NOMAD-based optimizations and Lazarus support for SimuSage
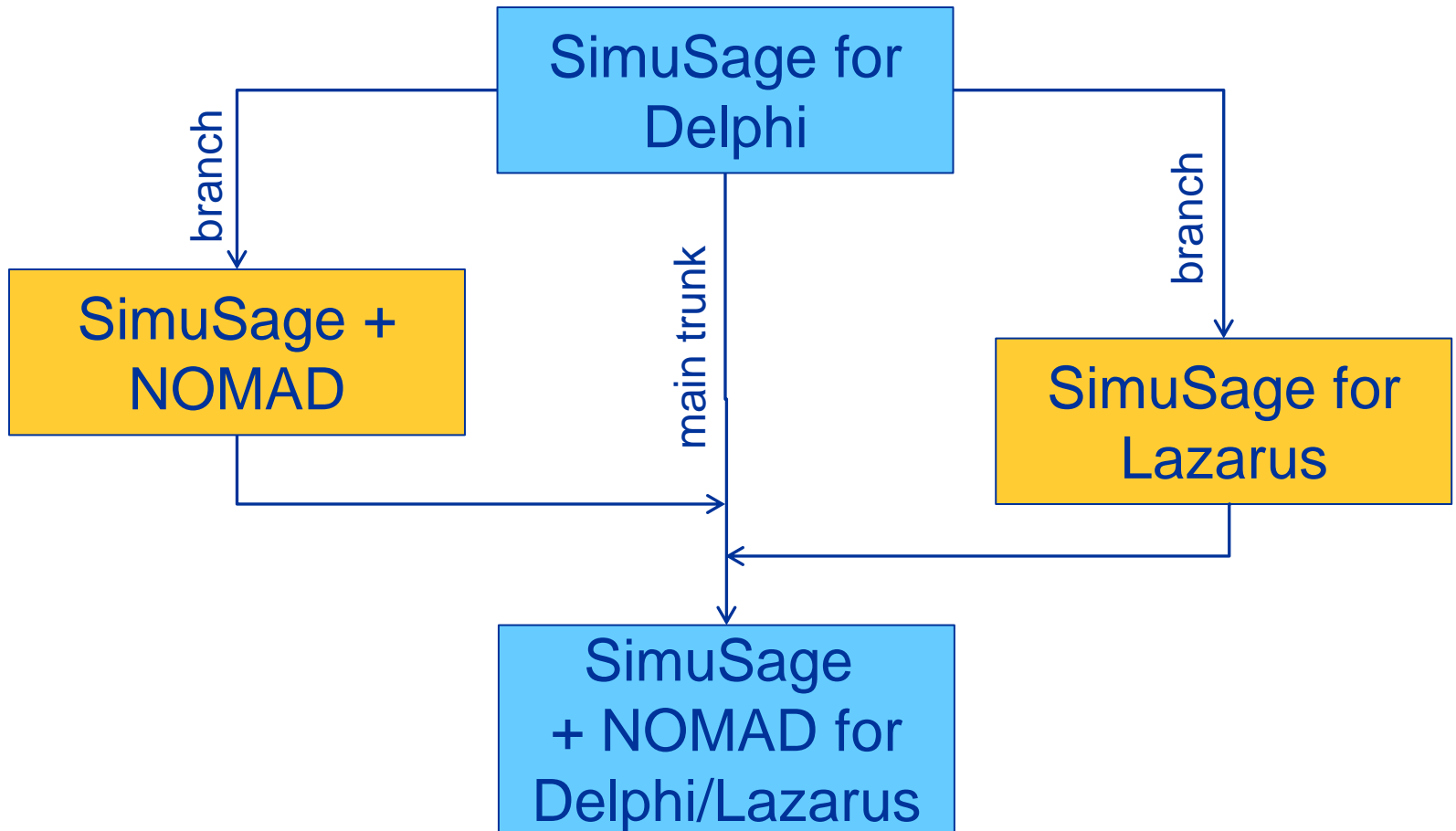
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GTT-Technologies, Herzogenrath, Germany

Latest SimuSage development

NOMAD in FactOptimal

NOMAD

- Nonlinear Optimization by Mesh Adaptive Direct Search

- C++ implementation of the Mesh Adaptive Direct Search (MADS) algorithm[*]

- Designed for constrained optimization blackbox functions in the form:
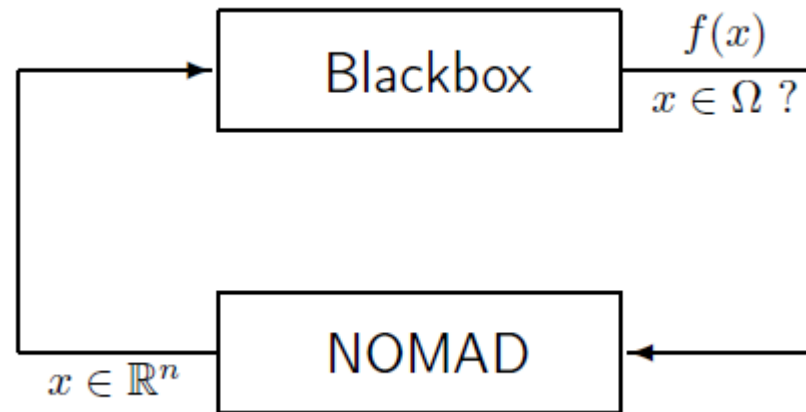
$$\min_{x \in \Omega} f(x)$$

[*] Auded, C., and Dennis, J. (2006). Mesh Adaptive Direct Search Algorithm for Constrained Optimization. SIAM J. Opt. 17, 1, 188-217

Blackbox Problems

- Unknown internal structure of the target problem

- Function can have unreliable properties

- NOMAD is intended for time-consuming blackbox simulations with a small number of variables

NOMAD integration in SimuSage

- NOMAD source code is compiled as stand-alone DLL

- All interaction between SimuSage flowsheet and NOMAD is done via the new TPbOptimizer component

- TPbOptimizer component provides graphical user interface to set objectives, variables, constraints, parameters, etc.

- No other coding necessary for "standard" optimizations of existing flowsheets

TPbOptimizer

- Component that links SimuSage with NOMAD for flowsheet optimizations

- Auxiliary SimuSage optimization design form opens when:

  - TPbOptimizer object is double clicked at design time

  - TPbOptimizer object is right clicked and the option "Edit …" is selected at design time

  - One of the following properties of TPbOptimizer are edited: OptObjective or OptVariable or OptConstraint at design time

  - TPbOptimizer object is clicked at run time

SimuSage and Delphi

- Initial SimuSage development was done for Delphi 5, 6, 7

- SimuSage is available for Delphi 7, 2005, 2006, 2007, 2009, 2010, XE, XE3, …

- At least the „Professional" version of Delphi is required or strongly recommended

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Lazarus

- Open Source „Delphi-compatible" development environment

- Based on Free Pascal

- LGPL licensed libraries, GPL licensed DIE

- (Cross Platform IDE, platform independent projects)

SimuSage and Lazarus

- Most existing SimuSage projects will likely compile with minor changes under Lazarus

- Converter tool available in Lazarus

- Most necessary code changes are due to graphical output or resource files

- One code base for a project that compiles both under Delphi and Lazarus is possible (SimuSage itself is one of them)
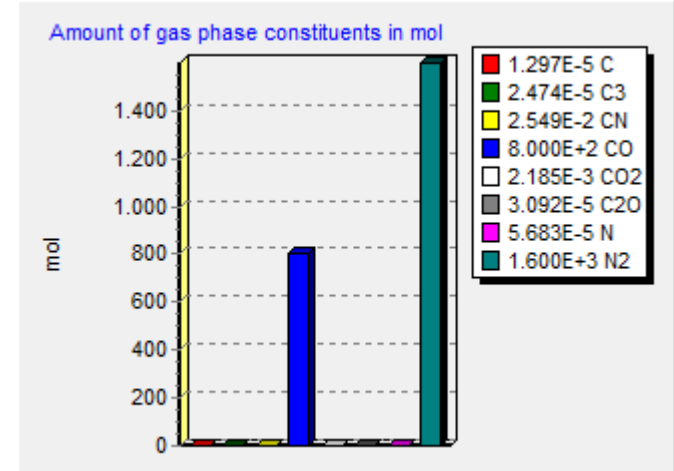
From Delphi to Lazarus
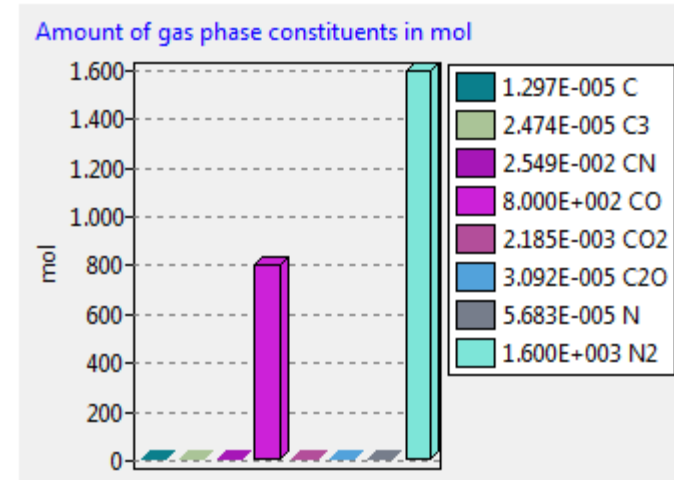
```
1    unit Graphs;
2
3    {$IFDEF FPC}
4        {$MODE Delphi}
5    {$ENDIF}
6
7    interface
8
9    uses
10   {$IFnDEF FPC}
11       Windows, TeEngine, Series, TeeProcs,
12       Chart,
13   {$ELSE}
14       LCLIntf, LCLType, LMessages, TAGraph,
15       TASeries, TACustomSeries, TATools,
16       TATransformations,
17   {$ENDIF}
18       Messages, SysUtils, Classes, Graphics,
19       Controls, Forms, Dialogs, ExtCtrls,
20       ComCtrls;
```
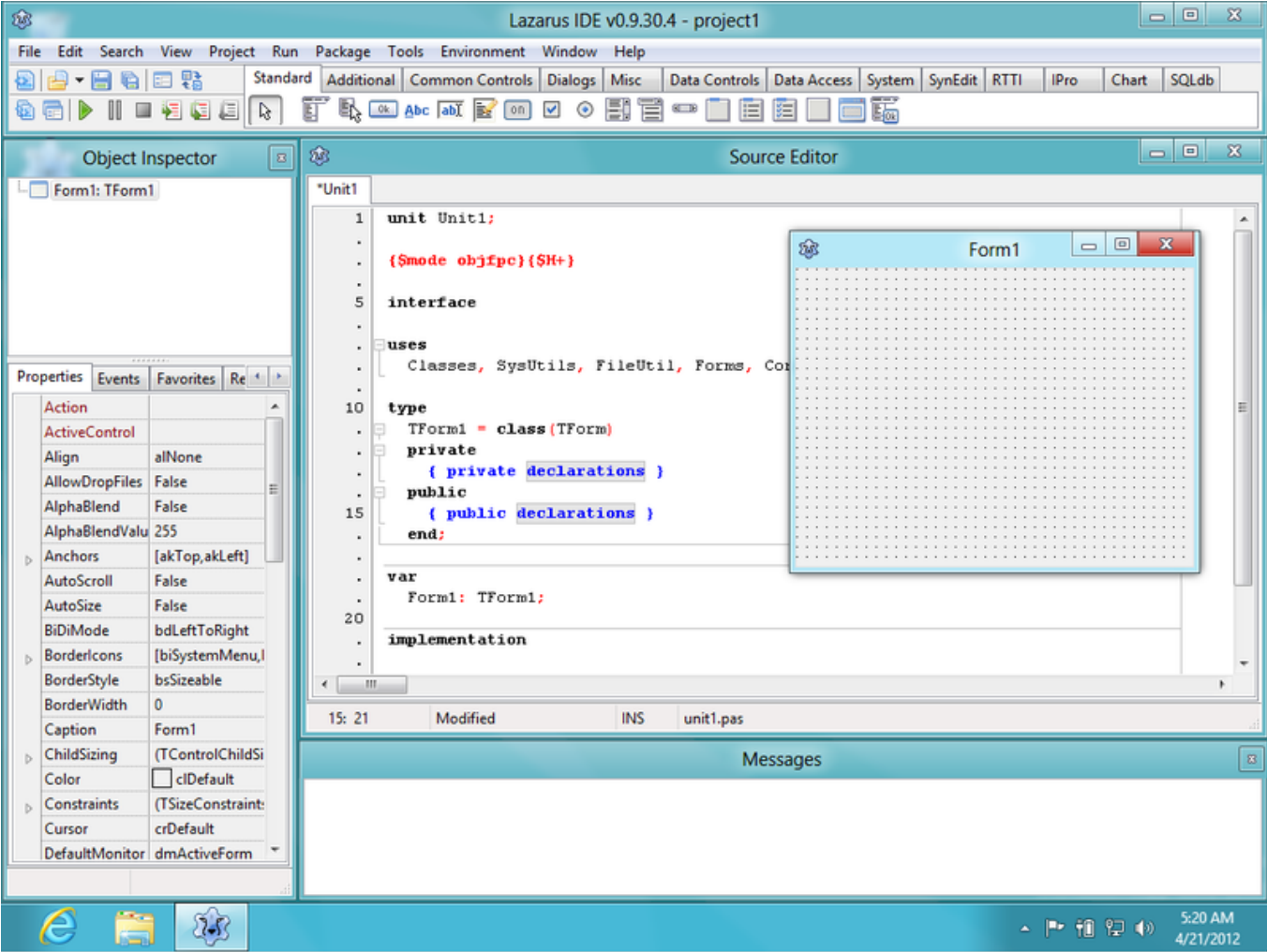
Amount of gas phase constituents in mol

■	1.297E-5 C
■	2.474E-5 C3
■	2.549E-2 CN
■	8.000E+2 CO
□	2.185E-3 CO2
■	3.092E-5 C2O
■	5.683E-5 N
■	1.600E+3 N2

TeeChart – Delphi

Amount of gas phase constituents in mol

■	1.297E-005 C
■	2.474E-005 C3
■	2.549E-002 CN
■	8.000E+002 CO
■	2.185E-003 CO2
■	3.092E-005 C2O
■	5.683E-005 N
■	1.600E+003 N2

TAChart – Lazarus

Lazarus IDE

SimuSage Optimization Form

- Objective

Choose a PbObject instance present in the designed flowsheet

In case of a target calculation a target value must be given

Select the type of optimization

Choose a property for the chosen PbObject

Close the form

Go to the Variables tab

SimuSage Optimization Form

- Variables

Clear the given variable parameters

Define a variable

1. PbObject present in the design form

2. Property of the PbObject

3. Minimum value for the variable

4. Maximum value for the variable

5. Initial value used by the optimizer

Add a variable

Delete a selected variable

Delete all defined variables

List of the defined variables

Close the form

Go to the Constraints tab

SimuSage Optimization Form

- Constraints

Clear the given constraint parameters

Define a constraint

1. PbObject present in the design form

2. Property of the PbObject

3. Mathematical symbol for the constraint equation

4. Value which the constraint must not exceed

5. Type of the constraint (Progressive Barrier or Extreme Barrier)

Add a constraint

Delete a selected constraint

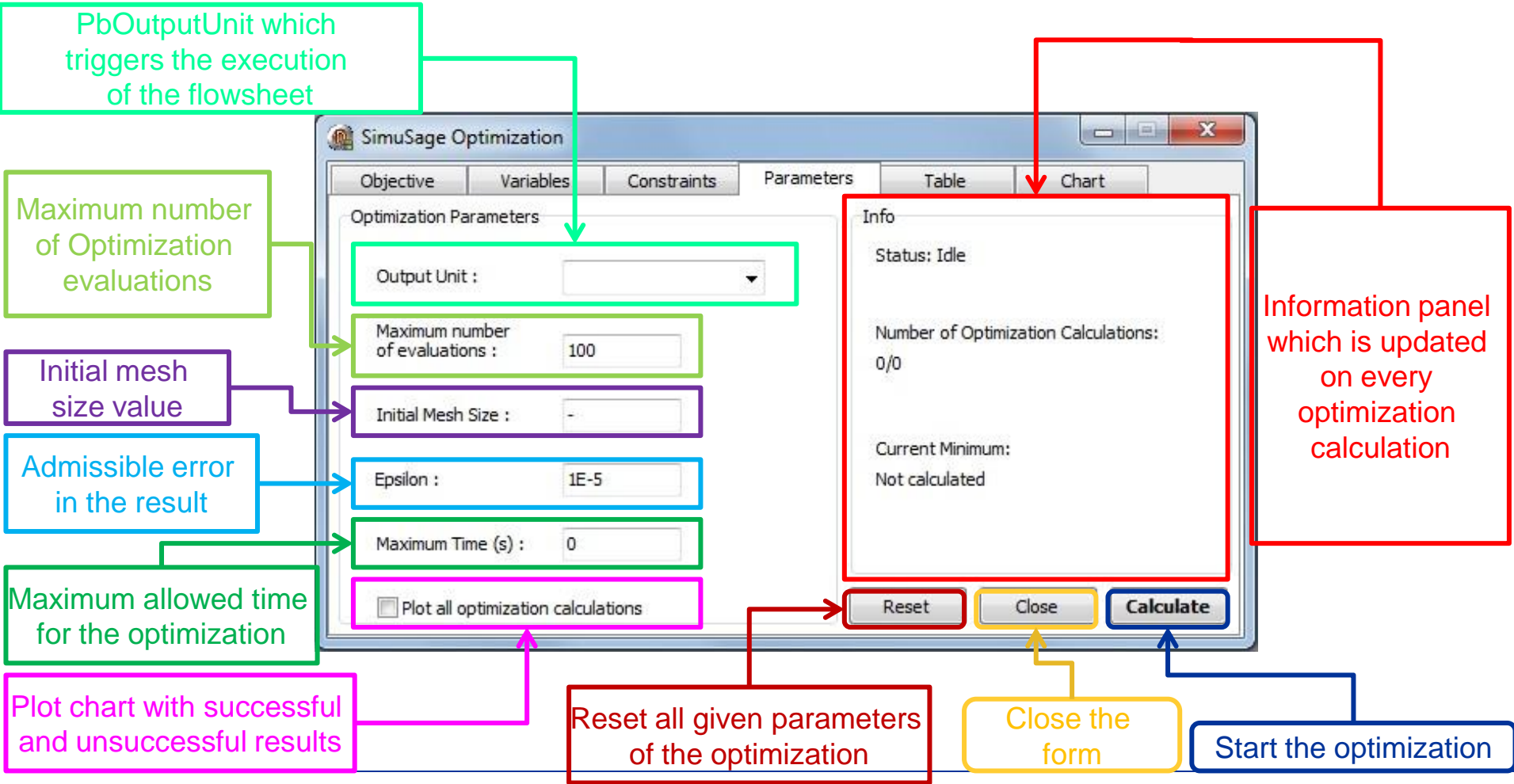Delete all defined constraints

List of the defined constraints

Close the form

Go to the Parameters tab

SimuSage Optimization Form

- Parameters

PbOutputUnit which triggers the execution of the flowsheet

Maximum number of Optimization evaluations

Initial mesh size value

Admissible error in the result

Maximum allowed time for the optimization

Plot chart with successful and unsuccessful results

SimuSage Optimization

| Objective | Variables | Constraints | Parameters | Table | Chart |

Optimization Parameters

Output Unit :

Maximum number of evaluations :   100

Initial Mesh Size :   -

Epsilon :   1E-5

Maximum Time (s) :   0

☐ Plot all optimization calculations

Info

Status: Idle

Number of Optimization Calculations:
0/0

Current Minimum:
Not calculated

Information panel which is updated on every optimization calculation

Reset   Close   **Calculate**

Reset all given parameters of the optimization

Close the form

Start the optimization

Thank you for your attention!