Adaptive DAE Model Reduction

J. D. Hedengren and T. F. Edgar
The University of Texas at Austin
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Topics

- Motivations
- Three Step Process for DAE Model Reduction
  1. Adaptive reduction of differential equations
  2. Partitioning and precedence ordering
  3. Adaptive reduction of algebraic equations with ISAT
- Three Examples
  1. Adaptive reduction of differential equations
  2. Object oriented modeling and model reduction
  3. A candidate to replace neural nets: ISAT

DAE model size

- Small (1-100 variables)
  - Single process units
  - $A \rightarrow B$
  - Useful for showing academic theory
- Medium (100-10,000 variables)
  - Multiple process units
  - Multicomponent modeling, reaction networks
  - Practical limit for real-time NMPC applications
- Large (10,000+ variables)
  - Plant wide dynamic models
  - Currently optimized at this level with steady state models (RTO)

Motivations

- Plant wide NMPC control (Large scale)
- Storage and retrieval of optimal control trajectories (Small and medium scale)
- Reveal underlying structure of the model
  - Determine dynamic degrees of freedom
  - Find source of DAE intialization / convergence problems

Adaptive DAE model reduction

1. Adaptive reduction of differential equations
2. Partitioning and precedence ordering
3. Adaptive reduction of algebraic equations with ISAT

ODE model reduction

- Semi-explicit ODE model form

$$\dot{x}(t) = f(x(t))$$

- Galerkin projection ($\widetilde{P}$)

$$x(t) = \widetilde{P}^T \overline{x}(t) + r(t)$$

- Substitution

$$\dot{\overline{x}}(t) = \widetilde{P} f(\widetilde{P}^T \overline{x}(t) + r(t)) + \widetilde{P} \dot{r}(t)$$

- Reduced model

$$\dot{\overline{x}}(t) = \widetilde{P} f(\widetilde{P}^T \overline{x}(t))$$

Model reduction error

- Variable error constraint

$$\left|\widetilde{P}^T \overline{x}(t) - x(t)\right| \le \varepsilon_{tol}$$

- Controlling variable error
  - ↓ model order, ↑ variable error
  - ↑ model order, ↓ variable error
- DOF
  - Total degrees of freedom (DOF) = model order
  - Dynamic degrees of freedom (DDOF) = reduced model order that satisfies the variable error constraint

Predicting DDOF

- Is there a way to predict the dynamic degrees of freedom?
  - Singular values (poor predictor)
  - Solve complete and reduced model at check points (inefficient)
  - Equation residuals (unexplored option)

Predicting DDOF

- Linearized system

$$\dot{x}(t) = Ax(t) + Bu(t)$$

- Galerkin projection

$$x(t) = \widetilde{P}^T \overline{x}(t) + r(t)$$

$$\dot{x}(t) = \widetilde{P}^T \dot{\overline{x}}(t) + \dot{r}(t)$$

- Substitute

$$\widetilde{P}^T \dot{\overline{x}}(t) = A\left(\widetilde{P}^T \overline{x}(t)\right) + Ar(t) - \dot{r}(t) + Bu(t)$$

- Predictor (*r(t)* = variable error, *R(t)* = equation residual)

$$R(t) = Ar(t) - \dot{r}(t) \cong Ar(t)$$

$r(t) \cong A^{-1}R(t)$ Variable error predictor

Adaptive ODE model reduction

- Variable error constraint

$$\left|\widetilde{P}^T \overline{x}(t) - x(t)\right| = \boxed{r(t) \cong A^{-1}R(t)} \le \varepsilon_{tol}$$

- Open equation format

$f(\dot{x}(t), x(t)) = 0$ Solution obtained by finding roots

$f(\widetilde{P}^T \dot{\overline{x}}(t), \widetilde{P}^T \overline{x}(t)) = R(t)$ Solution obtained by minimizing residuals

- Controlling variable error
  - When $A^{-1}R(t) \le \varepsilon_{tol}$, ↓ model order
  - When $A^{-1}R(t) > \varepsilon_{tol}$, ↑ model order
- Variable error predictor can also be used to improve reduced model accuracy

Adaptive DAE model reduction

1. Adaptive reduction of differential equations
2. <u>Partitioning and precedence ordering</u>
3. Adaptive reduction of algebraic equations with ISAT

Partioning and Precedence Ordering

- DAE model

$$f_{DAE}(\dot{z}, z, t) = 0 \quad \Longleftrightarrow \quad \begin{array}{l} f_{ODE}(\dot{x}, x, y, t) = 0 \\ f_{AE}(x, y, t) = 0 \end{array}$$

- Sparsity matrix

$$J_{ij} = \begin{cases} 1 & \text{if } y_j \text{ or } \dot{x}_j \text{ appears in } f_{DAE\,i} \\ 0 & \text{otherwise} \end{cases}$$

- Pairing equations and variables
  - Obtain a maximum transversal
  - Zero-free diagonal means that each variable is uniquely paired with each equation

Partitioning and Precedence Ordering

- Lower triangular block form
  - Each successive block of variables and equations can be solved independently
  - Inverting the sparsity matrix shows global variable dependencies
  - Binary distillation example (230 x 230 system):

<u>Original sparsity</u>

$$
\left[\begin{array}{cc|cccccccc}
X & 0 & X & 0 & 0 & X & 0 & 0 & 0 & 0 \\
0 & X & 0 & 0 & 0 & X & X & X & 0 & 0 \\
\hline
0 & 0 & X & 0 & 0 & 0 & 0 & 0 & X & 0 \\
0 & 0 & 0 & X & 0 & 0 & X & X & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & X & X \\
0 & 0 & 0 & X & 0 & X & 0 & 0 & 0 & 0 \\
0 & 0 & X & 0 & X & 0 & X & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & X & 0 & 0 & X & 0 & 0 \\
0 & 0 & 0 & 0 & X & 0 & 0 & 0 & X & 0 \\
0 & 0 & 0 & 0 & X & 0 & 0 & 0 & 0 & X
\end{array}\right]
\left[\begin{array}{c}
\dot{\mathbf{x}}_A \\ \dot{\mathbf{h}} \\ \hline \mathbf{y}_A \\ \mathbf{x}_L \\ \mathbf{T} \\ \dot{\mathbf{n}}_V \text{ or } \dot{\mathbf{n}}_L \\ \mathbf{h}_V \\ \mathbf{h}_L \\ \mathbf{P}_A^{sat} \\ \mathbf{P}_B^{sat}
\end{array}\right]
$$

<u>Lower triangular block form</u>

$$
\left[\begin{array}{cccccccc|cc}
X & X & X & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
X & X & X & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
X & X & X & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
X & X & X & X & 0 & 0 & 0 & 0 & 0 & 0 \\
X & X & X & 0 & X & 0 & 0 & 0 & 0 & 0 \\
X & X & X & 0 & X & X & 0 & 0 & 0 & 0 \\
X & X & X & X & X & X & X & 0 & 0 & 0 \\
X & X & X & X & X & X & X & X & 0 & 0 \\
\hline
X & X & X & X & X & X & X & X & X & 0 \\
X & X & X & X & X & X & X & X & 0 & X
\end{array}\right]
\left[\begin{array}{c}
\mathbf{T} \\ \mathbf{P}_A^{sat} \\ \mathbf{P}_B^{sat} \\ \mathbf{h}_L \\ \mathbf{y}_A \\ \mathbf{h}_V \\ \mathbf{x}_L \\ \dot{\mathbf{n}}_V \text{ or } \dot{\mathbf{n}}_L \\ \hline \dot{\mathbf{x}}_A \\ \dot{\mathbf{h}}
\end{array}\right]
$$

Scalability to large systems

- n – number of algebraic equations
- τ – number of non-zeros in the sparsity matrix
- The maximum transversal algorithm has a worst case bound of $O(nt)$ although typical examples are more like $O(n) + O(t)$ (Duff, 1981)
- The lower block triangular algorithm also exhibits excellent scaling for large problems with an upper bound of $O(n) + O(t)$ (Duff and Reid, 1978)

Adaptive DAE model reduction

1. Adaptive reduction of differential equations
2. Partitioning and precedence ordering
3. Adaptive reduction of algebraic equations with ISAT

Adaptive reduction of algebraic equations

- Explicit transformation of algebraic equations
  - Transform model equations in explicit form
    - Model equations can be proprietary
    - Re-code large number of equations by hand?
  - Neural networks
    - Extrapolation problems
    - No reliable error control strategy
  - In situ adaptive tabulation (ISAT)
    - Dynamic database with error control
    - Replacement for neural nets?

ISAT

- Proposed by Pope (1997) to decrease computing time of reacting turbulent gas simulations by 1000 times
- Extended by Hedengren and Edgar (2004a) to decrease computing time of NMPC calculations by 85 times
- Developed as a general storage and retrieval method that outperforms neural nets in interpolation (Hedengren and Edgar, 2004b) and extrapolation (Hedengren and Edgar, 2004c)

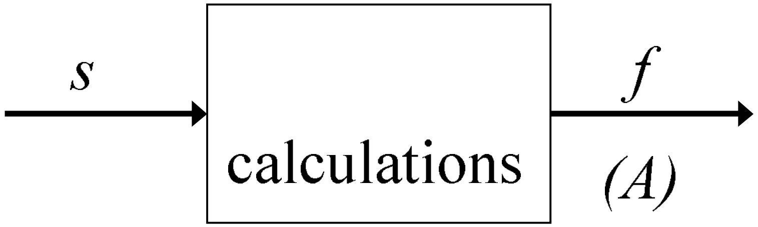
Overview of ISAT

- Black box function approximation

  s – vector of independent variables

  f – vector of dependent variables

  A – sensitivity matrix (if available)



- Automatic Error Control
  - Error tolerance ε_{tol} is the principal tuning parameter for ISAT

$$\left| f - f_{est} \right| \leq \varepsilon_{tol}$$

Example #1: Adaptive ODE reduction

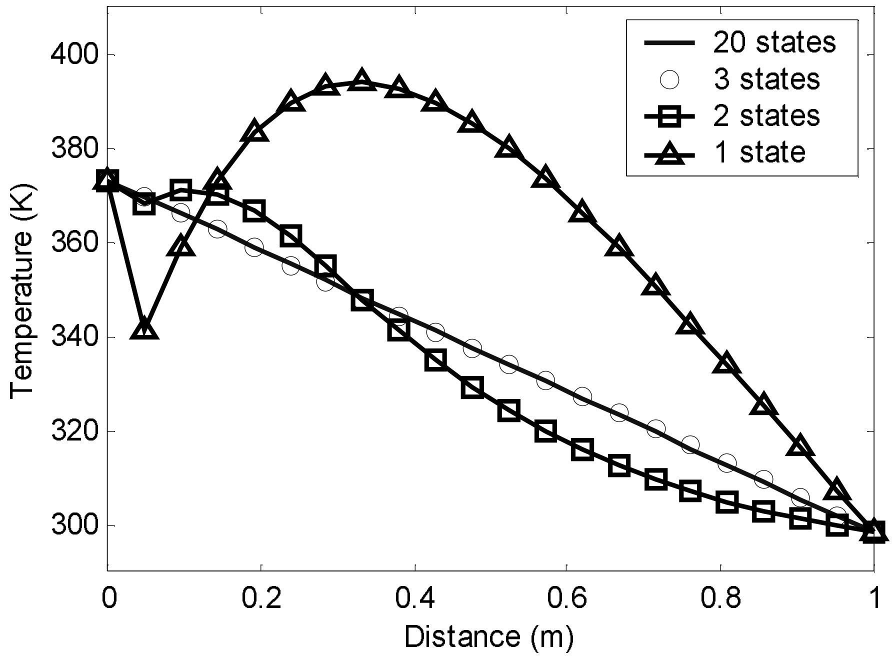
- 1-D unsteady heat conduction

$$\rho c \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x} \right)$$

- Discretizing the PDE results in a set of 20 ODEs
- Simulation:
  - Aluminum slab with thickness 1 m
  - Initially at 25 ºC
  - At $t = 0$ the left boundary is changed to 100 ºC
  - Tolerance set $\varepsilon_{tol} = 1$ ºC

Example #1 Results

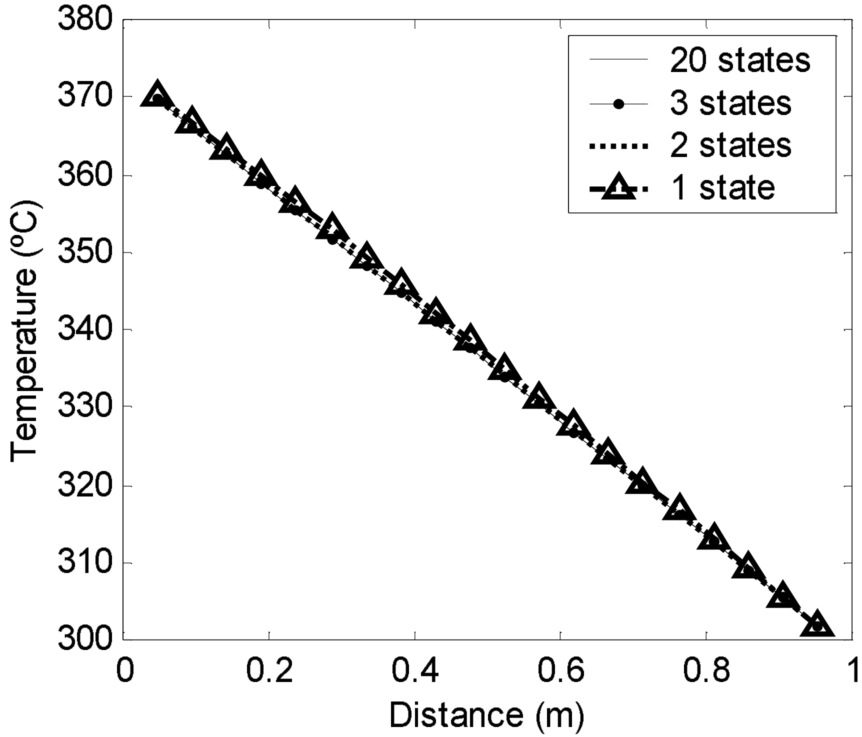
- After 100 minutes the temperature profile approaches steady state



- Variable error predictor indicates that at least 3 states are required to meet error tolerance

Example #1 Results

- Variable error predictor can also be used to improve the reduced model accuracy (1 state required with correction)



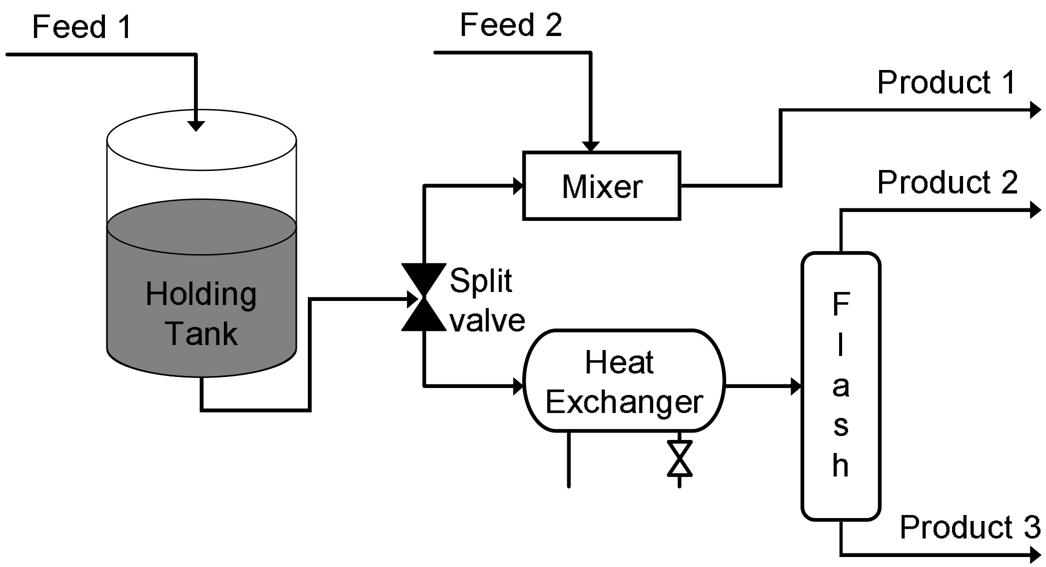
- Excellent prediction because the model is nearly linear and approaching steady state

Example #2: Object oriented modeling and model reduction

- Multicomponent, multiphase object oriented simulator
- FORTRAN 90 routines for fast execution
- DIPPR database with properties for >1700 compounds
- DASPK 3.0 for numerical integration and sensitivity analysis
- Current models are a compressor, splitter, mixer, vessel, heat exchanger, and flash column
- Developing models for continuous and batch distillation and reactors (integrate CANTERA)

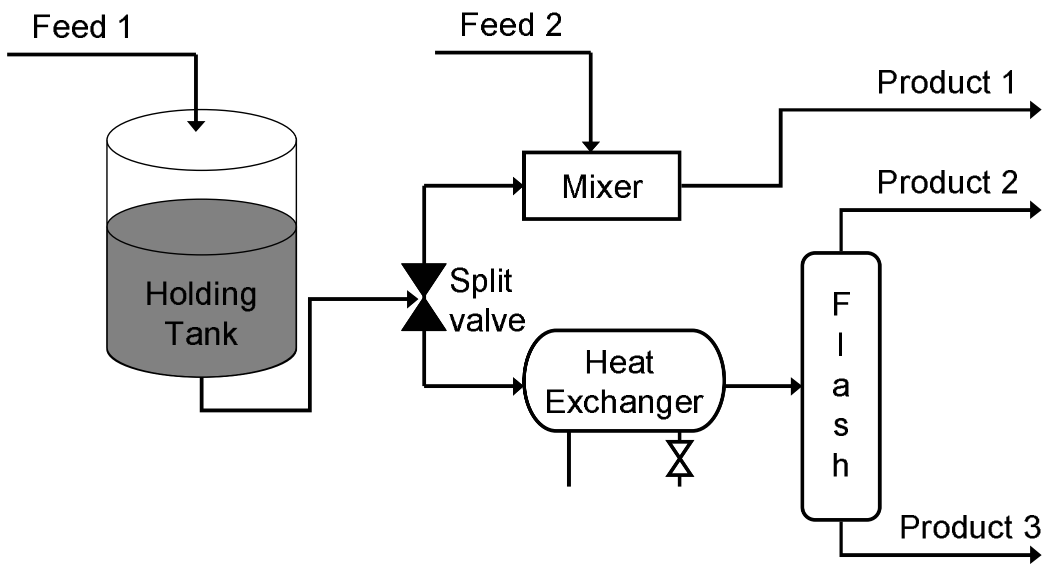
Example #2: Flow sheet model

- Blending and separation
  - Feed streams: butane, pentane, hexane, heptane, and octane
- DAE model
  - 12 differential equations
  - 217 algebraic equations



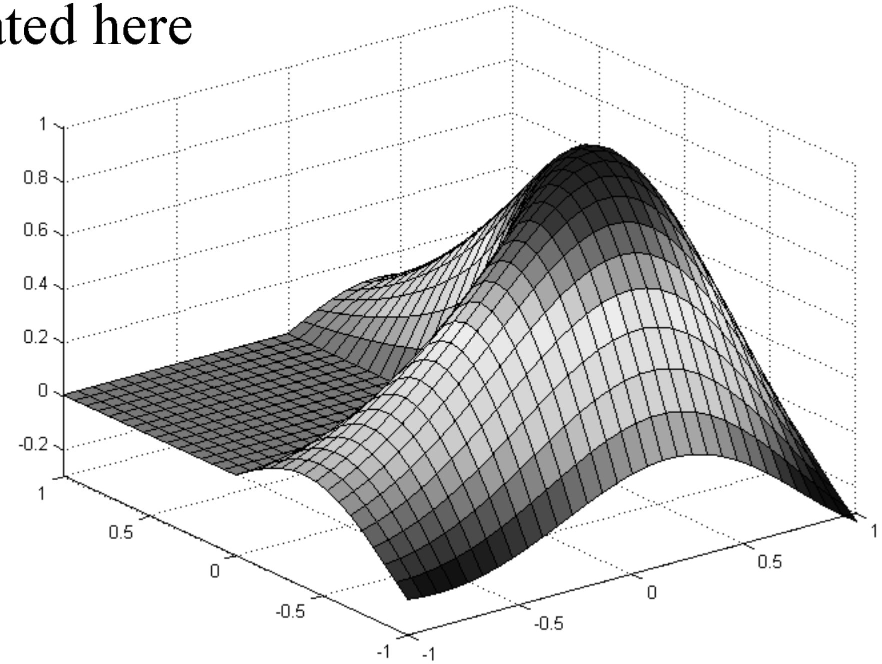
Example #2: Results

- Algebraic equation decomposition
  - 202 successively independent sets of variables and equations
  - One implicit set: 16 equations (flash column)
  - Model reduced from 229 to 28 states



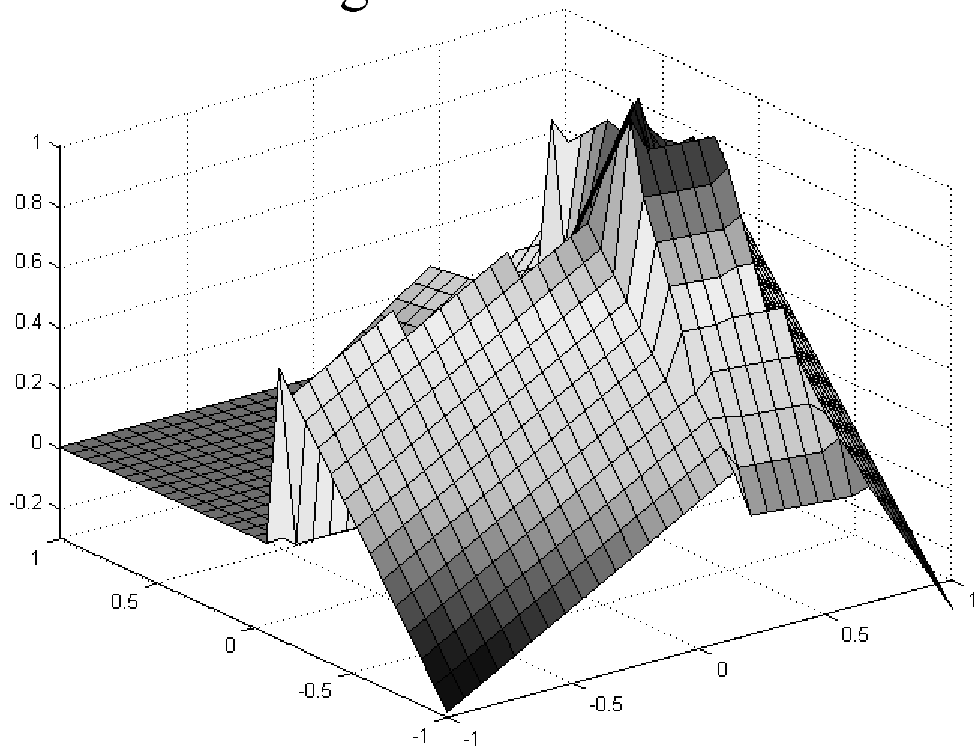
Example #3: ISAT vs neural nets

- Nonlinear function test case
  - 1st eigenfunction of an L-shaped membrane
  - 2nd and 3rd eigenfunctions also appear on Mathworks' publications
  - Linear and nonlinear regions
  - Points that are not continuously differentiable
  - ISAT also handles function discontinuities, although that capability is not demonstrated here



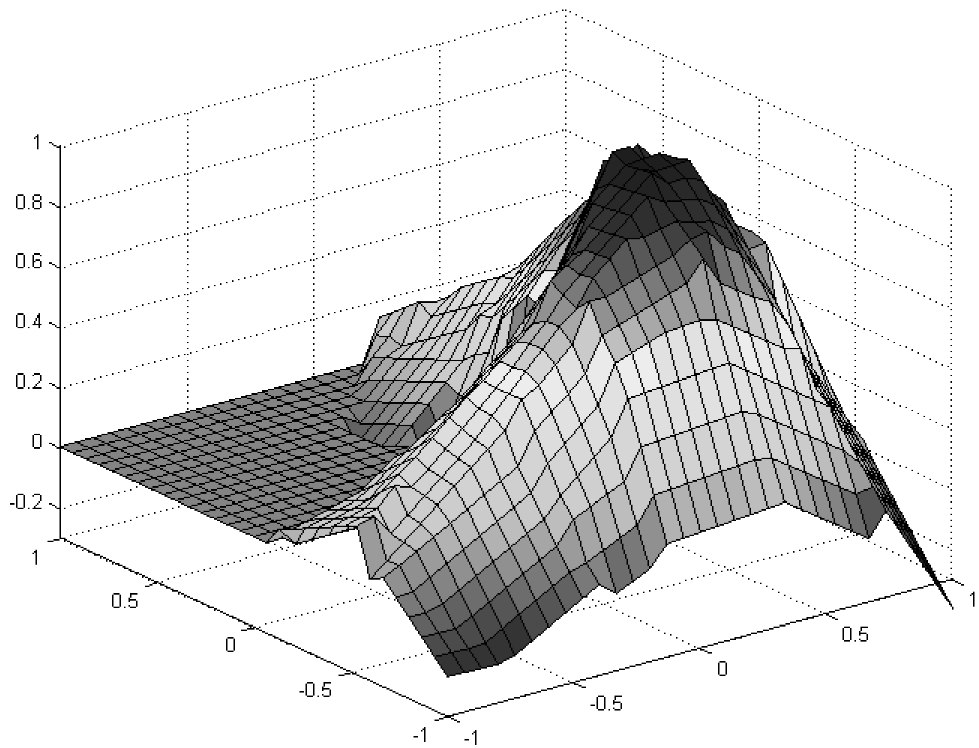
ISAT

- Principal tuning parameter
  - Set to $\varepsilon_{tol} = 0.5$ (extremely coarse)
  - Intuitive adjustable parameter – in this case little accuracy is required
  - ISAT created 12 linear regions



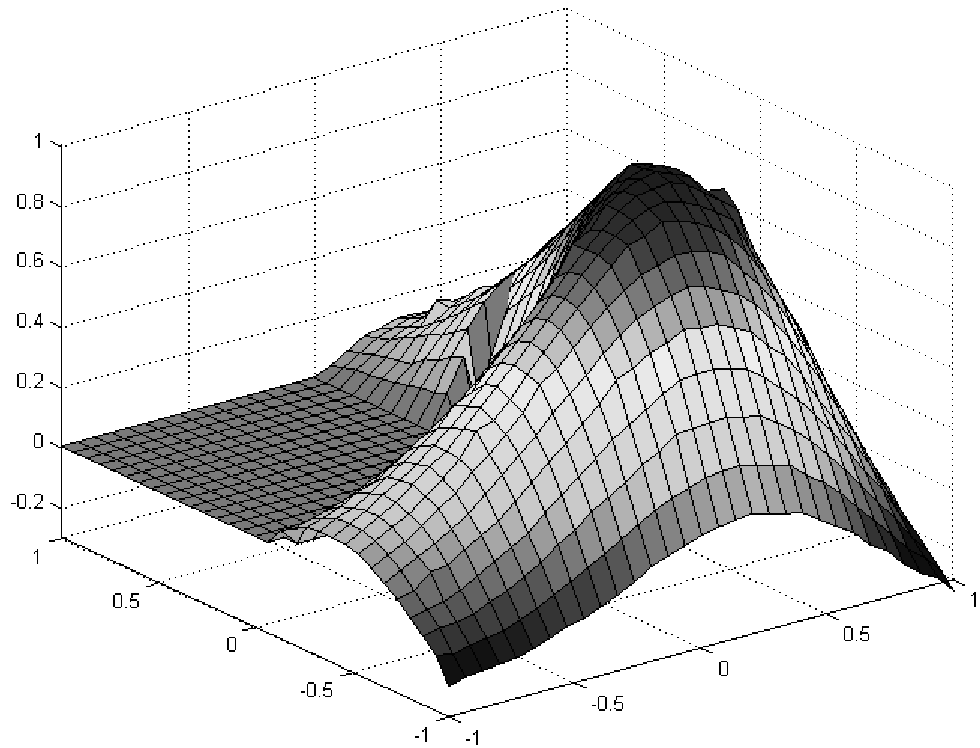
ISAT

- Principal tuning parameter
  - Set to $\varepsilon_{tol} = 0.1$
  - Moderate accuracy is required
  - ISAT created 48 linear regions



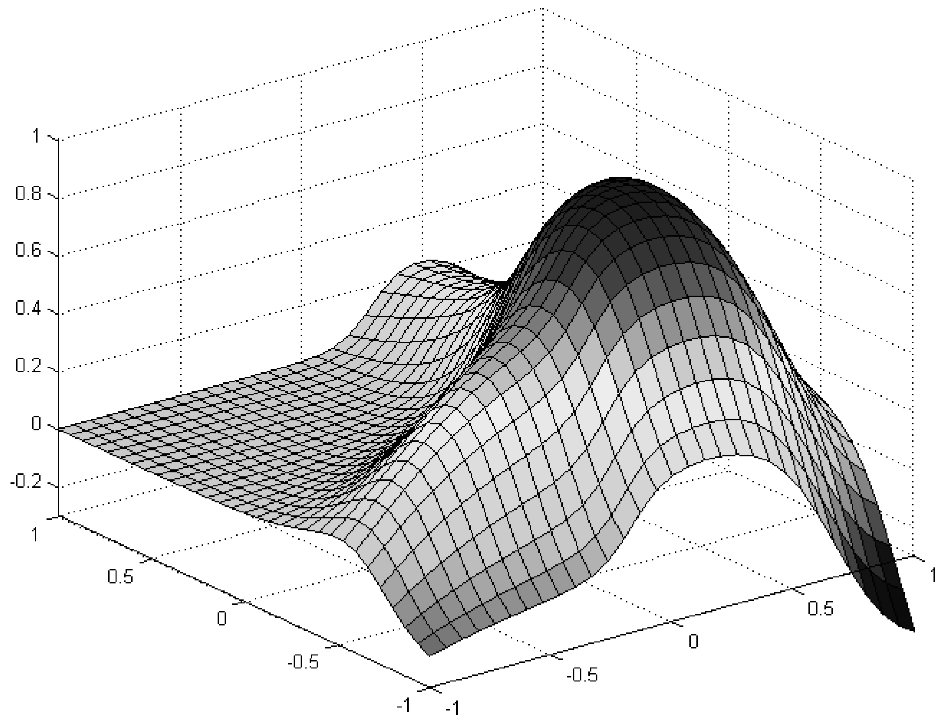
ISAT

- Principal tuning parameter
  - Set to $\varepsilon_{tol} = 0.01$
  - High accuracy is required
  - ISAT created 206 linear regions



Neural net

- Principal tuning parameters
  - Structure: 2 layers
    - Hidden layer: 4 neurons, tangent function
    - Output layer: 1 neuron, linear function
  - Optimization tolerances
- Generated with MATLAB's neural net toolbox



Example #3 Conclusions

- ISAT advantages
  - Fewer tuning parameters
  - More intuitive tuning parameters
  - Approximates discontinuous and non continuously differentiable functions
  - Builds *in situ,* with no global optimizations

Conclusions

- Three step DAE model reduction process
  1. Adaptive reduction of differential equations
     - Variable error predictor enables efficient adaptive ODE reduction
     - Predictor can also be used as a corrector (from example: 3 states $\rightarrow$ 1 state with no loss of accuracy)
  2. Partitioning and precedence ordering
     - Examples demonstrate ~10 times reduction in number of variables
     - Successful reduction of object-oriented flow sheet models with multicomponent processes
  3. Adaptive reduction of algebraic equations with ISAT
     - ISAT explicitly transforms sets of nonlinear equations with a given error tolerance
     - Suggested as a replacement for neural networks

Publications

Duff, I. S. On algorithms for obtaining a maximum transversal, ACM Transactions on Mathematical Software, **1981**, 7, 3, 315-330.

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Hedengren, J. D. and Edgar, T. F. *In situ* adaptive tabulation for real time control. *Proceedings of the ACC* **2004a**, Boston, MA, 2222-2228.

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