



Wrap-Up:

Improve automatic differentiation of object-oriented paradigms using Clad

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Original code

```
double f(double* x, double y) {
   g(x, y); // g(double*, double)
   return z;
}
```

```
void f_grad(...) {
  // forward pass
 // _t0 = x; ??
 g(x, y);
  // reverse pass
  // t0 = x; ??
 g_pullback(...);
```







Original code

```
double f(double* x, double y) {
   g(x, y); // g(double*, double)
   ...
   return z;
}
```

The argument is not fully copyable!

```
void f_grad(...) {
  // forward pass
  // t0 = x; ??
 g(x, y);
  // reverse pass
  // t0 = x; ??
 g_pullback(...);
```



What doesn't work



The same goes with all non-copyable types:

- std::initializer_list
- std::unique_ptr, std::shared_ptr, etc.
- Other STL and user-defined types.

Note: Methods of such classes follow the same logic as plain functions.







We introduced clad::restore_tracker (previously, clad::smart_tape) that can automatically store and restore multiple objects at the same time

Original code

```
double f(double* x, double y) {
   g(x, y); // g(double*, double)
   ...
   return z;
}
```

```
void f_grad(...) {
    clad::restore_tracker _tracker0 = {};
    g_reverse_forw(x, y, _d_x, *_d_y, _tracker0);
    ...
    // reverse pass
    _tracker0.restore();
    g_pullback(...);
    ...
}
```



Implemented solution



Original code

```
double g(double* x, double y) {
   for (int i = 0; i < 9; ++i) {
      x[i] *= y;
   }
   return x[3];
}</pre>
```

```
double g_reverse_forw(..., clad::restore_tracker &_tracker0) {
    unsigned long _t0 = 0UL;
    int _d_i = 0;
    for (int i = 0; i < 9; ++i) {
        _t0++;
        _tracker0.store(x[i]);
        x[i] *= y;
    }
    return x[3];
}</pre>
```



Implemented solution



- Already on Clad's master
- Well-tested with nested calls and local variables
- Fixed an example from ROOT
- The system is attached to TBR analysis to avoid unnecessary uses







It was meant to cover "nice" cases when the argument can be stored easily outside of the original function.

Original code

```
double f(double* x, double y) {
    g(x, y); // g(double*, double)
    ...
    return z;
}
```

```
void f_grad(...) {
  double _t0 = x[3];
  g(x, y);
  ...
  x[3] = _t0;
  ...
}
```



The second originally planned approach



- We decided that this feature is not currently needed as there are more relevant OOP-related issues
- Although we are halfway there as the approach relies on TBR analysis and most of the necessary improvements there were made





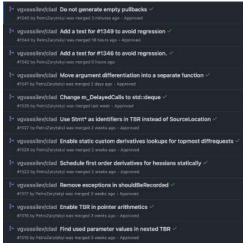


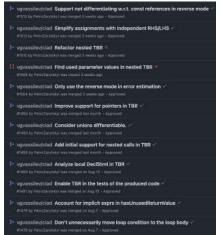


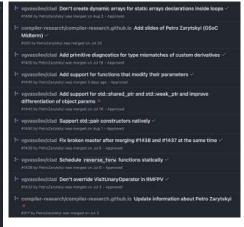




47 merged Pull Requests







vgvassilevicied Move VarData element access to VarData::operator[] <
vgvassilev/clad Rework SetisReq and overlay and combine them into a single function #1424 by PreniZhypsky) was neeged on Jun 29 1 Approved
vgyrassilev(clad Move ProfileID generation to a single point in TBR \$1622 by PetriZanyabyl was respect on Asr 26 - Approval
vgvassilev/clad Switch from Visit to Traverse functions in TBR #1421 to Princiary two margins on an 20 - Approved.
vgwassilev/clad. Perform lookups of reference variables in TBR::overlay 4:400 in ReinZerynkyl was renged in Jun 24 - Approved.
vgyrassilev/clad. Simplify getExprVar9ata in TBR and add a test \$1418 to Permiary (visit has transport in Jul 24 - Approved.
vgvassilev clad Update call argument storing in the reverse mode = state by feeoZaytiski wax marged in Jun 20 - Approved
vgvassilev/clind Move some tests from UserDefinedTypes.C to Constructor.C <
vgvassileviciad. Schedule simple partial derivatives statically × statically × statically statically as merged to Jun 15 - Approved.
vgyzastilevýclad Update the SmallPT ray tracer demo / #Mo2 by PstroZenytský, eva merged on Jun 16 - Aparovatí
vgvassiley/clad. Call UpdateDiffParamsinfo in the Diffplanner unconditionally

To vgvassilev/clad Don't store unused return values of reverse_forw v #1477 by PetraZarytskyi was merged on Aug 5 - Approved.

\$\text{vgvassilev/clad}\$ Schedule constructor pullbacks statically \(\square\text{#1391 by PetroZarytskyi was merged on May 28 \text{-} Approved \)

- vgvassilev/clad Enable static derivative scheduling in the forward mode by default
- #1400 by PetroZerytsky) was merged on Jun 11 - Approved

- vgvassilev/clad Fix the numeration in STLCustomDerivatives.C
- #1398 by PetroZerytsky) was merged on Jun 6 - Approved

- vgvassilev/clad Update a test of a break-stmt to avoid regression in #1123
- #1398 by PetroZerytsky) was merged on Jun 6 - Approved

vgvassilev/clad Automatically generate pullbacks of non-linear constructors #1286 by PetroZarytskyi was merged on Jun 18 • Approved





Summary: Improvements in TBR analysis

- Support for pointers: new operators, address and dereference operators (& and *), pointers are no longer always to-be-recorded.
- Support for nested function calls: information about variables is propagated between functions
- Improved OOP support leading to 17% less produced code and up to 44% speedup in OOP-specialized tests in Clad.
- Support for local declarations: in the reverse mode, they also require tapes and can be optimized by TBR
- Major code refactoring for better readability/maintainability (fixed some bugs automatically)





Summary: Improvements in OOP

- Automatic differentiation of constructors: general constructors are now supported (before, only linear), base-class constructors, delegating constructors, move-constructors constructor-exprs are supported on the same level as function call-exprs
- Improved reverse_forw functionality: fixed bugs and crashes, improved produced code, improved pointer support
- Diagnostics for custom derivatives: hints for the user if the custom derivative is written incorrectly and cannot be used by Clad.
- Other bugs/features: added support for std::pair, std::unique_ptr, std::shared_ptr, std::weak_ptr, etc.
- Related code maintenance: mostly moved to static scheduling of derivatives, etc.





Thank you! Questions?