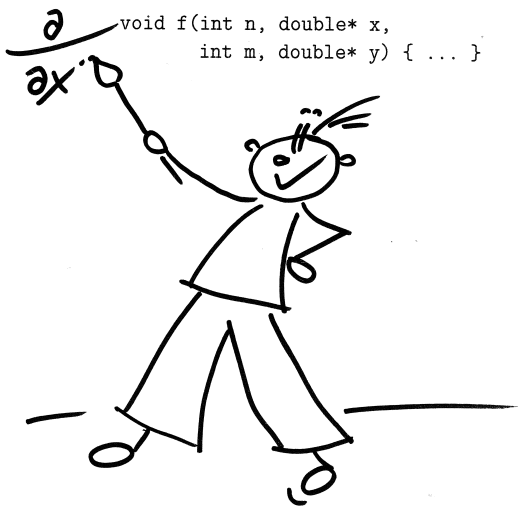
The Art of Differentiating Computer Programs

using Algorithmic Differentiation (AD)

Uwe Naumann



LuFG Informatik 12
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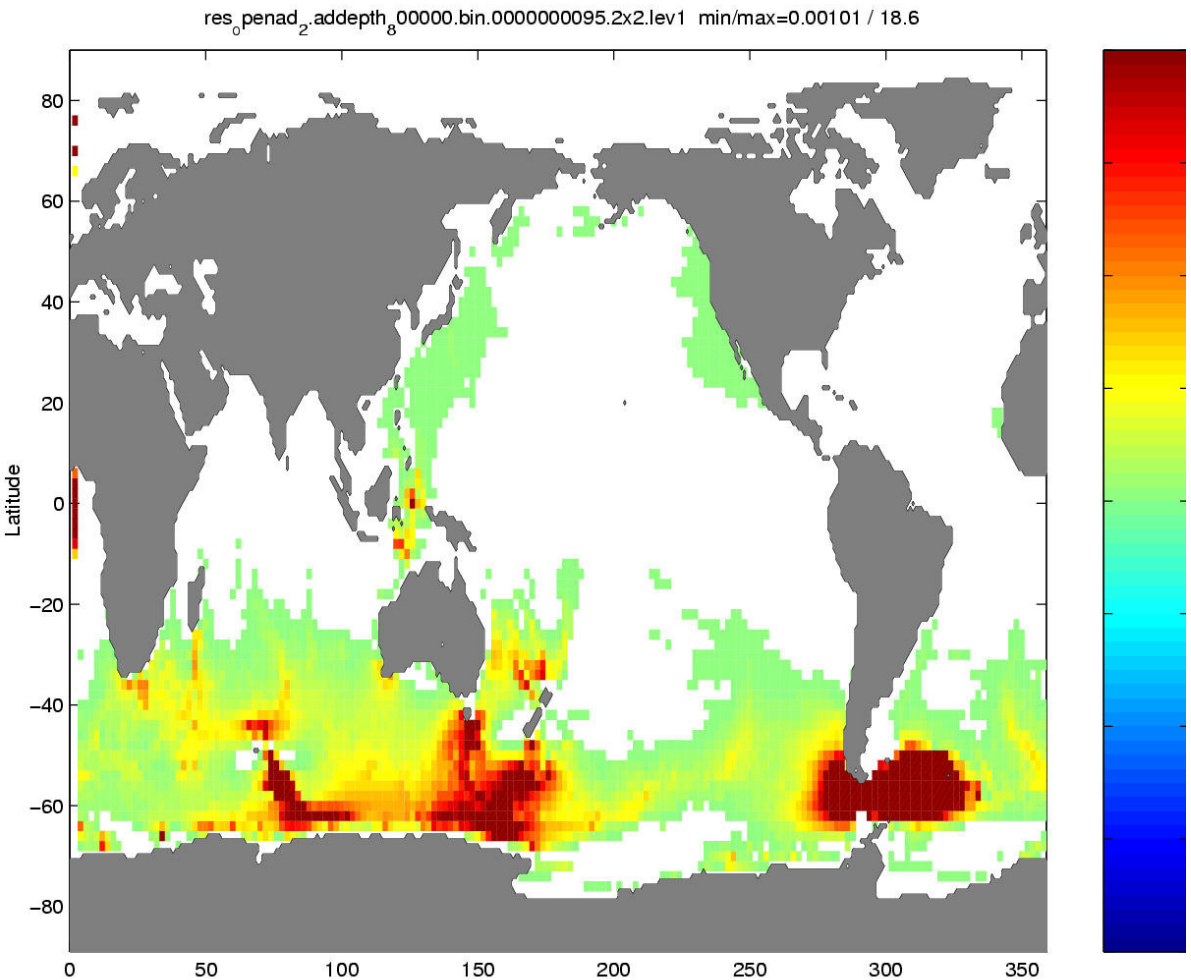
Motivation: Numerical Simulation e.g., MITgcm



Formally

Given: Numerical simulation program

$$F : \mathbb{R}^n \to \mathbb{R}^m, \quad \mathbf{y} = F(\mathbf{x})$$

Wanted: Sensitivity of outputs $\mathbf{y} \in \mathbb{R}^m$ on inputs $\mathbf{x} \in \mathbb{R}^n$ (Jacobian $\nabla F(\mathbf{x})$)

$$\nabla F(\mathbf{x}) \equiv \left(\frac{\partial y_j}{\partial x_i} \right)_{i=0,\ldots,n-1}^{j=0,\ldots,m-1}$$

Sensitivities / Derivatives

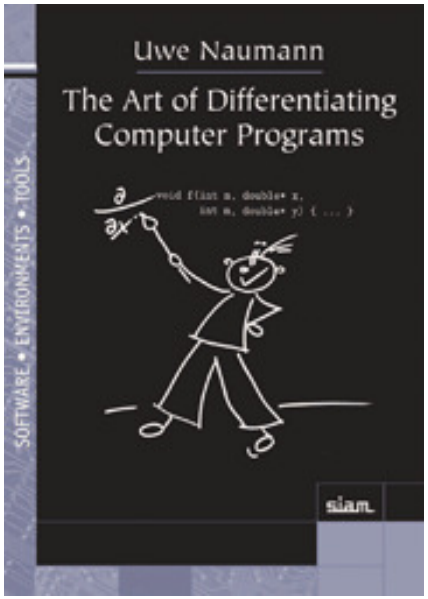
$y = f(x)$; effect of perturbation in x depending on $y' \equiv \frac{\partial y}{\partial x}$

- for large $y' > 0 \rightarrow$ large increase in y (instable)
- for small $y' > 0 \rightarrow$ small increase in y (stable)
- for large $y' < 0 \rightarrow$ large decrease in y (instable)
- for small $y' < 0 \rightarrow$ small decrease in y (stable)
- for $y' = 0 \rightarrow$ invariant

Outline

- 3 lectures
- 2 tutorials
- see tutorial sheet for contents

Literature



U. Naumann:
The Art of Differentiating Computer Programs.
An Introduction to Algorithmic Differentiation
Number 24 of Software, Environments, and Tools Series, SIAM, 2012.

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More ...

- Computational Differentiation (V3Ü1, Ba, WS)
- Combinatorial Problems in Scientific Computing (V2Ü2, Ma, SS)

Our Objective

For a given numerical simulation program, e.g.,

```
void f(int n, double *x, int m, double *y) {
  y[0]=x[0]*(x[0]+x[1]);
  y[1]=sin(x[1]);
}
```

build a program that can be used to compute the sensitivites of all outputs with respect to all inputs (Jacobian matrix).

Specific Objective: Tangent-Linear Code

$$\dot{\mathbf{y}} = \nabla F(\mathbf{x}) \cdot \dot{\mathbf{x}}$$
$$\mathbf{y} = F(\mathbf{x})$$

```
void f(int n, double *x, int m, double *y)
```

becomes

```
void df(int n, double *x, double *dx,
        int m, double *y, double *dy)
```

and computes product of the Jacobian with $\dot{\mathbf{x}}$ in $\dot{\mathbf{y}}$; not the Jacobian itself.

Example

```
void f(int n, double *x, int m, double *y) {
  y[0]=x[0]*(x[0]+x[1]);
  y[1]=sin(x[1]);
}
```

- Single Assignment Code (SAC)
- Directed Acyclic Graph (AST, DAG)
- Linearized SAC
- Linearized AST, DAG
- Local Tangent-Linear Code
- Chain Rule

Jacobian Computation and Validation

```
void f(int n, double *x, int m, double *y) {
  y[0]=x[0]*(x[0]+x[1]);
  y[1]=sin(x[1]);
}
```

- driver for tangent-linear code
- validation by finited differences

Validation through Approximation
Forward Finite Differences

Let $D \subseteq \mathbb{R}^n$ be an open domain and $F : D \to \mathbb{R}^m$ such that

$$F = \begin{pmatrix} F_0 \\ \vdots \\ F_{m-1} \end{pmatrix} \quad .$$

A *forward finite difference* approximation of the ith column of the Jacobian ∇F at point $\mathbf{x}^0$ is computed as

$$\frac{\partial F}{\partial x_i}(\mathbf{x}^0) \equiv \begin{pmatrix} \frac{\partial F_0}{\partial x_i}(\mathbf{x}^0) \\ \vdots \\ \frac{\partial F_{m-1}}{\partial x_i}(\mathbf{x}^0) \end{pmatrix} \approx_1 \frac{F(\mathbf{x}^0 + \mathbf{e}_i \cdot h) - F(\mathbf{x})}{h} \tag{1}$$

The *ith Cartesian basis vector in* $\mathbb{R}^n$ is denoted by $\mathbf{e}_i$.

However ...

Consider the approximation of the first derivative of $y = f(x) = x$ in single precision IEEE floating-point arithmetic on a 64 bit machine at $x = 10^6$ by the forward finite quotient

$$\nabla f(x) \approx \frac{f(x+h) - f(x)}{h}$$

with $h = 0.1$. Obviously, $\nabla f(x) = 1$ independent of x. The code

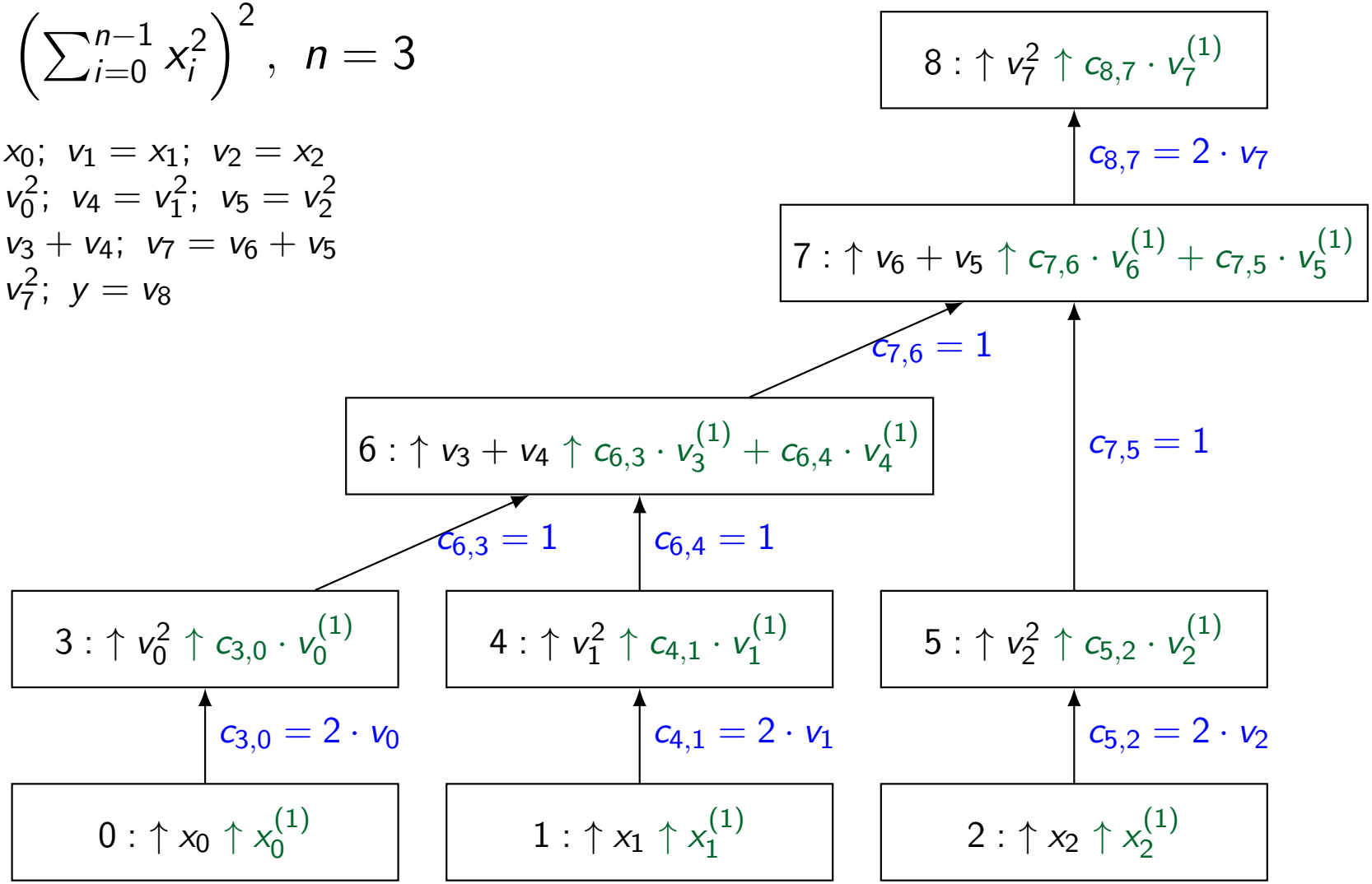
```
...
float x=1e6, h=1e-1;
cout << "(f(x+h)-f(x))/h=" << (x+h-x)/h << endl;
...
```

returns 1.25.

Tangent-Linear Code by Forward Mode AD

$$y = \left(\sum_{i=0}^{n-1} x_i^2 \right)^2, \quad n = 3$$

$v_0 = x_0;\ v_1 = x_1;\ v_2 = x_2$
$v_3 = v_0^2;\ v_4 = v_1^2;\ v_5 = v_2^2$
$v_6 = v_3 + v_4;\ v_7 = v_6 + v_5$
$v_8 = v_7^2;\ y = v_8$



Further Motivation
Nonlinear Optimization

Consider the nonlinear programming problem (NLP)

$$\min_{\mathbf{x}\in\mathrm{R}^n} f(\mathbf{x})$$

where, for example,

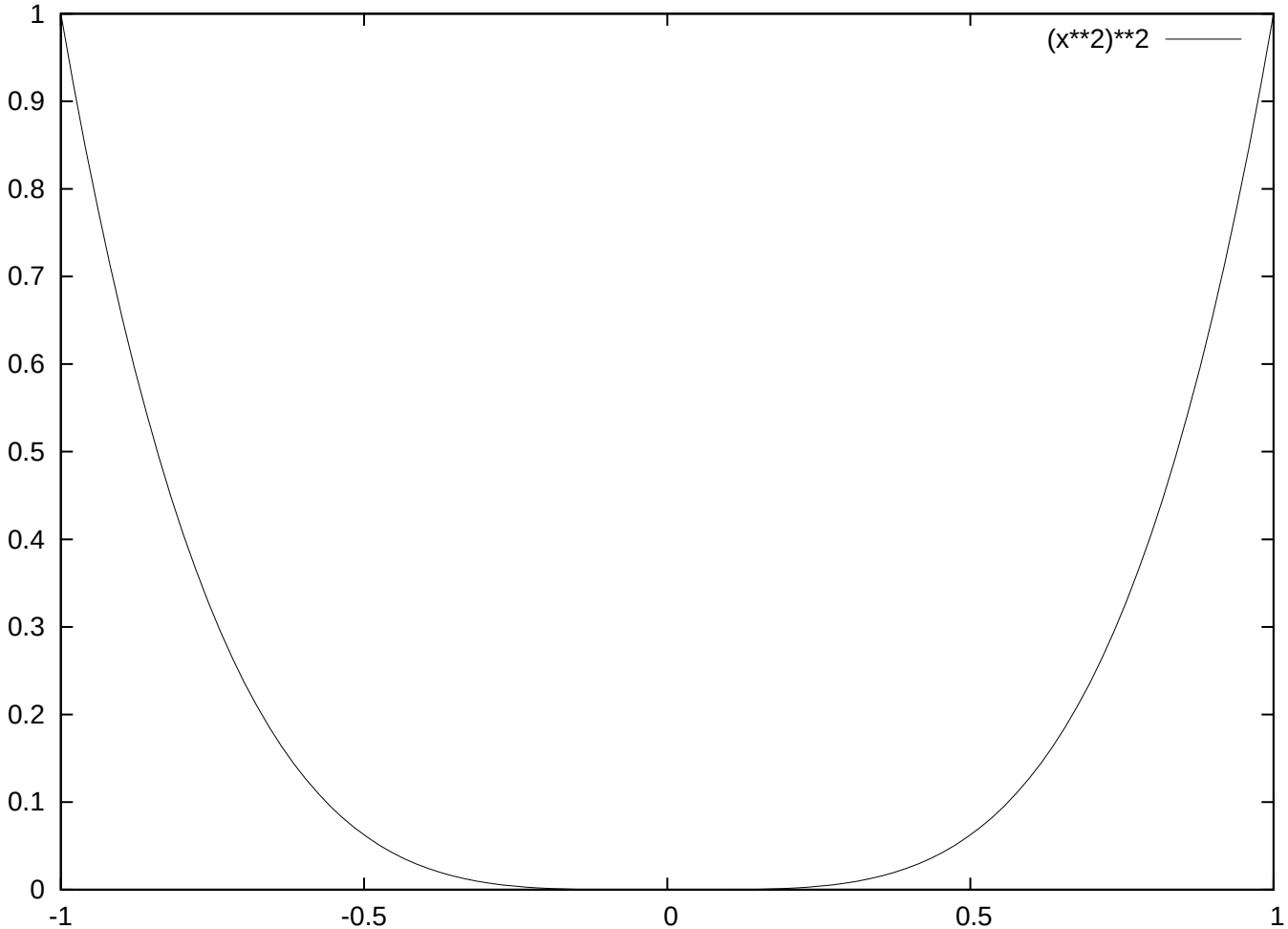
$$f(\mathbf{x}) = \left(\sum_{i=0}^{n-1} x_i^2\right)^2 \tag{2}$$

is implemented as

```
void f(int n, double *x, double &y)
{
   y=0;
   for (int i=0;i<n;i++) y=y+x[i]*x[i];
   y=y*y;
}
```

The function has a global minimum at $\mathbf{x} = 0$.

Nonlinear Optimization



Steepest Descent

... computes

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \alpha_k \cdot \nabla f(\mathbf{x}^k) \quad .$$

for some suitable starting value $\mathbf{x}^0 = (x_i^0)_{i=0,\ldots,n-1}$ and with a step length $\alpha_k > 0$, where $\nabla f(\mathbf{x}^k)$ denotes the gradient of f at the current iterate.

The step length $\alpha_k > 0$ is, for example, chosen by recursive bisection on α_k starting from $\alpha_k = 1$ $(0.5, 0.25, \ldots)$ and such that a decrease in the objective value is ensured

More Applications

...

Computational Finance

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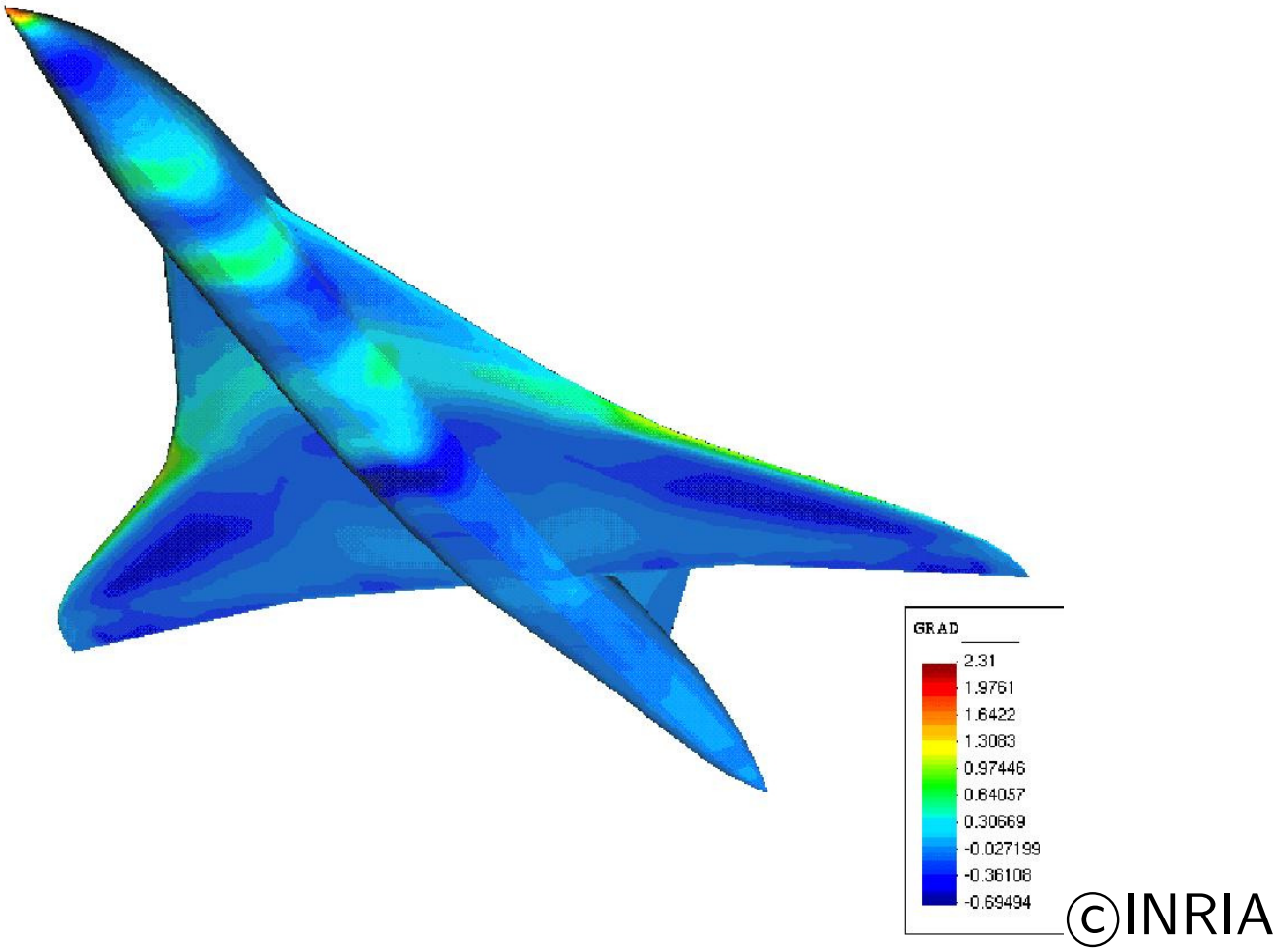
Aeroacoustics



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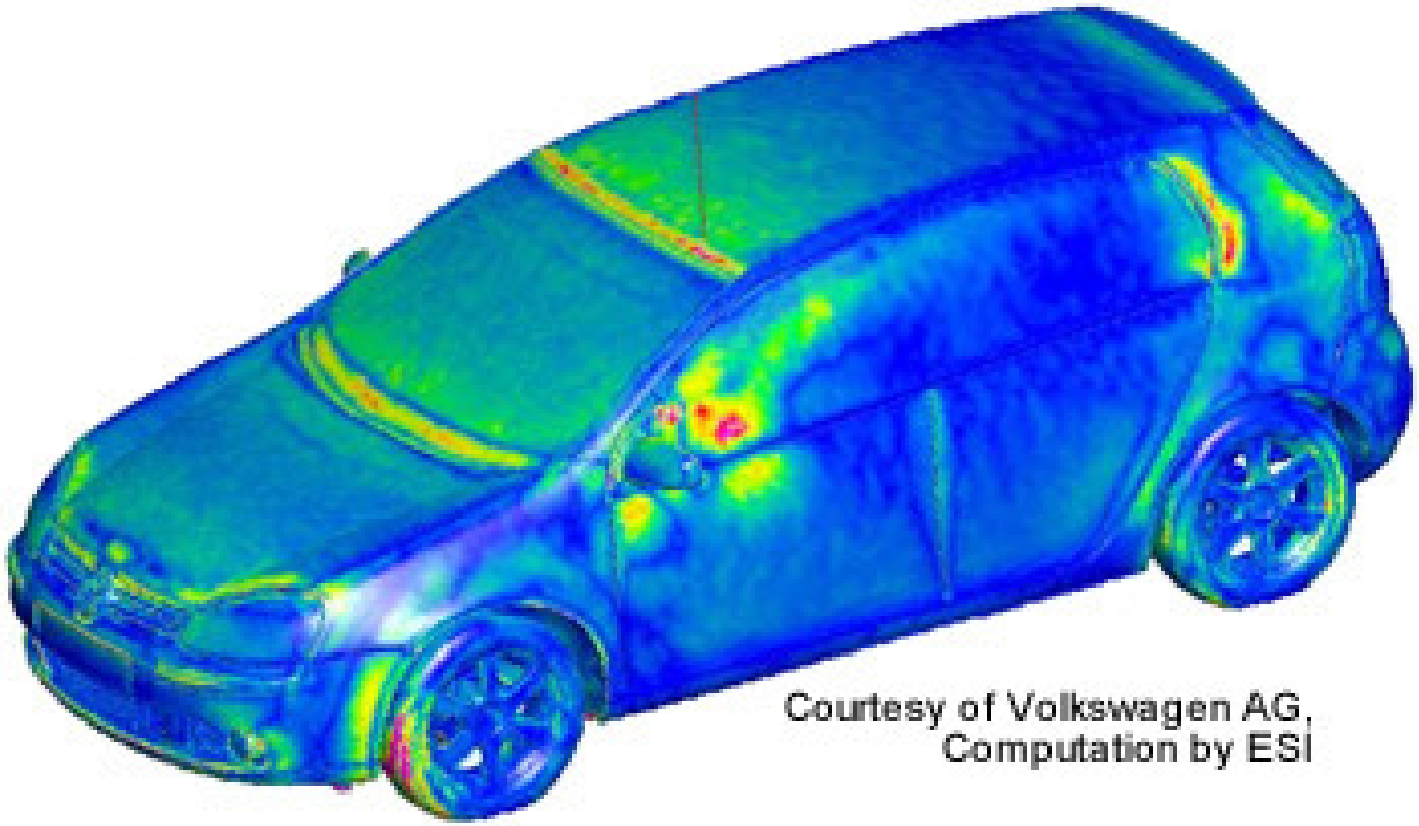
Automative Engineering



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dcc (version 0.9)

See

`www.siam.org/books/se24`

for

- source
- use guide
- Windows version

By The Way ...

It also works for, e.g.

```
void f(int n, double *x, double &y) {
  int i=0;
  while (i<n) {
    if (i==0) { y=x[i]*x[i]; }
    else { y=y+x[i]*x[i]; }
    i=i+1;
  }
  y=y*y;
}
```

as well as for interprocedural code etc.

Parsing SL^2

A *Straight-Line Simple Language* program is a sequence of statements described by the grammar $G = (V_n, V_t, P, s)$ with nonterminal symbols

$$V_n = \left\{ \begin{array}{ll} s & \text{(sequence of statements)} \\ a & \text{(assignment)} \\ e & \text{(expression)} \end{array} \right\}$$

terminal symbols

$$V_t = \left\{ \begin{array}{rl} V & \text{(program variables)} \\ C & \text{(constants)} \\ F & \text{(unary intrinsic)} \\ L & \text{(linear binary arithmetic operator)} \\ N & \text{(nonlinear binary arithmetic operator)} \\ ;\ )\ (\ = & \text{(remaining single character tokens)} \end{array} \right\}$$

... start symbol s, and production rules

$$P = \left\{ \begin{array}{llllll} (P1) & s : a & (P2) & s : as & (P3) & a : V = e; \\ (P4) & e : eLe & (P5) & e : eNe & (P6) & e : F(e) \\ (P7) & e : V & (P8) & e : C & & \end{array} \right\} .$$

Ambiguity

- Associativity?

$$a * b * c \stackrel{?}{=} (a * b) * c \stackrel{?}{=} a * (b * c)$$

- Operator Precedence?

$$a + b * c \stackrel{?}{=} (a + b) * c \stackrel{?}{=} a + (b * c)$$

... to be resolved by `bison`.

Parser → Parse Tree → Unparser

For example,

```
void f(int n, double *x, int m, double *y) {
  y[0]=x[0]*(x[0]+x[1]);
  y[1]=sin(x[1]);
}
```

- function body is word in G
- parser yields parse tree
- linearization annotates parse tree
- DFS tangent-linear code unparser

Unambiguous SL^2

An SL^2 *program* is a sequence of statements described by the grammar $G = (V_n, V_t, P, s)$ with nonterminal symbols

$$V_n = \left\{ \begin{array}{llllll} s & \text{(sequence of assignments)} & a & \text{(assignment)} & & \\ e & \text{(expression)} & t & \text{(term)} & f & \text{(factor)} \end{array} \right\}$$

terminal symbols

$$V_t = \left\{ \begin{array}{rl} V & \text{(program variables)} \\ C & \text{(constants)} \\ F & \text{(unary intrinsic)} \\ L & \text{(linear binary arithmetic operator)} \\ N & \text{(nonlinear binary arithmetic operator)} \\ ;\ )\ (\ = & \text{(remaining single character tokens)} \end{array} \right\}$$

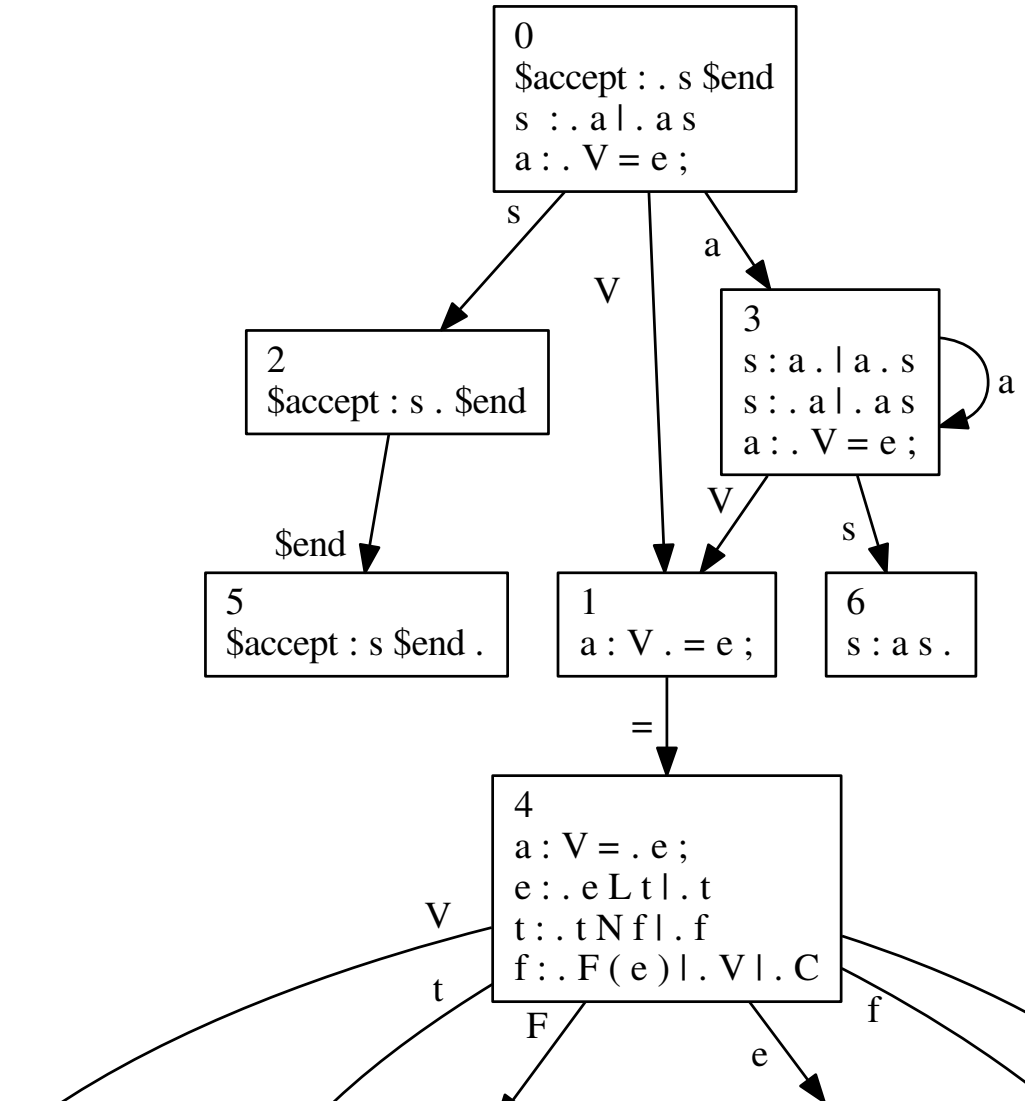
... start symbol s, and production rules

$$P = \left\{ \begin{array}{llllll} (P1) & s : a & (P2) & s : as & (P3) & a : V = e; \\ (P4) & e : eLt & (P5) & e : t & (P6) & t : tNf \\ (P7) & t : f & (P8) & f : F(e) & (P9) & f : V \\ (P10) & f : C & & & & \end{array} \right\} .$$

implies

- left-most bracketing for chained binary operations
- precedence of nonlinear over linear operations

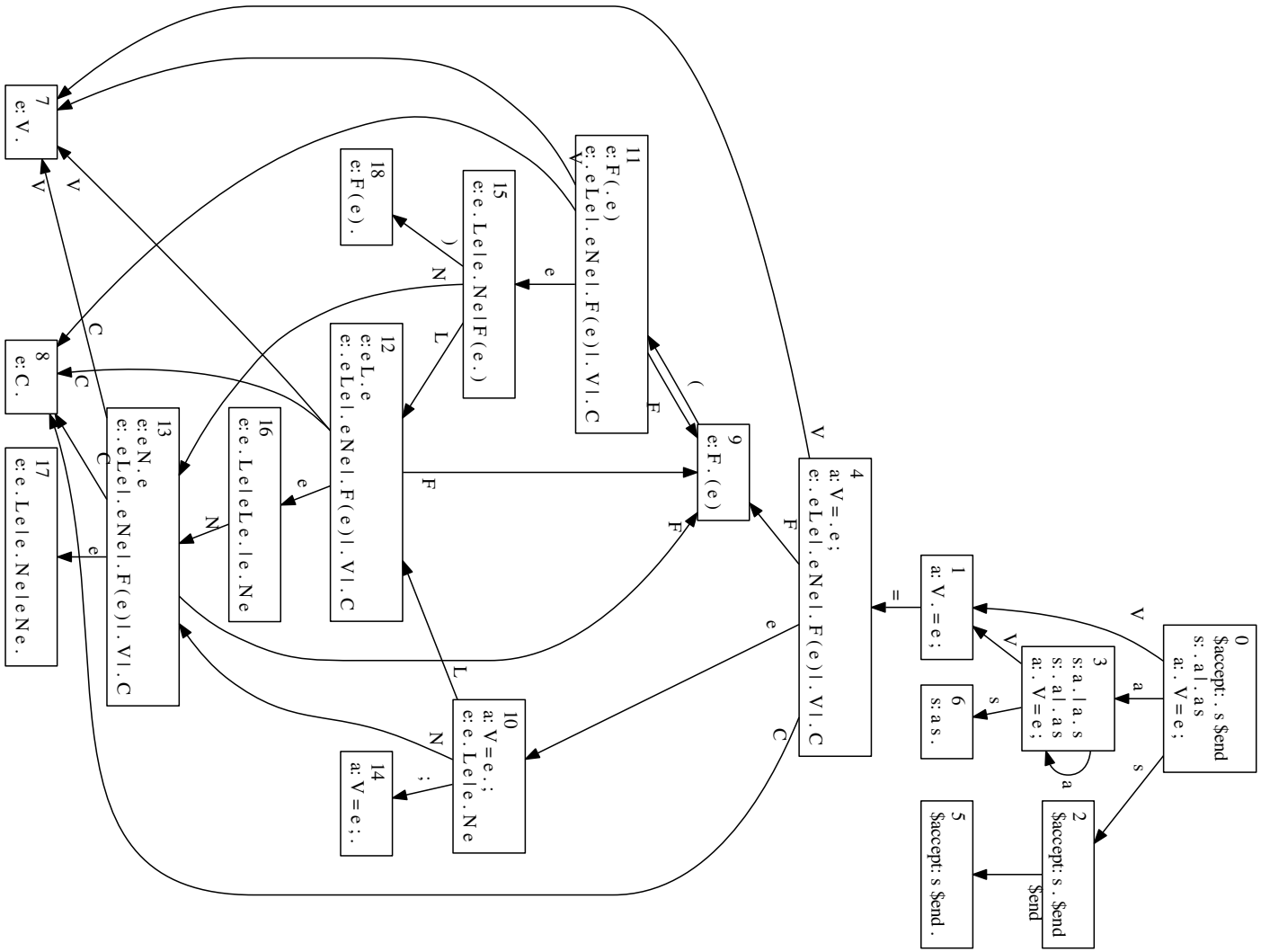
LR(0) Automaton



SLR Parsing
$V = F(VNC);$

	STACK	STATE	PARSED	INPUT	ACTION
1		0	V	$= F(VNC);$	S
2	0	1	$V =$	$F(VNC);$	S
3	0,1	4	$V = F$	$(VNC);$	S
4	0,1,4	9	$V = F($	$VNC);$	S
⋮					

Operator Precedence LR(0) Automaton



Operator Precedence Parsing
$V = F(VNC);$

	STACK	STATE	PARSED	INPUT	ACTION
1		0	V	$= F(VNC);$	S
2	0	1	$V =$	$F(VNC);$	S
3	0,1	4	$V = F$	$(VNC);$	S
4	0,1,4	9	$V = F($	$VNC);$	S
5	0,1,4,9	11	$V = F(V$	$NC);$	S
6	0,1,4,9,11	7		$NC);$	R($P6$)
7	0,1,4,9	11	$V = F(e$	$NC);$	S
8	0,1,4,9,11	15	$V = F(eN$	$C);$	S
9	0,1,4,9,11,15	13	$V = F(eNC$	$);$	S
10	0,1,4,9,11,15,13	8		$);$	R($P7$)
11	0,1,4,9,11,15	13	$V = F(eNe$	$);$	S
12	0,1,4,9,11,15,13	17		$);$	R($P4$)
13	0,1,4,9	11	$V = F(e$	$);$	S

	STACK	STATE	PARSED	INPUT	ACTION
14	0,1,4,9,11	15	$V = F(e)$	;	S
15	0,1,4,9,11,15	18		;	R($P5$)
16	0,1	4	$V = e$	;	S
17	0,1,4	10	$V = e;$		S
18	0,1,4,10	14			R($P3$)
19		0	a		S
20	0	3			R($P1$)
21		0	s		S
22	0	2	$\$end$		S
23	0,2	5			R($P0$)
24		0	$\$accept$		ACCEPT

Implementation with flex and bison
scanner.l

```
%{ #include "parser.tab.h" %}

whitespace      [ \t\n]+
variable        [a-z]
constant        [0-9]

%%

{whitespace}    { }
"sin"           { return F; }
"+"             { return L; }
"*"             { return N; }
{variable}      { return V; }
{constant}      { return C; }
.               { return yytext[0]; }

%%

void lexinit(FILE *source) { yyin=source; }
```

Implementation with flex and bison

parser.y

```
%token V C F L N

%left L
%left N

%%

s : a
  | a s
  ;
a : V '=' e ';' ;
e : e L e
  | e N e
  | F '(' e ')'
  | V
  | C
  ;

%%
...
```

Implementation with flex and bison
parser.y (Code Section)

```
...

#include<stdio.h>

int yyerror(char *msg) { printf("ERROR: %s \n",msg); return -1; }

int main(int argc,char** argv)
{
  FILE *source_file=fopen(argv[1],"r");
  lexinit(source_file);
  yyparse();
  fclose(source_file);
  return 0;
}
```

Toward Single-Pass Compilation

- Parse Tree Printer
  - data associated with parse tree nodes (**unsigned int** by default)
  - access to data corresponding to left-hand side of production rule by $$
  - access to data corresponding to symbols on right-hand side of production rule by postion, i.e. $1, $2, ...
  - see code
- Parser/Unparser
  - association of user-defined data (e.g. **char***) through redefinition of preprocessor macro YYSTYPE
  - see code