# Aggregated type handling in AD tape implementations

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# Overview

- Motivation - What are aggregated types and why do we need to handle them?
- Idea of handling them
- Implementation
- Performance example

# Motivation - Aggregated types

**Examples:**

- Complex numbers
- Matrices
- Vectors, arrays
- Tensors
- Computational grids
- Layers in neural networks
- etc.

**Aggregated type**

A structured type that can be represented by set of floating point values.

**AD handling:** e.g. `std::complex<adouble>`

# Motivation - Advantage of expression templates

**Example statement:**

```
w = sqrt(pow(u,2) + pow(v,2))
```

**Example statement with intermediates:**

```
t1 = pow(u,2);
t2 = pow(v,2);
t3 = t1 + t2;
w = sqrt(t3)
```

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|---|---|---|---|
| AD double with expression templates | 2 | 1 | 29 |
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Memory reduction by 70% (Just for this example.)

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Memory reduction by 50% (Just for this example.)

## Aggregated types - Expected memory increase

Let the aggregated type have $n$ entries.

**Jacobian taping** (Store $\frac{d\phi}{du}(u)$)

- *Per assignment:* Factor of $n$ for statements. (Each entry creates one statement.)
- *Per argument:* Factor of $n * n$ for Jacobians. (Each entry creates $n$ entries per argument for each statement.)

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- *Per argument:* Factor of $n$ for primal values. (Each entry creates $n$ entries per argument.)

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**For complex numbers:**

| | Per assignment | Per value |
|---|---|---|
| Jacobian taping | 2 | 4 |
| Primal value taping | 1 | 2 |

If aggregated types are not added to the expression templates, then memory usage increases further.

# Aggregated types - Handling idea

**Restrictions:**

- Use already available tape implementations.
  - No new fancy stuff or template meta programming magic.
- Make it “simple” to add custom aggregated types.
  - To the expression templates.
  - To the specialized handling.

# Aggregated types - Handling idea - Statement level handling

(Jacobian taping, Primal value taping)

**Assumption:** Aggregated types are already added to the expression framework.

**Assignment:** $w = expr$

- $w$ is an aggregated type with $n$ entries.
- $expr$ is an aggregated expression that matches $w$.

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**Idea:** Reduce to assignments of single entries.

```
// Recording:
for i = 1 ... n
  w[i] = expr[i]
end
```

- $w$ and $expr$ are treated as array types.

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- *expr* is an aggregated expression that matches $w$.

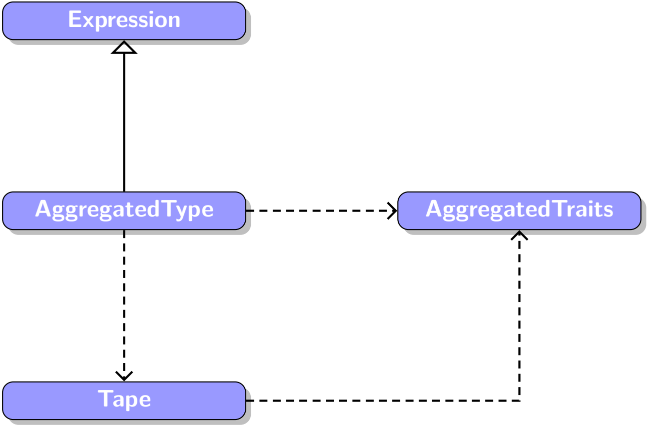
**Idea:** Store full expression on the tape, treat as array types in the reverse evaluation.

```
// Recording:
tape.store(w, expr);

// Reversal:
for i = 1 ... n
  expr[i].reverse(w_b[i]);
end
```

- Requires small changes on the tape layout for the primal value tape.

# Aggregated types - Implementation - Expression templates



# Aggregated types - Implementation - Expression templates

**Type for the integration into the expression template structure:**

```
<typename HOT> // HOT = HigherOrderType
struct AggregatedType : Expression {
  using Traits = AggregatedTraits<HOT>;
  HOT value_;
```

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  HOT value_;

  // Expression Interface
  Traits::ValueType getValue() const {return Traits::getValue(value_);}

  // Expression Interface
  void calcGradient(Traits::ValueType const& multiplier) const {
    for(int i = 0; i < Traits::nElements(value_); i += 1) {
      Traits::extract(value_, i).calcGradient(Traits::extract(multiplier, i));
    }
  }
```

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    }
  }

  <typename Arg>
  AggregatedType& operator=(Expression<Arg> const& arg) {
    Traits::getTape().store(*this, arg);
  }
};
```

- General implementation that uses the traits implementation for the logic.
- **AD handling:** e.g. `AggregatedType<std::complex<adouble>>`

# Aggregated types - Implementation - Expression templates

**General traits definition:**

```
template<typename _Type, typename = void>
struct AggregatedTypeTraits {

    using Type = CODI_DD(_Type, CODI_ANY);

    using ValueType; // Primal value representation
    using IdentifierType; // Identifier representation

    static size_t nElements(Type& type); // Number of elements

    static ValueType getValue(Type& type);
    static void setValue(Type& type, ValueType const& value);

    static IdentifierType getIdentifier(Type& type);
    static void setIdentifier(Type& type, IdentifierType consst& identifier);

    static double& extract(ValueType& value, size_t i);
    static int& extract(IdentifierType& value, size_t i);
};
```

- Needs to be specialized for each aggregated type – e.g. std::complex.

# Aggregated types - Implementation - Statement level handling

(Jacobian taping, Primal value taping)

**Specialize** the `store` method for aggregated types.

```
// In JacobianTape
<typename HOT, typename Rhs>
void store(AggregatedType<HOT>& lhs, Expression<Rhs> const& rhs) {
  using Traits = AggregatedTraits<HOT>;

  Traits::ValueType value = Traits::getValue(lhs.value_);
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  Traits::ValueType value = Traits::getValue(lhs.value_);
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  for(int i = 0; i < Traits::nElements(lhs.value_); i += 1) {
    RealReverseWrapper wrapper(Traits::extract(value, i),
                               Traits::extract(identifier, i));
    wrapper = ExtractExpression<Rhs>(rhs, i);
  }
```

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    RealReverseWrapper wrapper(Traits::extract(value, i),
                               Traits::extract(identifier, i));
    wrapper = ExtractExpression<Rhs>(rhs, i);
  }

  Traits::setValue(lhs.value_, value);
  Traits::setIdentifier(lhs.value_, identifier);
}
```

- For loop over entries.
- Value and identifier need to be extracted because of self assignments.
  - e.g. `a = a * a;`

# Aggregated types - Implementation - Expression level handling

(Primal value taping)

**Change** the tape structure:

- Old: $4 \cdot \text{nArgs} + 8 \cdot \text{nPas} + 8 \cdot \text{nCon} + 8 + 4 + 8 + 1$
- New: $4 \cdot \text{nArgs} + 8 \cdot \text{nPas} + 8 \cdot \text{nCon} + 8 \cdot \text{nOut} + 4 \cdot \text{nOut} + 8 + 1 + 1$
  - Store number of outputs: 1 byte (nOut)
  - Store a primal value for each entry: 8 byte each.
  - Store an identifier for each entry: 4 byte each.

**Implementation:**

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**Implementation:**

```
    // To much to show :(
```

# Performance example - Burgers equation

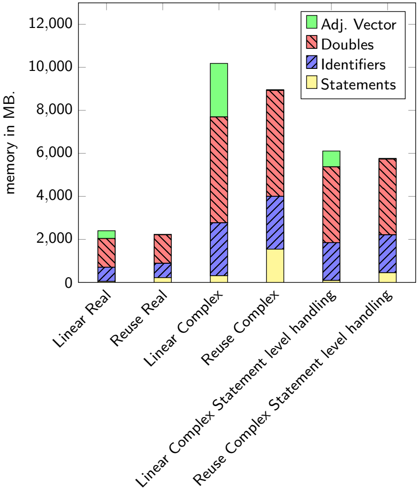
Performance test:

- Forward numerical scheme for the coupled Burgers's equation

$$u_t + uu_x + vu_y = \frac{1}{R}(u_{xx} + u_{yy})$$
$$v_t + uv_x + vv_y = \frac{1}{R}(v_{xx} + v_{yy})$$

- Solved on the unit square.
- Elwetritsch cluster compute node: Two Intel Xeon 6126 CPUs with a total of 24 cores and 384 GB of main memory.
- Solved with real and complex numbers.

# Performance example - Burgers equation - Memory




Jacobian taping

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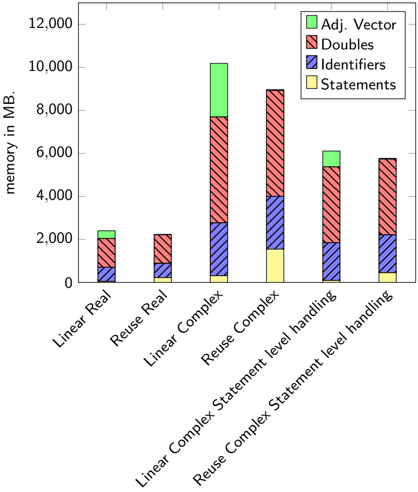
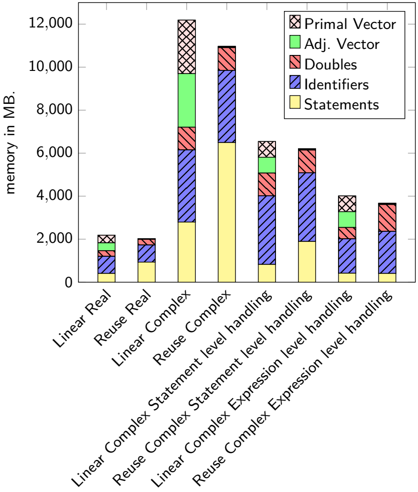
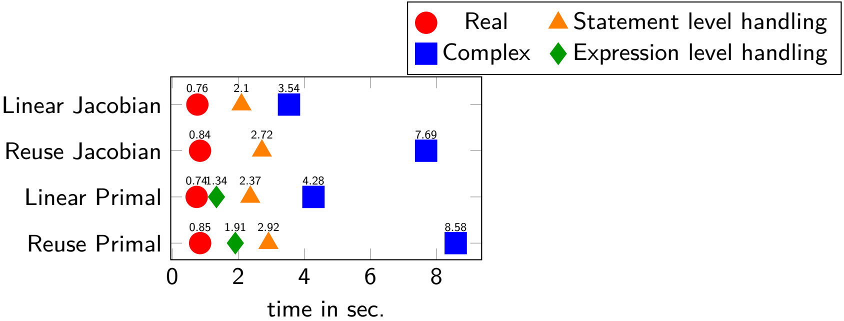



Jacobian taping




Primal value taping

# Performance example - Burgers equation - Timing




Recording time

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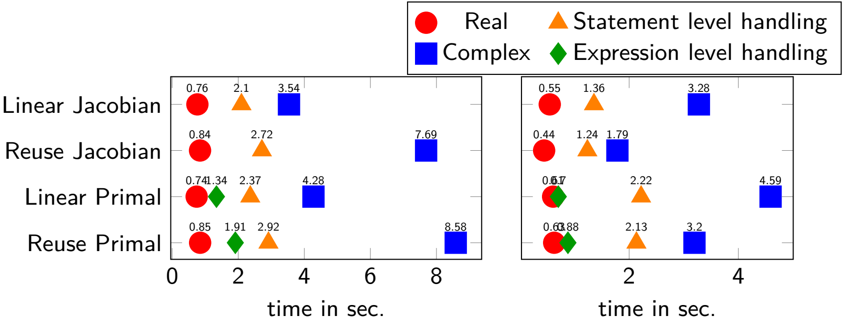


Recording time

Reversal time

# Conclusion & Outlook

**Conclusion:**

- Demonstration of overhead for aggregated types in expression template AD frameworks.
- Demonstration of aggregated type handling in standard AD tapes.
- Good memory and timing results.

**Outlook:**

- Member functions in expression template AD frameworks.
- Specialized tapes for aggregated type handling.

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**Thank you very much for your attention.**