Introduction to Algorithmic Differentiation

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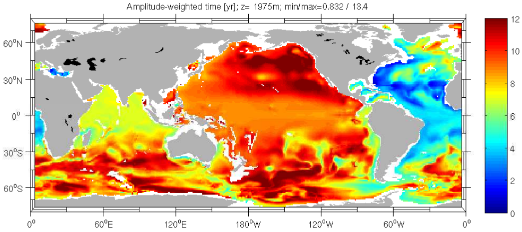
outline

- motivation
- basic principles
- tools and methods
- considerations for the user



why algorithmic differentiation?

given: some numerical model $\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}) : \mathbb{R}^n \mapsto \mathbb{R}^m$
implemented as a (large / volatile) program

wanted: sensitivity analysis, optimization, parameter (state) estimation, higher-order approximation...

1. don't pretend we know nothing about the program
(and take finite differences of an oracle)
2. get machine precision derivatives as $\boldsymbol{J}\dot{\boldsymbol{x}}$ or $\bar{\boldsymbol{y}}^T \boldsymbol{J}$ or ...
(avoid approximation-versus-roundoff problem)
3. the reverse (aka adjoint) mode yields "cheap" gradients
4. if the program is large, so is the adjoint program, and
so is the effort to do it manually ... easy to get wrong but hard to debug

$\Rightarrow$ use tools to do it **automatically!**

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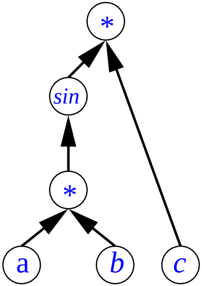
how does AD compute derivatives?

$f : y = sin(a * b) * c : \mathbb{R}^3 \mapsto \mathbb{R}$

yields a graph representing the order of computation:



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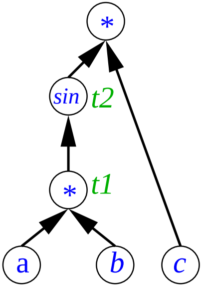

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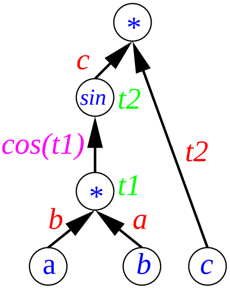

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- e.g. `sin(t1)` yields `p1=cos(t1)`
- in our example all others are already stored in variables

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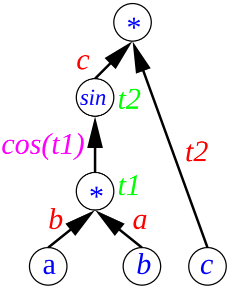

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What do we do with this?

forward mode with directional derivatives

- **associate** each variable v with a derivative $\dot{v}$
- take a point (a_0, b_0, c_0) and a direction $(\dot{a}, \dot{b}, \dot{c})$
- for each $v = \phi(w, u)$ propagate forward in order
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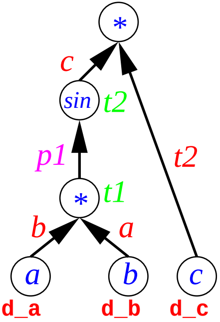

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  or *by address* [a%v,a%d]
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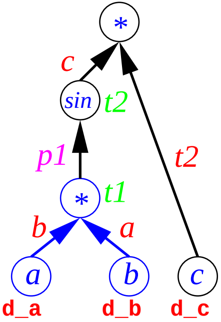

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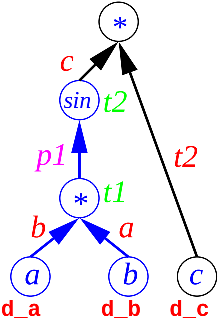

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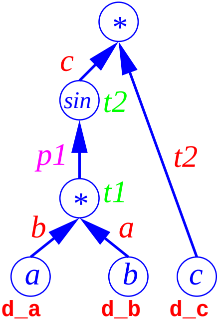

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d_y = d_t2*c + d_c*t2
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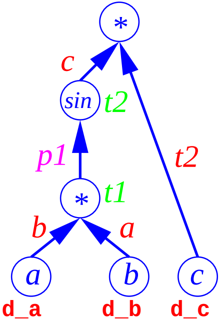

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What is in d_y ?

d_y contains a projection

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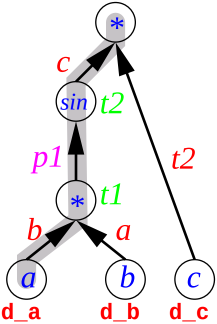

- yields the first element of the gradient
- all gradient elements cost $\mathcal{O}(n)$ function evaluations

applications

for instance

- ocean/atmosphere state estimation & uncertainty quantification, oil reservoir modeling
- computational chemical engineering
- CFD (airfoil shape optimization, suspended droplets e.g. by Dervieux, Forth, Gauger, Giles et al.)
- beam physics
- mechanical engineering (design optimization)

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- Jacobian projections
- Hessian projections
- higher order derivatives
  (full or partial tensors, univariate Taylor series)

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How do we get the cheap gradients?

higher order AD (1)

- propagation of (univariate) Taylor polynomials up to order o (in d directions) with coefficients $a_j^{(i)}, j = 1 \ldots o(, i = 1 \ldots d)$ around a common point $a_0 \equiv a_0^i$ in the domain

$$\phi(a_o + h) = \phi(a_0) + \phi\prime(a_0) \cdot h + \frac{\phi\prime\prime(a_0)}{2!} \cdot h^2 + \ldots + \frac{\phi^{(d)}(a_0)}{o!} \cdot h^o$$

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- but the propagation is applied to the sequence of programming language intrinsics
- and all relevant non-linear univariate (Fortran/C++) intrinsics ϕ can be seen as ODE solutions

higher order AD (2)

- using ODE approach permits (cheap) recurrence formulas for the coefficients, e.g. for $b = a^r$ we get

$$\tilde{b}_k = \frac{1}{a_o}\left(r \sum_{j=1}^{k} b_{k-j}\tilde{a}_j - \sum_{j=1}^{k-1} a_{k-j}\tilde{b}_j \right) \quad \text{with } \tilde{c}_j = j c_j$$

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- cost approx. $O(o^2)$ (arithmetic) operations
(for first order underlying ODE up to one nonlinear univariate)

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```
Tres += pk-1; Targ1 += pk-1; Targ2 += pk-1;
for (l=p-1; l>=0; l--)
  for (i=k-1; i>=0; i--) {
    *Tres = dp_T0[arg1]**Targ2-- + *Targ1--*dp_T0[arg2];
    Targ1OP = Targ1-i+1;
    Targ2OP = Targ2;
    for (j=0;j<i;j++) {
      *Tres += (*Targ1OP++) * (*Targ2OP--);
    }
    Tres--;
  }
dp_T0[res] = dp_T0[arg1] * dp_T0[arg2];
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  }
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```

- uses a work array and various pointers into it; the indices res, arg1, arg2 have been previously recorded; p = number of directions, k = derivative order
  makes compiler optimization difficult etc.; various AD tools

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- ... with emphasis on performance - Rapsodia (Charpentier, U.; OMS 2009) - example of generated code

```
r.v = a.v * b.v;
r.d1_1 = a.v * b.d1_1 + a.d1_1 * b.v;
r.d1_2 = a.v * b.d1_2 + a.d1_1 * b.d1_1 + a.d1_2 * b.v;
r.d1_3 = a.v * b.d1_3 + a.d1_1 * b.d1_2 + a.d1_2 * b.d1_1 + a.d1_3 * b.v;
r.d2_1 = a.v * b.d2_1 + a.d2_1 * b.v;
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```

- C++ active types called: `RAfloatS`, `RAfloatD`
- in Fortran: `RArealS`, `RArealD`, `RAcomplexS`, `RAcomplexD`
- are flat data structures with fields `v` and `d1_1`...`d2_3`
- code in Fortran: replace "." with "%"
- most differences are in the wrapping (also generated because of number the of interfaces, especially for Fortran)

Rapsodia Use Example

```
#include <iostream>
#include <cmath>

int main(void){



  double x,y;
  // the point at which we execute
  x=0.3;







  // compute sine
  y=sin(x);
  // print it
  std::cout << "y="<< y << std::endl;







  return 0; }
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- generate the library:

`generate -d 2 -o 3 -c Rlib`

Rapsodia Use Example

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- adjust the types/references

Rapsodia Use Example

```
#include <iostream>
#include <cmath>
#include "RAinclude.ipp"
int main(void){
  int i,j;
  const int directions=2;
  const int order=3;
  RAfloatD x,y;
  // the point at which we execute
  x=0.3;
  // initialize the input coefficients
  // in the 2 directions
  for( i=0;i<directions;i++) {
    for( j=0;j<order; j++) {
      if (j==0) x.set(i+1,j+1,0.1*(i+1));

      else x.set(i+1,j+1,0.0);
    } }
  // compute sine
  y=sin(x);
  // print it
  std::cout << "y="<< y.v << std::endl;
  // get the output Taylor coefficients
  // for each of the 2 directions
  for( i=0;i<directions;i++) {
    for( j=0;j<order; j++) {
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               << std::endl;
    } }
  return 0; }
```

- figure out what to compute
- generate the library:

`generate -d 2 -o 3 -c Rlib`

- adjust the types/references
- augment the “driver”

Rapsodia Use Example

```
#include <iostream>
#include <cmath>
#include "RAinclude.ipp"
int main(void){
  int i,j;
  const int directions=2;
  const int order=3;
  RAfloatD x,y;
  // the point at which we execute
  x=0.3;
  // initialize the input coefficients
  // in the 2 directions
  for( i=0;i<directions;i++) {
    for( j=0;j<order; j++) {
      if (j==0) x.set(i+1,j+1,0.1*(i+1));

      else x.set(i+1,j+1,0.0);
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- augment the “driver”
- compile and link everything

multivariate derivatives

have n inputs, coefficient multi-indices track differentiation with respect to individual inputs; exploit symmetry

- direct w multi index management: COSY, AD02,..

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- interpolation coefficients are precomputed
- practical advantage can be observed already for small $o > 3$
- interpolation error is typically negligible except in some cases; use modified schemes (Neidinger 2004 -)

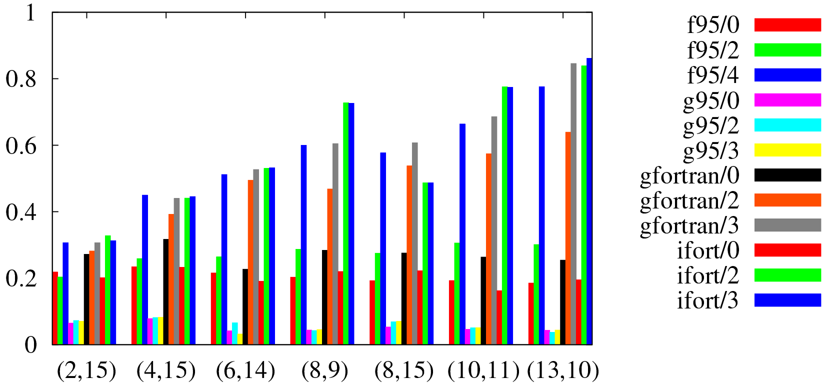
Rapsodia vs AD02

run time for derivative tensors of an ocean acoustics model;
DISCLAIMER: big advantage mostly due to univariate propagation!

		AD02				Rapsodia					
		g95	ifort	NAG				g95	ifort	NAG	
o	n	-O3	-O2	-O2	-O4	d^*	d	-O3	-O2	-O2	-O4
2	5	0.599	0.460	0.543	0.658	15	15	0.072	0.106	0.087	0.086
4	3	40.97	11.97	13.67	14.41	15	15	0.161	0.255	0.181	0.176
6	3	185.4	58.88	73.63	71.21	14	28	0.514	0.794	0.538	0.515
8	2	105.8	36.39	45.41	41.56	9	9	0.250	0.366	0.262	0.257
8	3	651.1	*	289.8	285.2	15	45	1.157	1.762	1.172	1.101
10	3	1958.	*	+	+	11	66	2.453	3.523	2.474	2.420
13	3	+	*	+	+	10	105	5.677	8.656	5.673	5.638

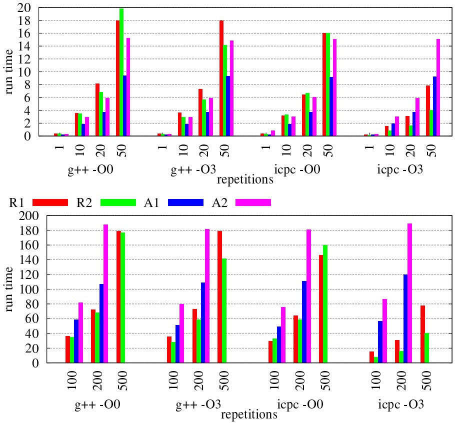
- o = derivative order, n = number of inputs
- $+$ = we did not wait for completion; * = aborted because of lack of memory;
- to see the difference to loops we had to hand-write our own test lib

Rapsodia vs Loops



run time ratios of Rapsodia vs. hand written library with loops over `PARAMETER`ized o and d^*

Rapsodia vs Adol-C



- simple model of volcanic eruption
- small set of active variables
- for the test: repeated evaluations
- R1: Rapsodia
- R2: Rapsodia inlined
- A1: `hov_forward`
- A2: taping + `hov_forward`
- Note: no "inline" directive for Fortran, need to rely on interprocedural optimization

Parallelization

- outer loop over d directions
- inner loop(s) over derivative order o
- identical amount of work in each direction
- all coefficients depend only on operation argument (result)
- no dependency between coefficients of different directions
- previously investigated with OpenMP by Bücker et al.
- only experimental prototypes (reuse?)
- have multicore hardware
- Can we parallelize:
  - within the library (w/o user code changes) ?
  - models with side effects?

to parallelize Rapsodia - limit the unrolling of the outer loop

limited unrolling

also aims at **constraining code bloat**, can help compiler optimization
Example: unrolled code for 4 directions:

```
r%v=a%v * b%v
r%d1_1=a%v * b%d1_1 + a%d1_1 * b%v
r%d1_2=a%v * b%d1_2 + a%d1_1 * b%d1_1 + a%d1_2 * b%v
r%d1_3=a%v * b%d1_3 + a%d1_1 * b%d1_2 + a%d1_2 * b%d1_1 + a%d1_3 * b%v
r%d2_1=a%v * b%d2_1 + a%d2_1 * b%v
r%d2_2=a%v * b%d2_2 + a%d2_1 * b%d2_1 + a%d2_2 * b%v
r%d2_3=a%v * b%d2_3 + a%d2_1 * b%d2_2 + a%d2_2 * b%d2_1 + a%d2_3 * b%v
r%d3_1=a%v * b%d3_1 + a%d3_1 * b%v
r%d3_2=a%v * b%d3_2 + a%d3_1 * b%d3_1 + a%d3_2 * b%v
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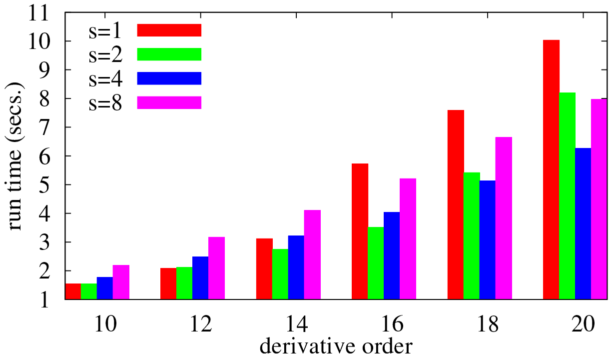
r%d4_1=a%v * b%d4_1 + a%d4_1 * b%v
r%d4_2=a%v * b%d4_2 + a%d4_1 * b%d4_1 + a%d4_2 * b%v
r%d4_3=a%v * b%d4_3 + a%d4_1 * b%d4_2 + a%d4_2 * b%d4_1 + a%d4_3 * b%v
```

vs. partially unrolled for 4 directions using 2 slices; stay **flat within slice**

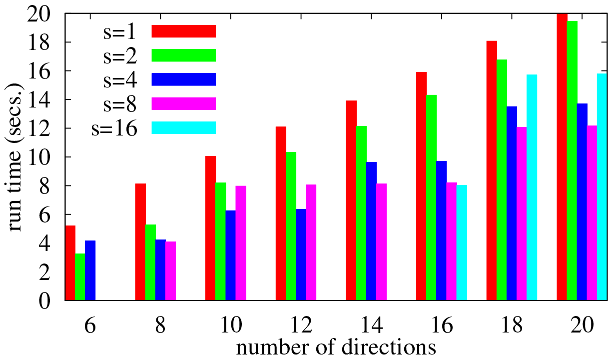
```
r%v=a%v * b%v
do i=1, 2, 1
 r%s(i)%d1_1=a%v*b%s(i)%d1_1 + a%s(i)%d1_1*b%v
 r%s(i)%d1_2=a%v*b%s(i)%d1_2 + a%s(i)%d1_1*b%s(i)%d1_1 + a%s(i)%d1_2*b%v
 r%s(i)%d1_3=a%v*b%s(i)%d1_3 + a%s(i)%d1_1*b%s(i)%d1_2 + a%s(i)%d1_2*b%s(i)%d1_1 + a%s(i)%d1_3*b%v
 r%s(i)%d2_1=a%v*b%s(i)%d2_1 + a%s(i)%d2_1*b%v
 r%s(i)%d2_2=a%v*b%s(i)%d2_2 + a%s(i)%d2_1*b%s(i)%d2_1 + a%s(i)%d2_2*b%v
 r%s(i)%d2_3=a%v*b%s(i)%d2_3 + a%s(i)%d2_1*b%s(i)%d2_2 + a%s(i)%d2_2*b%s(i)%d2_1 + a%s(i)%d2_3*b%v
end do
```

limited unrolling 2

- main problem: can only slice directions (not order),
- iteration complexity differs between ops.
- impact on register allocation differs between compilers/platforms

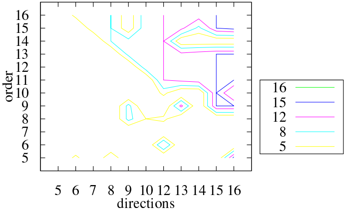


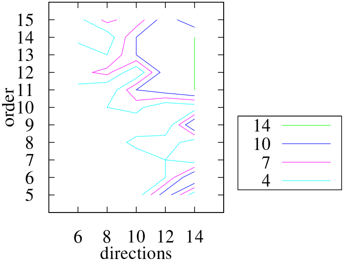
limited unrolling 3

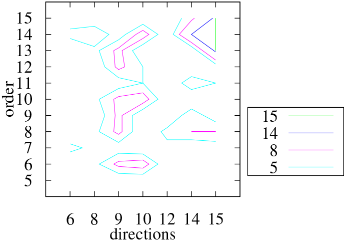


What is a good choice for the number of slices?

limited unrolling 4







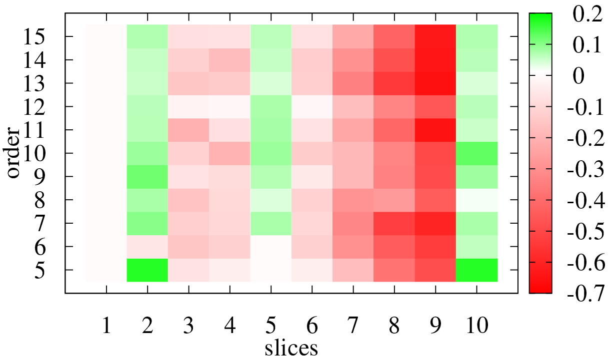
contours of optimal slices for test case with

1. mostly non-linear
2. mix linear/non-linear
3. mostly linear

operations

limited unrolling 5

(o, d)	5	6	7	8	9	10	11	12	13	14	15
5	5	3	1	4	2	2	11	2	13	2	3
6	5	2	7	4	9	10	11	2	13	2	5
7	5	6	1	4	3	2	11	4	13	2	3
8	5	2	7	4	9	2	11	6	13	8	8
9	5	2	7	2	9	2	11	2	13	7	3
10	5	2	7	4	9	10	11	2	13	2	3
11	5	2	7	2	3	5	11	2	13	7	5
12	5	2	7	2	9	5	11	2	13	2	3
13	5	2	1	4	9	2	11	4	13	2	15
14	5	6	7	8	3	10	11	2	13	14	15
15	5	3	7	2	3	2	11	2	13	7	15



Asynchronous parallel loops

OpenMP direction loop parallelization is not efficient on operator level
so lets do something else (i.e. much less convenient than OpenMP)

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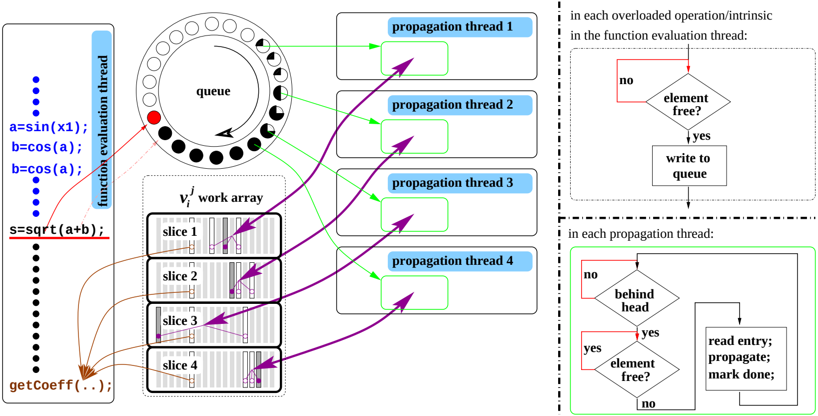

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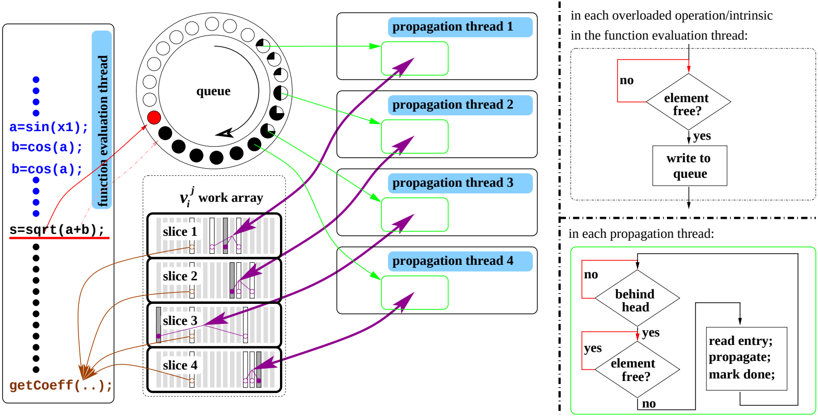
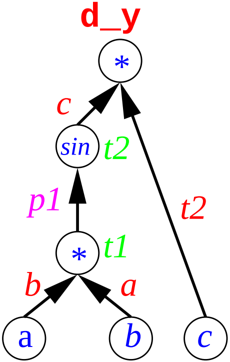


use of open portable atomics lib for spinlocks is crucial

reverse mode with adjoints

- same association model
- take a point (a_0, b_0, c_0), compute y, pick a weight $\bar{y}$
- for each $v = \phi(w, u)$ propagate backward
  $\bar{w} += \frac{\partial \phi}{\partial w}\ \bar{v}; \quad \bar{u} += \frac{\partial \phi}{\partial u}\ \bar{v}; \quad \bar{v} = 0$



backward propagation code appended:

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t1 = a*b
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y = t2*c
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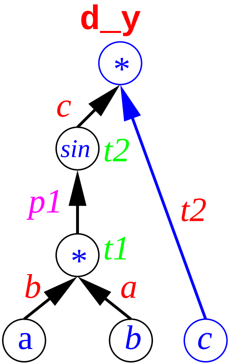

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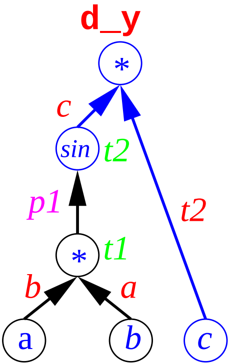

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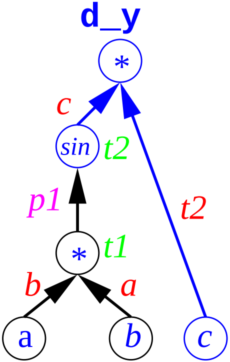

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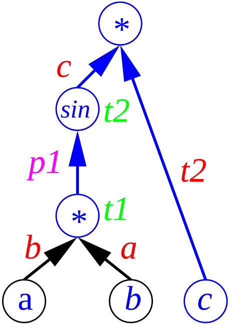

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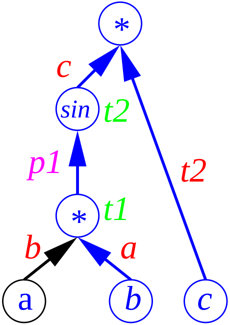

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d_t2 = c*d_y
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d_t1 = p1*d_t2
d_b = a*d_t1
```

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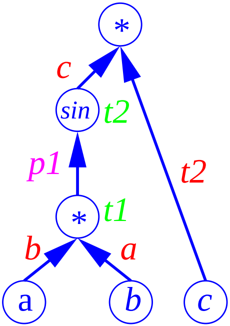

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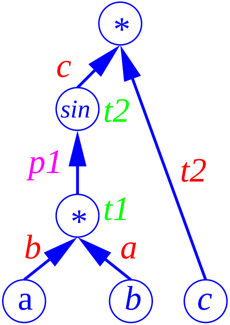

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d_t2 = c*d_y
d_y = 0
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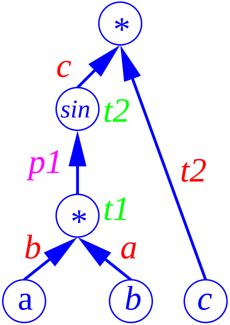
d_b = a*d_t1
d_a = b*d_t1
```

What is in (d_a,d_b,d_c)?

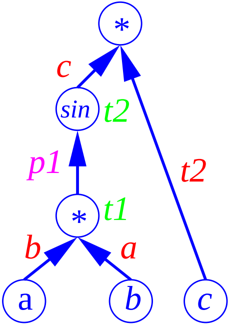
(d_a,d_b,d_c) contains a projection

- $\bar{\boldsymbol{x}} = \bar{\boldsymbol{y}}^T \boldsymbol{J}$ computed at $\boldsymbol{x}_0$



(d_a,d_b,d_c) contains a projection

- $\bar{\boldsymbol{x}} = \bar{\boldsymbol{y}}^T \boldsymbol{J}$ computed at $\boldsymbol{x}_0$
- for example for $\bar{y} = 1$ we have $[\bar{a}, \bar{b}, \bar{c}] = \nabla f$



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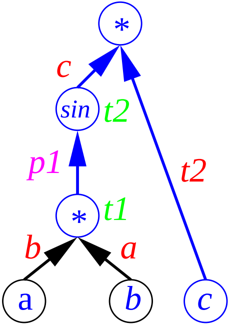

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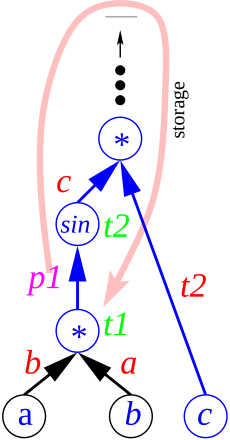

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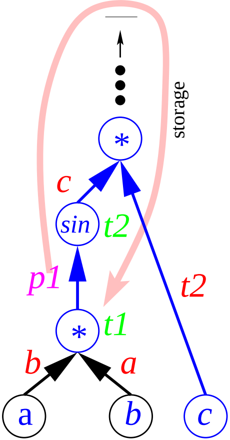

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Reverse mode with Adol-C.

ADOL-C

- http://www.coin-or.org/projects/ADOL-C.xml
- operator overloading creates an execution trace (also called 'tape')

Speelpenning example $y = \prod_i x_i$ evaluated at $x_i = \frac{i+1}{i+2}$

```
 double *x = new  double[n];
 double  t = 1;
 double y;

for(i=0; i<n; i++) {
  x[i]   = (i+1.0)/(i+2.0);
  t *= x[i]; }
y = t;

delete[] x;
```

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```
#include "adolc.h"
adouble *x = new adouble[n];
adouble  t = 1;
 double y;
trace_on(1);
for(i=0; i<n; i++) {
  x[i] <<= (i+1.0)/(i+2.0);
  t *= x[i]; }
t >>= y;
trace_off();
delete[] x;
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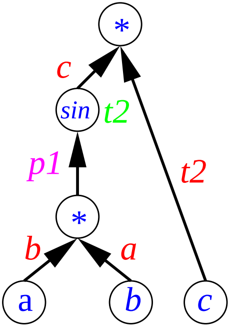
delete[] x;
```

use a driver :

```
  gradient(tag,
           n,
           x[n],
           g[n])
```

sidebar: preaccumulation & propagation

- build expression graphs (limited by aliasing, typically to a basic block)
- **preaccumulate** them to local Jacobians $\boldsymbol{J}$
- long program with control flow $\Rightarrow$ sequence of graphs $\Rightarrow$ sequence of $\boldsymbol{J}_i$



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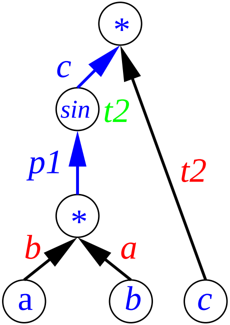

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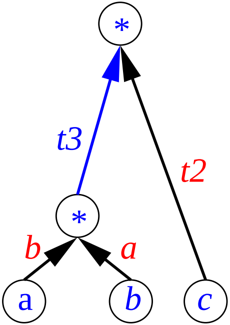

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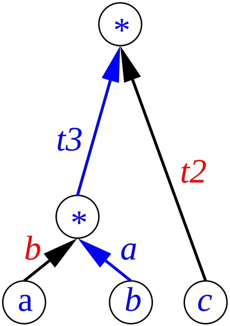

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t3 = c*p1
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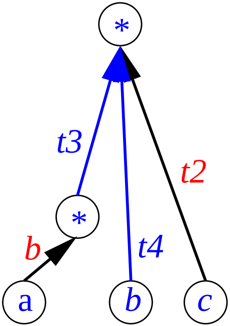

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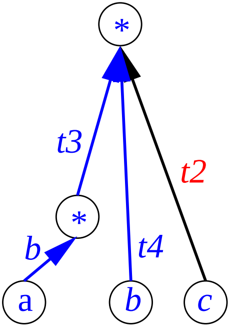

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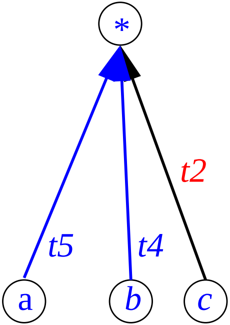


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t3 = c*p1
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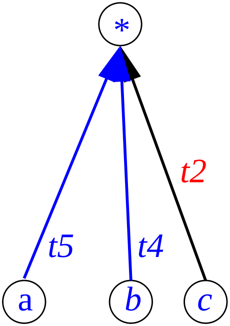


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- (t5,t4,t2) is the preaccumulated $\boldsymbol{J}_i$
- $\min_{ops}$(preacc.) ? a combinatorial problem
  $\Rightarrow$ compile time AD optimization!
- forward propagation of $\dot{\boldsymbol{x}}$
  $(\boldsymbol{J}_k \circ \ldots \circ (\boldsymbol{J}_1 \circ \dot{\boldsymbol{x}}) \ldots)$
- adjoint propagation of $\bar{\boldsymbol{y}}$
  $(\ldots(\bar{\boldsymbol{y}}^T \circ \boldsymbol{J}_k) \circ \ldots \circ \boldsymbol{J}_1)$

sidebar: toy example - source transformation reverse mode

code preparation

numerical "model" program:

```
         subroutine head(x,y)

double precision,intent(in) :: x

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         !$openad INDEPENDENT(x)
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code preparation ⇒ reverse mode OpenAD pipeline

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retrieve stored J_i & propagate:

```
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oadD_ptr = oadD_ptr-1
oadS_6 = oadD(oadD_ptr)
X%d = X%d+Y%d*oadS_6
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code preparation ⇒ reverse mode OpenAD pipeline

⇒ adapt the driver routine

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          end subroutine
```

driver modified for reverse mode:

```
        program driver
          use OAD_active
          implicit none
          external head
          type(active):: x, y
          x%v=.5D0
          y%d=1.0
          our_rev_mode%tape=.TRUE.
          call head(x,y)
          print *, "F(1,1)=",x%d
        end program driver
```

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```

forward vs. reverse

- simplest rule: given $y = f(x) : \mathbb{R}^n \mapsto \mathbb{R}^m$ use reverse if $n \gg m$ (gradient)
- what if $n \approx m$ and large
  - want only projections, e.g. $J\dot{x}$
  - sparsity (e.g. of the Jacobian)
  - partial separability (e.g. $f(x) = \sum(f_i(x_i)), x_i \in \mathcal{D}_i \Subset \mathcal{D} \ni x$)
  - intermediate interfaces of different size
- the above may make forward mode feasible (projection $\bar{y}^T J$ requires reverse)
- higher order tensors (practically feasible for small n) $\rightarrow$ forward mode (reverse mode saves factor n in effort only once)
- this determines overall propagation direction, not necessarily the local preaccumulation (combinatorial problem)

source transformation vs. operator overloading

- complicated implementation of tools
- especially for reverse mode
- full front end, back end, analysis
- efficiency gains from
  - compile time AD optimizations
  - activity analysis
  - explicit control flow reversal
- source transformation based type change & overloaded operators appropriate for higher-order derivatives.
- efficiency depends on analysis accuracy

- simple tool implementation
- reverse mode: generate & reinterpret an execution trace $\rightarrow$ inefficient
- implemented as a library
- efficiency gains from:
  - runtime AD optimization
  - optimized library
  - inlining (for low order)
- manual type change
  - $\lightning$ formatted I/O, allocation,...
  - matching signatures (Fortran)
  - easier with templates

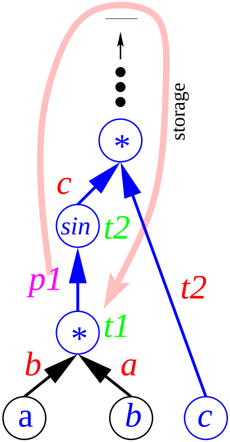
---

higher-order derivatives $\Rightarrow$ source transformation based type change + overloaded operators.

Reversal Schemes

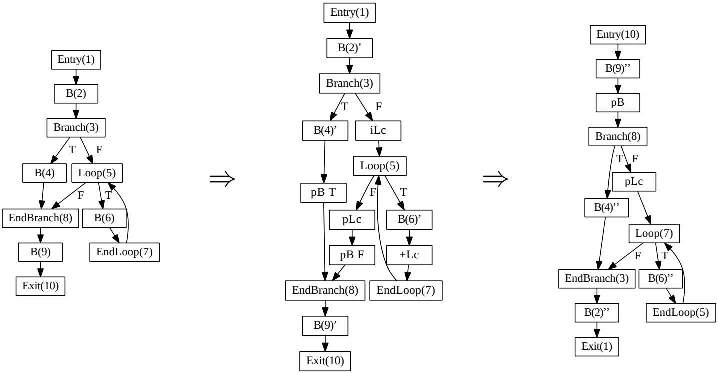
- why it is needed
- major modes
- alternatives

recap: store intermediate values / partials



storage also needed for control flow trace and addresses...

original CFG ⇒ record a path through the CFG ⇒ adjoint CFG

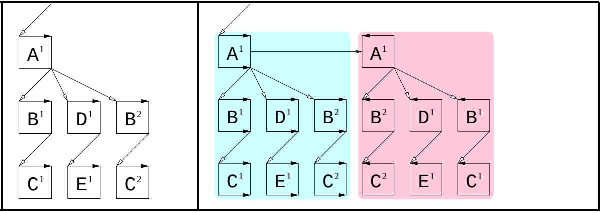


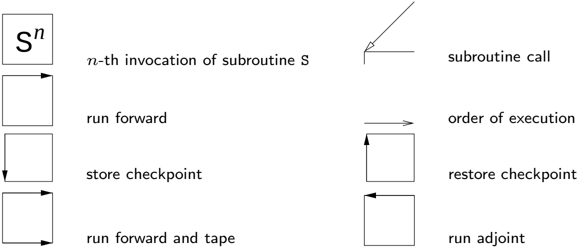
often cheap with structured control flow and simple address computations (e.g. index from loop variables)

unstructured control flow and pointers are expensive

trace all at once = global *split* mode

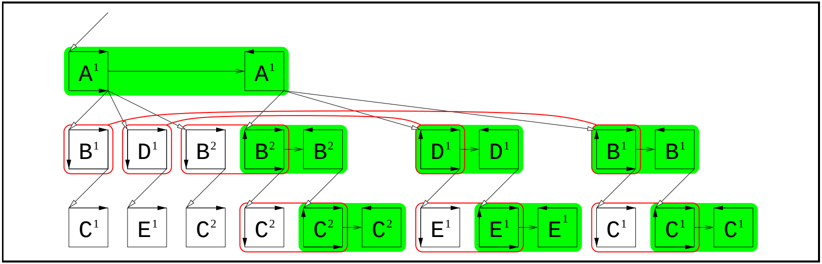
```
subroutine A()
   call B(); call
D(); call B();
end subroutine A
subroutine B()
   call C()
end subroutine B
subroutine C()
   call E()
end subroutine C
```





- have memory limits - need to create tapes for short sections in reverse order
- subroutine is "natural" checkpoint granularity, different mode...

trace one SR at a time = global *joint* mode



taping-adjoint pairs

checkpoint-recompute pairs

the deeper the call stack - the more recomputations
(unimplemented solution - result checkpointing)

familiar tradeoff between storing and recomputation at a higher level but in theory can be all unified.

in practice - hybrid approaches...

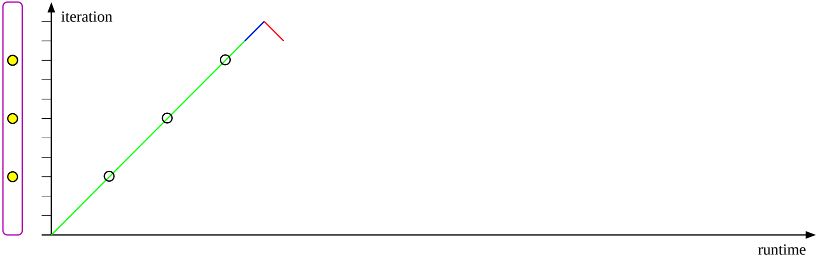
use of checkpointing to mitigate storage requirements

◇ 11 iters.

use of checkpointing to mitigate storage requirements

- 11 iters., memory limited to one iter. of storing $\boldsymbol{J}_i$
- run forward, store the last step, and adjoin

use of checkpointing to mitigate storage requirements



- 11 iters., memory limited to one iter. of storing $\boldsymbol{J}_i$ &
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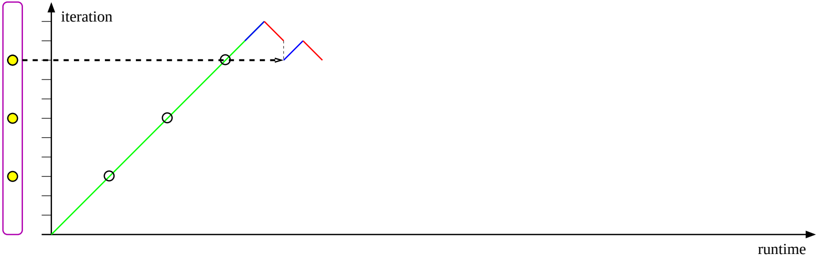

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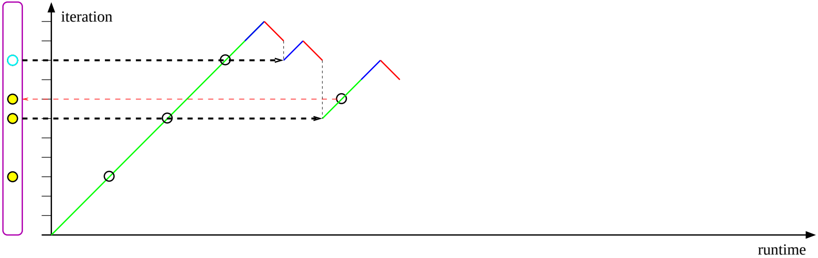

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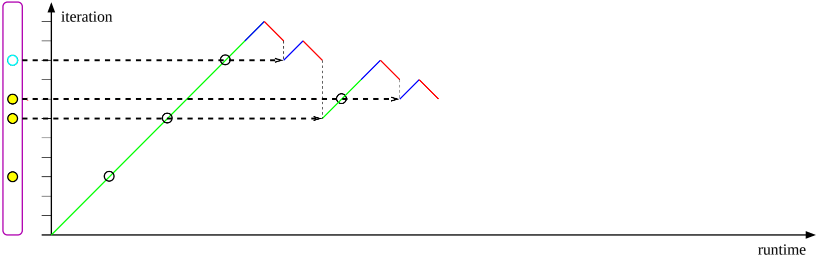

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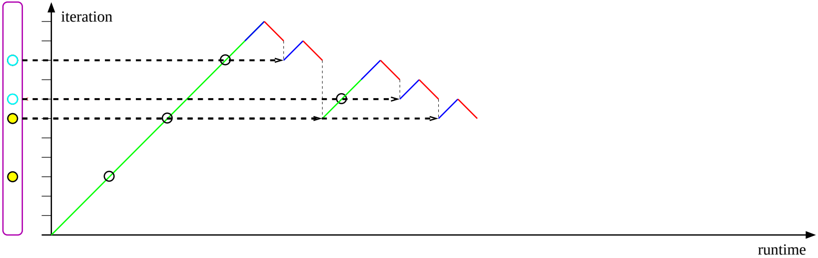

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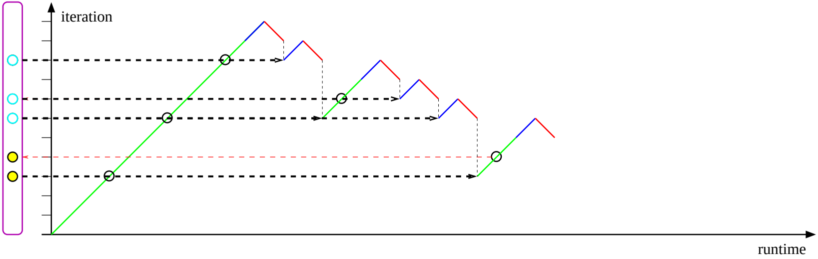

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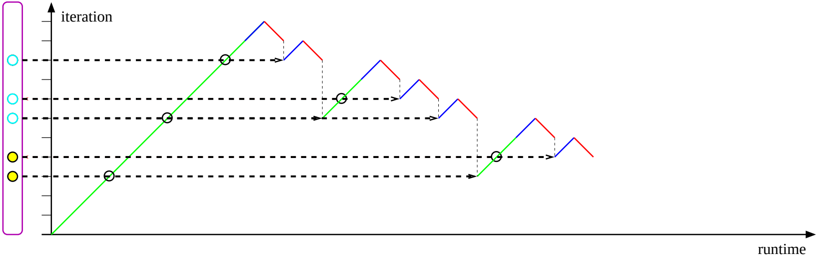

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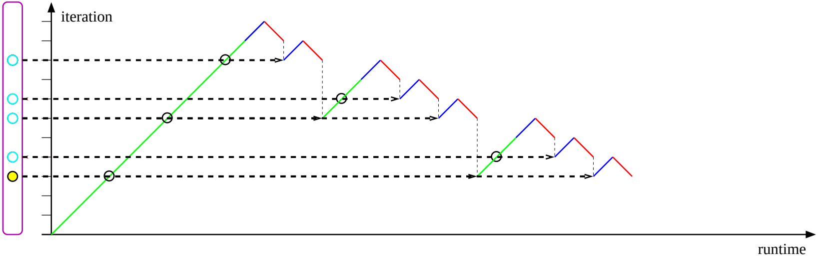

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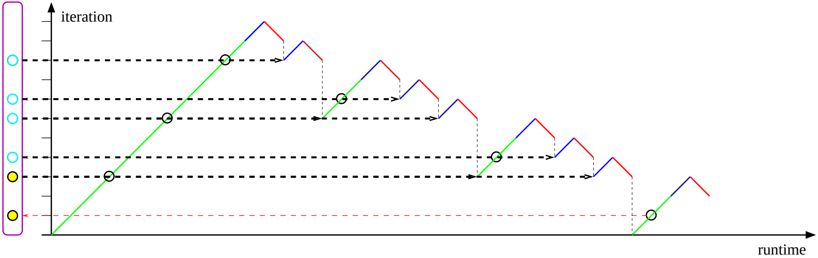

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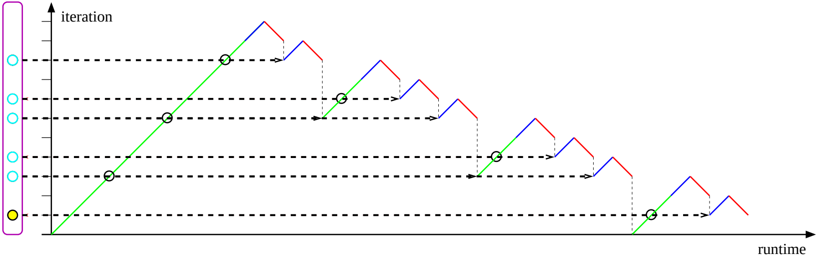

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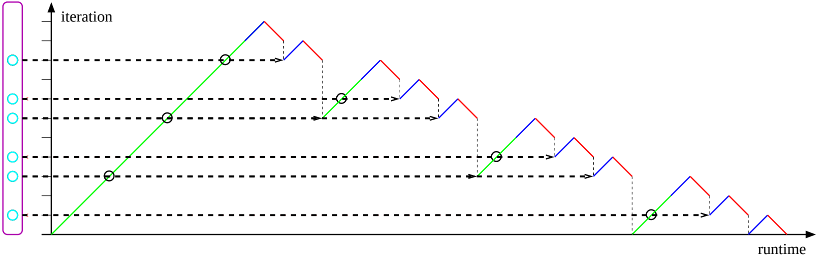

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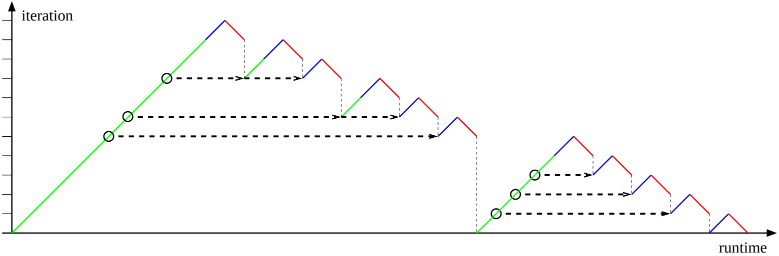

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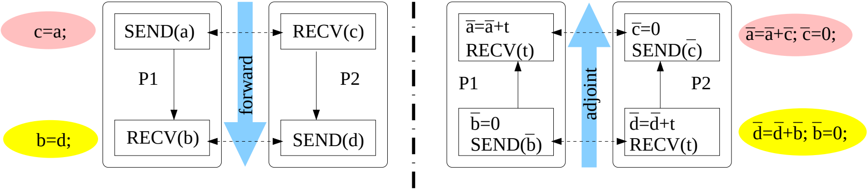
- optimal (binomial) scheme encoded in `revolve`; C++ and F9X implementation

MPI - parallelization

- simple MPI program needs 6 calls :

```
mpi_init      // initialize the environment
mpi_comm_size // number of processes in the communicator
mpi_comm_rank // rank of this process in the communicator
mpi_send      // send (blocking)
mpi_recv      // receive (blocking)
mpi_finalize  // cleanup
```

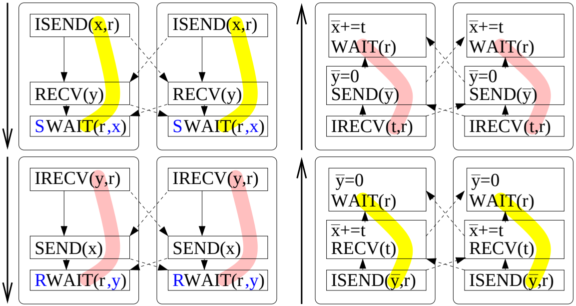
- example adjoining blocking communication between 2 processes and interpret as assignments



- use the communication graph as model

options for non-blocking reversal

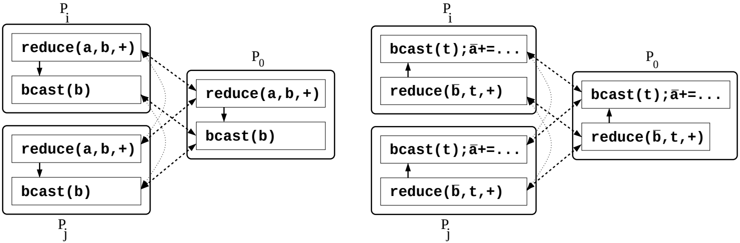
- ensure correctness ⇒ use nonblocking calls in the adjoint



- transformations are provably correct
- convey context ⇒ enables a transformation recipe per call (extra parameters and/or split interfaces into variants)
- promises to not read or **write** the respective buffer

collective communication

- example: reduction followed by broadcast
  $b_0 = \sum a_i$ followed by $b_i = b_0 \forall i$
- conceptually simple; `reduce` $\mapsto$ `bcast` and `bcast` $\mapsto$ `reduce`



- adjoint: $t_0 = \sum \bar{b}_i$ followed by $\bar{a}_i$+=$t_0 \forall i$
- has single transformation points (connected by hyper communication edge)
- efficiency for product reduction because of increment
  $\bar{a}_i$+=$\frac{\partial b_0}{\partial a_i} t_0, \forall i$

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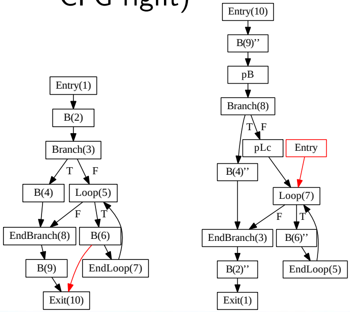

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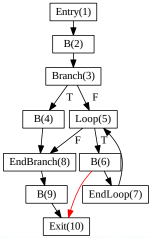
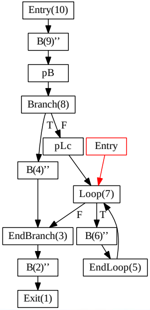
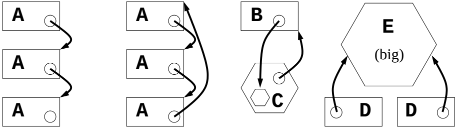




- OK without the red arrow
- some jumps are not permitted
- unstruct. control flow ↯ compiler opt.
- Fortran fallback: trace/replay enumerated basic blocks; for C++: hoist local variables inst.;
- exceptions: `catch` to undo `try` side effects

Checkpointing and non-contiguous data

checkpointing = saving program data (to disk)

- "contiguous" data: scalars, arrays (even with stride > 1), strings, structures,...
- "non-contiguous" data: linked lists, rings, structures with pointers,...
- checkpointing is very similar to "serialization"
- Problem: decide when to follow a pointer and save what we point to 

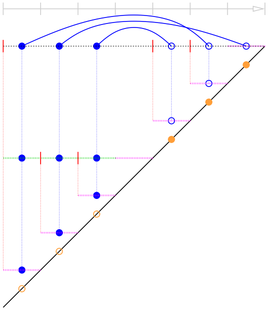
- unless we have extra info this is not decidable at source transformation time
- possible fallback: runtime bookkeeping of things that have been saved (is computationally expensive, cf. python `copy.deepcopy` or `pickle`)

Semantically Ambiguous Data

- e.g. `union` (or its Fortran counterpart `equivalence`)
  - data dependence analysis: dependencies propagate from one variable to **all** equivalenced variables
  - "activity" (i.e. the need to generate adjoint code for a variable) leaks to all equivalenced variables whether appropriate or not
  - certain technical problems with the use of an active type (as in OpenAD)
- work-arrays (multiple,0 semantically different fields are put into a (large) work-array); access via index offsets
  - data dependence analysis: there is *array section analysis* but in practice it is often not good enough to reflect the implied semantics
  - the entire work-array may become active / checkpointed
- programming patterns where the analysis has no good way to track the data dependencies:
  - data transfer via files (don't really want to assume all read data depends on all written data)
  - non-structured interfaces: exchanging data that is identified by a "key" but passed as `void*` or something equivalent.

Recomputation from Checkpoints and Program Resources

think of memory, file handles, sockets, MPI communicators,...



- problem when resource allocation and deallocation happen in different partitions (see hierarchical checkpointing scheme in the figure on the left)
- current AD checkpointing **does not track resources**
- dynamic memory is “easy” as long as nothing is deallocated before the adjoint sweep is complete.

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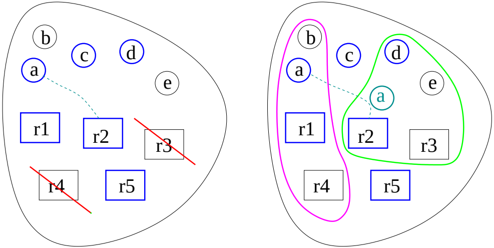

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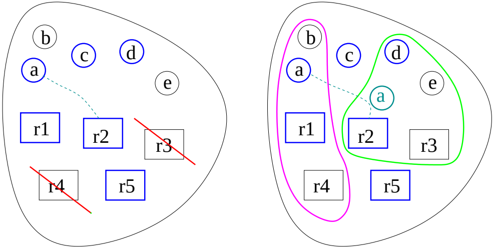

collaboration with Laurent Hascoët (Tapenade) at INRIA Sophia-Antipolis

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- effort for
  - initial implementation
  - **validation**
  - efficiency (generally - what is good for the adjoint is good for the model)
  - implement volatile parts with a domain-specific language (cf. ampl)?
  - **robustness**

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  - **smoothness of the model, utility of the cost function**

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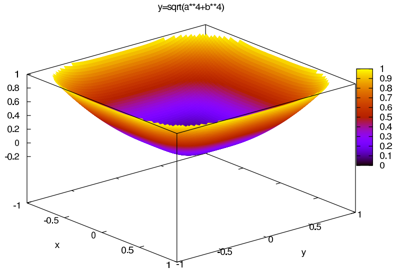
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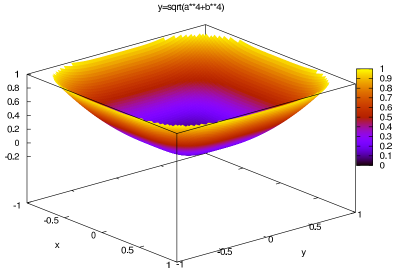

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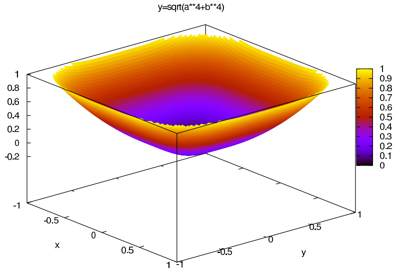

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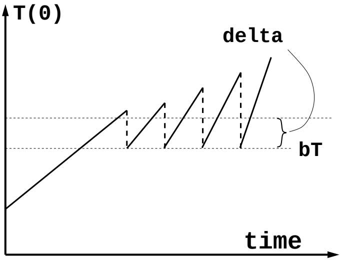
algorithmic differentiation computes derivatives of programs(!)

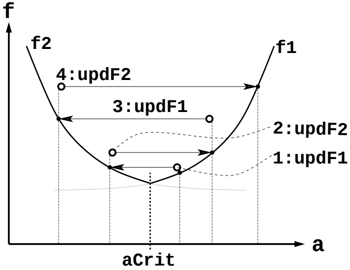
know your application e.g. fix point iteration, self adjoint, step size computation, convergence criteria
  ```

nonsmooth models

observed:

- `INF`, `NaN`, e.g. for $\sqrt{0 \pm 0}$; smoother in $[0, \varepsilon]$?
- oscillating derivatives (may be glossed over by FD) or derivatives growing out of bounds





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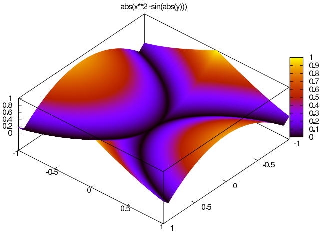
  - OpenAD (comparative tracing)

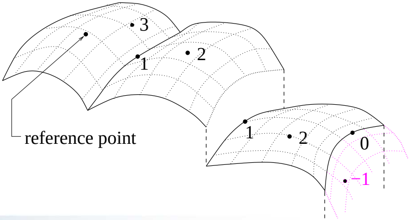
differentiability



piecewise differentiable function:
$|x^2 - sin(|y|)|$
is (locally) Lipschitz continuous;
almost everywhere differentiable
(except on the 6 critical paths)

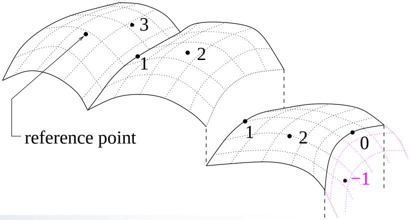
- Gâteaux: if $\exists\, \mathrm{d}f(x, \dot{x}) = \lim_{\tau \to 0} \frac{f(x+\tau\dot{x}) - f(x)}{\tau}$ for all directions $\dot{x}$
- Bouligand: Lipschitz continuous and Gâteaux
- Fréchet: $\mathrm{d}f(., \dot{x})$ continuous for every fixed $\dot{x}$ ... not generally
- in practice: often benign behavior, directional derivative exists and is an element of the generalized gradient.

case distinction



case distinction

3 locally analytic



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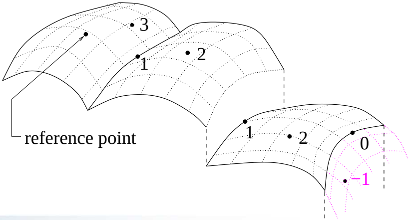

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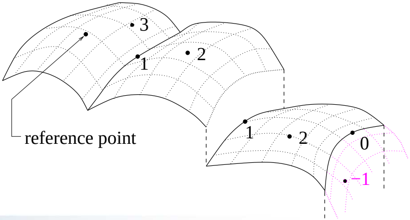

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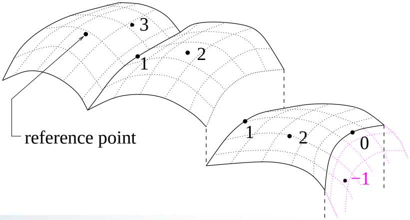

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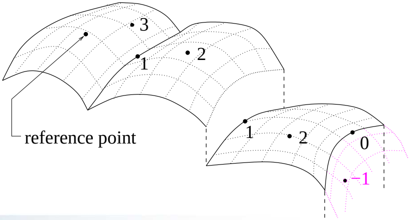
[-1 (operator overloading specific) arithmetic comparison yields a different value than before (tape invalid → sparsity pattern may be changed,...)]

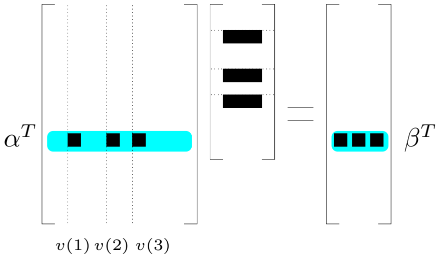


sparsity (1)

many repeated Jacobian vector products $\rightarrow$ compress the Jacobian
$F' \cdot S = B \in \mathbb{R}^{m\times q}$ using a seed matrix $S \in \mathbb{R}^{n\times q}$
What are S and q?
Row i in F' has ρ_i nonzeros in columns $v(1), \ldots, v(\rho_i)$
$F'_i = (\alpha_1, \ldots, \alpha_{\rho_i}) = \alpha^T$ and the compressed row is
$B_i = (\beta_1, \ldots, \beta_q) = \beta^T$ We choose S so we can solve:

$$\hat{S}_i \alpha = \beta$$

with $\hat{S}_i^T = (s_{v(1)}, \ldots, s_{v(\rho_i)})$

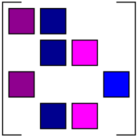


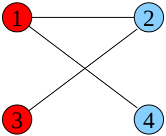
sparsity (2)

direct:

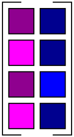
- Curtis/Powell/Reid: structurally orthogonal
- Coleman/Moré: column incidence graph coloring)

q is the color number in column incidence graph, each column in S represents a color with a 1 for each entry whose corresponding column in F' is of that color.





$$S = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$



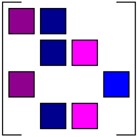
reconstruct F' by relocating nonzero elements (direct)

sparsity (3)

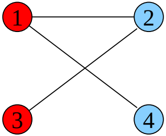
indirect:

- Newsam/Ramsdell: $q = \max_i \{\#nonzeros\} \leq \chi$
- S is a (generalized) Vandermonde matrix
  $\left[\lambda_i^{j-1}\right], \quad j = 1 \dots q, \quad \lambda_i \neq \lambda_{i'}$
- How many different λ_i ?

same example



$$S = \begin{bmatrix} \lambda_1^0 & \lambda_1^1 \\ \lambda_2^0 & \lambda_2^1 \\ \lambda_3^0 & \lambda_3^1 \\ \lambda_4^0 & \lambda_4^1 \end{bmatrix}$$



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all combinations of columns (= rows of S): $(1, 2), (2, 3), (1, 4)$
improved condition via generalization approaches

related notions: *partial separability, contraction points, scarcity*

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- efficiency considerations, see "delayed piggyback" e.g. for iterations $\boldsymbol{x}_{k+1} = \boldsymbol{f}(\boldsymbol{x}_k)$

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- advanced topics: Taylor coefficient recursions, mathematical mappings split over multiple library calls (reverse mode)

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