Block sequencing, partial derivatives and SG7

24th EuroAD Workshop

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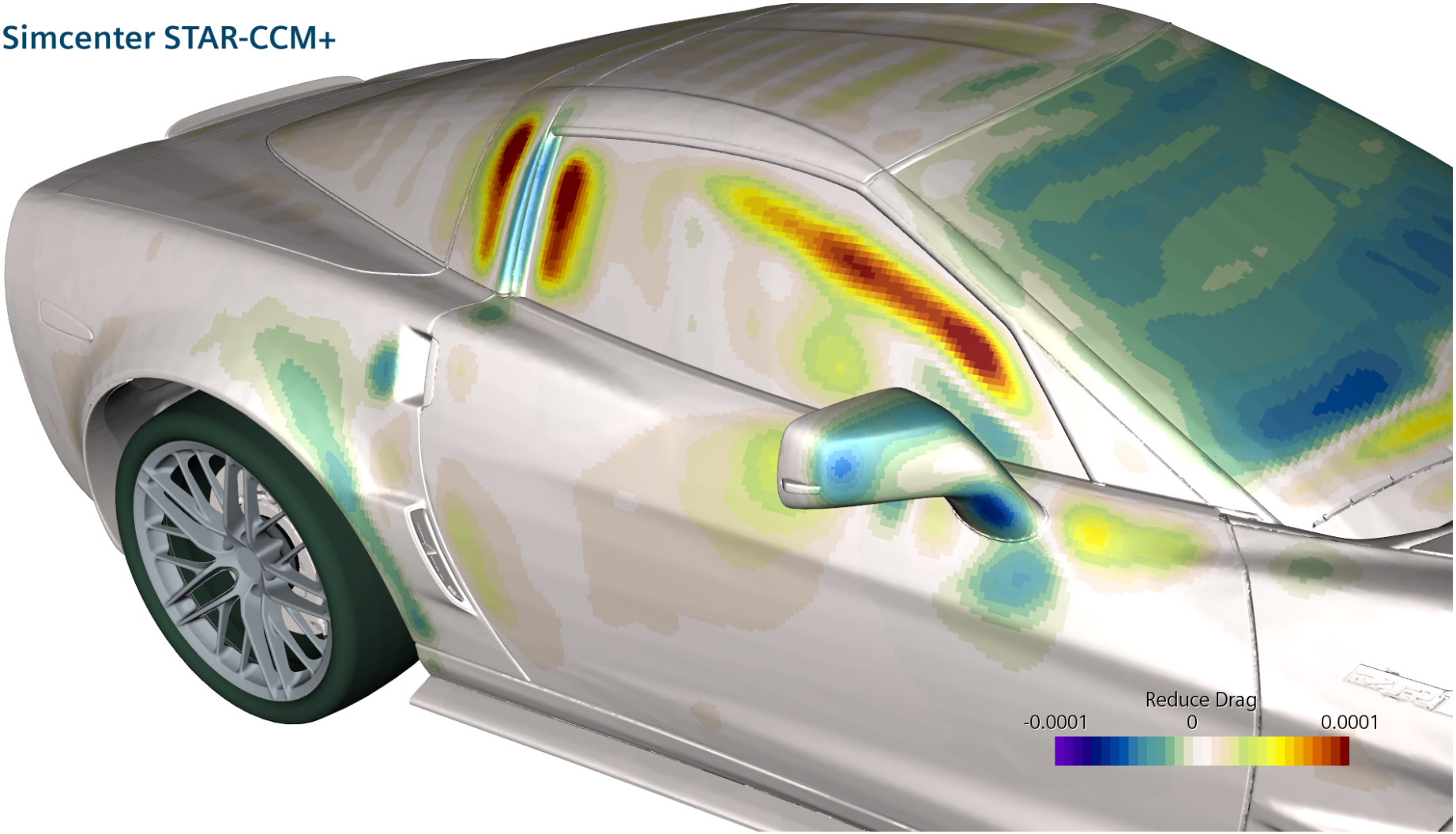
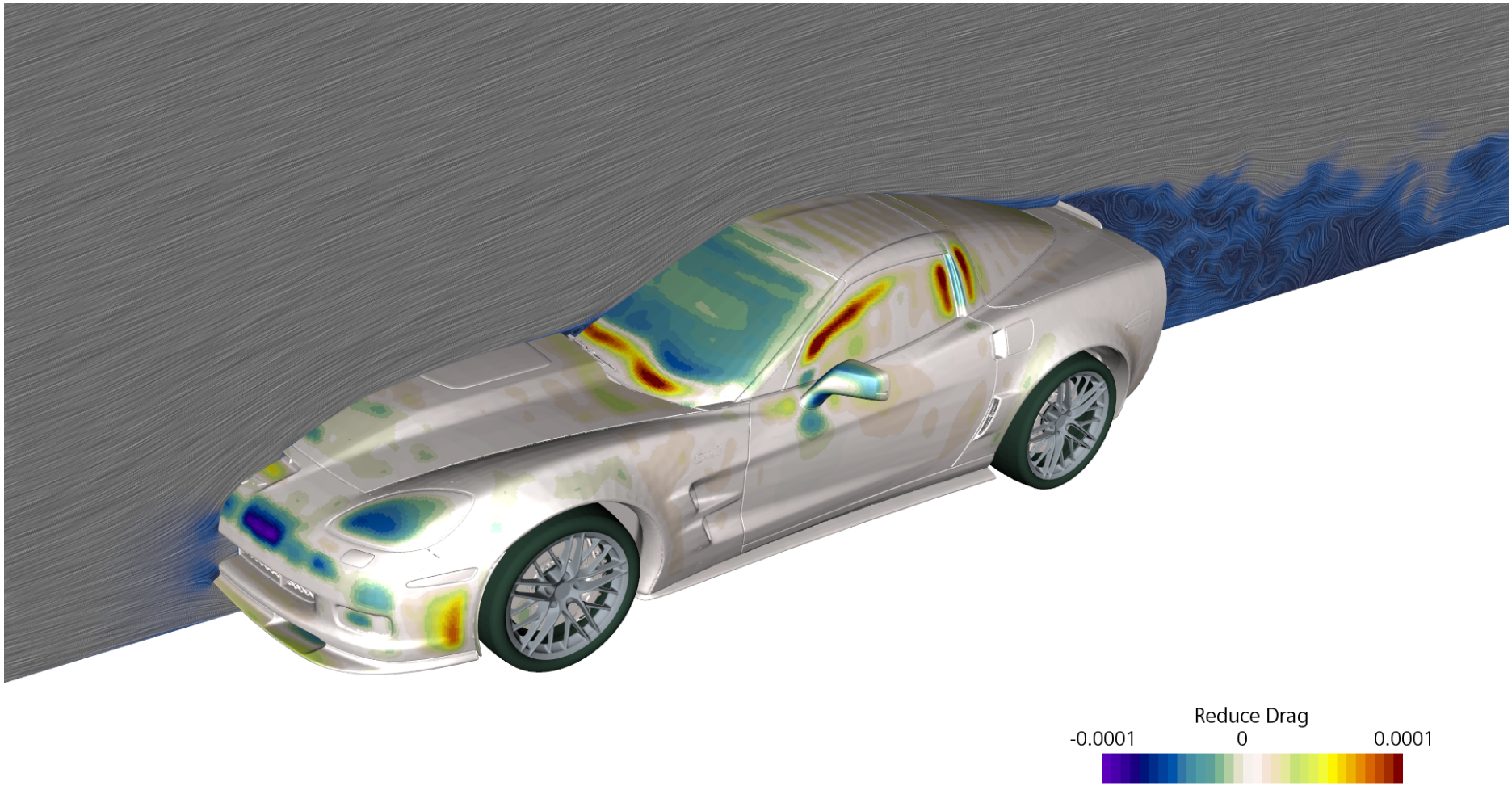
Introduction

- Siemen's Simcenter Star-CCM+ simulation software uses an in-house automatic differentiation tool to differentiate the coupled Naiver-Stokes solver, Spalart Allmaras turbulence model, and a significant amount of related code.
- The in-house route was taken due to the performance requirements of the resultant adjoint code (no taping is used, for example). Secondly, a tool was needed that would not conflict in presence of the PETE vector unrolling engine.
- In the course of applying AD to a large amount of code, a number of techniques have been devised. This talk will look at a couple of them.

Simcenter STAR-CCM+

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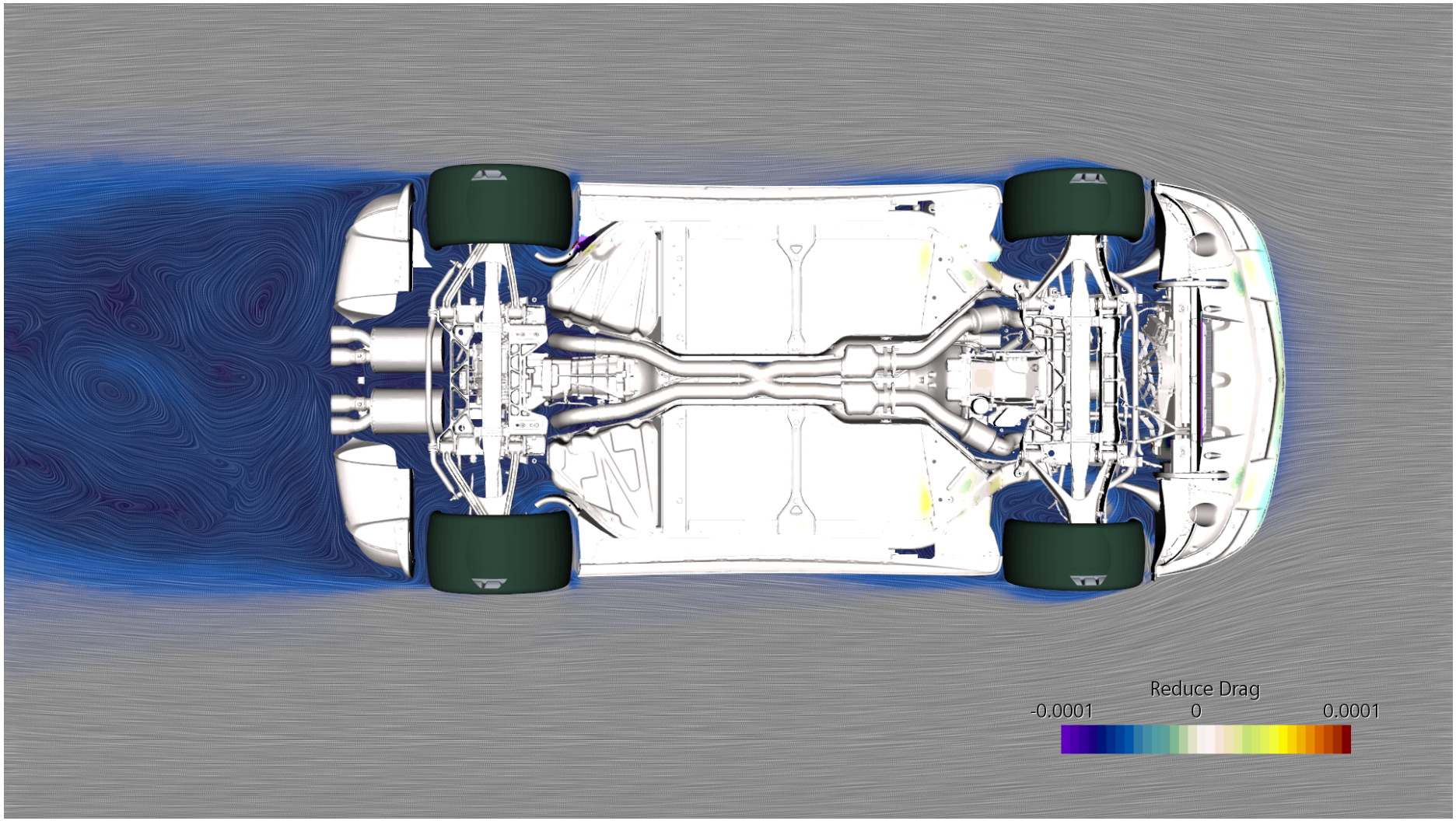
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Sequencing code blocks (1)

Non-RAII reversing

```
enum class direction : { forward, reverse };

void compute(direction d)
{
  sequence_begin(d)
  {
    std::cout << "block 1" << std::endl;
  }
  sequence_next()
  {
    std::cout << "block 2" << std::endl;
  }
  sequence_next()
  {
    std::cout << "block 3" << std::endl;
  }
  sequence_end();
}
```

sequence_begin

```
#define sequence_begin(mode)                                \
{                                                           \
  auto constexpr sequence_offset{__COUNTER__};              \
  auto const sequence_mode{mode};                           \
  auto sequence_case{int(0)};                               \
                                                            \
  if (mode == direction::reverse)                           \
    goto sequence_end_label;                                \
                                                            \
sequence_begin_label:                                       \
  switch (sequence_case) {                                  \
  case 0:                                                   \
  {
```

sequence_next

```
#define sequence_next()                                  \
  }                                                      \
  (sequence_mode == direction::reverse) ?                \
    sequence_case-- : sequence_case++;                   \
                                                         \
  goto sequence_begin_label;                             \
                                                         \
  case (__COUNTER__ - sequence_offset):                  \
  {
```

sequence_end

```
#define sequence_end()                                                  \
  }                                                                     \
  (sequence_mode == direction::reverse) ?                               \
    sequence_case-- : sequence_case++;                                  \
  goto sequence_begin_label;                                            \
                                                                        \
sequence_end_label:                                                     \
  default:                                                              \
  {                                                                     \
    auto constexpr size{__COUNTER__ - sequence_offset};                 \
    if (sequence_mode == direction::reverse &&                          \
        sequence_case >= 0)                                             \
    {                                                                   \
      sequence_case = size - 1;                                         \
      goto sequence_begin_label;                                        \
    }                                                                   \
  }                                                                     \
  break;                                                                \
  }                                                                     \
}
```

Sequencing code blocks (2)

RAII primal-adjoint pairs

```
void compute(X1 const &x1, X2 const &x2, Y &y)
{
  X1 t;

  IF (x1 > x2)
  {
    auto t0{x1 - x2};
    t = exp(t0);
  }
  ELSE
  {
    auto t0{x2 - x1};
    t = exp(t0);
  }
  ENDIF

  y = x1 * t;
}
```

Two lambdas from one

```
template<typename T1, typename T2, typename F>
struct BimodalLambda
{
  F f;
  BimodalLambda(F f) : f(f) { f(T1{}); }
  ~BimodalLambda()          { f(T2{}); }
};
```

C++20 template lambda

```
auto lambda = [&]<typename M>(M mode) // C++20
{
  auto eval = [mode]<typename E>(E const &expr)
  {
    if constexpr (sizeof(mode) == Primal::value)
      return ::eval_primal(expr);
    else
      return ::eval(expr);
  };

  // the 'lambda', e.g.
  {
    auto t0{eval(x1 - x2)}; // must wrap RHS with 'eval'
    t = exp(t0);
  }
});
```

Partial differentiation

Avoiding primitives

```
float a = 3, a_drv = 0;
float b = 4, b_drv = 0;
float        r_drv = 1;

Drv<Primal, float> a_{a, a_drv}; // passive but not primitive
Drv<Adjoint, float> b_{b, b_drv};
Drv<Adjoint, float&> r_{r_drv};

{
  auto a1 = drv::cos(a_);  // non-primitive argument required
  auto b1 = drv::sin(b_);
  r_ = drv::atan2(a1, b1); // at least one non-primitive req.
}

std::cout << a_drv << std::endl;
std::cout << b_drv << std::endl;
```

Permit mixed modes

- Operator overloading AD tools typically only accommodate the case where there can be only one permissible active type in a given context.
- Passive inputs may be made so by leaving their type as primitive, such as `float`.
- If, however, both a fully differentiated and a partially differentiated function are wanted, two versions of the code would be needed...
- ... unless we permit the co-existence of different active types, i.e. primal and tangent or primal and adjoint.

Expression node tagging

```
Drv<Primal, float> a_{a, a_drv}; // passive but not primitive
Drv<Adjoint, float> b_{b, b_drv};
Drv<Adjoint, float&> r_{r_drv};

{
  auto a1 = drv::cos(a_);  // non-primitive argument required
  auto b1 = drv::sin(b_);
  r_ = drv::atan2(a1, b1); // at least one non-primitive req.
}
```

Expression types:

```
{
  Unary<Primal, Cos, Drv<Primal, float>>    //  a1

  Unary<Adjoint, Sin, Drv<Adjoint, float>>  //  b1

  Binary<Adjoint, ATan2,                    //  r_ rhs
         Unary<Primal, Cos, Drv<Primal, float>>
         Unary<Adjoint, Sin, Drv<Adjoint, float>>>
}
```

Tag promotion

- If `a1` were a primitive then `drv::cos(a1)` would cause a compilation failure; unary operators only accept an active type.
- The tag for the expression `drv::atan2(a1, b1)` is deduced from its child nodes using promotion rules.

Compile time identity

A vexing problem

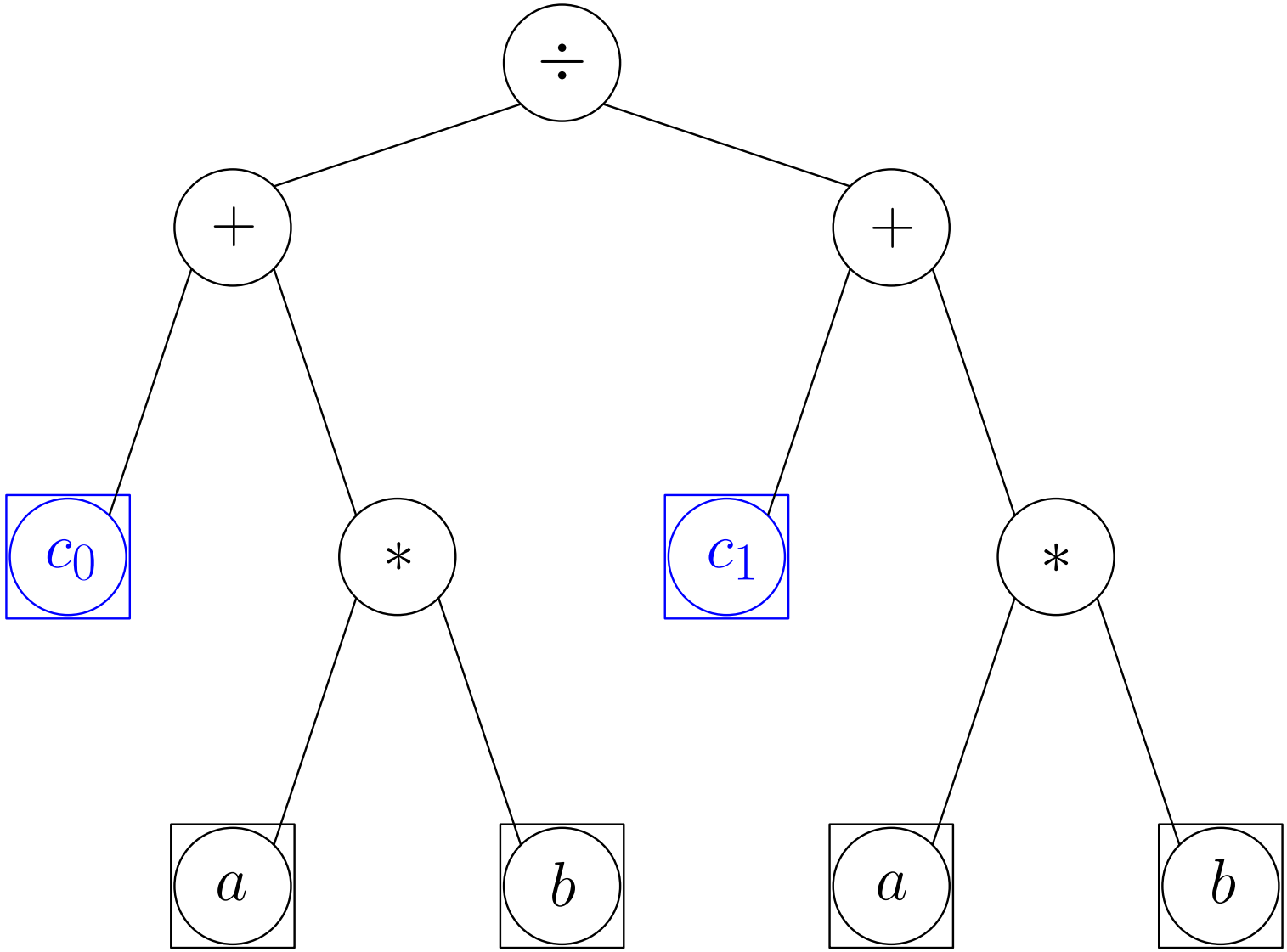
Can I query, at compile time, if the left branch identical to the right branch?

Apparently not, despite it being statically obvious.

```
template<typename A, typename B>
auto compute(A &&a, B &&b)
{
  float c0 = ...
  float c1 = ...

  auto ab    = a * b;
  auto left  = c0 + ab;
  auto right = c1 + ab;
  return left / right;
}
```

Same type, different names



Unique types

```
template<typename T, auto = []{}>  // lambda type is unique
struct Unique { T value; };

Unique<float> c0;
Unique<float> c1;

static_assert(!std::is_same_v<decltype(c0), decltype(c1)>);
```

Unique ‘addresses’

```
template<typename E0, typename E1>
auto constexpr isSame(E0 &&e0, E1 &&e1)
{ return &e0 == &e1; }

float c0;
float c1;

static_assert(isSame(c0, c0));
static_assert(!isSame(c0, c1));
```

Unique ‘addresses’: no good!

```
template<typename OP, typename E0, typename E1, bool IsSame>
struct Binary { ... };

template<typename E0, typename E1>
auto add(E0 &&e0, E1 &&e1)
 -> Binary<Add, E0, E1, isSame(e0, e1)>
{ ... }

float c0;
float c1;
add(c0, c1);  // error: non-type template argument
              //        is not a constant expression
```

C++ SG7 discussions

- I made a proposal to SG7, 'varid operator', December 2020, which drew some discussion.
- Andrew Sutton proposed a major revision of how reflection should be done around the same time. In P2237R0, 'Metaprogramming', p. 15, this paper describes a function, `meta::location_of(expr)`, returning line and column values.
- Marco Foco, et al, 'P2072R1: Differentiable programming for C++' provides a summary of the state of the art and a presentation on desirable language support.
- C++20 added `std::source_location`. I'm not sure how useful it is for this problem...

Summary

Summary

- An eclectic approach to differentiation has been taken, which is limited to what the language features permit, but excludes taping.
- The approach generally requires code to be written in a 'pure functional' manner.
- Template expressions are employed at the fine grain level, whereas at the coarse grain less formal approaches are used.
- Finding ways of constructing the efficient adjoint code within C++ would greatly help, even if this means influencing language changes. The reliance on taping is, in my opinion, a dead end.

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