Formal Identification of DC Operating Points in Integrated Circuits and some Lessons in (Ir)Reproducible Research in Computational Math

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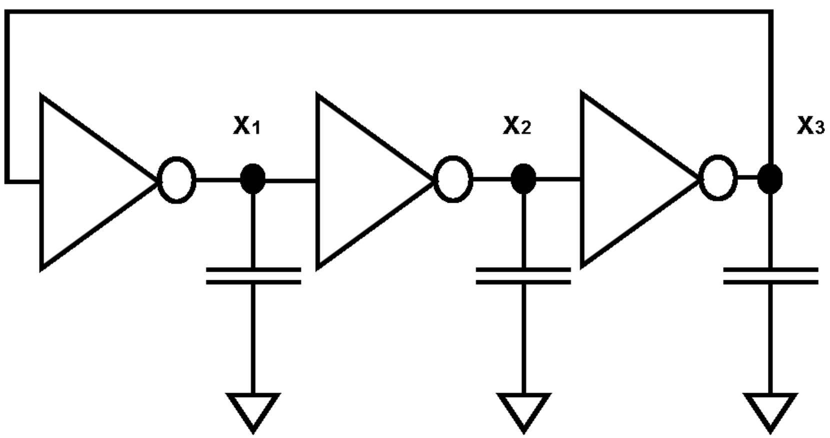
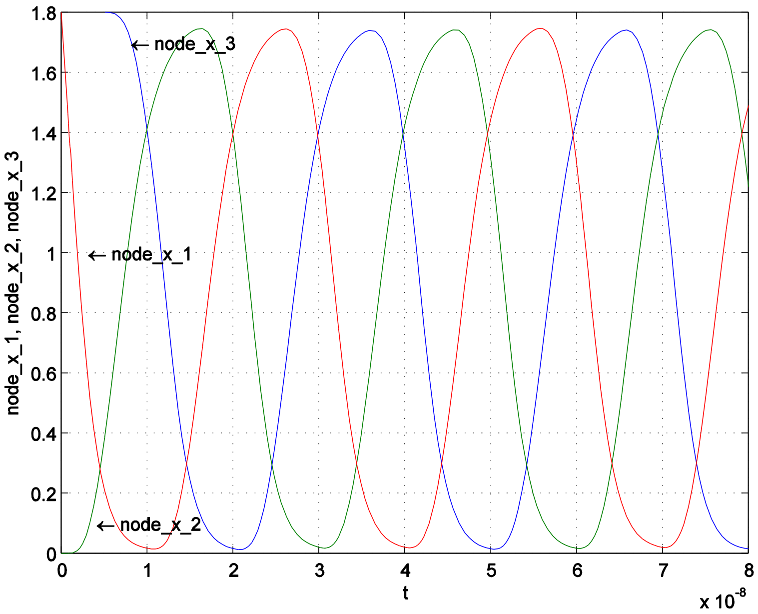
DC Operating Point(s) of a Circuit

- State (node voltages) towards which the system will settle when any inputs are held constant
  - Small perturbations of state will decay
- Inverter: A single known state
  - Output is high if input is low or vice versa
- Oscillator: No DC operating point(s)
  - Oscillation requires node voltages to keep changing
- D flip-flop: Depends on clock
  - Transparent: A single known state such that output matches D input
  - Latched: two possible states, depending on last D input
- Typical applications
  - Initial conditions for transient simulation
  - Linearization point for small signal analysis
  - Determine qualitative stable behaviour of the circuit (eg: memory or oscillator lockup)

Ring Oscillators

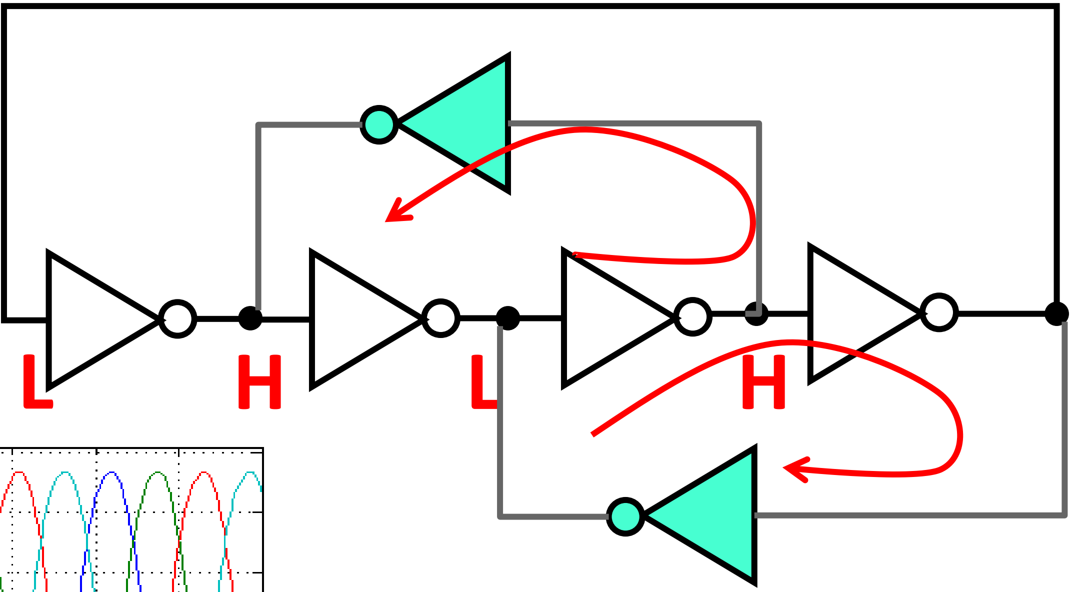
- Output oscillates between high and low values at fixed frequency
- Example implementation: Series inverters with feedback
  - No obvious stable state for odd number of inverters
  - Each inverter generates a signal with different phase

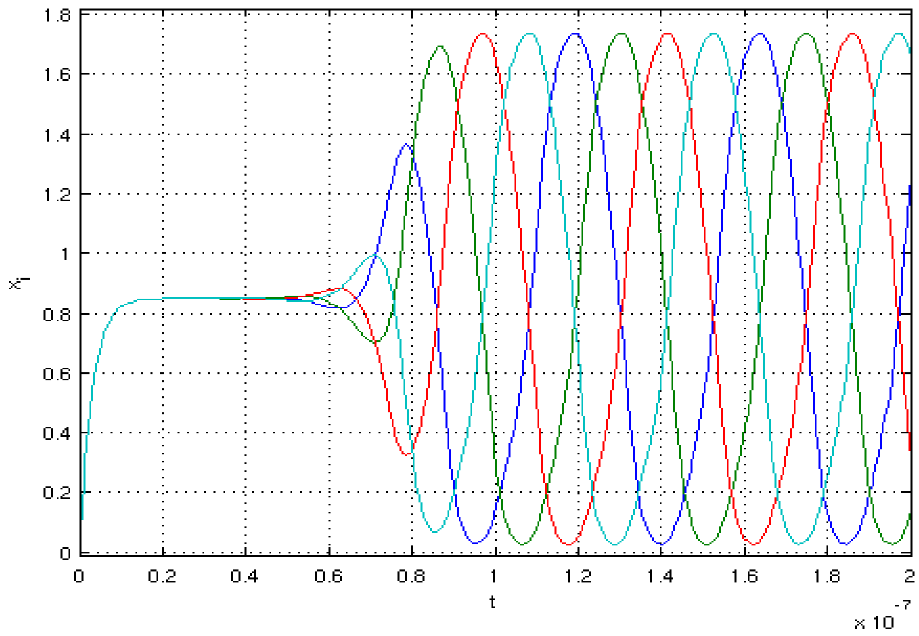




Rambus Ring Oscillator

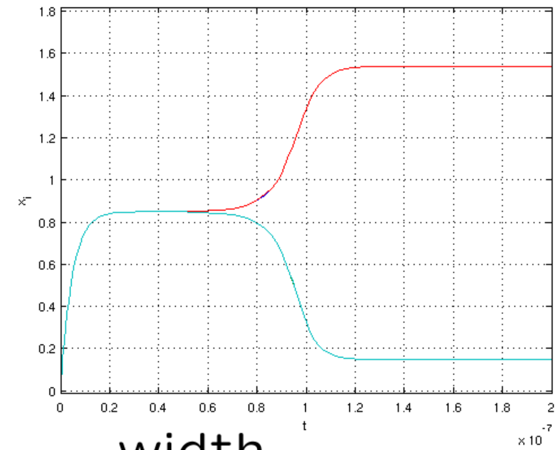
- Is it possible to generate a four phase signal?



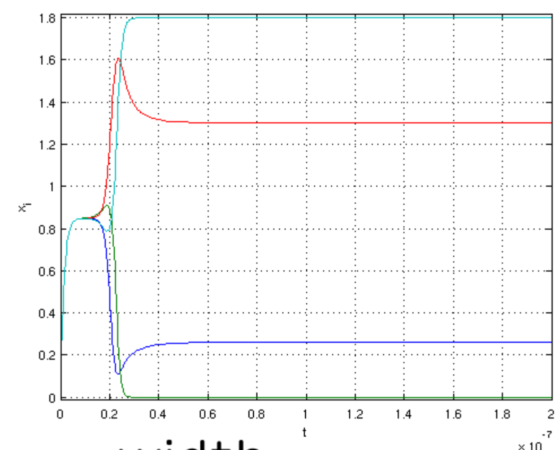


Rambus Ring Oscillator Failure Modes

- Behaviour depends critically on ratio of the widths of the ring and bridge inverters
  - Consistent oscillation if ratio is near one
  - Consistent failure to oscillate if ratio is very large or small
  - Behaviour depends on initial conditions for some ratios
- Example of actual design failure
  - Design passed typical analog validation procedure
  - Problems found during measurement of fabricated test chips



$$\frac{\text{width}_{\text{ring}}}{\text{width}_{\text{bridge}}} \gg 1$$



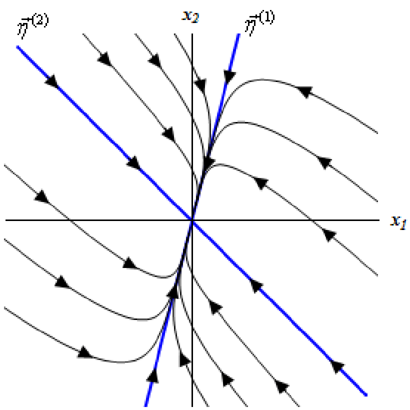
$$\frac{\text{width}_{\text{ring}}}{\text{width}_{\text{bridge}}} \ll 1$$

Outline (Part 1)

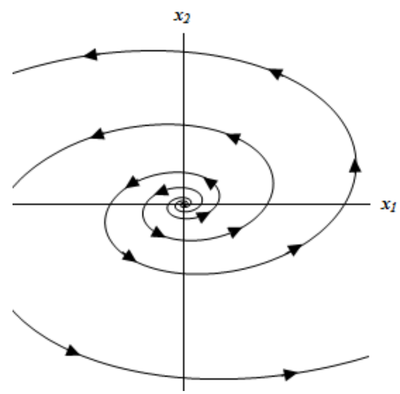
- Motivation
- Mathematical characterization of DC operating points
- Our approach
  - Circuit model construction with netlist & OOmspice / Chum
  - Analytic exclusion with symbolic model & HySAT
  - Numerical exclusion with interval model & IntLab
  - Stability analysis with pseudospectra & EigTool
- Examples
  - Schmitt trigger
  - Ring & Rambus oscillators

DC Operating Point Definition

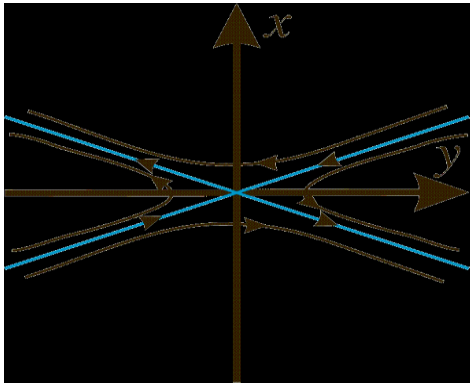
- Circuit modeled as an ordinary differential equation (ODE) with state $x(t)$: $dx(t) / dt = f(x(t))$
- Equilibrium state x_e such that: $f(x_e) = 0$
- DC operating point: Stable equilibrium state (toward which all neighbouring trajectories are attracted)
  – Stability determined by the sign of the real component of the eigenvalues $\boldsymbol{\lambda}_i$ of the Jacobian $\partial f(x_e) / \partial x$



Stable Equilibrium
(DC Operating point)
$\forall\lambda$ Re[λ] < 0



Unstable Equilibrium
$\forall\lambda$ Re[λ] > 0



Metastable Equilibrium
$\exists\lambda_1$ Re[λ_1] > 0 and
$\exists\lambda_2$ Re[λ_2] ≤ 0

Traditional DC Operating Point Analysis

- Solving non-convex, high-dimensional equation $f(x) = 0$ through traditional numerical methods is prone to failure
- Even if DC operating point is found, traditional numerical methods give no guarantee of uniqueness
- Common heuristic workarounds
  - Designer specifies the operating point
  - Transient simulation from powered off condition

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Our Approach (conceptually)

- Construct an analytic ODE circuit model $dx(t) / dt = f(x(t))$
  - Requires circuit netlist and analytic transistor models
  - Accomplished by in-house OOmspice & Chum tools
- Rigourously exclude regions containing no equilibria
  - No solution to $f(x_e) = 0$
  - Restricted to bounded region of state space (eg: 0 to V_{dd})
  - First pass with unsatisfiability solver HySAT
  - Output of HySAT further refined through interval arithmetic in IntLab
- Examine system stability in regions which must or may contain equilibria
  - Construct interval Jacobian matrix $\partial f(x_e) / \partial x$ within region using IntLab
  - Examine eigenvalues of interval Jacobian through matrix pseudospectra with EigTool

Circuit Model

- OOmspice tool takes a Spice-like netlist and synthesizes ODE as either symbolic equations or a Matlab function
- Each MOSFET transistor is modeled as a three terminal (gate, source and drain), nonlinear voltage controlled current source $i_{ds} = f(v_{gs}, v_{ds})$
- Circuit nodes have capacitance (such as connected transistor gates)
  - Currently all capacitance is assumed to be constant and to ground
- KCL implies $i_{\text{transistors}} + i_{\text{capacitors}} = 0$ and standard capacitor model is $i_{\text{capacitors}} = C({dv}/{dt})$, so circuit ODE is given by

$$\frac{dv}{dt} = -C^{-1} i_{\text{transistors}}$$

where $i_{\text{transistors}}$ is constructed from i_{ds} equations for each separate transistor

Transistor Model

- Chum tool samples Hspice current data on a fine grid of gate, source and drain voltages
- Data can be fit to several different models
  - First-order global transistor model (used in FAC paper)
  - Piecewise quadratic polynomial
  - Slightly simplified global EKV model [Enz, Krummenacher & Vittoz, *Analog Integrated Circuits and Systems*, 1995]
- Global model is pre-constructed
- Local models may be constructed within specified regions or with specified terminal values (eg: drain is grounded)
- Error bounds are also generated for each model

Unsatisfiability

- HySAT attempts to prove that $f(x_e) = 0$ cannot be satisfied within a specified state space region
  - Initial region that is a box; for example, each node is between 0 and V_{dd}
  - Uses symbolic model
- Typically fails and returns a subset of the region which may contain a solution
  - Subset is dispatched for further analysis
  - New region is constructed by excluding the subset
  - HySAT is called again with new region
- Process is repeated until HySAT finds some subset of the original box which contains no equilibria

Interval Arithmetic Analysis

- Intlab evaluates Matlab function model using interval arithmetic in regions proposed by HySAT
- Three possible outcomes
  - Refutation: One or more components of derivative do not change sign, so no equilibrium is possible
  - Confirmation: Subset of region is identified which definitely contains an equilibrium
  - Inconclusive: Region may or may not contain an equilibrium
- In the latter two cases, Intlab uses automatic differentiation on the Matlab function model to generate a Jacobian interval matrix

Matrix Pseudospectrum

- Spectrum of matrix A is the set of eigenvalues of A

$$\Lambda(A) = \{z \in \mathbb{C} \mid \det(zI - A) = 0\}$$

- ϵ-pseudospectrum (ϵ-ps) of A are the set of eigenvalues of neighbouring matrices

$$\Lambda_\epsilon(A) = \{z \in \mathbb{C} \mid z \in \Lambda(A + E) \text{ for some } \|E\| \leq \epsilon\}$$

- Eigtool package uses numerical continuation to plot contours of ϵ-ps for values of $\epsilon = 10^\eta$
- For more details, see Embree & Trefethen, Pseudospectra Gateway, `http://www.comlab.ox.ac.uk/pseudospectra`

Proving Equilibrium Stability / Instability

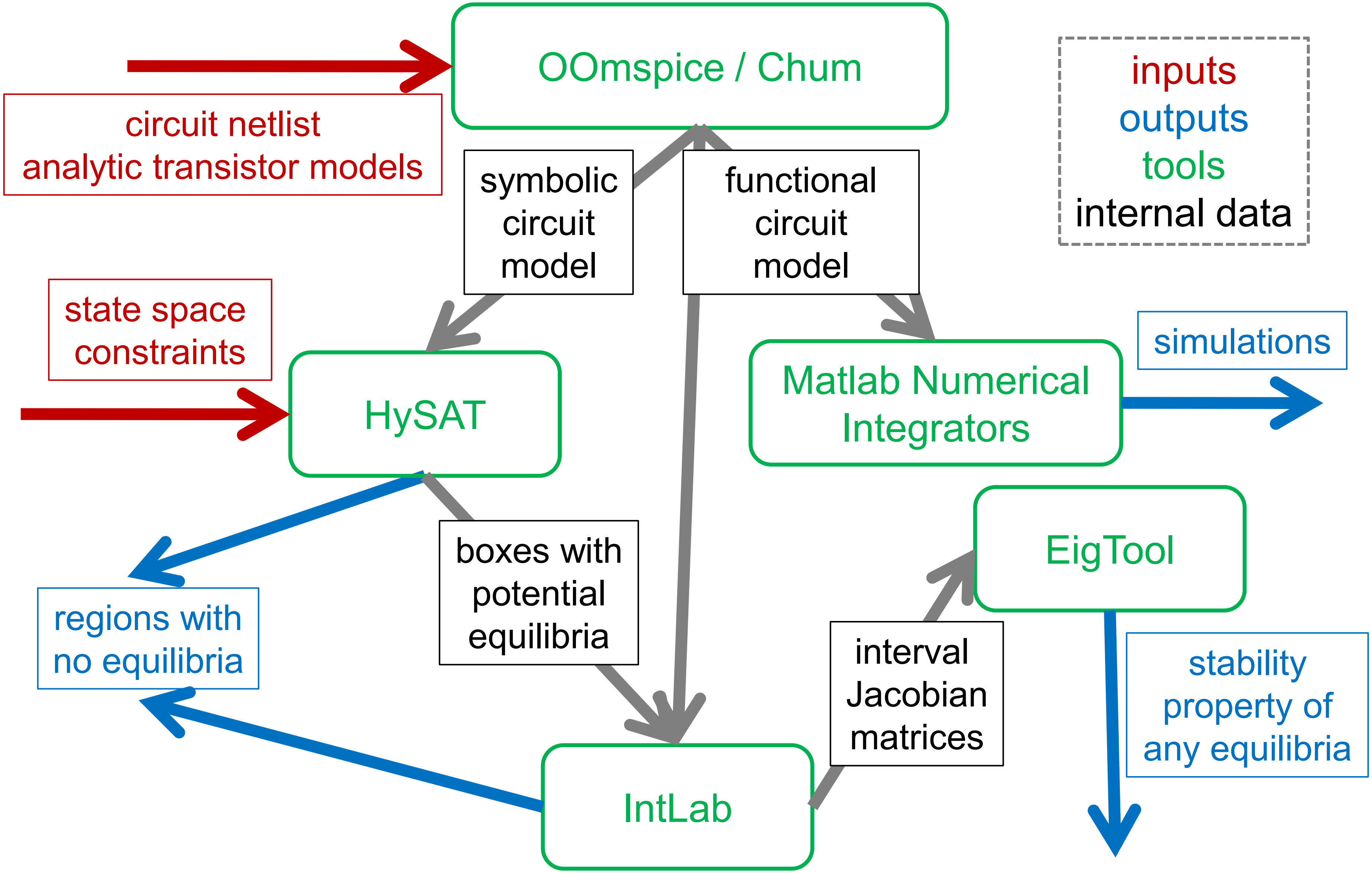
- For some region H of the state space, IntLab returns interval matrix $J_H = [A_C - \Delta, A_C + \Delta]$ containing $\partial f(\hat{x})/\partial x$ for all $\hat{x} \in H$
- Hurwitz test: J_H is stable if

$$\lambda_{\text{max}}(A_C^{(S)}) + \rho(\Delta^{(S)}) < 0$$

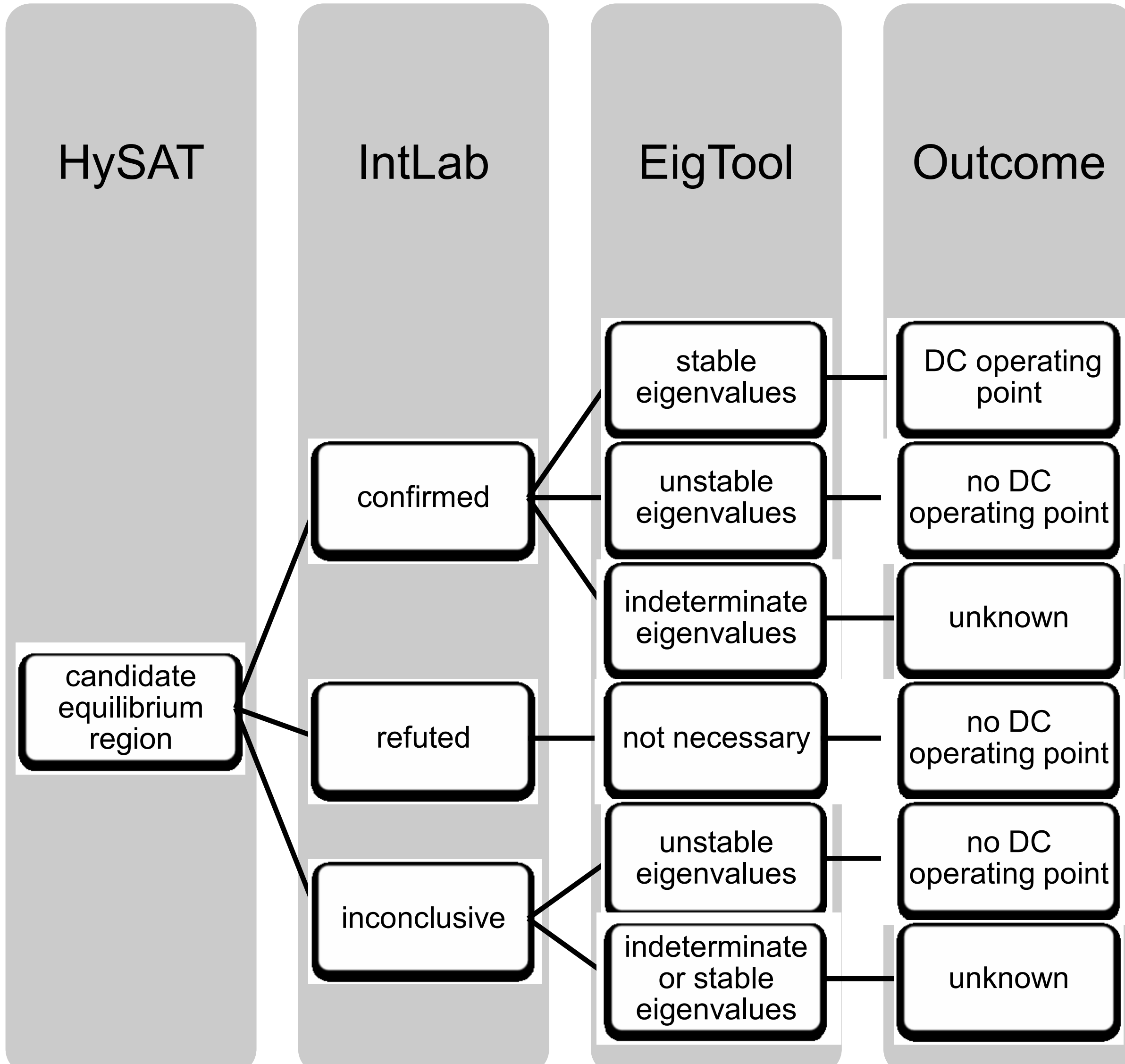
  where for matrix A, $A^{(S)} = \frac{1}{2}(A + A^T)$ and $\rho(A)$ is the spectral radius of A
- Can reach more general conclusions about stability / instability with ϵ-ps for $\epsilon_\Delta = \|\Delta\|_2$
  - No DC operating point: At least one isolated component of ϵ_Δ-ps in right-half plane
  - DC operating point(?): All ϵ_Δ-ps in left-half plane
  - Not a guarantee of a DC operating point:

$$\{A \mid A \in [A_C - \Delta, A_C + \Delta]\} \subset \{A_C + E \mid \|E\|_2 \leq \|\Delta\|_2\}$$

Our Approach (graphically)



Analysis Outcomes



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Schmitt Trigger Netlist

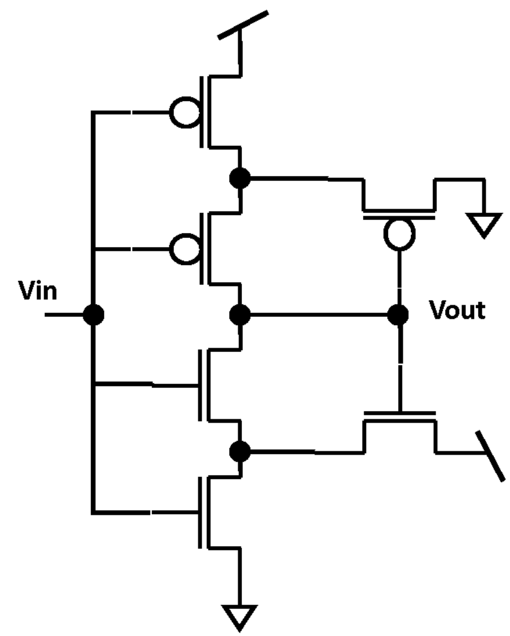
- Input to OOmspice

```
function   m = Schmitt_Trigger

%Parameters for First Order Transistors model
trn_params = 'Trans_params';
% Gate, Source and Drain Capacitance
C = [0.55e-15, 0.55e-15/2, 0.55e-15/2];
% Input Signal parameters
Pulse_params = 'pulse_param';

Vin1 = Voltage_Source_Pulse('Vin1', Pulse_params);
Vdd = Supply_Voltage('Vdd', 1.8);
Gnd = Ground('Gnd', 0);
NMos1 = NmosCell('NMos1', trn_params, C);
PMos1 = PmosCell('PMos1', trn_params, C);
PC = Trans_series('PC', trn_params, C, -1);
NC = Trans_series('NC', trn_params, C, 1);

m = connect_pins(m, Vdd, NMos1.D, 'node_vdd');
m = connect_pins(m, Vdd, PC.Vs);
m = connect_pins(m, Gnd, PMos1.D, 'node_gnd');
m = connect_pins(m, PC.Vgnd, Gnd);
m = connect_pins(m, NC.Vgnd, Gnd);
m = connect_pins(m, Gnd, Vin1.N);
m = connect_pins(m, Gnd, NC.Vs);
m = connect_pins(m, PC.Out, PMos1.S, 'node_y1');
m = connect_pins(m, NC.Out, NMos1.S, 'node_y2');
m = connect_pins(m, Vin1.P, PC.In, 'node_in');
m = connect_pins(m, Vin1.P, NC.In);
m = connect_pins(m, PMos1.G, PC.Vd, 'node_out');
m = connect_pins(m, NMos1.G, PC.Vd);
m = connect_pins(m, PC.Vd, NC.Vd);

m = end_circuit(m);
```

parameters

components

connectivity



Schmitt Trigger Circuit Model

- Output from OOmspice

```
function dydt = Schmitt_Trigger_model(t,y)

Cap_node_out_V_Port = y(1,:);
Cap_node_y2_V_Port = y(2,:);
Cap_node_y1_V_Port = y(3,:);

Vin1_V_Port = fun_pulse(t,'pulse_params')';
node_gnd_V = 0;
node_vdd_V = 1.80;
node_in_V = node_gnd_V+Vin1_V_Port;
node_y2_V = node_gnd_V+Cap_node_y2_V_Port;
node_y1_V = node_gnd_V+Cap_node_y1_V_Port;
node_out_V = node_gnd_V+Cap_node_out_V_Port;
Pmos1_PC_Ids = fun_mos(node_in_V,node_vdd_V,node_y1_V,-1,'Trans_Params');
Nmos1_NC_Ids = fun_mos(node_in_V,node_gnd_V,node_y2_V,1,'Trans_Params');
Nmos2_NC_Ids = fun_mos(node_in_V,node_y2_V,node_out_V,1,'Trans_Params');
Pmos2_PC_Ids = fun_mos(node_in_V,node_y1_V,node_out_V,-1,'Trans_Params');
PMos1_Ids = fun_mos(node_out_V,node_y1_V,node_gnd_V,-1,'Trans_Params');
NMos1_Ids = fun_mos(node_out_V,node_y2_V,node_vdd_V,1,'Trans_Params');
Cap_node_out_I_Port = -Pmos2_PC_Ids-Nmos2_NC_Ids;
Cap_node_y2_I_Port = -Nmos1_NC_Ids+Nmos2_NC_Ids+NMos1_Ids;
Cap_node_y1_I_Port = -Pmos1_PC_Ids+Pmos2_PC_Ids+PMos1_Ids;

dydt = [Cap_node_out_I_Port/1.650000e-15;...
        Cap_node_y2_I_Port/8.250000e-16;...
        Cap_node_y1_I_Port/8.250000e-16];
```

state space

provided by Chum

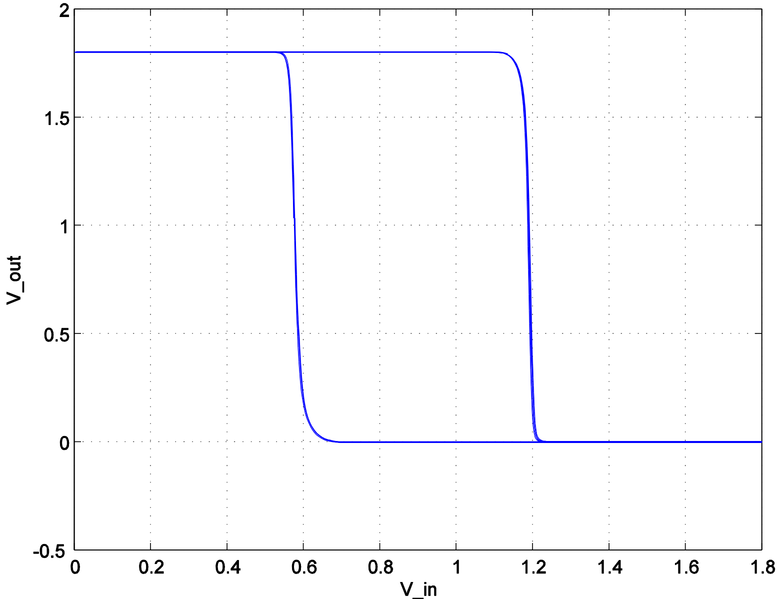
Equations

KCL

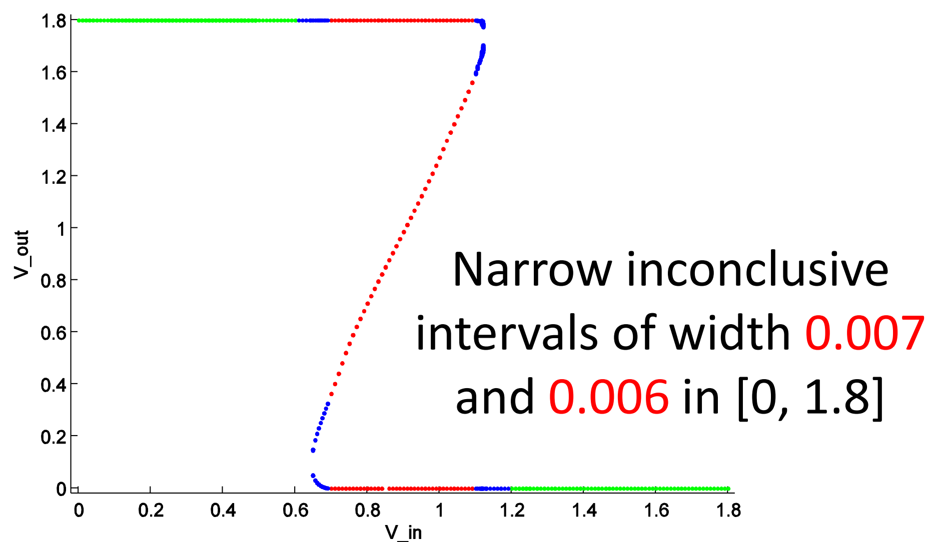
ODE

(Inverting) Schmitt Trigger Behaviour

- Input to output mapping is like an inverter, but with hysteresis
- Analysis determines location and stability of each equilibrium for each fixed input value
  - green: one equilibrium of known stability
  - red: three equilibria of known stability
  - blue: multiple equilibria of indeterminate stability



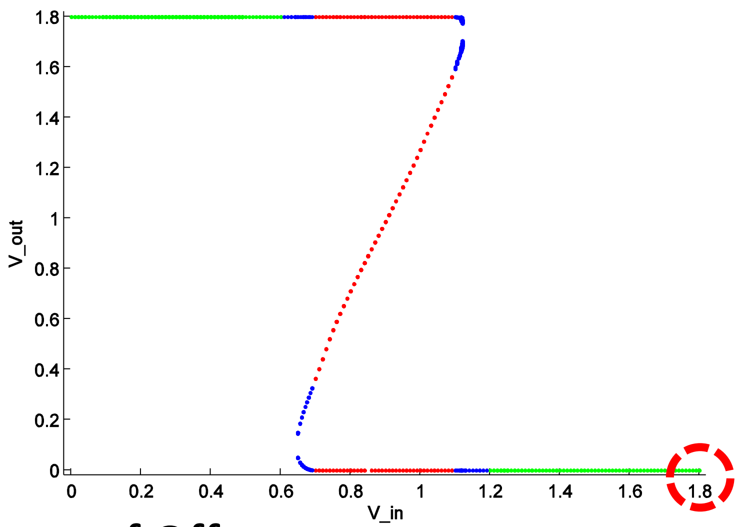
Simulation



DC equilibria detected

Schmitt Trigger Pseudospectrum V_{in} = 1.8

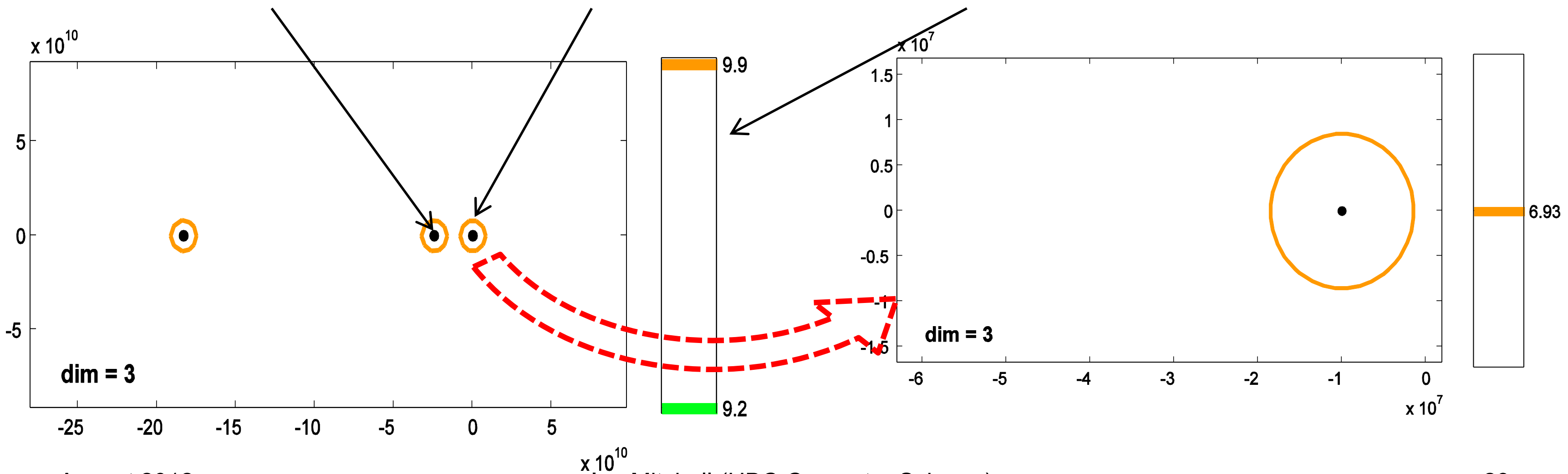
- Pseudospectrum of overapproximation of interval Jacobian lies in left half plane
- Equilibrium is a DC operating point



Eigenvalue of central matrix

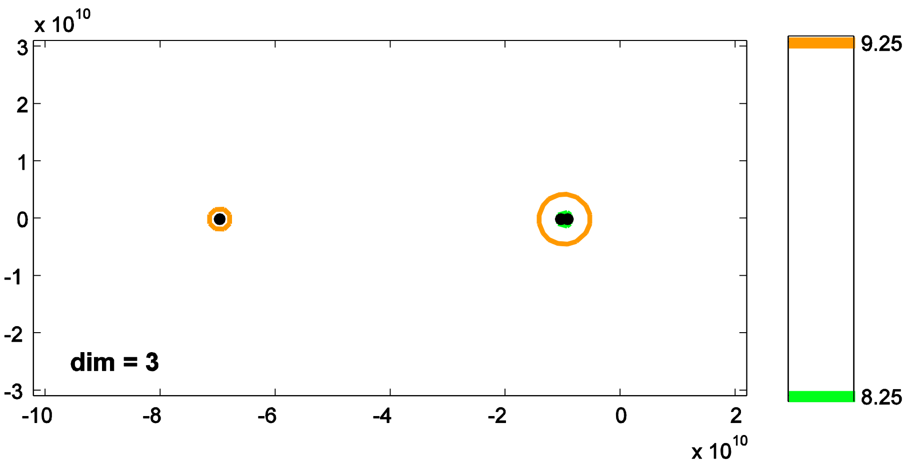
Bounds on eigenvalue

Norm of Offset Matrix (log scale)

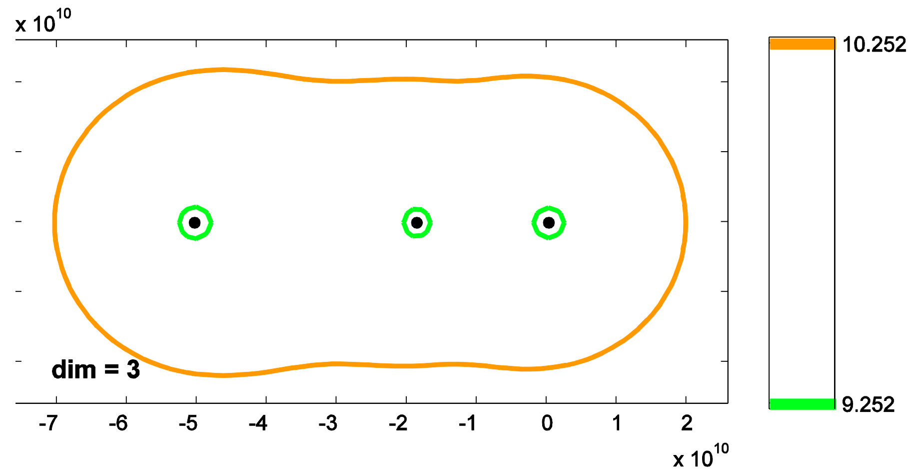


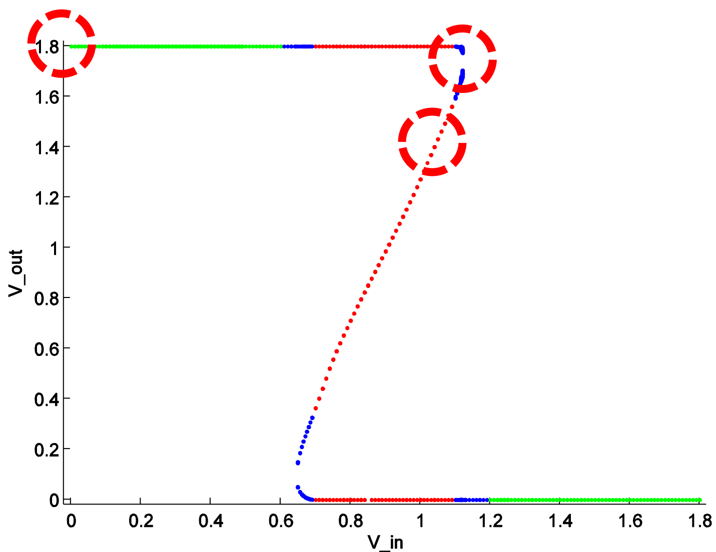
More Schmitt Trigger Pseudospectra

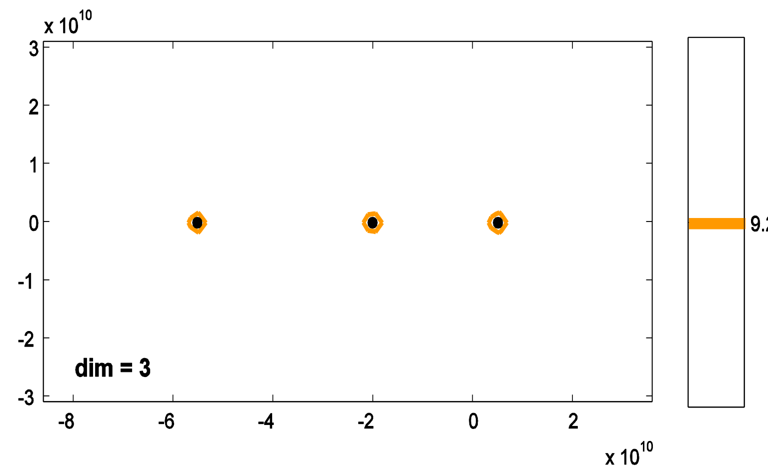
$V_{\text{in}} = 0$



$V_{\text{in}} = 1.124$ upper region



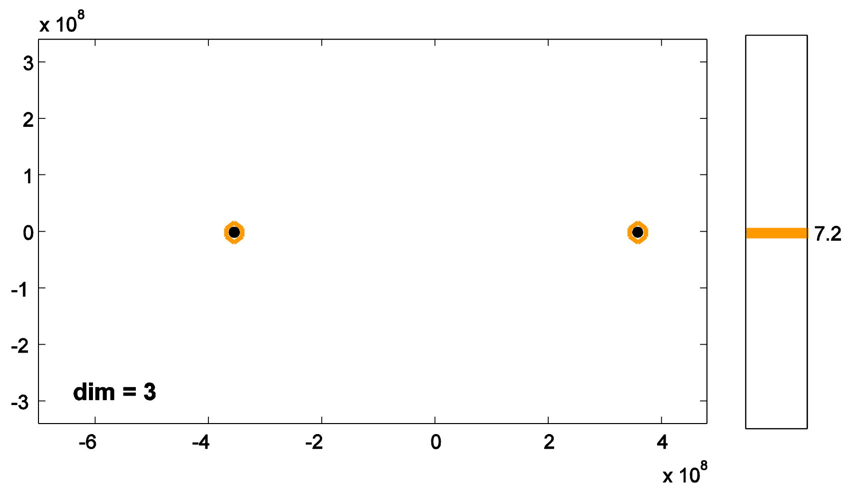




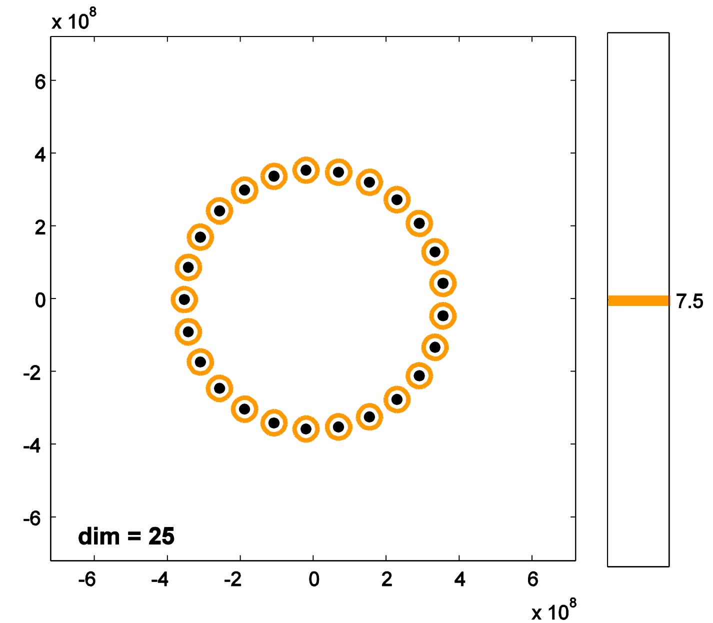
$V_{\text{in}} = 1$ middle equilibrium

Ring Oscillators' Results

- Ring oscillators with an odd number of inverters (up to 25) do not have DC operating points
  - However, a sufficiently large load capacitance on the output stage can create a DC operating point
- Ring oscillators with an even number of inverters (up to 24) always have DC operating points



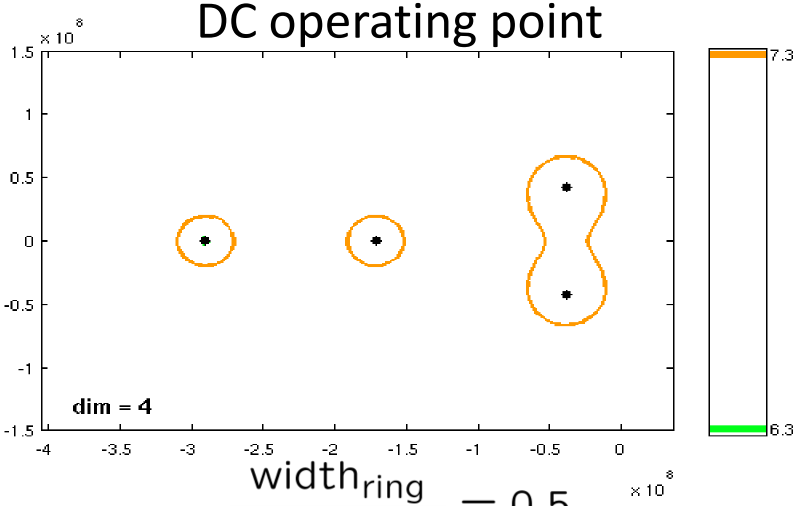
three inverters



25 inverters

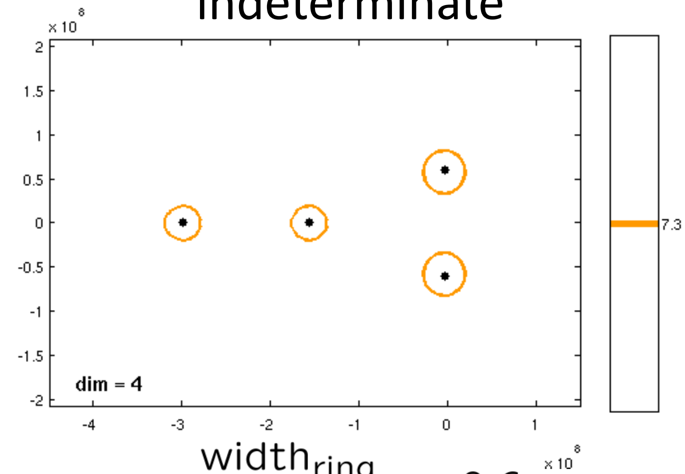
Rambus Oscillator’s Results

DC operating point



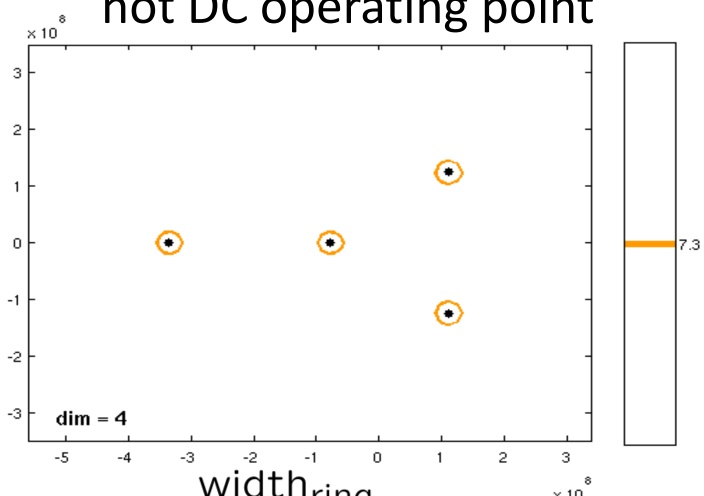
$$\frac{\text{width}_{\text{ring}}}{\text{width}_{\text{bridge}}} = 0.5$$

indeterminate



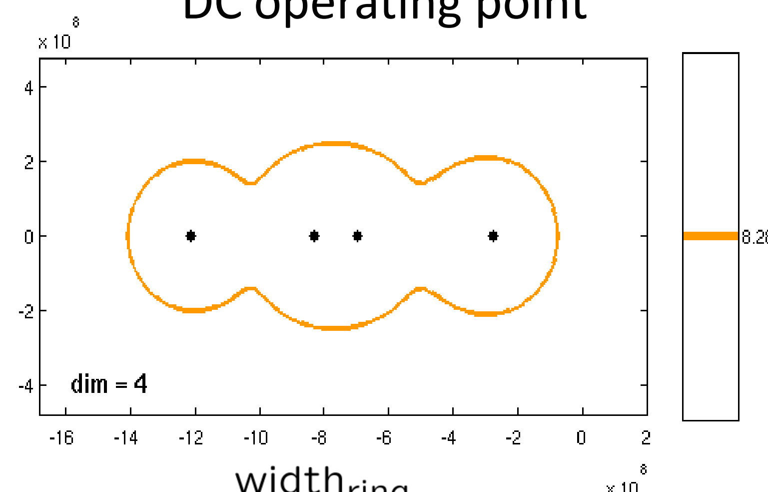
$$\frac{\text{width}_{\text{ring}}}{\text{width}_{\text{bridge}}} = 0.6$$

not DC operating point



$$\frac{\text{width}_{\text{ring}}}{\text{width}_{\text{bridge}}} = 0.9$$

DC operating point



$$\frac{\text{width}_{\text{ring}}}{\text{width}_{\text{bridge}}} = 3.5$$

Conclusions (Part 1)

- DC analysis can be approached formally and with rigour
- DC equilibria can be localized and their stability properties analyzed to find DC operating points using a collection of (almost) freely available tools
  - Models constructed by OOmspice / Chum (not released)
  - State space regions excluded by HySAT
  - Remaining regions confirmed or refuted (or not) by IntLab
  - Remaining regions’ stability examined by EigTool
- Demonstrated on Schmitt trigger, ring oscillators and Rambus oscillator
- Remaining challenges
  - Improved circuit models
  - Rigourous treatment of multiple roots
- Not a challenge: High dimensions

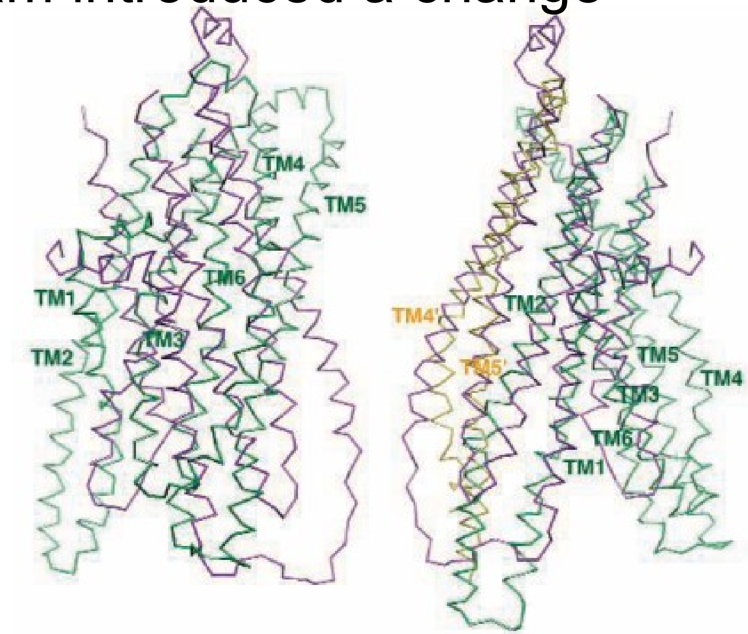
The Real Problem

- I can’t reproduce any of these results
- These aren’t my only such results
- I’m not alone

Accurate to within ±One (Hundred Percent)

- 2001–2005: Geoffrey Chang and colleagues published a number of high profile protein structures
  - 2001 paper on MsbA cited 360+ times by 2006
- September 2006: A dramatically different structure for a related protein is published
- December 2006: Chang et al retract five papers because "An in-house data reduction program introduced a change in sign…"

Image from:
Miller, "A Scientist's Nightmare: Software Problem leads to Five Retractions" in *Science* 314(5807): 1856-1857 (22 December 2006)



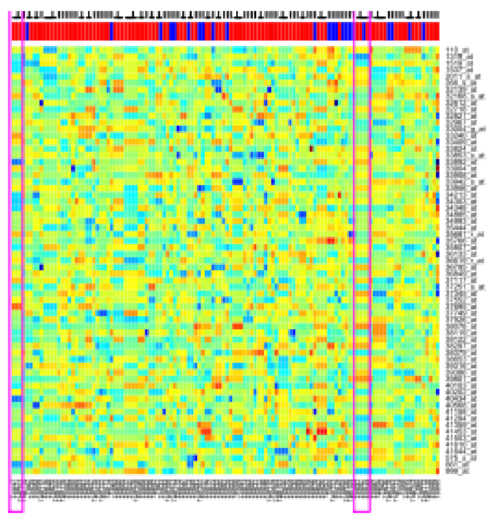
Flipping fiasco. The structures of MsbA (purple) and Sav1866 (green) overlap little (*left*) until MsbA is inverted (*right*).

A Simple Labelling Mistake?

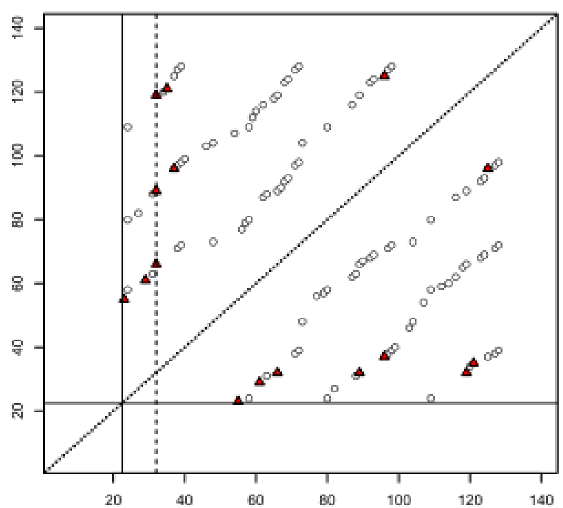
- 2006: Anil Potti and colleagues announce method for predicting patient response to chemotherapy drugs based on gene microarray data
  - 200+ citations by 2009
- 2007: Clinical trials begin
- 2007–2009: Baggerly, Coombes and colleagues try to reproduce results, but find frequent inconsistencies
- 2010–2011: Trials stopped, Potti resigns, 7+ retractions

Images from:
Baggerly & Coombes, "Deriving chemosensitivity from cell lines: Forensic bioinformatics and reproducible research in high-throughput biology" in *Annals of Applied Statistics* 3(4): 1309-1334 (2009)

Response Labelling +
Gene Expression Heatmap



Repeated Columns
(Δ: inconsistent labels)



Why so Secretive?

- 2005: Jelte Wicherts and colleagues requested data from 49 papers recently published in two highly ranked American Psychological Association journals (part of a larger study)
  - Corresponding authors had signed publication form agreeing to share data
  - 21 shared some data, 3 refused (lost or inaccessible data), 12 promised to later but did not, and 13 never responded
- 2011: Wicherts and colleagues analyze internal consistency of p-values reported from null hypothesis tests
  - Willingness to share is correlated with fewer reporting errors and relatively stronger evidence against NH

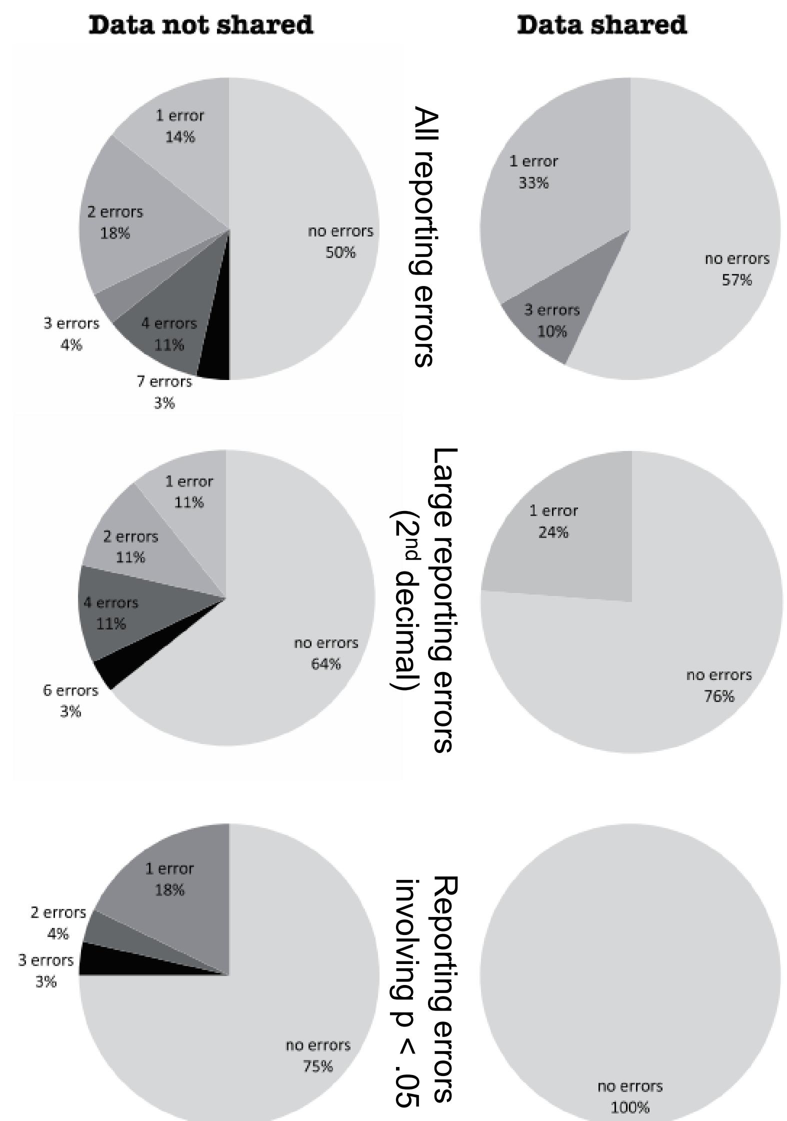


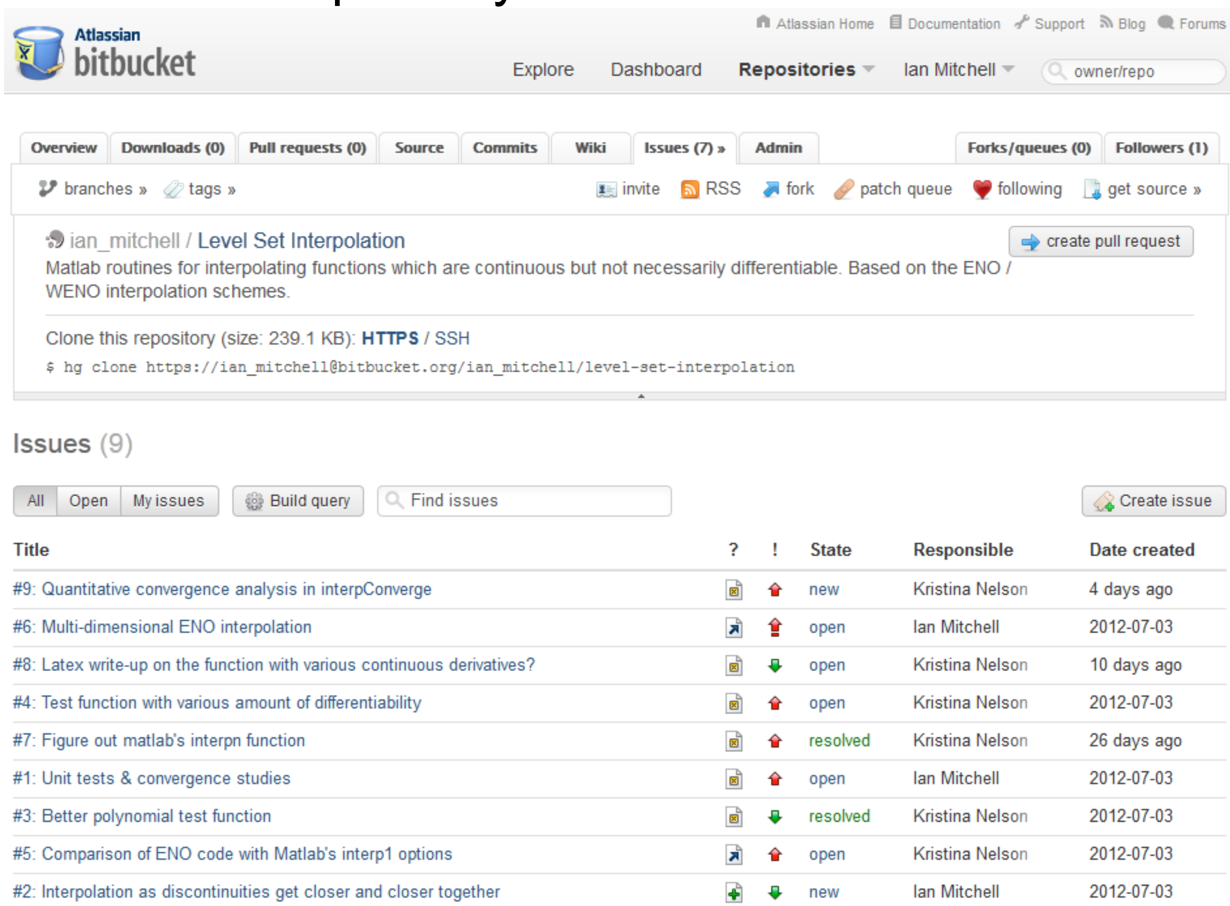
Image from:
Wicherts, Bakker & Molenaar, "Willingness to share research data is related to the strength of the evidence and the quality of reporting of statistical results" in *PLoS ONE* 6(11), Nov. 2011.

Some Suggestions for Doing It Better

- Use a (modern) version control system
  - Online repositories (eg: bitbucket, github, google code, sourceforge) include wikis and issue trackers
- Document with the data (and code is data)
  - You will forget how and why you did things, files and directories will get separated and lost
- Write tests first and run them often
  - Bugs are inevitable and “static” code isn’t
- If you do it twice, automate it
  - Computers are better at repetition, you can automate a person with a checklist, and automation is documentation
- Look at the code together
  - Code review and pair programming lead to demonstrable improvements in code quality
- Improve your process gradually, but continually
  - Every little bit helps

Example: Source and Issue Management

- Summer project with NSERC USRA Kristina Nelson: ENO interpolation in multiple dimensions
- Managed with Mercurial (hg) version control software and bitbucket online repository



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ian_mitchell / Level Set Interpolation

create pull request

Matlab routines for interpolating functions which are continuous but not necessarily differentiable. Based on the ENO / WENO interpolation schemes.

Clone this repository (size: 239.1 KB): **HTTPS** / SSH

```
$ hg clone https://ian_mitchell@bitbucket.org/ian_mitchell/level-set-interpolation
```

Issues (9)

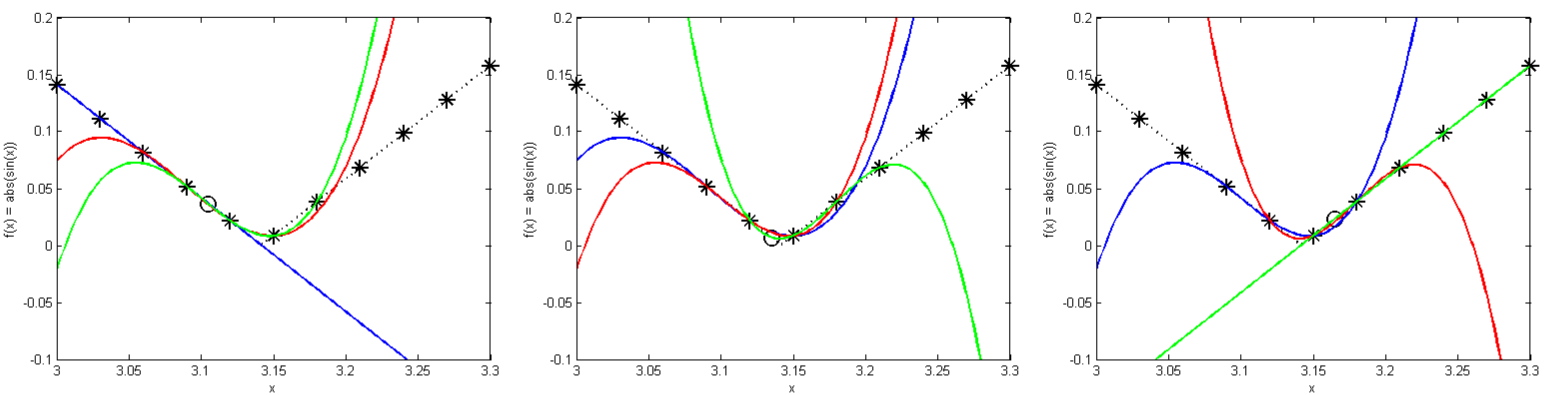
All · Open · My issues · Build query · Find issues · Create issue

Title	?	!	State	Responsible	Date created
#9: Quantitative convergence analysis in interpConverge			new	Kristina Nelson	4 days ago
#6: Multi-dimensional ENO interpolation			open	Ian Mitchell	2012-07-03
#8: Latex write-up on the function with various continuous derivatives?			open	Kristina Nelson	10 days ago
#4: Test function with various amount of differentiability			open	Kristina Nelson	2012-07-03
#7: Figure out matlab's interpn function			resolved	Kristina Nelson	26 days ago
#1: Unit tests & convergence studies			open	Ian Mitchell	2012-07-03
#3: Better polynomial test function			resolved	Kristina Nelson	2012-07-03
#5: Comparison of ENO code with Matlab's interp1 options			open	Kristina Nelson	2012-07-03
#2: Interpolation as discontinuities get closer and closer together			new	Ian Mitchell	2012-07-03

Example: Verifying Numerical Code

- For most scientific computing algorithms, testing for exact answers is not possible
  - Discretization, truncation and rounding are unavoidable
  - How can we automate testing?
- Background: Essentially Non-Oscillatory Interpolants
  - High order local polynomial interpolants for insufficiently smooth data often become oscillatory and hence inaccurate
  - ENO idea: Several different high order local polynomial interpolants can be constructed for a given set of data, so use the least oscillatory [Harten et. al., *J. Computational Physics* 71(2): 231–303, 1987]

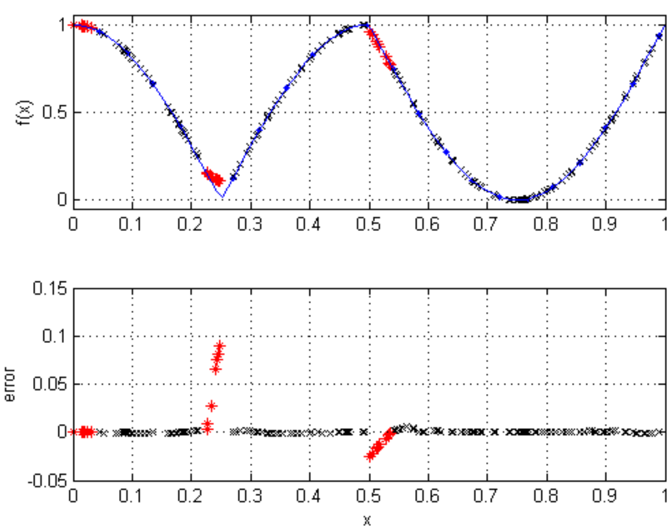
cubic polynomial interpolants of $|\sin(x)|$, $x_i = 3 + 0.03i$, for evaluation points in various intervals near $x = \pi$



Verification with Convergence Rate Test

- Theoretical order of accuracy for polynomial interpolants is easily derived (for smooth data)
- Given known test function, experimental order of accuracy for interpolants is easily measured
  - Experimental order of accuracy is very sensitive to bugs
  - Poor choice of test functions may not properly exercise code

test function & error (ENO3)

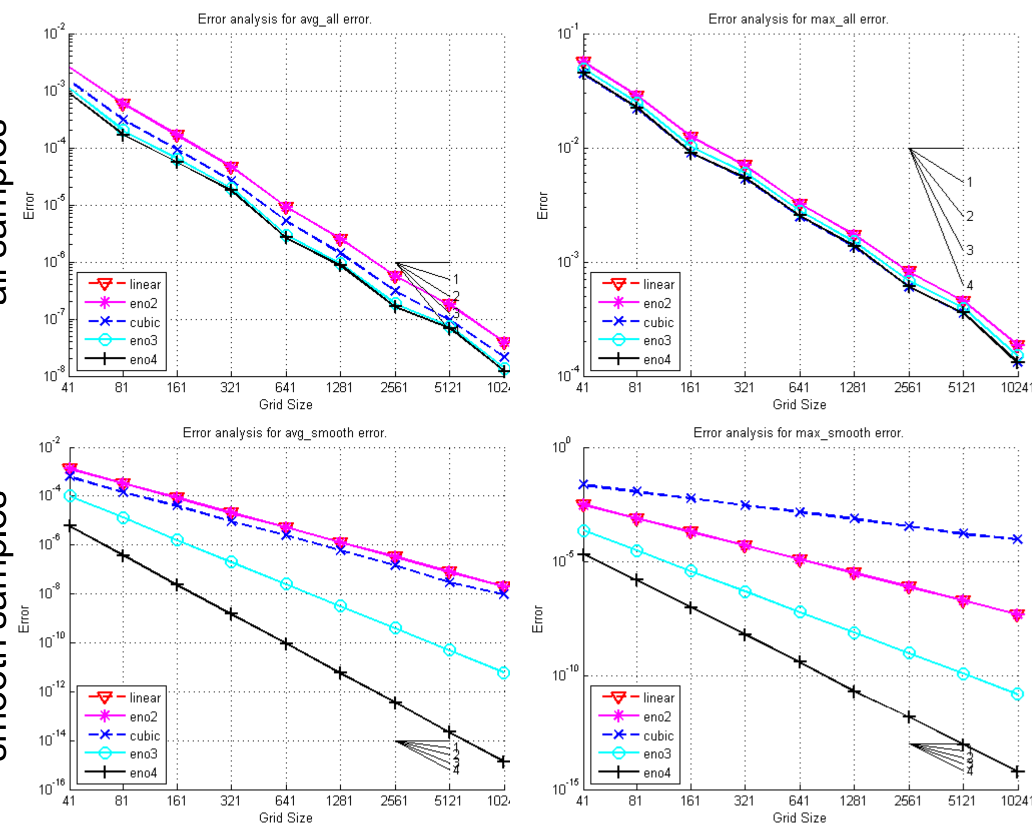


average error

maximum error

all samples

smooth samples



Citations and Links

- Software Carpentry website
  - Upcoming bootcamp at UBC October 18-19, 2012
- Ideas from software engineering
  - Heroux & Willenbring, "Barely Sufficient Software Engineering: 10 Practices to Improve Your CSE Software" in *ICSE Workshop on Software Engineering for Computational Science & Engineering*, pp.15-21 (2009)
  - Wilson et. al., "Best Practices for Scientific Computing" in preparation
  - Sink, *Version Control by Example*, 2011
- Testing differential equation codes
  - Oberkampf & Roy, *Verification and Validation in Scientific Computing*, 2010
  - Roy, "Review of Code and Solution Verification Procedures for Computational Simulation", *J. Comp. Physics* 205:131-156
  - Knupp & Salari, *Verification of Computing Codes in Computational Science and Engineering*, 2003
- Additional links and readings (CPSC 535Z at UBC): https://sites.google.com/site/ubccpsc535zwinter2011/

Formal Identification of DC Operating Points in Integrated Circuits and some Lessons in (Ir)Reproducible Research in Computational Math

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