Automatic Calibration of NAM Model
with
Multi-Objectives Consideration

D2K Technical Report 1298-1

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18th December 1998

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A Report on the research activities undertaken at DHI: (17th Aug – 18th Dec 98)

1 Introduction

In recent years, much research has been directed to developing global optimisation methods for automatic calibration of conceptual models as well as hydrodynamic models (Babovic et al., 1994). In this respect, population-based algorithms such as genetic algorithms (GA) (Goldberg, 1989), evolutionary strategy (ES) (Schwefel, 1981), shuffled complex evolution (SCE) (Duan, 1991) etc have shown to be effective and efficient in locating global optimum of a model with respect to single objective calibration (Duan et al., 1992; Wang, 1991).

In a recent R&D project at DHI, the SCE algorithm was applied as an automatic calibration of the NAM rainfall-runoff model (Madsen and Ammentorp, 1998). The preliminary applications demonstrated the two common "deficiency" of automatic calibration based on a single objective function: (1) there may be several important characteristics in the observations that are necessary to be modelled and any single objective function may not be adequate enough to represent the distinctions and similarities between the simulation and observation; and (2) both distributed and physically based hydrological model simulations usually involve the simulation of more than a single quality of measurement in the system and therefore several measurements of objective functions are necessary. This implies the need for a more elaborate formulation of the optimisation problem including multiple objective functions consideration.

Calibration of NAM model with multiple objective functions consideration can be formulated as a multiple objectives optimisation problem. A discussion on multiple objective optimisation and its relevance to model calibration is included in Appendix A. Once we are able to express the multiple objectives in a quantitative manner (in the form of fitness function), the next stage is to perform a search or optimisation in the fitness function space. In solving multi-objective problems, we are interested in obtaining a set of Pareto optimal solution points rather than a single solution point. The set of Pareto optimal solution points give the user a chance to select points that are "as good as" the other points in terms of fitness measurement but focusing on distinct characteristics of a hydrological process as reflected in the hydrograph. This report presents two such methods to calibrate the NAM model. Results presented herein are exploratory in nature and more work on comparative studies will be carried out from January 1999 to May 1999.

2 Objectives

The main objective of this stage is to formulate and implement different multi-objective calibration procedures for the automatic calibration of the NAM rainfall-runoff model. Specific aims would be to:

1. Implement the accelerated convergence genetic algorithm, ACGA, (Liong et al., 1998) formulated at the National University of Singapore (NUS) for the calibration of the NAM model;
2. Formulate different objectives that measures different characteristics of the hydrological response; and
3. Formulate a new process oriented approach for the automatic calibration of the NAM model.

3 Automatic calibration of NAM model using ACGA

The work during this phase was to couple NUS's ACGA (a modified multi-objective genetic algorithm) and DHI's NAM rainfall-runoff model and to implement a prototype window interface for. The objectives of this implementation are:

1. To provide a feasible tool for the automatic calibration of a rainfall-runoff model that takes into account of multi-objective calibration;
2. To provide a tool to explore the capability of the genetic algorithm in deriving a trade-off surface (or Pareto front) in the context of multiple objective optimisation;
3. To provide a tool to investigate the use of different quantitative measures describing the goodness-of-fit of the models' simulation; and

A prototype of the automatic calibration routine for NAM has been developed (Figure 1). This automatic calibration (window interface) has been programmed specifically for the NAM model. However, it can be modified (through hard coding) to suit other simulation models without changing the windows interface.

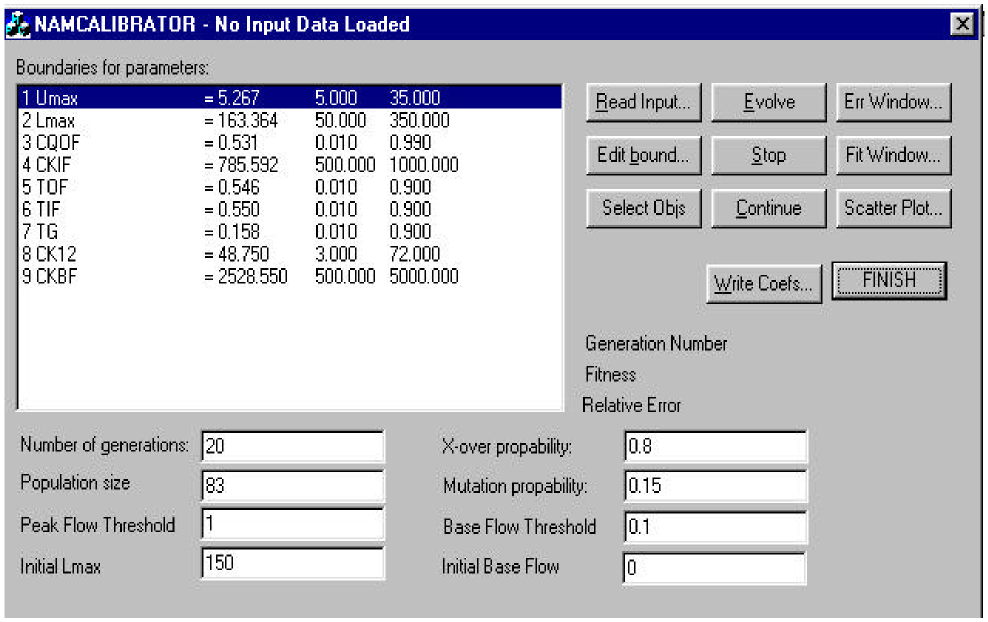

Figure 1: Main Input Dialog for the NAM-ACGA calibration routine.

The salient features of this implementation are:

1. The user can easily specify different catchments and the bounds of the calibration parameters;
2. The user can view the calibration process results such as simulation hydrograph (Figure 2), scatter plot of the simulated versus observed data (Figure 3) and the error window (Figure 4) as the calibration proceeds. Thus the user can choose to intervene with the calibration process as and when he preferred; and
3. The user can view the optimal set of calibration parameters as the calibration progresses (through the main input dialog) and store the optimal set of calibration parameters using the "write coefs" option.

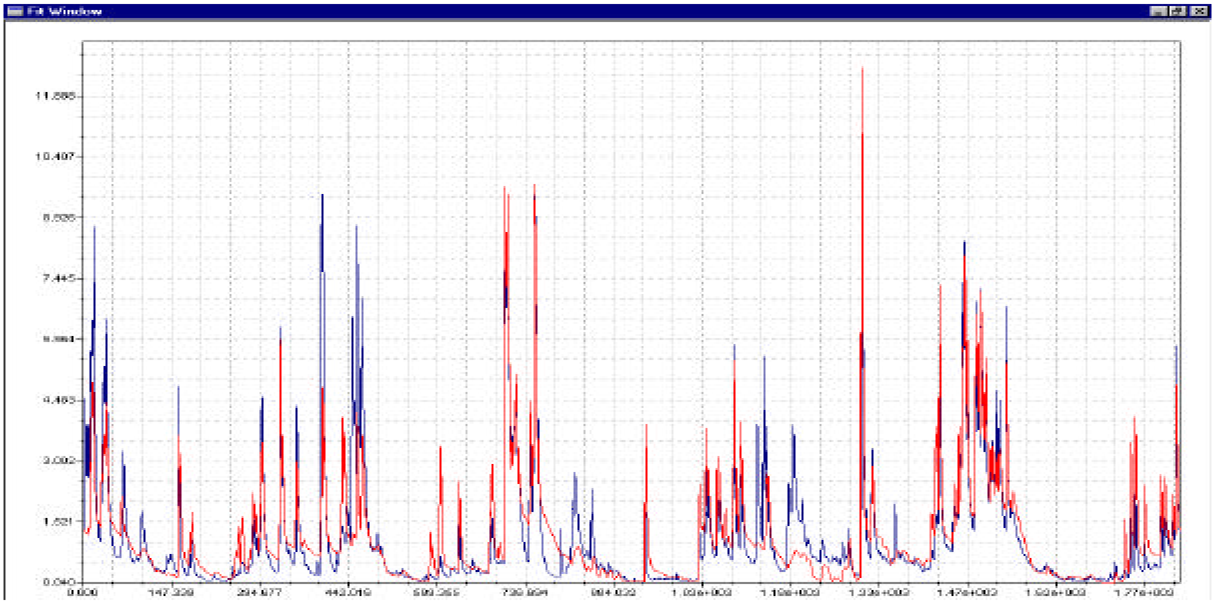

Figure 2: Simulated vs Observed Hydrograph

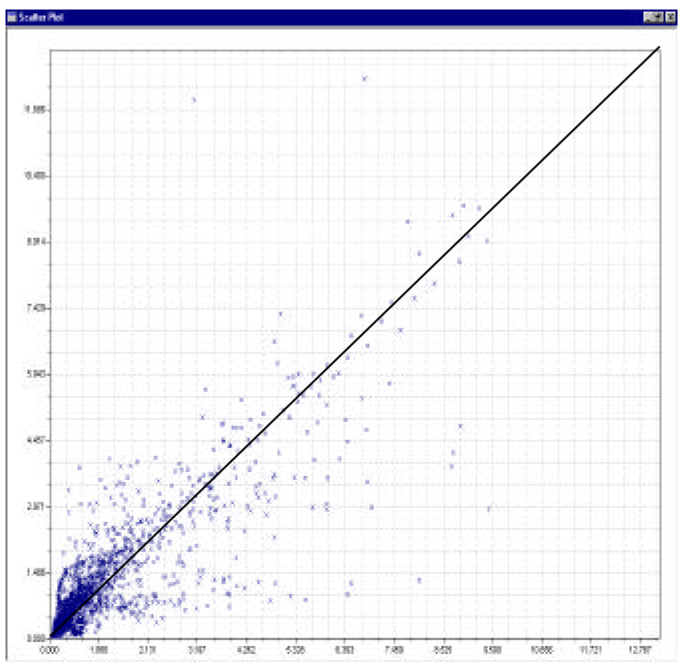

Figure 3: Scatter Plot of Observed vs. Simulated Flows

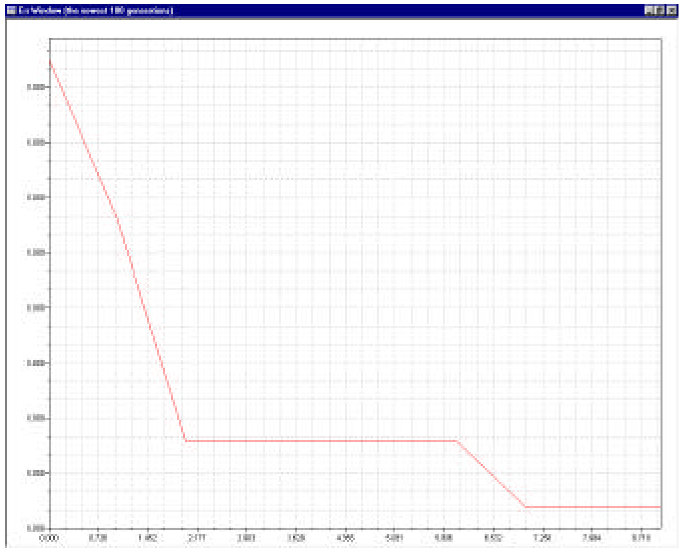

Figure 4: Plot of Prediction Error vs. Number of Generations

The main optimisation engine in this routine is the modified genetic algorithm known as accelerated convergence genetic algorithm (ACGA). A short description of ACGA will be given here and a more detailed description is included in Appendix B.

3.1 Accelerated Convergence Genetic Algorithm (ACGA)

The development of ACGA was initiated by the need to form a compact band of points around the Pareto front. This need arises because our study at NUS showed that optimal points were usually sparsely spaced along the Pareto front. It has been found that it is possible to reconstruct the Pareto front if the points around the front are sufficiently compacted. Thus ACGA was formulated to give a compact Pareto front, if the front exist. The ACGA mainly differs from the traditional simple GA (Goldberg, 1989) in the following two mechanisms:

1. Seeding of initial population:

   Fractional Factorial and Central Composite Designs (FFD-CCD), a response surface method, is used (instead of random data generator) to generate the initial sets of parameter combinations. The chosen initial seeding provides an extensive coverage of the parameter space as well as the objective function space; and

2. Selection Criterion:

   Only relatively fit populations (as measured by the distance function) are selectively chosen to generate the populations of the subsequent generations.

Thus, we would expect the resultant Pareto front, if any, to consist of relatively compact points.

4 Formulation of Different Objectives

The calibration routine allows the user to choose different objectives from the main input dialog (Figure 1). At present, the user can choose different combinations of any of these 5 objectives:

1. Peak flow magnitude;
2. Peak flow volume;
3. Base flow magnitude;
4. Total flow volume; and
5. Overall shape of the hydrograph.

The selection is done by placing a cross in the desired check-boxes next to the objectives (Figure 5). Besides specifying the objectives, there are also three options to specify the goodness-of-fit function to be associated with the objectives peak flow magnitude, base flow magnitude and overall shape of the hydrograph.

The user can select one of the following goodness-of-fit measures

- ***Root Mean Square Error (RMSE):***

$$RMSE = \left\{ \frac{1}{N} \sum_{i=1}^{N} \left[Q_{obs,i} - Q_{sim,i} \right]^2 \right\}^{1/2} \qquad (1)$$

- ***Nash-Sutcliffe coefficient (R^2):***

$$R^2 = 1 - \frac{\sum_{i=1}^{N} \left[Q_{obs,i} - Q_{sim,i} \right]^2}{\sum_{i=1}^{N} \left[Q_{obs,i} - \overline{Q} \right]^2} \qquad (2)$$

- ***Coefficient of variance:***

$$P = \frac{1}{\overline{Q}} \left(\frac{\sum_{i=1}^{N} \left[Q_{obs,i} - Q_{sim,i} \right]^2}{N} \right)^{1/2} \qquad (3)$$

- ***Reduced error estimate:***

$$REE = \left[\frac{\sum_{i=1}^{N} \left[Q_{obs,i} - Q_{sim,i} \right]^2}{\sum_{i=1}^{N} \left[Q_{obs,i} - \overline{Q} \right]^2} \right]^{1/2} \tag{4}$$

- ***Proportional error of estimate:***

$$PEE = \left\{ \sum_{i=1}^{N} \left(\frac{Q_{obs,i} - Q_{sim,i}}{Q_{obs,i}} \right)^2 \right\}^{1/2} \tag{5}$$

- ***Second Moment:***

$$M^2 = \frac{\sum_{i=1}^{N} \left(Q_{obs,i} \right)^2 - \sum_{i=1}^{N} \left(Q_{sim,i} \right)^2}{\sum_{i=1}^{N} \left(Q_{obs,i} \right)^2} \tag{6}$$

Each of the above equations shall be modified appropriately with the correct notation for different objective calculations i.e. for peak flow, base flow, or overall shape. For example Eq. (1) shall take the form:

(i) $$Peak_{RMSE} = \frac{1}{P} \sum_{j=1}^{P} \left\{ \frac{1}{M} \sum_{i=1}^{M} \left[Q_{obs,i} - Q_{sim,i} \right]^2 \right\}_j^{1/2} \qquad \textit{For } Q_{obs,i} \geq QT \tag{1a}$$

where Q_{obs} = observed flow (m^3/s);

Q_{sim} = simulated flow (m^3/s);

M = number of timestep in a particular peak event;

P = number of events with flow $Q_{,obs,i} \geq QT$; and

QT = threshold value of peak flow (m^3/s) .

(ii) $$BF_{RMSE} = \frac{1}{P} \sum_{j=1}^{P} \left\{ \frac{1}{M} \sum_{i=1}^{M} \left[Q_{obs,i} - Q_{sim,i} \right]^2 \right\}_j^{1/2} \qquad \textit{For } Q_{,obs,i} \leq QBF \tag{1a}$$

where Q_{obs} = observed flow (m^3/s);

Q_{sim} = simulated flow (m^3/s);

M = number of timestep in a particular low flow event;

P = number of events with flow $Q_{,obs,i}$ £ QBF; and

QBF = threshold value of low flow (m^3/s) .

The user can combine different objectives and also with different goodness-of-fit measures, thereby giving him a tool to calibrate the model that produces the "required" simulated hydrograph shape. A more detail description of the software interface can be found in Appendix C.

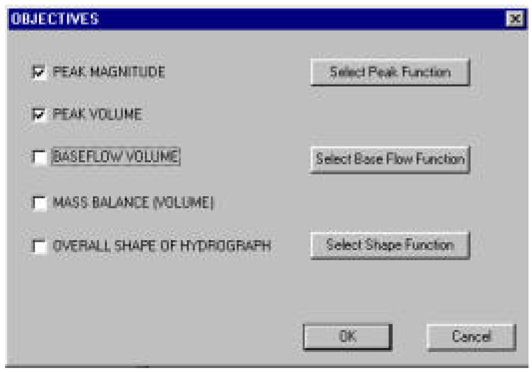

Figure 5: Dialog Box for the Selection of Objectives

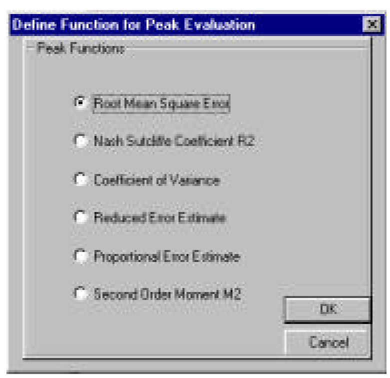

Figure 6: Dialog Box to Define the Function for Each Objective

By combining different objectives and goodness-of-fit measures, the effectiveness and efficiency of the calibration strategy can be studied based on a multi-objective approach. Thus, various studies such as the following can be performed:

- Effect of different objectives on the Pareto front;
- Effect of different goodness-of-fit on the Pareto front;
- their relationship with each other, if any; and

- interpretation of the amount of trade-off gained or lost when an alternate point on the Pareto front is chosen.

These studies should not only be looking at the goodness-of-fit measures but also on visual inspection of the hydrographs.

5 Formulation of a New Process Oriented Automatic Calibration (NPOC) Technique

The process oriented calibration, POC, scheme (Harlin, 1991) was first proposed by the Swedish Meteorological and Hydrological Institute to calibrate the HBV (Berstrom, 1976) model. In the original proposal, Harlin (1991) used the POC scheme to calibrate twelve parameters in two stages. Firstly, a recession analysis of observed runoff was carried out to determine the initial parameter values. Secondly, the parameters were calibrated individually by forming a loop over 3 processes: snow routine, soil routine, and flow routing. He found that the POC scheme yielded as good model performance as manual calibration.

Zhang and Lindstrom (1997) proposed a slightly different approach called Automatic Calibration Scheme for HBV (ASCH). In ASCH, the continuous hydrograph was split into different sub-periods, with the aim of making the runoff correspond to the rainfall in each sub-period. A two stage approach was proposed, first calibrating the soil moisture routine then the snow and flow routing routine. In the first stage, the parameters are determined in a 2 step process with the parameters split into 2 groups. The first step was to narrow the range of the group 1 parameters and the second step optimising on these narrow ranges. In the second stage, the parameters were determined in 4 steps, each step concentrating on a different objective function. The objective functions considered were the simple least squares, the total runoff volume prediction error and runoff volumes resulting from high and low flows of each sub-period. The optimisation routine used was the convergent descent method by Fletcher and Powell (1980).

The significance of the works of Harlin (1991) and Zhang and Lindstrom (1997) are that their calibration schemes gave special consideration to the human interpretation of parameter and response surface interaction. For example, the POC scheme had an automatic calibration looping that calibrates the parameters for 3 different processes, one at a time. This is similar to the present system of manually calibrating these processes, each time trying to increase the prediction accuracy. Another example is the stage 2 of ASCH scheme which divides the calibration period into sub-periods. Each period was then optimised individually with a different objective function. This is also similar to certain approaches used by practising engineers, whereby they would identify and isolate sub-periods of the hydrograph dominate by particular runoff mechanism and try to match them one at a time.

The proposed modified POC scheme is a hybrid of POC, ASCH, GA and the rule-based (Madsen and Ammentrop, 1998) schemes. The optimising routine is replaced with the Accelerated Convergence Genetic Algorithm, ACGA (Liong et al., 1998) and the determination of recession curve by the Master Recession Curve method (Lamb and Beven, 1997). The advantage of this methodology is that it minimises but does not eliminate the input required by the user thus ensuring that the user has sufficient control over the optimisation routine and the whole calibration process.

The proposed modified process oriented calibration (MPOC) scheme can be divided into 3 steps:

(i) Identification of calibration parameter ranges and initial values;

(ii) Optimisation Stage 1: optimising the water balance using multi-objective genetic algorithm;

(iii) Optimisation Stage 2: optimising the hydrograph shape using multi-objective genetic algorithm;

The main idea behind the formulation of the stage process is the direct translation of the human perceptive component in manual calibration to enhance existing automatic calibration. Manual calibration is a combination of trial and error method, multiple focus (multi-objectives) approach and the goodness-of-fit is measured qualitatively. The stage process that proposed is a combination of the first two qualities in the manual calibration process. The trial and error method (in manual calibration) will be replaced by automatic search. The multiple focus approach will be replace by the two stage approach (focusing on water balance and hydrograph shape) with the additional component of multi-objectives (focusing on both peak and base flows) in each stage.

6 Preliminary Results and Discussions

6.1 Automatic Calibration of NAM using ACGA

A preliminary study involving 2 objective functions: peak flow RMSE (Eq. (1a)) and overall RMSE (Eq. (1)) was performed. The catchment chosen is the Tryggevaelde catchment in Denmark. Table 1 shows the initial values of the state variables and Table 2 shows the bounds of the 9 calibration parameters. Tables 3 and 4 show a summary of the performance indicators and the respective optimal calibration parameter values of points along the Pareto front after running NAM for approximately 1500 simulations (with initial population size of 83 and for 18 generations) respectively.

Table 1: Initial Values of the State Variables

State Variables	Initial Values
SS	0.0
U	0.0
L	150
QR1	0.0
QR2	0.0
BF	0.9

Table 2: Bounds of the Calibration Parameters

Parameter	Upper Bound	Lower Bound
Umax (mm)	5	35
Lmax (mm)	50	350
CQOF	0.01	0.99
CKIF (hours)	500	1000
TOF	0.01	0.90
TIF	0.01	0.90
TG	0.01	0.90
CK12 (hours)	3	72
CKBF (hours)	500	5000

Table 3: Summary of Performance Indicators

Points on Pareto front	A	B	C	D
Nash Sutcliffe R^2	0.894	0.881	0.881	0.894
RMSE	0.795	0.776	0.755	0.770
Volume Error (%)	1.04	3.22	12.49	20.25
Volume Error (abs) (m^3)	2.6	7.9	30.8	49.9

Table 4: Optimal Parameters for Points on Pareto Front

Parameters	A	B	C	D
$\mathbf{U_{max}}$	14.3	25.6	13.2	9.4
$\mathbf{L_{max}}$	303	273	309	170
CQOF	0.500	0.594	0.953	0.729
CKIF	580	998	508	754
TOF	0.772	0.657	0.564	0.587
TIF	0.900	0.643	0.477	0.632
TG	0.775	0.696	0.424	0.318
CK12	37.5	29.0	27.4	27.4
CKBF	2750	3483	2043	2008

From Table 3, the goodness-of-fit measures (R^2 *and RMSE*) seemed to indicate that the performances of each set of parameters are comparable to each other. However, there is a noticeable trade-off between the points from the Pareto front plot (Figure 7) and there is significant variation in the parameter values between the points (Table 4). Figure 8 shows the difference in the resultant hydrograph of parameters obtained for point B and point C from the Pareto front of Figure 7.

6.2 New Process Oriented Automatic Calibration Technique

Based on the philosophy outlined in Section 4, a new process oriented calibration (NPOC) technique has been formulated for the calibration of the NAM model. Certain characteristics of the observed hydrograph such as peak flow volume, overall water balance, peak flow shape, low flow shape etc and the parameters that have most predominant effect on these characteristics have been identified (Table 5). From Table 5, the characteristics of the hydrographs are then lumped into two groups: one concerning water balance; and the other, shape of the hydrograph.

A calibration scheme was formed based on the above analysis. The details of the scheme is as follows:

(i) The values of parameters "CKIF", "CK12" and "CKBF" were fixed at default values given in MIKE11. The values correspond to 750, 30 and 2000 respectively.

(ii) Six parameters were chosen to be optimised. They were "U_{max}", "L_{max}", "CQOF", "TOF", "TIF" and "TG". They were the parameters in Table 5 that affects the water balance of the system. Initially, these 6 parameters were further subdivided into 2 groups: one concerning overall water balance and the other, peak and low flow water balance. Subsequent investigation showed that there was no necessity to have such fine division but rather include all three measurements of water balance in one optimisation process. However, since the purpose of optimisation was still to have good prediction on various portions of the hydrograph, there was a necessity to consider multi-objective optimisation. ACGA was used as the optimisation routine and approximately 500 NAM simulation runs were performed.

(iii) After the water balance has been optimised, the parameters affecting overall balance "U_{max}" and "L_{max}" were fixed. A new range of the upper and lower bounds of the remaining 4 parameters were identified (Table 6). The identification was based on the assumption that the overall target of water balance shall not be greater than ±5%. Thus, the worst combination of the upper and lower bounds of the 4 parameters shall not exceed the target of ±5% prediction error in any of the water balance criteria.

(iv) The next step was to calibrate the shape of the hydrograph. Based on the philosophy of process oriented approach, the shape was identified as consisting the shape of the peak flow events and low flow events. The peak flow and low flow events were given by certain threshold values calculated from statistical analysis of the observed data. The peak flow threshold was based on a 98% exceedance probability and the base flow threshold was based on the lowest 20% of the observed flow. ACGA was used as the optimisation routine and 500 NAM simulations runs were performed.

A preliminary study based on the above scheme was carried out to calibrate the Tryggevaelde catchment in Denmark. Figure 9 shows the resultant hydrograph, the scatter plot and the calibration parameters after stage 1 calibration (calibrate water balance). Figure 10 shows the results after stage 2 calibration where the ranges of parameters were narrower.

7 Proposed Work

7.1 Automatic calibration of NAM and other models

The preliminary investigations outlined in this report and the previous basis report #4730 (Henrik and Ammentrop, 1998) indicated that although algorithms such as ACGA and SCE are efficient and effective calibration schemes, the critical issue lies on the selection of objectives and goodness-of-fit criteria. The tool developed would enable users to select a variety of objectives and different combinations of goodness-of-fit measures. He would then

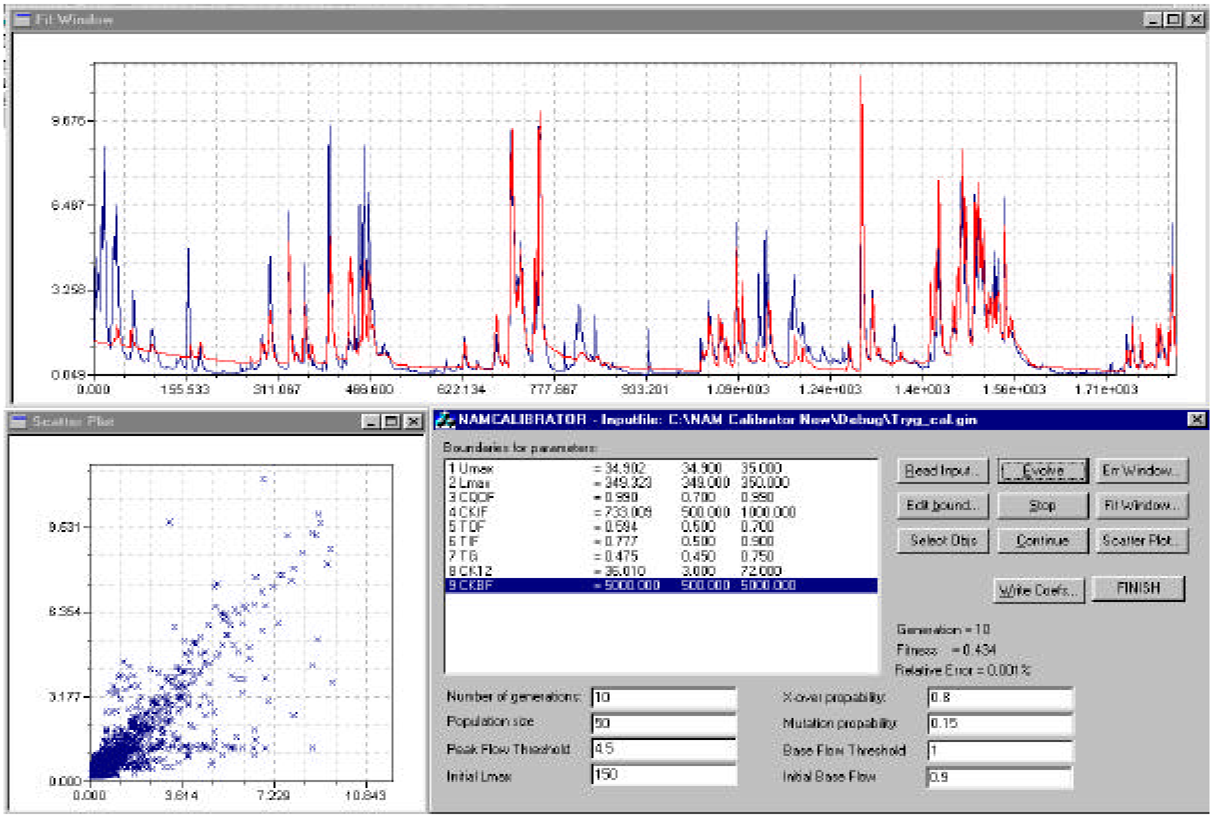

Figure 9: Results after Stage 1 NPOC Calibration

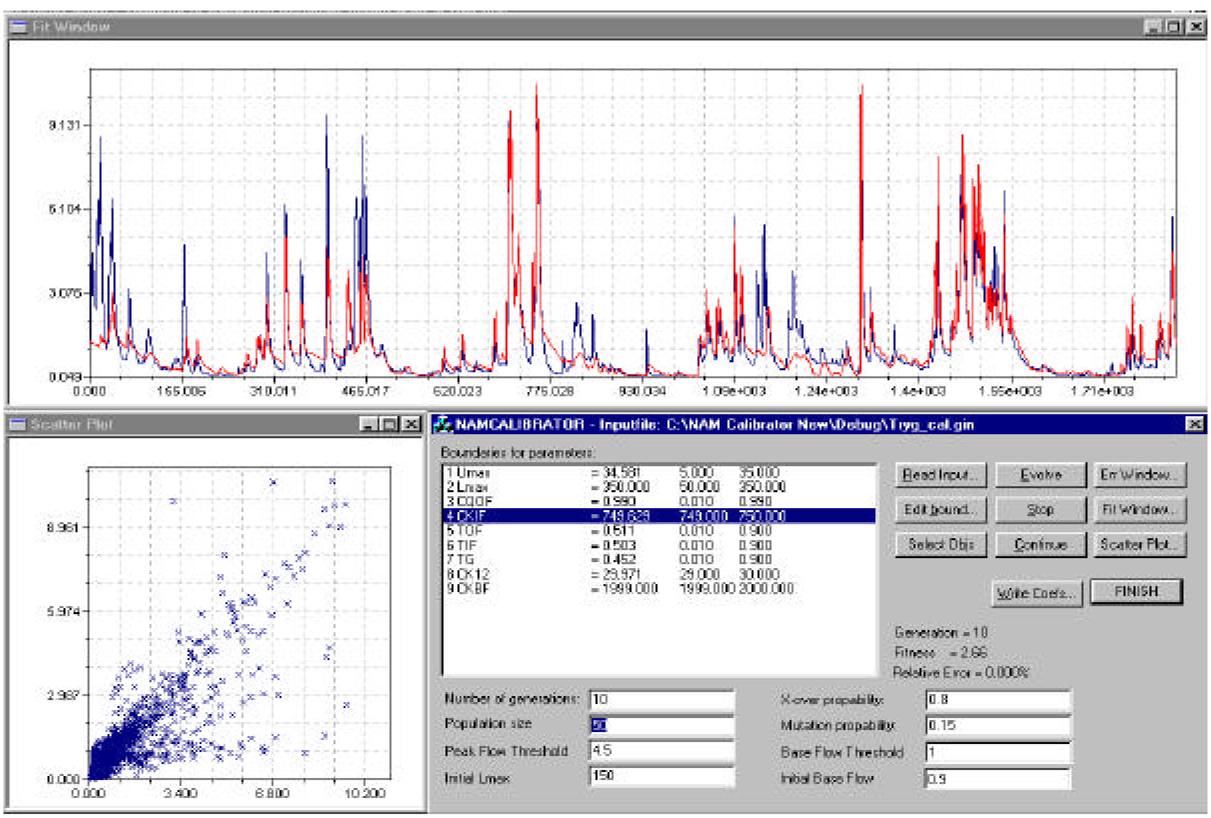

Figure 10: Results after Stage 2 NPOC Calibration

in a position to make critical assessment of the different results and select the desired combination. The subsequent work on the analysis of different combinations of objective functions will be carried out during the period February – May 1999 by a student from DTU.

The second task that needs to be performed is the application of ACGA and SCE to calibrate other existing hydrological or hydrodynamic models such as MOUSE and MIKE-SHE. There has been a previous attempt to calibrate the MOUSE model looking at single objective function (Babovic et al., 1994). It would be interesting to extend the study to include multi-objectives calibration. This issue will be examined further under one of the new DHI's internal R&D proposal by Henrik Madsen.

7.2 Implementation of NPOC scheme

The new process oriented calibration scheme in Section 6.2 indicated a direction towards the automatic calibration of models derived from manual calibration. The preliminary results are promising because it reduces the number of model simulations by up to 30%. This reduction in computational time could be extremely important for computational intensive simulation models such as MIKE21 and MIKE3. A lot of work is still required before a robust scheme can be devised. The areas of exploration includes:

(i) the sensitivity and determination of the default values used in the scheme outlined in Section 6.2. Experience indicates the most sensitive parameter is the baseflow time constant "CKBF". The work by Keith and Beven (1997) on "master recession curve" could shed some light in the determination of the initial value of "CKBF".

(ii) Although the outline of NPOC has been determined, it is model specified. The challenge is to devise a formal scheme which is generic and can be applied to calibrate other hydrological and/or hydrodynamic models.

The above areas of research will be examined by Soon-Thiam KHU at the National University of Singapore from the period January to May 1999.

7.3 Intelligent analysis of hydrological data

The research project outlined above focus on the application of advanced data analysis to the hydrological time series, under part of a larger project "**Data Mining in Hydroinformatics: D_2K**". The project on advanced application of data analysis tools will be conducted through several inter-linked stages. The first stage is oriented towards the automatic calibration of hydrological models. The second stage of the project will be oriented towards mining the same hydrological data. Techniques such as neural networks, polynomial networks, local –linear models and genetic programming will be investigated. Work in the area of local-linear models and genetic programming has already started and results of some applications in hydrology can be expected in April 1999. Based on these results, new R&D directions and strategies have to be made and more extensive applications of these techniques should begin from June 1999 onwards.

8 Conclusions

By considering the multi-objective aspect of model calibration, we are able to obtain a set of Pareto optimal solution points rather than a single solution point. The set of Pareto optimal solution points give the user a chance to select points that are "as good as" the other points in terms of fitness measurement but focusing on distinct characteristics of a hydrological process as reflected in the hydrograph. This report presents two such methods to calibrate the NAM model. The first method is a straightforward application of multi-objective optimisation technique such as ACGA. The study focus on the formulation of an overall calibration strategy, from data quality assessment to choice of objective functions, based on a multi-objective perspective. The second method is a new process oriented approach, which gave special consideration to the human interpretation of parameter and response surface interaction. This approach required the optimisation to be performed in a multiple objective domain. Preliminary results although exploratory, seems to indicate that the study objectives can be met but more work on comparative studies will be carried out from January 1999 to May 1999.

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APPENDIX A:

Explanatory Note on Window Interface for ACGA-NAM Calibrator

I Main Input Dialog

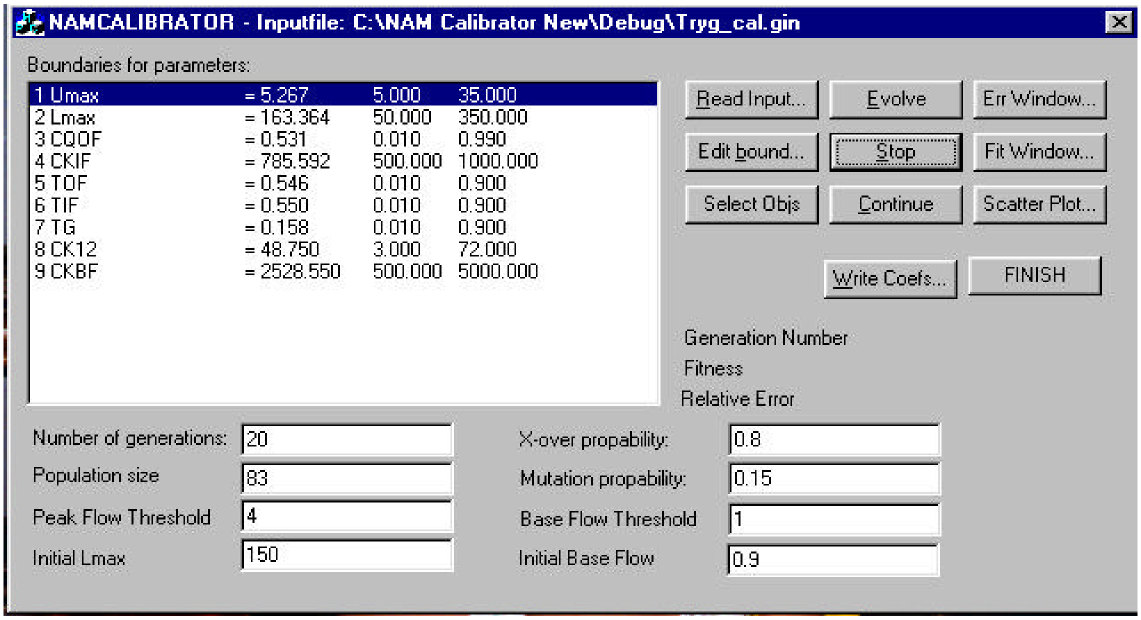

Figure A.1: Main Input Dialog of NAM Calibrator

Function Keys appearing On Main Input Dialog	Description of Function
`Read Input….`	This is an essential step to run the model. Figure A.2 will appear prompting user to enter the desired input filename with extension "gin". This file should contain the number of observed discharges and the values of each discharge. At the moment, another file with default filename of "nam.cal" is required. This file should contain the catchment size, the observed discharge, precipitation, evaporation and temperature measurements at each timestep.
`Edit bound…`	Prompts the user to state the new upper and lower bounds of the highlighted parameters in the "Boundaries for Parameters" box.
`Select Objs….`	Allows the user to specify any combination of these five objectives : 1. Peak magnitude; 2. Peak volume; 3. Base flow volume; 4. Overall volume or water balance; 5. Overall hydrograph shape.

	Figure A.3 will appear prompting user to select (mark a cross by clicking the mouse) the appropriate objective(s). Select of the objective functions to be associated with each objective can be done another dialog (Figure A.4).
Evolve	Initiates the calibration process.
Stop	Temporary halt to the calibration process. The initial calibration parameter values can be changed at this stage.
Continue	Continues the halted calibration process.
Err Window	Display the error function window as shown in Figure A.5.
Fit Window	Display the observed (in blue) and simulated (in red) hydrographs as shown in Figure A.6.
Scatter Plot…	Display the scatter plot of each observed discharge (x-axis) and simulated discharge (y-axis) as show in Figure A.7.
Write Coeffs…	Enables the user to save the best parameter combination so far to a file (Figure A.8).
FINISH	Terminated the calibration process and close all windows.

Initial parameter values for NAM calibrator	Explanation
Number of generations	Specify the number of generation as the termination criteria. The size of one generation is equal to the population size.
Population size	Specify the maximum number of NAM evaluations per generation.
Peak Flow Threshold	Specify the peak flow threshold.
Initial Lmax	Specify the initial value of the water content in the lower storage zone (catchment specific).
X-over probability	Specify the crossover rate of ACGA. A simple one point crossover is used.
Mutation probability	Specify the mutation rate of ACGA. The rate is given as number of bits.
Base Flow Threshold	Specify the base flow threshold.

`Initial Base Flow`	Specify the initial value of the base flow runoff coefficient (catchment specific).

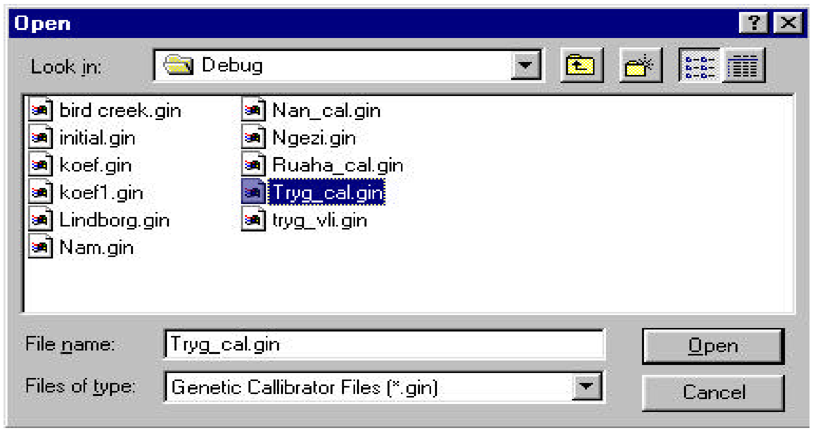

Figure A.2: Selection of input filename.

II Selection of Objectives and Measurements of goodness-of-fit

Selection of objectives is performed through the "Select Objs…" function key (Figure A.1). Figure A.3 will appear when the function key is selected. The user can select any combination of the five objectives listed by marking the box associated with the objective. The user can also specify the desired goodness-of-fit functions corresponding to the selected objective (Figure A.4). The definitions of the desired functions are as follows:

- ***Root Mean Square Error (RMSE):***

$$RMSE = \left\{ \frac{1}{N} \sum_{i=1}^{N} \left[Q_{obs,i} - Q_{sim,i} \right]^2 \right\}^{1/2} \qquad \text{(A.1)}$$

- ***Nash-Sutcliffe coefficient (R^2):***

$$R^2 = 1 - \frac{\sum_{i=1}^{N} \left[Q_{obs,i} - Q_{sim,i} \right]^2}{\sum_{i=1}^{N} \left[Q_{obs,i} - \overline{Q} \right]^2} \qquad \text{(A.2)}$$

- ***Coefficient of variance:***

$$P = \frac{1}{\overline{Q}} \left(\frac{\sum_{i=1}^{N} \left[Q_{obs,i} - Q_{sim,i} \right]^2}{N} \right)^{1/2} \qquad \text{(A.3)}$$

- ***Reduced error estimate:***

$$REE = \left[\frac{\sum_{i=1}^{N} \left[Q_{obs,i} - Q_{sim,i} \right]^2}{\sum_{i=1}^{N} \left[Q_{obs,i} - \overline{Q} \right]^2} \right]^{1/2} \qquad \text{(A.4)}$$

- ***Proportional error of estimate:***

$$PEE = \left\{ \sum_{i=1}^{N} \left(\frac{Q_{obs,i} - Q_{sim,i}}{Q_{obs,i}} \right)^2 \right\}^{1/2} \qquad \text{(A.5)}$$

- ***Second Moment:***

$$M^2 = \frac{\sum_{i=1}^{N} \left(Q_{obs,i} \right)^2 - \sum_{i=1}^{N} \left(Q_{sim,i} \right)^2}{\sum_{i=1}^{N} \left(Q_{obs,i} \right)^2} \qquad \text{(A.6)}$$

Each of the above equations shall be modified appropriately with the correct notation for different objective calculations i.e. for peak flow, base flow, or overall shape. For example Eq. (1) shall take the form:

(i) $$Peak_{RMSE} = \frac{1}{P} \sum_{j=1}^{P} \left\{ \frac{1}{M} \sum_{i=1}^{M} \left[Q_{obs,i} - Q_{sim,i} \right]^2 \right\}_j^{1/2} \qquad For\ Q_{,obs,i} \geq QT$$

(A.7)

where Q_{obs} = observed flow (m^3/s);

Q_{sim} = simulated flow (m^3/s);

M = number of timestep in a particular peak event;

P = number of events with flow $Q_{,obs,i} \geq QT$; and

QT = threshold value of peak flow (m^3/s) .

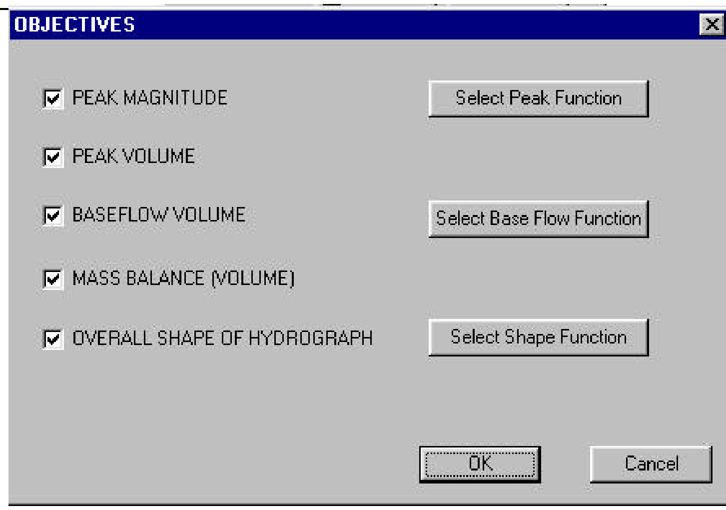

Figure A.3: Selection of Objectives.

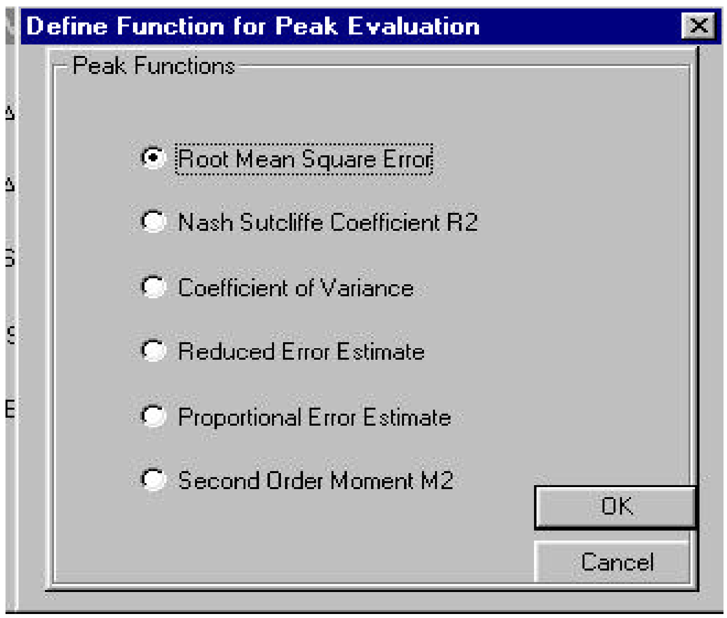

Figure A.4: Selection of Goodness-of-Fit Functions

III Saving and Visualisation of Results

The results can be view both online and offline. The online facilities includes:

1. Error plot of the performance of the ACGA (Figure A.5);
2. Plot of observed (in blue) vs. simulated (in red) hydrograph for the best parameter combination obtained so far (Figure A.6);
3. Scatter plot showing the observed (x-axis) vs. the simulated (y-axis) runoff of each point on the hydrograph (Figure A.7);
4. Values of the best calibration parameter set obtained so far are shown in the “Boundaries for parameters” window (Figure A.1).

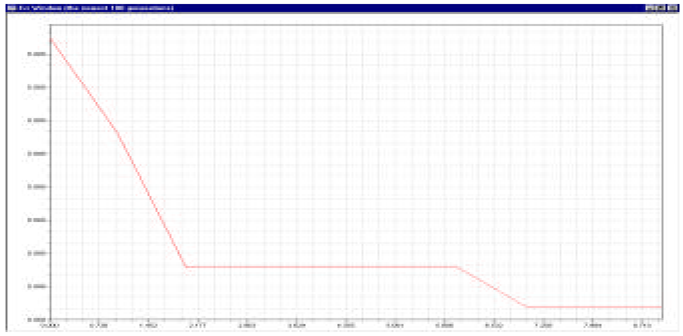

Figure A.5: Plot of Prediction Error vs. Number of Generations

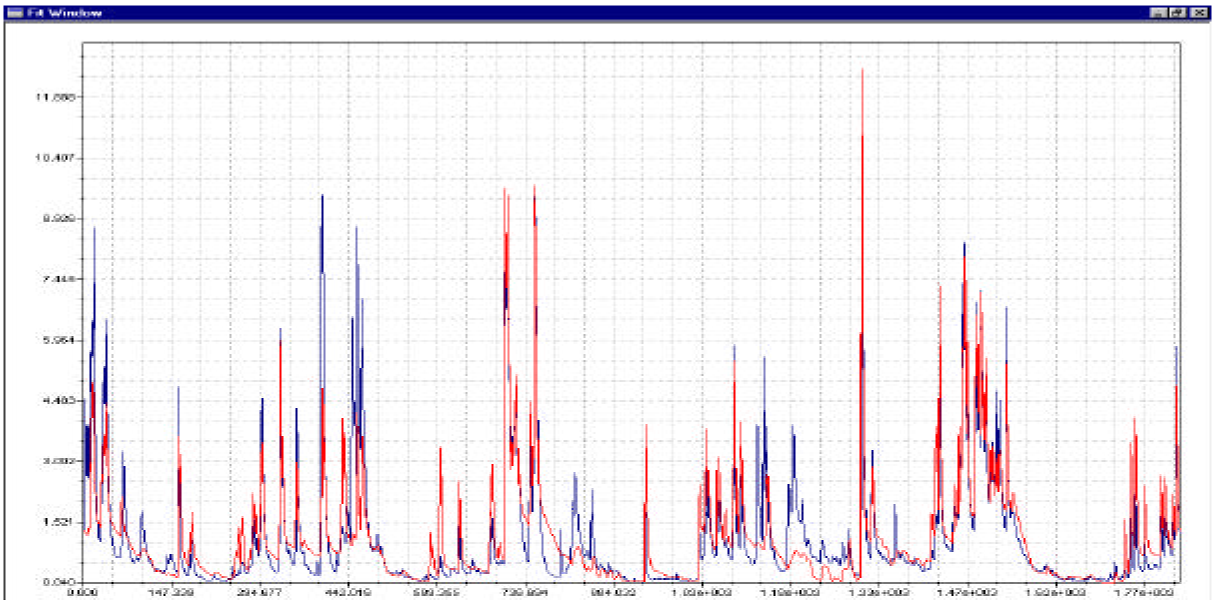

Figure A.6: Simulated vs Observed Hydrograph

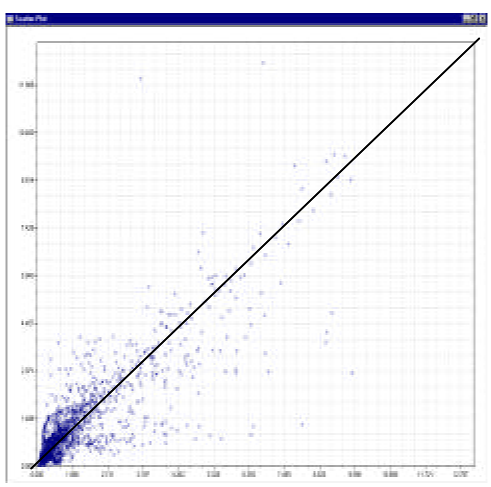

Figure A.7: Scatter Plot of Observed vs Simulated Flows

The best calibration parameter set also be saved using the "Write Coeffs.." function key (Figure A.8). All the calibration parameters are also saved in the text file "**vector.out**" and all the performance of each objective selected are saved in the text file "**results.out**".

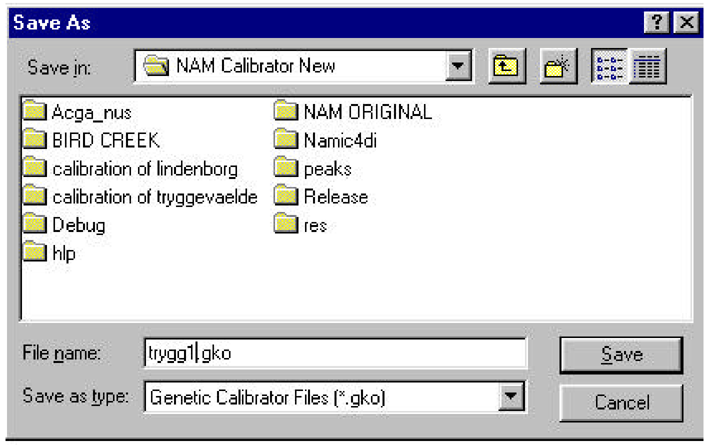

Figure A.8: Saving the best calibration parameter set

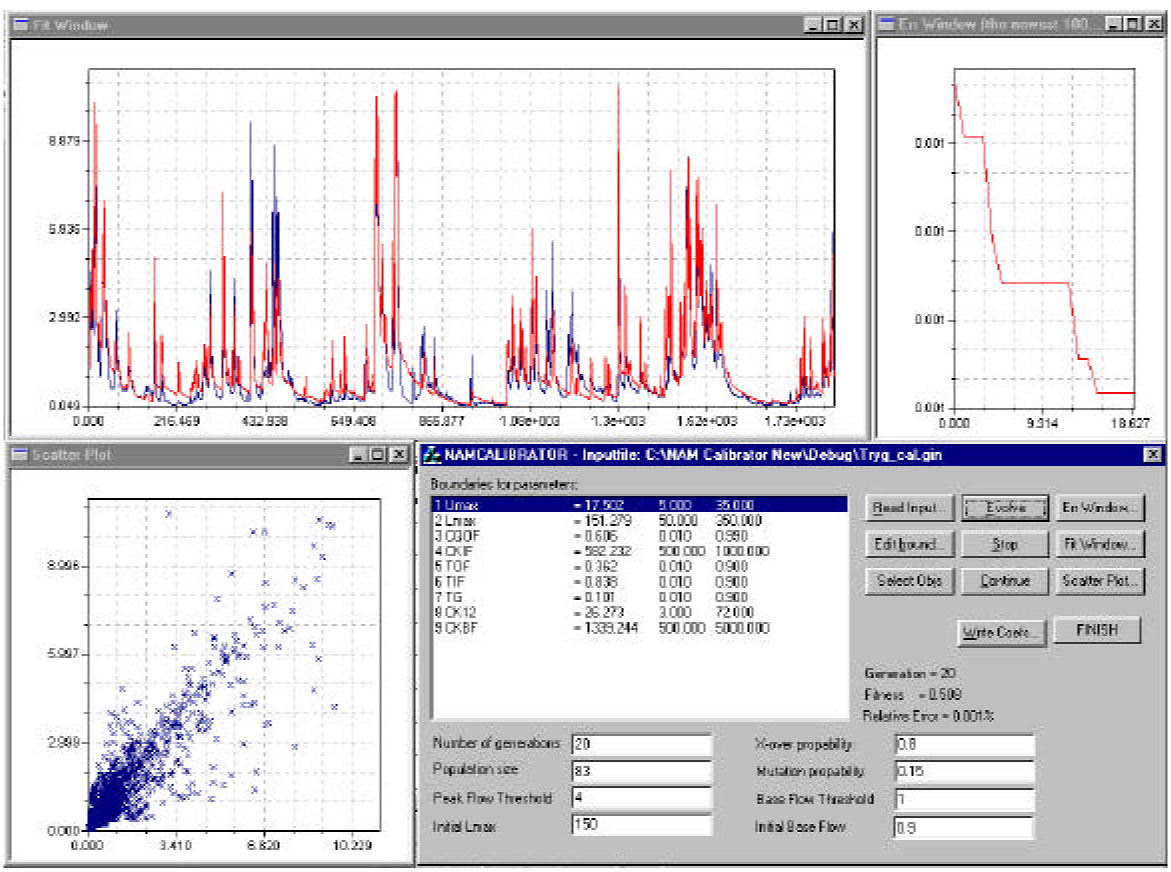

Figure A.9: Visualisation of Results

APPENDIX B:

ACCELERATED CONVERGENCE GENETIC ALGORITHM

It is still quite common to consider one catchment response at a time in calibrating multi-objective catchment problems. This approach frequently yields totally different optimal sets of calibration parameter values for different objectives. Thus, designers have to resort to compromise in the accuracy levels of the various objectives considered. Generating a trade-off curve for the performance levels of the considered objectives is therefore highly desirable. We present here a modified genetic algorithm known as accelerated convergence genetic algorithm (ACGA). The modified GA mainly differs from the traditional simple GA (Goldberg, 1989) in the following two mechanisms:

1. Fractional Factorial and Central Composite Designs ,FFD-CCD, (Liong et al., 1995) a response surface method, is used (instead of random data generator) to generate the initial sets of parameter combinations; and
2. Only relatively fit populations are selectively chosen to generate the populations of the subsequent generations.

The primary function of ACGA is to accelerate the convergence rate of GA and generate a more complete trade-off curve. The proposed GA, Accelerated Convergence GA (ACGA) mainly contains the following modifications:

1. instead of generating the chromosomes of the first generation through a random data generator, a more systematic FFD-CCD method is employed; and
2. a new chromosome selection method is suggested; the selection method considers only the fitter chromosomes for mating and ensures that no inbreeding occurs.

It should be noted that in ACGA, the objective function of interest is the distance function expressed as:

$$\boldsymbol{D} = \left[(\boldsymbol{Obj_1})^2 + (\boldsymbol{Obj_2})^2 + \ldots + (\boldsymbol{Obj_n})^2\right]^{1/2} \tag{B.1}$$

where Obj_n = prediction error of objective n.

The FFD-CCD ensures that data from the upper and lower bounds, and within the bounds are present in the initial population. For a problem with 9 parameters, for instance, FFD-CCD requires a total of 83 sets of parameter combinations. To further enhance the acceleration of the convergence rate, the optimal point resulting from the FFD-CCD optimisation process is included in the pool of chromosomes of the initial population. The inclusion of this optimal point allows ACGA to consider one of the very fit chromosomes from the beginning of the process as well.

Unlike the selection engine of traditional GA, ACGA selects only more fit chromosomes for mating. The selection procedure is as follows:

a) Compute the centroid of the prediction errors in the objective function space.

b) Compute the value of the distance function of the centroid, D_c:

$$D_c = \left[\left\{ \frac{\sum_{i=1}^{n} |Obj_1|}{m} \right\}^2 + \left\{ \frac{\sum_{i=1}^{n} |Obj_n|}{m} \right\}^2 \right]^{1/2} \tag{B.2}$$

where m is the population size.

c) Construct a 45°-line passing through the centroid. Data within the triangle OAB, Figure A.1, are the fitter chromosomes than those outside the triangle.

d) Construct another 45° line passing through a point on the OC line, of a distance $1.05D_c$. The chromosomes lie within the triangle ODE are the ones selected into the temporary mating pool. The reason for the inclusion of more points (lying in the region ADEB), in addition to those lying in the triangle OAB, is to minimise inbreeding and yet to avoid the inclusion of too many not-so-fit chromosomes (lying outside of the triangle ODE).

e) The number of chromosomes lying in the ODE triangle should be at least 80% of the total population size. This is required to ascertain that there is no inbreeding problem. Should the target of 80% be reached, the usual GA crossover and mutation operations continue. If the number of chromosomes is, however, less than 80%, additional chromosomes will be selected randomly from those lying outside of the triangle ODE to make up the 80% target size criterion.

f) Assign fitnesses to the selected chromosomes in the temporary mating pool.

After performing the chromosome selection, the conventional crossover and mutation operations are carried out. A simple one-point crossover is then performed on pairs of randomly selected chromosomes in the mating pool. The mutation operation is also carried out with the mutation rate fixed at 0.1%. The chromosome selection and reproduction operations are carried out until a pre-determined stopping criterion is met.

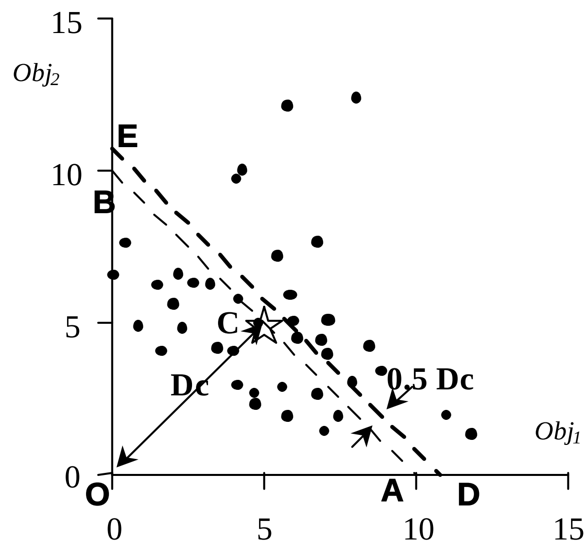

Figure B.1: Construction of Proposed Region, ODE, for Chromosome Selection

Reference:

1. Liong, S. Y., ShreeRam, J. and Ibrahim, Y., (1995). Catchment calibration using fractional-factorial and central-composite-designs-based response surface, *Journal of Hydraulic Engineering, ASCE, Vol. 121, No. 6,* pp 507-510.

2. Goldberg, D. E., (1989). *Genetic Algorithms in Search, Optimisation and Machine Learning,* Addison-Wesley, Reading, Mass.

Appendix C:
Multi-objective Optimisation and Its relevance to Model Calibration

A Short Technical Note *by* Soon Thiam Khu

1. Introduction

The quest for solutions to engineering problems involving multiple measurements of performance to be optimised simultaneously has been a long time dream. This dream is fast becoming a reality due to various factors, among them are (1) the exponential increase in computing power; (2) the drop in the cost of computers; and (3) the emergence of new solvers or algorithms.

Many real engineering problems involve the determination of solution sets, which satisfy one or more measurement of performance (objectives). This is a process commonly known as multi-objective optimisation in the fields of operational research, computer science and engineering. The process of parameter value estimation or calibration can be viewed as an optimisation process.

In optimisation, we seek to find the set of solution, which gives an optimal value to the objective function. This is similar to calibration where we seek to find the set of parameters that represent the catchment characteristics and in doing so, should give an optimal value between the discrepancy of the observed and measured quantity. This process could be extended to cover multi-objective calibration which is essentially the same as multi-objective optimisation.

The most common method of handling multiple objectives or multiple criterion, with or without employing evolutionary algorithms as search methods, is to aggregate the multiple objectives and evaluate the performance based on a single fitness function. Aggregation methods can be further divided into three approaches: (1) order-aggregation (non-scalar); (2) choice-aggregation; and (3) scalar-aggregation. These three approaches will be discussed in Section 3.

Once we are able to express the multiple objectives in a quantitative manner (in the form of fitness function), the next stage is to perform a search or optimisation in the fitness function space. In solving multi-objective problems, we are interested in obtaining a set of Pareto optimal solution points rather than a single solution point. Thus, the logical approach is to use population-based optimisation techniques such as evolutionary algorithms. An excellent overview of many evolutionary algorithms in multi-objective optimisation is given by Fonseca and Fleming (1997). A brief review of the techniques that are mentioned in Fonseca and Fleming (1997) and other more recent methods are included on Section 4.

2. Pareto Optimality

In single objective optimisation, we seek to optimise a single fitness function which represents the objective of the problem. Optimality can be defined when a solution is able to give the best (highest or lowest) fitness value achieved so far is found. In multiple objective optimisation, the notion of optimality is not that obvious. A new definition of optimality is required, which will respect the integrity of each of the objectives considered. The concept of Pareto optimality, proposed by a French economist Vilfredo Pareto (Pareto, 1896), offers such a definition.

A formal definition of Pareto optimality can be defined as follows: consider without loss of generality, the minimisation of the N components f_k, $k = 1, 2, \ldots, N$, of a vector objective function f of a set of solution variables X where

$$f(X) = \{f_1(X), \quad .... \quad f_N(X)\}$$

Then, the solution set X^u is said to be Pareto optimal if and only if there is no X^v for which $f(X^v)$ dominates $f(X^u)$, i.e. there is no $f(X^v)$ such that

$$\forall i \in \{1,........,N\}, \quad f_i(X^v) \le f_i(X^u)$$

$$\wedge$$

$$\exists i \in \{1,........,N\}, \quad f_i(X^v) < f_i(X^u)$$

The set of all Pareto optimal or non-dominated objective function vectors f(X) forms points on the Pareto front in the multiple objective function space. The corresponding solution variables, X, are the set of Pareto optimal solutions.

The notion of Pareto optimality can best be illustrated with a simple example (Goldberg, 1989). Suppose a water resources engineer wanted to optimise (minimise) the size of the retention pond to be built and the size of the canal leading to the pond because of cost. Both of these criteria are important because they are related to direct and indirect costs and the time of completion of the project. Suppose further that the engineer has worked out five combinations of sizes of pond and canal which result in the following pond cost and canal cost:

A = ($2m, $7.5m) (pond cost, canal cost)
B = ($3.5m, $6m)
C = ($6.5m, $3m)
D = ($4.5m, $6.5m)
E = ($8m, $3.5m)

These data are plotted in Figure 3.4, from which it can be seen that cases A, B and C are possible solutions even though none of these three points is best along both dimensions. Among these three points, it is difficult to judge which is superior because none of these points is better than the others in both cost criteria. These points are called *non-dominated* or *non-inferior* points. Case D ($4.5m, $6.5m) is bettered by case B ($3.5m, $6m) in all criteria and case E ($8m, $3.5m) is bettered by case C ($6.5m, $3m). Points D and E are known as *dominated* points. The condition of Pareto optimality pertains to a given set of vectors or points in the multi-objective space. All non-dominated points or vectors form the Pareto optimal set and are used to construct the Pareto front (two-dimensional) or surface (multi-dimensional).

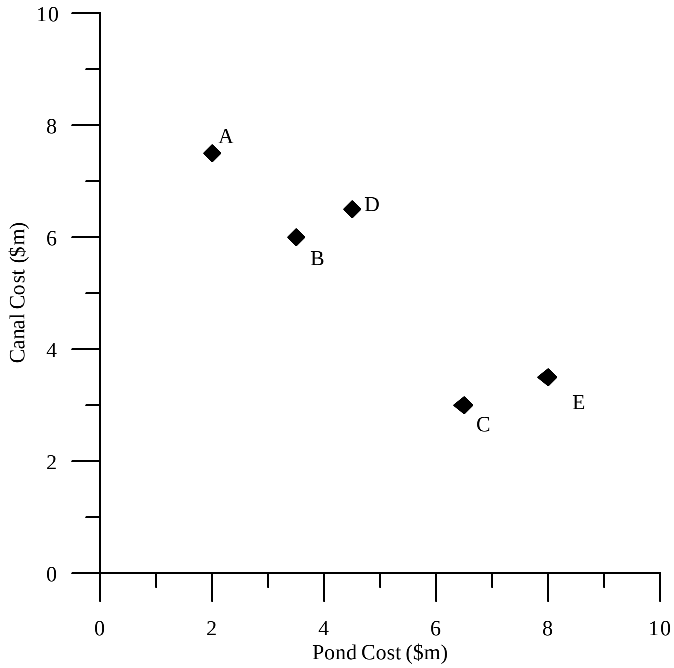

Figure: Illustration of Pareto Optimality (Adapted from Goldberg, 1989)

3. Model Calibration and Multi-objective Optimisation

The objectives of performing numerical simulations using rainfall- runoff models can be manifolds. Conventionally, rainfall- runoff modelling can be divided into continuous and event-based simulation depending on the simulation time scale.

Continuous simulation involves the determination of the quantity of water regular time intervals over a long duration, usually in the order of months or years. Thus, the primary objective of this type of simulation concerns the long-term behaviour of the catchment's hydrologic system. More specifically, we are concerned with continuous discharge over time, ground water levels, concentration of water quality measurements etc.

Event-based simulation is mostly used for stormwater and flood studies. The objectives of event-based simulation are the determination of peak discharges, total runoff volume, hydrograph shape or time-to-peak resulting from an isolated storm event or a combination of several of these objectives. These properties are useful in the design or analysis of stormwater systems.

Thus, there is a need to consider multiple objectives calibration for both continuous and event-based simulation although the objectives may be different.

4. Fitness Measurement

As mentioned in the introduction, there are three approaches commonly used when assigning fitness value to evaluate the worth of a given solution set. This fitness value is a single scalar measurement that reflects the performance of the solution set in the multi-objective environment. The three approached are:

1. Order-aggregate approach;
2. Choice-aggregate approach; and
3. Scalar-aggregate approach.

4.1 Order-aggregate approach

This approach treats the different objectives as separate entities, without combining them. For example, the lexicographic ordering approach (Ben-Tal, 1980) assumed that each solution set can be arranged according to their performance in each objective. As in a dictionary, lexicographic ordering assigns priority to the most important objective. The fitness value will be assigned based on the chosen objective. However, fitness value can also be assigned based on a randomly selected objective (voting scheme) (Fourman, 1985). This approach has a distinct disadvantage that suitable solution sets to the overall problem can seldom be found except for trivial cases.

More than often, optimal solution set for one objective gives poor performance on some or all of the rest of the objectives. Under such situations, we are forced to accept compromising solution set that "satisfy" all the objectives. This "compromising" solution set is usually sub-optimal in the solution space of each objective and also possibly in the overall objective space. However, the introduction of population-based optimisation techniques brought new ideas to this approach. Because population-based techniques start the search at different locations in the solution space, there is a high chance to find suitable solution sets for the overall problem.

Once such population-based technique is the vector evaluated genetic algorithm (VEGA) (Schaffer, 1984). VEGA starts by dividing the initial population into *N* different sub-populations where *N* is the number of objectives to be optimised. The fitness value of individuals in each sub-population is assigned based on a predefined objective for this sub-population. In this manner, no scalarisation of multiple objectives is required. Other examples using order-aggregate approach in population-based searches are by Fourman (1985) and Kursawe (1991), which will be discussed in Section 5.

4.2 Choice-aggregate approach

This approach requires the user to chose one objective as the dominating objective and regards the other objectives as a supporting role. One such example is to treat the other objectives as constraints (Davis and Streenstrup, 1987). In this way, the violation of any constraints can be defined by penalties to the overall fitness value. Thus the pressure of the search is moving towards the direction of optimising the chosen objective while satisfying the other objectives.

In a slightly different approach, the fitness value could be derived from the maximum value by comparing each of the objectives (Osyczka, 1984). This approach is known as the minimax or MinMax formulation and can be formulated as:

$$\text{Minimise } Z = \mathit{maximum}\ [f_i(X)]$$

In this formulation, it is important to normalise the different objective functions so that there will be no scaling problem.

The resultant solution set would probably be a sub-optimal solution optimised for the chosen objective function. Additional search can be done to consider each objective in turn while treating the others as constraints. After all the objectives has been considered, a compromise solution set is then derived. This approach can be coupled with population-based search algorithms to increase its efficiency.

4.3 Scalar-aggregate approach

This is perhaps the most commonly used aggregate method. It combined the various objectives into a single scalar fitness value, reflecting the multi-objective trade-off preference of the user. The simplest representation of the scalar fitness value is a linear function (or weighted sum) combining the various objectives. The optimal point obtained on the trade-off surface is dependent on the weights assigned to the objectives. Mathematically, the new objective function is given by:

$$Z = \sum_{i=1}^{N} w_i f_i(X) \qquad (i=1, \ldots\ldots, N)$$

where w_i = weight assigned to the i-th objective,

$$0 \le w \le 1 \text{ subjected to } \sum_{i=1}^{N} w_i = 1;$$

$f_i(X)$ = the i-th objective function; and

X = the parameter considered.

This method allows the user to reflect the relative priority of a list of objectives by assigning the appropriate weights. The method known as the Tschebcheff's method (Steuer, 1986) essentially utilises the same concept.

Alternatively, the distance function can be used for fitness representation. Mathematically, the objectives is given by:

$$D = \left[\sum_{i=1}^{N} \left| f_i(X) - T_i \right|^r \right]^{1/r}$$

where $f_i(X)$ = the i-th objective function;

T_i = the target or goal of i-th objective; and

r = shape constant, $0 < r < \infty$.

In the decision analysis community, the concept of multi-attribute utility analysis (MAUA) (Keeney and Raiffa, 1976) can be used to scalarise the multiple objectives. In MAUA, separate utility functions for each objective are determined by the user. The user can thus choose to incorporate uncertainty into the utility function. The individual utility functions are then combined by multiplication (rather than addition) to determine the fitness value.

Recently, the genetic algorithm community used the concept of Pareto optimality to determine the fitness value of the solution set. The concept of ranking in accordance to Pareto optimality was introduced (Goldberg, 1989; Fonseca and Fleming, 1993). Goldberg (1989) used the method of "onion peeling" when assigning the rank of any solution set in a population of solution sets. All the non-dominated points in the population were given the best ranking and were removed from the population temporarily. The remaining solution sets were ranked again with the new non-dominated points given the second best ranking. This process continued until all the solution sets were ranked. Fonseca and Fleming (1993) ranked the population in a slightly different manner, according to the "degree of domination". The ranking assignment was based on the following expression:

$R_i = 1 + p(i)$

Where R_i = rank of solution set i; and

$p(i)$ = number of points dominating point i.

5. Evolutionary Algorithms for Multi-objective Optimisation

The use of evolutionary algorithms (EAs) such as genetic algorithm (GA) (Holland, 1975), evolutionary programming (EP) (Fogel et al., 1966), evolutionary strategy (ES) (Schwefel, 1981) and genetic programming (GP) (Koza, 1992) for multi-objective optimisation is a natural one since EAs are multi-start and parallel search algorithms. EAs essentially start searching with a population of possible solution set and hence the name, population-based search.

Cohon and Marks (1975) reviewed a number of numerical techniques fot heir suitability in solving multi-objective problems in water resources planning. They found that many of those techniques reviewed were not applicable to multi-objective water resources problems. They suggested that either the weighted sum method, constraint method or surrogate worth trade-off method should be used instead. With hindsight, we can say that the methods reviewed by Cohon and Marks (1975) are methods to solve the representing objective function problem and not intended to produce multiple Pareto optimal solutions to the problem.

We can classify population-based search into 2 main categories: (I) non-Pareto approach; and (ii) Pareto approach. In non-Pareto approach, the optimisation technique ignores the information regarding the Pareto optimality of each solution set but choose to optimise according to the information given by the fitness function alone. In Pareto approach, the information about the Pareto optimality are often embedded into the fitness function.

5.1 Non-Pareto Multi-objective approach

Non-Pareto multi-objective optimisation techniques essentially combines the search strategies of genetic algorithm or evolutionary strategy with some form of aggregated fitness function approach (Section 4.1 and 4.2) except that of Pareto ranking.

5.1.1 <u>Coupled with order-aggregate approach</u>

As mentioned earlier, Schaffer (1984) combined the concept of order-aggregate approach with genetic algorithm and called it vector evaluated genetic algorithm (VEGA). The fitness value of each solution set in the sub-population was assigned according to the objective of that sub-population. Potentially good solution sets were subsequently pooled together regardless of their performance in other objective. This method of pooling resources created a population of solution sets with expertise dealing with different objectives. Recombination and mutation were then performed in the traditional manner according to probability. The newly formed generation would then be sub-divided into different sub-population.

Fourman (1985) implemented a scheme that combined binary tournament selection with order-aggregate assignment. In his scheme, a pair of solution sets were chosen (hence the name binary tournament) and were evaluated based on a randomly chosen objective. If there is a tie, another objective would be selected as the evaluation criterion. Recombination and mutation were subsequent carried out.

Kursawe (1991) implemented a scheme similar to Fourman's but coupled with evolutionary strategy (ES) rather than GA. However, instead of choosing the objectives randomly, each objective is assigned a probability vector which determined the chances of this objective being chosen for evaluation.

These researchers had shown that it is possible to combine population-based search algorithms with order-aggregate approach of assigning fitness to multiple objectives. However, the main criticism of these methods were that the search tends to locate the extrema (corners) of the Pareto front or trade-off surface.

5.1.2 <u>Coupled with choice aggregate approach</u>

Research into this form of search has been very limited. Most of the works employed methods similar to that of Davis and Streenstrup (1987), where the search is concentrated on one objective and the other objectives are acting as constraints. The constraints were handled by GA in the form of penalty functions. In their work, the search is performed by GA but without exploring the full potential of GA's multi-search capability. Ritzel et al. (1994) modified David and Streenstrup (1987) approach to include multiple searches for different constraints. They run GA a number of times, and each time, they varied the weights in the penalty function in an attempt to obtain more points on the Pareto front.

A scheme similar to that of VEGA would be an appropriate way to vary the weights of the constraints.

5.1.3 <u>Coupled with scalar-aggregate approach (excluding Pareto ranking)</u>

The method of combining population-based search with scalar-aggregate approach is intuitively simple. However, it was not until the early 1990's that successful attempts to coupled them were reported. Swswerda and Palmucci (1991) successfully optimised the weighted sum of several objectives for scheduling applications using GA. Jakob et al. (1992) were successful in applying the same strategy for the purpose of task planning.

Hajela and Lin (1992) proposed to include the weights in the objective function in the search and letting them evolve with the parameter sets Thus, the solution set comprised of the parameter values and the weights of each objective. Murata and Ishibuchi (1995) allowed the weights in the fitness criterion to be adjusted randomly instead of evolving. Other researchers have adopted a passive approach by varying the weights in an orderly manner and in equal increments (Cieniawski, 1993; Tsoi et al., 1995; Chang et al., 1995).

GA was coupled with the distance function in fields of physics and engineering (Wienke et al., 1992; Wilson and Macleod, 1993; Liong et al., 1998). GA was also coupled with the MAUA approach (Horn and Nafpliotis, 1993) but no real world application was given.

5.2 Pareto-based Multi-objective Search

When Goldberg (1989) discussed the concept of Pareto ranking, it was set in the context of implementing it in a population-based search algorithm. Hillard et al. (1989) were among the first researchers to coupled GA search with Pareto ranking. Their implementation was a simple non-dominated selection but without niching (Goldberg, 1989). Other researchers has since coupled other forms of GA selection schemes with Pareto ranking (Liepins et al., 1990; Ritzel et al., 1994). In order to obtain an even distribution of solution sets spread along the Pareto front, a method known as niching (through sharing or crowding) was often included in the selection scheme (Eheart et al., 1993; Horn et al., 1994; Srinivas and Deb, 1995; Tamaki et al., 1995; Tanaka et al., 1996). More recently, Yapo et al. (1998) coupled the shuffled complex evolution algorithm (SCE-UA) (Duan et al., 1992) with Pareto ranking.

The multi-objective GA (MOGA) of Fonseca and Fleming (1993) coupled GA with the ranking approach based on "degree of domination". Shaw and Fleming (1996) applied MOGA to a scheduling problem with 3 objective functions. The selections were included both niching and without niching. There are many more examples that utilise Pareto optimality as the basis of assigning fitness and coupled them with EA. However, since these methods involve a modification of various GA mechanisms, they are not included in this discussion. Readers are referred to Horn (1997) for further reading on this subject matter.

6. Future Perspective

The trend in multi-objective optimisation is moving towards a hybrid approach: combining different search strategies with different fitness assignment approach; and/ or applying different optimisation techniques at different stages of the search.

In the area of automatic model calibration using evolutionary techniques, the trend moving towards a more complete approach with the merger of expert system and evolutionary algorithms. There is also a need to incorporate measurements of prediction accuracy, such as level of confidence, in calibration. Population-based optimisation technique such as MOCOM-UA (Yapo et al., 1998) and ACGA (Liong et al., 1998) have shown to produce better Pareto optimal solutions compared to VEGA (Schaffer, 1984). The inclusion of expert knowledge and decision making-like processes in these techniques should be able to enhance the local search capabilities of these methods. Consequently, the user acceptance level of these methods would be improved.

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