

# Investigating Model Behavioural Analysis: A Critical Examination of Two Methods

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## ***Abstract***

*Two methods for model behavioural analysis are implemented on a simple 2<sup>nd</sup> order non-linear model. The results of applying Ford's behavioral approach are compared with those obtained using both system-wide and variable-specific loop eigenvalue elasticity analysis. Differences in the division of the time span into analysis intervals are identified as are discrepancies in the outcomes. The effort required for implementation and the necessity for automation also differ substantially. We consider Ford's method readily understandable, whereas the mathematically more powerful eigenvalue elasticity analysis poses difficulties*

*in this regard. Future directions for research on model behavioural analysis are identified based on the results of this critical comparison and the learning associated with our development of a prototypical automated model behavioural analysis framework.*

**Keywords :** Loop dominance, nonlinear dynamics, eigenvalue elasticity analysis, formal model analysis, model structure

## **1 Introduction**

The endeavour to explain model behaviour in terms of system structure lies at the heart of the System Dynamics methodology. Yet as recently as 2000, Sterman (2000) identified the development of tools to aid understanding model behaviour as an outstanding problem for the future of System Dynamics emphasizing that “Technical support for understanding the connections between model structure and behavior is weak to the point of being almost nonexistent” (Sterman 2000, page 897).

Although this still is an outstanding issue, significant research effort has been and still is being invested in addressing this issue. Since Nathan Forrester (Forrester 1982) first proposed model analysis based on eigenvalue elasticities attention has been devoted to the development of formal methods for model behavioural analysis. These include the pathway participation metric (Mojtahedzadeh 1997), based on a definition of loop polarity, and its implementation within the DIGEST software package (Mojtahedzadeh, Andersen et al. 2004) as well as Kampmann’s (1996) formalization of model structure using graph theory. The latter enabled the identification of an independent loop set (ILS) for a model, laying the foundation for further progress in loop eigenvalue elasticity analysis. Oliva’s subsequent introduction of the shortest independent loop set (SILS) solved some of the problems associated with a non-unique independent loop set, leading to an improved structural analysis foundation for loop eigenvalue elasticity analysis (Oliva 2004; Kampmann and Oliva 2005). Recently, Saleh and Güneralp were able to relate eigenvalue elasticity analysis to the behaviour of specific state variables and to automate this (Saleh 2002; AbdelGawad 2005; Güneralp 2005). In addition, Ford (1999) proposed a non structurally-based method of analyzing model behaviour using unique atomic behaviour patterns of variables of interest.

In this paper, we will report upon our progress in consistently applying and comparing the model behavioural analysis methods proposed by Ford (1999), Kampmann (Kampmann 1996; Kampmann and Oliva 2005) and Güneralp (2005). The implementation of these methods on one and the same model is described and the outcomes compared. The reliability of the methods, their implementation requirements and their explanatory power are evaluated. Finally, promising directions for future research in this field are identified.

## **2 Method**

The long term goal of our research is consistent implementation, effective intercomparison and improvement of formal model behavioural analysis methods. To this end, an automated model behavioural analysis framework (AMBA) is undergoing development. For a more detailed description see Appendix A and Appendix C. Eventually, it will be feasible to plug in different methods and apply each of them to a selection of (the same) models.

### **2.1 Selection of model analysis methods for comparison**

We distinguish two broad classes of methods, namely (i) those proposed by Mojtahedzadeh and Ford and (ii) eigenvalue elasticity analysis. Owing primarily to its inability to deal effectively with oscillations (Kampmann and Oliva 2005), the pathway participation metric (Mojtahedzadeh 1997; Mojtahedzadeh, Andersen et al. 2004) was excluded from further implementation at an early stage of this research. Consequently, we choose to compare Ford with a selection of two eigenvalue elasticity analysis based methods. Further, the Kampmann variant of eigenvalue elasticity analysis is selected for implementation since it takes the system-wide perspective. The Güneralp variant is considered representative of the methods that relate elasticities to specific state variables. Comparable methods include that outlined in Abdelgawad (2005).

In this paper, we use the full AMBA framework to automate the implementation of eigenvalue elasticity analysis (Kampmann 1996; Güneralp 2005; Kampmann and Oliva 2005), but apply Ford's behavioural analysis (Ford 1999) using only some sections of the framework.

### **2.2 Selection of the Yeast model**

To facilitate comparison of the different model behavioural analysis methods, these had to be applied to the same models. In this paper, we choose to discuss only their application to the Yeast model (Figure 1). This is a relatively simple second order overshoot and decline model, which has also been used by other authors as a test case for loop dominance analysis (Saleh 2002; Güneralp 2005).

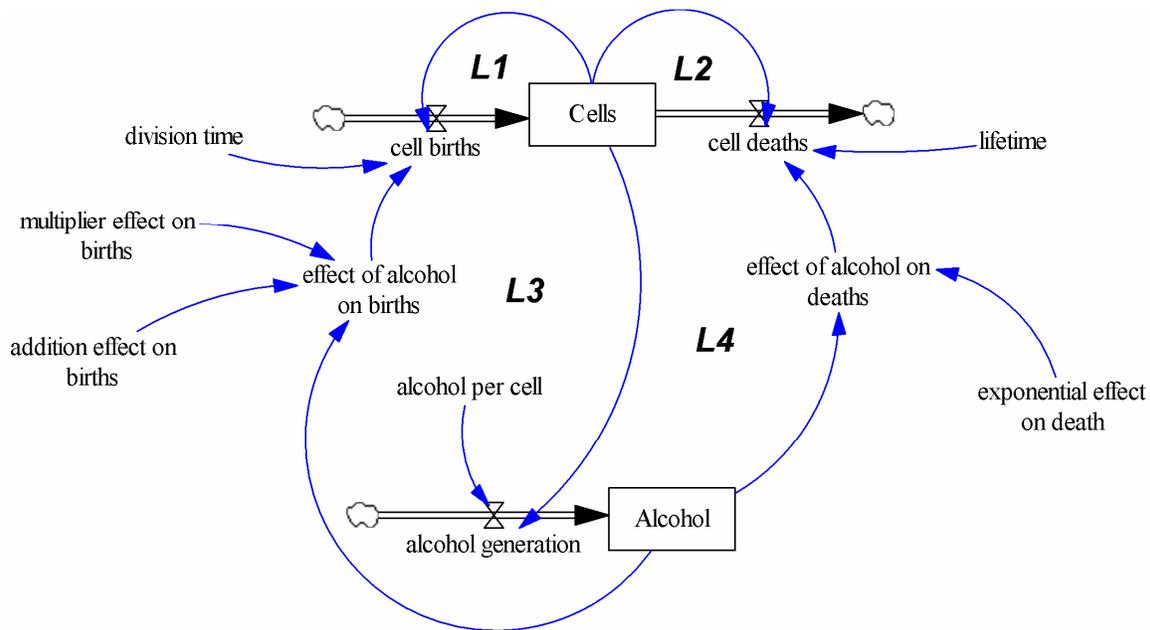


Figure 1: Diagram of the Yeast model showing the loops in the model.

The Yeast model (Figure 1) represents the growth of Yeast cells in a vat. The cells multiply and eventually die off as a result of the alcohol they produce. There are very few Cells present and there is virtually no Alcohol at the outset. This allows an almost exponential increase in the number of Cells. As the cell numbers increase, the Alcohol concentration also increases. The influence of Alcohol on the deaths of the cells eventually constrains the growth of cells causing the amount of Cells to reach a maximum. From then on the effect of Alcohol on the death of cells is so large that these decline in number until the number of Cells approaches zero.

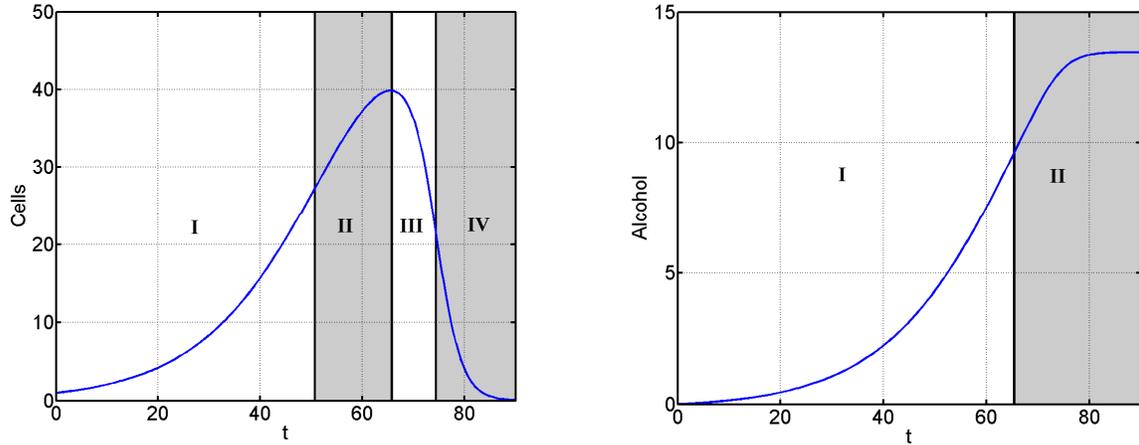
The behaviour of the variables Cells and Alcohol is depicted in Figure 4.

### 3 Results

#### 3.1 Ford's behavioural approach

Ford (1999) assesses the role of a particular loop by deactivating it. To do this, he selects a variable of interest and divides its behaviour up into different phases characterized by an atomic behavior pattern. This is determined according to the slope of the magnitude of the net rate of change of the variable of interest. He then assesses the role of each loop in determining the behaviour of the variable of interest by eliminating loops or combinations of loops and observing the change in behaviour.

We now apply the method of Ford to the Yeast model. Our variable of interest is the number of Cells. The graphs of its behaviour and that of Alcohol, divided into phases according to their atomic behavior patterns, are depicted in Figure 2.



(a) Behavior of Cells in the Yeast model.

(b) Behavior of Alcohol in the Yeast model.

Figure 2: Behavior of the Yeast Model. Division into phases based on Ford’s atomic behaviour pattern.

### Implementation requirements

In seeking to apply Ford’s method consistently, we had first to define a standard method for eliminating a loop. This issue is mentioned in Ford’s description of the method. We chose to deactivate links by modifying the equation of the dependent variable (the “to” variable) by setting the value of the independent variable (the “from” variable) in that equation to that at the beginning of the interval to be analysed. The option of setting the link under consideration to infinity or zero was eliminated because this sometimes means that one cannot remove a loop uniquely. For instance, if we wish to take out the effect of L2 in the Yeast model, setting the value of Cells to zero in Cell deaths would also eliminate L4. Another option of setting the gain of an edge to steady state was also dismissed since it is questionable whether steady state gain is applicable when the relation between the structure of the model in its current state is under investigation.

By imposing this consistency, we could easily adjust the time at which a loop was turned off and efficiently do the analysis for one loop over several intervals, thereby speeding up the behavioural analysis process. Note that although the execution is done per loop the results are analysed per phase. A difficulty with Ford’s approach is that the results of this behavioural analysis method might differ depending on the method selected for eliminating loops.

Furthermore, we restricted the search for sets of shadow loops dominating behavior to the intervals where no dominant loop was found. This reduced the time required for method application. Ford defines a set of shadow loops as two or more dominant loops that

generate the same atomic behaviour pattern, so that taking out one of the loops does not cause the atomic behavior pattern to change because the other loop continues to generate this. Consequently, a set of shadow loops has been found if the behavior pattern only changes when two loops are eliminated<sup>1</sup>. See Table 1.

Table 1: Unambiguous conditions for a set of shadow loops

Loop A	Loop B	Result
Inactive	Active	No change in behavior patter
Active	Inactive	No change in behavior pattern
Inactive	Inactive	Behavior pattern changes

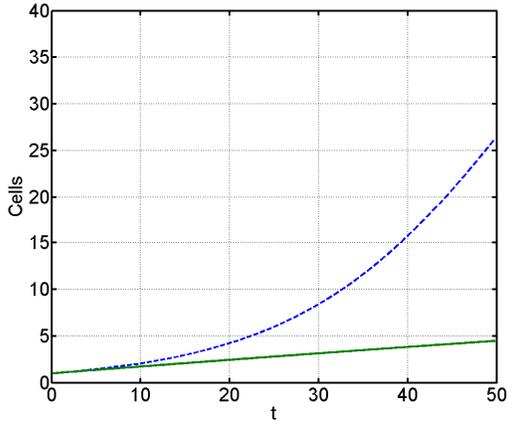
According to the atomic behaviour pattern, the behaviour of the variable Cells can be divided into four phases (Figure 2). For each of the phases we eliminated each loop in turn to see if this caused the atomic behavior pattern of the variable of interest to alter. The loops are taken out at the beginning of each interval. The equations used in eliminating each loop are listed in Table 2.

Table 2: Changes applied to the Yeast model in order to perform Ford's behavioral approach to loop dominance. The  $s$  subscript refers to the value of the variable at the start of the interval analyzed

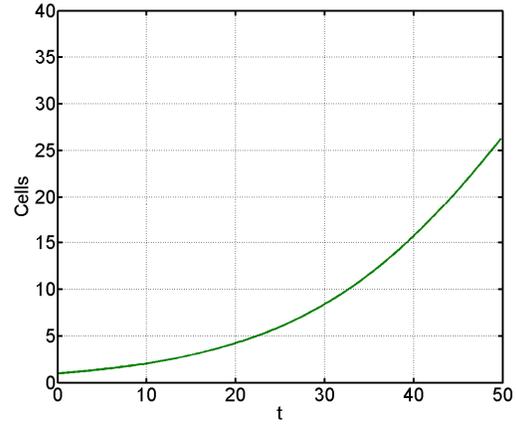
Loop	Edge	Original Equation	Modified equation
L1	Cells $\rightarrow$ Cell Births	$\frac{Cells}{divisionTime} effAlcB$	$\frac{Cells_s}{divisionTime} effAlcB$
L2	Cells $\rightarrow$ Cell Death	$\frac{Cells}{lifeTime} effAlcD$	$\frac{Cells_s}{lifeTime} effAlcD$
L3	Eff. Alc. Births $\rightarrow$ Cell Births	$\frac{Cells}{divisionTime} effAlcB$	$\frac{Cells}{divisionTime} effAlcB_s$
L4	Eff. Alc. Death $\rightarrow$ Cell Deaths	$\frac{Cells}{lifeTime} effAlcD$	$\frac{Cells}{lifeTime} effAlcD_s$

### Results from the analysis of the Yeast Model

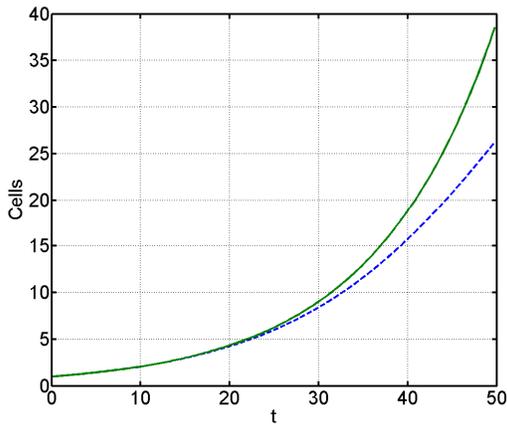
The growth loop is clearly dominant in the first phase with the birth loop L1 causing the atomic behaviour pattern of exponential growth (Figure 3 (a)). Taking out the third loop reveals that it functions as a brake on the growth of the Cells (Figure 3(c)). During phase I, the effect of Alcohol via the two death loops (L2 and L4) is so small that the reference run and the run with the loops eliminated are visually indistinguishable (Figure 3(b) & (d)).



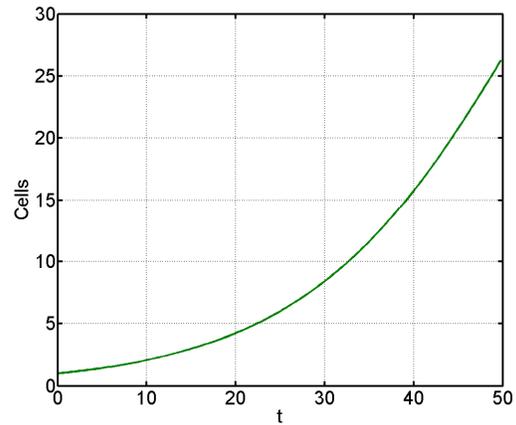
(a) L1



(b) L2



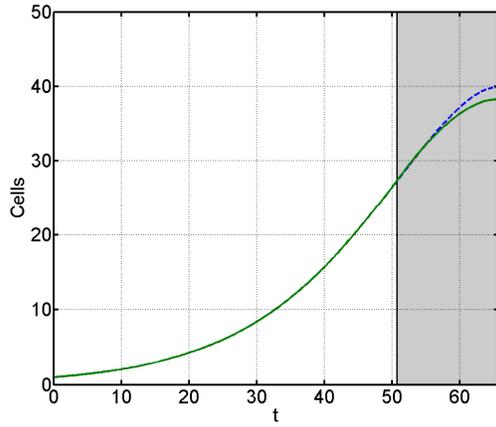
(c) L3



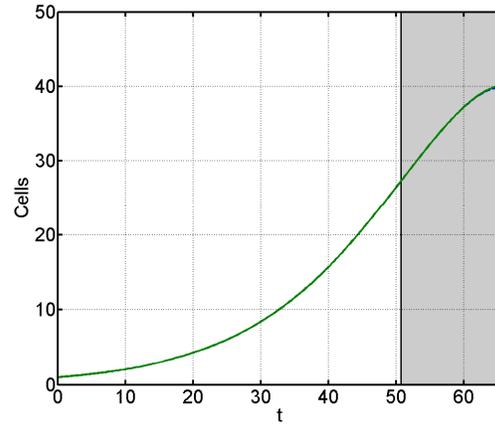
(d) L4

Figure 3: Effects of eliminating the different loops during phase I of the Yeast model. The dashed blue line is the original behavior of the model. The gray areas denote the intervals where the behavioral pattern of Cells is negative in the original model, the white areas denote a positive behavioral pattern.

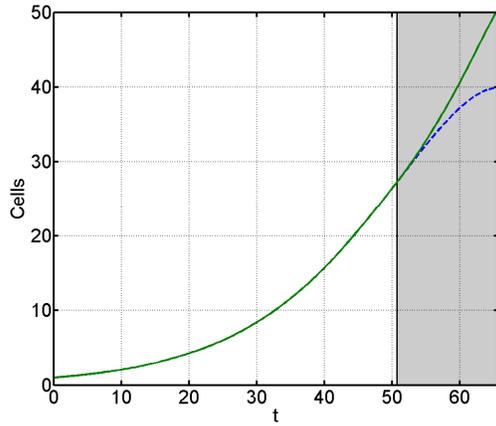
During phase II, the loop L3 containing the constraining effect of alcohol on birth is responsible for the balancing growth behaviour (Figure 4 (c)). Its effect on the growth of the number of cells is so large that the growth rate declines. The elimination of L1, which was dominant in the previous phase results only in slower growth and no longer causes a switch in the sign of the atomic behavior pattern.



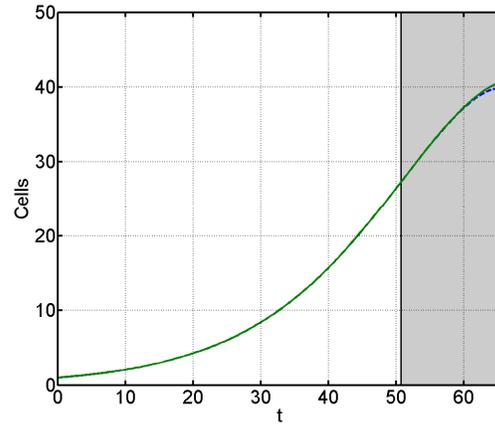
(a) *L1*



(b) *L2*



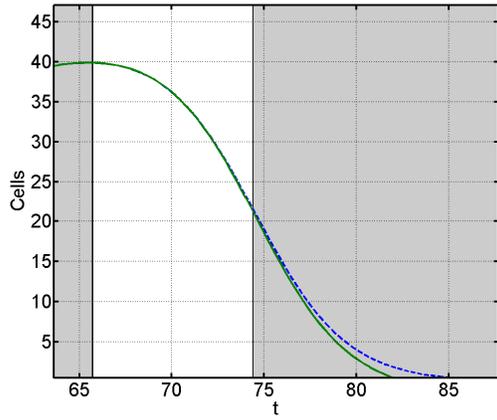
(c) *L3*



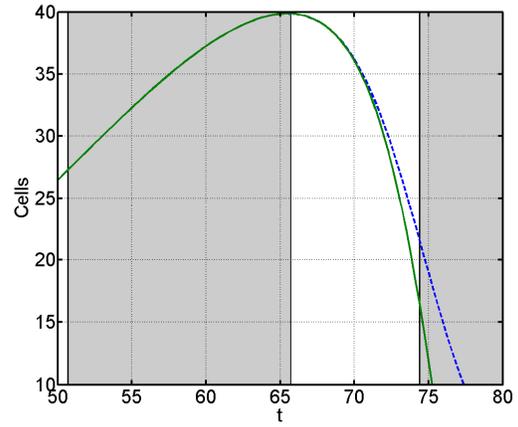
(d) *L4*

Figure 4: Effects of eliminating the different loops during phase II of the Yeast model.

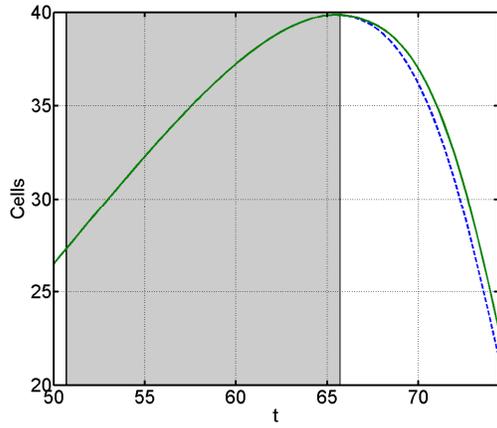
In the third phase, no dominant loop was identified in the first round of analysis involving the removal of individual loops (Figure 5), so we looked for a set of shadow loops. The effects of removing combinations of loops are displayed in Figure 6. Only when loops L3 and L4 were both removed did the atomic behavior pattern change from exponential decline to logarithmic with a very large time constant. According to Ford, this means that loops L3 and L4 form a pair of shadow loops causing the exponential decline of phase III.



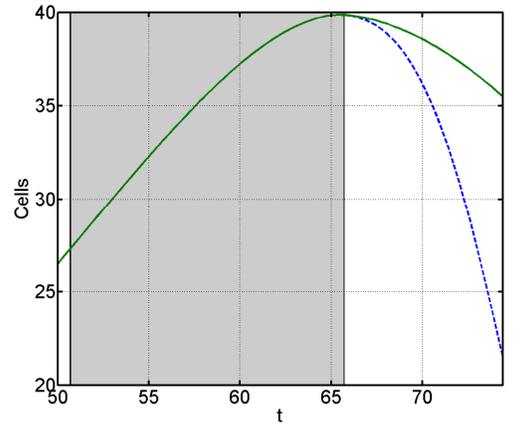
(a) L1



(b) L2

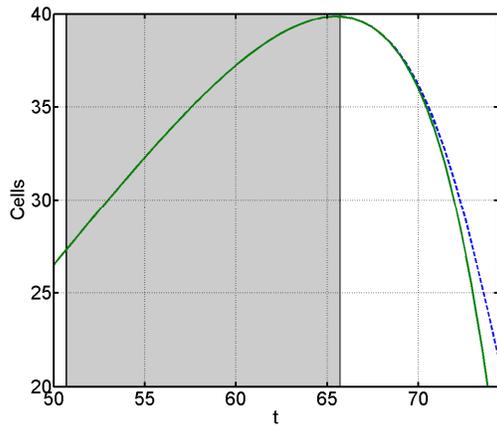


(c) L3

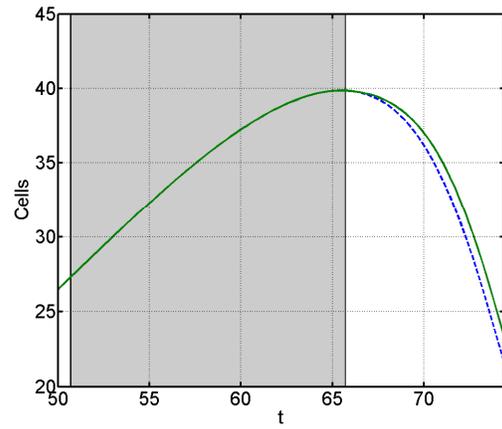


(d) L4

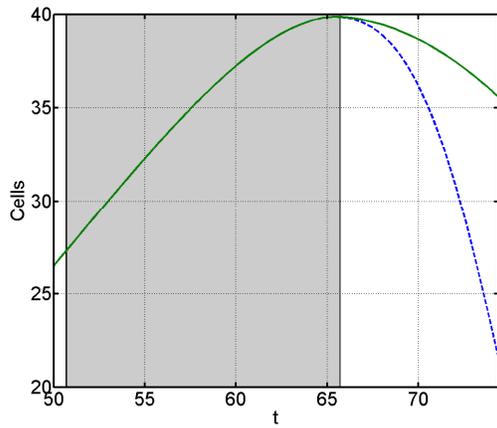
Figure 5: First round of analysis for phase III



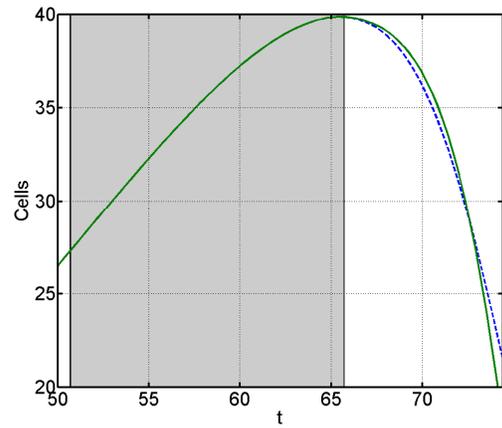
(a)  $L1$  &  $L2$



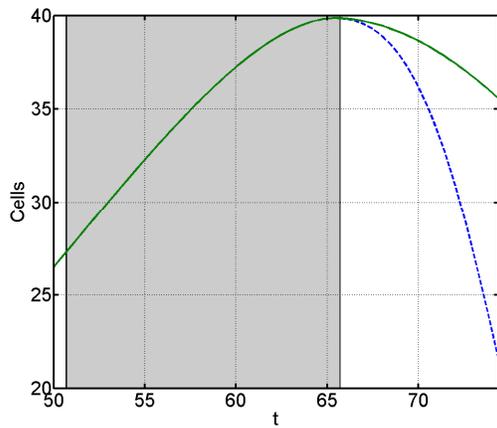
(b)  $L1$  &  $L3$



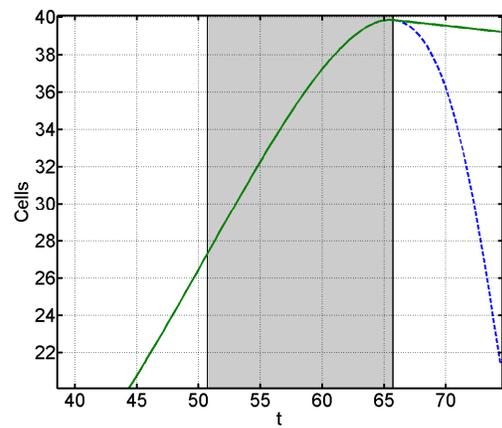
(c)  $L1$  &  $L4$



(d)  $L2$  &  $L3$



(e)  $L2$  &  $L4$



(f)  $L3$  &  $L4$

Figure 6: Checking for shadow loops during phase III of the Yeast model

During phase IV, L2 is found to dominate the behaviour (Figure 9(b)). The eventual decline towards zero is caused by the death of Cells.

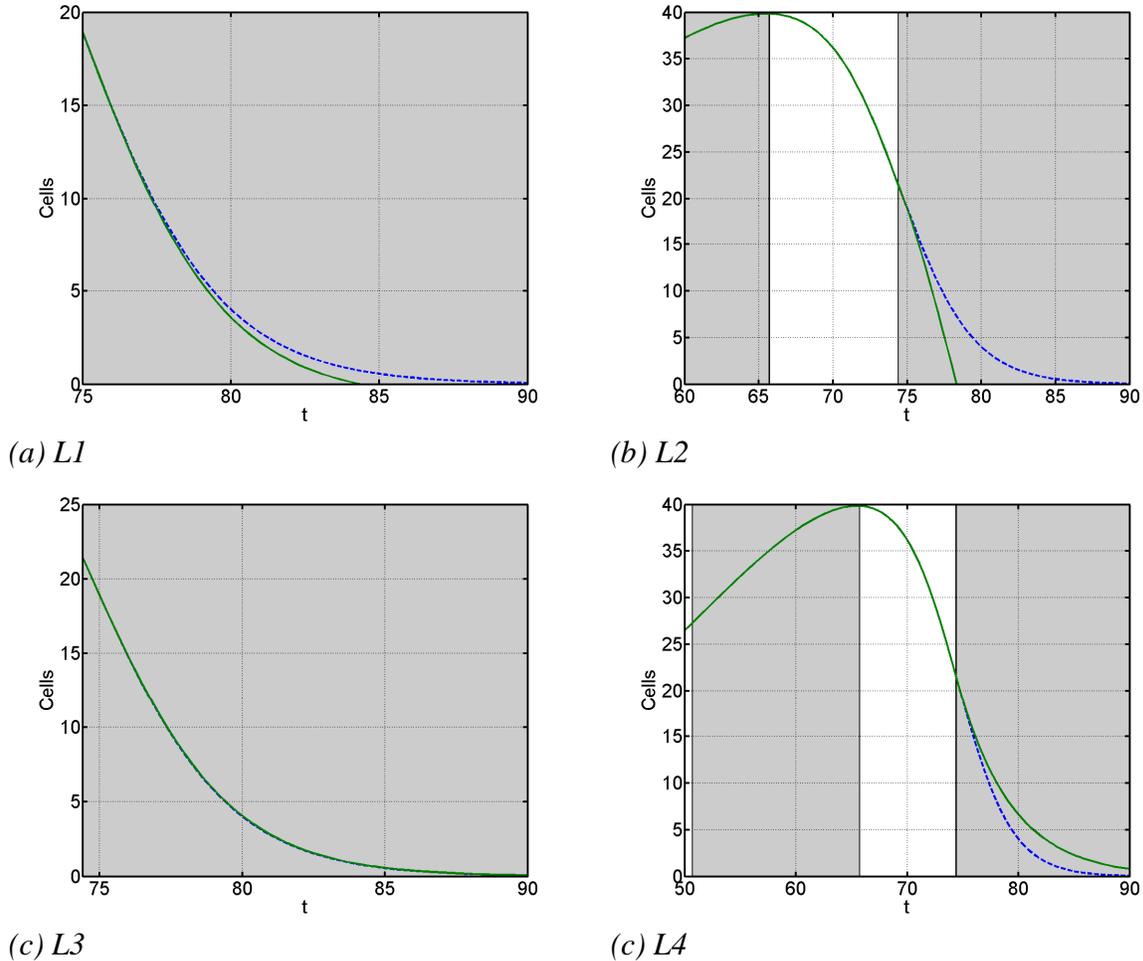


Figure 7: Effects of eliminating the different loops during phase IV of the Yeast model.

In summary, on the basis of Ford’s method, L1 dominates in the exponential growth phase, L3 dominates the balancing growth phase, L3 and L4 form a shadow pair responsible for phase III and L2 dominates the decline of Phase IV.

### 3.2 Eigenvalue Elasticity Analysis

The methods of Kampmann (Kampmann 1996; Kampmann and Oliva 2005) and Güneralp (2005) were applied to the Yeast model using the AMBA framework. These methods calculate loop eigenvalue elasticities. The elasticities represent a relative change in an eigenvalue induced by changes in a particular loop of the model. The eigenvalues are descriptors of the behaviour of the model. Consequently, the influence of the loops of the model on eigenvalues relate model structure and behavior. For instance, a loop with a

positive elasticity to a positive, real eigenvalue drives the exponential growth represented by that eigenvalue.

The adjacency matrix of the Yeast model was generated by the model routine of the AMBA framework and passed to the behavioural analysis routine for structural analysis as described by Oliva (2004)<sup>2</sup>. This structural analysis is required for the calculation of eigenvalue elasticities as described by (Kampmann 1996; Güneralp 2005). In our application, edge gains were perturbed to numerically determine individual edge elasticities. By performing the behavioural analyses at snapshots sufficiently close together we are able to generate eigenvalue elasticities for the entire simulation period and present these in the form of graphs such as those in Figure 9<sup>3</sup>.

The behavioural analysis is separated into time intervals based on the behaviour of the eigenvalues of the Yeast model, not on the basis of the behavior of a specific variable as is the case with the Ford method (Figure 8). Note that this division into phases does not coincide with the identification of phases based on the atomic behaviour pattern of the state variable Cells, except at the point where the imaginary pair of eigenvalues changes sign at  $t \approx 65$  (Figure 8). The first phase is characterized by divergent behavior without oscillation (positive, real eigenvalues). This changes to divergent oscillatory behavior in Phase II (complex pair of eigenvalues with a positive real part). However, when the real part of the complex conjugate pair drops below zero, the behaviour alters to dampened oscillation (Phase III). At this time, the variable Cells displays non balancing behavior (the atomic behaviour pattern is exponential). At  $t \approx 78$ , the imaginary pair of eigenvalues bifurcates into two negative real eigenvalues and Phase IV is characterized by convergent behaviour.

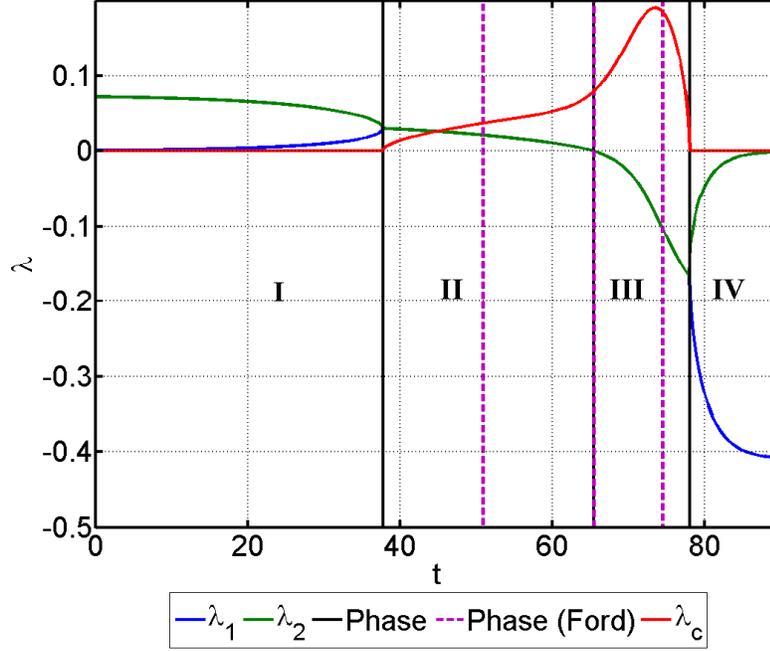


Figure 8: Eigenvalues of the Yeast Model.  $\lambda_1$  and  $\lambda_2$  describe the real parts,  $\lambda_c$  the imaginary part. These eigenvalues are obtained using the gain matrix of the linearised model at the defined snapshot times. The purple dashed lines represent the changes in phases according to Ford's atomic behavior pattern. The changes in phases only coincide at the transition from phase II to phase III.

### Loop based Eigenvalue Elasticity Analysis

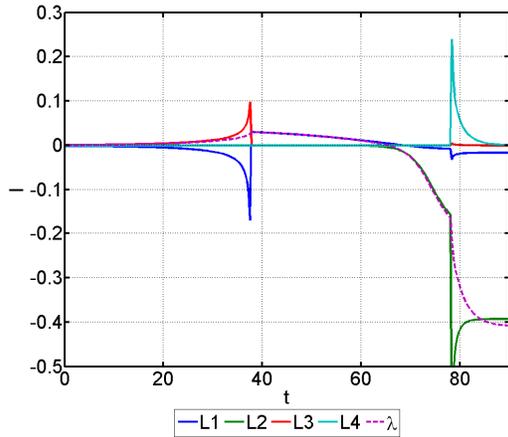
Using the shortest independent loop set<sup>4</sup> (SILS) of the Yeast model, the loop eigenvalue elasticities are calculated (see Appendix B for the loop set). This analysis was performed with a snapshot interval of .3 time units (see Appendix A), while the integration was performed using a timestep of .1 time units. We used as the measure of elasticity the loop influence as defined by (Kampmann and Oliva 2005):

$$l_{i,g(c)} = \frac{\partial \lambda_i}{\partial g(c)} g(c)$$

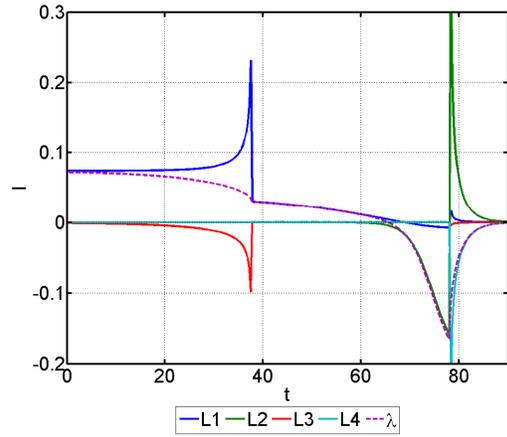
where  $l_{i,g(c)}$  is the influence of a loop  $c$  on a particular eigenvalue and  $g(c)$  is the gain of the loop. The main reason for using this formulation is its ability to deal with eigenvalues that are close to zero. The real part of  $l_{i,g(c)}$  measures the influence of loop  $c$  on the exponential envelope, while the imaginary part of  $l_{i,g(c)}$  provides a measure of the effect of loop  $c$  on the frequency of oscillation. The magnitude of  $l_{i,g(c)}$  provides an indication of

the overall influence of a loop, the overall elasticity. The elasticities for all of the eigenvalues over the full time interval of the simulation can be found in Figure 9.

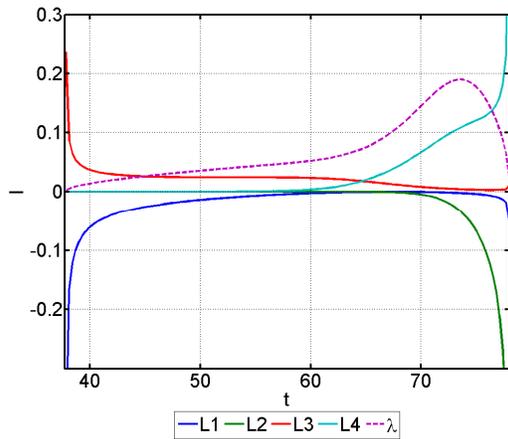
All of these graphs exhibit peaks near  $t = 38$  and  $t = 78$ . It turns out that the closer the analysis comes to either of these points, the higher the values of the elasticities. These are the times at which two real eigenvalues join into a complex pair, or where an imaginary pair bifurcates into two real eigenvalues. The peaks represent the efforts of numerical methods to simulate accurately in the neighbourhood of singularities. As noted in (Kampmann and Oliva 2005), the eigenvalue elasticity analysis method cannot deal with repeated eigenvalues and linearly dependent eigenvectors<sup>5</sup>.



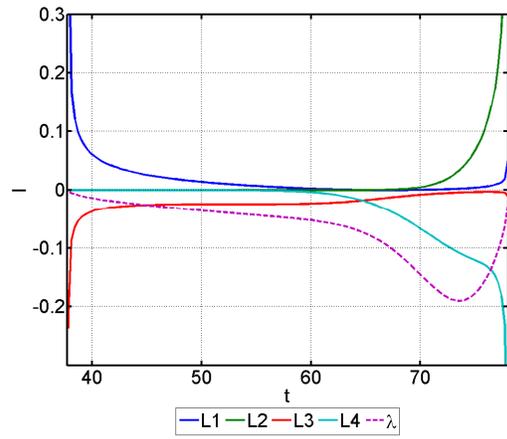
(a) Real elasticities of eigenvalue 1



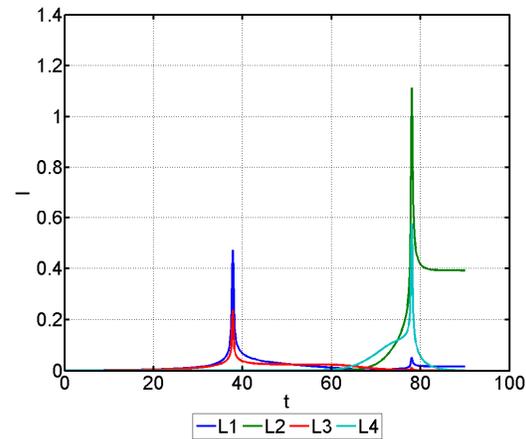
(b) Real elasticities of eigenvalue 2



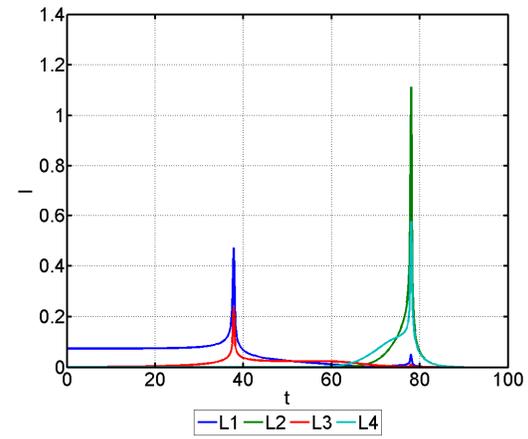
(c) Imaginary elasticities of eigenvalue 1



(d) Imaginary elasticities of eigenvalue 1



(e) Overall elasticities of eigenvalue 1



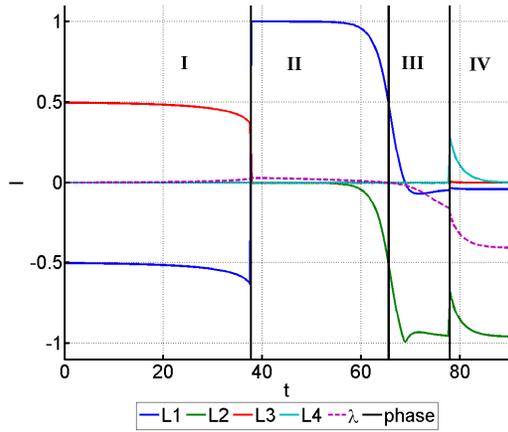
(f) Overall elasticities of eigenvalue 2

Figure 9: Elasticities in the Yeast Model for the loops L1, L2, L3 and L4

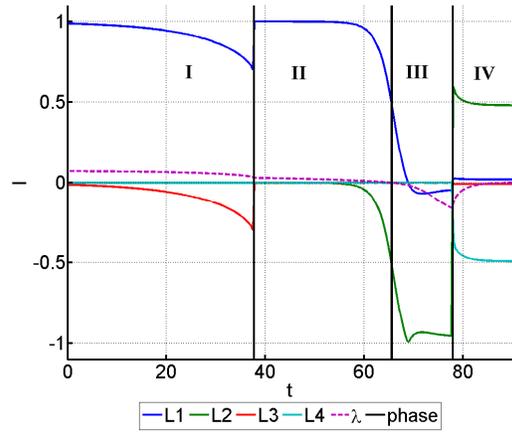
In the Yeast model, the eigenvalues are unique and the eigenvectors linearly independent, except at points such as  $t = 38$ , where, as we approach the point where the eigenvalues

merge into the pair, they are almost equal. At the merge point, the eigenvalues are non-unique, the right eigenvectors form a singular matrix. At these points, the eigenvalue elasticities are undetermined. The fact that loop eigenvalue elasticity analysis cannot deal with a singular matrix of right eigenvectors was mentioned by (Kampmann and Oliva 2005). Not only does this influence the scalability of the method<sup>6</sup>, but it also restricts the domain of the analysis to open intervals on which there is no switch from real, non-equal eigenvalues to a pair of complex conjugates or vice versa. To keep the results of the analysis readable we scaled the elasticities to values between -1 and 1 by dividing them by the sum of the absolute values of all elasticities as does Güneralp (2005). We also subdivide the domain of the analysis into open time intervals on the basis of these singularities in the eigenvalue elasticities. Also, note that the gain matrix has poorly conditioned eigenvalues round these points (Deuffhard and Hohmann 1995). Consequently, not only are the elasticities high, but so are the potential errors in calculating the eigenvalues in the neighbourhood of these points owing to round-off errors, for instance. Since the entire analysis relies on the calculation of the eigenvalues of the gain matrix, its validity becomes questionable in the neighbourhood of these singularities.

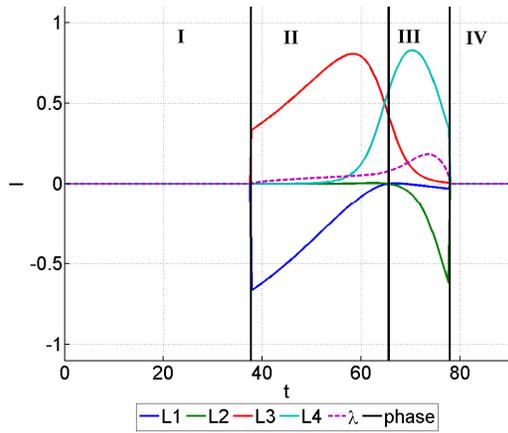
The analysis is divided into four phases, with the transition from phase I to phase II defined as the time at which the eigenvalues merge into a complex pair near  $t = 38$ . The transition from phase II to III is defined as the time at which the real part of the complex conjugate pair becomes negative. The final transition occurs when the complex conjugate pair of eigenvalues bifurcates.



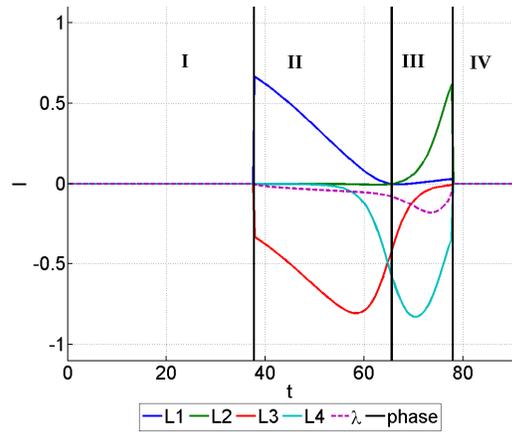
(a) Real elasticities of eigenvalue 1



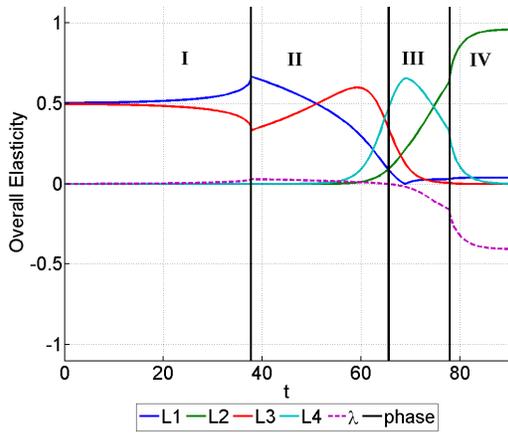
(b) Real elasticities of eigenvalue 2



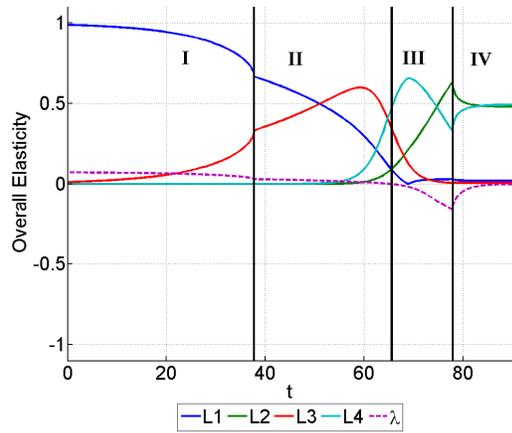
(c) Imaginary elasticities of eigenvalue 1



(d) Imaginary elasticities of eigenvalue 1



(e) Overall elasticities of eigenvalue 1



(f) Overall elasticities of eigenvalue 2

Figure 10: Rescaled loop eigenvalue elasticities for the Yeast Model

The loops L1 and L3 (Figure 10) play a significant role in determining the behavior of the Yeast model in Phase I, with L3 exerting an influence opposite to L1 on both eigenvalues.

The first eigenvalue is, for most of the interval, much smaller than the second, and exerts little effect on overall behavior. L1 is primarily responsible for the exponential growth of Phase I, with L3 restraining the growth. While the overall elasticities give an indication of the magnitude of the influence of the loops, they tell us nothing about the direction of that influence.

In the second phase, the real part of the eigenvalue elasticity is still dominated by the first loop L1. However, the third loop exerts a strong influence on the imaginary part. Both the influence of the first loop on the imaginary part of the complex pair and the absolute value of the real part of the complex pair decline over time and the overall elasticity of the third loop is larger than that of the first loop from  $t = 50$  onwards.

In phase III, the elasticity analysis assigns the most importance to L2 and L4, the two death loops responsible for the exponential decline of Cells.

During the fourth phase, the absolute value of the first eigenvalue quickly becomes much larger than the second one. Consequently, we consider the first eigenvalue to determine the model behaviour during this phase. L2 has by far the largest elasticity for this eigenvalue with L4 having an opposite elasticity, but quickly decreasing to zero. We conclude that L2 is the loop responsible for the last phase of exponential decline.

#### ***Relating the elasticities to specific states***

It is possible to link eigenvalue elasticities to the behavior of states in a model. The algorithms we used for this are based on Güneralp (2005).

The elasticity measure used by Güneralp (2005) is

$$e_1 = \frac{\partial \operatorname{Re}(\lambda_i)}{\partial g} \frac{g}{\operatorname{Re}(\lambda_i)} \quad , \quad e_2 = \frac{\partial \operatorname{Im}(\lambda_i)}{\partial g} \frac{g}{\operatorname{Im}(\lambda_i)}$$

where  $e_1$  is the real elasticity,  $e_2$  the imaginary elasticity,  $g$  the gain of the loop, and  $\operatorname{Re}(\lambda_i)$  and  $\operatorname{Im}(\lambda_i)$  the real and imaginary part of the eigenvalue respectively. The measure used by Kampmann and Saleh (Kampmann 1996; Saleh 2002) is

$$e_1 = \frac{\partial \operatorname{Re}(\lambda_i)}{\partial g} \frac{g}{|\lambda_i|} \quad , \quad e_2 = \frac{\partial \operatorname{Im}(\lambda_i)}{\partial g} \frac{g}{|\lambda_i|}$$

which divides  $g$  by the magnitude of  $\lambda_i$  for both elasticities.

The Güneralp measure has two advantages. First, the sign of the elasticity is defined relative to the eigenvalue. Consequently, if a loop or a parameter pulls the eigenvalue towards zero, decreasing the magnitude of its effect, the elasticity is negative. This definition of elasticity relative to the sign of the eigenvalue makes it suited for determining the influence of a particular loop to the behavior of a state (Güneralp 2005). Secondly, the

change in the exponential envelope or the frequency of oscillation is measured relative to the appropriate component of the eigenvalue. So, even if the eigenvalue has a very small real part (that is the exponential envelope has a large time constant), a loop that has a large relative impact on that time constant, is given a large elasticity. The same applies to the imaginary part of the elasticity and the associated frequency of oscillation.

However, there is a disadvantage to this measure of eigenvalue elasticity. If an eigenvalue has a real part that is close to zero while the imaginary part is significantly larger, the real part has relatively little influence over the associated dynamics in the short term. Applying this measure can result in any loop having a significant impact on the real part of the eigenvalue being attributed a large elasticity, while its influence on the dynamics of the model may be small.

Given these issues, we decided to apply both the Güneralp (Güneralp 2005) and Kampmann (Kampmann 1996) elasticity measures and compare the outcomes. The Kampmann (Kampmann 1996) measure for eigenvalue elasticity does not relate an elasticity to the sign of the eigenvalue. To make it suitable for relating the slope contributions of the eigenvalues, we multiplied it with the sign of the eigenvalue, such that

$$e_1 = \frac{\partial \operatorname{Re}(\lambda_i)}{\partial g} \frac{g}{|\lambda_i|} \operatorname{sgn}(\operatorname{Re}(\lambda_i)) , \quad e_2 = \frac{\partial \operatorname{Im}(\lambda_i)}{\partial g} \frac{g}{|\lambda_i|} \operatorname{sgn}(\operatorname{Im}(\lambda_i))$$

where  $|\lambda_i|$  is the magnitude of the eigenvalue. The contribution of each eigenvalue to the behavior of the selected state variable is calculated in similar fashion to Güneralp (2005), but the solution of the slope equations for the linear system is kept in complex form. This form can be extended for more complex systems (e.g. higher order systems) without modification (Appendix C).

The contributions of the different eigenvalues to the change in slope differ somewhat from the graph presented in Güneralp (2005) (Figure 11). Whereas Güneralp (2005) keeps the contributions of the conjugate pair together to form a single positive contribution of one, we assign a contribution of  $\frac{1}{2}$  to each member of the pair. This is due to differences in calculating these contributions (see Appendix C.2), since our method calculates the partial contribution per individual eigenvalue. The other discrepancy lies in the change of sign of the contributions of the eigenvalues between the inflection points of Cells at  $t = 50$  and  $t = 75$ <sup>7</sup>.

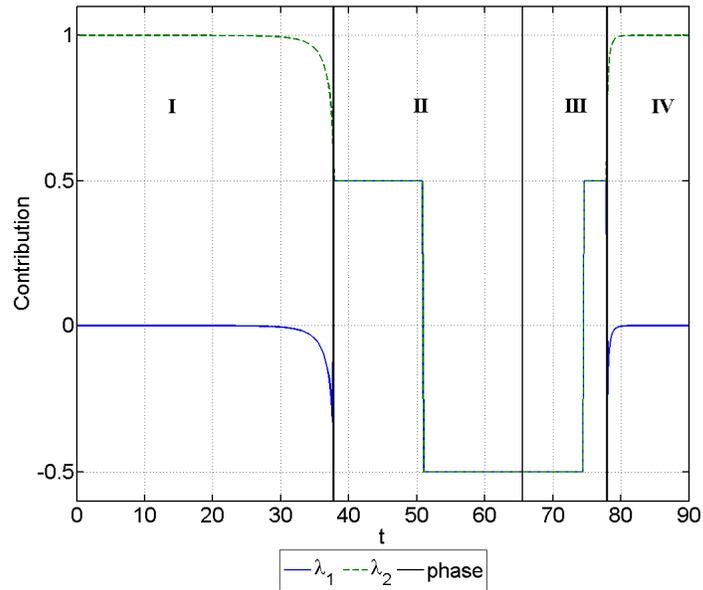
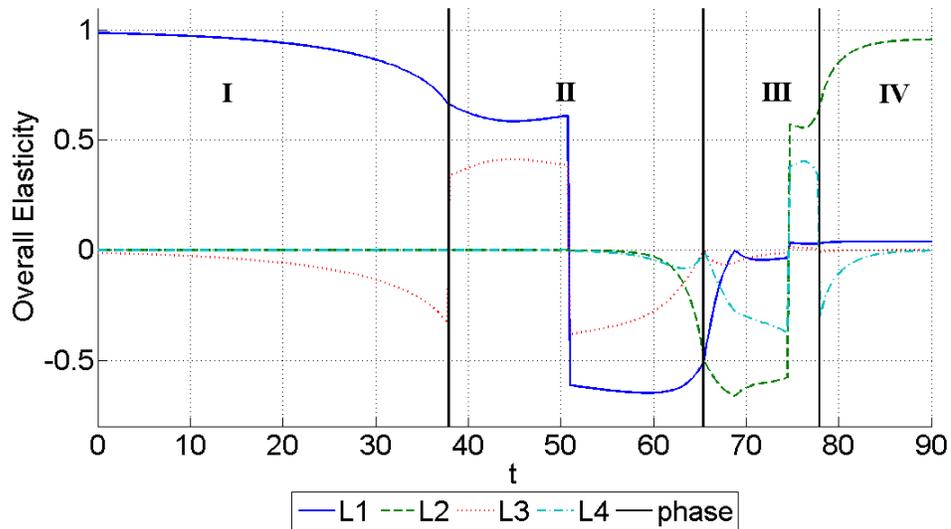
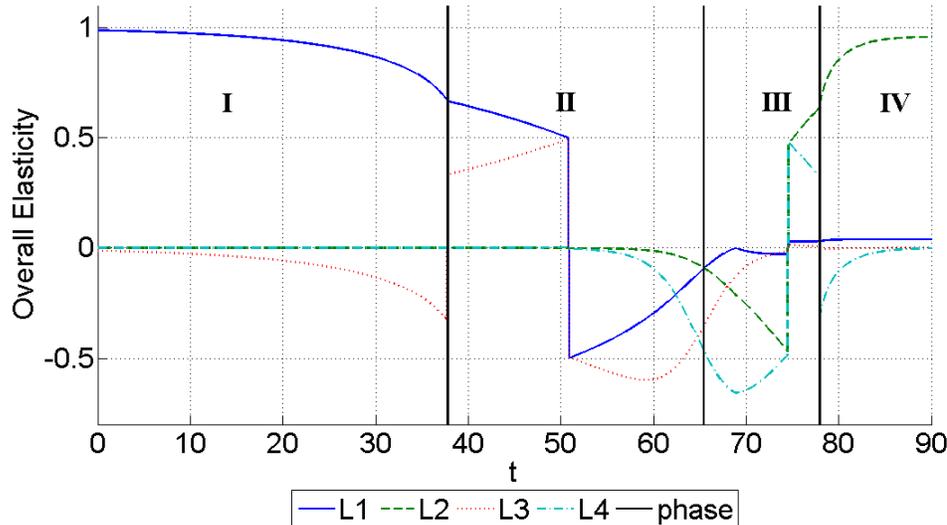


Figure 11: Contributions of the eigenvalues to the rate of change of Cells

The overall elasticity (Güneralp 2005) is used to calculate the relative influence of each loop on the behavior of the rate of change of state variable Cells. The results of implementing both the Kampmann definition of elasticity and the Güneralp one are shown in Figure 12.



(a) Loop dominance dynamics for Cells in the Yeast model calculated as in Güneralp (2005)



(a) Loop dominance dynamics for Cells in the Yeast model using the overall Kampmann elasticities

Figure 12: Loop dominance dynamics in the Yeast model

In contrast to the original results, the second measure attributes dominance to L2 in the end of phase II and L4 in phase III, in agreement with the system wide analysis using loop influence presented in the previous paragraph. With regards to the dominance of L4, the effect of alcohol on Cell Death displays a sharp increase over the third phase. This is one of the reasons for the exponential decline as seen in phase III, providing yet another argument for identifying the loop containing this variable as dominant. This analysis (Figure 12) shows that there can be significant differences in outcomes depending on which elasticity measure the analyst chooses to use.

## 4 Comparative Analysis

### 4.1 Disparities in results

The eigenvalue elasticity analysis provides us with a mathematical criterion for dividing the continuous time span of the analysis into specific phases. These phases are determined on the basis of overall model behavior rather than the behavior of a single variable. In contrast, Ford's method focuses on the behavior of a single variable and on this basis determines its time intervals for analysis. This means that the analysis of second or further variables of interest could result in different time intervals (that is, different phases) and make for lack of clarity in interpreting the results. See Figure 8 for the differences in phase determination between the two methods.

Ford's method ascribes dominance to L1 in the exponential growth phase of Cells, L3 in the balancing growth phase, L3 and L4 - as a shadow pair - in phase III and L2 in phase IV. However, the loop based eigenvalue elasticity analysis related to the variable Cells indicates that the loops L1 and L3 (Figure 10) play a significant role in determining

behavior in Phase I, with L3 exerting an influence opposite to L1. L1 is primarily responsible for the exponential growth of Phase I, with L3 restraining the growth. At the start of phase II, L1 still dominates behavior, but L3 becomes increasingly dominant towards the end of the phase. In strong contrast to Ford, the elasticity analysis for phase III assigns the most importance to L2 and L4, the two death loops responsible for the exponential decline of Cells. During phase IV, L2 is considered most influential in determining the balancing decline of cells. The results of the eigenvalue elasticity analysis relating the elasticities to the behavior of the state Cells agree with the results from the system wide analysis.

Clearly, there are discrepancies in the outcomes of the two methods, particularly in phase III. Whereas the eigenvalue elasticity method identifies the two death loops L2 and L4 as responsible for the decline of Cells after  $t \approx 66$ , the Ford method points to loops L3 and L4. In obtaining these results, the lack of single loop dominance in phase III meant that the Ford method required elimination of pairs of loops. We find the difference between the original model and the model with one loop taken out small enough to be acceptable. In contrast, a model with two loops eliminated is so different from the original model that it is doubtful whether the conclusions based on the modified model can be translated directly to the original model. In the case of the Yeast model, this was equivalent to reducing the second order non-linear model to a linear first order model and drawing conclusions regarding the original based on the behavior of the linear first order system in phase III.

## 4.2 Implementation requirements

For Ford's behavioural analysis, two modifications to the prescribed procedure were required for efficient implementation. These included a consistent means of deactivating a loop and an unambiguous definition of shadow loops. We did not fully automate Ford, but used both the model representation and solver routine of the AMBA in executing the analysis. However, we consider full automation to be feasible.

An additional argument for this automation is that, currently, applying the method to a larger model makes the required effort significantly larger<sup>8</sup>. While Ford suggests that the method can be adjusted to include only those loops that the analyst suspects to be influential, this approach is methodologically weaker, because there is no test that loops outside of the set of loops regarded as influential are correctly excluded.

No standard, readily available software exists for implementing eigenvalue elasticity analysis. So, it was necessary to automate model behavioural analysis to obtain the results presented in this paper. We chose to develop a prototypical generic framework for this purpose because we intend to proceed further with the comparison of different behavioural analysis methods. Once the AMBA framework was operational, it became possible to perform the steps required by eigenvalue elasticity analysis (namely structural analysis, linearizations and the computation of the elasticities themselves) in a standard fashion. Until such software becomes commonplace, significant effort and investment is required

for the implementation of eigenvalue elasticity analysis. However, within the AMBA framework, the application of the method to a given model is relatively easy.

### 4.3 Explanatory power

Since the definition of the atomic behavioral pattern accords well with an intuitive understanding of model behavior and the mechanism of deactivating loops is readily explicable, Ford's method is understandable. This is the strongest argument for the routine application of Ford's method.

The restriction of the analysis to separate time intervals limits its explanatory power for an oscillating model. Its conclusions are confined to time intervals displaying one atomic behavior pattern, causing effects spanning more than one interval to be ignored. In the case of a model with dampened oscillation, where one loop is responsible for the speed of dampening, Ford's approach will have difficulty in distinguishing this effect, since it is restricted to time intervals in which the dampening cannot show.

In contrast, the method of eigenvalue elasticity analysis determines the relative contribution of loops to the behaviour of eigenvalues or specific state variables in an almost continuous fashion. This means that it has no trouble identifying system-wide effects and is the analytically stronger method. However, understanding and interpreting the results of the analysis requires in-depth knowledge of the method and its mathematical basis. It is difficult to explain even to *analysts* who are not familiar with the method. This currently restricts its application to experts in the field of model behavioural analysis.

In our view, the strongest contribution of the eigenvalue elasticity analysis method to date is its visualization of the fractional influence of loops on eigenvalues and state variables. We suggest that the term "fractional influence of a loop" be adopted as a descriptor of the role that system structure plays in determining model behaviour instead of the term "loop dominance", which implies that a single loop is responsible for model behaviour. This may help to improve the explanatory power of eigenvalue elasticity analysis.

## 5 Future Research

This research confirms that eigenvalue elasticity analysis holds promise as a tool for powerful model behavioural analysis despite the difficulties associated with understanding and explaining the method itself and its results. In developing the method further, there are a few hiccoughs that need to be addressed. These include:

- Analytically determining individual edge elasticities. Using structural analysis it is possible to identify the pathways between different states, as in the identification of pathways in DIGEST (Mojtahedzadeh, Andersen et al. 2004) and in (AbdelGawad 2005). Once these are identified, the pathways of which each causal link is a member can be listed<sup>9</sup> and their gains as well as their elasticities can then be calculated analytically.

- Edges in some models are not always active. It is possible that a loop included in the shortest independent loop set becomes inactive at some time during a simulation while another loop, excluded from the SILS, yet forming an alternative path, remains active. This poses a problem if the original SILS is used throughout the analysis of the eigenvalue elasticities. By checking for such a condition and re-executing a structural analysis when it occurs (Güneralp 2006), this problem can be resolved. Current developments as mentioned in (Goncalves, Lerpattarapong et al. 2000) are making progress in this area.
- Quantifying the contributions of real and imaginary parts of the complex eigenvalues. The eigenvalue elasticities are hardest to interpret when there is a complex conjugate pair of eigenvalues. Currently the real and imaginary parts of the elasticities of the pair of eigenvalues are separated, but the relative contributions of the real and imaginary parts of the eigenvalues to the behavior of the state variable of interest are not. This limits the insights derived. By quantifying the contributions of real and imaginary parts of the complex eigenvalues, this problem can also be addressed.

With increasing model size, the applicability of the system-wide variant of eigenvalue elasticity analysis decreases. The larger the size of the model, the more difficult the system-wide variant becomes to interpret. In the case of high order, nonlinear models, a variant that relates model structure to the behavior of specific variables is potentially more powerful than a system-wide variant (Kampmann and Oliva 2005). Also, numerical issues may arise as model size increases. Further analysis is needed to address and resolve this issue. For example, a plot of either the condition number or the determinant (Appendix B.2) can reveal how close the matrix of right eigenvectors is to being singular. Such information accompanying the eigenvalue and contribution plots would enable the analyst to make a better judgment of whether a singularity should be expected or is purely a characteristic feature of the model under study.

We plan to contribute to endeavours in this field of research by developing the AMBA framework further. This development will include implementations of the algorithms not analyzed in this paper (Goncalves, Lerpattarapong et al. 2000; AbdelGawad 2005; Saleh 2005) and the automation of Ford's method.

Eigenvalue elasticity analysis and the automated application of Ford's behavioural analysis are still in the development phase. However with the extension of the AMBA framework, it should be feasible to expand testing and comparison to more and larger models. We concur with Diker (Diker 2006) that a standard, formal way of representing models would be of significant help in performing this type of research.

Furthermore, the explanatory power of eigenvalue elasticity analysis can be improved by the design of alternative approaches to the communication and visualization of results<sup>10</sup>. Research on this aspect is necessary. We also consider that a consistent and more insightful

terminology for describing the relationships between model behaviour and structure would be useful for explaining the method and its results.

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<sup>1</sup> In this paper it is assumed that a shadow feedback structure resulted in the atomic behavior patten (ABP) not changing by removing each loop separately, but changing if we eliminate both loops. That is, two dominant loops generate the same behavior, one taking over if the other is eliminated. However, according to Ford's Long Wave example in his paper (Ford, 1999) it appears to be the case that a shadow feedback loop is found by first taking out a dominant loop and than determining if other loops are dominant in the model that is missing the dominant loop. So, in this example, Loop B is said to be a shadow loop of A if the ABP generated over a given time interval by eliminating loop B and Loop A is different from the ABP generated by the model if only Loop A is eliminated. In other words, the result of the dominance test for A changes if B is also eliminated. If this is the case, A can still be a shadow loop of B. This line of reasoning is *not* used in this paper.

<sup>2</sup> The functions were obtained via [R. Oliva's resource page](#). Their output contains descriptions of all loops, but not in the form of a Directed Cycle Matrix. The output had to be rewritten to a form usable for the rest of the analysis.

<sup>3</sup> The time between the different points of analysis does not need to be kept constant during the analysis. For instance, AMBA enabled us to increase the granularity of the analysis of the more dynamic phases of behavior of the Long Wave model.

<sup>4</sup> The shortest independent loop set is a subset of the loops in the model is defined as [...] consisting entirely of geodetic loops where the path between any two variables in the loop is also te shortest pah between those variables. [...] (Kampmann and Oliva, 2005)

<sup>5</sup> This is clear from the analytical formulation for an influence on  $\lambda_i$  of a particular element at the position (p,q)  $g_{pq}$  in the gain matrix  $G$ , for which

$$\frac{\partial \lambda_i}{\partial g_{pq}} g_{pq} = \mathbf{l}'_i(p) \mathbf{r}_i(q) g_{pq}$$

where  $\mathbf{l}_i$  is the left eigenvector associated with  $\lambda_i$  and  $\mathbf{r}_i$  the right eigenvector (Saleh, 2002) Since,

$$\mathbf{L} = \mathbf{R}^{-1}$$

where  $\mathbf{R}$  is the matrix composed of right eigenvectors and  $\mathbf{L}$  the matrix of left eigenvectors. The left eigenvectors are undetermined when  $\mathbf{R}$  has linearly dependent columns.

<sup>6</sup> Larger matrices are more likely to have singular or close to singular matrices of right eigenvectors.

<sup>7</sup> This is due to a minor error in calculation in the Gunealp paper. The current results are consistent with the definition of the contribution of an eigenvalue to the behavior of the state variable of interest.

<sup>8</sup> In his own application of the method on the Long Wave model, Ford only tests the role of those loops already identified as dominant by Kampmann, using the EEA as a guideline for selecting loops. If we have  $n$  loops in our ILS, there are  $2^n$  possible combinations of eliminated or active loops. The analysis of the Yeast model required 22 different model runs on a second order model with four different phases of behavior. This includes rewriting equations to support the switching off of loops. Analysing a second variable in the same model would require comparable effort, although some work can be reused.

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<sup>9</sup> The end result would be hash table with the edges in the model as keys and the pathways they belong to as values. Once this has been obtained, figuring out the gains of the individual pathways during the elasticity analysis is trivial. Assuming the rest of the analysis remains the same, the search only needs to be performed once, in the structural phase of the analysis.

<sup>10</sup> One tool that seems promising for developing static visualizations and perhaps even animations is the Java Universal Network/Graph framework. (JUNG). JUNG is “a software library that provides a common and extendible language for the modeling, analysis, and visualization of data that can be represented as a graph or network”. The homepage for this project is <http://jung.sourceforge.net>.

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