- **30.10.2018: Release v1.7**
  - Forward evaluation of tapes (full support)
  - Primal evaluation of tapes
- **07.01.2019: Release v1.8**
  - Automatic Jacobian combination for statements
  - Dropped tape modules approach, switched to inheritance of structures
- **10.10.2019: Release v1.9**
  - EvaluationHelper
  - TapeHelper
  - Expression logic definition rework
History of CoDiPack

- **19.06.2015**: Initial release v1.0
  - Jacobian taping approach with linear index management
  - External function support
- **23.12.2015**: Release v1.1
  - Jacobian taping approach with reuse index management
  - Preaccumulation support
  - Template files for binary and unary operators
- **07.04.2016**: Release v1.2
  - ReferenceActiveReal
  - Reuse index management with assign optimization
  - Full vector support
  - Module based implementation of tapes
- **14.09.2016**: Release v1.3
  - Primal value taping approach
- **16.02.2017**: Release v1.4
  - Higher order derivative helper
  - Read/write tapes from files
  - Management of multiple tapes
- **18.12.2017**: Release v1.5
  - Custom adjoint vector support
  - TapeVectorHelper
  - ExternalFunctionHelper
  - PreaccumulationHelper
  - StatementPushHelper
- **15.03.2018**: Release v1.6
  - Forward evaluation of tapes (basic support)
  - Generalized function for stack evaluation
- **30.10.2018**: Release v1.7
  - Forward evaluation of tapes (full support)
  - Primal evaluation of tapes
- **07.01.2019**: Release v1.8
  - Automatic Jacobian combination for statements
  - Dropped tape modules approach, switched to inheritance of structures
- **10.10.2019**: Release v1.9
  - EvaluationHelper
  - TapeHelper
  - Expression logic definition rework
History of CoDiPack

- **19.06.2015**: Initial release v1.0
  - Jacobian taping approach with linear index management
  - External function support

- **23.12.2015**: Release v1.1
  - Jacobian taping approach with reuse index management
  - Preaccumulation support
  - Template files for binary and unary operators

- **07.04.2016**: Release v1.2
  - ReferenceActiveReal
  - Reuse index management with assign optimization
  - Full vector support
  - Module based implementation of tapes

- **14.09.2016**: Release v1.3
  - Primal value taping approach

- **16.02.2017**: Release v1.4
  - Higher order derivative helper
  - Read/write tapes from files
  - Management of multiple tapes

- **18.12.2017**: Release v1.5
  - Custom adjoint vector support
  - TapeVectorHelper
  - ExternalFunctionHelper
  - PreaccumulationHelper
  - StatementPushHelper

- **15.03.2018**: Release v1.6
  - Forward evaluation of tapes (basic support)
  - Generalized function for stack evaluation

- **30.10.2018**: Release v1.7
  - Forward evaluation of tapes (full support)
  - Primal evaluation of tapes

- **07.01.2019**: Release v1.8
  - Automatic Jacobian combination for statements
  - Dropped tape modules approach, switched to inheritance of structures

- **10.10.2019**: Release v1.9
  - EvaluationHelper
  - TapeHelper
  - Expression logic definition rework
History of CoDiPack

- **19.06.2015**: Initial release v1.0
  - Jacobian taping approach with linear index management
  - External function support
- **23.12.2015**: Release v1.1
  - Jacobian taping approach with reuse index management
  - Preaccumulation support
  - Template files for binary and unary operators
- **07.04.2016**: Release v1.2
  - ReferenceActiveReal
  - Reuse index management with assign optimization
  - Full vector support
  - Module based implementation of tapes
- **14.09.2016**: Release v1.3
  - Primal value taping approach
- **16.02.2017**: Release v1.4
  - Higher order derivative helper
  - Read/write tapes from files
  - Management of multiple tapes
- **18.12.2017**: Release v1.5
  - Custom adjoint vector support
  - TapeVectorHelper
  - ExternalFunctionHelper
  - PreaccumulationHelper
  - StatementPushHelper
- **15.03.2018**: Release v1.6
  - Forward evaluation of tapes (basic support)
  - Generalized function for stack evaluation
- **30.10.2018**: Release v1.7
  - Forward evaluation of tapes (full support)
  - Primal evaluation of tapes
- **07.01.2019**: Release v1.8
  - Automatic Jacobian combination for statements
  - Dropped tape modules approach, switched to inheritance of structures
- **10.10.2019**: Release v1.9
  - EvaluationHelper
  - TapeHelper
  - Expression logic definition rework
CoDiPack tape layout

- TapeBaseModule
- ExternalFunctionModule
- StatementModule
- JacobiModule
- IoModule
- JacobiTape
- TapInterface
- JacobiIndexTape
- LinearIndexHandler
- ReuseIndexHandler
- ReuseIndexHandlerUseCount
CoDiPack tape layout - Changes for mixed AD types

What do we want to support?

```cpp
AReal r;       // Active Real
AComplex c;    // Active Complex
ASimd s;       // Active Simd

GlobalTape::registerInput(r, c, s);

AComplex w1 = r * c;        // Mixed type computations
ASimd w2 = (norm(c) + r) * s;

GlobalTape::registerOutput(w1, w2);
w1.gradient() = 2.0 + 3.0 * I;
w2.gradient() = {1.0, 1.0, 1.0, 1.0};

GlobalTape::evaluate();
```
CoDiPack tape layout - Changes for mixed AD types

- **TapeBaseModule**
- **ExternalFunctionModule**
- **StatementModule**
- **JacobiModule**
- **IoModule**
- **TapeBaseMixedModule**
- **StatementMixedModule**
- **JacobiMixedModule**

- **TapeInterface**
- **JacobiTape**
- **LinearIndexHandler**
- **TapeInterface**
- **JacobiIndexTape**
- **ReuseIndexHandler**
- **ReuseIndexHandlerUseCount**
- **JacobiIndexMixedTape**
CoDiPack tape layout - Modular approach

Drawbacks:
- Difficult to find function implementation (Which module?)
- IDE support (e.g. auto completion) only partly working
- Hard to understand
  - Module A calls module B calls module C calls module A calls module D
- Difficult to generalize
  - Module needs to cover all different usecases
    - Normal, Mixed, Threaded, OpenMP, etc.
  - Mostly contradicting requirements

Advantages:
- No code copy
- Faster
  - w.r.t compile time, evaluation time
  - (Original motivation for modularized approach)
CoDiPack tape layout - CoDiPack 2.0 approach

- Traditional inheritance strategy
- Basic implementation contains only:
  - Forward function
  - Self contained data structures
- Each taping approach has a single implementation file
CoDiPack statement handling

How is a statement stored?

\[ w = (a + b) \times (c - d); \]

The call hierarchy is:

ActiveReal → Tape → Expression → Tape

operator = → store → calcGradient → pushJacobi
CoDiPack statement handling

How is a statement stored?

\[ w = (a + b) \times (c - d); \]

The call hierarchy is:

- ActiveReal → Tape → Expression → Tape
- operator = → store → calcGradient → pushJacobi

- Expression can be:
  - UnaryExpression, BinaryExpression11, BinaryExpression01, BinaryExpression10, ActiveReal, RefActiveReal
  \( \Rightarrow \) 6 different implementation of calcGradient

- Primal value tapes require additional functions:
  - getValueStatic, calcGradientStatic, perValueAction, perConstantAction, pushLazyJacobies
  \( \Rightarrow \) In total 36 different method implementations
CoDiPack statement handling

Drawbacks:
- Code copy (Especially function definitions)
- Difficult to know all Expression implementations
- Difficult to add new Expression implementation
- Hard to understand (Large call hierarchy)
- Tape specific logic in expression implementation

Advantages:
- No template magic
- Faster
  - w.r.t compile time, evaluation time
  - (Original motivation for deep call hierarchy)
CoDiPack statement handling - CoDiPack 2.0 approach

General idea:
- Make it possible to evaluate custom logic operations on an expression graph
CoDiPack statement handling - CoDiPack 2.0 approach

General idea:
- Make it possible to evaluate custom logic operations on an expression graph

Statement:
\[ w = (a + b) \times (c - d); \]

Graph:
CoDiPack statement handling - CoDiPack 2.0 approach

General idea:
- Make it possible to evaluate custom logic operations on an expression graph

Statement:
\[ w = (a + b) \times (c - d); \]

Graph:

User needs to be able to declare logic for each:
- Node
- Link
- Termination node
CoDiPack statement handling - CoDiPack 2.0 approach

General idea:
- Make it possible to evaluate custom logic operations on an expression graph

Statement:
\[ w = (a + b) \times (c - d); \]

Graph:

```
struct TraversalLogic {
    template<typename Node, typename ... Args>
    void node(Node const& node, Args&& ... args);

    template<typename Node, typename ... Args>
    void term(Node const& node, Args&& ... args);

    template<size_t LeafNumber, typename Leaf, typename Root, typename ... Args>
    void link(Leaf const& leaf, Root const& root, Args&& ... args);
};
```
CoDiPack statement handling - CoDiPack 2.0 approach

Example: Jacobian computation and storing

```cpp
template<typename Real>
struct JacobianLogic : public TraversalLogicBase {

    template<size_t LeafNumber, typename Leaf, typename Root, typename ... Args>
    void link(Leaf const& leaf, Root const& root, Real const& jacobian, Args&& ... args) {
        Real curJacobian = root.template getJacobian<LeafNumber>() * jacobian;
        toNode(leaf, curJacobian, std::forward<Args>(args)...);
    }

    template<typename Node, typename DataVector>
    enableIfLhsExpression<Node> term(Node const& node, Real jacobian, DataVector& dataVector) {
        dataVector.pushData(jacobian, node.getIdentifier());
    }
};
```

- `link`: Accesses the Jacobian with respect to this link
- `term`: Stores the computed Jacobian
- `node`: Using default logic (Forward to all links)
- `enableIfLhsExpression`: Only evaluate this for active types
CoDiPack statement handling - CoDiPack 2.0 approach

Drawbacks:
  - Lots of template magic
  - Difficult to select correct termination pointer (SFINAE principle)
  - Lots of steps with debugger

Advantages:
  - No code copy
  - Implementation local to tape
  - Easy to understand

Observations:
  - No compile time drawback
  - No performance drawback
CoDiPack expression implementation

CoDiPack: 6 classes, 11 functions

- Classes: UnaryExpression, BinaryExpression11, BinaryExpression10, BinaryExpression01, ActiveReal, RefActiveReal
- Functions: calcGradient(), calcGradient(multiplier), derv11, devr01, derv10, derv11M, derv01M, derv10M, gradientA, gradientB, gradient

Drawbacks:
- Several variations on the same logic
- Special handling of the constant case

Goal:
- Minimize user required implementations
- Remove hand optimizations
- Add constant values to the expressions

\[ w = (a + b) \times (c - 4.0); \]
CoDiPack expression implementation - CoDiPack 2.0 approach

CoDiPack 2.0: 4 classes, 5 functions

- Classes: UnaryExpression, BinaryExpression, LhsExpressionInterface, ConstantExpression
- Functions: getJacobian<link>, forEachLink, gradientA, gradientB, gradient

Advantages:
- New binary operator: Only two function implementations from user
- New expression: Only two function implementations from developer

Observations:
- No performance changes
CoDiPack - Misc changes

- New folder Structure
  - Old: Grown over time, lots of files in single folder
  - New: More context specific folders, extra traits folder

- Declaration of `const` values:
  - `const` is a left binding operator
  - Right binding is legacy behavior
  - Wrong intuition for:

```cpp
using T = int*;
using D1 = const T;  // Intuition: pointer to const int (Wrong)
using D2 = T const;  // const pointer to modifyable int
```
CoDiPack 2.0 programming guidelines - Template arguments

What about them?

- Hard to document - What range of types is allowed? (C++20 concepts)
- How to name them - With or without type suffix?
- How to declare them in the structure?
- No IDE support - auto completion
  - IDE does not know the type range
  - C++20 concept support will take quite a while.
CoDiPack 2.0 programming guidelines - Template arguments

What about them?

- Hard to document - What range of types is allowed? (C++20 concepts)
- How to name them - With or without type suffix?
- How to declare them in the structure?
- No IDE support - auto completion
  - IDE does not know the type range
  - C++20 concept support will take quite a while.

- CoDiPack 2.0 guideline:
  - Template arguments are declared with an underscore prefix
  - Template arguments are declared with `using` inside the structure without the prefix
  - They need to be declared with a default interface
CoDiPack 2.0 programming guidelines - Template arguments

Example:

```cpp
template<typename _Tape>
struct ActiveType {
    using Tape = DECLARE_DEFAULT(
        _Tape,
        TEMPLATE(FullTapeInterface<double, double, ANY, ANY>));

    ...
};
```

- DECLARE_DEFAULT is a preprocessor switch
- In an IDE, the second argument is used
- Auto completion based on interface definition
CoDiPack 2.0 performance measurements - Burgers test case

Coupled Burgers equations test case:

\[
\begin{align*}
    u_t + uu_x + vu_y &= \frac{1}{R}(u_{xx} + u_{yy}) \\
    v_t + uv_x + vv_y &= \frac{1}{R}(v_{xx} + v_{yy})
\end{align*}
\]

- Evaluated on 601x601 grid with 32 time steps
- Run with two Intel Xeon SP 6126 CPUs on HPC cluster Elwetritsch of TU Kaiserslautern
- Two load cases:
  - Sequential (1 process on the node)
  - Bandwidth limited (24 process on the node)
CoDiPack 2.0 performance measurements - Offset computation

CoDiPack:

```c
for(StatementInt curVar = 0; curVar < activeVariables; ++curVar) {
    --dataPos;
    adjoints[indices[dataPos]] += adj * jacobians[dataPos];
}
```

CoDiPack 2.0: (with offset computation)

```c
dataPos -= activeVariables;

for(StatementInt curVar = 0; curVar < activeVariables; curVar += 1) {
    size_t curOffset = dataPos + curVar;
    adjoints[indices[curOffset]] += adj * jacobians[curOffset];
}
```
CoDiPack 2.0 performance measurements - Offset computation

Burgers test tape reversal sequential case
CoDiPack 2.0 performance measurements - Offset computation

- CoDiPack
- CoDiPack2 with offset computation
- CoDiPack2 not offset computation

Burgers test tape reversal bandwidth limited case
CoDiPack 2.0 performance measurements - while loop optimization

CoDiPack:

```c
for(StatementInt curVar = 0; curVar < activeVariables; ++curVar) {
    --dataPos;
    adjoints[indices[dataPos]] += adj * jacobians[dataPos];
}
```

CoDiPack 2.0:

```c
size_t endDataPos = dataPos - activeVariables;

while(endDataPos < dataPos) {
    dataPos -= 1;
    adjoints[indices[dataPos]] += adj * jacobians[dataPos];
}
```
CoDiPack 2.0 performance measurements - while loop optimization

Burgers test tape reversal sequential case
CoDiPack 2.0 performance measurements - while loop optimization

CoDiPack 2.0: Lessons learned and new ideas

Burgers test tape reversal bandwidth limited case
CoDiPack 2.0 performance measurements - current status

- Burgers test tape record sequential case
CoDiPack 2.0 performance measurements - current status

- Burgers test tape reversal sequential case
CoDiPack 2.0 performance measurements - current status

- Burgers test tape record bandwidth limited case
CoDiPack 2.0 performance measurements - current status

- Burgers test tape reversal bandwidth limited case
CoDiPack 2.0 - Conclusion & release

Conclusion:
- Performance gain in nearly all cases
- Simpler development of new tapes
- Simpler maintenance due to more code locality
- Consistent naming schemes
- Consistent coding style

Road map:
- Todo:
  - Port EvaluationHelper
  - User documentation
  - Developer documentation
- Release:
  - End of this year