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Selection and Calibration of Numerical Modeling in Flow and Water Quality

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Abstract

Numerical modeling is frequently used in coastal engineering research and application. One possible issue associated with using this method however, is that initial outcomes might differ from expectation. Modeling manipulation addresses this issue by changing the initial parameters which in turn affects the final output results.

The advancement of modeling techniques in recent years has seen a gradual but steady accruement of knowledge regarding the relationship between input parameters and possible outputs, which has resulted in improved accuracy and efficiency methods. The advancements within this field have predominantly occurred on an individual basis and as such lack standardisation. An expert numerical modeler may use this knowledge subconsciously, yet may not know how to convey it to the model users. This paper has been written to introduce a systematic intelligent coding schema designed to organise current coastal engineering modeling manipulation knowledge into a standardised format. This system is relevant to the development of appropriate strategies for improved accuracy and efficiency as well as model modification to simulate specific real phenomena in prototype application cases.

Introduction

Numerical modeling is frequently used in coastal engineering research and application. Typically, a comprehensive coastal engineering numerical model software package contains several modules: transport-dispersion; hydrodynamics; water quality; sediment; wind and wave effects. The modern modeling systems tend to include more modules dealing with different coastal processes, as well as encapsulate more contemporary knowledge in order to provide assistance to engineers who may not be expert numerical modelers.

As described by Abbott [2], numerical modeling is a process which transforms the knowledge of natural water phenomena into digital forms, allows for a complete computer simulation and then translates the digital experimental results into new knowledge. Through this process, our understanding can be heightened. To clarify, numerical modeling can be considered as the interaction between knowledge and information in the form of:

Knowledge → Information → Knowledge

In this context, *knowledge* exists in a format comprehensible to people whilst *information* is in a primitive code solely for use in computer processing.

For numerical modeling in coastal zones, the first step from *knowledge* to *information* is the selection of a suitable model together with model parameters, whilst the second step from information to knowledge includes the post-processing of result data. The term ‘modeling manipulation’ is a process of feed back and modification comprising the above two steps. It is possible that modeling manipulation exists as a lengthy process and whether or not it finally results in satisfactory simulation is very much dependent on the experience of the modeler. In this context, satisfactory simulation means that the simulation results are within acceptable error tolerances regarding the verification of real phenomena or measurement data. Ragas et al. [15] have compared eleven UK and USA water quality models used in establishing discharge criteria and found that model selection is a complicated process of matching model features with particular situations. If the selection of the numerical model and the values of the model parameters have been obtained with a high degree of accuracy, the process from *knowledge* to *information* has been completed. It is possible, however, especially for non-expert users of the numerical model, that the selection of modeling parameters is accompanied with a moderate degree of accuracy. In this context, the degree of accuracy is measured inversely in terms of the error between the simulation results and the verifying data - a higher degree of accuracy represents smaller error and vice versa. The user’s selection of model parameters may be modified many times before they can attain satisfactory simulation results.

In modeling manipulation, knowledge is integrated together. Knowledge in a modeling process context, refers to: real physical observations; mathematical description of the water movement or water quality; the discretization of governing equations for the physical and chemical processes; the numerical algorithm; and, the analysis of various numerical modeling outputs. For experts in numerical modeling, the knowledge mentioned above may be used subconsciously, as they would know most of the domain knowledge on selection and calibration of numerical modeling in flow and water quality. Experts within this field however, may not know how to convey their knowledge to the model users and/or how to apply recent artificial intelligence (AI) technology to bridge the existing gap between modelers and practitioners in this field.

According to Abbott [1], numerical modeling system developments regarding a user-friendly interface and post-processing were undertaken in the fourth generation system with AI technology to be integrated in the fifth generation to provide assistance for non-experienced users. Successful applications of expert system technology have been reported on the selection of numerical model in coastal engineering [4, 10, 11]. If the knowledge relating to modeling manipulation is encapsulated in the form of a knowledge base and then integrated into a schema, the fifth generation system will be more powerful. The principal objective of this study is to develop a systematic intelligent coding schema to represent and organise current coastal engineering modeling manipulation knowledge into a standardised format with a modern shell.

Procedure of modeling manipulation

The manipulation process begins from the selection of a random model and ends with the satisfactory simulation of a specific real phenomenon. The intermediate process comprises the determination of the direction to improve the modeling simulation by changing some of the model parameters. The usual detailed process can be delineated as:

randomly select a numerical model → run it → estimate the accuracy of the model results

→ find a direction to modify some parameters → revise the parameters
→ raise the pertaining accuracy.

After several iterative cycles when the model results meet the threshold of error tolerance specified by the user, the process is considered completed.

Experts themselves usually keep some fundamental modeling selections unchanged during the manipulation. For example, after it was reported in the literature [13] that ADI modeling could be applied in two-dimensional computational space for many two dimensional tidal dynamics modeling, an ADI model was used. The discretization method and algorithm scheme of the model were kept unchanged. Previously, when researchers used two-dimensional modeling in coastal engineering, only the bottom friction coefficient was varied [6]. Presently, although researchers frequently use three dimensional modeling, they normally keep some fundamental parameters of popular models unchanged to ensure that the lowest number of parameters are changed. For example, engineers often employ the widely accepted POM model [14] to coastal dynamics simulation. The co-ordinate system, grid setting, numerical scheme in both time and space are kept the same with the original POM model, whilst only the turbulence coefficients in the vertical and horizontal directions are changed to seek better simulation results [5]. Another example is in dispersion-transport modeling. After the ELM model [12] was reported to increase accuracy, the numerical schemes were kept the same, with only the dispersion coefficient being changed. One more example is in water quality modeling. Researchers endeavouring to simulate eutrophication (red tide) took sun light variation into consideration as the current literature suggested that algal behaviour was closely related to respiration and water temperature [3].

These examples reflect that human intelligence uses existing knowledge to reduce the number of choices in modeling manipulation. Accordingly, it tends to change one or two parameters in the process rather than changing many parameters simultaneously. It is possible that if the model users modify many parameters at the same time, they may easily get lost regarding the direction of the modification. Many traditional modeling systems have integrated a vast quantity of field data to describe real phenomena for verifying numerical simulation results. In some fourth generation modeling systems, automatic checking and warning prompts are designed to facilitate verification between modeling results and real observation data, thus in turn to improve modeling manipulation.

Balance between accuracy and efficiency

A numerical model is a tool to simulate a physical problem by solving differential equations. It is often constructed on the basis of some ideal physical and chemical equations. However, model parameters such as the bottom frictional coefficient, turbulence and kinetic coefficients, to name a few, can be adjusted within a certain range in order to mimic the real environmental phenomena. Modeling accuracy is then determined by comparing simulation results with field data. In modeling manipulation of coastal engineering, the final aim is to obtain a satisfactory simulation, however, since the number of computers used, in conjunction with the memory and computer speed is often limited, we have to strike a balance between modeling accuracy and efficiency. In this situation, efficiency is measured in terms of the time taken by a numerical modeler to complete the modeling process with a desired degree of accuracy. For some engineering problems, accuracy is very important. For some research problems, to understand the general process of the phenomenon and mechanism, modeling efficiency becomes more important. In other words, the term ‘satisfactory’ depends largely on the user’s requirement in the relationship between modeling accuracy and efficiency, which form the two directions in the manipulation process. There exist methods to change the parameters to improve modeling accuracy as shown in Figure 1 and also methods to enhance modeling efficiency, as shown in Figure 2.

Expert system shell

The knowledge-based system development environment for this prototype intelligent system is VISUAL RULE STUDIO (VRS), which acts as an ActiveX Designer under the Microsoft Visual Basic programming environment [16]. VRS is an application development environment that combines expert system technologies with object-oriented programming, relational database, graphics capabilities and debugging tools. It incorporates a variety of knowledge representation schemes, different inference mechanisms and capabilities to interface with external programs in the windows environment. VRS provides an interactive windows-based user interface that runs under the conventions of Microsoft Windows. This common graphical user interface enables the user to: open multiple windows; size and arrange; and, have multiple software applications opened simultaneously. Under this system, any types of display windows can be represented as objects, each with its own private data and information. Various types of displays - checkbox group, list box, command button, textbox, option button and picture box - can be defined as different classes inheriting common characteristics and possessing their own special properties.

Components integrated into the system

VRS allows the expertise knowledge rules to be written in Production Rule Language, which is integrated easily into the intelligent system. In the fourth generation modeling system, some helpful tools were integrated with the main processor, however, the fifth generation modeling system further incorporates four independent components with different functions: knowledge base; main processor; user interface; and, toolbox. Figure 3 shows the structure of the system with relationships amongst various components.

1. Knowledge base

The encapsulation of a knowledge base relating to modeling manipulation is one of the most important tasks in this study. A literature review has been undertaken to research knowledge on modeling application and selection [1, 3, 5, 6, 7, 8, 9, 12, 13, 14, 15]. Moreover, in order to establish this knowledge base, interviews with numerical modelers have been undertaken. In the interviews the major factors discussed included: the order of importance of the parameters; the sequence of decision making on parameter selections; personal experience in selecting parameters; and, personal opinion on difficulties of model selections. Experienced modelers can duely combine both written and practical knowledge to obtain a more acceptable result in model simulation, with a relatively reasonable balance of accuracy and efficiency. Observation data of both a numerical and descriptive nature is useful to understand the real situation. This data includes information about current, tidal elevation, water depth, temperature, salinity, dissolved oxygen, phosphorus, nitrogen, sediment, and their subsequent variations with time and locations.

The relationship between human intelligence and modeling manipulation is extracted and described in the form of rules. Rules describe the operational logic and cause-and-effect relationships, which are needed to make decisions and to implement certain events or actions during execution. In general, production rules (IF-THEN-ELSE) are considered an intuitive means for representation of heuristic knowledge. If the antecedent of a rule in the IF statement is determined to be true, the inference engine may implement the rule, inferring the THEN statements to be true, which is then added to the working memory. The ELSE statement works similar to the THEN statement, except on this occasion it is invoked only if the antecedent part of the rule is FALSE. Such rules are activated whenever certain conditions become true in a cyclic manner. During each cycle, the conditions of each rule are matched against the current state of domain contexts. When rules and conditions match one another, actions are implemented. These actions alter the current state of contexts, invoking in turn new rule matching. The knowledge base incorporates the whole set of inference rules relating to manipulation direction and user's requirements. The following example gives a typical inference production rule:

> RULE to manipulate scheme: 5 of 12
> IF a first order scheme is currently used AND
>   Computed error > preset threshold of error tolerance AND
>   demand on efficiency is low
> THEN a higher order scheme is chosen.

After the expertise is encapsulated into the programming code in the form of a database or rule base, non-experienced users benefit from the assistance provided by the system. Good combinations of parameters are suggested in accordance with heuristic rules in the knowledge base. Templates are prepared as a kind of model frame. The 'table' consists of many 'input fields', which represent the modeling parameters. Some input fields in the table are fixed whilst the others can be modified to suit the specific environment. Thus the manipulation process seeks suitable input fields so that modeling results coincide well with real phenomena. The knowledge base is also comprised of several sub-bases which need to be discussed: relation base; selection base; question base; rule base; and, model base.

The relation base describes the structure of a relation tree, which in turn describes how many factors one parameter is related to. The tree nodes are generally in a single layer but may consist of two layers if the factor is related to others. The selection base describes the structure of a selection tree, which in turn describes how many forms or values of selections can be suggested for a parameter. Each node of the selection tree represents a parameter and its subsequent branches represent its possible selections. The question base stores questions by asking users for their specifications in regard to the factors related to the parameter. The rule base describes inference rules from the user's specification to the parameter selection. The model base stores certain popular models in coastal simulation and examples of case studies in the world.

In the knowledge base, all the parameters for a numerical model can be classified into six main types: scheme; method and dimensions; driving force and boundary condition; turbulence, grid; and, initial conditions. The details of the classification system are shown in Table 1. This kind of classification system not only facilitates the formulation and search of a knowledge and rule base, but also reflects important branches in numerical modeling research. As the driving force for selection and calibration of numerical model comes from the needs of its user, the selection of modeling parameters is a function of four aspects: the purpose of the user; the physical conditions in the specific problem; the modeling experience of the user; and, the insight of the user about the possible model results.

Users can specify their preference to accuracy and/or efficiency, and a set of suggested parameters would be listed in the interface for modification. In the intelligent system, the parameters allowed for modification are represented in the form of a parameter tree. After the manipulation process is completed, the tree skeleton becomes a solid tree with fixed branches. The tree is managed and controlled by the rules in the knowledge base. It has a full skeleton during modeling selection. Some branches will be cut off after users have specified their preference of accuracy and/or efficiency. Figure 4 shows an example of the tree formation in the manipulation process.

After users have selected a model prototype and have specified their preference for model accuracy and/or efficiency, VRS inference engine can use the mixed strategy of the back and forward chaining inference mechanism to give the suggested direction of manipulation. An inference engine controls the selection of procedural methods and production rules from the knowledge base to derive a conclusion or design context. An event-driven inference processing mechanism has been adopted so that the ensuing action of the system will depend on the input made by the user.

2. Main processor

The central programme component, termed the main processor, which can be executed to produce numerical simulations of real phenomena, is a key component of a modeling system. In a traditional system, only this component exists. In this intelligent system, the main processor is designed in a form of ActiveX Control. It is an OCX programme, ready to operate with various properties including modeling parameters and various methods of action such as initialization, execution, stop, pause, recording, comparison and warning, to name a few. The selection of the modeling parameters then becomes crucial to setting the properties and methods of the main processor. The properties related to modeling are classified into six classes consistent with the knowledge base: scheme; method and dimensions; driving force and boundary condition; turbulence; grid; and, initial conditions. The methods related to the result display consist of but are not limited to: saving the data file; comparing with the existing data information; monitoring the results under limitations; and, recording the images to show the animation display of modeling results.

Figure 5 shows a flow chart displaying the methods of selection and calibration of numerical modeling. The main processor is designed to run with a set of default values and is purposely designed as an independent module in the system. This main processor is encapsulated as a control with only the properties and methods exposed to changes in modeling manipulation. The major advantage of this arrangement is that part of the team can concentrate their efforts on the main processor design while the remaining members can work separately on the design of the knowledge base integration.

3. User interface

The user interface in this system represents the platform displaying modeling results, in conjunction with interacting or exchanging information with the user. It is used to converse with the user, ask question, and record the answers in order to acquire the user's demand on accuracy and/or efficiency, as well as, the physical conditions of the simulating environment. It provides the required information for the system to infer from the rule base through backward and forward chaining inference mechanisms. Figure 6 shows an example of the input user interface.

4. Toolbox

The toolbox provides a comparison between simulation results and real observation data. The improvement in estimating modeling results depends on a performance indicator through pattern recognition technology. In this system, the normalised mean square error (NMSE) between the key model results and the associated observation data is employed as the performance indicator. It represents the sum of squared errors normalised by the number of patterns over all output data and the estimated variance of the data. An NMSE of zero indicates a perfect fit of the model to the recorded field data, while an NMSE of infinity suggests the worst fit possible. If the NMSE is subtracted by unity, the result would be a statistic similar to the coefficient of determination.

In addition, the toolbox includes other helpful tools for pre-processing, such as drawing a boundary with a mouse and drawing a time variation curve of a tidal boundary condition. Furthermore, the toolbox can be used to monitor the manipulation process by prompting warning message if simulation results exceed the pre-set limitation. This limitation can be based on a variety of controls, such as the maximum value control for alerting the user.

Case application in modeling of Hong Kong coastal areas

Numerical model can only be verified by simulating real phenomena for a particular application. The results can provide additional knowledge and in fact, one of the purposes of employing this model is to obtain new understanding on real water environment. Knowledge encapsulation into the knowledge base and integration into the modeling system may assist novice users to seek the appropriate direction of modeling manipulation. Without this, only an expert or model developer is able to manipulate the model to obtain satisfactory simulation results.

Modeling in the Hong Kong area has been used to test the performance of the intelligent system. The improvements in accuracy and efficiency have been employed in two cases of target manipulation. A numerical model on tidal and water quality computations in the Hong Kong coastal areas has been built. It covers several strategic study areas including Tolo Harbour [6, 7, 8], Pearl River Estuary [5], and Shing Mun River [9]. Tolo Harbour is a nearly land-locked sea inlet with a narrow outlet. The water quality of Tolo Harbour in recent years has declined dramatically. The water body can be regarded as highly eutrophic which exhibits high algal growth. The Pearl River is the largest river system in South China. With the economic boom of the Pearl River Delta Region, the resources of the estuary have been exploited. Additionally, water quality is deteriorating and red tides have occurred several times in the past two years.

Shing Mun River is the major river channel flowing into Tolo Harbour. The detailed description and results of mathematical modeling for these study areas can be obtained from the above literature.

Through the use of this system, a number of experiments were then performed on these study areas to investigate the effects of applying different methods to manipulate either accuracy and/or efficiency. The improvement in accuracy was measured by comparing the NMSE for the two cases with and without the specified method applied, expressed in a percentage format. The improvement in efficiency was measured by comparing the required computer processing unit time on a pentium for the two cases, also expressed in a percentage format. Table 2 shows a summary of comparisons in selected experiments regarding accuracy and/or efficiency improvement resulting from this work.

With all other parameters kept constant, the use of a fully three-dimensional finite difference model instead of the depth-averaged two-dimensional staggered grid finite difference model can be seen to improve the accuracy by 10%. The decreases in a time step size from 10 minutes to 5 minutes and a horizontal grid spacing size from 1000m to 500m have the effects of 6% and 5% improvement, respectively. A cubic order error scheme has also been used to replace the first order error scheme and it resulted in a 4% improvement in accuracy. The direction on the improvement in efficiency has also been studied.

Again, for each time, only one design parameter was varied in order to study its effect. When the four-point operators Preissmann one-dimensional implicit finite difference model was used to replace the depth-averaged two-dimensional finite difference model, the improvement in efficiency was found to be up to 50%. The use of only four major tidal constituents instead of forty-two tidal constituents as the open boundary condition sped up the computation by 8%. When the implicit finite difference model was replaced by the conditionally stable explicit finite difference model, the result was a 20% increase in efficiency. The reduction in the number of variables in the water quality model from nine water quality variables to only two of the most important variables (BOD and DO) resulted in an improvement of efficiency by 10%. When the density and salinity were assumed to be constant with respect to time, the improvement in computational time was 12%.

In applying the intelligent system to simulate case studies in Hong Kong coastal areas, it was found that the processes used in hydro-informatics and manipulation direction, were reasonable. In all the case studies, the most appropriate selection and manipulation of numerical model was effective, with regard to: bathymetry; data availability; demand on accuracy; demand on efficiency; and, numerical stability. Similar manipulation processes by human expert counterparts have also been undertaken.

Conclusions

Numerical modeling can generate a large quantity of digital sets at different times and spatial locations. Manipulation processes are employed to improve modeling results for representation of real phenomena. Expertise in numerical modeling includes knowledge on an appropriate direction to affect manipulation. It has proved very useful to apply the engineering knowledge advancements into a knowledge base and subsequent integration into numerical modeling for the assistance of novice users. Up to the present, there has been a shortage of relevant literature reporting on expert system application in this domain. In this paper, a systematic intelligent coding schema to organise current coastal engineering modeling manipulation knowledge into a standardised format has been implemented. It has been demonstrated to have the capability to aid users in modeling manipulation. It is understood that the manipulation process may deviate amongst different experts and that it is not easy to extract all available knowledge into rules. Nevertheless, there is a potential need to bridge the existing gap between numerical modelers and practitioners in this field. It is strongly believed that this is the correct direction for future development of numerical modeling.

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Table 1. Table listing salient properties of main processor

category	*Salient properties*
Scheme	stability, explicit or implicit, algorithm, advection term, alternating direction or not, error of scheme
Method and dimensions	numerical method, co-ordinate system, dimensions, vertical co-ordinate, numerical method in vertical direction
Driving force and boundary condition	river discharge at open boundary, tide at open boundary, wind at surface, value and variation at open boundary, high order variation at boundary, value and variation at close boundary
Turbulence	vertical eddy diffusion, vertical eddy viscosity, horizontal eddy diffusion, horizontal eddy viscosity, turbulence model, bottom drag coefficient
Grid	x-grid spacing, y-grid spacing, vertical grid spacing, type of point setting, grid uniform or not, grid shape
Initial conditions	initial current conditions, initial elevation conditions, initial conditions of water quality variables

Table 2. Examples of comparison of accuracy or efficiency improvement from this case study

Method	*Improvement in accuracy*	*Improvement in efficiency*
use 3-d instead of 2-d	10%	-60%
decrease time step size	6%	-30%
decrease horizontal grid spacing	5%	-35%
use higher order scheme	4%	-25%
use 1-d instead of 2-d	-11%	50%
incorporate major tidal constituent only	-7%	8%
use explicit scheme instead of implicit scheme	-3%	20%
consider minimum number of variables of interest	-5%	10%
assume some physical variables to be constant	-6%	12%

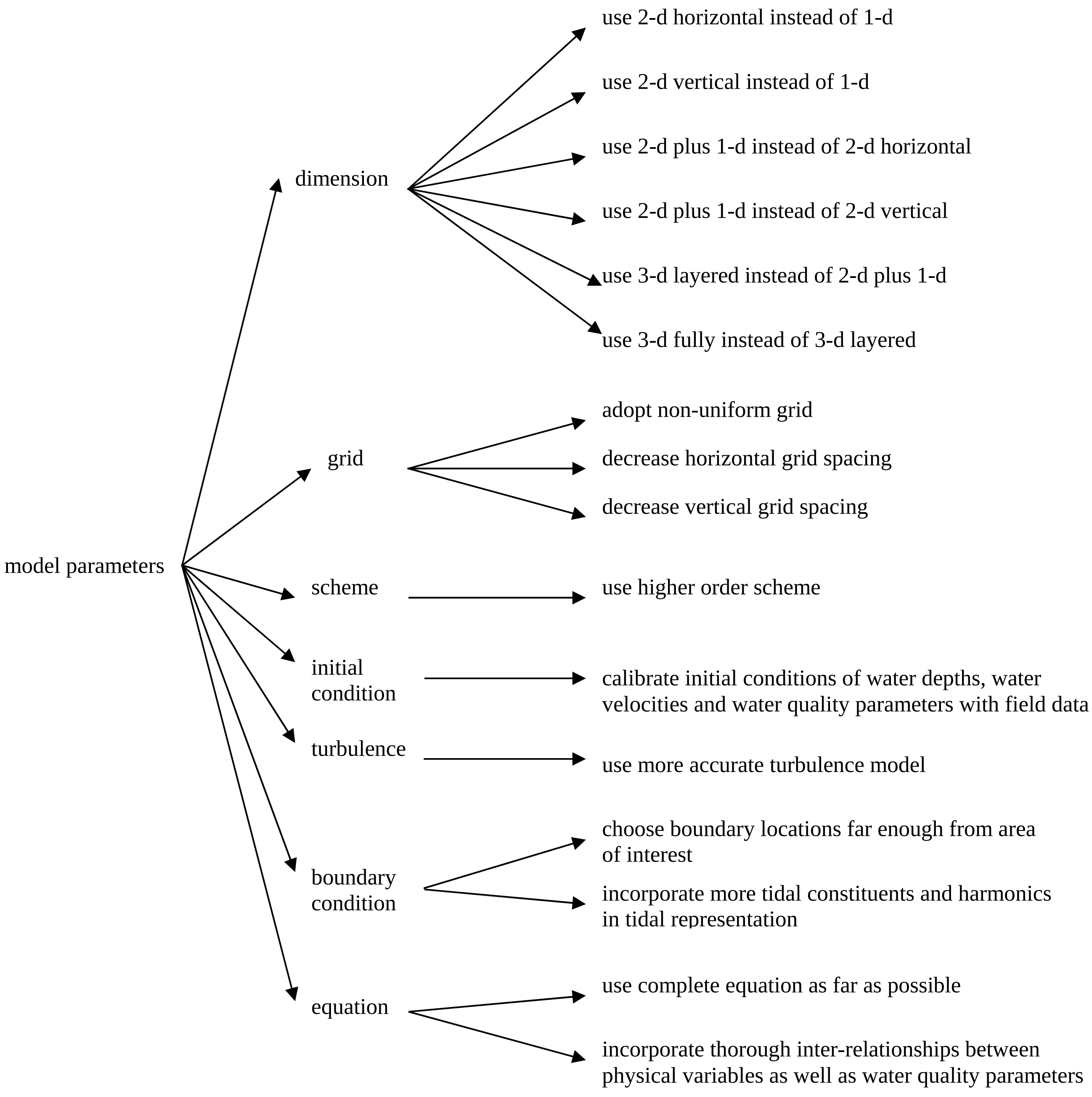

Figure 1. Some methods to raise modeling accuracy

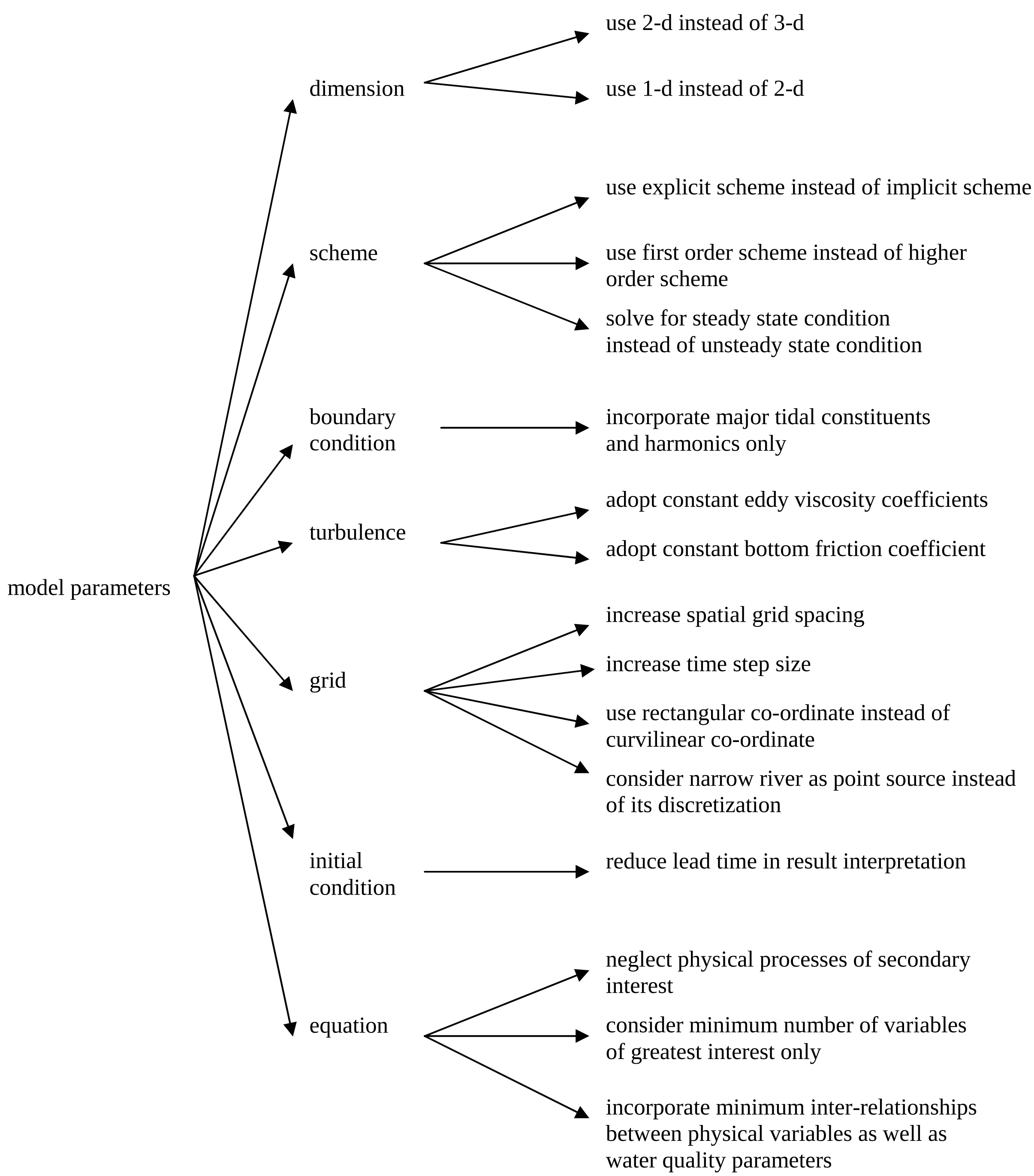

Figure 2. Some methods to raise modeling efficiency

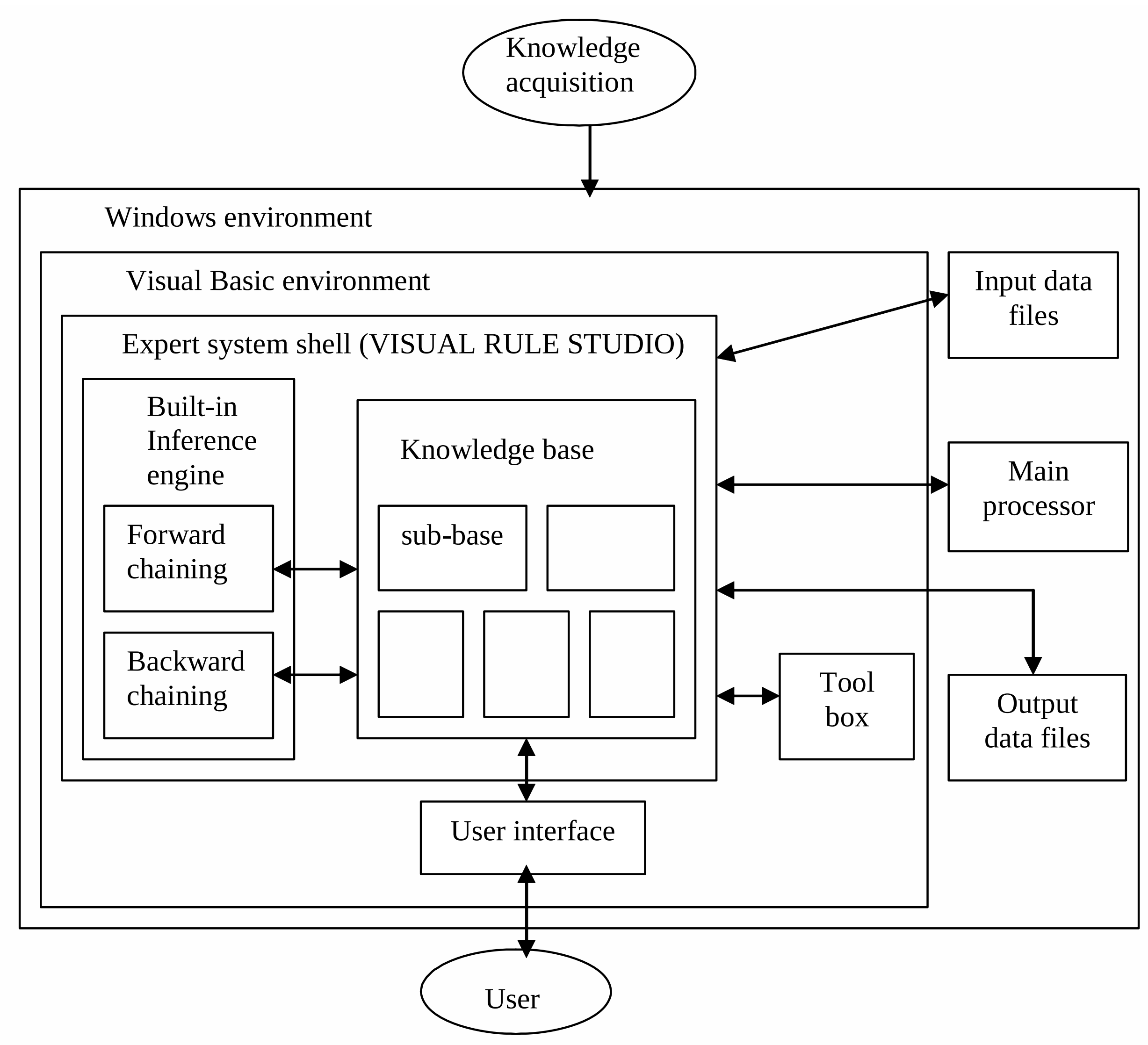

Figure 3. Structure of system showing relationships amongst various components

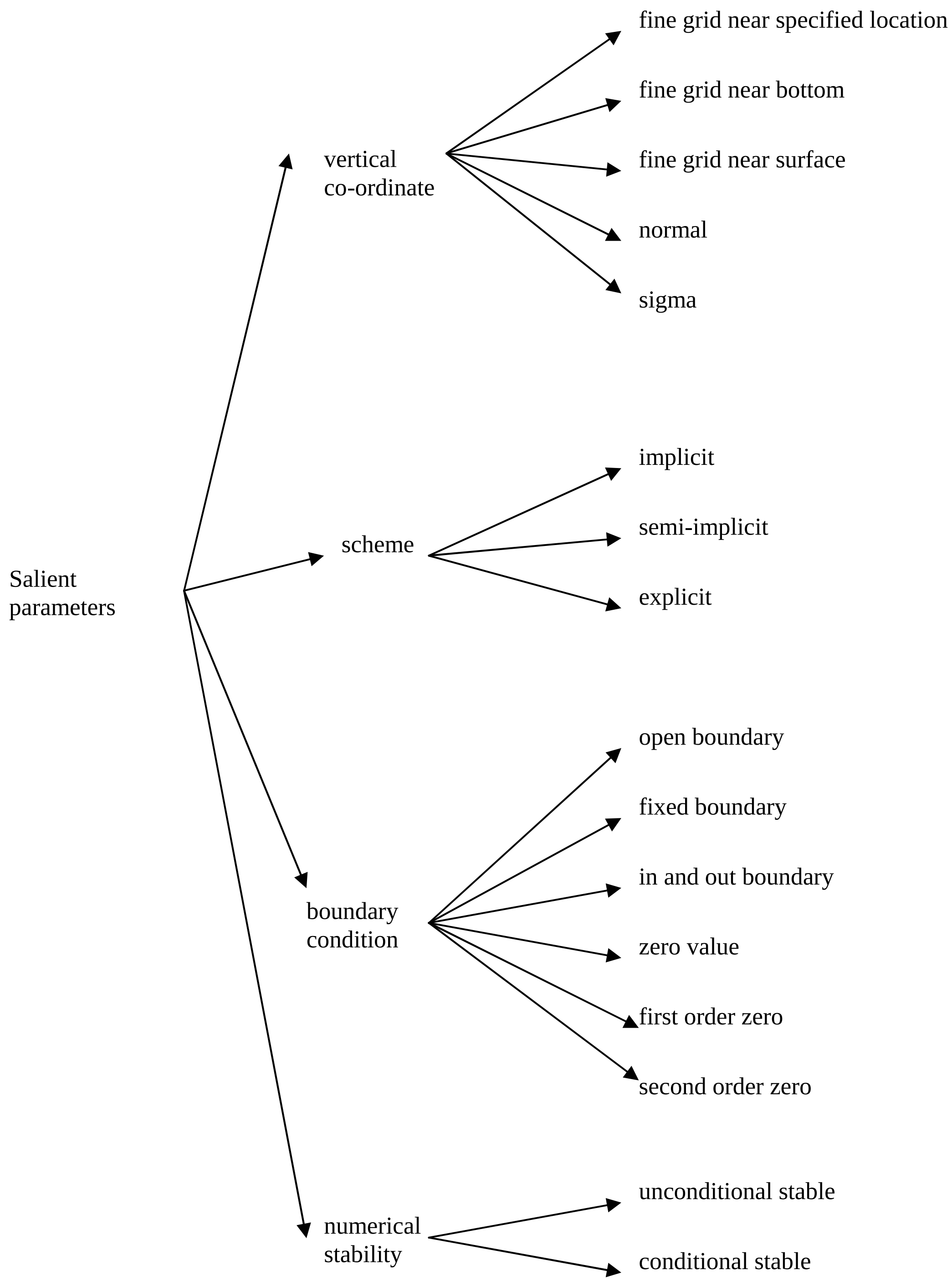

Figure 4. Example of tree formation in manipulation process

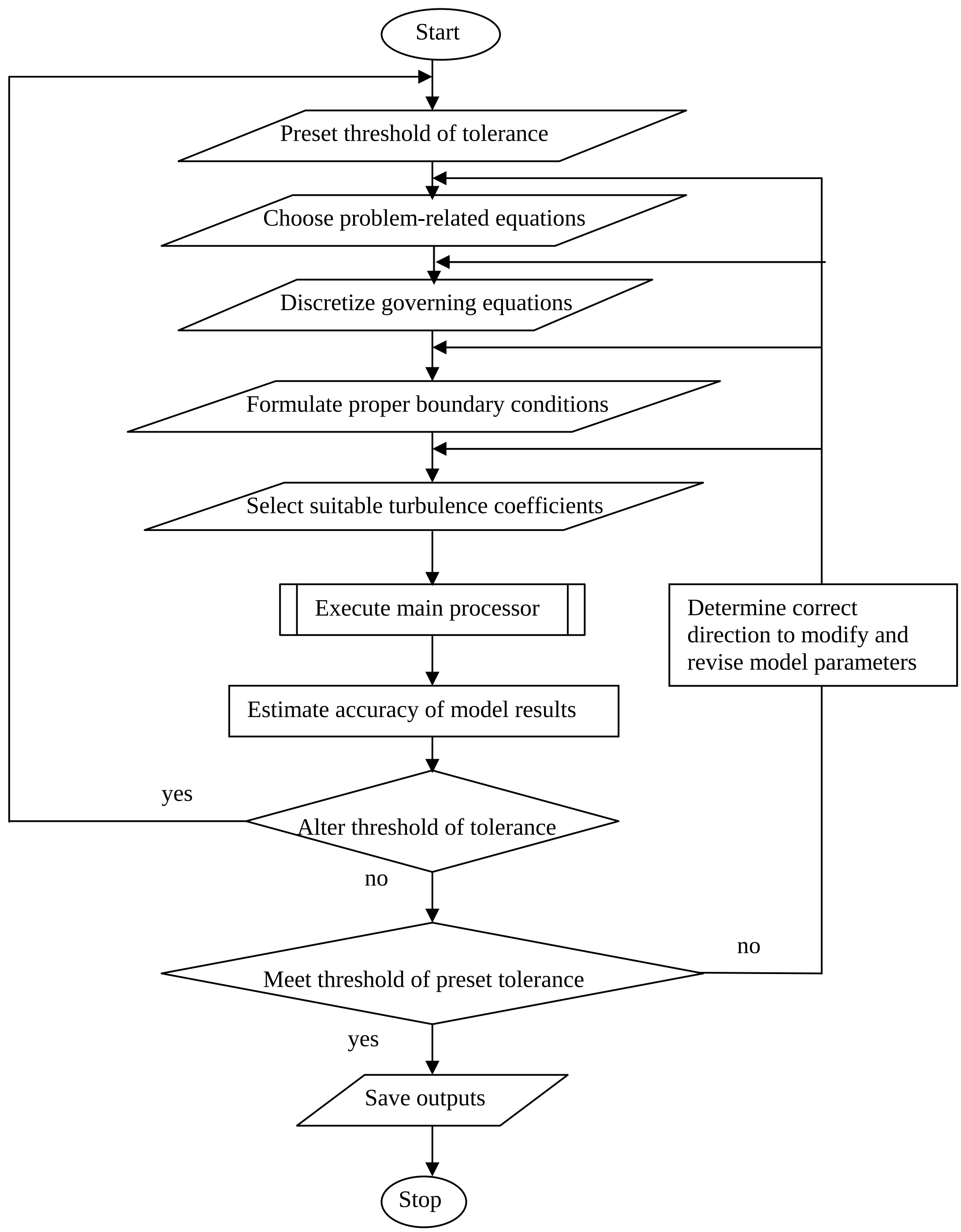

Figure 5. Flow chart showing methods of selection and calibration of numerical modeling

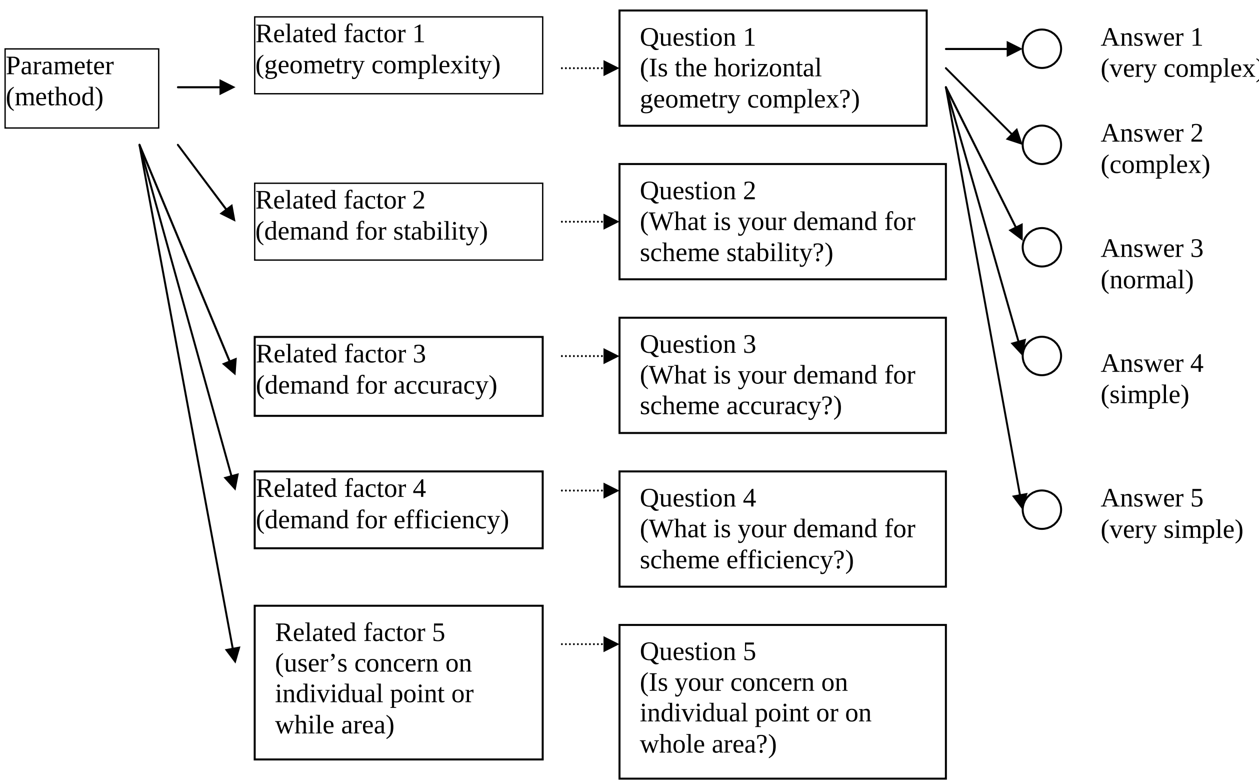

Figure 6. An example of the input user interface