INTRODUCTION AND METHODOLOGICAL APPROACH

The main concept explored in this document is the potential usefulness of a Monte Carlo simulation as an analysis tool aiming to capture the properties and patterns of change for sequences of events, and to generate scenarios and classifications of water quality change (WQC) in the Great Barrier Region of Australia.

Examples of such properties are rare events that occur in time and affect the capacity for resilient characteristics of systemic perturbations (Adger et al., 2005). In other cases, they can also represent a major flood event or storm event, a major polluting event and so on. Beyond these major and genuine natural events, many researchers have identified additional extraordinary societal events that cannot be treated or measured directly using traditional risk analysis as they involve substantial levels of uncertainty and complexity (Alacs, 2004; Lökvist-Andersen et al., 2004).

Extreme events have serious impacts on policy, social and economic characteristics of the systems they affect, and often go beyond the limited spatial (geographic) and temporal boundaries of their immediate physical presence (Ayres, 2000; Brown et al., 2002).

Treating water quality parameters as endogenous probability density functions used in model construction is not a new idea. The methodology has been identified and established in the relevant scientific literature. Thierfelder (1999) uses calibrated normal distributions to describe the distribution of the mean of seven key water quality measurements such as pH, alkalinity, conductivity, hardness, color, Secchi depth, and Total Phosphorous in pre- and post-treatment or management regimes in lake ecosystems (Thierfelder, 1999). Similarly, Uddameri (2007) uses normal Bayesian priors for estimating the quality parameters of a groundwater water system in a semi-arid coastal ecosystem in US.

The use of probabilistic distributions to predict unfavorable water quality events is also documented in the relevant literature. Dolgonosov and Korchagin (2005) use this approach to estimate a probabilistic deviance from regularities in water quality characteristics such as flow.
turbidity, color index, oxidability, ammonia and phytoplankton concentrations in river systems. They argue that the probability of observing an unfavorable value of these parameters can be modeled using power law approximations and their associated distributions, using a general density function of the form (Dolgonosov and Korchagin, 2005):

\[ P\{X > x\} = \int_x^\infty p(x')dx' = A\alpha^{-1}x^{-\alpha} \]  
(Eq. 1)

where,

\[ P\{X > x\} \]: the probability that a random water quality characteristic variable, \( X \) exceeds a threshold value of \( x \).

\( A, \alpha \): parameters describing the properties of the water quality characteristics from a set of Fokker-Plank stochastic differential equations of water flow.

For other water quality characteristics, such as biochemical indicators, bacterial contaminants and microorganisms often similar log-normal distributions have been used to approximate their measured values against some non-arbitrarily chosen threshold values (El-Shaarawi and Marsalek, 1999). For large enough sample sizes, these log-normal distributions also provide indicators for the presence of power-law relationships in contaminant concentrations (Ruggeri and Sivaganesan, 2005). In the case of some water quality characteristic that exhibit the presence of single or multiple chemical equilibria, the use of both finite Furrier distributions and three parameter Gamma distributions have been proven to provide acceptable and useful approximation of contaminant loads in the Mississippi River in US (Tsai et al., 2001). For anthropogenic microbiological contaminants a Normalized Laplace transformation of distribution density has been used to predict the level of contaminant in the Moskva River in Russia (Dolgonosov et al., 2006). Some peripheral parameter distributions that indirectly affect the values of key water quality characteristics (such as hydraulic conductivity, pore size distributions, degradation rate coefficients) can be estimated directly from preexisting theoretical and empirical distributions. For example, Sohrabi et al. (2002) uses a combination of triangular, normal and lognormal distributions to represent these input parameters for a non-point source water quality model. Using a statistical starting point, Van Buren et al. (1997) evaluate the suitability of the lognormal and normal distributions to model storm water quality parameters and they provide a series of goodness-of-fit tests and techniques for assessing candidate distributions (Van Buren et al., 1997, p. 99).

Sadiq et al. (2006) provide a methodological probabilistic approach to the estimation of water quality parameters, especially in the face of uncertainty about their distribution. They demonstrate their approach using evidential belief reasoning and the Dempster-Shafer (DS) inference theory for the evaluation of potential risk of two key water quality characteristics, namely the total coliform level (TC) and the heterotrophic plate counts (HPCs) in a water distribution network. Non-distributional probabilistic assessment of water quality data was provided by Preston and Shackelford (2002), where the probability of an acute or toxic ecotoxicological threshold of heavy metal contaminants were estimated from empirical evidence and spatially-explicit data collection in North Carolina’s surface waters. Empirical distributions of evidential data can be tested and evaluated for their fit against known probabilistic distributions. Borsuk et al. (2003) used a number of probability elicitation techniques to
estimate the components of a water quality Bayesian probability network model for predicting key water quality parameters in a river estuary in North Carolina (Borsuk et al., 2003, p. 275). King and Richardson (2003) use numerical probabilistic bioassessment of water quality criteria to estimate cumulative probabilities of cut-off or change-point values, and indicative and defendable ecological thresholds. Thompson et al. (2002) use a Markov Chain Monte Carlo (MCMC) probabilistic analysis of Gaussian random mixing distributions for estimating the temporal distribution of tidal cycles. Borsuk and Stow (2000) demonstrate the usefulness of a Bayesian approach to estimate the posterior distribution of a nonlinear mixed-order BOD decay model from a set of marginal priors in North Carolina’s river systems.

Beyond the dominant temporal distribution of the water quality characteristics, as they are determined by the distribution and flow networks, two additional factors contribute to the level of uncertainty and variability of these values. These factors are the spatial configuration of the region under study (i.e., landscape homogeneity and heterogeneity), and the seasonal variation of contaminant loads (i.e., annual, monthly and daily cycles). Many of these variations require monitoring and analysis while others exhibit a predictable regularity across various scales of analysis (Danielsson et al., 2004; Hall and Anderson, 2003). Some of the contaminant and key water quality characteristics are subject to global, regional and local biogeochemical cycles and hydrological processes (Harris et al., 2004; Kucharik et al., 2000; Kundzewicz and Somlyódy, 1997; Vanni, 2002). Robarts et al. (2005) use empirical data from a Canadian hypertrophic prairie lake to estimate seasonal variation of dissolved oxygen characteristics, and their associated risk threshold probabilistic criteria (Robarts et al., 2005). Giri et al. (2001) tested four alternative distributions, namely, the uniform, normal, exponential, and log-normal distributions for estimating key random parameters and their monthly variability of a biochemical pollutant (TCDD) transport concentration levels in a shallow river system, using Monte Carlo techniques.

Measuring and predicting probabilities of events allow us to avoid many important pitfalls on modeling the dynamics of whole systems (e.g., a river or water distribution system) across various spatial and temporal scales. The heterogeneity of water uses and water quality parameters used to assess the suitability and threshold values of the water, would otherwise require a very large variety of models including stochastic and dynamic equations, mass conservation, momentum and energy conservation, thermodynamic equilibrium equations, hydraulic and engineering flows, chemical and biological reactions, climatic interaction equations, to name a few (Chiang and Gates, 2004). Simplification and transparency of modeling assumptions thus, becomes a central element for the ability of decision makers and stakeholders to monitor, evaluate and adopt different management regimes. The level of detail to which the state of water quality of a river or river catchment becomes a single dimensional element of decision making and as such is often sought to be captured by probabilistic assessment techniques (Briske et al., 2006; Rogerson, 2005; Sohrabi et al., 2002), or probabilistic inference algorithms (C. F. Chen et al., 2007; da Conceição Cunha, 1999).

When the level of uncertainty is large, or the available data for assessing scale or latent probabilistic relationships with thresholds, the use of simplified binary responses (e.g., success-failure) and their derivatives (e.g., time-to-failure, success thresholds), have been modeled and represented using discrete probabilistic binary distributions. Hamed and El-Beshry use probabilistic uncertainty analysis to estimate a normal binary success-failure response distribution of the dissolved oxygen (BOD) concentrations in steams (Hamed and El-Beshry, 2004). Worrall et al. (1998) use a logistic distribution (output of a logit regression analysis) for the probabilistic threshold estimation of three key water quality characteristics: dissolved
oxygen, biochemical oxygen demand and ammonia levels in a river system in Northumberland, UK (Worrall et al., 1998).

The above described distributions and probabilistic approaches to modeling key water quality characteristics, mostly describes a closed system of distributions that model endogenous parameters of the water quality characteristics (i.e., physical, chemical, and biological), and its properties across space, time and scales (shown as the first nested box in Figure 1, labeled “Key water system characteristics”).

![Figure 1: Key systemic characteristics of probabilistic assessment of the water quality system](image)

Beyond this rather limiting view of water systems and their qualitative characteristics, a series of events and their characteristics affect the magnitude, scale and distributions across space and time of the water quality values. Events such as floods, extreme rainfalls or draughts, accidents, industrial and agricultural runoffs, often magnify, multiply and propagate the water quality characteristics, exceed threshold levels and diffuse many of the undesired pollutant levels across spatial and temporal scales. In many other cases, whilst the actual values of pollutant loads within the closed system do not change, any changes in the rate to which these runoffs are delivered across different end-points of the water distribution system, directly or indirectly affect the quality and health of the ecosystem within which the water system is embedded (Heathcote, 1998; Lake and Bond, 2007; Moran et al., 2006). The inclusion of these key events and their characteristics into a modeling regime allows us to treat the water quality system as an open system with exogenous modeling parameters (shown with the second nested box in Figure
1, labeled “Key event characteristics”). The use of the term “open system” here, signifies the fact that not only the key water quality characteristics and their distributions affect the state of the water system, but also a series of event-type characteristics contribute to the systems’ state.

The relevant literature provides some applications of assessing the water quality implications under the presence and occurrence of events. Guo and Urbonas (2002) provide quantitative probabilistic estimates of the runoff and delivery curves for storm water quality events such as extreme rainfall. They focus in events that cannot be classify as extreme (as their long-term appearance is within the expected range of the event horizon), but they exhibit an exponential distribution over time and runoff volume. Both Van Buren et al. (1997) and Chen and Adams (2007) showed that when assessing storm water regimes, the nature of the underlying distribution changes from a normal distribution under base flow conditions (normal expected runoff and its effect to key pollutant loads), to log-normal distribution under event conditions (intense or extreme rainfall, extreme slopes and wastewater flow), thus altering the physical and chemical composition of water quality characteristics (Van Buren et al., 1997, p. 101).

Finally, beyond both the key water quality characteristic distributions and the event characteristic distributions, a number of key considerations are important determinants and inflectors of the state of a water system and its water quality values. These factors include considerations of uncertainty and randomness entering the system (i.e., in cases where empirical distributions are estimated from uncertain data, or where event occurrences cannot be predicted with a reasonable confidence), variable levels of stochasticity (i.e., in cases where varying the level of stochasticity and specificity of our assumptions allow us to capture boundary distributions and events), alternative scenarios for modeling, or ranges of target maximum loads, management goals and objectives. These factors, although non-explicit in terms of a water system and its water quality characteristics, are implicit on many of our modeling assumptions and distributional representations of water quality values and events. Any modeling regime that explicitly accounts and tests such factors as inclusive to a water system, allows us to address such a system as an open system with endogenous modeling parameters (shown with the outer nested box in Figure 1, labeled “key inference characteristics”).

estimating algal mass occurrences in a lake water system. Revelli and Ridolfi (2004) also provide further verification of the important role of stochasticity and randomness in studying water quality system parameters. Mailhot and Villeneuve (2003) demonstrate the value of uncertainty analysis and its applications to probabilistic water quality modeling. Finally Varis (1998) showcases the use of Bayesian probabilistic belief estimation for water quality characteristics optimization by matching management and control targets and goals.

The benefits of using alternative and complementary approaches to modeling water quality parameters and the state of the associated water systems is shown by Stow et al. (2003), by analyzing and comparing the advantages and disadvantages of alternative modeling techniques for estimating TDML eutrophication levels in river estuaries in the US. They recognize the importance of recognizing that “each model is an extremely crude representation of complex system behavior, based on an incomplete understanding of the system. There are likely to be unexpected feedbacks and changes in system behavior with time that are not captured in any of these models. (…)” (Stow et al., 2003, p. 313).

SIMULATION TOOLS
For the purpose of this analysis the Crystal Ball Monte-Carlo simulation framework is used. The concept development includes (a) the generation of a simulation model of probability density functions and the development of a series of risk factors of these events; (b) the replication of the water quality characteristics of distribution flows for hundreds or thousands of times; and (c) the study and analysis of the results.

MONTE CARLO SIMULATION MODEL CHARACTERISTICS

A. EXTREME EVENT DISTRIBUTION
The model considered in this example is inspired from the natural hazards type of process modeling. The general idea involves the simulation of a process framework of the form:

\[ \text{Natural Hazard} \rightarrow \text{Damage} \rightarrow \text{Loss} \quad \text{(Eq. 2)} \]

We can represent this hazard as an *extreme events’ occurrence* probability distribution. In other words, the distribution denotes the probabilities for the occurrence of an extreme event within a finite time horizon. The longer the time that intervenes between the two events is, the smaller is the frequency of events for a given time interval. Despite the fact that extreme events in general are the result of complex (and often unobservable) dynamics across multiple scales (Adger et al., 2005; Rosenzweig et al., 2001), according to Altmann et al., “(…) the characterization of extreme events is usually done in a single scientifically or socially relevant observable (dimension) (…)” (Altmann et al., 2006, p. 435). We can use a number of distributions to generate the probabilistic frequencies of these events.

We can use a *maximum extreme value type I distribution* to generate the probability density function. It is also known as a *Gumbel (maximum) distribution* function, and it represents the distribution of the maximum value of an extreme event over a given period of time (Gumbel,
It has been proven useful for the probabilistic prediction of extreme events (such as earthquakes, floods or other naturally occurring extreme events).

The following example represents the simulation of the probability of an extreme event. The likeliest probability of the event’s occurrence is 25%, and the scale of the events’ occurrence is 0.1 (e.g., a 100-year storm event occurring in the next 10 years). Symbolically, we can represent this distribution as,

\[\xi(n) = MaxExtremeValue(Likeliest, Scale) = Gumbel(0.25, 0.1)\]  
(Eq. 3)

Using the parameters of the above distribution to generate a Monte Carlo simulation, produces the following empirical distribution shown in Figure 2.

Figure 2: A Gumbel (maximum extreme event) probability distribution example

The probability for an extreme event such as the one described above represents an uncertain assumption variable (independent) in the model.

**B. VULNERABILITY PARAMETER (IMPACT OR DAMAGE)**

This is a second component in the model considered in this approach. If the natural hazard (i.e., extreme event occurrence) leads to some form of damage, then such a damage (especially its observable impacts) is a significant part of the analysis. Nevertheless, although damage and impact are not entirely dependent to each other, different types or characteristics of events generate different, and often uncertain types of impacts. On the other hand, also similar characteristics of events (e.g., extreme events happening in the same time frequency), might also generate different and uncertain types of impacts. Thus, a significant part of the observed and realized impacts in the society is an uncertain, independent variable.

We can simulate such a distribution with a *Beta* density function in which we can model probabilities based on Bayesian statistics, and can predict the random behavior of percentages and fractions. A *Beta distribution* ranges between two possible values (*a-alpha* and *b-beta*), and has a minimum and maximum range.
For a standardized distribution we need a Beta distribution with the following characteristics:

\[ C(n) = Beta(\text{min}, \text{max}, \alpha, \beta) = Beta(0,1,3,3) \quad (\text{Eq. 4}) \]

Where, \(-\infty \leq Beta(0,1,3,3) \leq \infty\). Such a distribution is shown in the next Figure 3.

![Figure 3: A Beta probability distribution for vulnerability (impact or damage)](image)

Similarly, this variable (distribution) will also be represented with an assumption parameter, since it is also an uncertain (independent) variable or model component, and we do not have any control over its values.

Nevertheless as seen previously, there is also a significant relationship between an extreme event and the impact it generates. This relationship is causal, synergistic, and/or symbiotic. Arbitrarily (or intuitively) a correlation coefficient is chosen to represent this relationship \((r = -0.75)\). In this relationship between extreme events' time-to-failure (higher time-to-failure mean less time between events, or less events per unit of time), and impact magnitude (higher impact means more damage) the correlation coefficient is negative. Also, this correlation has a non-linear form, since the distributions chosen to represent the extreme events’ time-to-failure and vulnerability have different slope characteristics. The correlation coefficient is shown in the following figure.

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C. EXPOSURE PARAMETER (PREPAREDNESS)

This is the third component of the model. As seen in the hazard type of model (Eq.1), the hazard-damage coupling leads to a higher level of loss from damage. This loss is affected by the amount of exposure the damage is facing, in other words, the degree of preparedness to which, for example, a society or a system in general is subjected to. A system that its functionality is designed to withstand and absorb the damages caused by the occurrence of an extreme event, will present less losses than a system that exhibits a very low degree of preparedness.

The degree of preparedness, $\alpha$, unlike the previous two variables (distributions) is not something that is beyond our control, but it is determined by our actions and responses (individually and collectively) to changes, damages, and extreme event occurrences. Any uncertainty involved in its determination will only be related to the degree in which we are uncertain about the extreme events that are likely to occur, and the magnitude of damages or impact that they may cause. In other words, for a given frequency of occurrence of extreme events, and a given magnitude of impacts observed, we are certain about the degree of preparedness or exposure we have in place.

We conceptualize a continuous range of preparedness degree, from 0.0 to 1.0 (a consistent scale with the previous two variables). The simulation in Crystal Ball will not directly alter the degree of preparedness, but will compute the forecasted risk level (see next session) for a given preparedness threshold. We know in advance that higher levels of preparedness can ameliorate the effects of low frequency of event occurrences and high impact levels. Consequently, our global optimum preparedness threshold is 1 (corresponding to a 100% preparedness to any frequency and magnitude of event occurrence and impact respectively). Yet, we do not know how this threshold is and can be reached, and what different levels and patterns of thresholds mean in terms of their respective risks.

We can study these effects by looking at different scenarios for this decision variable (preparedness). In other words, we will be constructing a scenario ensemble based on realistic, simulated values of the constructed model.
Finally, in a sub-optimal world many different reasons render the achievement of the globally optimal threshold of preparedness (=1.0) as unrealistic or even impossible. Some of these reasons include limited amount and availability of resources, increased or unreal costs involved, or simply because we cannot imagine, visualize and be prepared for, event horizons and futures that never have been observed in the past. In a modeling paradigm, the later can be calibrated further using an empirical assessment that aims to identify a reasonable sub-optimal (local optima) threshold for which a social target can be set.

The degree of preparedness is represented in the simulated model by a decision parameter, i.e., a variable for which we have control over its achieved values.

Following a similar logic, we can define a second decision parameter, $\beta$, to represent the degree of decision fading in the model. In the context of the model we are examining, fading represents an inherent systemic property: if a sequence of events have a lower magnitude than the ones expected (or prepared for), then fading indicates the probability of incremental lowering of the threshold values.

D. Risk Event Assessment (Moving Threshold)

The notion of risk has very solid grounds in the theory of probabilistic assessment and reasoning. In probabilistic terms, given an uncertain event, risk can be defined as the product of
the probability of occurrence and the consequences of occurrence (Lökvist-Andersen et al., 2004). Symbolically,

\[ q(n) = \text{pdf} \left( d(n) \times C_n, \gamma \right) \]  
(Eq. 5)

where,

- \( q(n) \): a risk factor (threshold);
- \( n \): an uncertain event;
- \( P(n) \): the probability of event occurrence;
- \( C_n \): a consequence or cost or loss function, and;
- \( \gamma \): an uncertainty parameter (similar to the parameters \( \alpha \) and \( \beta \) above, indicating our level of certainty on our expected risk assessment).

For the purpose of this model example, the risk assessment threshold function is simulated as a normal distribution with mean the product of \( d(n) \) and \( C_n \), and standard deviation the uncertainty parameter, \( \gamma \).

In the constructed model the risk event threshold is actively dependent on a series of additional parameters that are simultaneously forecasted. The first one is the dominant threshold value, \( d(n) \) that allow us to determine whether or not the expected probability of an extreme events’ occurrence exceeds the expected or perceived risk threshold value.

\[ d(n) = \max \{ \xi(n), q(n + 1) \} \]  
(Eq. 6)

The expected or perceived risk threshold value can be calculated from the bimodal distribution:

\[ q(n + 1) = \begin{cases} 
\max \{ a\xi(n), \beta q(n) \} & \text{if } \xi(n) > q(n) \\
\beta q(n) & \text{otherwise}
\end{cases} \]  
(Eq. 7)

The equations 5, 6 and 7 allow us to compute iteratively and estimate the probability distributions of the risk threshold values.

The following figures showcase the simulated model estimates for the example considered in this document. A more intuitive and perhaps more interesting indicator of the model performance (adaptivity) is the computation of the event barrier difference, \( y(n) \), as the difference between the probabilities of observed events and expected risk threshold preparedness, post-estimated from the data. In other words,

\[ y(n) = \xi(n) - q(n) \]  
(Eq. 8)
Figure 7: Forecasted probability distribution for the dominant adaptation threshold

Figure 8: Simulated forecast of the extreme events’ barrier difference threshold. Values of the threshold above 0 indicate positive response feedback (adaptation).
SYNTHESIS OF SIMULATION RUNS

Synthesizing the results of the Monte Carlo simulation runs described in the previous paragraphs, we can see how the model allow us to estimate the adaptive dynamics of a moving risk threshold in the presence of extreme, uncertain and turbulent events entering the water quality system. From the following Figure 11, we can see that the risk event assessment threshold trails successfully the dominant threshold, and the cases where the difference between observed (extreme) and expected (prepared for) events occurs mainly where threshold values are negative (the present risk threshold exceeds the extreme event frequency). By looking also the assumption parameters in the cross-tabulation matrix of Figure 12, we can see that the moving threshold is very responsive to changes in assumed event frequencies (relatively clustered data cloud). On the other hand, the moving threshold seems to be less responsive to vulnerabilities inherent in the system. The gray lines in the cross-tabulation matrix represent response curves among any two pairs of parameters.

This analysis does not include the study of the dynamic behavior of the three decision parameters included in the model (α, β, γ). Initial repeated tournaments of simulation results confirmed the sensitivity of results to these decision parameters, and more successful response curves under varying combinations of these parameters is very possible to indicate a strong policy mix associated with them. The mix between exposure (degree of inherent preparedness of the water quality management system), fading (degree of inherent relaxation of policies, regulations, etc.), and uncertainty (degree of inherent uncertainty about estimated risk assessment) represents a very important aspect of this modeling exercise and deserves a closer examination in future implementations.

Figure 9: Risk event assessment of moving threshold distribution for the Monte Carlo simulation. Threshold values above the mean threshold value are likely to increase the adaptive capacity of the response system.
Figure 11: Overlay of Monte Carlo simulation forecasts for the adaptive threshold model

Figure 10: Matrix cross-tabulation of simulation assumptions (green) to Monte Carlo simulation forecasts for the model’s moving threshold.


