OBJECT ORIENTED IMPLEMENTATION OF A SECOND-ORDER OPTIMIZATION METHOD

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OPTIMIZATION APPROACH

- Nonlinear program
- Second-order approximation
- Integrated formulation
- All the problem variables are present in the nonlinear program
- No sensitivity analysis

OPTIMIZATION SOFTWARE

- General purpose code
- Lagrange-Newton method
- Symbolic manipulation of all the functions
- Exact 1st and 2nd derivatives
- Object oriented approach
- Language: **C++**

OBJECT ORIENTED PROGRAMMING

- What we gain
  - Higher abstraction level
  - Encapsulation of lower level complexities
  - Code maintenance and reuse is facilitated
- What we lose
  - Performance
  - Straightforward coding

OBJECT ORIENTED FEATURES

- Classes
- Function and operator overloading
- Inheritance
- Polymorphism
- Templates
- Exception handling

NONLINEAR PROGRAMMING

Minimize $f(\underset{\sim}{x})$

subject to

$$\underset{\sim}{g}(\underset{\sim}{x}) \le \underset{\sim}{0} \quad \rightarrow \quad g_i(\underset{\sim}{x}) + s_i^2 = 0$$

$$\underset{\sim}{h}(\underset{\sim}{x}) = \underset{\sim}{0}$$

- Variables / functions ⇨ real and continuous
- Generic functions can be treated

LAGRANGIAN

$$L\left(\underset{\sim}{X}\right) = f\left(\underset{\sim}{x}\right) + \sum_{k=1}^{m} \lambda_k^g \left[g_k\left(\underset{\sim}{x}\right) + s_k^2 \right] + \sum_{k=1}^{p} \lambda_k^h h_k\left(\underset{\sim}{x}\right)$$

VARIABLES

$$\underset{\sim}{X} = \left(\underset{\sim}{x}, \underset{\sim}{s}, \underset{\sim}{\lambda}^g, \underset{\sim}{\lambda}^h\right)$$

SOLUTION

- Stationary point of the Lagrangian

SYSTEM OF NONLINEAR EQUATIONS

$$\nabla L\left(\underset{\sim}{X}\right) = \underset{\sim}{0} \quad \Rightarrow \quad \left| \begin{array}{ll} 2 s_i \lambda_i^g = 0 & (i = 1, \ldots, m) \\ g_i + s_i^2 = 0 & (i = 1, \ldots, m) \\ \dfrac{\partial f}{\partial x_i} + \sum_{k=1}^{m} \lambda_k^g \dfrac{\partial g_k}{\partial x_i} + \sum_{k=1}^{p} \lambda_k^h \dfrac{\partial h_k}{\partial x_i} = 0 & (i = 1, \ldots, n) \\ h_i = 0 & (i = 1, \ldots, p) \end{array} \right.$$

- The solution of the system is a KKT solution when

$$\boxed{\underset{\sim}{\lambda}^g \geq 0}$$

LAGRANGE-NEWTON METHOD

- The system of nonlinear equations

$$\nabla L(\underset{\sim}{X}) = \underset{\sim}{0}$$

is solved by the Newton method

- In each iteration the following system of linear equations has to be solved

$$\underset{\sim}{H}\left(\underset{\sim}{X}^{q-1}\right)\Delta\underset{\sim}{X}^{q} + \nabla L\left(\underset{\sim}{X}^{q-1}\right) = \underset{\sim}{0}$$

- H is the Hessian of the Lagrangian
- Second derivatives of all the functions are required

SYSTEM OF LINEAR EQUATIONS

- Gaussian elimination
  - adapted to the sparsity pattern of the Hessian matrix

- Conjugate gradients
  - diagonal preconditioning
  - adapted to an indefinite Hessian matrix

LINE SEARCH

$$\underset{\sim}{X}^{q} = \underset{\sim}{X}^{q-1} + \alpha \, \Delta \underset{\sim}{X}^{q}$$

- The value of α minimizes the error in $\Delta \underset{\sim}{X}^{q}$ direction
  - the value of α is often close to one
  - faster convergence
  - process may fail
- The value of α is made considerably smaller (e.g. α = 0.1)
  - stable convergence
  - more iterations - slower

AUTOMATIC DIFFERENTIATION

- Expression evaluation
- Partial derivative calculation (first, second, ...)
- Each function is parsed and stored as a tree of tokens (constants, variables and operators)
- Automatic differentiation is based on Rall numbers

RALL NUMBERS

- A Rall number is a class that encapsulates the numerical value of the function, its gradient vector and its Hessian matrix
- All the operators are overloaded in order to apply the differentiation rules
- With Rall numbers automatic differentiation can be efficiently performed

RALL NUMBERS

Example:

Functions $f(x_1, x_2)$ and $g(x_1, x_2)$

Derivatives of the product:

$$\frac{\partial}{\partial x_1}(f\,g) = \frac{\partial f}{\partial x_1} g + f \frac{\partial g}{\partial x_1}$$

$$\frac{\partial^2}{\partial x_1 \partial x_2}(f\,g) = \frac{\partial^2 f}{\partial x_1 \partial x_2} g + \frac{\partial f}{\partial x_2}\frac{\partial g}{\partial x_1} + \frac{\partial f}{\partial x_1}\frac{\partial g}{\partial x_2} + f \frac{\partial^2 g}{\partial x_1 \partial x_2}$$

RALL NUMBERS

```
class CRall {
  double x; // Operand value
  double v[2]; // df/dx1, df/dx2
  double m[2][2]; // d2f/dxi dxj
public:
  CRall CRall::operator* (const CRall & g) const {
    CRall t;
    t.x = x * g.x;

    t.v[0] = v[0]*g.x + x*g.v[0];
    t.v[1] = v[1]*g.x + x*g.v[1];

    t.m[0][0] = m[0][0]*g.x+v[0]*g.v[0]+v[0]*g.v[0]+x*g.m[0][0];
    t.m[0][1] = m[0][1]*g.x+v[0]*g.v[1]+v[1]*g.v[0]+x*g.m[0][1];
    t.m[1][0] = m[1][0]*g.x+v[1]*g.v[0]+v[0]*g.v[1]+x*g.m[1][0];
    t.m[1][1] = m[1][1]*g.x+v[1]*g.v[1]+v[1]*g.v[1]+x*g.m[1][1];

    return t;
  }
};
```

RALL NUMBERS

```
x = constant value;
   v = [0,0];
      m = [[0,0],[0,0]]
```

x = value of x_1;

```
   v = [1,0];
      m = [[0,0],[0,0]]
```

x = value of x_2;

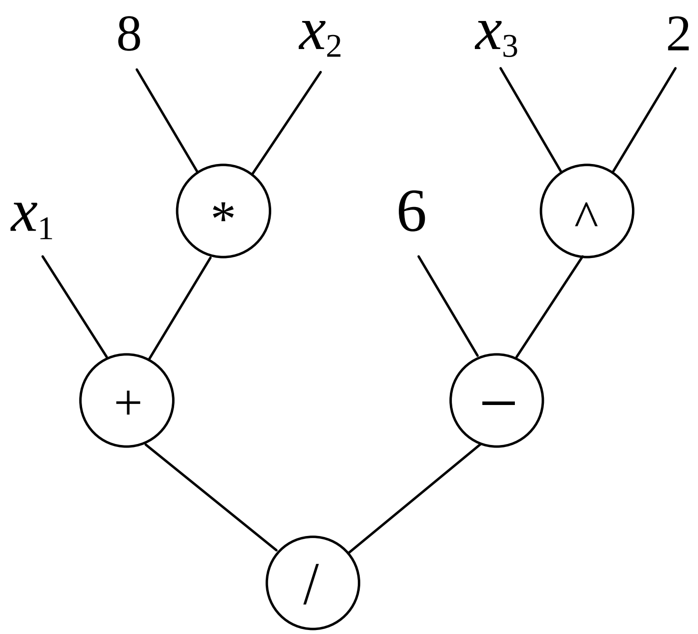
```
   v = [0,1];
      m = [[0,0],[0,0]]
```

EXPRESSION PARSER

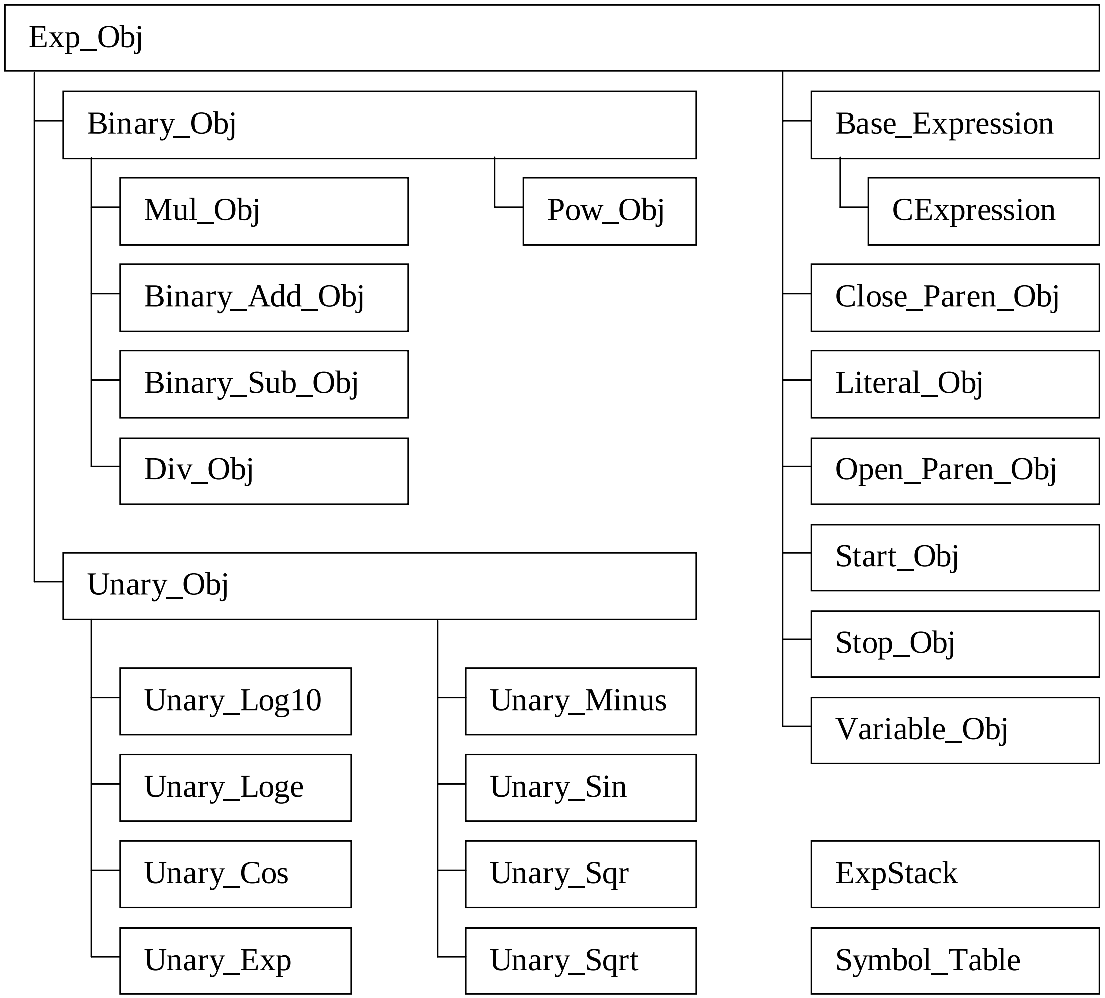
- A binary tree is constructed according to the operator precedence
- Each tree node is a Rall number
- A symbol table is initialized with the values of the variables and constants
- The tree traversal causes an evaluation of the function, gradient and Hessian

EXPRESSION PARSER

- Example: $f\left(x_1, x_2, x_3\right) = (x_1 + 8\,x_2)/(6 - x_3^2)$



EXPRESSION PARSER



SCALING

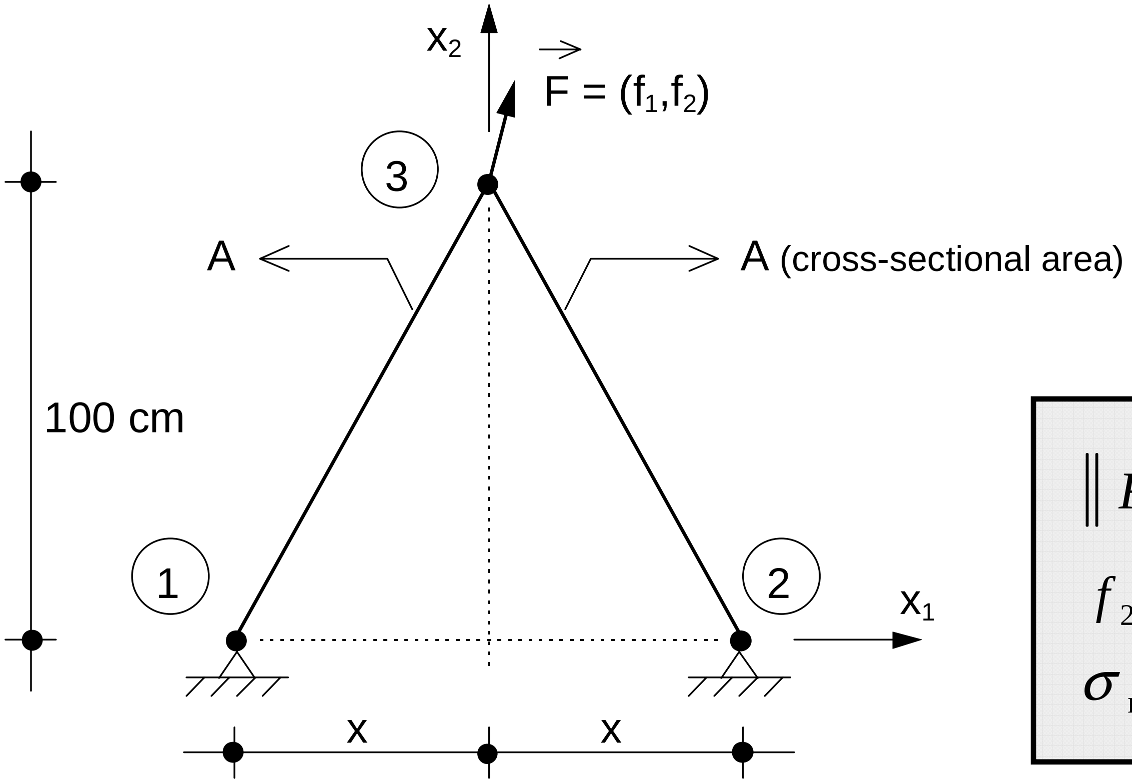
- Variable substitution: $x_i = c\ \bar{x}_i$
- Constraint normalization: $g_i = c\ \bar{g}_i$

$$\begin{aligned} &Min.\ \ 2000\,x_1 \\ &\quad subject\ to \\ &\qquad -x_1 + 200 + x_3^2 = 0 \\ &\qquad x_2 - 0.2 + x_4^2 = 0 \\ &\qquad -10\,x_1\,x_2 + 500 = 0 \end{aligned}$$

$$\Rightarrow$$

$$\begin{aligned} &Min.\ \ y_1 \\ &\quad subject\ to \\ &\qquad -0.640\,y_1 + 0.256 + 0.384\,y_3^2 = 0 \\ &\qquad 0.447\,y_2 - 0.894 + 0.447\,y_4^2 = 0 \\ &\qquad -0.707\,y_1\,y_2 + 0.707 = 0 \end{aligned}$$

NUMERICAL EXAMPLE



$$\| \vec{F} \| = 200\, kN$$

$$f_2 = 8\, f_1$$

$$\sigma_{max} = 100\ kN / cm^2$$

- Variables: A , x
- Svanberg's solution confirmed

NONLINEAR PROGRAM

$$Min.\;\; w(x_1, x_2) = C_1\, x_1 \sqrt{1 + x_2^2}$$

subject to

$$\sigma_1(x_1, x_2) = C_2 \sqrt{1 + x_2^2}\left(\frac{8}{x_1} + \frac{1}{x_1\, x_2}\right) \le 1$$

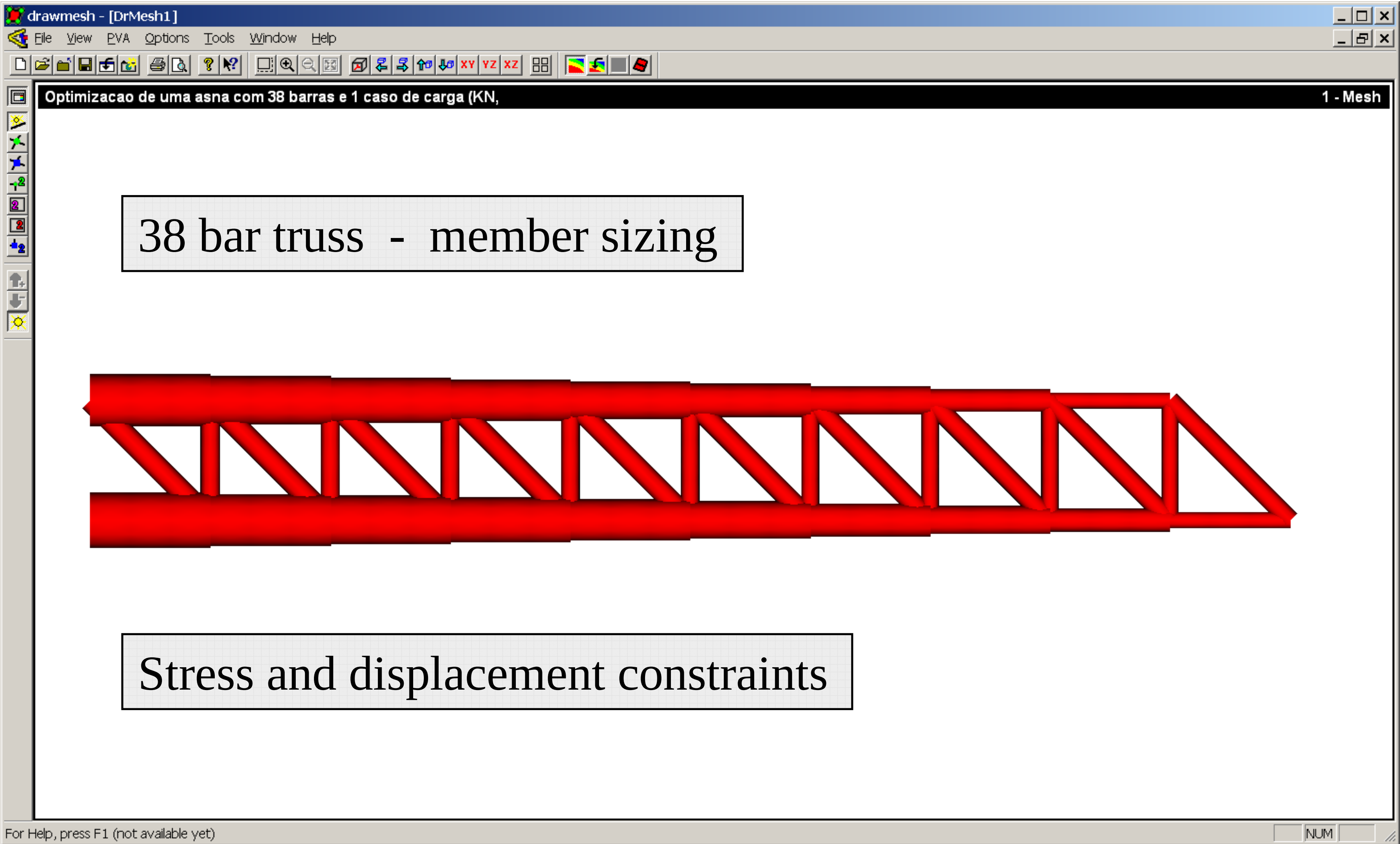
$$\sigma_2(x_1, x_2) = C_2 \sqrt{1 + x_2^2}\left(\frac{8}{x_1} - \frac{1}{x_1\, x_2}\right) \le 1$$

$$0.2 \le x_1 \le 4.0 \;\; ; \;\; 0.1 \le x_2 \le 1.6$$

DATA FILE

```
# Main title
Shape optimization of a two bar truss

# N. of eq. constr.; N. of ineq. constr.
                 0                    6

# Objective Function
  C1 * x1 * sqrt(1+x2^2);

# Allowable stress - bar 1
  C2 * sqrt(1+x2^2) * (8/x1+1/x1/x2) - 1;

# Allowable stress - bar 2
  C2 * sqrt(1+x2^2) * (8/x1-1/x1/x2) - 1;
```

```
# Minimum x1
  -x1 + 0.2;

# Maximum x1
  x1 - 4.0;

# Minimum x2
  -x2 + 0.1;

# Maximum x2
  x2 - 1.6;

# N. of variables
  4

SUBSTITUTED, 1.000, C1;
SUBSTITUTED, 0.124, C2;
INDEPENDENT, 1.5, x1;
INDEPENDENT, 0.5, x2;
```


drawmesh - [DrMesh1]
File View PVA Options Tools Window Help
Optimizacao de uma asna com 38 barras e 1 caso de carga (KN,
1 - Mesh
38 bar truss - member sizing
Stress and displacement constraints
For Help, press F1 (not available yet)
NUM

CONCLUSIONS

- Code maintenance
- Efficiency and accuracy in the evaluation of derivatives
- Easy inclusion of alternative numerical techniques
- Not efficient in the OO manipulation of the Hessian matrix
- Friendly user interface is still required