Scientific Computing
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Simultaneous Preaccumulations in OpenMP-Parallel Automatic Differentiation

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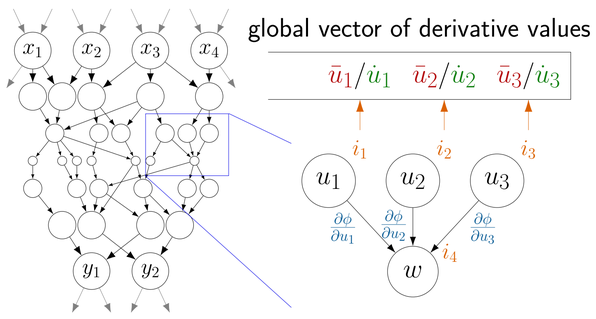
Automatic Differentiation (AD)



(sub)graph/program G individual statement

primal program

$w = \phi(u) \qquad y = G(x)$

reverse mode

$\bar{u}_i \mathrel{+}= \frac{\partial\phi}{\partial u_i}(u)\bar{w} \;\forall i$

$\bar{x} = \frac{\partial}{\partial x}G(x)^\mathsf{T}\bar{y}$

forward mode

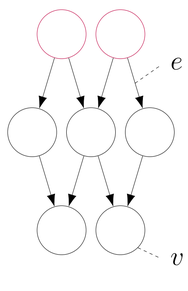
$\dot{w} = \Sigma_i \frac{\partial\phi}{\partial u_i}(u)\dot{u}_i$

$\dot{y} = \frac{\partial}{\partial x}G(x)\dot{x}$

- recorded computational graph with values as nodes, direct dependencies as edges [11]
  - edges annotated with partials, nodes annotated with identifiers (virtual addresses)
  - identifiers address into memory for adjoint values or tangent values
- compute derivatives based on graph, using the rules for the forward or reverse mode
- **preaccumulation:** precompute Jacobians of subgraphs to save memory [11]
  - apply the same techniques recursively during recording

Model for Simultaneous Preaccumulations

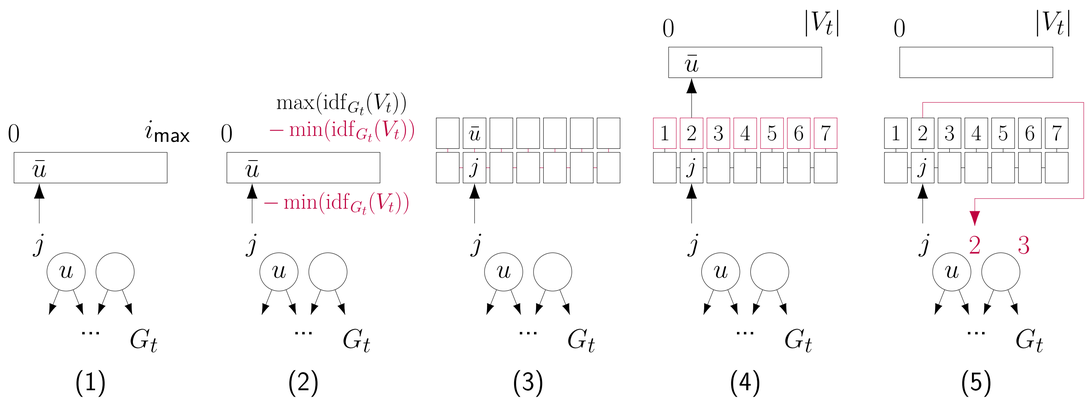
```
#pragma omp parallel
{
  // thread-local preaccumulation of subgraph G_t
}
```



- isomorphic subgraphs $G_t = (V_t, E_t)$
  - identical structure, different data/identifiers
  - input nodes may be shared among graphs
  - identifiers $\mathrm{idf}_{G_t}\colon V_t \to \mathbb{N}$
  - w.l.o.g. $|\mathrm{idf}_{G_t}(V_t)| = |V_t|$
- preaccumulated in parallel with T threads
- i_max largest identifier among all G_t and already recorded prior parts of the global graph

- simultaneous preaccs. with a shared vector of derivative values are subject to **data races**
- threads place/combine unrelated values in derivative memory for shared inputs
- use **thread-local derivative memory** instead [4]

Alternatives for Thread-Local Derivative Memory

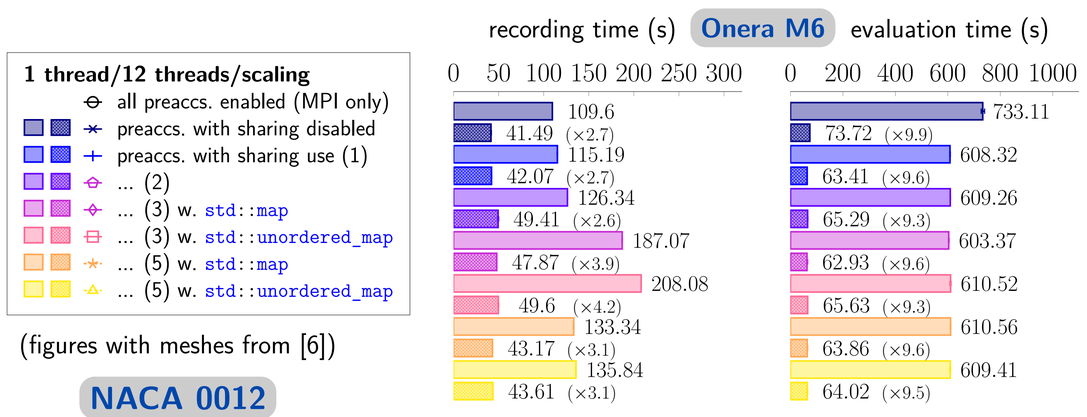


	runtime for single adjoint access	runtime for memory allocation (one thread)	memory consumption (all threads)	remarks/further costs
(1) large vector	$\mathcal{O}(1)$	$\mathcal{O}(i_\mathsf{max})$ (worst case)	$\mathcal{O}(i_\mathsf{max} \cdot T)$	vectors may persist across preaccs., reallocation not always required
(2) large vector with offset	$\mathcal{O}(1)$	$\mathcal{O}(i_\mathsf{max})$ (worst case)	$\mathcal{O}(i_\mathsf{max} \cdot T)$ (worst case)	same as (1), $\mathcal{O}(\lvert V_t\rvert)$ runtime to compute min, max
(3) map, `std::map`	$\mathcal{O}(\log \lvert V_t\rvert)$ (upper bound)	included in access times	$\mathcal{O}(\lvert V_t\rvert \cdot T)$	maps can be populated dynamically
(3) map, `std::unordered_map`	$\mathcal{O}(1)$ (average) $\mathcal{O}(\lvert V_t\rvert)$ (worst case)	included in access times	$\mathcal{O}(\lvert V_t\rvert \cdot T)$	same as (3) w. `std::map`, also applies to other maps below additional indirection, memory for both map and vector, compute $\lvert V_t\rvert$ (might be known)
(4) remap identifiers, `std::map`, small vector	$\mathcal{O}(\log \lvert V_t\rvert)$ (upper bound)	included in access times (map) $\mathcal{O}(\lvert V_t\rvert)$ (vector)	$\mathcal{O}(\lvert V_t\rvert \cdot T)$	
(4) remap identifiers, `std::unordered_map`, small vector	$\mathcal{O}(1)$ (average) $\mathcal{O}(\lvert V_t\rvert)$ (worst case)	included in access times (map) $\mathcal{O}(\lvert V_t\rvert)$ (vector)	$\mathcal{O}(\lvert V_t\rvert \cdot T)$	same as (4) w. `std::map`
(5) map to edit graph, `std::map`, small vector	$\mathcal{O}(1)$	$\mathcal{O}(\lvert V_t\rvert)$ (vector)	$\mathcal{O}(\lvert V_t\rvert \cdot T)$	editing has same map-related time complexity and temporary memory consumption as one evaluation in (4) w. `std::map`
(5) map to edit graph, `std::unordered_map`, small vector	$\mathcal{O}(1)$	$\mathcal{O}(\lvert V_t\rvert)$ (vector)	$\mathcal{O}(\lvert V_t\rvert \cdot T)$	analogous to (5) w. `std::map`, but w.r.t. (4) w. `std::unordered_map`

- (1) consumes too much memory, (2) could save memory but is often as bad in practice
- (3) has unfavourable runtime, (4) has no advantages compared to (3)
- (5) advances (4), combines advantages of (1) and (3) in case of multiple evaluations

Benchmarking in SU2

- open-source multiphysics simulation-suite **SU2** [9, 10]
  - discrete adjoints by means of reverse AD [1, 2]
  - operator overloading (OO) AD with **CoDiPack** [12]
  - **MeDiPack** for OO AD of MPI
- **OpDiLib** provides OO AD of OpenMP [7, 3]
- our prior work enables OpenMP-parallel discrete adjoints in SU2 with OpDiLib [6, 5]
- **goal:** preaccs. with sharing disabled in [6], re-enable them using local adjoints [5, 4]
- benchmarks with three test cases from [6], Elwetritsch cluster at RPTU
  - aerodynamic lift as objective, mesh coordinates as parameters
  - SU2 uses **reverse accumulation**, an iterative AD approach for differentiating fixed-points [8]
  - primary recording, multiple evaluations for rev. acc.; secondary recording, 1 evaluation
  - Intel Xeon Gold 6126 (each 12 cores, 1 NUMA domain), dual-socket nodes
  - ⊖ is MPI-only, one proc. per core; others: 1 proc. per socket, 1 thread per core
  - (5) applied only to preaccs. with multiple evaluations, otherwise use corresponding variant of (3)



(figures with meshes from [6])

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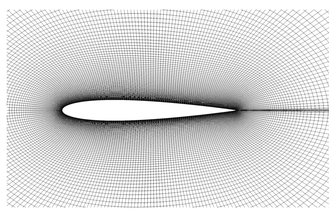
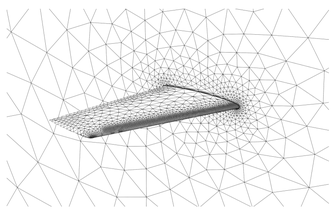


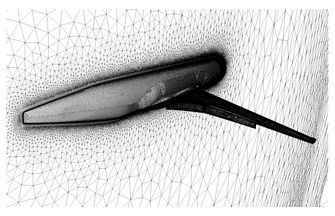
75140 quad.
300 fixed-point iter.

Onera M6

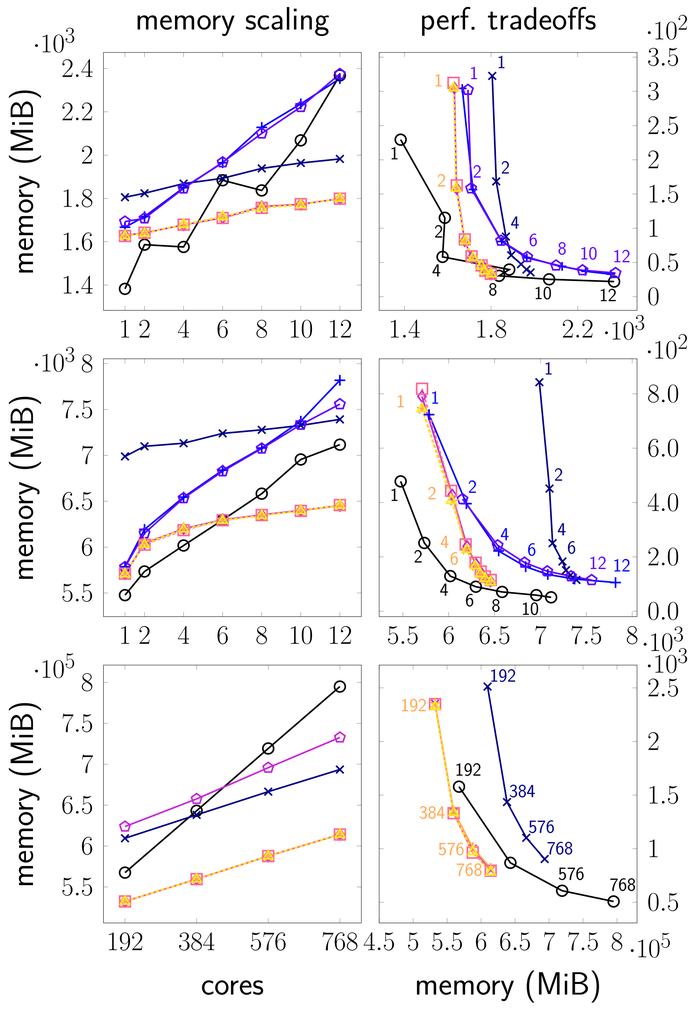


258969 tetr.
300 Krylov iter.

NASA HL-CRM



18 Mio. cells/8.3 Mio. nodes
1000 Krylov iter.



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Primary reference.
See also references cited therein.

Software

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