Automatic Differentiation of the Kokkos framework and the STL with Clad

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Clang

Source

```
double fn(double x, double y) {
   double t = 2*x + y*y;
   return t;
}
```

Compiled

Clad

Derivatives

```
void fn_grad(double x, double y,
double *_d_x, double *_d_y) {
   double _d_t = 0.;
   double t = 2 * x + y * y;
   _d_t += 1;
   {
      *_d_x += 2 * _d_t;
      *_d_y += _d_t * y;
      *_d_y += y * _d_t;
   }
}
```

Making an efficient language efficiently differentiable

This allows template usage!

Making STL differentiable
(C++ Standard Template Library)

```
double fnVec6(double x, double y) {
    std::vector<double> v(3, y);

    v.pop_back();
    double res = v.size()*x;

    v.erase(v.begin());
    res += v.size()*x;

    std::vector<double> w;
    w = v;
    w.clear();
    res += w.size()*x + v.size()*x;

    w.insert(w.end(), 5);
    res += w.size()*x;

    w.insert(w.end(), {y, x, y});
    w.insert(w.end(), v.begin(), v.end());

    w.assign(2, y);
    res += (w[0] == y && w[1] == y)*x;

    v[0] = x;
    w.assign(v.begin(), v.end());
    res += w[0];

    w.assign({3*x, 2*x, 4*x});
    res += w[1];

    return res;
}
```

Methods
Operators
Constructors

Library-specific extensions for Clad
(my job)

```
double fn(double x, double y) {
    double t = 2*x + y*y;
    return t;
}
```

```
void fn_grad(double x, double y,
double *_d_x, double *_d_y) {
    double _d_t = 0.;
    double t = 2 * x + y * y;
    _d_t += 1;
    {
        *_d_x += 2 * _d_t;
        *_d_y += _d_t * y;
        *_d_y += y * _d_t;
    }
}
```

```
double fn_darg0(double x, double y) {
    double _d_x = 1;
    double _d_y = 0;
    double _d_t = 0 * x + 2 * _d_x + _d_y * y + y * _d_y;
    double t = 2 * x + y * y;
    return _d_t;
}
```

```
double fn(double x, double y) {
    double t = 2*x + y*y;
    return t;
}
```

Gradient (reverse mode)

```
void fn_grad(double x, double y,
double *_d_x, double *_d_y) {
    double _d_t = 0.;
    double t = 2 * x + y * y;
    _d_t += 1;
    {
        *_d_x += 2 * _d_t;
        *_d_y += _d_t * y;
        *_d_y += y * _d_t;
    }
}
```

df/dx (forward mode)

```
double fn_darg0(double x, double y) {
    double _d_x = 1;
    double _d_y = 0;
    double _d_t = 0 * x + 2 * _d_x + _d_y * y + y * _d_y;
    double t = 2 * x + y * y;
    return _d_t;
}
```

`f(...)` calls `g(...)`

`f_darg0(...)` calls `g_pushforward(...)`

`g(...)`

`value`

`g_pushforward(...)`

`{value, d_value}`

```
double fn(double x, double y) {
    double t = 2*x + y*y;
    return t;
}
```

```
void fn_grad(double x, double y,
double *_d_x, double *_d_y) {
    double _d_t = 0.;
    double t = 2 * x + y * y;
    _d_t += 1;
    {
        *_d_x += 2 * _d_t;
        *_d_y += _d_t * y;
        *_d_y += y * _d_t;
    }
}
```

```
double fn_darg0(double x, double y) {
    double _d_x = 1;
    double _d_y = 0;
    double _d_t = 0 * x + 2 * _d_x + _d_y * y + y * _d_y;
    double t = 2 * x + y * y;
    return _d_t;
}
```

```
double fn(double x, double y) {
    double t = 2*x + y*y;
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Gradient (reverse mode)

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void fn_grad(double x, double y,
double *_d_x, double *_d_y) {
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    {
        *_d_x += 2 * _d_t;
        *_d_y += _d_t * y;
        *_d_y += y * _d_t;
    }
}
```

df/dx (forward mode)

```
double fn_darg0(double x, double y) {
    double _d_x = 1;
    double _d_y = 0;
    double _d_t = 0 * x + 2 * _d_x + _d_y * y + y * _d_y;
    double t = 2 * x + y * y;
    return _d_t;
}
```

`f(...)` calls `g(...)`

`f_grad(...)` calls `g_reverse_forw(...)`
and `g_pullback(...)`

`f(...)` calls `g(...)`

(for OOP)

`f_grad(...)` calls `g_reverse_forw(...)`
and `g_pullback(...)`

`f(...)` calls `g(...)`

`f_grad(...)` calls `g_reverse_forw(...)`
and `g_pullback(...)`

Can provide a better pullback than the generated one? Prove your own!

```
namespace clad::custom_derivatives {

    void g_pullback(double v, double u,
                    double d_y,
                    double * d_v, double * d_u) {
        ...
    }

}
```

```
namespace clad::custom_derivatives {

    void g_pullback(double v, double u,
                    double d_y,
                    double * d_v, double * d_u) {
        ...
    }

}
```

```
namespace clad::custom_derivatives {

    void g_pullback(double v, double u,
                    double d_y,
                    double * d_v, double * d_u) {
        ...
    }

}
```

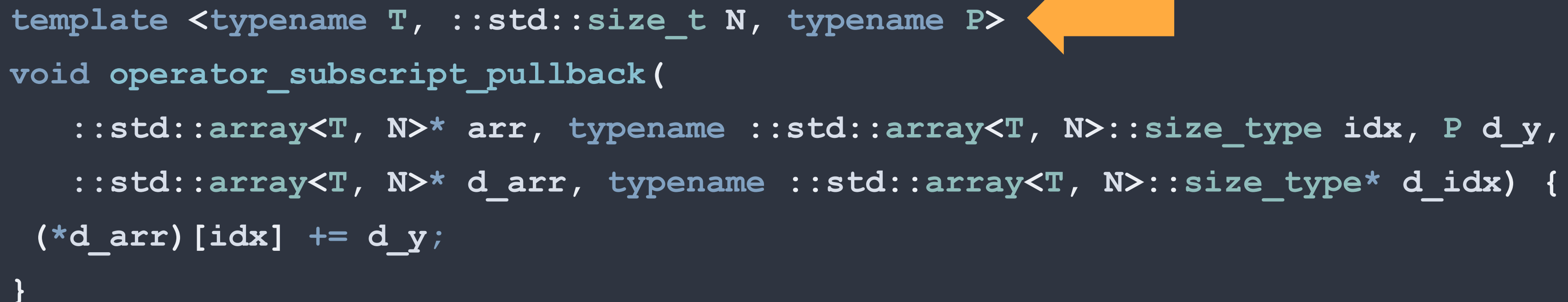
```
namespace clad::custom_derivatives {

    void g_pullback(double v, double u,
                    double d_y,
                    double * d_v, double * d_u) {
        ...
    }

}
```

```
namespace clad::custom_derivatives {

    void g_pullback(double v, double u,
                    double d_y,
                    double * d_v, double * d_u) {
        ...
    }

}
```

Methods?
Operators?
Constructors?

```
namespace clad::custom_derivatives::class_functions {
    ...
}
```

```cpp
template <typename T, ::std::size_t N, typename P>
void operator_subscript_pullback(
    ::std::array<T, N>* arr, typename ::std::array<T, N>::size_type idx, P d_y,
    ::std::array<T, N>* d_arr, typename ::std::array<T, N>::size_type* d_idx) {
 (*d_arr)[idx] += d_y;
}
```



template <typename T, ::std::size_t N, typename P>
void operator_subscript_pullback(
::std::array<T, N>* arr, typename ::std::array<T, N>::size_type idx, P d_y,
::std::array<T, N>* d_arr, typename ::std::array<T, N>::size_type* d_idx) {
(*d_arr)[idx] += d_y;
}

No class modification
No Clad codebase modification ↦ **Easy support**

No class modification
No Clad codebase modification $\mapsto$ **Easy support**
(almost)

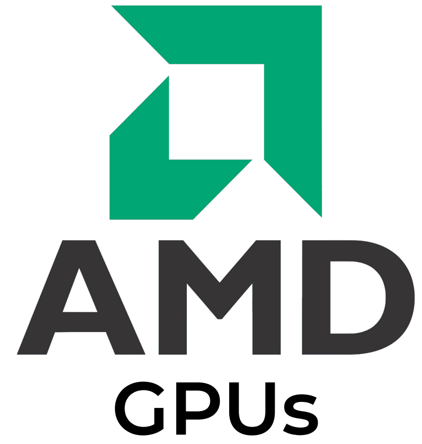
kokkos

Source ↦ Source
Parallel ↦ Parallel

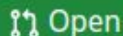
```
Kokkos::parallel_for("name", Policy, f);
```

```
Kokkos::parallel_for("name", Policy, f);
Kokkos::parallel_for("d_name", Policy, d_f);
```

Performance Portable Gradient Computations Using Source Transformation
(a paper)


AMD
GPUs

Kokkos-aware Clad #783

 kliegeois wants to merge 75 commits into `vgvassilev:master` from `kliegeois:kokkos-PR`

Conversation 20 Commits 75 Checks 80 Files changed 13

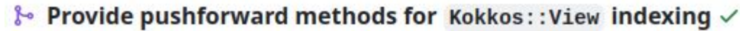
kliegeois commented on Feb 22 — First-time contributor

This PR provides the implementation of a first set of features for the automatic generation of gradients of Kokkos-based code.

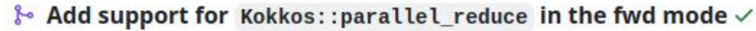
The content of this PR supports reverse mode of Kokkos `parallel_for`, `deep_copy`, and view accesses.

@vgvassilev **@brian-kelley**

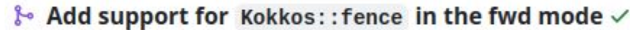
#1063 by gojakuch was merged last month



#1061 by gojakuch was merged last month

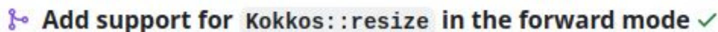


#1056 by gojakuch was merged last month

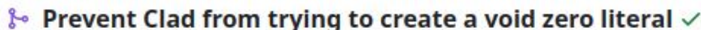


#1048 by gojakuch was merged on Aug 21 • Approved

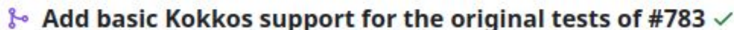
#1022 by gojakuch was merged on Aug 21



#999 by gojakuch was merged on Jul 24



#989 by gojakuch was merged on Jul 21 • Approved



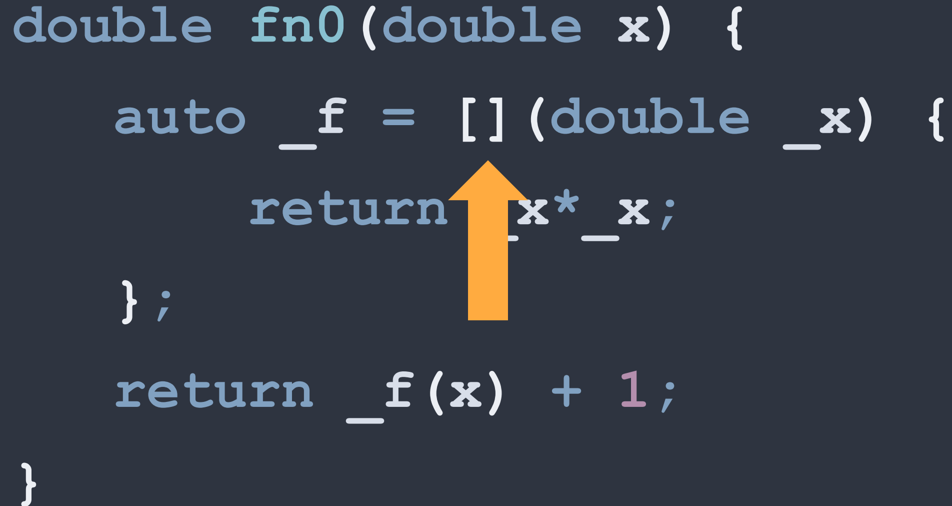
#977 by gojakuch was merged on Jul 22 • Approved

#967 by gojakuch was merged on Jul 4 • Approved

#826 by gojakuch was merged on Apr 19 • Approved

Rough edges
(ongoing work)

No captures here yet.



```
auto pack(double x) {
    return std::make_tuple(x, 2*x, 3*x);
}

double fnTuple1(double x, double y) {
    double u, v = 288*x, w;

    std::tie(u, v, w) = pack(x+y);

    return v;
} // = 2x + 2y
```

No reverse mode support yet.

Try it out!
(we’re use-case driven)