Model Diagnostics for Equation Oriented Models: Roadblocks and the Path Forward

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Introduction

Equation Oriented (EO) modeling techniques are **powerful tools** for solving complex **process engineering** models. However, EO-based tools come with several **challenges**, especially when applied to large models

Structural issues

- Incorrect degrees of freedom
- Inconsistent units
- Structural rank deficiencies

Numerical issues

- Local infeasibility
- Function evaluation errors
- Numeric rank deficiencies
- Ill-conditioning

User Research

We interviewed 13 users of the IDAES platform about diagnosing model issues

Most users did not have formal training in diagnosing issues.

Many useful diagnostics tools were already available.

There was no common workflow for diagnosing the same types of issues.

Types of issues experienced

Scaling	8/13
Degeneracy, Evaluation Errors, DoF, or Infeasibility	4/13
Initialization	3/13
Incorrect Assumptions	1/13

No user was aware of all available tools.

Degeneracy Hunter/Model Stats	8/13
Solver Options/Jacobian Inspection	4/13
Solver Log	3/13
Other Tools	2/13

Many users overlooked valuable information.

Solver Logs	8/13
Model Statistics	4/13
Jacobian Inspection	2/13
Other	1/13

Needs identified

Standard workflow for diagnosing issues

Centralized toolbox of useful diagnosis methods

Automatically diagnosing arbitrary issues with nonlinear optimization problems is a Holy Grail of Operations Research.

Can You Find All 6 Potential Issues?

8 Variables:

v_1 - [m]
v_2 - [m]
v_3 - $0 \leq v_3 \leq 5$
v_4
v_5 - $0 \leq v_5 \leq 1$
v_6
v_7 - [m], $0\ \mathrm{m} \leq v_7 \leq 1\mathrm{m}$
v_8

4 Constraints:

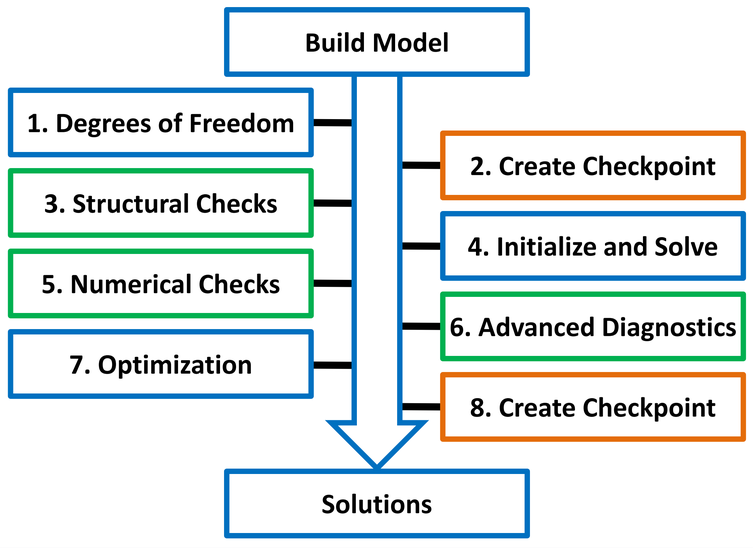
c1: $v_1 + v_2 = 10$
c2: $v_3 = v_4 + v_5$
c3: $2v_3 = 3v_4 + 4v_5 + v_6$
c4: $v_7 = 1 \times 10^{-8}\ v_1$

3 Fixed Variables:

$v_4 = 2,\ v_5 = 2,\ v_6 = 0$

```
import pyomo.environ as pyo

m = pyo.ConcreteModel()

m.v1 = pyo.Var(units=pyo.units.m)
m.v2 = pyo.Var(units=pyo.units.m)
m.v3 = pyo.Var(bounds=(0, 5))
m.v4 = pyo.Var()
m.v5 = pyo.Var(bounds=(0, 5))
m.v6 = pyo.Var()
m.v7 = pyo.Var(units=pyo.units.m, bounds=(0, 1))
m.v8 = pyo.Var()

m.c1 = pyo.Constraint(expr=m.v1 + m.v2 == 10)
m.c2 = pyo.Constraint(expr=m.v3 == m.v4 + m.v5)
m.c3 = pyo.Constraint(expr=2*m.v3 == 3*m.v4 + 4*m.v5 + m.v6)
m.c4 = pyo.Constraint(expr=m.v7 == 2e-8*m.v1)

m.v4.fix(2)
m.v5.fix(2)
m.v6.fix(0)
```

Diagnostics Workflow



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Diagnostics Toolbox

Applicable to any Pyomo model:

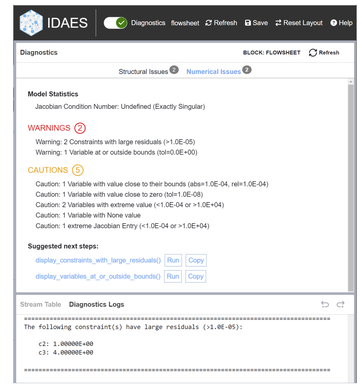
```
from idaes.core.util import DiagnosticsToolbox

dt = DiagnosticsToolbox(model)
dt.report_structural_issues()
```

Documentation

Modeling issue	Tool to identify
Incorrect degrees of freedom	Dulmage-Mendelsohn decomposition
Structural rank deficiency	
Inconsistent units of measure	Pyomo units system
Potential function evaluation errors	Bound propagation
Numeric rank deficiency	Parallel row/column identification
Ill-conditioning	Singular value decomposition, ill-conditioning certificate

- Automated issue detection
  - Run multiple tests with one command
- Concise summary of issues
  - **Warnings**: must-fix issues
  - **Cautions**: potential additional issues
- Suggested next steps
  - Workflow integrated into Toolbox
- Additional detail available
  - Display methods for each issue type
  - Provide in-depth information
- Continuing improvement



Success Stories

- Structural singularity in fluidized bed reactor model
- Inconsistent boundary conditions in large PDAE system
- Degenerate recycle loops
- Ill-conditioned Jacobian in solvent absorption column

Future Work

- Seek feedback from users to refine tools and workflow.
- Identifying issues is relatively easy, fixing them is hard.
- Need to assist users with correcting identified issues.
- Documentation is needed to help educate users.