NOMAD-based optimizations and Lazarus support for SimuSage

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Latest SimuSage development

- SimuSage for Delphi
- SimuSage + NOMAD
- SimuSage + NOMAD for Delphi/Lazarus
- SimuSage for Lazarus

Branches and main trunk connections.
NOMAD in FactOptimal

Number of FactSage calculations: 150
Best answer so far:
Temperature: 436.77°C

Last solution:

<table>
<thead>
<tr>
<th>Species</th>
<th>mol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>0.11539</td>
</tr>
<tr>
<td>Cu</td>
<td>0.02</td>
</tr>
<tr>
<td>Mg</td>
<td>0.75</td>
</tr>
<tr>
<td>Zn</td>
<td>0.11461</td>
</tr>
</tbody>
</table>

Constraints:
- Al+Cu=0.11539
- Density=2.19982
- Cost $=2856.28075

Results:

<table>
<thead>
<tr>
<th>Temperature (C)</th>
<th># of Calculations</th>
</tr>
</thead>
<tbody>
<tr>
<td>448</td>
<td>120</td>
</tr>
<tr>
<td>446</td>
<td></td>
</tr>
<tr>
<td>444</td>
<td></td>
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<tr>
<td>442</td>
<td></td>
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<tr>
<td>440</td>
<td></td>
</tr>
<tr>
<td>438</td>
<td></td>
</tr>
<tr>
<td>436</td>
<td></td>
</tr>
</tbody>
</table>

UNITS: Temperature: C, Mass: mol
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:

\[
\min_{x \in \Omega} f(x)
\]

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

```delphi
unit Graphs;

{$IFDEF FPC}
  {$MODE Delphi}
{$ENDIF}

interface

uses

{$IFDEF FPC}
  Windows, TeEngine, Series, TeeProcs, Chart,
{$ELSE}
  LCLIntf, LCLType, LMessages, TATGraph, TASeries, TACustomSeries, TATools, TATransformations,
{$ENDIF}

Messages, SysUtils, Classes, Graphics, Controls, Forms, Dialogs, ExtCtrls, ComCtrls;
```
Lazarus IDE
SimuSage Optimization Form

- Objective

  - Select the type of optimization
  - Choose a PbObject instance present in the designed flowsheet
  - Choose a property for the chosen PbObject
  - In case of a target calculation a target value must be given

Go to the Variables tab
Close the form
SimuSage Optimization Form

- **Variables**

1. **Define a variable**
   - 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**

- List of the defined variables
- Close the form
- Go to the Constraints tab
- Add a variable
- Clear all defined variables
- Delete all selected variables
- Delete all defined variables
- Clear the given variable parameters
SimuSage Optimization Form

- Constraints

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)

[Diagram showing a form with tabs for Objective, Variables, Constraints, Parameters, Table, and Chart.

- Go to the Parameters tab
- Close the form
- Clear the given constraint parameters
- Add a constraint
- Delete a selected constraint
- Delete all defined constraints
- List of the defined constraints]
SimuSage Optimization Form

- **Parameters**

  - **PbOutputUnit** which triggers the execution of the flowsheet
  - **Initial mesh size value**
  - **Admissible error in the result**
  - **Maximum number of Optimization evaluations**
  - **Maximum allowed time for the optimization**
  - **Plot chart with successful and unsuccessful results**
  - **Plot chart with successful and unsuccessful results**
  - **Reset all given parameters of the optimization**
  - **Close the form**
  - **Start the optimization**
  - **Information panel which is updated on every optimization calculation**

  - **Output Unit:**
    - **Maximum number of evaluations:** 100
    - **Epsilon:** 1E-5
    - **Maximum Time (s):** 0
    - **Plot all optimization calculations**

  - **Information:**
    - **Status:** Idle
    - **Number of Optimization Calculations:** 0/0
    - **Current Minimum:** Not calculated
Thank you for your attention!